

**Wechselspiel zwischen Basizität und  
Nucleophilie  
von Alkyllithiumverbindungen:  
Ungewöhnliche Reaktionen an Organosilanen**

**ANHANG**

**Dissertation**  
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## 10. Anhang

## 10.1. Weitere Angaben zu den Einkristallröntgenstrukturanalysen

10.1.1. Benzylmethyldiphenylsilan (**42**)Tabelle 10.1 Kristallographische Daten und Strukturverfeinerung von **42**.

Verbindung	<b>42</b>
CCDC Nummer	1005509
Empirische Formel	C <sub>20</sub> H <sub>20</sub> Si
Formelmasse [g/mol]	288.45
Temperatur [K]	173(2)
Wellenlänge [Å]	0.71073
Kristallsystem	monoklin
Raumgruppe	<i>P</i> 2 <sub>1</sub> / <i>c</i> (14)
<i>a</i> [Å]	12.6846(4)
<i>b</i> [Å]	17.5223(5)
<i>c</i> [Å]	7.6447(2)
$\beta$ [°]	107.002(3)°
Zellvolumen [Å <sup>3</sup> ]	1624.87(8)
Formeleinheit pro Zelle	Z = 4
Berechnete Dichte [g/cm <sup>3</sup> ]	1.179
Absorptionskoeffizient $\mu$ [mm <sup>-1</sup> ]	0.136
F(000)	616
Kristallgröße [mm <sup>3</sup> ]	0.30 x 0.20 x 0.10
Messbereich $\Theta$ [°]	2.32 – 27.00
	-16 $\leq h \leq$ 16
Index-Breite	-22 $\leq k \leq$ 22
	-9 $\leq l \leq$ 9
Gemessene Reflexe	35024
Unabhängige Reflexe	3547 ( <i>R</i> <sub>int</sub> = 0.0445)
Daten / Restraints / Parameter	3547 / 0 / 199
Goodness-of-fit an F <sup>2</sup>	1.035
Endgültige R-Werte [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	<i>R</i> 1 = 0.0362, <i>wR</i> 2 = 0.0853
<i>R</i> -Werte (sämtliche Daten)	<i>R</i> 1 = 0.0555, <i>wR</i> 2 = 0.0885
Restelektronendichte [e/Å <sup>3</sup> ]	0.322 und -0.234

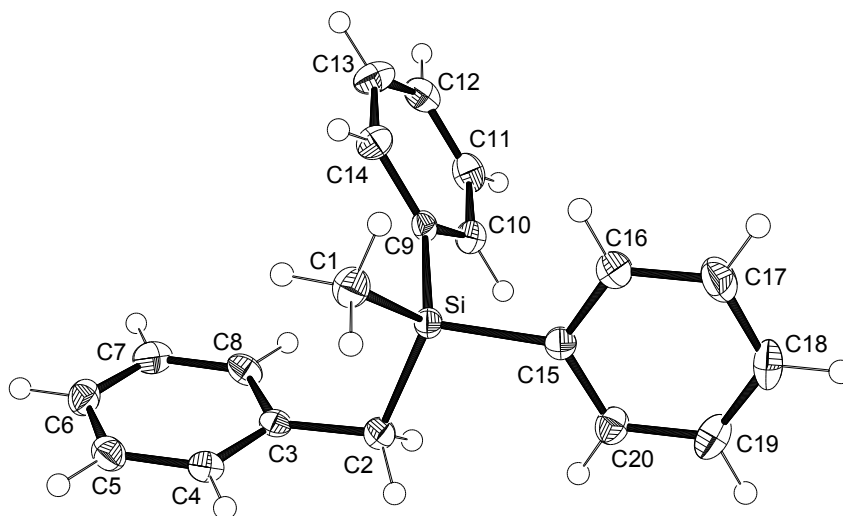


Abbildung 10.1 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von **42** im Kristall (ORTEP-Darstellung<sup>[206,207]</sup>). Das Nummerierungsschema der Wasserstoffatome wurde der Übersichtlichkeit halber weggelassen. Ausgewählte Bindungslängen [Å] und -winkel [°]: Si(1)-C(1) 1.8533(14), Si(1)-C(2) 1.8760(15), Si(1)-C(9) 1.8687(14), Si(1)-C(15) 1.8727(14), C(2)-C(3) 1.502(2), C(1)-Si(1)-C(2) 110.42(7), C(1)-Si(1)-C(9) 109.79(6), C(1)-Si(1)-C(15) 110.06(7), C(2)-Si(1)-C(9) 108.26(7), C(9)-Si(1)-C(15) 108.30(6), C(15)-Si(1)-C(2) 109.96(6), C(3)-C(2)-Si(1) 110.46(10).

Tabelle 10.2 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{Å}^2 \cdot 10^3$ ] von **42**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\ddot{}}$ -Tensors.

	x	y	z	$U(\text{eq})$
Si(1)	2584(1)	3909(1)	3641(1)	18(1)
C(9)	2348(1)	4805(1)	4795(2)	18(1)
C(3)	4087(1)	3268(1)	6697(2)	20(1)
C(15)	1276(1)	3658(1)	1840(2)	19(1)
C(6)	6213(1)	3569(1)	8964(2)	28(1)
C(12)	1958(1)	6144(1)	6519(2)	28(1)
C(8)	4266(1)	3794(1)	8113(2)	24(1)
C(4)	5000(1)	2891(1)	6446(2)	23(1)
C(2)	2958(1)	3131(1)	5403(2)	23(1)
C(7)	5320(1)	3943(1)	9236(2)	28(1)
C(13)	2771(1)	6126(1)	5661(2)	31(1)
C(1)	3711(1)	4057(1)	2586(2)	27(1)
C(20)	616(1)	3042(1)	1998(2)	24(1)
C(14)	2958(1)	5465(1)	4805(2)	25(1)
C(5)	6048(1)	3040(1)	7571(2)	26(1)
C(16)	907(1)	4116(1)	292(2)	29(1)
C(19)	-370(1)	2898(1)	679(2)	30(1)
C(11)	1342(1)	5498(1)	6546(2)	29(1)

C(10)	1539(1)	4839(1)	5703(2)	25(1)
C(18)	-722(1)	3367(1)	-826(2)	29(1)
C(17)	-82(1)	3974(1)	-1029(2)	32(1)
H(2A)	2919(12)	2618(10)	4720(20)	41(5)
H(2B)	2412(12)	3119(8)	6070(20)	27(4)

Tabelle 10.3 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **42**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Si(1)	16(1)	19(1)	18(1)	1(1)	4(1)	-1(1)
C(9)	16(1)	21(1)	15(1)	2(1)	0(1)	1(1)
C(3)	23(1)	18(1)	18(1)	6(1)	5(1)	0(1)
C(15)	19(1)	20(1)	19(1)	-2(1)	6(1)	1(1)
C(6)	24(1)	32(1)	23(1)	8(1)	-1(1)	-5(1)
C(12)	36(1)	25(1)	19(1)	-3(1)	3(1)	7(1)
C(8)	29(1)	23(1)	18(1)	3(1)	6(1)	7(1)
C(4)	27(1)	19(1)	22(1)	1(1)	7(1)	1(1)
C(2)	22(1)	22(1)	23(1)	3(1)	4(1)	-1(1)
C(7)	39(1)	24(1)	19(1)	0(1)	4(1)	-3(1)
C(13)	41(1)	23(1)	29(1)	-3(1)	12(1)	-9(1)
C(1)	24(1)	30(1)	28(1)	-2(1)	10(1)	-1(1)
C(20)	24(1)	28(1)	20(1)	-1(1)	5(1)	-3(1)
C(14)	27(1)	26(1)	24(1)	-1(1)	11(1)	-3(1)
C(5)	23(1)	26(1)	28(1)	7(1)	9(1)	4(1)
C(16)	29(1)	27(1)	27(1)	4(1)	1(1)	-2(1)
C(19)	26(1)	37(1)	28(1)	-8(1)	10(1)	-11(1)
C(11)	24(1)	37(1)	26(1)	0(1)	10(1)	6(1)
C(10)	21(1)	26(1)	28(1)	1(1)	7(1)	-1(1)
C(18)	17(1)	44(1)	23(1)	-10(1)	1(1)	1(1)
C(17)	30(1)	38(1)	24(1)	4(1)	-1(1)	5(1)

### 10.1.2. Hydrochlorid **54**

Tabelle 10.4 Kristallographische Daten und Strukturverfeinerung von **54**.

Verbindung	<b>54</b>
Empirische Formel	$C_{25}H_{32}ClNOSi$

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Formelmasse [g/mol]	426.06
Temperatur [K]	173(2)
Wellenlänge [Å]	0.71073
Kristallsystem	monoklin
Raumgruppe	P2 <sub>1</sub> /c (14)
<i>a</i> [Å]	13.7008(10)
<i>b</i> [Å]	12.5893(5)
<i>c</i> [Å]	14.7890(9)
$\beta$ [°]	115.956(9)
Zellvolumen [Å <sup>3</sup> ]	2293.5(2)
Formeleinheit pro Zelle	4
Berechnete Dichte [g/cm <sup>3</sup> ]	1.234
Absorptionskoeffizient $\mu$ [mm <sup>-1</sup> ]	0.235
F(000)	912
Kristallgröße [mm <sup>3</sup> ]	0.20 x 0.20 x 0.10
Messbereich $\Theta$ [°]	2.23 – 27.00
	-17 $\leq$ h $\leq$ 17
Index-Breite	-16 $\leq$ k $\leq$ 16
	-18 $\leq$ l $\leq$ 18
Gemessene Reflexe	20157
Unabhängige Reflexe	4970 (R <sub>int</sub> = 0.04849)
Daten / Restraints / Parameter	4970 / 0 / 274
Goodness-of-fit an F <sup>2</sup>	1.050
Endgültige R-Werte [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	R1 = 0.0432, wR2 = 0.0982
R-Werte (sämtliche Daten)	R1 = 0.0702, wR2 = 0.1113
Restelektronendichte [e/Å <sup>3</sup> ]	0.331 and -0.243 e.Å <sup>-3</sup>

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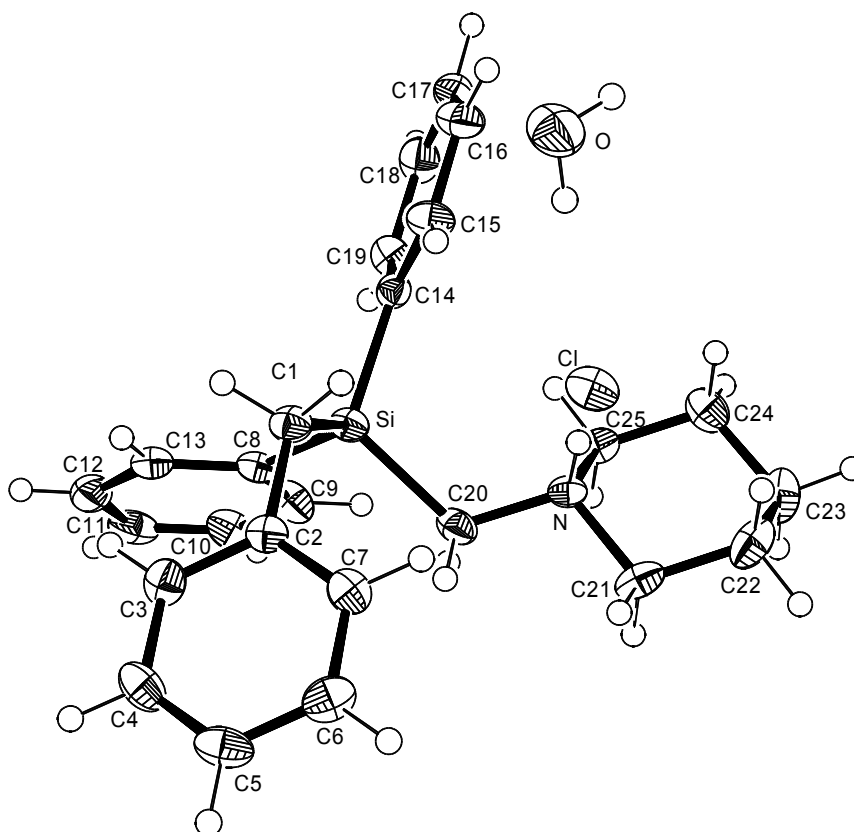


Abbildung 10.2 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von **54** im Kristall (ORTEP-Darstellung<sup>[206,207]</sup>). Das Nummerierungsschema der Wasserstoffatome wurde der Übersichtlichkeit halber weggelassen.

Tabelle 10.5 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **54**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\ddot{}}$ -Tensors.

	x	y	z	$U(\text{eq})$
Si	3180(1)	2359(1)	7871(1)	23(1)
N	900(1)	2416(1)	7544(1)	21(1)
C(1)	3265(2)	1936(2)	6688(1)	26(1)
C(2)	3038(2)	781(2)	6385(1)	24(1)
C(3)	3865(2)	37(2)	6655(2)	30(1)
C(4)	3643(2)	-1015(2)	6373(2)	35(1)
C(5)	2587(2)	-1352(2)	5819(2)	35(1)
C(6)	1754(2)	-624(2)	5543(2)	34(1)
C(7)	1977(2)	439(2)	5817(2)	30(1)
C(8)	4315(2)	1824(2)	9037(1)	26(1)
C(9)	4196(2)	1755(2)	9927(2)	35(1)
C(10)	5017(2)	1368(2)	10806(2)	38(1)

C(11)	5977(2)	1037(2)	10815(2)	38(1)
C(12)	6131(2)	1105(2)	9956(2)	38(1)
C(13)	5304(2)	1492(2)	9074(2)	29(1)
C(14)	3198(2)	3851(2)	7908(1)	23(1)
C(15)	2770(2)	4455(2)	7023(2)	30(1)
C(16)	2813(2)	5556(2)	7047(2)	35(1)
C(17)	3287(2)	6083(2)	7951(2)	34(1)
C(18)	3703(2)	5515(2)	8838(2)	35(1)
C(19)	3661(2)	4411(2)	8817(2)	30(1)
C(20)	1895(2)	1746(2)	7857(2)	28(1)
C(21)	-109(2)	1747(2)	7209(2)	33(1)
C(22)	-1110(2)	2433(2)	6856(2)	38(1)
C(23)	-1049(2)	3179(2)	7682(2)	39(1)
C(24)	-22(2)	3847(2)	8034(2)	34(1)
C(25)	977(2)	3160(2)	8364(1)	24(1)
Cl	341(1)	3006(1)	5351(1)	32(1)
O	1078(2)	4986(2)	4420(1)	48(1)
H(26)	790(15)	2777(15)	7000(15)	21(5)
H(27A)	750(20)	5530(20)	4530(20)	73(10)
H(27B)	870(20)	4470(20)	4670(20)	56(9)

Tabelle 10.6 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **54**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Si	30(1)	21(1)	21(1)	1(1)	13(1)	1(1)
N	28(1)	20(1)	18(1)	1(1)	10(1)	-3(1)
C(1)	34(1)	24(1)	24(1)	1(1)	17(1)	-1(1)
C(2)	31(1)	25(1)	18(1)	-2(1)	14(1)	-2(1)
C(3)	29(1)	33(1)	28(1)	-6(1)	13(1)	-1(1)
C(4)	45(1)	31(1)	31(1)	-4(1)	18(1)	8(1)
C(5)	55(2)	25(1)	26(1)	-6(1)	20(1)	-5(1)
C(6)	36(1)	37(1)	27(1)	-6(1)	10(1)	-10(1)
C(7)	33(1)	30(1)	25(1)	1(1)	12(1)	3(1)
C(8)	33(1)	19(1)	25(1)	-1(1)	10(1)	0(1)
C(9)	44(1)	34(1)	27(1)	2(1)	16(1)	9(1)
C(10)	53(2)	31(1)	24(1)	2(1)	12(1)	6(1)
C(11)	39(1)	25(1)	30(1)	2(1)	-2(1)	-5(1)
C(12)	27(1)	30(1)	46(1)	1(1)	8(1)	-5(1)
C(13)	32(1)	22(1)	33(1)	-1(1)	15(1)	-5(1)

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C(14)	23(1)	23(1)	24(1)	-2(1)	12(1)	-1(1)
C(15)	40(1)	25(1)	25(1)	0(1)	14(1)	-2(1)
C(16)	44(1)	25(1)	37(1)	5(1)	20(1)	0(1)
C(17)	32(1)	21(1)	53(1)	-6(1)	23(1)	-2(1)
C(18)	34(1)	33(1)	37(1)	-14(1)	14(1)	-2(1)
C(19)	32(1)	31(1)	27(1)	-2(1)	13(1)	1(1)
C(20)	36(1)	22(1)	31(1)	6(1)	20(1)	5(1)
C(21)	37(1)	33(1)	32(1)	-7(1)	18(1)	-14(1)
C(22)	27(1)	56(2)	31(1)	-2(1)	11(1)	-10(1)
C(23)	28(1)	54(2)	33(1)	3(1)	13(1)	5(1)
C(24)	43(1)	31(1)	29(1)	0(1)	17(1)	7(1)
C(25)	28(1)	25(1)	20(1)	-5(1)	11(1)	-4(1)
Cl	45(1)	29(1)	22(1)	2(1)	15(1)	2(1)
O	62(1)	47(1)	47(1)	14(1)	36(1)	11(1)

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10.1.3. Hydrochlorid **60**Tabelle 10.7 Kristallographische Daten und Strukturverfeinerung von **60**.

Verbindung	<b>60</b>
Empirische Formel	C <sub>15</sub> H <sub>26</sub> ClNSi
Formelmass [g/mol]	283.91
Temperatur [K]	173(2)
Wellenlänge [Å]	0.71073
Kristallsystem	triklin
Raumgruppe	<i>P1</i> (2)
<i>a</i> [Å]	7.0162(4)
<i>b</i> [Å]	10.6029(6)
<i>c</i> [Å]	12.2372(8)
$\alpha$ [°]	67.423(6)
$\beta$ [°]	74.773(5)
$\gamma$ [°]	85.123(5)
Zellvolumen [Å <sup>3</sup> ]	810.94(8)
Formeleinheit pro Zelle	2
Berechnete Dichte [g/cm <sup>3</sup> ]	1.163
Absorptionskoeffizient $\mu$ [mm <sup>-1</sup> ]	0.295
F(000)	308
Kristallgröße [mm <sup>3</sup> ]	0.20 x 0.20 x 0.05
Messbereich $\Theta$ [°]	3.01 – 27.00
	-8 ≤ <i>h</i> ≤ 8
Index-Breite	-13 ≤ <i>k</i> ≤ 13
	-15 ≤ <i>l</i> ≤ 15
Gemessene Reflexe	17947
Unabhängige Reflexe	3525 ( <i>R</i> <sub>int</sub> = 0.0433)
Daten / Restraints / Parameter	3525 / 0 / 169
Goodness-of-fit an <i>F</i> <sup>2</sup>	1.020
Endgültige <i>R</i> -Werte [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	<i>R</i> 1 = 0.0354, <i>wR</i> 2 = 0.0807
<i>R</i> -Werte (sämtliche Daten)	<i>R</i> 1 = 0.0495, <i>wR</i> 2 = 0.0882
Restelektronendichte [e/Å <sup>3</sup> ]	0.281 and -0.205 e.Å <sup>-3</sup>

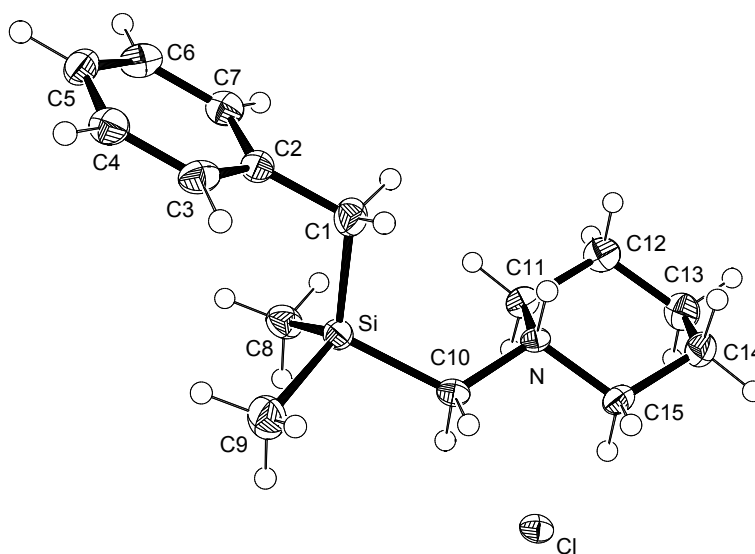


Abbildung 10.3 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von **60** im Kristall (ORTEP-Darstellung<sup>[206,207]</sup>). Das Nummerierungsschema der Wasserstoffatome wurde der Übersichtlichkeit halber weggelassen.

Tabelle 10.8 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **60**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\text{ij}}$ -Tensors.

	x	y	z	$U(\text{eq})$
Si	3330(1)	3407(1)	2878(1)	22(1)
N	3139(2)	6101(1)	3099(1)	18(1)
C(1)	871(2)	3709(2)	2490(2)	32(1)
C(2)	356(2)	2690(2)	2023(2)	25(1)
C(3)	-594(2)	1457(2)	2823(2)	28(1)
C(4)	-1115(3)	531(2)	2397(2)	29(1)
C(5)	-674(2)	823(2)	1154(2)	29(1)
C(6)	290(2)	2036(2)	343(2)	30(1)
C(7)	800(2)	2959(2)	776(2)	28(1)
C(8)	5339(3)	3512(2)	1509(2)	32(1)
C(9)	3376(3)	1707(2)	4111(2)	39(1)
C(10)	3725(2)	4635(2)	3589(1)	22(1)
C(11)	4288(2)	6849(2)	1810(1)	23(1)
C(12)	3703(3)	8337(2)	1345(2)	30(1)
C(13)	3973(3)	9050(2)	2168(2)	33(1)
C(14)	2801(3)	8276(2)	3469(2)	30(1)
C(15)	3382(2)	6794(2)	3926(2)	23(1)
Cl	8731(1)	6547(1)	3159(1)	25(1)
H(16)	1820(30)	6131(19)	3128(16)	29(5)

Tabelle 10.9 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **60**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Si	23(1)	22(1)	21(1)	-8(1)	-6(1)	2(1)
N	15(1)	22(1)	18(1)	-7(1)	-5(1)	-1(1)
C(1)	24(1)	35(1)	45(1)	-25(1)	-10(1)	4(1)
C(2)	17(1)	30(1)	33(1)	-16(1)	-8(1)	4(1)
C(3)	23(1)	37(1)	24(1)	-12(1)	-5(1)	0(1)
C(4)	26(1)	27(1)	32(1)	-7(1)	-8(1)	-3(1)
C(5)	26(1)	34(1)	33(1)	-19(1)	-9(1)	1(1)
C(6)	24(1)	43(1)	24(1)	-14(1)	-4(1)	-1(1)
C(7)	21(1)	29(1)	30(1)	-7(1)	-5(1)	-4(1)
C(8)	29(1)	37(1)	28(1)	-13(1)	-6(1)	7(1)
C(9)	55(1)	26(1)	32(1)	-5(1)	-11(1)	-2(1)
C(10)	23(1)	23(1)	18(1)	-4(1)	-8(1)	2(1)
C(11)	23(1)	26(1)	18(1)	-5(1)	-2(1)	-4(1)
C(12)	36(1)	23(1)	24(1)	-1(1)	-6(1)	-7(1)
C(13)	36(1)	24(1)	39(1)	-9(1)	-10(1)	-6(1)
C(14)	31(1)	28(1)	35(1)	-17(1)	-10(1)	1(1)
C(15)	21(1)	30(1)	21(1)	-12(1)	-7(1)	0(1)
Cl	16(1)	31(1)	27(1)	-9(1)	-5(1)	1(1)

#### 10.1.4. Hydrochlorid **61**

Tabelle 10.10 Kristallographische Daten und Strukturverfeinerung von **61**.

Verbindung	<b>61</b>
Empirische Formel	$C_{12}H_{28}ClNSi$
Formelmasse [g/mol]	249.89
Temperatur [K]	173(2)
Wellenlänge [ $\text{\AA}$ ]	0.71073
Kristallsystem	monoklin
Raumgruppe	$P2_1/c$
$a$ [ $\text{\AA}$ ]	7.0110(6)
$b$ [ $\text{\AA}$ ]	9.3151(12)

$c$ [Å]	23.383(2)
$\beta$ [°]	92.143(8)
Zellvolumen [Å <sup>3</sup> ]	1526.1(3)
Formeleinheit pro Zelle	4
Berechnete Dichte [g/cm <sup>3</sup> ]	1.088
Absorptionskoeffizient $\mu$ [mm <sup>-1</sup> ]	0.305
F(000)	552
Kristallgröße [mm <sup>3</sup> ]	0.50 x 0.05 x 0.03
Messbereich $2\theta$ [°]	2.35 – 26.99
	$-8 \leq h \leq 8$
Index-Breite	$-11 \leq k \leq 10$
	$-29 \leq l \leq 29$
Gemessene Reflexe	11161
Unabhängige Reflexe	3303 ( $R_{\text{int}} = 0.0535$ )
Daten / Restraints / Parameter	3303 / 0 / 143
Goodness-of-fit an $F^2$	1.093
Endgültige R-Werte [ $I > 2\sigma(I)$ ]	$R1 = 0.0505$ , $wR2 = 0.1209$
R-Werte (sämtliche Daten)	$R1 = 0.0680$ , $wR2 = 0.1333$
Restelektronendichte [e/Å <sup>3</sup> ]	0.470 and $-0.289$ e.Å <sup>-3</sup>

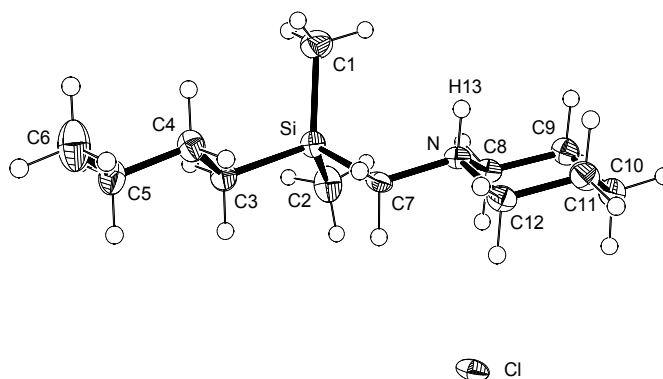


Abbildung 10.4 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von **61** im Kristall (ORTEP-Darstellung<sup>[206,207]</sup>). Das Nummerierungsschema der Wasserstoffatome wurde der Übersichtlichkeit halber weggelassen.

Tabelle 10.11 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{Å}^2 \cdot 10^3$ ] von **61**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\text{ij}}$ -Tensors.

	x	y	z	$U(\text{eq})$
Si	2469(1)	3506(1)	8731(1)	25(1)
N	2211(3)	3795(2)	7467(1)	20(1)
C(1)	-100(4)	3065(3)	8793(1)	38(1)

C(2)	3981(4)	1877(3)	8837(1)	37(1)
C(3)	3280(3)	4860(3)	9277(1)	30(1)
C(4)	2191(4)	6281(3)	9296(1)	31(1)
C(5)	2959(4)	7298(3)	9758(1)	33(1)
C(6)	1886(5)	8713(3)	9769(1)	49(1)
C(7)	2955(3)	4413(3)	8023(1)	23(1)
C(8)	2857(3)	2281(3)	7382(1)	23(1)
C(9)	2199(3)	1709(3)	6802(1)	28(1)
C(10)	2846(3)	2664(3)	6319(1)	33(1)
C(11)	2113(3)	4183(3)	6410(1)	30(1)
C(12)	2823(3)	4748(3)	6987(1)	25(1)
Cl	7850(1)	3525(1)	7295(1)	30(1)
H(13)	910(40)	3800(30)	7458(10)	31(7)

Tabelle 10.12 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **61**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Si	27(1)	21(1)	26(1)	0(1)	1(1)	1(1)
N	18(1)	14(1)	27(1)	0(1)	2(1)	-1(1)
C(1)	35(1)	42(2)	38(1)	4(1)	5(1)	-9(1)
C(2)	49(2)	27(2)	35(1)	0(1)	-3(1)	10(1)
C(3)	31(1)	28(2)	30(1)	-2(1)	-1(1)	6(1)
C(4)	34(1)	28(2)	30(1)	-3(1)	-2(1)	6(1)
C(5)	40(1)	32(2)	27(1)	-5(1)	0(1)	8(1)
C(6)	75(2)	32(2)	39(2)	-6(1)	-6(1)	11(2)
C(7)	21(1)	21(1)	28(1)	-2(1)	1(1)	-3(1)
C(8)	23(1)	15(1)	32(1)	0(1)	0(1)	1(1)
C(9)	26(1)	23(1)	34(1)	-7(1)	-1(1)	0(1)
C(10)	30(1)	39(2)	29(1)	-5(1)	1(1)	-5(1)
C(11)	32(1)	31(2)	28(1)	5(1)	-2(1)	-5(1)
C(12)	26(1)	21(1)	29(1)	5(1)	1(1)	-5(1)
Cl	18(1)	26(1)	47(1)	-4(1)	0(1)	0(1)

10.1.5. Hydrochlorid *rac*-**84**Tabelle 10.13 Kristallographische Daten und Strukturverfeinerung von *rac*-**84**.

Verbindung	<i>rac</i> - <b>84</b>
Empirische Formel	C <sub>17</sub> H <sub>30</sub> ClNSi
Formelmass [g/mol]	311.96
Temperatur [K]	173(2) K
Wellenlänge [Å]	0.71073 Å
Kristallsystem	monoklin
Raumgruppe	P2 <sub>1</sub> /n (14)
<i>a</i> [Å]	14.6577(14)
<i>b</i> [Å]	7.1815(6)
<i>c</i> [Å]	17.7092(18)
$\beta$ [°]	101.251(9)
Zellvolumen [Å <sup>3</sup> ]	1828.3(3)
Formeleinheit pro Zelle	4
Berechnete Dichte [g/cm <sup>3</sup> ]	1.133
Absorptionskoeffizient $\mu$ [mm <sup>-1</sup> ]	0.267
F(000)	680
Kristallgröße [mm <sup>3</sup> ]	0.30 x 0.30 x 0.20
Messbereich 2 $\theta$ [°]	2.35 – 26.00
Index-Breite	-18 ≤ <i>h</i> ≤ 18 -8 ≤ <i>k</i> ≤ 8 -19 ≤ <i>l</i> ≤ 21
Gemessene Reflexe	13648
Unabhängige Reflexe	3582 (R <sub>int</sub> = 0.0541)
Daten / Restraints / Parameter	3582 / 0 / 187
Goodness-of-fit an F <sup>2</sup>	1.063
Endgültige R-Werte [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	R1 = 0.0618, wR2 = 0.1394
R-Werte (sämtliche Daten)	R1 = 0.0993, wR2 = 0.1585
Restelektronendichte [e/Å <sup>3</sup> ]	0.514 and -0.342 e.Å <sup>-3</sup>

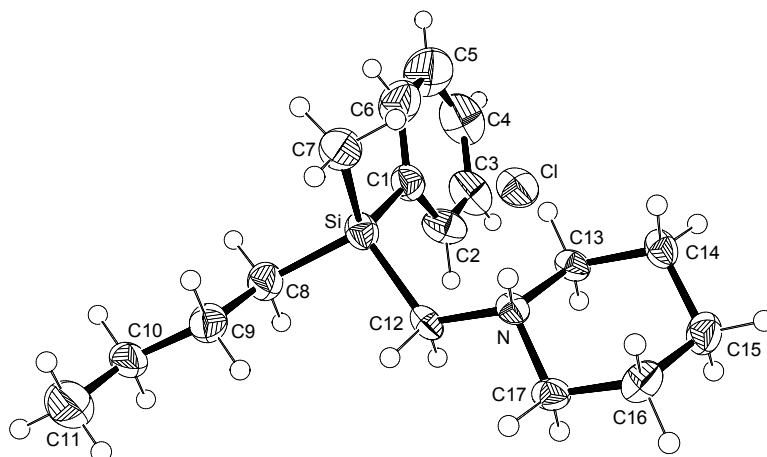


Abbildung 10.5 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von *rac*-**84** im Kristall (ORTEP-Darstellung<sup>[206,207]</sup>). Das Nummerierungsschema der Wasserstoffatome wurde der Übersichtlichkeit halber weggelassen.

Tabelle 10.14 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von *rac*-**84**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\text{ij}}$ -Tensors.

	x	y	z	U(eq)
Si	8800(1)	7710(1)	1563(1)	35(1)
N	10667(2)	7226(4)	1175(2)	27(1)
C(1)	9061(2)	8799(5)	2548(2)	40(1)
C(2)	9474(3)	10540(5)	2665(2)	47(1)
C(3)	9626(3)	11406(7)	3397(2)	59(1)
C(4)	9363(3)	10517(8)	4000(3)	69(1)
C(5)	8949(4)	8785(9)	3903(3)	75(2)
C(6)	8796(3)	7958(7)	3175(2)	58(1)
C(7)	8600(3)	5178(5)	1645(2)	51(1)
C(8)	7749(2)	8916(5)	1003(2)	42(1)
C(9)	7372(2)	8125(5)	213(2)	42(1)
C(10)	6491(3)	9109(6)	-218(2)	50(1)
C(11)	6168(3)	8262(7)	-993(2)	68(1)
C(12)	9730(2)	8165(4)	976(2)	30(1)
C(13)	11187(2)	7781(5)	1956(2)	31(1)
C(14)	12118(2)	6779(5)	2148(2)	35(1)
C(15)	12708(2)	7133(5)	1541(2)	41(1)
C(16)	12151(2)	6610(5)	747(2)	40(1)
C(17)	11235(2)	7633(5)	576(2)	35(1)
Cl	683(1)	2896(1)	1178(1)	35(1)
H(25)	10590(20)	6070(50)	1181(17)	21(9)

Tabelle 10.15 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von *rac*-**84**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Si	34(1)	31(1)	39(1)	0(1)	2(1)	3(1)
N	31(2)	19(2)	30(2)	2(1)	0(1)	-2(1)
C(1)	37(2)	47(2)	36(2)	1(2)	8(2)	10(2)
C(2)	60(3)	44(2)	38(2)	-1(2)	14(2)	11(2)
C(3)	67(3)	60(3)	47(3)	-11(2)	4(2)	19(2)
C(4)	73(3)	95(4)	42(3)	-14(3)	15(2)	26(3)
C(5)	80(4)	103(4)	47(3)	-3(3)	26(2)	-3(3)
C(6)	51(3)	78(3)	47(3)	-3(2)	15(2)	-7(2)
C(7)	49(2)	40(2)	62(3)	9(2)	7(2)	4(2)
C(8)	36(2)	40(2)	48(2)	2(2)	1(2)	2(2)
C(9)	40(2)	37(2)	47(2)	3(2)	5(2)	-1(2)
C(10)	53(2)	46(2)	44(2)	12(2)	-5(2)	-14(2)
C(11)	72(3)	71(3)	53(3)	10(2)	-9(2)	-18(2)
C(12)	34(2)	23(2)	31(2)	1(1)	-1(1)	1(1)
C(13)	36(2)	27(2)	26(2)	1(1)	-1(1)	-3(1)
C(14)	34(2)	31(2)	37(2)	2(2)	-4(2)	-1(1)
C(15)	33(2)	41(2)	49(2)	-1(2)	5(2)	-6(2)
C(16)	39(2)	41(2)	42(2)	-6(2)	13(2)	-9(2)
C(17)	40(2)	33(2)	30(2)	4(1)	4(1)	-8(2)
Cl	42(1)	22(1)	38(1)	1(1)	-1(1)	-4(1)

10.1.6. (R,R)-**91**Tabelle 10.16 Kristallographische Daten und Strukturverfeinerung von (R,R)-**91**.

Verbindung	(R,R)- <b>91</b>
CCDC Nummer	1005510
Empirische Formel	$C_{30}H_{41}LiN_2Si$
Formelmasse [g/mol]	464.68
Temperatur [K]	173(2)
Wellenlänge [ $\text{\AA}$ ]	0.71073
Kristallsystem	monoklin
Raumgruppe	$P2_1$ (4)
$a$ [ $\text{\AA}$ ]	9.7688(4)
$b$ [ $\text{\AA}$ ]	18.6214(8)
$c$ [ $\text{\AA}$ ]	15.1899(8)

$\theta$ [°]	90.859(4)
Zellvolumen [Å <sup>3</sup> ]	2762.8(2)
Formeleinheit pro Zelle	Z = 4
Berechnete Dichte [g/cm <sup>3</sup> ]	1.117
Absorptionskoeffizient $\mu$ [mm <sup>-1</sup> ]	0.105
F(000)	1008
Kristallgröße [mm <sup>3</sup> ]	0.40 x 0.30 x 0.20
Messbereich $\Theta$ [°]	2.35 – 26.00
	-12 ≤ h ≤ 12
Index-Breite	-22 ≤ k ≤ 22
	-17 ≤ l ≤ 18
Gemessene Reflexe	22783
Unabhängige Reflexe	10464 ( $R_{int} = 0.0377$ )
Daten / Restraints / Parameter	10464 / 1 / 631
Goodness-of-fit an $F^2$	1.000
Endgültige R-Werte [ $I > 2\sigma(I)$ ]	$R1 = 0.0408$ , $wR2 = 0.0554$
R-Werte (sämtliche Daten)	$R1 = 0.0740$ , $wR2 = 0.0578$
Absoluter Strukturparameter	-0.31(11)
Restelektronendichte [e/Å <sup>3</sup> ]	0.433 und -0.323

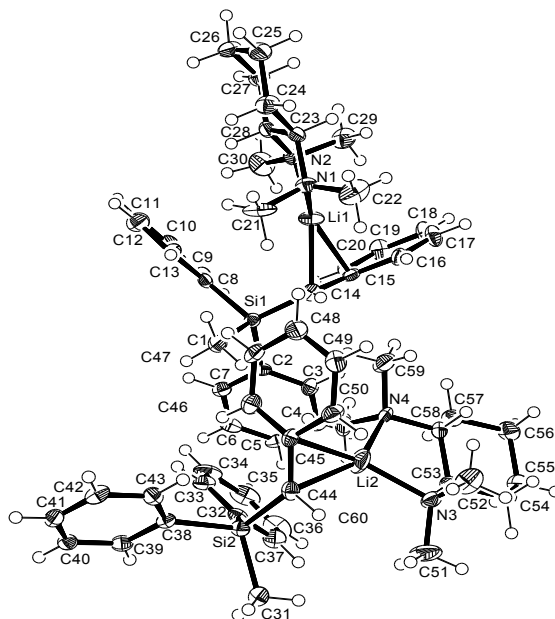


Abbildung 10.6 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von (*R,R*)-**91** im Kristall, zwei Moleküle in der asymmetrischen Einheit (ORTEP-Darstellung<sup>[206,207]</sup>). Das Nummerierungsschema der Wasserstoffatome wurde der Übersichtlichkeit halber weggelassen.

Tabelle 10.17 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von (R,R)-**91**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\text{H}}$ -Tensors.

	x	y	z	$U(\text{eq})$
C(1)	3719(3)	8046(2)	6540(2)	27(1)
C(2)	2966(3)	9470(2)	7374(2)	21(1)
C(3)	3647(3)	10120(2)	7255(2)	24(1)
C(4)	2965(3)	10757(2)	7096(2)	29(1)
C(5)	1557(3)	10751(2)	7072(2)	30(1)
C(6)	849(3)	10125(2)	7190(2)	30(1)
C(7)	1542(3)	9489(2)	7347(2)	24(1)
C(8)	3043(3)	8113(2)	8451(2)	22(1)
C(9)	2366(3)	8445(2)	9131(3)	27(1)
C(10)	1770(3)	8069(2)	9809(3)	34(1)
C(11)	1815(3)	7337(2)	9820(3)	36(1)
C(12)	2456(4)	6974(2)	9145(3)	36(1)
C(13)	3060(3)	7359(2)	8476(3)	30(1)
C(14)	5742(3)	8745(2)	7756(3)	23(1)
C(15)	6391(3)	9194(2)	8390(3)	23(1)
C(16)	7836(3)	9290(2)	8436(3)	25(1)
C(17)	8473(3)	9672(2)	9107(3)	31(1)
C(18)	7754(4)	9985(2)	9772(3)	34(1)
C(19)	6331(4)	9910(2)	9751(3)	35(1)
C(20)	5684(3)	9529(2)	9094(3)	26(1)
C(21)	6976(4)	6809(2)	7599(3)	43(1)
C(22)	9183(3)	7361(2)	7749(2)	48(1)
C(23)	8212(3)	6740(2)	9017(2)	24(1)
C(24)	8498(3)	5945(2)	8850(3)	33(1)
C(25)	8815(3)	5547(2)	9706(2)	37(1)
C(26)	7660(3)	5622(2)	10354(2)	40(1)
C(27)	7416(3)	6414(2)	10533(2)	30(1)
C(28)	7078(3)	6831(1)	9696(2)	23(1)
C(29)	7889(3)	7991(2)	10319(2)	37(1)
C(30)	5504(3)	7722(2)	10288(3)	45(1)
C(31)	3624(3)	9169(2)	1575(2)	26(1)
C(32)	2979(3)	9084(2)	3487(2)	22(1)
C(33)	2344(3)	8739(2)	4191(3)	28(1)
C(34)	1817(3)	9120(2)	4891(3)	36(1)
C(35)	1905(4)	9871(3)	4896(3)	40(1)
C(36)	2500(4)	10215(2)	4217(3)	39(1)
C(37)	3031(3)	9827(2)	3519(3)	31(1)
C(38)	2878(3)	7733(2)	2384(2)	19(1)

C(39)	1444(3)	7740(2)	2303(2)	24(1)
C(40)	711(3)	7130(2)	2084(2)	25(1)
C(41)	1400(3)	6491(2)	1927(2)	27(1)
C(42)	2803(3)	6472(2)	2006(2)	27(1)
C(43)	3531(3)	7088(2)	2234(2)	24(1)
C(44)	5680(3)	8446(2)	2770(3)	23(1)
C(45)	6344(3)	7992(2)	3392(3)	21(1)
C(46)	5663(3)	7614(2)	4076(3)	28(1)
C(47)	6349(3)	7213(2)	4687(3)	30(1)
C(48)	7758(3)	7143(2)	4692(3)	34(1)
C(49)	8457(3)	7499(2)	4034(3)	30(1)
C(50)	7779(3)	7899(2)	3413(3)	28(1)
C(51)	7029(4)	10392(2)	2469(3)	49(1)
C(52)	9074(3)	9880(2)	3082(2)	42(1)
C(53)	7531(3)	10584(2)	4035(2)	23(1)
C(54)	8389(3)	11268(2)	3995(2)	29(1)
C(55)	8152(3)	11750(2)	4774(2)	33(1)
C(56)	8438(3)	11357(1)	5636(2)	33(1)
C(57)	7547(3)	10688(2)	5687(2)	28(1)
C(58)	7800(3)	10191(1)	4907(2)	22(1)
C(59)	7785(3)	8984(2)	5509(3)	36(1)
C(60)	5631(3)	9565(2)	5218(3)	38(1)
Li(1)	6788(6)	8028(4)	8626(4)	31(2)
Li(2)	6756(6)	9170(4)	3682(5)	39(2)
N(1)	7917(3)	7168(2)	8223(2)	26(1)
N(2)	6801(3)	7605(2)	9843(2)	26(1)
N(3)	7647(3)	10094(2)	3263(2)	30(1)
N(4)	7068(2)	9498(2)	4921(2)	24(1)
Si(2)	3874(1)	8591(1)	2571(1)	21(1)
Si(1)	3948(1)	8611(1)	7545(1)	20(1)
H(14)	6220(20)	8641(16)	7351(18)	13(9)
H(44)	6320(20)	8621(15)	2186(18)	23(8)

Tabelle 10.18 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von  $(R,R)$ -**91**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
C(1)	35(2)	24(2)	21(2)	-3(2)	-3(2)	-5(2)
C(2)	26(2)	23(2)	13(2)	1(2)	0(2)	4(2)
C(3)	24(2)	23(2)	26(2)	-1(2)	4(2)	-1(2)
C(4)	39(2)	21(2)	27(2)	2(2)	-1(2)	-1(2)

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C(5)	47(2)	20(2)	22(2)	5(2)	4(2)	10(2)
C(6)	29(2)	40(2)	20(2)	-3(2)	-5(2)	10(2)
C(7)	32(2)	20(2)	21(2)	1(2)	-1(2)	1(2)
C(8)	19(2)	25(2)	21(2)	-2(2)	-5(2)	-3(2)
C(9)	22(2)	29(3)	31(3)	3(2)	-2(2)	-3(2)
C(10)	25(2)	55(3)	21(3)	-6(2)	2(2)	-8(2)
C(11)	31(2)	46(3)	29(3)	16(2)	4(2)	-13(2)
C(12)	51(2)	31(3)	26(3)	-1(2)	-3(2)	-4(2)
C(13)	35(2)	25(3)	30(3)	5(2)	4(2)	-2(2)
C(14)	25(2)	24(2)	19(3)	-2(2)	6(2)	2(2)
C(15)	26(2)	20(2)	21(3)	9(2)	1(2)	2(2)
C(16)	17(2)	23(2)	34(3)	6(2)	5(2)	-3(2)
C(17)	17(2)	34(3)	42(3)	-5(2)	0(2)	-2(2)
C(18)	34(2)	30(3)	36(3)	-10(2)	-8(2)	-10(2)
C(19)	33(2)	34(2)	37(3)	-4(2)	4(2)	1(2)
C(20)	18(2)	25(2)	33(3)	-4(2)	-1(2)	-4(2)
C(21)	69(3)	35(2)	24(2)	7(2)	-8(2)	23(2)
C(22)	51(2)	47(3)	47(3)	6(2)	25(2)	12(2)
C(23)	23(2)	26(2)	24(2)	0(1)	-6(2)	2(1)
C(24)	39(2)	22(2)	37(3)	-1(2)	-1(2)	9(2)
C(25)	40(2)	18(2)	52(3)	-1(2)	-15(2)	7(2)
C(26)	50(2)	29(2)	39(2)	14(2)	-14(2)	-5(2)
C(27)	31(2)	31(2)	27(2)	4(2)	0(2)	2(2)
C(28)	19(2)	23(2)	26(2)	-1(1)	-2(1)	0(1)
C(29)	48(2)	21(2)	41(3)	-5(2)	1(2)	4(2)
C(30)	33(2)	52(3)	49(3)	-6(2)	9(2)	11(2)
C(31)	30(2)	24(2)	24(3)	-3(2)	3(2)	0(2)
C(32)	21(2)	28(3)	17(2)	-4(2)	-3(2)	3(2)
C(33)	28(2)	31(3)	24(3)	7(2)	-2(2)	6(2)
C(34)	35(2)	57(3)	16(2)	3(2)	0(2)	14(2)
C(35)	39(2)	57(3)	25(3)	-13(2)	-3(2)	21(2)
C(36)	43(2)	26(3)	50(3)	-22(2)	-5(2)	20(2)
C(37)	33(2)	33(3)	27(3)	-1(2)	2(2)	3(2)
C(38)	26(2)	17(2)	14(2)	-1(2)	2(2)	2(2)
C(39)	26(2)	24(2)	21(3)	1(2)	2(2)	6(2)
C(40)	24(2)	30(2)	20(2)	5(2)	0(2)	-2(2)
C(41)	41(2)	24(2)	16(2)	-1(2)	-2(2)	-11(2)
C(42)	39(2)	19(2)	24(2)	1(2)	8(2)	6(2)
C(43)	23(2)	28(2)	20(2)	-1(2)	2(2)	0(2)
C(44)	24(2)	23(2)	22(3)	-4(2)	2(2)	-4(2)
C(45)	24(2)	13(2)	25(3)	-2(2)	3(2)	1(2)

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C(46)	30(2)	24(2)	31(3)	-4(2)	2(2)	-1(2)
C(47)	38(2)	21(2)	31(3)	7(2)	4(2)	-4(2)
C(48)	33(2)	25(2)	43(3)	3(2)	-6(2)	2(2)
C(49)	26(2)	18(2)	47(3)	-5(2)	-1(2)	5(2)
C(50)	31(2)	22(2)	31(3)	7(2)	2(2)	2(2)
C(51)	75(3)	51(3)	21(2)	9(2)	-11(2)	1(2)
C(52)	58(2)	39(2)	30(2)	-6(2)	15(2)	-1(2)
C(53)	27(2)	22(2)	18(2)	-1(1)	-1(2)	-2(1)
C(54)	34(2)	28(2)	25(2)	7(2)	-5(2)	-5(2)
C(55)	44(2)	23(2)	31(2)	-1(2)	-9(2)	-4(2)
C(56)	42(2)	31(2)	25(2)	-7(2)	-6(2)	-3(2)
C(57)	36(2)	27(2)	20(2)	-3(2)	-4(2)	-1(2)
C(58)	20(2)	23(2)	23(2)	1(1)	-1(1)	-4(1)
C(59)	48(2)	27(2)	34(3)	8(2)	-1(2)	-5(2)
C(60)	37(2)	40(2)	38(3)	-1(2)	-1(2)	-19(2)
Li(1)	42(4)	34(4)	17(4)	1(3)	-3(3)	9(3)
Li(2)	52(4)	25(4)	41(5)	-4(3)	4(4)	-12(3)
N(1)	34(2)	26(2)	19(2)	3(1)	-1(1)	3(1)
N(2)	23(1)	31(2)	24(2)	1(1)	2(1)	7(1)
N(3)	40(2)	28(2)	20(2)	6(2)	-2(1)	-8(1)
N(4)	27(1)	19(2)	24(2)	6(1)	3(1)	-9(1)
Si(2)	24(1)	19(1)	19(1)	-2(1)	-2(1)	2(1)
Si(1)	23(1)	16(1)	21(1)	0(1)	0(1)	1(1)

## 10.1.7. 94a

Tabelle 10.19 Kristallographische Daten und Strukturverfeinerung von **94a**.

Verbindung	<b>94a</b>
Empirische Formel	C <sub>21</sub> H <sub>40</sub> LiN <sub>3</sub> Si
Formelmass [g/mol]	369.59
Temperatur [K]	173.15
Wellenlänge [Å]	0.71073
Kristallsystem	monoklin
Raumgruppe	<i>P</i> 2 <sub>1</sub> / <i>n</i> (14)
<i>a</i> [Å]	17.2976(17)
<i>b</i> [Å]	17.0490(9)
<i>c</i> [Å]	17.6035(17)
$\beta$ [°]	116.317(12)

Zellvolumen [ $\text{\AA}^3$ ]	4653.3(8)
Formeleinheit pro Zelle	Z = 8
Berechnete Dichte [ $\text{g/cm}^3$ ]	1.055
Absorptionskoeffizient $\mu$ [ $\text{mm}^{-1}$ ]	0.110
F(000)	1632.0
Kristallgröße [ $\text{mm}^3$ ]	$0.3 \times 0.2 \times 0.2$
Messbereich $2\theta$ [ $^\circ$ ]	4.778 – 51.996
Index-Breite	$-21 \leq h \leq 18$ $-21 \leq k \leq 21$ $-21 \leq l \leq 21$
Gemessene Reflexe	34111
Unabhängige Reflexe	9134 ( $R_{\text{int}} = 0.0562$ )
Daten / Restraints / Parameter	9134 / 0 / 489
Goodness-of-fit an $F^2$	1.028
Endgültige R-Werte [ $I > 2\sigma(I)$ ]	$R1 = 0.0526$ , $wR2 = 0.1236$
R-Werte (sämtliche Daten)	$R1 = 0.0970$ , $wR2 = 0.1481$
Restelektronendichte [ $\text{e}/\text{\AA}^3$ ]	0.38 und $-0.25$

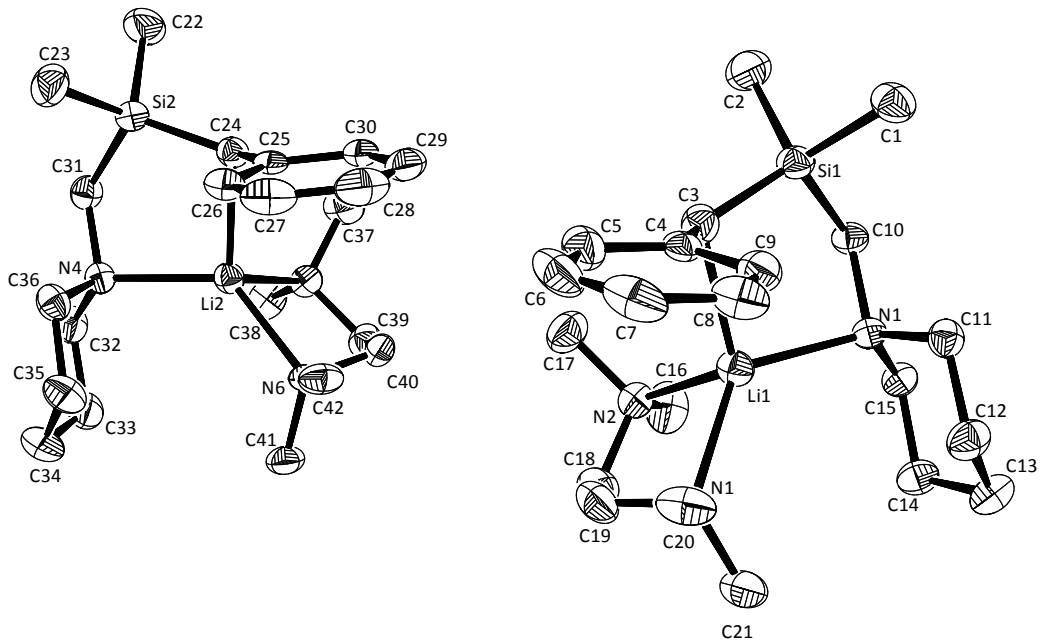


Abbildung 10.7 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von **94a** im monoklinen Kristallsystem (links). Die Abbildung der Wasserstoffatome der Übersichtlichkeit halber weggelassen (ORTEP-Darstellung<sup>[206,207]</sup>).

Tabelle 10.20 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **94a**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\text{H}}$ -Tensors.

	x	y	z	$U(\text{eq})$
H3	6462(17)	5716(14)	8234(15)	47(7)
H24	1975(14)	6206(12)	8215(14)	28(6)
Li1	7452(3)	7025(2)	8531(2)	28.8(8)
Li2	1630(2)	7523(2)	7552(2)	27.7(8)
C1	8701.7(16)	4691.1(13)	9546.4(15)	36.3(6)
C2	7181.0(18)	4918.0(15)	9921.2(17)	45.4(7)
C3	7092.7(17)	5706.2(13)	8338.5(15)	33.1(6)
C4	7117.7(15)	5537.8(11)	7545.3(14)	26.8(5)
C5	6349.9(17)	5437.0(13)	6785.8(16)	40.2(6)
C6	6355(2)	5289.6(14)	6015.2(16)	46.4(7)
C7	7108(2)	5235.1(14)	5951.5(16)	46.5(7)
C8	7881.8(19)	5334.0(14)	6681.3(16)	42.3(7)
C9	7883.5(17)	5478.7(13)	7451.2(15)	34.9(6)
C10	8275.8(15)	6283.4(12)	10116.6(14)	26.8(5)
C11	9334.6(15)	6678.4(13)	9654.3(15)	29.0(5)
C12	9651.2(16)	7318.9(13)	9271.2(16)	36.5(6)
C13	9873.0(17)	8063.5(14)	9804.0(17)	39.7(6)
C14	9126.7(16)	8294.0(13)	9999.6(16)	33.3(6)
C15	8837.2(15)	7605.5(12)	10353.2(14)	27.7(5)
C16	6531.0(18)	8144.3(16)	9299.3(18)	51.6(7)
C17	5662.7(17)	7168.2(15)	8326.8(18)	44.5(7)
C18	6180.3(18)	8275.8(14)	7826.7(17)	43.8(7)
C19	6387.2(17)	7948.7(16)	7150.2(16)	44.6(7)
C20	7409.3(19)	7355.6(14)	6769.5(16)	43.9(7)
C21	7812.0(18)	8498.7(13)	7616.1(16)	40.8(6)
C22	392.6(18)	5353.5(16)	7929.6(18)	54.2(8)
C23	197.7(18)	5341.8(15)	6142.5(17)	48.0(7)
C24	1762.3(15)	6193.2(13)	7622.5(15)	27.8(5)
C25	2430.4(15)	6016.1(11)	7378.4(14)	26.8(5)
C26	2296.8(16)	5911.9(13)	6530.9(15)	33.4(6)
C27	2980(2)	5757.1(14)	6339.3(19)	45.6(7)
C28	3816(2)	5697.1(15)	6962(2)	51.0(8)
C29	3966.9(17)	5792.7(14)	7795(2)	45.0(7)
C30	3304.1(15)	5941.4(12)	7997.7(16)	33.4(6)
C31	-52.2(15)	6842.5(13)	6976.6(15)	31.3(5)
C32	-281.5(16)	8230.9(13)	6695.5(16)	34.9(6)
C33	8.7(18)	8970.9(14)	6436.0(17)	44.4(7)
C34	-33(2)	8885.7(15)	5562.5(18)	53.0(8)

C35	440.9(19)	8144.9(15)	5516.6(17)	45.8(7)
C36	152.4(16)	7432.1(14)	5835.6(14)	34.0(6)
C37	2310.6(19)	7387.1(15)	9434.6(15)	47.3(7)
C38	1367.2(17)	8486.9(15)	8898.6(17)	44.9(7)
C39	2780.6(16)	8520.5(14)	8936.8(15)	34.9(6)
C40	3234.7(15)	8220.5(14)	8433.3(15)	33.3(6)
C41	2477.6(16)	9053.8(13)	7219.8(16)	37.5(6)
C42	3117.7(17)	7867.9(13)	7072.1(16)	37.2(6)
N1	8575.7(11)	6934.7(10)	9762.2(11)	23.3(4)
N2	6386.0(12)	7711.4(11)	8530.6(12)	32.1(5)
N3	7309.4(13)	7773.2(10)	7450.4(12)	30.6(5)
N4	244.8(12)	7551.2(10)	6698.8(11)	26.5(4)
N5	2033.9(13)	8023.1(11)	8805.3(12)	30.7(5)
N6	2668.4(12)	8240(1)	7516.5(12)	26.9(4)
Si1	7808.0(4)	5396.8(3)	9400.8(4)	28.53(17)
Si2	635.4(4)	5926.9(4)	7149.5(4)	30.75(17)

Tabelle 10.21 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **94a**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	U33	U23	U13	U12		
C1	42.2(16)	28.0(12)	33.8(14)	-2.2(11)	12.3(12)	2.8(11)
C2	47.5(18)	40.6(15)	47.1(17)	0.4(13)	20.0(14)	-8.3(13)
C3	30.9(14)	31.4(13)	33.1(14)	-3.4(11)	10.7(12)	-0.7(11)
C4	31.8(14)	14.9(10)	30.6(13)	1.5(9)	11.2(11)	1.8(10)
C5	40.6(16)	30.1(13)	39.9(15)	-2.0(12)	8.9(13)	3.8(12)
C6	61(2)	34.5(14)	27.0(14)	2.8(11)	4.2(13)	9.9(14)
C7	80(2)	29.9(13)	27.4(14)	0.4(11)	22.1(15)	9.1(14)
C8	58.2(19)	31.7(13)	40.7(16)	4.4(12)	25.3(14)	5.0(13)
C9	38.6(15)	31.5(13)	31.6(14)	0.4(11)	12.8(12)	-0.6(11)
C10	31.9(13)	26.2(11)	23.9(12)	0.9(10)	13.9(10)	-1.1(10)
C11	27.3(13)	29.2(12)	30.7(13)	-2.3(10)	12.9(11)	1.5(10)
C12	36.1(15)	36.0(13)	46.8(15)	-1.4(12)	26.8(13)	-1.1(11)
C13	39.0(16)	37.9(14)	47.3(16)	-5.0(12)	23.7(13)	-11.1(12)
C14	40.2(15)	27.1(12)	35.0(14)	-5.7(11)	18.8(12)	-6.5(11)
C15	30.3(13)	25.7(11)	27.6(12)	-4.8(10)	13.5(11)	-2.9(10)
C16	46.0(18)	56.9(17)	54.7(18)	-15.8(15)	24.8(15)	4.5(14)
C17	34.8(16)	43.2(15)	59.8(18)	-1.9(14)	24.8(14)	-5.0(13)
C18	38.5(16)	36.3(14)	58.0(18)	10.7(13)	22.7(14)	10.3(12)
C19	43.6(17)	48.4(16)	35.5(15)	14.7(13)	11.9(13)	7.9(13)

C20	72(2)	29.2(13)	37.0(15)	2.0(11)	30.7(15)	0.3(13)
C21	52.3(18)	31.6(13)	34.7(14)	4.8(11)	15.7(13)	-1.7(12)
C22	44.5(18)	56.6(18)	61.5(19)	24.5(15)	23.6(16)	-1.7(14)
C23	42.1(17)	37.2(14)	51.9(17)	-11.7(13)	9.3(14)	-2.9(13)
C24	32.2(14)	26.0(12)	24.1(13)	0.4(10)	11.6(11)	0.1(10)
C25	31.9(13)	13.1(10)	34.1(13)	3.0(9)	13.5(11)	0.2(9)
C26	40.7(15)	24.7(12)	37.0(14)	2.6(10)	19.2(12)	1.8(11)
C27	67(2)	30.8(13)	56.7(18)	2.7(13)	43.6(17)	2.6(14)
C28	50.0(19)	32.7(14)	90(2)	8.8(15)	48.9(19)	6.1(13)
C29	33.9(16)	26.5(13)	72(2)	8.5(13)	21.1(15)	-0.5(12)
C30	32.6(14)	20.4(11)	43.7(15)	5.9(11)	13.7(12)	-1.3(10)
C31	29.0(14)	35.5(13)	31.2(13)	-1.1(11)	14.9(11)	-1.1(11)
C32	28.4(14)	32.3(13)	39.4(14)	-6.1(11)	10.8(11)	6.1(11)
C33	38.9(16)	30.1(13)	52.2(17)	0.7(12)	9.3(13)	8.1(12)
C34	55.4(19)	39.0(15)	55.7(19)	18.8(14)	16.8(15)	9.9(14)
C35	54.1(19)	49.1(16)	36.0(15)	11.3(13)	21.7(14)	6.4(14)
C36	35.9(15)	36.9(13)	26.8(13)	-0.4(11)	11.8(11)	3.8(11)
C37	66(2)	47.8(16)	27.4(14)	0.0(12)	20.4(14)	-7.9(14)
C38	47.5(17)	50.3(16)	47.6(17)	-16.3(13)	30.7(14)	-4.8(13)
C39	36.1(15)	34.0(13)	31.5(14)	-6.6(11)	12.2(12)	-5.9(11)
C40	26.1(14)	31.0(12)	38.8(14)	-0.8(11)	10.9(11)	-4.3(11)
C41	37.5(15)	24.2(12)	52.9(16)	6.9(11)	21.9(13)	-0.5(11)
C42	45.0(16)	30.5(13)	49.9(16)	7.2(12)	33.5(14)	1.2(11)
Li1	32(2)	28.7(19)	25(2)	-0.6(16)	12.3(17)	0.1(17)
Li2	28(2)	31(2)	24.6(19)	1.3(16)	12.3(17)	0.5(17)
N1	26.9(11)	21.4(9)	23.4(10)	-2.0(8)	12.8(8)	-1.6(8)
N2	29.8(12)	32.8(10)	33.6(11)	0.3(9)	14.1(9)	-1.7(9)
N3	39.3(13)	26.4(10)	26.9(10)	3.4(8)	15.5(9)	4.4(9)
N4	26.7(11)	26.6(10)	25.9(10)	-1.5(8)	11.3(9)	2.3(8)
N5	34.4(12)	33.5(10)	27.4(11)	-3.3(9)	16.4(9)	-3.7(9)
N6	30.9(11)	20.6(9)	34.3(11)	2.2(8)	19.0(9)	0.2(8)
Si1	32.8(4)	22.7(3)	27.6(4)	-1.0(3)	11.1(3)	-1.9(3)
Si2	31.6(4)	26.7(3)	32.9(4)	1.8(3)	13.4(3)	-2.3(3)

### 10.1.8. (*R,R*)-**94b** und (*S,R,R*)-**94b**

Tabelle 10.22 Kristallographische Daten und Strukturverfeinerung von (*R,R*)-**94b** und (*S,R,R*)-**94b**.

Verbindung	( <i>R,R</i> )- <b>94b</b>	( <i>S,R,R</i> )- <b>94b</b>
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CCDC Nummer	1005511	./.
Empirische Formel	C <sub>25</sub> H <sub>46</sub> LiN <sub>3</sub> Si	C <sub>25</sub> H <sub>46</sub> LiN <sub>3</sub> Si
Formelmasse [g/mol]	423.68	423.68
Temperatur [K]	173(2)	173(2)
Wellenlänge [Å]	0.71073	0.71073
Kristallsystem	triklin	monoklin
Raumgruppe	<i>P</i> 1 (1)	<i>P</i> 2 <sub>1</sub> (4)
<i>a</i> [Å]	8.9540(6)	9.707(3)
<i>b</i> [Å]	9.7970(6)	14.4272(12)
<i>c</i> [Å]	15.6114(11)	10.1090(18)
$\alpha$ [°]	89.457(6)	90
$\beta$ [°]	80.566(6)	115.73(3)
$\gamma$ [°]	73.495(6)	90
Zellvolumen [Å <sup>3</sup> ]	1294.28(16)	1275.4(5)
Formeleinheit pro Zelle	Z = 2	Z = 2
Berechnete Dichte [g/cm <sup>3</sup> ]	1.087	1.103
Absorptionskoeffizient $\mu$ [mm <sup>-1</sup> ]	0.106	0.108
F(000)	468	468
Kristallgröße [mm <sup>3</sup> ]	0.20 x 0.20 x 0.10	0.50 x 0.30 x 0.30
Messbereich $\Theta$ [°]	2.17 – 25.00	2.43 – 27.00
	-10 ≤ <i>h</i> ≤ 10	-12 ≤ <i>h</i> ≤ 11
Index-Breite	-11 ≤ <i>k</i> ≤ 11	-18 ≤ <i>k</i> ≤ 18
	-18 ≤ <i>l</i> ≤ 18	-12 ≤ <i>l</i> ≤ 12
Gemessene Reflexe	15594	10532
Unabhängige Reflexe	8906 ( <i>R</i> <sub>int</sub> = 0.0396)	5492 ( <i>R</i> <sub>int</sub> = 0.0224)
Daten / Restraints / Parameter	8906 / 3 / 560	5492 / 1 / 289
Goodness-of-fit an <i>F</i> <sup>2</sup>	0.924	0.965
Endgültige <i>R</i> -Werte [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	<i>R</i> 1 = 0.0508, <i>wR</i> 2 = 0.0936	<i>R</i> 1 = 0.0333, <i>wR</i> 2 = 0.0681
<i>R</i> -Werte (sämtliche Daten)	<i>R</i> 1 = 0.0955, <i>wR</i> 2 = 0.0991	<i>R</i> 1 = 0.0412, <i>wR</i> 2 = 0.0694
Absoluter Strukturparameter	0.19(17)	0.07(7)
Restelektronendichte [e/Å <sup>3</sup> ]	0.339 und -0.312	0.221 und -0.182

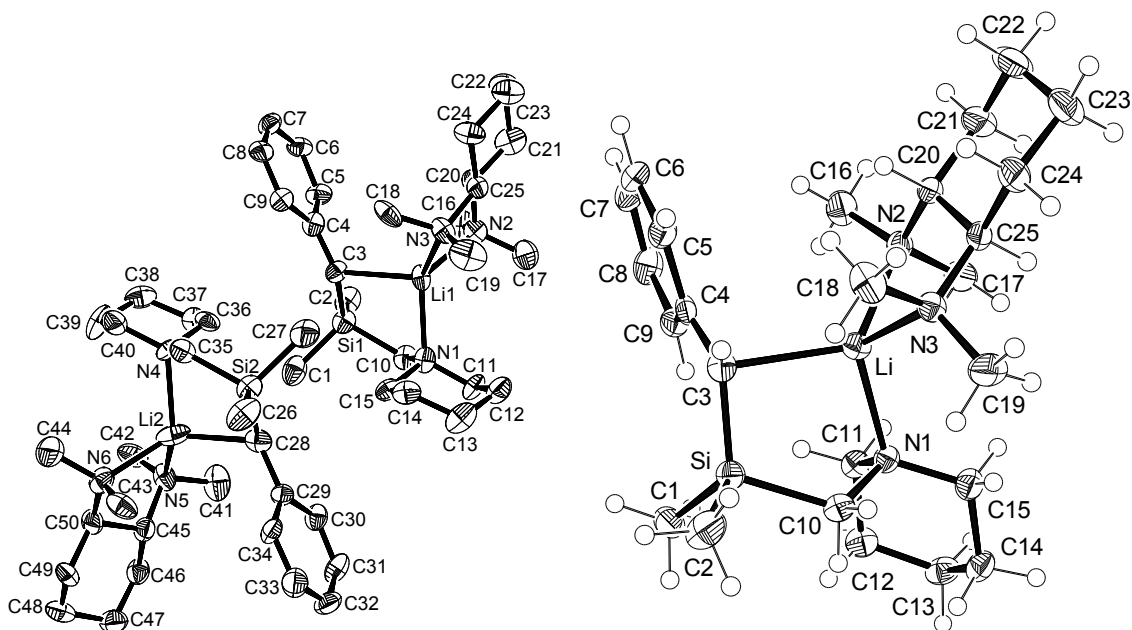


Abbildung 10.8 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von *(R,R)*-**94b** im triklinen Kristallsystem(links) und *(S,R,R)*-**94b** im monoklinen Kristallsystem (rechts). Die Abbildung der Wasserstoffatome bzw. Nummerierungsschema der Wasserstoffatome wurde der Übersichtlichkeit halber weggelassen (ORTEP-Darstellung<sup>[206,207]</sup>).

Tabelle 10.23 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von *(R,R)*-**94b**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\text{ij}}$ -Tensors.

	x	y	z	$U(\text{eq})$
H(3)	5400(60)	2980(50)	7670(30)	38
H(28)	6130(50)	2240(40)	4940(30)	11(8)
C(1)	8480(7)	3844(6)	6833(4)	53(2)
C(2)	8682(7)	3924(6)	8686(4)	48(2)
C(3)	5737(7)	3245(6)	8162(4)	32(2)
C(4)	4557(7)	4321(6)	8671(4)	35(2)
C(5)	4715(6)	4960(6)	9439(4)	40(2)
C(6)	3508(7)	5934(6)	9966(4)	40(2)
C(7)	2027(7)	6413(6)	9736(4)	41(2)
C(8)	1810(7)	5836(6)	8969(4)	37(2)
C(9)	3002(7)	4853(6)	8459(4)	34(2)
C(10)	9045(6)	1133(6)	7794(4)	36(2)
C(11)	9253(6)	-1326(5)	7527(4)	36(2)
C(12)	8474(7)	-2413(6)	7295(4)	48(2)
C(13)	7979(7)	-2114(6)	6411(4)	52(2)
C(14)	7030(7)	-591(6)	6371(4)	40(2)
C(15)	7896(6)	405(6)	6642(4)	34(2)

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C(16)	7001(7)	1260(7)	10191(4)	54(2)
C(17)	7189(7)	-1131(6)	9822(4)	56(2)
C(18)	2966(7)	1410(7)	8489(4)	43(2)
C(19)	3874(7)	-1150(6)	8245(4)	61(2)
C(20)	4584(5)	586(5)	10188(3)	35(1)
C(21)	4329(7)	208(7)	11142(4)	53(2)
C(22)	2557(7)	570(6)	11548(3)	58(2)
C(23)	1689(6)	-127(6)	10997(3)	55(2)
C(24)	1958(7)	241(7)	10071(4)	43(2)
C(25)	3700(5)	-148(5)	9674(3)	35(1)
Li(1)	6125(11)	858(9)	8503(6)	29(2)
N(1)	8235(5)	124(5)	7537(3)	35(1)
N(2)	6253(5)	327(5)	9790(3)	36(1)
N(3)	4010(5)	93(5)	8746(3)	37(1)
Si(1)	7847(2)	3097(2)	7888(1)	37(1)
C(26)	2877(7)	1171(6)	3931(4)	52(2)
C(27)	3191(6)	1344(6)	5800(4)	47(2)
C(28)	5822(7)	1902(7)	4409(4)	35(2)
C(29)	6993(6)	788(6)	3853(4)	31(1)
C(30)	8544(7)	198(6)	4026(4)	37(2)
C(31)	9701(7)	-785(6)	3496(4)	46(2)
C(32)	9410(7)	-1308(6)	2758(4)	46(2)
C(33)	7865(8)	-781(7)	2571(4)	48(2)
C(34)	6724(7)	241(5)	3074(4)	34(2)
C(35)	2613(7)	3989(6)	4780(4)	36(2)
C(36)	3824(6)	4737(6)	5887(3)	36(2)
C(37)	4682(6)	5739(6)	6164(4)	37(2)
C(38)	3774(7)	7282(6)	6105(4)	46(2)
C(39)	3244(7)	7548(6)	5217(4)	51(2)
C(40)	2426(7)	6482(6)	4995(4)	45(2)
C(41)	8684(7)	3773(6)	4238(4)	58(2)
C(42)	7557(6)	6225(6)	4045(3)	48(2)
C(43)	4930(7)	3783(6)	2343(4)	46(2)
C(44)	3829(7)	6295(7)	2681(4)	61(2)
C(45)	8018(5)	4479(5)	2812(3)	36(1)
C(46)	9613(6)	4666(6)	2394(4)	41(2)
C(47)	9932(6)	4478(5)	1427(3)	47(1)
C(48)	8625(6)	5458(5)	1034(3)	49(1)
C(49)	7082(7)	5147(7)	1385(3)	44(2)
C(50)	6676(5)	5342(5)	2355(3)	38(1)
Li(2)	5509(12)	4232(12)	4042(7)	51(3)

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N(4)	3438(5)	4993(5)	5015(3)	29(1)
N(5)	7580(5)	4793(5)	3784(3)	39(1)
N(6)	5156(5)	5042(5)	2757(3)	40(1)
Si(2)	3750(2)	2054(2)	4720(1)	35(1)

Tabelle 10.24 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von  $(R,R)$ -**94b**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
C(1)	44(4)	40(4)	78(5)	7(3)	-15(4)	-14(3)
C(2)	47(4)	39(4)	64(5)	-6(3)	-16(4)	-20(3)
C(3)	30(4)	26(4)	40(4)	-3(3)	-5(3)	-10(3)
C(4)	32(4)	36(4)	40(4)	2(3)	-13(3)	-11(3)
C(5)	21(3)	57(4)	40(4)	-1(3)	-8(3)	-8(3)
C(6)	42(4)	44(4)	30(3)	-8(3)	3(3)	-12(3)
C(7)	27(3)	34(4)	55(4)	2(3)	0(3)	-3(3)
C(8)	21(3)	48(4)	42(4)	8(3)	-1(3)	-15(3)
C(9)	30(4)	35(4)	38(4)	-2(3)	-9(3)	-11(3)
C(10)	20(3)	43(4)	48(4)	5(3)	-14(3)	-11(3)
C(11)	29(3)	25(4)	51(4)	-6(3)	-16(3)	0(3)
C(12)	50(4)	33(4)	53(4)	-7(3)	-10(3)	-2(3)
C(13)	44(4)	45(4)	66(5)	-17(3)	-23(3)	-7(3)
C(14)	33(3)	50(4)	39(4)	-6(3)	-6(3)	-12(3)
C(15)	32(3)	30(4)	40(4)	-10(3)	-5(3)	-7(3)
C(16)	56(4)	61(4)	56(4)	-1(3)	-25(3)	-24(3)
C(17)	60(4)	61(4)	45(4)	12(3)	-19(3)	-10(3)
C(18)	33(3)	76(5)	32(3)	22(3)	-13(2)	-31(3)
C(19)	66(4)	78(4)	53(4)	-12(3)	-11(3)	-40(4)
C(20)	40(3)	40(3)	26(3)	8(2)	-11(2)	-9(3)
C(21)	48(4)	60(4)	53(4)	-11(3)	-14(3)	-17(3)
C(22)	76(4)	65(4)	28(3)	-9(3)	-4(3)	-15(3)
C(23)	44(3)	65(4)	52(4)	-3(3)	4(3)	-16(3)
C(24)	36(4)	61(4)	34(4)	-5(3)	-1(3)	-21(3)
C(25)	40(3)	32(3)	30(3)	3(2)	-4(2)	-6(3)
Li(1)	32(5)	29(6)	37(6)	10(4)	-17(5)	-18(4)
N(1)	37(3)	33(3)	40(3)	3(2)	-18(3)	-12(3)
N(2)	38(3)	40(3)	33(3)	0(2)	-11(2)	-15(2)
N(3)	39(3)	46(3)	34(3)	10(2)	-12(2)	-22(2)
Si(1)	29(1)	39(1)	47(1)	1(1)	-10(1)	-12(1)
C(26)	28(4)	50(4)	80(5)	-11(4)	-17(4)	-10(3)

C(27)	24(3)	54(4)	64(4)	6(3)	-7(3)	-12(3)
C(28)	32(4)	51(4)	26(4)	-3(3)	-12(3)	-13(3)
C(29)	24(3)	33(4)	34(4)	3(3)	0(3)	-8(3)
C(30)	28(4)	37(4)	45(4)	6(3)	-13(3)	-7(3)
C(31)	33(4)	35(4)	65(5)	0(3)	-16(3)	2(3)
C(32)	36(4)	35(4)	55(4)	-4(3)	12(3)	-2(3)
C(33)	52(4)	42(4)	49(4)	5(3)	-11(3)	-11(3)
C(34)	39(4)	24(3)	36(4)	-4(3)	-15(3)	2(3)
C(35)	42(4)	38(4)	32(4)	0(3)	-3(3)	-16(3)
C(36)	21(3)	55(4)	29(4)	9(3)	1(3)	-11(3)
C(37)	40(4)	37(4)	38(4)	0(3)	-12(3)	-14(3)
C(38)	39(4)	51(5)	48(4)	-16(3)	2(3)	-17(3)
C(39)	43(4)	26(4)	88(5)	-6(3)	-33(4)	-3(3)
C(40)	45(4)	55(5)	31(4)	6(3)	-7(3)	-9(4)
C(41)	48(4)	65(5)	78(5)	20(4)	-36(3)	-26(4)
C(42)	55(4)	58(4)	37(3)	-4(3)	2(3)	-33(3)
C(43)	44(3)	74(5)	28(3)	6(3)	-9(3)	-27(3)
C(44)	49(4)	69(4)	56(4)	7(3)	-15(3)	2(3)
C(45)	35(3)	32(3)	38(3)	3(2)	-11(2)	-4(2)
C(46)	30(3)	40(4)	52(4)	10(3)	-7(3)	-9(3)
C(47)	40(3)	53(4)	42(3)	-4(3)	2(2)	-9(3)
C(48)	57(3)	61(4)	28(3)	-5(3)	5(2)	-19(3)
C(49)	49(4)	53(4)	25(3)	11(3)	-4(3)	-7(3)
C(50)	34(3)	44(3)	34(3)	8(3)	-13(2)	-7(3)
Li(2)	27(6)	63(8)	56(7)	-18(6)	6(5)	-6(5)
N(4)	18(2)	28(3)	38(3)	-3(2)	-5(2)	1(2)
N(5)	32(3)	52(3)	40(3)	14(2)	-18(2)	-16(2)
N(6)	27(3)	44(3)	47(3)	2(2)	-15(2)	-3(2)
Si(2)	28(1)	36(1)	42(1)	-2(1)	-10(1)	-10(1)

Tabelle 10.25 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von *(S,R,R)*-**94b**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\text{ij}}$ -Tensors.

	x	y	z	$U(\text{eq})$
Si	2739(1)	2341(1)	6663(1)	24(1)
N(1)	125(1)	1170(1)	6140(1)	22(1)
N(2)	2173(1)	-699(1)	8676(1)	23(1)
N(3)	1824(1)	926(1)	10154(1)	23(1)
C(1)	2848(2)	2426(1)	4859(2)	34(1)
C(2)	3012(2)	3542(1)	7450(2)	43(1)

C(3)	4018(2)	1536(1)	7992(2)	23(1)
C(4)	4961(2)	817(1)	7867(2)	22(1)
C(5)	6240(2)	476(1)	9131(2)	29(1)
C(6)	7097(2)	-267(1)	9074(2)	35(1)
C(7)	6770(2)	-728(1)	7772(2)	37(1)
C(8)	5582(2)	-392(1)	6518(2)	34(1)
C(9)	4712(2)	355(1)	6551(2)	27(1)
C(10)	663(2)	2144(1)	6299(2)	24(1)
C(11)	120(2)	731(1)	4821(2)	24(1)
C(12)	-1026(2)	1150(1)	3382(2)	29(1)
C(13)	-2635(2)	1151(1)	3292(2)	31(1)
C(14)	-2665(2)	1554(1)	4666(2)	29(1)
C(15)	-1436(2)	1105(1)	6043(2)	28(1)
C(16)	3274(2)	-1217(1)	8319(2)	34(1)
C(17)	627(2)	-1055(1)	7765(2)	32(1)
C(18)	3275(2)	1384(1)	11075(2)	34(1)
C(19)	574(2)	1518(1)	10076(2)	37(1)
C(20)	2593(2)	-734(1)	10271(2)	23(1)
C(21)	2430(2)	-1695(1)	10833(2)	36(1)
C(22)	2848(2)	-1704(1)	12464(2)	44(1)
C(23)	1898(2)	-1010(1)	12827(2)	44(1)
C(24)	2138(2)	-54(1)	12350(2)	34(1)
C(25)	1694(2)	-12(1)	10696(2)	23(1)
Li	2050(3)	711(2)	8139(3)	24(1)
H(3)	4415(17)	1792(11)	8930(18)	25(4)
H(20)	3671(17)	-569(10)	10798(16)	19(4)
H(25)	573(16)	-172(10)	10157(14)	14(4)

Tabelle 10.26 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von *(S,R,R)*-**94b**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Si	23(1)	21(1)	25(1)	-1(1)	8(1)	-3(1)
N(1)	19(1)	24(1)	21(1)	-1(1)	7(1)	-1(1)
N(2)	23(1)	22(1)	26(1)	-2(1)	12(1)	-2(1)
N(3)	26(1)	24(1)	22(1)	-1(1)	12(1)	1(1)
C(1)	32(1)	35(1)	31(1)	7(1)	10(1)	-6(1)
C(2)	29(1)	26(1)	62(1)	-9(1)	9(1)	-3(1)
C(3)	23(1)	27(1)	16(1)	-5(1)	7(1)	-4(1)

C(4)	20(1)	28(1)	22(1)	1(1)	11(1)	-7(1)
C(5)	22(1)	37(1)	26(1)	0(1)	10(1)	-2(1)
C(6)	19(1)	45(1)	39(1)	12(1)	11(1)	6(1)
C(7)	30(1)	39(1)	52(1)	2(1)	25(1)	7(1)
C(8)	34(1)	41(1)	36(1)	-7(1)	23(1)	1(1)
C(9)	26(1)	34(1)	23(1)	2(1)	11(1)	-1(1)
C(10)	23(1)	23(1)	23(1)	-2(1)	7(1)	2(1)
C(11)	23(1)	22(1)	26(1)	-3(1)	9(1)	0(1)
C(12)	31(1)	33(1)	21(1)	-2(1)	8(1)	0(1)
C(13)	24(1)	28(1)	29(1)	-1(1)	1(1)	0(1)
C(14)	20(1)	33(1)	33(1)	-1(1)	8(1)	0(1)
C(15)	24(1)	34(1)	28(1)	0(1)	11(1)	-1(1)
C(16)	39(1)	26(1)	47(1)	-3(1)	26(1)	1(1)
C(17)	31(1)	28(1)	30(1)	0(1)	7(1)	-5(1)
C(18)	42(1)	35(1)	26(1)	-8(1)	15(1)	-12(1)
C(19)	45(1)	40(1)	32(1)	6(1)	23(1)	16(1)
C(20)	17(1)	24(1)	24(1)	4(1)	6(1)	-2(1)
C(21)	39(1)	29(1)	40(1)	10(1)	16(1)	1(1)
C(22)	53(1)	38(1)	39(1)	17(1)	18(1)	-1(1)
C(23)	48(1)	56(1)	34(1)	15(1)	21(1)	-4(1)
C(24)	36(1)	45(1)	26(1)	5(1)	17(1)	1(1)
C(25)	18(1)	30(1)	22(1)	3(1)	9(1)	-1(1)
Li	26(1)	23(1)	22(1)	1(1)	11(1)	1(1)

## 10.1.9. 95

Tabelle 10.27 Kristallographische Daten und Strukturverfeinerung von **95**.

Verbindung	<b>95</b> · 2 <i>n</i> -
CCDC Nummer	1005512
Empirische Formel	C <sub>43</sub> H <sub>78</sub> Li <sub>2</sub> N <sub>4</sub> Si <sub>2</sub>
Formelmasse [g/mol]	721.15
Temperatur [K]	173(2)
Wellenlänge [Å]	0.71073
Kristallsystem	monoklin
Raumgruppe	C <sub>2</sub> (5)
<i>a</i> [Å]	22.973(6)

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$b$ [Å]	11.338(2)
$c$ [Å]	19.2030(18)
$\beta$ [°]	102.603(14)
Zellvolumen [Å <sup>3</sup> ]	4881.2(16)
Formeleinheit pro Zelle	$Z = 4$
Berechnete Dichte [g/cm <sup>3</sup> ]	0.981
Absorptionskoeffizient $\mu$ [mm <sup>-1</sup> ]	0.102
F(000)	1592
Kristallgröße [mm <sup>3</sup> ]	0.60 x 0.30 x 0.20
Messbereich $\Theta$ [°]	2.38 – 26.00
	$-27 \leq h \leq 28$
Index-Breite	$-13 \leq k \leq 13$
	$-19 \leq l \leq 23$
Gemessene Reflexe	18801
Unabhängige Reflexe	9208 ( $R_{\text{int}} = 0.0410$ )
Daten / Restraints / Parameter	9208 / 1 / 480
Goodness-of-fit an $F^2$	1.038
Endgültige R-Werte [ $I > 2\sigma(I)$ ]	$R1 = 0.0555, wR2 = 0.1414$
R-Werte (sämtliche Daten)	$R1 = 0.0635, wR2 = 0.1469$
Absoluter Strukturparameter	-0.07(11)
Restelektronendichte [e/Å <sup>3</sup> ]	0.278 und -0.192

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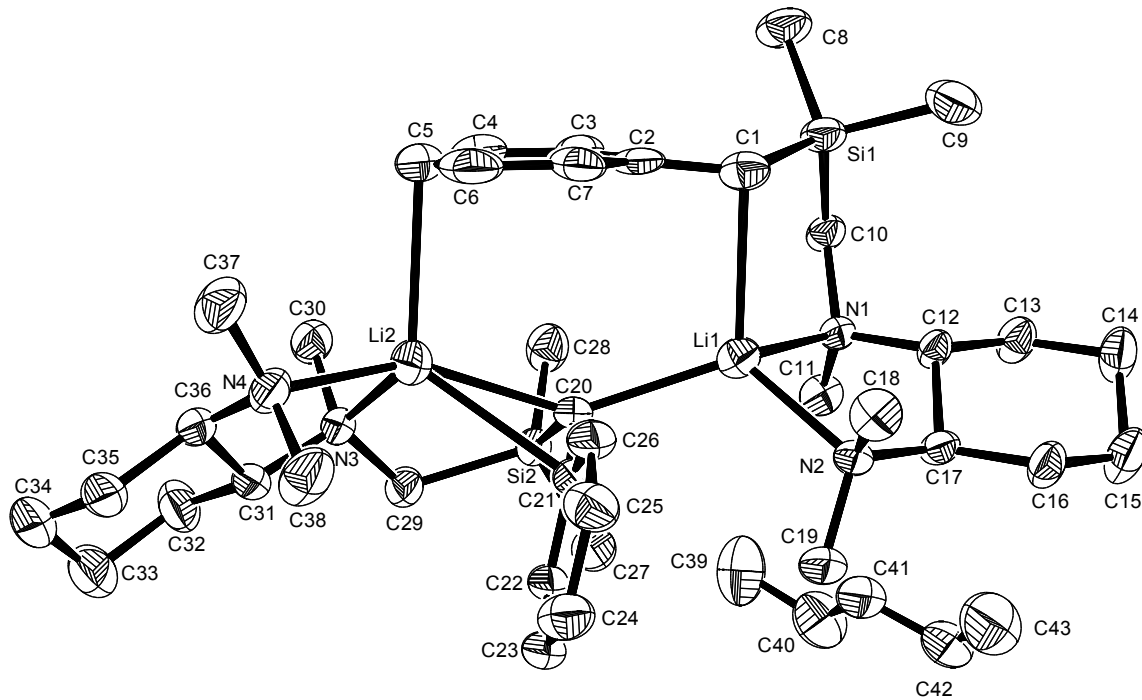


Abbildung 10.9 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von **95** · 2 *n*-Pentan im Kristall (ORTEP-Darstellung<sup>[206,207]</sup>). Ein Molekül Pentan wurde mit dem SQUEEZE Werkzeug der PLATON Software Suite<sup>[179]</sup> entfernt. Wasserstoffatome wurden der Übersichtlichkeit halber entfernt.

Tabelle 10.28 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **95**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\text{ij}}$ -Tensors.

	x	y	z	$U(\text{eq})$
H(1)	8032(16)	10440(40)	1871(18)	57(10)
H(20)	7785(13)	7290(30)	2208(15)	34(8)
C(1)	8335(1)	9806(3)	1906(2)	37(1)
C(2)	8150(1)	8897(3)	1408(2)	37(1)
C(3)	8487(1)	7863(3)	1363(2)	40(1)
C(4)	8271(2)	6936(4)	928(2)	54(1)
C(5)	7698(2)	6966(4)	484(2)	55(1)
C(6)	7366(2)	8002(4)	480(2)	55(1)
C(7)	7588(1)	8915(3)	913(2)	41(1)
C(8)	9719(2)	9787(4)	1908(2)	52(1)
C(9)	9171(2)	11727(3)	2612(2)	54(1)
C(10)	9312(1)	9167(3)	3220(1)	32(1)
C(11)	9035(1)	8140(3)	4208(2)	38(1)
C(12)	8736(1)	10211(3)	3966(1)	27(1)
C(13)	9255(1)	10679(3)	4533(2)	39(1)

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C(14)	9119(1)	11877(3)	4821(2)	47(1)
C(15)	8559(1)	11801(4)	5127(2)	51(1)
C(16)	8038(1)	11394(3)	4545(2)	39(1)
C(17)	8156(1)	10183(3)	4240(1)	29(1)
C(18)	7353(1)	10644(3)	3197(2)	40(1)
C(19)	7217(1)	9096(3)	4005(2)	42(1)
C(20)	7596(1)	6861(3)	2540(2)	31(1)
C(21)	6992(1)	7200(3)	2533(1)	30(1)
C(22)	6623(1)	6588(3)	2923(1)	32(1)
C(23)	6044(1)	6901(3)	2905(2)	36(1)
C(24)	5785(2)	7865(3)	2512(2)	44(1)
C(25)	6130(1)	8487(3)	2128(2)	44(1)
C(26)	6710(1)	8150(3)	2129(2)	37(1)
C(27)	8014(2)	5272(3)	3924(2)	46(1)
C(28)	8745(1)	5434(3)	2795(2)	46(1)
C(29)	7520(1)	4166(3)	2519(2)	35(1)
C(30)	7779(1)	3910(3)	1369(2)	41(1)
C(31)	6733(1)	3612(3)	1472(2)	38(1)
C(32)	6804(2)	2273(3)	1473(2)	53(1)
C(33)	6196(2)	1656(4)	1254(2)	70(1)
C(34)	5872(2)	2070(4)	530(2)	66(1)
C(35)	5801(2)	3417(4)	511(2)	56(1)
C(36)	6410(1)	4044(3)	731(2)	37(1)
C(37)	6252(2)	5729(4)	-54(2)	53(1)
C(38)	5914(2)	5837(4)	1036(2)	56(1)
C(39)	9678(3)	4634(5)	5926(3)	103(2)
C(40)	9513(2)	5496(5)	6455(3)	77(1)
C(41)	9256(2)	6620(4)	6148(2)	63(1)
C(42)	9121(2)	7517(4)	6676(2)	65(1)
C(43)	8838(2)	8607(5)	6351(3)	92(2)
Li(1)	8042(2)	8679(5)	2952(2)	34(1)
Li(2)	7148(2)	6014(5)	1417(3)	39(1)
N(1)	8856(1)	9051(2)	3659(1)	27(1)
N(2)	7658(1)	9713(2)	3679(1)	28(1)
N(3)	7299(1)	4264(2)	1731(1)	32(1)
N(4)	6380(1)	5340(3)	695(1)	38(1)
Si(1)	9094(1)	10119(1)	2384(1)	36(1)
Si(2)	7964(1)	5512(1)	2935(1)	32(1)

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Tabelle 10.29 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **95**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
C(1)	29(2)	48(2)	35(2)	5(1)	11(1)	0(1)
C(2)	30(2)	59(2)	26(1)	11(1)	15(1)	-8(1)
C(3)	38(2)	54(2)	32(2)	3(1)	17(1)	-8(2)
C(4)	60(2)	66(3)	46(2)	1(2)	32(2)	-7(2)
C(5)	61(2)	73(3)	35(2)	-7(2)	21(2)	-31(2)
C(6)	46(2)	88(3)	31(2)	18(2)	10(2)	-21(2)
C(7)	35(2)	57(2)	31(1)	14(2)	9(1)	-12(2)
C(8)	37(2)	83(3)	41(2)	-3(2)	19(1)	-12(2)
C(9)	53(2)	53(2)	58(2)	8(2)	18(2)	-15(2)
C(10)	24(1)	43(2)	31(1)	-7(1)	11(1)	-3(1)
C(11)	39(2)	38(2)	36(2)	4(1)	9(1)	6(1)
C(12)	23(1)	32(2)	28(1)	-8(1)	7(1)	1(1)
C(13)	28(2)	50(2)	39(2)	-15(2)	6(1)	-2(1)
C(14)	37(2)	48(2)	56(2)	-26(2)	8(2)	-4(2)
C(15)	41(2)	64(2)	49(2)	-30(2)	10(2)	-2(2)
C(16)	31(2)	43(2)	44(2)	-19(2)	14(1)	-2(1)
C(17)	27(1)	37(2)	25(1)	-2(1)	10(1)	-1(1)
C(18)	30(2)	48(2)	40(2)	1(2)	1(1)	5(1)
C(19)	37(2)	51(2)	43(2)	-6(2)	20(1)	-11(2)
C(20)	36(2)	33(2)	28(1)	-1(1)	15(1)	-9(1)
C(21)	36(2)	34(2)	21(1)	-1(1)	7(1)	-9(1)
C(22)	38(2)	34(2)	26(1)	1(1)	11(1)	-9(1)
C(23)	39(2)	40(2)	31(1)	-1(1)	14(1)	-12(1)
C(24)	36(2)	59(2)	38(2)	2(2)	11(1)	-2(2)
C(25)	40(2)	50(2)	39(2)	8(2)	4(1)	-6(2)
C(26)	43(2)	40(2)	30(1)	5(1)	12(1)	-6(1)
C(27)	58(2)	52(2)	26(1)	6(1)	2(1)	-10(2)
C(28)	38(2)	52(2)	45(2)	-9(2)	5(1)	1(2)
C(29)	44(2)	34(2)	28(1)	-1(1)	7(1)	-4(1)
C(30)	38(2)	46(2)	41(2)	-9(2)	12(1)	-3(1)
C(31)	38(2)	50(2)	28(1)	-4(1)	9(1)	-19(2)
C(32)	65(2)	43(2)	44(2)	4(2)	-1(2)	-22(2)
C(33)	86(3)	69(3)	54(2)	0(2)	13(2)	-41(2)
C(34)	54(2)	90(3)	52(2)	-14(2)	10(2)	-40(2)
C(35)	40(2)	90(3)	38(2)	-12(2)	9(2)	-32(2)
C(36)	33(2)	51(2)	29(1)	-9(1)	12(1)	-12(1)
C(37)	47(2)	76(3)	31(2)	-8(2)	1(1)	-5(2)
C(38)	32(2)	89(3)	48(2)	-23(2)	10(2)	3(2)

C(39)	126(5)	69(4)	114(4)	-27(3)	23(4)	0(3)
C(40)	68(3)	70(3)	89(3)	5(3)	8(2)	-3(2)
C(41)	62(2)	73(3)	59(2)	-5(2)	24(2)	-17(2)
C(42)	49(2)	71(3)	76(3)	-4(2)	18(2)	-17(2)
C(43)	83(3)	63(3)	138(5)	-4(3)	44(3)	10(3)
Li(1)	32(3)	40(3)	30(2)	0(2)	7(2)	2(2)
Li(2)	41(3)	44(3)	31(2)	-3(2)	4(2)	-9(2)
N(1)	26(1)	29(1)	26(1)	-2(1)	9(1)	-1(1)
N(2)	24(1)	31(1)	30(1)	-1(1)	10(1)	-3(1)
N(3)	34(1)	37(1)	26(1)	-7(1)	8(1)	-7(1)
N(4)	32(1)	54(2)	29(1)	-11(1)	8(1)	-4(1)
Si(1)	31(1)	49(1)	31(1)	-1(1)	13(1)	-8(1)
Si(2)	36(1)	34(1)	26(1)	-3(1)	6(1)	-6(1)

10.1.10. (R<sub>N</sub>,R,R,R)-96Tabelle 10.30 Kristallographische Daten und Strukturverfeinerung (R<sub>N</sub>,R,R,R)-96a und (R<sub>N</sub>,R,R,R)-96b.

Verbindung	(R <sub>N</sub> ,R,R,R)-96a	(R <sub>N</sub> ,R,R,R)-96b
CCDC Nummer	1005513	1005514
Empirische Formel	C <sub>23</sub> H <sub>43</sub> LiN <sub>2</sub> OSi	C <sub>24</sub> H <sub>45</sub> LiN <sub>2</sub> OSi
Formelmass [g/mol]	398.62	412.65
Temperatur [K]	173(2)	173(2)
Wellenlänge [Å]	0.71073	0.71073
Kristallsystem	orthorombisch	orthorombisch
Raumgruppe	P <sub>2</sub> <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (19)	P <sub>2</sub> <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (19)
a [Å]	8.9067(9)	8.8020(13)
b [Å]	16.1715(19)	15.9171(19)
c [Å]	17.505(2)	18.343(2)
Zellvolumen [Å <sup>3</sup> ]	2521.4(5)	2570.0(6)
Formeleinheit pro Zelle	Z = 4	Z = 4
Berechnete Dichte [g/cm <sup>3</sup> ]	1.050	1.067
Absorptionskoeffizient μ [mm <sup>-1</sup> ]	0.107	0.107
F(000)	880	912
Kristallgröße [mm <sup>3</sup> ]	0.20 x 0.10 x 0.05	0.20 x 0.06 x 0.02
Messbereich Θ [°]	2.33 – 26.00	2.56 – 24.99
	-10 ≤ h ≤ 10	-10 ≤ h ≤ 10
	-19 ≤ k ≤ 19	-18 ≤ k ≤ 18
	-21 ≤ l ≤ 21	-21 ≤ l ≤ 21

Gemessene Reflexe	15091	17960
Unabhängige Reflexe	4950 ( $R_{\text{int}} = 0.0407$ )	4537 ( $R_{\text{int}} = 0.0867$ )
Daten / Restraints / Parameter	4950 / 0 / 264	4537 / 0 / 275
Goodness-of-fit an $F^2$	1.013	1.011
Endgültige R-Werte [ $I > 2\sigma(I)$ ]	$R1 = 0.0499$ , $wR2 = 0.1093$	$R1 = 0.0539$ , $wR2 = 0.0856$
R-Werte (sämtliche Daten)	$R1 = 0.0749$ , $wR2 = 0.1217$	$R1 = 0.1013$ , $wR2 = 0.1009$
Absoluter Strukturparameter	-0.18(17)	-0.18(18)
Restelektronendichte [ $e/\text{\AA}^3$ ]	0.285 und -0.206	0.192 und -0.235

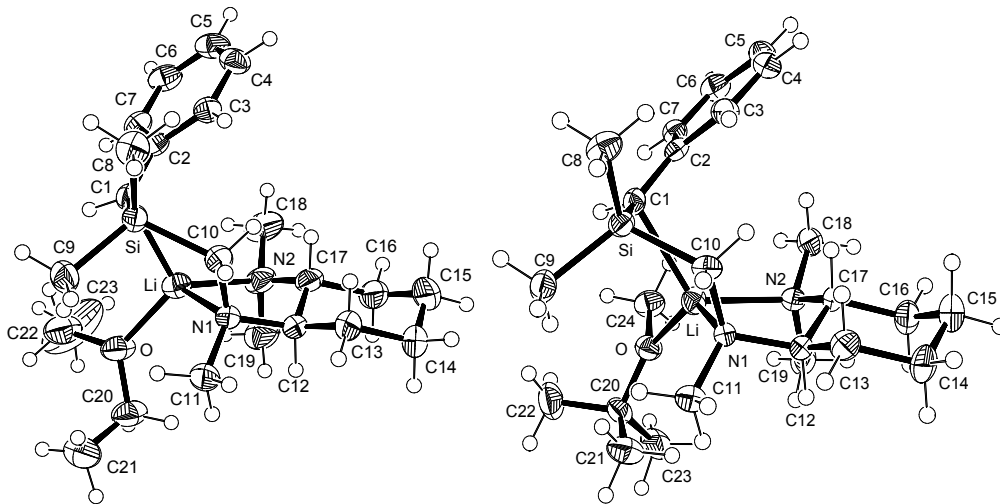


Abbildung 10.10 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von  $(R_N,R,R,R)$ -**96a** (links) und  $(R_N,R,R,R)$ -**96b** (rechts) im Kristall (ORTEP-Darstellung<sup>[206,207]</sup>). Das Nummerierungsschema der Wasserstoffatome wurde der Übersichtlichkeit halber weggelassen.

Tabelle 10.31 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von  $(R_N,R,R,R)$ -**96a**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\text{ij}}$ -Tensors.

	x	y	z	$U(\text{eq})$
H(1)	9850(30)	-1504(15)	7783(13)	21(6)
Li	9620(5)	19(3)	7624(3)	38(1)
C(1)	9293(3)	-1327(2)	7346(1)	29(1)
C(2)	9994(3)	-1530(2)	6635(1)	28(1)
C(3)	9266(3)	-1463(2)	5919(1)	33(1)
C(4)	9977(3)	-1649(2)	5230(2)	42(1)
C(5)	11450(3)	-1914(2)	5219(2)	45(1)
C(6)	12201(3)	-1986(2)	5903(2)	43(1)
C(7)	11513(3)	-1802(2)	6586(2)	35(1)
C(8)	5978(3)	-1959(2)	7013(2)	44(1)
C(9)	6953(3)	-1288(2)	8555(2)	44(1)

C(10)	6687(3)	-156(2)	7107(2)	36(1)
C(11)	6653(3)	827(2)	8150(2)	41(1)
C(12)	7722(3)	1277(2)	6944(1)	42(1)
C(13)	6327(4)	1554(2)	6518(2)	57(1)
C(14)	6625(5)	2341(2)	6042(2)	71(1)
C(15)	7903(6)	2174(2)	5486(2)	79(1)
C(16)	9315(5)	1898(2)	5898(2)	65(1)
C(17)	9040(4)	1118(2)	6389(2)	47(1)
C(18)	11465(4)	423(2)	6264(2)	63(1)
C(19)	11212(4)	1488(2)	7209(2)	61(1)
C(20)	10230(4)	933(2)	9124(2)	51(1)
C(21)	9388(5)	792(3)	9857(2)	70(1)
C(22)	11387(4)	-423(2)	9037(2)	62(1)
C(23)	12936(5)	-229(3)	8933(4)	145(3)
N(1)	7478(2)	558(1)	7464(1)	33(1)
N(2)	10403(3)	826(1)	6791(1)	45(1)
O	10408(2)	188(1)	8679(1)	48(1)
Si	7292(1)	-1209(1)	7497(1)	30(1)

Tabelle 10.32 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von  $(R_N, R, R, R)96a$ . Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
C(1)	30(1)	26(1)	31(1)	3(1)	-5(1)	2(1)
C(2)	30(1)	19(1)	36(1)	-1(1)	0(1)	-6(1)
C(3)	31(1)	31(2)	36(1)	-3(1)	-1(1)	-3(1)
C(4)	50(2)	42(2)	33(2)	-7(1)	0(1)	-15(1)
C(5)	47(2)	43(2)	46(2)	-13(2)	20(2)	-12(2)
C(6)	34(2)	38(2)	57(2)	-10(1)	10(1)	-1(1)
C(7)	29(2)	29(1)	48(2)	0(1)	-1(1)	-2(1)
C(8)	36(2)	45(2)	50(2)	2(2)	-2(1)	-5(1)
C(9)	51(2)	47(2)	35(1)	6(1)	9(1)	7(2)
C(10)	39(2)	35(2)	34(1)	-1(1)	0(1)	9(1)
C(11)	47(2)	42(2)	34(2)	-2(1)	9(1)	10(1)
C(12)	71(2)	28(1)	28(1)	1(1)	5(1)	11(2)
C(13)	89(3)	45(2)	37(2)	2(2)	-3(2)	28(2)
C(14)	129(3)	46(2)	38(2)	7(2)	-8(2)	28(2)
C(15)	154(4)	49(2)	33(2)	11(2)	8(2)	7(3)
C(16)	121(3)	35(2)	40(2)	6(2)	23(2)	6(2)
C(17)	83(2)	24(2)	36(2)	-1(1)	18(2)	-1(2)

C(18)	71(2)	42(2)	77(2)	-7(2)	40(2)	-14(2)
C(19)	76(2)	38(2)	69(2)	0(2)	16(2)	-17(2)
C(20)	52(2)	43(2)	57(2)	-18(2)	-12(2)	5(2)
C(21)	89(3)	70(3)	50(2)	-11(2)	-1(2)	14(2)
C(22)	63(2)	57(2)	65(2)	-19(2)	-19(2)	18(2)
C(23)	57(3)	82(4)	294(9)	-8(5)	10(4)	15(3)
Li	39(2)	33(2)	41(3)	-5(2)	1(2)	-2(2)
N(1)	43(1)	29(1)	27(1)	-1(1)	4(1)	6(1)
N(2)	57(2)	29(1)	51(2)	-2(1)	16(1)	-6(1)
O	49(1)	44(1)	51(1)	-18(1)	-14(1)	12(1)
Si	31(1)	30(1)	31(1)	3(1)	2(1)	1(1)

Tabelle 10.33 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von  $(R_M, R, R, R)$ -**96b**.  $U_{eq}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{ij}$ -Tensors.

	x	y	z	$U_{eq}$
Si	7362(1)	2478(1)	2486(1)	27(1)
O	11540(2)	1236(1)	1734(1)	32(1)
N(1)	7792(3)	709(1)	2661(1)	24(1)
N(2)	10708(3)	570(2)	3395(1)	26(1)
Li	9955(6)	1310(3)	2522(3)	29(1)
C(1)	9326(4)	2708(2)	2659(2)	26(1)
C(2)	9987(4)	2935(2)	3346(2)	26(1)
C(3)	9192(4)	2879(2)	4019(2)	31(1)
C(4)	9863(4)	3051(2)	4683(2)	36(1)
C(5)	11360(4)	3305(2)	4729(2)	35(1)
C(6)	12170(4)	3400(2)	4083(2)	35(1)
C(7)	11509(4)	3225(2)	3416(2)	27(1)
C(8)	5860(4)	3199(2)	2857(2)	38(1)
C(9)	7068(4)	2455(2)	1467(1)	37(1)
C(10)	6891(4)	1432(2)	2945(2)	28(1)
C(11)	6991(4)	351(2)	2021(2)	33(1)
C(12)	8056(4)	29(2)	3213(2)	27(1)
C(13)	6614(4)	-253(2)	3617(2)	38(1)
C(14)	6919(4)	-977(2)	4140(2)	44(1)
C(15)	8131(4)	-734(2)	4682(2)	46(1)
C(16)	9573(4)	-471(2)	4285(2)	39(1)
C(17)	9300(4)	265(2)	3761(2)	26(1)
C(18)	11684(4)	1035(2)	3911(2)	34(1)
C(19)	11613(4)	-112(2)	3067(2)	37(1)

C(20)	11718(4)	828(2)	1030(2)	32(1)
C(21)	10234(4)	364(2)	927(2)	47(1)
C(22)	11949(4)	1484(2)	440(2)	52(1)
C(23)	13031(4)	199(2)	1059(2)	50(1)
C(24)	12819(4)	1720(2)	1973(2)	37(1)

Tabelle 10.34 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von  $(R_N, R, R, R)$ -**96b**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Si	28(1)	23(1)	29(1)	-1(1)	-4(1)	2(1)
O	34(1)	31(1)	29(1)	-3(1)	2(1)	0(1)
N(1)	31(2)	20(1)	19(1)	1(1)	-1(1)	-1(1)
N(2)	28(2)	25(2)	24(1)	-2(1)	2(1)	1(1)
C(1)	31(2)	24(2)	25(2)	5(2)	1(2)	-4(2)
C(2)	29(2)	17(2)	31(2)	0(2)	0(2)	4(2)
C(3)	33(2)	29(2)	31(2)	-3(2)	4(2)	-2(2)
C(4)	47(3)	32(2)	28(2)	-4(2)	5(2)	2(2)
C(5)	42(2)	35(2)	28(2)	-4(2)	-15(2)	7(2)
C(6)	29(2)	29(2)	46(2)	-4(2)	-7(2)	1(2)
C(7)	27(2)	24(2)	29(2)	0(2)	-1(2)	-1(2)
C(8)	33(2)	31(2)	52(2)	-4(2)	-5(2)	0(2)
C(9)	46(2)	30(2)	36(2)	7(2)	-11(2)	-7(2)
C(10)	26(2)	27(2)	29(2)	-7(2)	-1(2)	2(2)
C(11)	36(2)	32(2)	31(2)	-6(2)	-2(2)	-2(2)
C(12)	39(2)	19(2)	23(2)	1(1)	-2(2)	0(2)
C(13)	47(2)	31(2)	36(2)	0(2)	2(2)	-11(2)
C(14)	54(3)	37(2)	41(2)	13(2)	14(2)	-14(2)
C(15)	58(3)	43(2)	36(2)	14(2)	1(2)	-1(2)
C(16)	45(3)	37(2)	35(2)	11(2)	-2(2)	-1(2)
C(17)	36(2)	20(2)	21(2)	4(2)	2(2)	2(2)
C(18)	35(2)	35(2)	31(2)	1(2)	-9(2)	2(2)
C(19)	42(2)	32(2)	37(2)	6(2)	6(2)	9(2)
C(20)	37(2)	37(2)	21(2)	-2(2)	2(2)	-2(2)
C(21)	49(3)	50(2)	43(2)	-15(2)	-2(2)	-10(2)
C(22)	64(3)	58(3)	34(2)	14(2)	-1(2)	-5(2)
C(23)	59(3)	58(3)	31(2)	-8(2)	10(2)	21(2)
C(24)	31(2)	36(2)	44(2)	-5(2)	-5(2)	-6(2)
Li	30(3)	29(3)	28(3)	2(3)	5(3)	2(3)
H(1)	9860(30)	2904(16)	2275(13)	18(8)	H(1)	9860(30)

10.1.11. Ammoniumiodid (*S,R,R*)-**100**Tabelle 10.35 Kristallographische Daten und Strukturverfeinerung von (*S,R,R*)-**100**.

Verbindung	( <i>S,R,R</i> )- <b>100</b>
CCDC Nummer	1005515
Empirische Formel	C <sub>23</sub> H <sub>45</sub> IN <sub>2</sub> SiSn
Formelmasse [g/mol]	623.29
Temperatur [K]	173(2)
Wellenlänge [Å]	0.71073
Kristallsystem	monoklin
Raumgruppe	P 1 21 1
<i>a</i> [Å]	8.7778(6)
<i>b</i> [Å]	10.5752(11)
<i>c</i> [Å]	15.399(2)
$\beta$ [°]	92.113(9)
Zellvolumen [Å <sup>3</sup> ]	1428.4(3)
Formeleinheit pro Zelle	Z = 2
Berechnete Dichte [g/cm <sup>3</sup> ]	1.449
Absorptionskoeffizient $\mu$ [mm <sup>-1</sup> ]	2.028
F(000)	628
Kristallgröße [mm <sup>3</sup> ]	0.30 x 0.20 x 0.10
Messbereich $\Theta$ [°]	2.32 – 25.00
	-10 ≤ <i>h</i> ≤ 8
Index-Breite	-12 ≤ <i>k</i> ≤ 12
	-18 ≤ <i>l</i> ≤ 18
Gemessene Reflexe	9807
Unabhängige Reflexe	5050 ( <i>R</i> <sub>int</sub> = 0.0396)
Daten / Restraints / Parameter	5050 / 1 / 262
Goodness-of-fit an F <sup>2</sup>	1.047
Endgültige R-Werte [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	<i>R</i> 1 = 0.0540, <i>wR</i> 2 = 0.1190
<i>R</i> -Werte (sämtliche Daten)	<i>R</i> 1 = 0.0696, <i>wR</i> 2 = 0.1292
Absoluter Strukturparameter	0.01(4)
Restelektronendichte [e/Å <sup>3</sup> ]	1.644 und -0.993

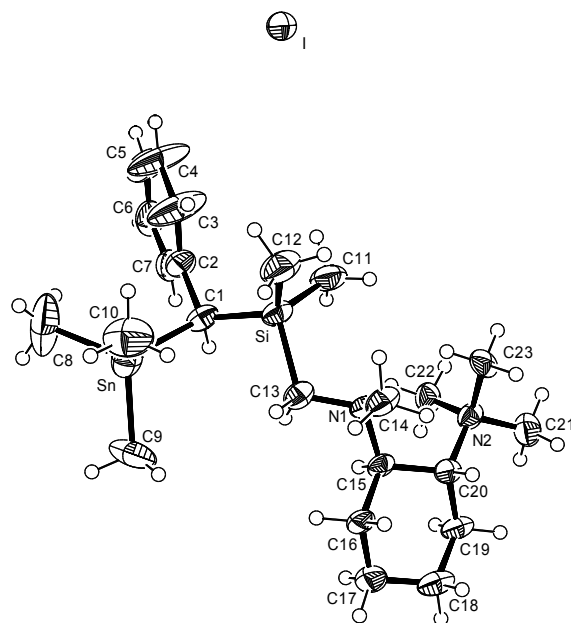


Abbildung 10.11 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von (*S,R,R*)-**100** im Kristall (ORTEP-Darstellung<sup>[206,207]</sup>). Das Nummerierungsschema der Wasserstoffatome wurde der Übersichtlichkeit halber weggelassen.

Tabelle 10.36 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von (*S,R,R*)-**100**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\text{ij}}$ -Tensors.

	x	y	z	$U_{\text{eq}}$
I	7685(1)	8586(1)	3957(1)	50(1)
Sn	7455(1)	880(1)	637(1)	59(1)
Si	4942(3)	1899(2)	2162(2)	42(1)
N(1)	3046(8)	-49(6)	2788(5)	33(2)
N(2)	2241(8)	-150(7)	4646(5)	36(2)
C(1)	6955(10)	1819(9)	1856(6)	40(2)
C(2)	7857(10)	3024(9)	1936(7)	45(2)
C(3)	7380(15)	4128(13)	1547(12)	107(6)
C(4)	8159(17)	5228(13)	1623(12)	115(7)
C(5)	9457(15)	5270(12)	2134(9)	80(4)
C(6)	9965(12)	4184(11)	2528(8)	59(3)
C(7)	9140(10)	3097(10)	2471(7)	48(2)
C(8)	9558(17)	1600(20)	194(11)	127(7)
C(9)	7718(17)	-1081(10)	942(9)	87(4)
C(10)	5754(15)	1198(13)	-337(8)	87(4)
C(11)	4837(13)	2743(9)	3199(7)	60(3)
C(12)	3642(13)	2719(11)	1367(9)	71(3)
C(13)	4397(10)	182(8)	2290(6)	42(2)

C(14)	1683(11)	20(9)	2234(7)	48(3)
C(15)	3191(8)	-1244(8)	3289(6)	33(2)
C(16)	2991(10)	-2415(8)	2714(7)	40(2)
C(17)	3350(11)	-3611(9)	3210(7)	50(2)
C(18)	2377(11)	-3688(9)	3980(7)	53(3)
C(19)	2512(11)	-2532(8)	4569(7)	43(2)
C(20)	2148(8)	-1339(9)	4055(5)	34(2)
C(21)	1565(11)	-406(11)	5509(7)	51(3)
C(22)	3841(9)	263(9)	4827(7)	44(2)
C(23)	1339(8)	927(9)	4259(6)	42(2)

Tabelle 10.37 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von  $(S,R,R)$ -**100**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U_{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U_{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
I	25(1)	47(1)	79(1)	6(1)	-2(1)	-2(1)
Sn	52(1)	71(1)	53(1)	-8(1)	6(1)	-21(1)
Si	41(1)	33(1)	52(2)	5(1)	-1(1)	-10(1)
N(1)	32(4)	25(4)	42(5)	8(3)	-3(3)	-4(3)
N(2)	28(4)	38(4)	42(5)	7(4)	0(3)	-4(3)
C(1)	46(5)	37(5)	37(5)	7(4)	-8(4)	-14(4)
C(2)	41(5)	38(5)	56(6)	-2(5)	2(5)	-13(4)
C(3)	72(9)	71(9)	175(17)	64(10)	-53(10)	-38(7)
C(4)	103(11)	59(8)	177(18)	56(10)	-56(11)	-54(8)
C(5)	84(9)	58(8)	98(11)	3(7)	5(8)	-44(7)
C(6)	48(6)	67(7)	64(8)	-19(6)	12(5)	-20(5)
C(7)	35(5)	54(6)	55(6)	-4(5)	7(4)	-4(4)
C(8)	90(11)	200(20)	99(12)	-20(12)	55(9)	-38(12)
C(9)	122(11)	41(8)	97(10)	-16(6)	-1(9)	25(6)
C(10)	121(11)	72(9)	67(8)	4(7)	-20(7)	1(8)
C(11)	83(8)	33(5)	66(8)	-1(5)	8(6)	-13(5)
C(12)	72(7)	58(7)	82(9)	30(7)	0(7)	-4(6)
C(13)	43(5)	41(5)	42(6)	12(4)	-2(4)	-4(4)
C(14)	47(5)	43(6)	53(7)	18(5)	-3(5)	-7(5)
C(15)	24(3)	28(5)	47(5)	2(4)	-3(3)	-9(4)
C(16)	31(5)	29(5)	61(6)	-2(4)	5(4)	-11(4)
C(17)	48(5)	37(5)	64(7)	-6(5)	4(5)	-9(4)
C(18)	55(6)	33(5)	70(7)	8(5)	-9(5)	-13(4)
C(19)	43(5)	28(5)	59(7)	8(5)	-6(5)	-8(4)
C(20)	27(3)	31(4)	44(5)	3(5)	-4(3)	0(4)

C(21)	43(6)	61(7)	51(6)	4(5)	8(5)	6(5)
C(22)	29(4)	53(6)	52(6)	-5(5)	4(4)	-3(4)
C(23)	21(4)	40(5)	65(6)	-9(5)	-2(4)	5(4)

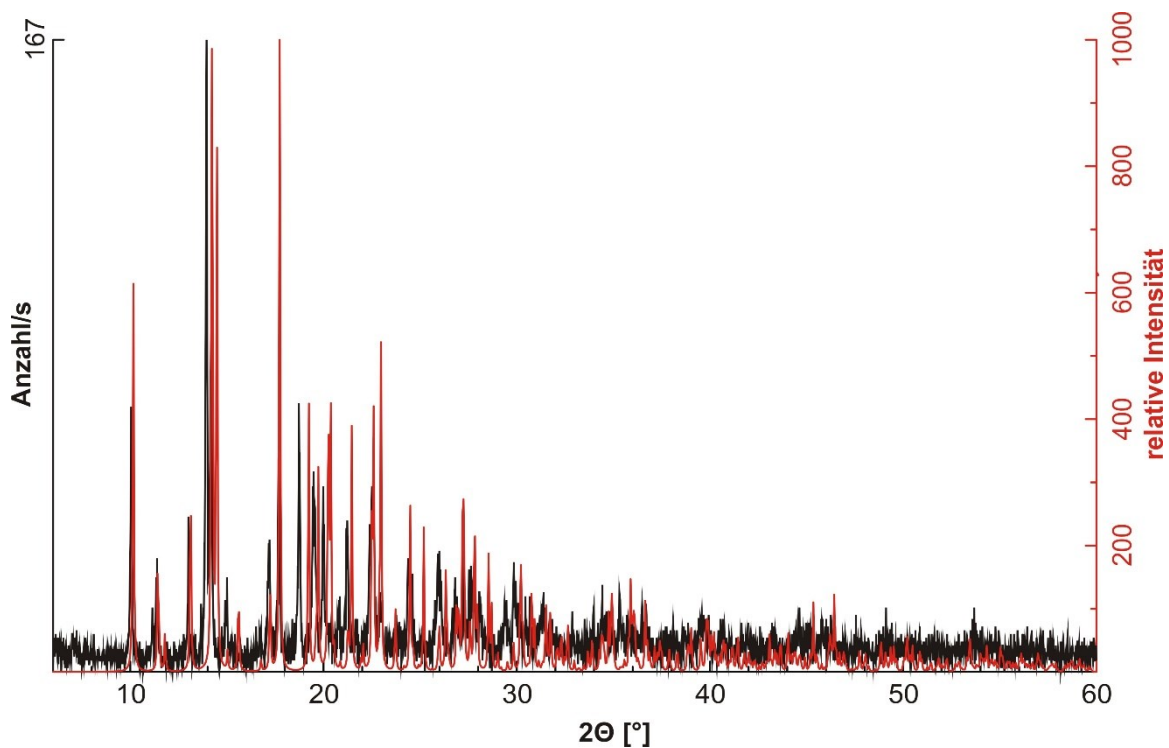


Abbildung 10.12 Pulverdiffraktogramm von (*S,R,R*)-**100** (schwarz) mit dem berechneten Diffraktogramm (rot).

### 10.1.12. Dimeres lithiiertes Benzylsilan **102**

Tabelle 10.38 Kristallographische Daten und Strukturverfeinerung von **102**.

Verbindung	<b>102</b>
Empirische Formel	C <sub>56</sub> H <sub>62</sub> Li <sub>2</sub> N <sub>2</sub> Si <sub>2</sub>
Formelmasse [g/mol]	833.14
Temperatur [K]	173(2) K
Wellenlänge [Å]	0.71073
Kristallsystem	triklin
Raumgruppe	<i>P</i> 1 (2)

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$a$ [Å]	9.8012(2)
$b$ [Å]	11.4279(3)
$c$ [Å]	11.7747(4)
$\alpha$ [°]	111.464(3)
$\beta$ [°]	102.524(2)
$\gamma$ [°]	93.586(2)
Zellvolumen [Å <sup>3</sup> ]	1183.48(6)
Formeleinheit pro Zelle	1
Berechnete Dichte [g/cm <sup>3</sup> ]	1.169
Absorptionskoeffizient $\mu$ [mm <sup>-1</sup> ]	0.114
F(000)	446
Kristallgröße [mm <sup>3</sup> ]	0.20 x 0.20 x 0.05
Messbereich $\Theta$ [°]	2.49 – 25.99
	-12 $\leq h \leq$ 12
Index-Breite	-14 $\leq k \leq$ 14
	-14 $\leq l \leq$ 14
Gemessene Reflexe	45611
Unabhängige Reflexe	4643 ( $R_{\text{int}} = 0.0381$ )
Daten / Restraints / Parameter	4643 / 0 / 284
Goodness-of-fit an $F^2$	1.064
Endgültige R-Werte [ $I > 2\sigma(I)$ ]	R1 = 0.0498, wR2 = 0.1360
R-Werte (sämtliche Daten)	R1 = 0.0647, wR2 = 0.1411
Restelektronendichte [e/Å <sup>3</sup> ]	1.062 und -0.295

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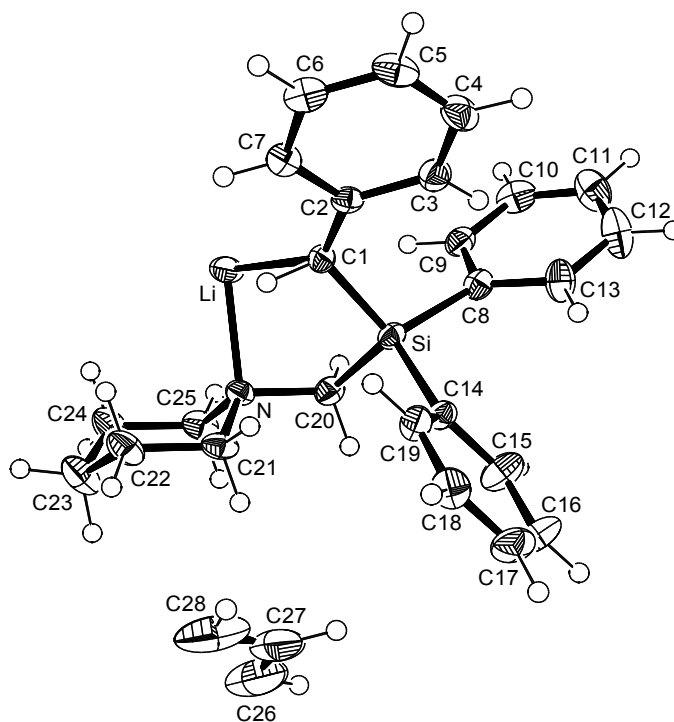


Abbildung 10.13 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von **102** im Kristall (ORTEP-Darstellung<sup>[206,207]</sup>). Das Nummerierungsschema der Wasserstoffatome wurde der Übersichtlichkeit halber weggelassen.

Tabelle 10.39 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **102**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\text{ij}}$ -Tensors.

	x	y	z	$U(\text{eq})$
Si	9365(1)	1345(1)	8420(1)	20(1)
N	9039(2)	2599(2)	10905(1)	21(1)
C(1)	8561(2)	-32(2)	8608(2)	21(1)
C(2)	7969(2)	-1261(2)	7546(2)	21(1)
C(3)	8418(2)	-1679(2)	6426(2)	28(1)
C(4)	7886(2)	-2862(2)	5470(2)	33(1)
C(5)	6909(2)	-3698(2)	5589(2)	32(1)
C(6)	6437(2)	-3316(2)	6673(2)	29(1)
C(7)	6931(2)	-2122(2)	7615(2)	25(1)
C(8)	11056(2)	1020(2)	7916(2)	24(1)
C(9)	12228(2)	881(2)	8743(2)	27(1)
C(10)	13417(2)	471(2)	8363(2)	35(1)
C(11)	13453(2)	166(2)	7133(2)	42(1)
C(12)	12326(2)	331(3)	6293(2)	45(1)
C(13)	11153(2)	762(2)	6686(2)	34(1)

C(14)	8239(2)	1904(2)	7269(2)	23(1)
C(15)	8769(2)	2868(2)	6948(2)	37(1)
C(16)	7905(3)	3309(2)	6142(2)	44(1)
C(17)	6499(3)	2798(2)	5653(2)	39(1)
C(18)	5943(2)	1845(2)	5948(2)	35(1)
C(19)	6813(2)	1407(2)	6752(2)	28(1)
C(20)	9910(2)	2699(2)	10051(2)	24(1)
C(21)	7586(2)	2805(2)	10439(2)	27(1)
C(22)	6656(2)	2673(2)	11268(2)	33(1)
C(23)	7255(3)	3601(2)	12630(2)	42(1)
C(24)	8791(2)	3486(2)	13082(2)	36(1)
C(25)	9644(2)	3590(2)	12189(2)	28(1)
Li	9503(4)	847(3)	10839(3)	29(1)
C(26)	6183(4)	5655(4)	9967(5)	75(1)
C(27)	5457(5)	4611(4)	8929(4)	80(1)
C(28)	4278(5)	3972(3)	8988(4)	75(1)
H(1)	7890(20)	200(20)	9110(20)	30(6)

Tabelle 10.40 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **102**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Si	23(1)	21(1)	18(1)	10(1)	3(1)	4(1)
N	24(1)	21(1)	17(1)	6(1)	4(1)	8(1)
C(1)	23(1)	23(1)	19(1)	10(1)	6(1)	5(1)
C(2)	20(1)	21(1)	20(1)	9(1)	1(1)	6(1)
C(3)	32(1)	26(1)	25(1)	11(1)	7(1)	4(1)
C(4)	42(1)	31(1)	21(1)	4(1)	6(1)	10(1)
C(5)	31(1)	24(1)	26(1)	0(1)	-6(1)	4(1)
C(6)	20(1)	27(1)	34(1)	11(1)	-5(1)	-2(1)
C(7)	22(1)	28(1)	21(1)	9(1)	0(1)	4(1)
C(8)	23(1)	23(1)	23(1)	9(1)	3(1)	-2(1)
C(9)	32(1)	24(1)	28(1)	13(1)	7(1)	2(1)
C(10)	24(1)	31(1)	45(1)	17(1)	0(1)	-2(1)
C(11)	25(1)	46(1)	47(2)	9(1)	16(1)	-1(1)
C(12)	32(1)	66(2)	29(1)	9(1)	12(1)	-2(1)
C(13)	26(1)	48(1)	23(1)	12(1)	5(1)	-1(1)
C(14)	28(1)	24(1)	20(1)	11(1)	4(1)	6(1)
C(15)	32(1)	38(1)	40(1)	24(1)	-5(1)	-5(1)
C(16)	51(2)	39(1)	50(2)	32(1)	0(1)	1(1)

C(17)	45(1)	41(1)	33(1)	20(1)	0(1)	15(1)
C(18)	24(1)	47(1)	32(1)	16(1)	3(1)	9(1)
C(19)	26(1)	33(1)	29(1)	16(1)	8(1)	4(1)
C(20)	26(1)	23(1)	24(1)	10(1)	5(1)	1(1)
C(21)	27(1)	24(1)	25(1)	7(1)	0(1)	10(1)
C(22)	24(1)	40(1)	33(1)	10(1)	7(1)	13(1)
C(23)	39(1)	51(2)	31(1)	7(1)	12(1)	20(1)
C(24)	39(1)	42(1)	19(1)	2(1)	6(1)	12(1)
C(25)	29(1)	23(1)	22(1)	1(1)	-1(1)	4(1)
Li	36(2)	24(2)	27(2)	9(1)	8(2)	12(1)
C(26)	60(2)	58(2)	128(4)	60(2)	21(2)	18(2)
C(27)	128(3)	64(2)	79(3)	48(2)	45(2)	62(2)
C(28)	93(3)	32(2)	77(3)	19(2)	-19(2)	10(2)

### 10.1.13. Lithiiertes Benzylphenylsulfan **104**

Tabelle 10.41 Kristallographische Daten und Strukturverfeinerung von **104**.

Verbindung	<b>104</b>
Empirische Formel	C <sub>25</sub> H <sub>35</sub> LiO <sub>3</sub> S
Formelmasse [g/mol]	422.53
Temperatur [K]	173(2)
Wellenlänge [Å]	0.71073
Kristallsystem	orthorombisch
Raumgruppe	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (19)
<i>a</i> [Å]	9.2133(11)
<i>b</i> [Å]	15.0160(10)
<i>c</i> [Å]	16.7712(11)
Zellvolumen [Å <sup>3</sup> ]	2320.3(3)
Formeleinheit pro Zelle	4
Berechnete Dichte [g/cm <sup>3</sup> ]	1.210
Absorptionskoeffizient $\mu$ [mm <sup>-1</sup> ]	0.162
F(000)	912
Kristallgröße [mm <sup>3</sup> ]	0.40 x 0.20 x 0.10
Messbereich $\theta$ [°]	2.43 – 26.00
	-11 ≤ <i>h</i> ≤ 6
Index-Breite	-14 ≤ <i>k</i> ≤ 18
	-20 ≤ <i>l</i> ≤ 20
Gemessene Reflexe	9784

Unabhängige Reflexe	4559 ( $R_{\text{int}} = 0.0297$ )
Daten / Restraints / Parameter	4559 / 0 / 275
Goodness-of-fit an $F^2$	1.004
Endgültige R-Werte [ $I > 2\sigma(I)$ ]	$R1 = 0.0369$ , $wR2 = 0.0575$
R-Werte (sämtliche Daten)	$R1 = 0.0547$ , $wR2 = 0.0592$
Absoluter Strukturparameter	0.06(6)
Restelektronendichte [ $e/\text{\AA}^3$ ]	0.344 and $-0.227 e\cdot\text{\AA}^{-3}$

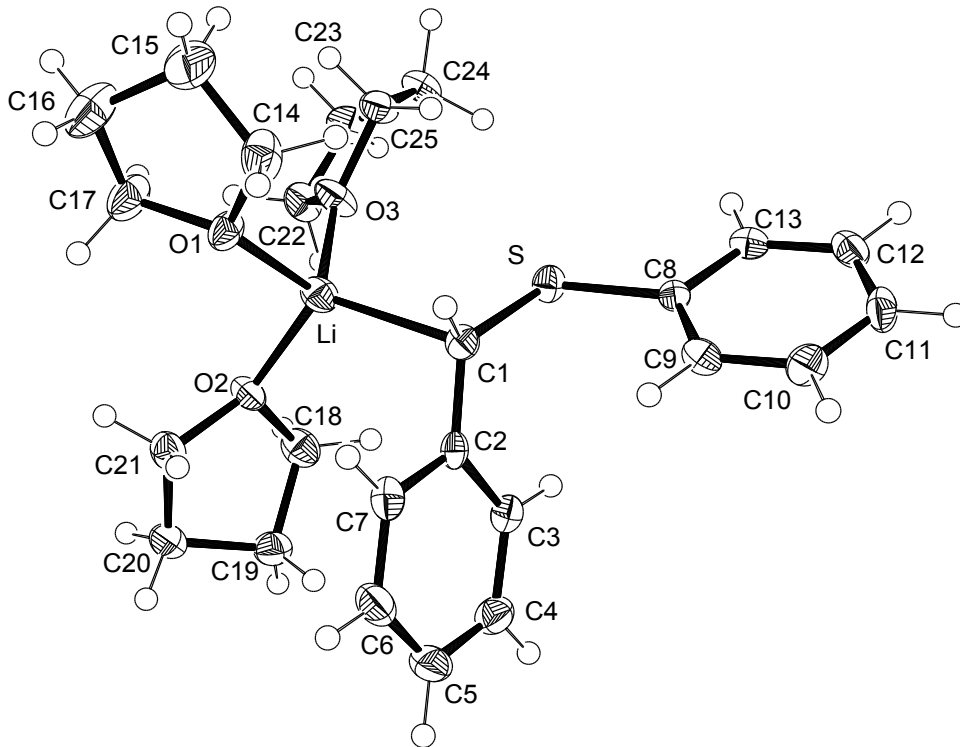


Abbildung 10.14 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von **104** im Kristall (ORTEP-Darstellung<sup>[206,207]</sup>). Das Nummerierungsschema der Wasserstoffatome wurde der Übersichtlichkeit halber weggelassen.

Tabelle 10.42 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **104**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\text{ij}}$ -Tensors.

	x	y	z	$U(\text{eq})$
H(1)	1634(19)	5358(10)	7259(9)	11(5)
C(1)	2275(2)	5763(1)	7503(1)	22(1)
C(2)	1730(2)	6161(1)	8223(1)	20(1)
C(3)	2220(2)	6979(1)	8533(1)	25(1)
C(4)	1699(2)	7315(1)	9241(1)	31(1)
C(5)	645(3)	6873(2)	9666(1)	36(1)

C(6)	136(2)	6071(2)	9376(1)	34(1)
C(7)	664(2)	5723(1)	8673(1)	26(1)
C(8)	2453(2)	7159(1)	6337(1)	18(1)
C(9)	1039(2)	7394(1)	6513(1)	24(1)
C(10)	356(2)	8061(1)	6092(1)	29(1)
C(11)	1071(2)	8494(1)	5482(1)	29(1)
C(12)	2458(2)	8255(1)	5297(1)	27(1)
C(13)	3152(2)	7596(1)	5721(1)	22(1)
C(14)	1985(2)	3351(1)	6999(1)	39(1)
C(15)	2515(3)	2463(2)	6720(1)	59(1)
C(16)	2886(3)	1988(2)	7454(1)	48(1)
C(17)	3451(3)	2715(1)	7976(1)	38(1)
C(18)	5016(2)	5487(1)	9308(1)	30(1)
C(19)	4290(2)	5691(1)	10082(1)	30(1)
C(20)	3964(3)	4777(1)	10404(1)	32(1)
C(21)	3576(2)	4265(1)	9662(1)	29(1)
C(22)	7006(2)	4464(2)	7684(1)	30(1)
C(23)	8044(2)	4552(2)	6995(1)	34(1)
C(24)	7088(2)	4828(1)	6306(1)	32(1)
C(25)	5665(2)	4415(1)	6521(1)	27(1)
Li	3727(4)	4657(2)	7920(2)	26(1)
O(1)	2741(1)	3523(1)	7730(1)	26(1)
O(2)	4332(1)	4691(1)	9018(1)	25(1)
O(3)	5566(2)	4530(1)	7358(1)	31(1)
S(1)	3428(1)	6318(1)	6863(1)	23(1)

Tabelle 10.43 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **104**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
C(1)	24(1)	18(1)	23(1)	-1(1)	-1(1)	-6(1)
C(2)	18(1)	19(1)	22(1)	6(1)	-5(1)	4(1)
C(3)	27(1)	20(1)	28(1)	3(1)	0(1)	0(1)
C(4)	40(1)	25(1)	29(1)	-4(1)	-4(1)	4(1)
C(5)	45(2)	42(2)	21(1)	1(1)	1(1)	13(1)
C(6)	34(1)	41(2)	27(1)	10(1)	7(1)	5(1)
C(7)	28(1)	23(1)	28(1)	5(1)	-5(1)	-1(1)
C(8)	23(1)	16(1)	16(1)	-2(1)	-5(1)	-4(1)
C(9)	19(1)	30(1)	22(1)	1(1)	2(1)	-5(1)
C(10)	21(1)	33(1)	34(1)	0(1)	-1(1)	7(1)

C(11)	35(1)	24(1)	27(1)	7(1)	-11(1)	1(1)
C(12)	36(2)	27(1)	20(1)	2(1)	0(1)	-8(1)
C(13)	20(1)	25(1)	21(1)	-4(1)	1(1)	-5(1)
C(14)	45(2)	33(1)	40(1)	7(1)	-21(1)	-3(1)
C(15)	100(2)	32(2)	43(2)	-10(1)	-12(2)	-9(2)
C(16)	46(2)	30(1)	67(2)	-9(1)	-19(2)	9(1)
C(17)	45(1)	27(1)	42(1)	-2(1)	-16(1)	13(1)
C(18)	28(1)	35(2)	27(1)	2(1)	1(1)	-7(1)
C(19)	34(1)	28(1)	26(1)	-4(1)	2(1)	-2(1)
C(20)	44(2)	30(1)	24(1)	0(1)	6(1)	-4(1)
C(21)	34(1)	27(1)	27(1)	3(1)	4(1)	-7(1)
C(22)	22(1)	41(1)	28(1)	6(1)	-2(1)	8(1)
C(23)	23(1)	46(2)	32(1)	-3(1)	1(1)	0(1)
C(24)	39(1)	38(2)	20(1)	1(1)	8(1)	1(1)
C(25)	26(1)	35(2)	20(1)	-1(1)	1(1)	7(1)
Li	27(2)	30(2)	20(2)	0(2)	-4(2)	-2(2)
O(1)	30(1)	21(1)	29(1)	-1(1)	-9(1)	6(1)
O(2)	29(1)	29(1)	17(1)	2(1)	2(1)	-6(1)
O(3)	23(1)	51(1)	19(1)	6(1)	3(1)	5(1)
S(1)	19(1)	22(1)	26(1)	3(1)	0(1)	1(1)

#### 10.1.14. Lithiertes *N,N*-Dimethyl-*o*-toluidin **105**

Tabelle 10.44 Kristallographische Daten und Strukturverfeinerung von **105**.

Verbindung	105
Empirische Formel	C <sub>36</sub> H <sub>48</sub> Li <sub>4</sub> N <sub>4</sub>
Formelmasse [g/mol]	564.54
Temperatur [K]	173(2) K
Wellenlänge [Å]	0.71073
Kristallsystem	tetragonal
Raumgruppe	<i>P</i> 4 <sub>2</sub> <sub>1</sub> <i>c</i> (114)
<i>a</i> [Å]	14.1540(5)
<i>b</i> [Å]	14.1540(5)
<i>c</i> [Å]	8.1543(7)
Zellvolumen [Å <sup>3</sup> ]	1633.60(16)
Formeleinheit pro Zelle	2
Berechnete Dichte [g/cm <sup>3</sup> ]	1.148
Absorptionskoeffizient $\mu$ [mm <sup>-1</sup> ]	0.065

F(000)	608
Kristallgröße [mm <sup>3</sup> ]	0.20 x 0.10 x 0.05
Messbereich $\Theta$ [°]	2.88 – 25.99
	-17 $\leq h \leq$ 14
Index-Breite	-15 $\leq k \leq$ 17
	-10 $\leq l \leq$ 10
Gemessene Reflexe	11038
Unabhängige Reflexe	1601 ( $R_{\text{int}} = 0.0550$ )
Daten / Restraints / Parameter	1601 / 0 / 110
Goodness-of-fit an $F^2$	1.016
Endgültige R-Werte [ $I > 2\sigma(I)$ ]	$R1 = 0.0364$ , $wR2 = 0.0534$
R-Werte (sämtliche Daten)	$R1 = 0.0571$ , $wR2 = 0.0557$
Restelektronendichte [ $e/\text{\AA}^3$ ]	0.115 und -0.134

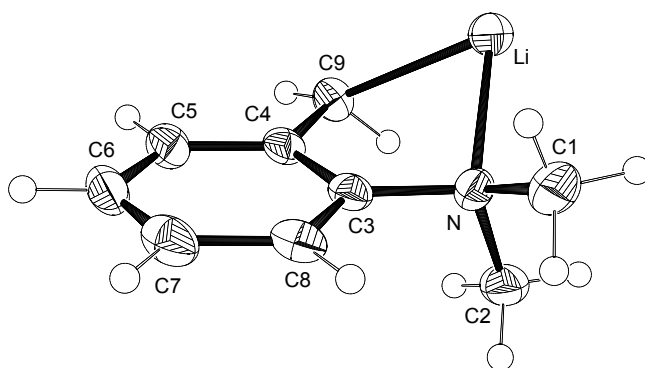


Abbildung 10.15 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von **105** im Kristall (ORTEP-Darstellung<sup>[206,207]</sup>). Das Nummerierungsschema der Wasserstoffatome wurde der Übersichtlichkeit halber weggelassen.

Tabelle 10.45 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von XXX.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\text{ij}}$ -Tensors.

	x	y	z	$U(\text{eq})$
N	6043(1)	7175(1)	973(2)	26(1)
C(1)	5752(1)	7626(1)	2505(2)	39(1)
C(2)	7074(1)	7309(1)	772(2)	37(1)
C(3)	5539(1)	7513(1)	-467(2)	25(1)
C(4)	5470(1)	6873(1)	-1804(2)	26(1)
C(5)	4965(1)	7197(1)	-3176(2)	31(1)
C(6)	4566(1)	8089(1)	-3248(2)	35(1)
C(7)	4654(1)	8694(1)	-1935(3)	37(1)
C(8)	5145(1)	8402(1)	-545(2)	31(1)
C(9)	5837(1)	5920(1)	-1703(2)	28(1)

Li	5630(2)	5718(2)	1078(3)	30(1)
H(9A)	5882(9)	5627(9)	-2741(17)	23(4)
H(9B)	6472(10)	5889(9)	-1250(18)	24(4)

Tabelle 10.46 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von XXX. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
N	26(1)	28(1)	24(1)	-2(1)	-2(1)	-2(1)
C(1)	47(1)	39(1)	33(1)	-8(1)	-4(1)	-10(1)
C(2)	29(1)	36(1)	46(1)	11(1)	-6(1)	-6(1)
C(3)	22(1)	26(1)	28(1)	5(1)	4(1)	-3(1)
C(4)	23(1)	30(1)	24(1)	4(1)	6(1)	-3(1)
C(5)	32(1)	38(1)	25(1)	4(1)	4(1)	-2(1)
C(6)	26(1)	43(1)	36(1)	19(1)	1(1)	2(1)
C(7)	27(1)	31(1)	54(1)	15(1)	5(1)	7(1)
C(8)	30(1)	26(1)	37(1)	4(1)	8(1)	-3(1)
C(9)	33(1)	28(1)	23(1)	-3(1)	5(1)	4(1)
Li	31(2)	31(2)	29(2)	-3(1)	2(1)	-2(1)

### 10.1.15. Lithiiertes *N,N*-Dimethyl-*o*-toluidin **106**

Tabelle 10.47 Kristallographische Daten und Strukturverfeinerung von **106**.

Verbindung	<b>106</b>
Empirische Formel	$C_{19}H_{34}LiN_3$
Formelmass [g/mol]	311.43
Temperatur [K]	173(2) K
Wellenlänge [ $\text{\AA}$ ]	0.71073
Kristallsystem	monoklin
Raumgruppe	$P2_1$ (4)
$a$ [ $\text{\AA}$ ]	8.3473(4)
$b$ [ $\text{\AA}$ ]	14.2312(6)
$c$ [ $\text{\AA}$ ]	16.2504(8)
Zellvolumen [ $\text{\AA}^3$ ]	1901.54(16)
Formeleinheit pro Zelle	4
Berechnete Dichte [ $\text{g/cm}^3$ ]	1.088
Absorptionskoeffizient $\mu$ [ $\text{mm}^{-1}$ ]	0.063

F(000)	688
Kristallgröße [mm <sup>3</sup> ]	0.30 x 0.10 x 0.10
Messbereich $\Theta$ [°]	2.48 – 26.00
	-10 $\leq h \leq$ 10
Index-Breite	-17 $\leq k \leq$ 17
	-20 $\leq l \leq$ 20
Gemessene Reflexe	25652
Unabhängige Reflexe	7466 ( $R_{\text{int}} = 0.0434$ )
Daten / Restraints / Parameter	7466 / 1 / 443
Goodness-of-fit an $F^2$	1.018
Endgültige R-Werte [ $I > 2\sigma(I)$ ]	$R1 = 0.0377$ , $wR2 = 0.0576$
R-Werte (sämtliche Daten)	$R1 = 0.0665$ , $wR2 = 0.0596$
Absoluter Strukturparameter	0.3(17)
Restelektronendichte [ $e/\text{\AA}^3$ ]	0.139 and -0.153 $e.\text{\AA}^{-3}$

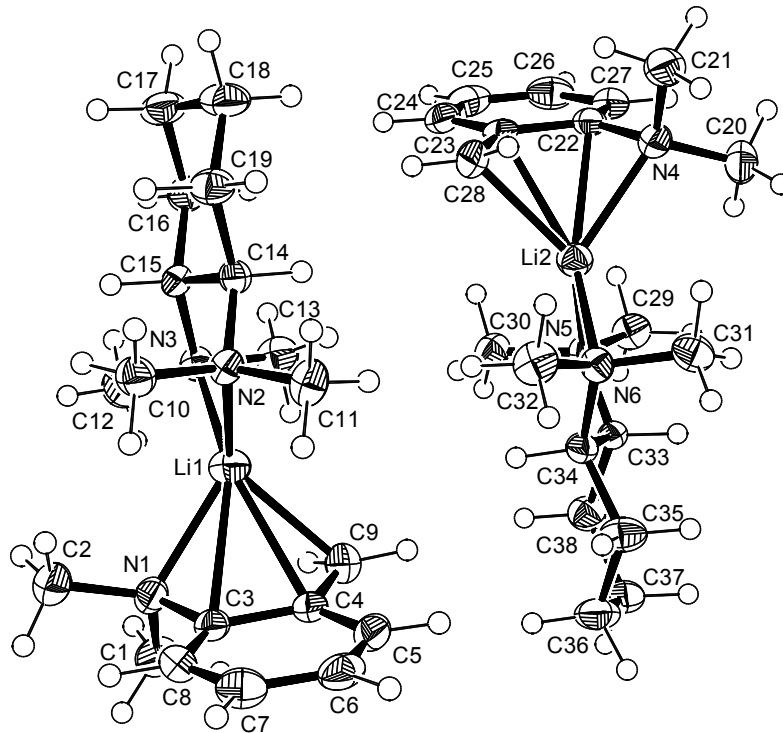


Abbildung 10.16 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von **106** im Kristall (ORTEP-Darstellung<sup>[206,207]</sup>). Das Nummerierungsschema der Wasserstoffatome wurde der Übersichtlichkeit halber weggelassen.

Tabelle 10.48 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **106**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U_{ij}$ -Tensors.

	x	y	z	$U_{\text{eq}}$
N(1)	8344(2)	7957(1)	-555(1)	29(1)

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N(2)	9910(2)	6647(1)	1438(1)	23(1)
N(3)	6464(2)	6677(1)	997(1)	25(1)
C(1)	7145(3)	8596(2)	-1031(1)	39(1)
C(2)	8578(3)	7154(2)	-1089(1)	39(1)
C(3)	9805(3)	8446(1)	-185(1)	27(1)
C(4)	9666(3)	9010(2)	529(1)	30(1)
C(5)	11171(3)	9433(2)	907(1)	38(1)
C(6)	12610(3)	9306(2)	627(1)	39(1)
C(7)	12688(3)	8749(2)	-58(2)	38(1)
C(8)	11267(3)	8327(2)	-460(1)	32(1)
C(9)	8252(3)	9092(2)	880(2)	39(1)
C(10)	10678(2)	6051(2)	879(1)	33(1)
C(11)	11190(2)	7203(2)	1956(1)	34(1)
C(12)	5304(2)	6403(2)	247(1)	39(1)
C(13)	5638(3)	7272(2)	1533(1)	37(1)
C(14)	8915(2)	6117(1)	1955(1)	25(1)
C(15)	7278(2)	5845(1)	1436(1)	24(1)
C(16)	6225(3)	5313(1)	1968(1)	32(1)
C(17)	7104(3)	4460(2)	2388(1)	41(1)
C(18)	8688(3)	4759(2)	2926(1)	43(1)
C(19)	9763(3)	5255(1)	2392(1)	34(1)
Li(1)	8282(4)	7549(3)	730(2)	33(1)
N(4)	6735(2)	8261(1)	5563(1)	31(1)
N(5)	5002(2)	9619(1)	3685(1)	24(1)
N(6)	8395(2)	9392(1)	3800(1)	24(1)
C(20)	6508(3)	9101(2)	6049(1)	41(1)
C(21)	7923(3)	7641(2)	6072(1)	40(1)
C(22)	5252(3)	7768(1)	5217(1)	27(1)
C(23)	5362(3)	7165(2)	4519(1)	29(1)
C(24)	3853(3)	6739(2)	4157(1)	38(1)
C(25)	2432(3)	6900(2)	4435(2)	44(1)
C(26)	2369(3)	7481(2)	5104(2)	41(1)
C(27)	3793(3)	7912(2)	5490(1)	33(1)
C(28)	6764(3)	7061(2)	4169(2)	37(1)
C(29)	3754(2)	9985(2)	4145(1)	33(1)
C(30)	4205(2)	9003(2)	3008(1)	33(1)
C(31)	9263(2)	9876(2)	4544(1)	35(1)
C(32)	9519(3)	8796(2)	3436(1)	37(1)
C(33)	5943(2)	10396(1)	3393(1)	23(1)
C(34)	7531(2)	10043(1)	3157(1)	25(1)
C(35)	8547(3)	10875(2)	2947(1)	38(1)

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C(36)	7632(3)	11455(2)	2230(1)	43(1)
C(37)	6021(3)	11792(1)	2444(1)	38(1)
C(38)	5016(3)	10972(2)	2663(1)	34(1)
Li(2)	6663(4)	8613(3)	4254(2)	30(1)
H(9A)	7200(20)	8960(15)	565(11)	29(7)
H(9B)	8300(30)	9447(17)	1389(15)	65(8)
H(28A)	6720(20)	6682(14)	3708(12)	28(6)
H(28B)	7820(30)	7136(17)	4507(13)	57(8)

Tabelle 10.49 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **106**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
N(1)	33(1)	23(1)	30(1)	-2(1)	4(1)	0(1)
N(2)	19(1)	22(1)	29(1)	-3(1)	7(1)	0(1)
N(3)	23(1)	25(1)	26(1)	-1(1)	2(1)	5(1)
C(1)	35(2)	38(2)	42(2)	4(1)	-2(1)	-4(1)
C(2)	45(2)	33(1)	38(1)	-5(1)	4(1)	-4(1)
C(3)	32(1)	23(1)	24(1)	3(1)	1(1)	-4(1)
C(4)	43(2)	21(1)	24(1)	4(1)	3(1)	-2(1)
C(5)	57(2)	24(1)	29(1)	2(1)	-3(1)	-4(1)
C(6)	43(2)	32(2)	35(2)	11(1)	-10(1)	-12(1)
C(7)	33(2)	40(2)	40(2)	11(1)	6(1)	2(1)
C(8)	42(2)	32(2)	25(1)	1(1)	7(1)	-2(1)
C(9)	53(2)	33(2)	33(2)	-4(1)	13(2)	1(1)
C(10)	33(1)	34(1)	33(1)	0(1)	10(1)	3(1)
C(11)	26(1)	33(1)	43(1)	-9(1)	10(1)	0(1)
C(12)	36(1)	43(1)	36(1)	1(1)	-3(1)	2(1)
C(13)	32(1)	34(1)	46(2)	4(1)	12(1)	8(1)
C(14)	29(1)	24(1)	24(1)	-1(1)	9(1)	3(1)
C(15)	27(1)	19(1)	26(1)	-1(1)	5(1)	1(1)
C(16)	35(1)	30(1)	34(1)	1(1)	9(1)	-3(1)
C(17)	54(2)	29(1)	45(2)	10(1)	24(1)	-1(1)
C(18)	50(2)	37(1)	43(2)	17(1)	10(1)	10(1)
C(19)	34(1)	31(2)	36(1)	8(1)	4(1)	7(1)
Li(1)	33(2)	32(2)	36(2)	5(2)	9(2)	1(2)
N(4)	33(1)	26(1)	31(1)	0(1)	2(1)	-3(1)
N(5)	23(1)	25(1)	24(1)	-3(1)	3(1)	-1(1)
N(6)	23(1)	25(1)	26(1)	-2(1)	6(1)	7(1)
C(20)	50(2)	39(2)	34(1)	-10(1)	6(1)	-9(1)

C(21)	39(2)	38(2)	38(2)	5(1)	-5(1)	-5(1)
C(22)	31(1)	25(1)	24(1)	6(1)	2(1)	-4(1)
C(23)	41(2)	19(1)	27(1)	9(1)	1(1)	1(1)
C(24)	53(2)	24(1)	33(1)	6(1)	-7(1)	-5(1)
C(25)	41(2)	36(2)	50(2)	16(1)	-10(1)	-11(1)
C(26)	31(2)	46(2)	48(2)	17(1)	9(1)	-1(1)
C(27)	39(2)	31(2)	31(1)	5(1)	8(1)	-3(1)
C(28)	53(2)	25(2)	33(2)	-4(1)	6(2)	4(1)
C(29)	27(1)	34(1)	41(1)	2(1)	13(1)	2(1)
C(30)	32(1)	29(1)	37(1)	0(1)	1(1)	-1(1)
C(31)	32(1)	40(1)	32(1)	5(1)	2(1)	3(1)
C(32)	27(1)	37(1)	47(2)	1(1)	10(1)	9(1)
C(33)	26(1)	19(1)	23(1)	1(1)	5(1)	1(1)
C(34)	31(1)	23(1)	22(1)	1(1)	4(1)	2(1)
C(35)	35(1)	40(2)	43(2)	10(1)	17(1)	-2(1)
C(36)	56(2)	35(2)	42(2)	11(1)	19(1)	-3(1)
C(37)	51(2)	29(1)	32(1)	9(1)	3(1)	5(1)
C(38)	37(1)	31(2)	34(1)	4(1)	6(1)	7(1)
Li(2)	32(2)	29(2)	29(2)	2(2)	6(2)	3(2)

### 10.1.16. Cyclopentadienyl-Komplex **108**

Tabelle 10.50 Kristallographische Daten und Strukturverfeinerung von **108**.

Verbindung	<b>108</b>
CCDC Nummer	1009747
Empirische Formel	C <sub>24</sub> H <sub>29</sub> NPdSi
Formelmasse [g/mol]	465.97
Temperatur [K]	123(2)
Wellenlänge [Å]	0.71073
Kristallsystem	tetragonal
Raumgruppe	<i>P</i> 4 <sub>3</sub> 2 <sub>1</sub> 2 (96)
<i>a</i> [Å]	11.9477(2)
<i>c</i> [Å]	32.6793(10)
Zellvolumen [Å <sup>3</sup> ]	4664.91(18)
Formeleinheit pro Zelle	Z = 8
Berechnete Dichte [g/cm <sup>3</sup> ]	1.327
Absorptionskoeffizient $\mu$ [mm <sup>-1</sup> ]	0.855
F(000)	1920

Kristallgröße [mm <sup>3</sup> ]	0.30 x 0.30 x 0.30
Messbereich $\Theta$ [°]	2.41 – 27.98°
Index-Breite	-15 $\leq h \leq$ 15 -15 $\leq k \leq$ 15 -43 $\leq l \leq$ 43
Gemessene Reflexe	58301
Unabhängige Reflexe	5626 ( $R_{\text{int}} = 0.0394$ )
Daten / Restraints / Parameter	5626 / 0 / 244
Goodness-of-fit an $F^2$	1.034
Endgültige R-Werte [ $I > 2\sigma(I)$ ]	$R1 = 0.0228$ , $wR2 = 0.0612$
R-Werte (sämtliche Daten)	$R1 = 0.0247$ , $wR2 = 0.0621$
Absoluter Strukturparameter	0.01(2)
Restelektronendichte [ $e/\text{\AA}^3$ ]	0.396 und -0.320

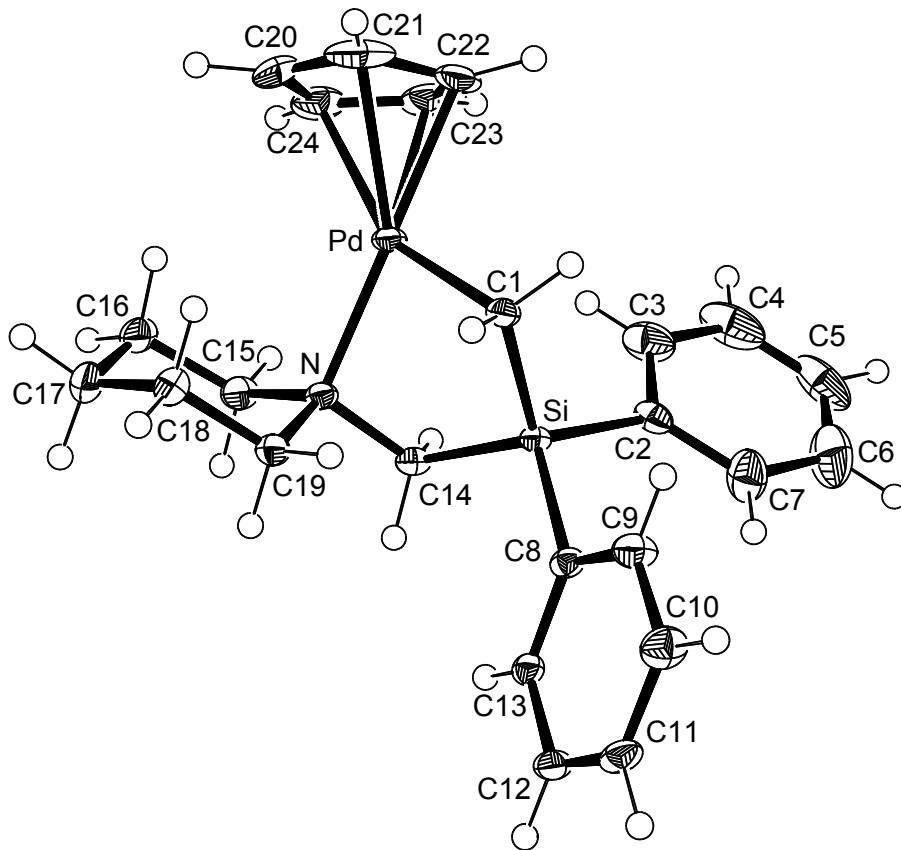


Abbildung 10.17 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von **108** im Kristall (ORTEP-Darstellung<sup>[206,207]</sup>). Das Nummerierungsschema der Wasserstoffatome wurde der Übersichtlichkeit halber weggelassen.

Tabelle 10.51 Atomkoordinaten [ $\cdot 10^4$ ] und isotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **108**.  $U_{\text{eq}}$  berechnet sich als Drittel der Spur des orthogonalisierten  $U^{\text{ij}}$ -Tensors.

	x	y	z	$U(\text{eq})$
Pd	5822(1)	9086(1)	2313(1)	17(1)
Si	3642(1)	9892(1)	1921(1)	14(1)
N	4370(1)	9255(2)	2692(1)	17(1)
C(1)	4761(2)	8853(2)	1825(1)	17(1)
C(2)	3927(2)	11236(2)	1643(1)	20(1)
C(3)	4884(2)	11869(2)	1730(1)	35(1)
C(4)	5112(3)	12848(3)	1515(1)	49(1)
C(5)	4382(3)	13218(2)	1210(1)	48(1)
C(6)	3451(3)	12623(3)	1127(1)	50(1)
C(7)	3213(3)	11637(2)	1343(1)	35(1)
C(8)	2233(2)	9370(2)	1750(1)	16(1)
C(9)	2139(2)	8782(2)	1383(1)	24(1)
C(10)	1107(2)	8393(2)	1245(1)	27(1)
C(11)	158(2)	8561(2)	1477(1)	22(1)
C(12)	225(2)	9136(2)	1843(1)	22(1)
C(13)	1255(2)	9543(2)	1978(1)	17(1)
C(14)	3699(2)	10158(2)	2494(1)	17(1)
C(15)	4652(2)	9591(2)	3121(1)	23(1)
C(16)	5254(2)	8661(2)	3353(1)	27(1)
C(17)	4584(2)	7581(2)	3349(1)	30(1)
C(18)	4285(2)	7264(2)	2911(1)	24(1)
C(19)	3671(2)	8225(2)	2708(1)	18(1)
C(20)	7625(2)	8344(3)	2593(1)	36(1)
C(21)	7525(2)	8131(3)	2188(1)	43(1)
C(22)	7376(2)	9171(4)	1978(1)	48(1)
C(23)	7512(2)	10040(3)	2271(1)	43(1)
C(24)	7583(2)	9517(3)	2653(1)	36(1)

Tabelle 10.52 Anisotrope Auslenkungsparameter [ $\text{\AA}^2 \cdot 10^3$ ] von **108**. Der Exponent des anisotropen Auslenkungsparameters hat die Form:  $-2\pi^2 \cdot (2h^2 \cdot a^* \cdot U^{11} + \dots + 2h \cdot k \cdot a^* \cdot b^* \cdot U^{12})$ .

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Pd	9(1)	26(1)	15(1)	-3(1)	0(1)	2(1)
Si	10(1)	16(1)	16(1)	-1(1)	1(1)	0(1)
N	11(1)	24(1)	15(1)	-1(1)	-1(1)	1(1)
C(1)	13(1)	22(1)	16(1)	-2(1)	1(1)	1(1)
C(2)	20(1)	18(1)	23(1)	-2(1)	7(1)	0(1)

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C(3)	28(1)	28(1)	51(2)	1(1)	8(1)	-6(1)
C(4)	45(2)	27(2)	74(2)	-5(2)	27(2)	-16(1)
C(5)	68(2)	20(1)	56(2)	4(1)	39(2)	0(1)
C(6)	71(2)	34(2)	43(2)	17(1)	1(2)	2(2)
C(7)	44(2)	26(1)	34(1)	8(1)	-4(1)	-6(1)
C(8)	13(1)	14(1)	21(1)	2(1)	-1(1)	-1(1)
C(9)	17(1)	29(1)	25(1)	-5(1)	1(1)	-1(1)
C(10)	23(1)	30(1)	27(1)	-5(1)	-5(1)	-3(1)
C(11)	13(1)	22(1)	32(1)	4(1)	-6(1)	-4(1)
C(12)	13(1)	22(1)	29(1)	7(1)	2(1)	2(1)
C(13)	15(1)	15(1)	20(1)	4(1)	-1(1)	1(1)
C(14)	13(1)	19(1)	20(1)	-3(1)	1(1)	1(1)
C(15)	19(1)	34(1)	15(1)	-6(1)	-1(1)	2(1)
C(16)	21(1)	47(2)	14(1)	-1(1)	-3(1)	7(1)
C(17)	29(1)	42(2)	21(1)	10(1)	1(1)	10(1)
C(18)	21(1)	27(1)	24(1)	6(1)	-2(1)	3(1)
C(19)	15(1)	23(1)	17(1)	0(1)	0(1)	0(1)
C(20)	13(1)	51(2)	44(2)	11(1)	-5(1)	6(1)
C(21)	13(1)	61(2)	55(2)	-28(2)	1(1)	4(1)
C(22)	11(1)	112(3)	21(1)	6(2)	2(1)	8(2)
C(23)	13(1)	45(2)	70(2)	12(2)	4(1)	-3(1)
C(24)	16(1)	62(2)	31(1)	-16(1)	-5(1)	2(1)

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## 10.2. Details zu den quantenchemischen Rechnungen

### 10.2.1. Details zu den Evaluations-Rechnungen von Kapitel 3.2

#### 10.2.1.1. Aggregation von Lithiumchlorid

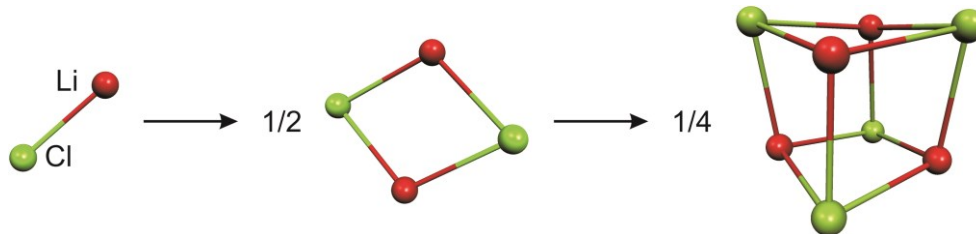


Abbildung 10.18 Aggregation von Lithiumchlorid bis hin zu einem Tetramer.

Tabelle 10.53 Berechnete Energien der optimierten Strukturen zur Aggregation von Lithiumchlorid in der jeweils höchsten möglichen Punktgruppe (Monomer:  $C_{\infty v}$ ; Dimer:  $D_{2h}$ ; Tetramer  $T_d$ ).

	Method	Basissatz	SCF [Hartree]	ZPE [Hartree]
LiCl	SVWN	6-31+G(d)	-466.5514285	-466.550003
(LiCl) <sub>2</sub>	SVWN	6-31+G(d)	-933.1892143	-933.184242
(LiCl) <sub>4</sub>	SVWN	6-31+G(d)	-1866.467389	-1866.454838
LiCl	PBE	6-31+G(d)	-467.5604043	-467.559016
(LiCl) <sub>2</sub>	PBE	6-31+G(d)	-935.2007517	-935.195935
(LiCl) <sub>4</sub>	PBE	6-31+G(d)	-1870.474734	-1870.462814
LiCl	TPSS	6-31+G(d)	-467.7989629	-467.797566
(LiCl) <sub>2</sub>	TPSS	6-31+G(d)	-935.6776322	-935.672837
(LiCl) <sub>4</sub>	TPSS	6-31+G(d)	-1871.428395	-1871.416082
LiCl	PBE0	6-31+G(d)	-467.6042727	-467.602856
(LiCl) <sub>2</sub>	PBE0	6-31+G(d)	-935.2898714	-935.284964
(LiCl) <sub>4</sub>	PBE0	6-31+G(d)	-1870.653935	-1870.641932
LiCl	TPSSh	6-31+G(d)	-467.7933078	-467.7919
(LiCl) <sub>2</sub>	TPSSh	6-31+G(d)	-935.6668668	-935.662033
(LiCl) <sub>4</sub>	TPSSh	6-31+G(d)	-1871.407281	-1871.394889
LiCl	B3LYP	6-31+G(d)	-467.7998561	-467.798448
(LiCl) <sub>2</sub>	B3LYP	6-31+G(d)	-935.6783966	-935.673526
(LiCl) <sub>4</sub>	B3LYP	6-31+G(d)	-1871.42444	-1871.412776
LiCl	B3LYP	6-311+G(d,p)	-467.8338013	-467.832345
(LiCl) <sub>2</sub>	B3LYP	6-311+G(d,p)	-935.7452462	-935.740245
(LiCl) <sub>4</sub>	B3LYP	6-311+G(d,p)	-1871.553292	-1871.541403
LiCl	M052X	6-31+G(d)	-467.7693486	-467.767914
(LiCl) <sub>2</sub>	M052X	6-31+G(d)	-935.6220183	-935.617098
(LiCl) <sub>4</sub>	M052X	6-31+G(d)	-1871.323991	-1871.311068
LiCl	M052X	6-31+G(d,p)	-467.7693486	-467.767914
(LiCl) <sub>2</sub>	M052X	6-31+G(d,p)	-935.6220183	-935.617098
(LiCl) <sub>4</sub>	M052X	6-31+G(d,p)	-1871.323991	-1871.311068
LiCl	M052X	6-311+G(d,p)	-467.8066539	-467.805218
(LiCl) <sub>2</sub>	M052X	6-311+G(d,p)	-935.6959838	-935.69092
(LiCl) <sub>4</sub>	M052X	6-311+G(d,p)	-1871.467845	-1871.454679
LiCl	M052X	6-311+G(3df,3pd)	-467.808903	-467.80747

(LiCl) <sub>2</sub>	M052X	6-311+G(3df,3pd)	-935.7012422	-935.696172
(LiCl) <sub>4</sub>	M052X	6-311+G(3df,3pd)	-1871.479004	-1871.466048
LiCl	M06L	6-31+G(d)	-467.7837511	-467.782405
(LiCl) <sub>2</sub>	M06L	6-31+G(d)	-935.6472131	-935.64264
(LiCl) <sub>4</sub>	M06L	6-31+G(d)	-1871.37328	-1871.361163
LiCl	M06	6-31+G(d)	-467.7646612	-467.763303
(LiCl) <sub>2</sub>	M06	6-31+G(d)	-935.608978	-935.604286
(LiCl) <sub>4</sub>	M06	6-31+G(d)	-1871.292867	-1871.283452
LiCl	M06	6-31+G(d,p)	-467.7646612	-467.763303
(LiCl) <sub>2</sub>	M06	6-31+G(d,p)	-935.608978	-935.604286
(LiCl) <sub>4</sub>	M06	6-31+G(d,p)	-1871.292867	-1871.283452
LiCl	M06	6-311+G(d,p)	-467.7937015	-467.792284
(LiCl) <sub>2</sub>	M06	6-311+G(d,p)	-935.6658072	-935.661082
(LiCl) <sub>4</sub>	M06	6-311+G(d,p)	-1871.403437	-1871.393902
LiCl	M062X	6-31+G(d)	-467.7571747	-467.755733
(LiCl) <sub>2</sub>	M062X	6-31+G(d)	-935.5979542	-935.592961
(LiCl) <sub>4</sub>	M062X	6-31+G(d)	-1871.277339	-1871.264022
LiCl	M062X	6-31+G(d,p)	-467.7571747	-467.755733
(LiCl) <sub>2</sub>	M062X	6-31+G(d,p)	-935.5979542	-935.592961
(LiCl) <sub>4</sub>	M062X	6-31+G(d,p)	-1871.277339	-1871.264022
LiCl	M062X	6-311+G(d,p)	-467.7948464	-467.793376
(LiCl) <sub>2</sub>	M062X	6-311+G(d,p)	-935.6727696	-935.667609
(LiCl) <sub>4</sub>	M062X	6-311+G(d,p)	-1871.423269	-1871.409876
LiCl	MP2	6-31+G(d)	-467.1498855	-467.148453
(LiCl) <sub>2</sub>	MP2	6-31+G(d)	-934.3854111	-934.380436
(LiCl) <sub>4</sub>	MP2	6-31+G(d)	-1868.850632	-1868.838601
LiCl	MP2	6-311+G(d,p)	-467.1885752	-467.187072
(LiCl) <sub>2</sub>	MP2	6-311+G(d,p)	-934.4636466	-934.45841
(LiCl) <sub>4</sub>	MP2	6-311+G(d,p)	-1869.00481	-1868.99224
LiCl	G3			-467.632458
(LiCl) <sub>2</sub>	G3			-935.345574
(LiCl) <sub>4</sub>	G3			-1870.765167

Tabelle 10.54 Standardorientierung von LiCl (C<sub>∞v</sub>) [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
Cl	-0.9739847208	-1.4128856952	0.
Li	0.9739847208	-0.8183883048	0.

Tabelle 10.55 Standardorientierung von (LiCl)<sub>2</sub> (D<sub>2h</sub>) [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
Li	0.	1.3039910795	0.
Cl	0.	0.	1.7678762504
Li	0.	-1.3039910795	0.
Cl	0.	0.	-1.7678762504

Tabelle 10.56 Standardorientierung von (LiCl)<sub>4</sub> (T<sub>d</sub>) [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
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Li	-0.0000000035	0.0000000082	1.7479243548
Li	-0.0000000007	-1.6479588831	-0.5826414434
Li	1.427174263	0.8239794354	-0.5826414486
Li	-1.4271742524	0.8239794496	-0.5826414543
Cl	0.0000000087	2.0472051029	0.7237962991
Cl	-1.7729316282	-1.0236025353	0.7237963056
Cl	0.0000000043	-0.0000000046	-2.1713889088
Cl	1.7729316151	-1.023602553	0.7237963127

Tabelle 10.57 Standardorientierung von LiCl ( $C_{\infty v}$ ) [globales Minimum; PBE/6-31+G(d)].

	x	y	z
Cl	-0.9854826737	-1.4163947354	0.
Li	0.9854826737	-0.8148792646	0.

Tabelle 10.58 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; PBE/6-31+G(d)].

	x	y	z
Li	0.	1.312321248	0.
Cl	0.	0.	1.8056875195
Li	0.	-1.312321248	0.
Cl	0.	0.	-1.8056875195

Tabelle 10.59 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; PBE/6-31+G(d)].

	x	y	z
Li	-0.0000000035	0.0000000083	1.7742060902
Li	-0.0000000072	-1.6727375409	-0.5914020218
Li	1.4486332101	0.8363687641	-0.591402027
Li	-1.4486331994	0.8363687785	-0.5914020328
Cl	0.000000009	2.1006262105	0.7426835126
Cl	-1.8191956646	-1.0503130888	0.7426835193
Cl	0.0000000044	-0.0000000048	-2.2280505499
Cl	1.8191956511	-1.0503131069	0.7426835265

Tabelle 10.60 Standardorientierung von LiCl ( $C_{\infty v}$ ) [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
Cl	-0.9853253695	-1.416346728	0.
Li	0.9853253695	-0.814927272	0.

Tabelle 10.61 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
Li	0.	1.3143683184	0.
Cl	0.	0.	1.8036024872
Li	0.	-1.3143683184	0.
Cl	0.	0.	-1.8036024872

Tabelle 10.62 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
Li	-0.0000000035	0.0000000083	1.7754970604
Li	-0.0000000072	-1.6739546793	-0.5918323452
Li	1.4496872829	0.8369773333	-0.5918323504
Li	-1.4496872722	0.8369773477	-0.5918323562
Cl	0.0000000009	2.096044514	0.7410636383
Cl	-1.815227799	-1.0480222406	0.741063645
Cl	0.0000000044	-0.0000000047	-2.2231909269
Cl	1.8152277856	-1.0480222587	0.7410636522

Tabelle 10.63 Standardorientierung von  $\text{LiCl}$  ( $C_{\infty v}$ ) [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
Cl	-0.9814187056	-1.41515446	0.
Li	0.9814187056	-0.81611954	0.

Tabelle 10.64 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
Li	0.	1.314867879	0.
Cl	0.	0.	1.7916099012
Li	0.	-1.314867879	0.
Cl	0.	0.	-1.7916099012

Tabelle 10.65 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
Li	-0.0000000035	0.0000000083	1.7716547582
Li	-0.0000000071	-1.670332122	-0.5905515777
Li	1.4465500562	0.8351660546	-0.590551583
Li	-1.4465500455	0.835166069	-0.5905515888
Cl	0.0000000089	2.0855648927	0.7373585327
Cl	-1.8061521807	-1.04278243	0.7373585393
Cl	0.0000000044	-0.0000000047	-2.21207561
Cl	1.8061521674	-1.042782448	0.7373585465

Tabelle 10.66 Standardorientierung von  $\text{LiCl}$  ( $C_{\infty v}$ ) [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
Cl	-0.98379192	-1.4158787372	0.
Li	0.98379192	-0.8153952628	0.

Tabelle 10.67 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
Li	0.	1.3149691682	0.
Cl	0.	0.	1.7984576608

Li	0.	-1.3149691682	0.
Cl	0.	0.	-1.7984576608

Tabelle 10.68 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
Li	-0.0000000035	0.0000000083	1.7752107867
Li	-0.0000000072	-1.6736847778	-0.5917369206
Li	1.4494535414	0.8368423826	-0.5917369259
Li	-1.4494535307	0.836842397	-0.5917369317
Cl	0.0000000089	2.090430828	0.7390789006
Cl	-1.8103662044	-1.0452153976	0.7390789073
Cl	0.0000000044	-0.0000000047	-2.2172367138
Cl	1.810366191	-1.0452154157	0.7390789145

Tabelle 10.69 Standardorientierung von  $\text{LiCl}$  ( $C_{\infty v}$ ) [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
Cl	-0.9823369476	-1.4154346967	0.
Li	0.9823369476	-0.8158393033	0.

Tabelle 10.70 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
Li	0.	1.3101829844	0.
Cl	0.	0.	1.8022815039
Li	0.	-1.3101829844	0.
Cl	0.	0.	-1.8022815039

Tabelle 10.71 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
Li	1.0259385049	1.0259385049	1.0259385049
Li	-1.0259385049	-1.0259385049	1.0259385049
Li	1.0259385049	-1.0259385049	-1.0259385049
Li	-1.0259385049	1.0259385049	-1.0259385049
Cl	1.2853458839	1.2853458839	-1.2853458839
Cl	-1.2853458839	1.2853458839	1.2853458839
Cl	-1.2853458839	-1.2853458839	-1.2853458839
Cl	1.2853458839	-1.2853458839	1.2853458839

Tabelle 10.72 Standardorientierung von  $\text{LiCl}$  ( $C_{\infty v}$ ) [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
Cl	-0.9682213969	-1.4111267965	0.
Li	0.9682213969	-0.8201472035	0.

Tabelle 10.73 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
Li	0.	1.2831107565	0.
Cl	0.	0.	1.7866266096
Li	0.	-1.2831107565	0.
Cl	0.	0.	-1.7866266096

Tabelle 10.74 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
Li	-0.0000000035	0.0000000082	1.7486037374
Li	-0.000000007	-1.6485994112	-0.5828679042
Li	1.4277289765	0.8242996994	-0.5828679095
Li	-1.427728966	0.8242997136	-0.5828679151
Cl	0.0000000089	2.0848546056	0.7371074083
Cl	-1.8055370541	-1.0424272865	0.7371074149
Cl	0.0000000044	-0.0000000047	-2.2113222368
Cl	1.8055370408	-1.0424273044	0.7371074221

Tabelle 10.75 Standardorientierung von  $\text{LiCl}$  ( $C_{\infty v}$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Cl	-0.984798659	-1.4161859821	0.
Li	0.984798659	-0.8150880179	0.

Tabelle 10.76 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	0.	1.3199547681	0.
Cl	0.	0.	1.7942327459
Li	0.	-1.3199547681	0.
Cl	0.	0.	-1.7942327459

Tabelle 10.77 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	-0.0000000035	0.0000000083	1.7745545996
Li	-0.0000000072	-1.6730661187	-0.5915181916
Li	1.4489177668	0.836533053	-0.5915181969
Li	-1.4489177562	0.8365330674	-0.5915182026
Cl	0.0000000089	2.0870371812	0.7378790653
Cl	-1.80742722	-1.0435185743	0.7378790719
Cl	0.0000000044	-0.0000000047	-2.2136372078
Cl	1.8074272067	-1.0435185923	0.7378790791

Tabelle 10.78 Standardorientierung von  $\text{LiCl}$  ( $C_{\infty v}$ ) [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
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Cl	-0.984798659	-1.4161859821	0.
Li	0.984798659	-0.8150880179	0.

Tabelle 10.79 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
Li	0.	1.3199547696	0.
Cl	0.	0.	1.7942327392
Li	0.	-1.3199547696	0.
Cl	0.	0.	-1.7942327392

Tabelle 10.80 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
Li	-0.0000000035	0.0000000083	1.7745545997
Li	-0.0000000072	-1.6730661188	-0.5915181916
Li	1.4489177669	0.8365330531	-0.5915181969
Li	-1.4489177563	0.8365330675	-0.5915182027
Cl	0.0000000089	2.0870371812	0.7378790653
Cl	-1.80742722	-1.0435185743	0.7378790719
Cl	0.0000000044	-0.0000000047	-2.2136372078
Cl	1.8074272067	-1.0435185922	0.7378790791

Tabelle 10.81 Standardorientierung von  $\text{LiCl}$  ( $C_{\infty v}$ ) [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
Cl	-0.9710097612	-1.4119777725	0.
Li	0.9710097612	-0.8192962275	0.

Tabelle 10.82 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
Li	0.	1.2865220122	0.
Cl	0.	0.	1.7801477363
Li	0.	-1.2865220122	0.
Cl	0.	0.	-1.7801477363

Tabelle 10.83 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
Li	-0.0000000035	0.0000000082	1.7415758531
Li	-0.000000007	-1.6419734583	-0.5805252761
Li	1.421990733	0.820986723	-0.5805252813
Li	-1.4219907225	0.8209867371	-0.580525287
Cl	0.0000000089	2.0724784595	0.7327317799
Cl	-1.7948189971	-1.0362392135	0.7327317865
Cl	0.0000000044	-0.0000000047	-2.1981953515
Cl	1.7948189838	-1.0362392313	0.7327317936

Tabelle 10.84 Standardorientierung von LiCl ( $C_{\infty v}$ ) [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
Cl	-0.9699973405	-1.4116687936	0.
Li	0.9699973405	-0.8196052064	0.

Tabelle 10.85 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
Li	0.	1.2804801265	0.
Cl	0.	0.	1.7832869922
Li	0.	-1.2804801265	0.
Cl	0.	0.	-1.7832869922

Tabelle 10.86 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
Li	-0.0000000035	0.0000000082	1.7319965311
Li	-0.000000007	-1.6329419869	-0.5773321689
Li	1.4141692493	0.8164709873	-0.577332174
Li	-1.4141692389	0.8164710014	-0.5773321797
Cl	0.0000000089	2.0792639635	0.7351308179
Cl	-1.8006954159	-1.0396319654	0.7351308244
Cl	0.0000000044	-0.0000000047	-2.2053924653
Cl	1.8006954027	-1.0396319833	0.7351308316

Tabelle 10.87 Standardorientierung von LiCl ( $C_{\infty v}$ ) [globales Minimum; M06L/6-31+G(d)].

	x	y	z
Cl	-0.983412892	-1.4157630623	0.
Li	0.983412892	-0.8155109377	0.

Tabelle 10.88 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; M06L/6-31+G(d)].

	x	y	z
Li	0.	1.3437190979	0.
Cl	0.	0.	1.787089627
Li	0.	-1.3437190979	0.
Cl	0.	0.	-1.7870896269

Tabelle 10.89 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; M06L/6-31+G(d)].

	x	y	z
Li	-0.0000000036	0.0000000084	1.8219017228
Li	-0.0000000073	-1.7177054146	-0.6073005658
Li	1.4875765312	0.8588527007	-0.6073005713
Li	-1.4875765203	0.8588527155	-0.6073005772
Cl	0.0000000089	2.0866783581	0.7377522022
Cl	-1.80711647	-1.0433391627	0.7377522088
Cl	0.0000000044	-0.0000000047	-2.2132566184
Cl	1.8071164567	-1.0433391807	0.737752216

Tabelle 10.90 Standardorientierung von LiCl ( $C_{\infty v}$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Cl	-0.98666253	-1.4167548136	0.
Li	0.98666253	-0.8145191864	0.

Tabelle 10.91 Standardorientierung von (LiCl)<sub>2</sub> ( $D_{2h}$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	0.	1.3472191857	0.
Cl	0.	0.	1.7992920648
Li	0.	-1.3472191857	0.
Cl	0.	0.	-1.7992920648

Tabelle 10.92 Standardorientierung von (LiCl)<sub>4</sub> ( $T_d$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	-0.0000000037	0.0000000085	1.8304833818
Li	-0.0000000074	-1.7257962802	-0.6101611188
Li	1.4945834264	0.8628981335	-0.6101611242
Li	-1.4945834154	0.8628981483	-0.6101611302
Cl	0.0000000009	2.1079926637	0.7452879471
Cl	-1.8255752002	-1.0539963154	0.7452879538
Cl	0.0000000045	-0.0000000048	-2.2358638534
Cl	1.8255751867	-1.0539963335	0.7452879611

Tabelle 10.93 Standardorientierung von LiCl ( $C_{\infty v}$ ) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Cl	-0.98666253	-1.4167548136	0.
Li	0.98666253	-0.8145191864	0.

Tabelle 10.94 Standardorientierung von (LiCl)<sub>2</sub> ( $D_{2h}$ ) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Li	0.	1.3472209924	0.
Cl	0.	0.	1.7992911275
Li	0.	-1.3472209924	0.
Cl	0.	0.	-1.7992911275

Tabelle 10.95 Standardorientierung von (LiCl)<sub>4</sub> ( $T_d$ ) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Li	-0.0000000037	0.0000000085	1.8304833576
Li	-0.0000000074	-1.7257962575	-0.6101611107
Li	1.4945834067	0.8628981221	-0.6101611162
Li	-1.4945833957	0.862898137	-0.6101611221
Cl	0.0000000009	2.107992639	0.7452879384

Cl	-1.8255751788	-1.053996303	0.7452879451
Cl	0.0000000045	-0.0000000048	-2.2358638272
Cl	1.8255751654	-1.0539963212	0.7452879524

Tabelle 10.96 Standardorientierung von LiCl ( $C_{\infty v}$ ) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Cl	-0.98666253	-1.4167548136	0.
Li	0.98666253	-0.8145191864	0.

Tabelle 10.97 Standardorientierung von (LiCl)<sub>2</sub> ( $D_{2h}$ ) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Li	0.	1.3472209924	0.
Cl	0.	0.	1.7992911275
Li	0.	-1.3472209924	0.
Cl	0.	0.	-1.7992911275

Tabelle 10.98 Standardorientierung von (LiCl)<sub>4</sub> ( $T_d$ ) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Li	-0.0000000037	0.0000000085	1.8304833576
Li	-0.0000000074	-1.7257962575	-0.6101611107
Li	1.4945834067	0.8628981221	-0.6101611162
Li	-1.4945833957	0.862898137	-0.6101611221
Cl	0.000000009	2.107992639	0.7452879384
Cl	-1.8255751788	-1.053996303	0.7452879451
Cl	0.0000000045	-0.0000000048	-2.2358638272
Cl	1.8255751654	-1.0539963212	0.7452879524

Tabelle 10.99 Standardorientierung von LiCl ( $C_{\infty v}$ ) [globales Minimum; M062X/6-31+G(d)].

	x	y	z
Cl	-0.9805990395	-1.4149043076	0.
Li	0.9805990395	-0.8163696924	0.

Tabelle 10.100 Standardorientierung von (LiCl)<sub>2</sub> ( $D_{2h}$ ) [globales Minimum; M062X/6-31+G(d)].

	x	y	z
Li	0.	1.3170440339	0.
Cl	0.	0.	1.7832674983
Li	0.	-1.3170440339	0.
Cl	0.	0.	-1.7832674983

Tabelle 10.101 Standardorientierung von (LiCl)<sub>4</sub> ( $T_d$ ) [globales Minimum; M062X/6-31+G(d)].

	x	y	z
Li	-0.0000000035	0.0000000083	1.7761492041

Li	-0.0000000072	-1.6745695262	-0.5920497264
Li	1.4502197559	0.8372847567	-0.5920497317
Li	-1.4502197453	0.8372847712	-0.5920497375
Cl	0.0000000089	2.0723545511	0.7326879717
Cl	-1.7947116893	-1.0361772593	0.7326879783
Cl	0.0000000044	-0.0000000047	-2.1980639268
Cl	1.7947116761	-1.0361772772	0.7326879854

Tabelle 10.102 Standardorientierung von LiCl ( $C_{\infty v}$ ) [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
Cl	-0.9805990408	-1.414904308	0.
Li	0.9805990408	-0.816369692	0.

Tabelle 10.103 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
Li	0.	1.3170440343	0.
Cl	0.	0.	1.7832674977
Li	0.	-1.3170440343	0.
Cl	0.	0.	-1.7832674977

Tabelle 10.104 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
Li	-0.0000000035	0.0000000083	1.7761492798
Li	-0.0000000072	-1.6745695976	-0.5920497516
Li	1.4502198178	0.8372847925	-0.5920497569
Li	-1.4502198071	0.8372848069	-0.5920497627
Cl	0.0000000089	2.072354605	0.7326879908
Cl	-1.794711736	-1.0361772862	0.7326879973
Cl	0.0000000044	-0.0000000047	-2.198063984
Cl	1.7947117227	-1.0361773041	0.7326880045

Tabelle 10.105 Standardorientierung von LiCl ( $C_{\infty v}$ ) [globales Minimum; M062X/6-311+G(d,p)].

	x	y	z
Cl	-0.9666929906	-1.4106603448	0.
Li	0.9666929906	-0.8206136552	0.

Tabelle 10.106 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; M062X/6-311+G(d,p)].

	x	y	z
Li	0.	1.2846242723	0.
Cl	0.	0.	1.7705716829
Li	0.	-1.2846242723	0.
Cl	0.	0.	-1.7705716829

Tabelle 10.107 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; M062X/6-311+G(d,p)].

	x	y	z
Li	-0.0000000035	0.0000000082	1.7432577199
Li	-0.000000007	-1.6435591375	-0.5810858984
Li	1.4233639715	0.8217795626	-0.5810859036
Li	-1.423363961	0.8217795768	-0.5810859093
Cl	0.0000000088	2.0596206403	0.7281858544
Cl	-1.783683799	-1.029810304	0.7281858609
Cl	0.0000000044	-0.0000000046	-2.1845575748
Cl	1.7836837859	-1.0298103217	0.7281858681

Tabelle 10.108 Standardorientierung von  $\text{LiCl}$  ( $C_{\infty v}$ ) [globales Minimum; MP2/6-31+G(d)].

	x	y	z
Cl	-0.9858177382	-1.4164969931	0.
Li	0.9858177382	-0.8147770069	0.

Tabelle 10.109 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; MP2/6-31+G(d)].

	x	y	z
Li	0.	1.3275101966	0.
Cl	0.	0.	1.7934471428
Li	0.	-1.3275101966	0.
Cl	0.	0.	-1.7934471428

Tabelle 10.110 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; MP2/6-31+G(d)].

	x	y	z
Li	-0.0000000036	0.0000000083	1.7937285124
Li	-0.0000000072	-1.691143457	-0.5979094959
Li	1.4645732011	0.8455717222	-0.5979095011
Li	-1.4645731904	0.8455717366	-0.5979095069
Cl	0.0000000088	2.081973774	0.7360888807
Cl	-1.8030421807	-1.0409868708	0.7360888871
Cl	0.0000000044	-0.0000000046	-2.2082666535
Cl	1.8030421675	-1.0409868886	0.7360888943

Tabelle 10.111 Standardorientierung von  $\text{LiCl}$  ( $C_{\infty v}$ ) [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
Cl	0.	0.	0.2895492925
Li	0.	0.	-1.7325362925

Tabelle 10.112 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
Li	0.	1.2829736098	0.
Cl	0.	0.	1.7692823049

Li	0.	-1.2829736098	0.
Cl	0.	0.	-1.7692823049

Tabelle 10.113 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
Li	1.0033227965	1.0033227965	1.0033227965
Li	-1.0033227965	-1.0033227965	1.0033227965
Li	1.0033227965	-1.0033227965	-1.0033227965
Li	-1.0033227965	1.0033227965	-1.0033227965
Cl	1.2596051079	1.2596051079	-1.2596051079
Cl	-1.2596051079	1.2596051079	1.2596051079
Cl	-1.2596051079	-1.2596051079	-1.2596051079
Cl	1.2596051079	-1.2596051079	1.2596051079

Tabelle 10.114 Standardorientierung von  $\text{LiCl}$  ( $C_{\infty v}$ ) [globales Minimum; G3].

	x	y	z
Cl	-0.9871208944	-1.4168947011	0.
Li	0.9871208944	-0.8143792989	0.

Tabelle 10.115 Standardorientierung von  $(\text{LiCl})_2$  ( $D_{2h}$ ) [globales Minimum; G3].

	x	y	z
Li	0.	1.3264846775	0.
Cl	0.	0.	1.796829474
Li	0.	-1.3264846775	0.
Cl	0.	0.	-1.796829474

Tabelle 10.116 Standardorientierung von  $(\text{LiCl})_4$  ( $T_d$ ) [globales Minimum; G3].

	x	y	z
Li	1.0334899282	1.0334899282	1.0334899282
Li	-1.0334899282	-1.0334899282	1.0334899282
Li	1.0334899282	-1.0334899282	-1.0334899282
Li	-1.0334899282	1.0334899282	-1.0334899282
Cl	1.276349377	1.276349377	-1.276349377
Cl	-1.276349377	1.276349377	1.276349377
Cl	-1.276349377	-1.276349377	-1.276349377
Cl	1.276349377	-1.276349377	1.276349377

## 10.2.1.2. Aggregation von Methyllithium

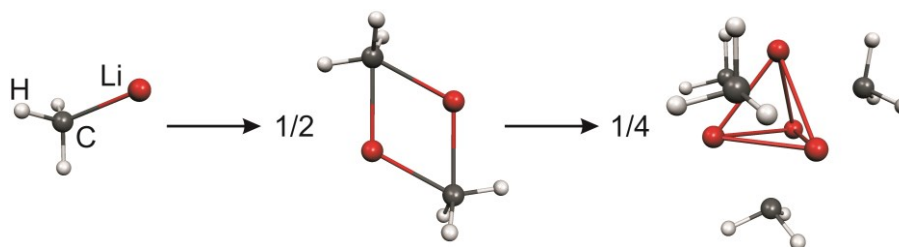


Abbildung 10.19 Von monomeren Methyllithium ( $\text{MeLi}$ ,  $C_{3v}$ ) über das dimere Aggregat  $[(\text{MeLi})_2]$ ,  $C_{2h}$ ] zum Methyllithiumtetramer  $[(\text{MeLi})_4]$ ,  $T_d$ ].

Tabelle 10.117 Vergleich unterschiedlicher Konformere dimeren Methyllithiums. Alle Berechnungen wurden mit dem 6-31+G(d)-Baissatz durchgeführt.

Methode	Punktgruppe	Konformation	Zahl		
			imaginärer Frequenzen	SCF [Hartree]	ZPE [Hartree]
MP2	$C_{2h}$	ekliptisch	2	-94.1014908	-94.33262
MP2	$C_{2h}$	gestaffelt	0	-94.1014498	-94.332461
MP2	$C_{2v}$	ekliptisch	2	-94.1014793	-94.332586
MP2	$C_{2v}$	gestaffelt	0	-94.1014608	-94.332474
B3LYP	$C_{2h}$	ekliptisch	0	-94.8770151	-94.808088
B3LYP	$C_{2h}$	gestaffelt	2	-94.877009	-94.808182
B3LYP	$C_{2v}$	ekliptisch	0	-94.877014	-94.808123
B3LYP	$C_{2v}$	gestaffelt	2	-94.8770192	-94.808197
M052X	$C_{2h}$	ekliptisch	0	-94.8383207	-94.768096
M052X	$C_{2h}$	gestaffelt	2	-94.8383155	-94.768337
M052X	$C_{2v}$	ekliptisch	0	-94.8383208	-94.768083
M052X	$C_{2v}$	gestaffelt	2	-94.8383126	-94.768345

Tabelle 10.118 Standardorientierung von  $(\text{MeLi})_2$  ( $C_{2h}$ , gestaffelt) [global Minimum; MP2/6-31+G(d)].

	x	y	z
Li	0.	0.	-1.0972249213
C	-0.0156578047	-1.8342635739	0.
Li	0.	0.	1.0972249213
C	0.0156578047	1.8342635739	0.
H	-0.5657820382	-2.2537320099	-0.8632012773
H	0.9561481741	-2.3528385014	0.
H	-0.5657820382	-2.2537320099	0.8632012773
H	-0.9561481741	2.3528385014	0.
H	0.5657820382	2.2537320099	-0.8632012773
H	0.5657820382	2.2537320099	0.8632012773

Tabelle 10.119 Standardorientierung von (MeLi)<sub>2</sub> (C<sub>2h</sub>, ekliptisch) [lokales Minimum; MP2/6-31+G(d)].

	x	y	z
Li	0.9401653989	0.5641306609	0.
C	-0.9266919063	1.5836542189	0.
Li	-0.9401653989	-0.5641306609	0.
C	0.9266919063	-1.5836542189	0.
H	-0.7602681606	2.2281135325	0.8797250978
H	-0.7602681606	2.2281135325	-0.8797250978
H	-2.0221301367	1.4225508321	0.
H	2.0221301367	-1.4225508321	0.
H	0.7602681606	-2.2281135325	-0.8797250978
H	0.7602681606	-2.2281135325	0.8797250978

Tabelle 10.120 Standardorientierung von (MeLi)<sub>2</sub> (C<sub>2v</sub>, ekliptisch) [lokales Minimum; MP2/6-31+G(d)].

	x	y	z
Li	0.	0.	1.097267719
C	0.	1.8351382962	0.0072078458
Li	0.	0.	-1.0947233217
C	0.	-1.8351382962	0.0072078458
H	-0.8796974009	2.2974401332	0.4863409188
H	0.8796974009	2.2974401332	0.4863409188
H	0.	2.2706502759	-1.010502512
H	0.	-2.2706502759	-1.010502512
H	-0.8796974009	-2.2974401332	0.4863409188
H	0.8796974009	-2.2974401332	0.4863409188

Tabelle 10.121 Standardorientierung von (MeLi)<sub>2</sub> (C<sub>2v</sub>, gestaffelt) [lokales Minimum; MP2/6-31+G(d)].

	x	y	z
Li	0.	-1.0971508581	-0.0266004451
C	1.8338948046	0.	0.0040631082
Li	0.	1.0971508581	-0.0266004451
C	-1.8338948046	0.	0.0040631082
H	2.2530868194	-0.8632532958	0.5539937222
H	2.3521130967	0.	-0.9680825474
H	2.2530868194	0.8632532958	0.5539937222
H	-2.3521130967	0.	-0.9680825474
H	-2.2530868194	0.8632532958	0.5539937222
H	-2.2530868194	-0.8632532958	0.5539937222

Tabelle 10.122 Standardorientierung von (MeLi)<sub>2</sub> (C<sub>2h</sub>, ekliptisch) [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
Li	0.9285749901	0.5570424737	0.
C	-0.9262171467	1.5627819285	0.
Li	-0.9285749901	-0.5570424737	0.
C	0.9262171467	-1.5627819285	0.
H	-0.753893286	2.2125501579	0.8792406589

H	-0.753893286	2.2125501579	-0.8792406589
H	-2.0286034668	1.4340489291	0.
H	2.0286034668	-1.4340489291	0.
H	0.753893286	-2.2125501579	-0.8792406589
H	0.753893286	-2.2125501579	0.8792406589

Tabelle 10.123 Standardorientierung von (MeLi)<sub>2</sub> (C<sub>2h</sub>, gestaffelt) [lokales Minimum; B3LYP/6-31+G(d)].

	x	y	z
Li	0.	0.	-1.0828285709
C	-0.0316011483	-1.8163772965	0.
Li	0.	0.	1.0828285709
C	0.0316011483	1.8163772965	0.
H	-0.5682764043	-2.2622648983	-0.861895955
H	0.9543226114	-2.3167609016	0.
H	-0.5682764043	-2.2622648983	0.861895955
H	-0.9543226114	2.3167609016	0.
H	0.5682764043	2.2622648983	-0.861895955
H	0.5682764043	2.2622648983	0.861895955

Tabelle 10.124 Standardorientierung von (MeLi)<sub>2</sub> (C<sub>2v</sub>, ekliptisch) [lokales Minimum; B3LYP/6-31+G(d)].

	x	y	z
Li	0.	0.	1.07893001
C	0.	1.8167198286	0.0033218149
Li	0.	0.	-1.0863438362
C	0.	-1.8167198286	0.0033218149
H	-0.8793018083	2.2823495199	0.4882026523
H	0.8793018083	2.2823495199	0.4882026523
H	0.	2.2794062525	-1.0053608365
H	0.	-2.2794062525	-1.0053608365
H	-0.8793018083	-2.2823495199	0.4882026523
H	0.8793018083	-2.2823495199	0.4882026523

Tabelle 10.125 Standardorientierung von (MeLi)<sub>2</sub> (C<sub>2v</sub>, gestaffelt) [lokales Minimum; B3LYP/6-31+G(d)].

	x	y	z
Li	0.	-1.085698444	-0.003658557
C	1.8140546921	0.	0.0116878712
Li	0.	1.085698444	-0.003658557
C	-1.8140546921	0.	0.0116878712
H	2.2652643699	-0.8617073865	0.5441570796
H	2.3051020834	0.	-0.9789759134
H	2.2652643699	0.8617073865	0.5441570796
H	-2.3051020834	0.	-0.9789759134
H	-2.2652643699	0.8617073865	0.5441570796
H	-2.2652643699	-0.8617073865	0.5441570796

Tabelle 10.126 Standardorientierung von  $(\text{MeLi})_2$  ( $C_{2h}$ , ekliptisch) [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	0.9318895447	0.5624107673	0.
C	-0.9302909999	1.5630547114	0.
Li	-0.9318895447	-0.5624107673	0.
C	0.9302909999	-1.5630547114	0.
H	-0.7499822192	2.2036945704	0.8765727615
H	-0.7499822192	2.2036945704	-0.8765727615
H	-2.0265510544	1.4351807002	0.
H	2.0265510544	-1.4351807002	0.
H	0.7499822192	-2.2036945704	-0.8765727615
H	0.7499822192	-2.2036945704	0.8765727615

Tabelle 10.127 Standardorientierung von  $(\text{MeLi})_2$  ( $C_{2h}$ , gestaffelt) [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	0.	0.	-1.0884708157
C	-0.0327812309	-1.818823911	0.
Li	0.	0.	1.0884708157
C	0.0327812309	1.818823911	0.
H	-0.5667048284	-2.2569951219	-0.8597663152
H	0.9515110022	-2.3083024226	0.
H	-0.5667048284	-2.2569951219	0.8597663152
H	-0.9515110022	2.3083024226	0.
H	0.5667048284	2.2569951219	-0.8597663152
H	0.5667048284	2.2569951219	0.8597663152

Tabelle 10.128 Standardorientierung von  $(\text{MeLi})_2$  ( $C_{2v}$ , gestaffelt) [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	0.	-1.0885500391	0.0016215619
C	1.8189046101	0.	0.0125738456
Li	0.	1.0885500391	0.0016215619
C	-1.8189046101	0.	0.0125738456
H	2.2640081439	-0.8597211843	0.540687175
H	2.2952528123	0.	-0.9782021974
H	2.2640081439	0.8597211843	0.540687175
H	-2.2952528123	0.	-0.9782021974
H	-2.2640081439	0.8597211843	0.540687175
H	-2.2640081439	-0.8597211843	0.540687175

Tabelle 10.129 Standardorientierung von  $(\text{MeLi})_2$  ( $C_{2v}$ , ekliptisch) [global Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	0.	0.	1.0823939694
C	0.	1.8190865484	0.0016778266
Li	0.	0.	-1.0940774423
C	0.	-1.8190865484	0.0016778266
H	-0.8766852616	2.2729630355	0.4882572509
H	0.8766852616	2.2729630355	0.4882572509
H	0.	2.278744163	-1.0016912219

H	0.	-2.278744163	-1.0016912219
H	-0.8766852616	-2.2729630355	0.4882572509
H	0.8766852616	-2.2729630355	0.4882572509

Tabelle 10.130 Berechnete Energien der optimierten Strukturen zur Aggregation von Methyllithium

	Method	Basissatz	Zahl imaginärer Frequenzen	SCF [Hartree]	ZPE [Hartree]
MeLi	SVWN	6-31+G(d)	0	-47.08501548	-47.052185
(MeLi) <sub>2</sub>	SVWN	6-31+G(d)	0	-94.24708382	-94.179131
(MeLi) <sub>4</sub>	SVWN	6-31+G(d)	0	-188.5815953	-188.439627
MeLi	PBE	6-31+G(d)	0	-47.3059557	-47.27318
(MeLi) <sub>2</sub>	PBE	6-31+G(d)	2	-94.68056609	-94.613118
(MeLi) <sub>4</sub>	PBE	6-31+G(d)	0	-189.4336981	-189.292858
MeLi	TPSS	6-31+G(d)	0	-47.40581922	-47.372684
(MeLi) <sub>2</sub>	TPSS	6-31+G(d)	2	-94.87989107	-94.811767
(MeLi) <sub>4</sub>	TPSS	6-31+G(d)	0	-189.8317811	-189.689565
MeLi	PBE0	6-31+G(d)	0	-47.31802407	-47.28429
(MeLi) <sub>2</sub>	PBE0	6-31+G(d)	0	-94.70702206	-94.637418
(MeLi) <sub>4</sub>	PBE0	6-31+G(d)	0	-189.4882856	-189.343351
MeLi	TPSSh	6-31+G(d)	0	-47.40093973	-47.367464
(MeLi) <sub>2</sub>	TPSSh	6-31+G(d)	2	-94.87107549	-94.802209
(MeLi) <sub>4</sub>	TPSSh	6-31+G(d)	0	-189.8146789	-189.670933
MeLi	B3LYP	6-31+G(d)	0	-47.40498741	-47.3715
(MeLi) <sub>2</sub>	B3LYP	6-31+G(d)	0	-94.87700608	-94.808074
(MeLi) <sub>4</sub>	B3LYP	6-31+G(d)	0	-189.8210239	-189.677353
MeLi	B3LYP	6-311+G(d,p)	0	-47.42002482	-47.387023
(MeLi) <sub>2</sub>	B3LYP	6-311+G(d,p)	2	-94.90908912	-94.841086
(MeLi) <sub>4</sub>	B3LYP	6-311+G(d,p)	0	-189.8836225	-189.7413
MeLi	M052X	6-31+G(d)	0	-47.38350213	-47.349444
(MeLi) <sub>2</sub>	M052X	6-31+G(d)	0	-94.83832071	-94.768096
(MeLi) <sub>4</sub>	M052X	6-31+G(d)	0	-189.7570285	-189.610766
MeLi	M052X	6-31+G(d,p)	0	-47.38822629	-47.35438
(MeLi) <sub>2</sub>	M052X	6-31+G(d,p)	0	-94.84786758	-94.778105
(MeLi) <sub>4</sub>	M052X	6-31+G(d,p)	0	-189.7763775	-189.630799
MeLi	M052X	6-311+G(d,p)	0	-47.39812565	-47.364551
(MeLi) <sub>2</sub>	M052X	6-311+G(d,p)	2	-94.86991163	-94.800763
(MeLi) <sub>4</sub>	M052X	6-311+G(d,p)	0	-189.8184013	-189.673614
MeLi	M052X	6-311+G(3df,3pd)	0	-47.40199504	-47.368494
(MeLi) <sub>2</sub>	M052X	6-311+G(3df,3pd)	2	-94.87804692	-94.809
(MeLi) <sub>4</sub>	M052X	6-311+G(3df,3pd)	0	-189.8352032	-189.690378
MeLi	M06L	6-31+G(d)	0	-47.39333687	-47.359771
(MeLi) <sub>2</sub>	M06L	6-31+G(d)	1	-94.85614774	-94.78685
(MeLi) <sub>4</sub>	M06L	6-31+G(d)	0	-189.7871062	-189.643481
MeLi	M06	6-31+G(d)	0	-47.36210865	-47.328699
(MeLi) <sub>2</sub>	M06	6-31+G(d)	1	-94.79210579	-94.723301
(MeLi) <sub>4</sub>	M06	6-31+G(d)	0	-189.6532275	-189.510879
MeLi	M06	6-31+G(d,p)	0	-47.36661154	-47.333372
(MeLi) <sub>2</sub>	M06	6-31+G(d,p)	0	-94.80100277	-94.732414

	Method	Basissatz	Zahl imaginärer Frequenzen	SCF [Hartree]	ZPE [Hartree]
(MeLi) <sub>4</sub>	M06	6-31+G(d,p)	0	-189.6712405	-189.529621
MeLi	M06	6-311+G(d,p)	0	-47.37652102	-47.343519
(MeLi) <sub>2</sub>	M06	6-311+G(d,p)	2	-94.82254528	-94.754525
(MeLi) <sub>4</sub>	M06	6-311+G(d,p)	0	-189.7124347	-189.571118
MeLi	M062X	6-31+G(d)	0	-47.36633722	-47.33244
(MeLi) <sub>2</sub>	M062X	6-31+G(d)	0	-94.80463329	-94.734687
(MeLi) <sub>4</sub>	M062X	6-31+G(d)	0	-189.6906301	-189.54481
MeLi	M062X	6-31+G(d,p)	0	-47.37026836	-47.336562
(MeLi) <sub>2</sub>	M062X	6-31+G(d,p)	0	-94.81257152	-94.743061
(MeLi) <sub>4</sub>	M062X	6-31+G(d,p)	0	-189.7067525	-189.56159
MeLi	M062X	6-311+G(d,p)	0	-47.38112855	-47.347673
(MeLi) <sub>2</sub>	M062X	6-311+G(d,p)	2	-94.83643678	-94.767507
(MeLi) <sub>4</sub>	M062X	6-311+G(d,p)	0	-189.7523732	-189.607962
MeLi	MP2	6-31+G(d)	0	-47.16682204	-47.132616
(MeLi) <sub>2</sub>	MP2	6-31+G(d)	2	-94.40305077	-94.33262
(MeLi) <sub>4</sub>	MP2	6-31+G(d)	0	-188.8851563	-188.737863
MeLi	MP2	6-311+G(d,p)	0	-189.0610442	-188.916393
(MeLi) <sub>2</sub>	MP2	6-311+G(d,p)	2	-94.49231434	-94.423194
(MeLi) <sub>4</sub>	MP2	6-311+G(d,p)	0	-47.21054968	-47.176978
MeLi	G3	G3	0		-47.328543
(MeLi) <sub>2</sub>	G3	G3	0		-94.726997
(MeLi) <sub>4</sub>	G3	G3	0		-189.528567

Tabelle 10.131 Standardorientierung von MeLi (C<sub>3v</sub>) [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
C	-0.0242145242	0.1203112494	-0.3610061182
Li	0.1002374289	-0.4980405155	1.4944185585
H	0.3067367792	-0.6503248678	-1.086512714
H	0.6001704437	1.0169651283	-0.5505419837
H	-1.060086229	0.3944417075	-0.6466473511

Tabelle 10.132 Standardorientierung von (MeLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
Li	0.9059543826	0.5767968135	0.
C	-0.9399585553	1.5087463268	0.
Li	-0.9059543826	-0.5767968135	0.
C	0.9399585553	-1.5087463268	0.
H	-0.7535535306	2.1596615673	0.8838395916
H	-0.7535535306	2.1596615673	-0.8838395916
H	-2.0496744715	1.4097012318	0.
H	2.0496744715	-1.4097012318	0.
H	0.7535535306	-2.1596615673	-0.8838395916
H	0.7535535306	-2.1596615673	0.8838395916

Tabelle 10.133 Standardorientierung von (MeLi)<sub>4</sub> (T<sub>d</sub>) [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
Li	1.179278989	-0.6808570443	0.4814386291
Li	-0.0000000043	0.0000000005	-1.4443158903
Li	0.0000000028	1.3617140808	0.4814386351
Li	-1.1792789875	-0.680857042	0.4814386361
C	0.0000000064	-0.0000000039	2.1367557155
C	-0.0000000041	-2.0145526062	-0.7122519043
C	-1.7446537351	1.0072763042	-0.7122518954
C	1.7446537328	1.0072763009	-0.7122519057
H	-0.8663551314	-0.5001903763	2.6318229446
H	0.0000000088	1.0003807407	2.6318229439
H	0.8663551461	-0.500190378	2.6318229395
H	-0.0000000075	-2.1478462144	-1.8204423251
H	-0.8663551426	-2.6480365879	-0.4056903058
H	0.866355135	-2.6480365896	-0.4056903109
H	-1.8600893852	2.074303854	-0.405690297
H	-2.7264445254	0.573732737	-0.4056902962
H	-1.8600893904	1.0739231105	-1.8204423156
H	1.8600893816	1.0739231069	-1.8204423267
H	2.7264445241	0.5737327317	-0.4056903125
H	1.8600893868	2.0743038504	-0.405690308

Tabelle 10.134 Standardorientierung von MeLi (C<sub>3v</sub>) [globales Minimum; PBE/6-31+G(d)].

	x	y	z
C	-0.0246459458	0.1224548102	-0.367438081
Li	0.1018638101	-0.5061213504	1.5186658904
H	0.3068196331	-0.6495598025	-1.0928997643
H	0.6006484928	1.0199756926	-0.5562071909
H	-1.0618442065	0.39661386	-0.6524419927

Tabelle 10.135 Standardorientierung von (MeLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; PBE/6-31+G(d)].

	x	y	z
Li	0.9248201635	0.5745742333	0.
C	-0.9508101539	1.5503315363	0.
Li	-0.9248201635	-0.5745742333	0.
C	0.9508101539	-1.5503315363	0.
H	-0.781795053	2.2079862606	0.8840085198
H	-0.781795053	2.2079862606	-0.8840085198
H	-2.0609950103	1.4254166484	0.
H	2.0609950103	-1.4254166484	0.
H	0.781795053	-2.2079862606	-0.8840085198
H	0.781795053	-2.2079862606	0.8840085198

Tabelle 10.136 Standardorientierung von (MeLi)<sub>4</sub> (T<sub>d</sub>) [globales Minimum; PBE/6-31+G(d)].

	x	y	z
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Li	1.2026461631	-0.6943480886	0.4909782379
Li	-0.0000000044	0.0000000006	-1.4729347169
Li	0.0000000028	1.3886961693	0.4909782441
Li	-1.2026461616	-0.6943480863	0.490978245
C	0.0000000065	-0.000000004	2.1962763814
C	-0.0000000042	-2.0706692282	-0.7320921264
C	-1.7932521553	1.0353346153	-0.7320921171
C	1.793252153	1.0353346118	-0.7320921278
H	-0.8682020232	-0.5012566799	2.6901976171
H	0.000000009	1.0025133477	2.6901976164
H	0.8682020382	-0.5012566816	2.6901976119
H	-0.0000000076	-2.2021715144	-1.8419111906
H	-0.8682020346	-2.7034281914	-0.4241432094
H	0.8682020268	-2.7034281931	-0.4241432145
H	-1.907136475	2.1035991111	-0.4241432003
H	-2.7753385072	0.5998290835	-0.4241431996
H	-1.9071364802	1.1010857606	-1.8419111808
H	1.9071364714	1.1010857569	-1.8419111922
H	2.7753385059	0.5998290781	-0.4241432161
H	1.9071364766	2.1035991074	-0.4241432117

Tabelle 10.137 Standardorientierung von MeLi ( $C_{3v}$ ) [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
C	-0.0245884947	0.1221693586	-0.3665815557
Li	0.1022264863	-0.5079233426	1.5240729434
H	0.3049747714	-0.6445569425	-1.0934351507
H	0.5974053514	1.0170335281	-0.5592966024
H	-1.0571758388	0.3966381643	-0.6550734398

Tabelle 10.138 Standardorientierung von (MeLi)<sub>2</sub> ( $C_{2h}$ ) [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
Li	0.9293342628	0.572311758	0.
C	-0.9490845616	1.5582646635	0.
Li	-0.9293342628	-0.572311758	0.
C	0.9490845616	-1.5582646635	0.
H	-0.7876902402	2.2162431831	0.8805170256
H	-0.7876902402	2.2162431831	-0.8805170256
H	-2.0550193934	1.4206533341	0.
H	2.0550193934	-1.4206533341	0.
H	0.7876902402	-2.2162431831	-0.8805170256
H	0.7876902402	-2.2162431831	0.8805170256

Tabelle 10.139 Standardorientierung von (MeLi)<sub>4</sub> ( $T_d$ ) [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
Li	1.206315518	-0.6964665916	0.4924762457
Li	-0.0000000044	0.0000000006	-1.4774287405
Li	0.0000000028	1.3929331753	0.4924762519

Li	-1.2063155164	-0.6964665893	0.4924762529
C	0.0000000066	-0.000000004	2.2023743594
C	-0.0000000042	-2.076418457	-0.7341247857
C	-1.7982311335	1.0382092297	-0.7341247765
C	1.7982311312	1.0382092262	-0.7341247872
H	-0.8661520201	-0.50007311	2.6929409249
H	0.000000009	1.000146208	2.6929409242
H	0.8661520351	-0.5000731117	2.6929409197
H	-0.0000000076	-2.2055469763	-1.8405938658
H	-0.8661520315	-2.7056200835	-0.4261735257
H	0.8661520237	-2.7056200852	-0.4261735308
H	-1.9100597109	2.1029197024	-0.4261735166
H	-2.7762117399	0.6027003844	-0.4261735159
H	-1.910059716	1.1027734916	-1.840593856
H	1.9100597072	1.1027734879	-1.8405938674
H	2.7762117385	0.602700379	-0.4261735324
H	1.9100597124	2.1029196987	-0.426173528

Tabelle 10.140 Standardorientierung von MeLi ( $C_{3v}$ ) [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
C	-0.0244739411	0.1216001878	-0.3648737034
Li	0.1013155369	-0.5033972011	1.5104918153
H	0.3040091425	-0.64277148	-1.0883188957
H	0.5954280487	1.0130706604	-0.5560282184
H	-1.0534290601	0.394821576	-0.6514737124

Tabelle 10.141 Standardorientierung von (MeLi)<sub>2</sub> ( $C_{2h}$ ) [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
Li	0.9223129935	0.5723446191	0.
C	-0.9465797673	1.5438991231	0.
Li	-0.9223129935	-0.5723446191	0.
C	0.9465797673	-1.5438991231	0.
H	-0.7769084669	2.1948968385	0.8781329694
H	-0.7769084669	2.1948968385	-0.8781329694
H	-2.0478549609	1.4153312607	0.
H	2.0478549609	-1.4153312607	0.
H	0.7769084669	-2.1948968385	-0.8781329694
H	0.7769084669	-2.1948968385	0.8781329694

Tabelle 10.142 Standardorientierung von (MeLi)<sub>4</sub> ( $T_d$ ) [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
Li	1.1950254666	-0.6899482774	0.4878671016
Li	-0.0000000044	0.000000006	-1.4636013079
Li	0.0000000028	1.3798965469	0.4878671077
Li	-1.195025465	-0.6899482751	0.4878671087
C	0.0000000065	-0.000000004	2.1869402043

C	-0.000000042	-2.061866996	-0.7289800673
C	-1.7856291986	1.0309334992	-0.7289800582
C	1.7856291963	1.0309334958	-0.7289800688
H	-0.8628035528	-0.4981398715	2.6736890609
H	0.0000000089	0.996279731	2.6736890602
H	0.8628035678	-0.4981398732	2.6736890557
H	-0.0000000076	-2.1886849705	-1.8305312283
H	-0.8628035642	-2.6868248392	-0.4215789124
H	0.8628035564	-2.6868248409	-0.4215789175
H	-1.8954567855	2.0906222225	-0.4215789034
H	-2.7582603472	0.5962026199	-0.4215789027
H	-1.8954567906	1.0943424886	-1.8305312186
H	1.8954567819	1.094342485	-1.8305312299
H	2.7582603459	0.5962026146	-0.4215789191
H	1.895456787	2.0906222188	-0.4215789147

Tabelle 10.143 Standardorientierung von MeLi (C<sub>3v</sub>) [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
C	-0.0245209226	0.1218336198	-0.3655741387
Li	0.1019699814	-0.5066488732	1.520248774
H	0.3040330571	-0.6423335695	-1.091568598
H	0.5956389368	1.0145709544	-0.5589364045
H	-1.054276074	0.3959252032	-0.6544431361

Tabelle 10.144 Standardorientierung von (MeLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
Li	0.9277324859	0.5718997375	0.
C	-0.9478815807	1.5547992876	0.
Li	-0.9277324859	-0.5718997375	0.
C	0.9478815807	-1.5547992876	0.
H	-0.785072345	2.2100754936	0.8784942937
H	-0.785072345	2.2100754936	-0.8784942937
H	-2.0507122967	1.4177150824	0.
H	2.0507122967	-1.4177150824	0.
H	0.785072345	-2.2100754936	-0.8784942937
H	0.785072345	-2.2100754936	0.8784942937

Tabelle 10.145 Standardorientierung von (MeLi)<sub>4</sub> (T<sub>d</sub>) [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
Li	1.2038336694	-0.6950336956	0.4914630353
Li	-0.0000000044	0.0000000006	-1.4743891091
Li	0.0000000028	1.3900673834	0.4914630414
Li	-1.2038336678	-0.6950336933	0.4914630424
C	0.0000000065	-0.0000000004	2.198062676
C	-0.0000000042	-2.0723533629	-0.7326875579
C	-1.7947106587	1.0361766827	-0.7326875487

C	1.7947106564	1.0361766792	-0.7326875594
H	-0.8641397805	-0.498911343	2.6863184319
H	0.000000009	0.9978226739	2.6863184311
H	0.8641397956	-0.4989113447	2.6863184267
H	-0.0000000076	-2.2000777414	-1.8361957192
H	-0.8641397919	-2.6989890815	-0.4250613525
H	0.8641397842	-2.6989890832	-0.4250613576
H	-1.9053232145	2.0978615508	-0.4250613434
H	-2.769463004	0.6011275339	-0.4250613427
H	-1.9053232196	1.1000388741	-1.8361957094
H	1.9053232108	1.1000388704	-1.8361957208
H	2.7694630026	0.6011275285	-0.4250613592
H	1.905323216	2.0978615471	-0.4250613548

Tabelle 10.146 Standardorientierung von MeLi ( $C_{3v}$ ) [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
C	-0.024724885	0.1228470274	-0.3686149668
Li	0.1013572854	-0.503604633	1.5111142349
H	0.3048983594	-0.6451761474	-1.0881041992
H	0.5969934795	1.01450824	-0.5545783846
H	-1.0556896681	0.394824559	-0.6502453522

Tabelle 10.147 Standardorientierung von (MeLi)<sub>2</sub> ( $C_{2h}$ ) [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
Li	-0.0204050957	1.0824189998	0.
C	-1.8171525985	-0.0253960538	0.
Li	0.0204050957	-1.0824189998	0.
C	1.8171525985	0.0253960538	0.
H	-2.301426275	0.4404070819	0.8791363048
H	-2.301426275	0.4404070819	-0.8791363048
H	-2.2397060272	-1.0523376698	0.
H	2.2397060272	1.0523376698	0.
H	2.301426275	-0.4404070819	-0.8791363048
H	2.301426275	-0.4404070819	0.8791363048

Tabelle 10.148 Standardorientierung von (MeLi)<sub>4</sub> ( $T_d$ ) [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
Li	1.1995286995	-0.6925482202	0.4897055387
Li	-0.0000000044	0.0000000006	-1.4691166194
Li	0.0000000028	1.3850964324	0.4897055449
Li	-1.199528698	-0.6925482178	0.4897055458
C	0.0000000065	-0.000000004	2.191859181
C	-0.0000000042	-2.0665046517	-0.7306197262
C	-1.7896455262	1.0332523271	-0.7306197171
C	1.789645524	1.0332523236	-0.7306197277
H	-0.8640934215	-0.4988845775	2.6777862108

H	0.000000089	0.997769143	2.6777862101
H	0.8640934363	-0.4988845792	2.6777862057
H	-0.0000000076	-2.1920513299	-1.8333011761
H	-0.8640934328	-2.6909359046	-0.4222425135
H	0.864093425	-2.6909359063	-0.4222425187
H	-1.8983721382	2.0937948142	-0.4222425045
H	-2.7624655685	0.5971410937	-0.4222425038
H	-1.8983721433	1.0960256684	-1.8333011664
H	1.8983721346	1.0960256646	-1.8333011776
H	2.7624655672	0.5971410882	-0.4222425202
H	1.8983721398	2.0937948104	-0.4222425158

Tabelle 10.149 Standardorientierung von MeLi ( $C_{3v}$ ) [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
C	-0.0243556854	0.1210126228	-0.3631106575
Li	0.1008369796	-0.5010194421	1.5033571177
H	0.3031634591	-0.6409295431	-1.0856405583
H	0.5937898061	1.010409276	-0.5547975287
H	-1.0505829783	0.3938416166	-0.6499834438

Tabelle 10.150 Standardorientierung von (MeLi)<sub>2</sub> ( $C_{2h}$ ) [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
Li	0.9216935432	0.5556253193	0.
C	-0.9292931845	1.5492174624	0.
Li	-0.9216935432	-0.5556253193	0.
C	0.9292931845	-1.5492174624	0.
H	-0.7828941914	2.2050298133	0.8748653012
H	-0.7828941914	2.2050298133	-0.8748653012
H	-2.0240696528	1.3811087778	0.
H	2.0240696528	-1.3811087778	0.
H	0.7828941914	-2.2050298133	-0.8748653012
H	0.7828941914	-2.2050298133	0.8748653012

Tabelle 10.151 Standardorientierung von (MeLi)<sub>4</sub> ( $T_d$ ) [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
Li	1.1963231782	-0.6906975116	0.4883968901
Li	-0.0000000044	0.0000000006	-1.4651906736
Li	0.0000000028	1.3813950152	0.4883968963
Li	-1.1963231767	-0.6906975092	0.4883968973
C	0.0000000065	-0.000000004	2.1829637805
C	-0.0000000042	-2.0581179877	-0.7276545927
C	-1.7823824622	1.029058995	-0.7276545836
C	1.7823824598	1.0290589916	-0.7276545942
H	-0.862187871	-0.4977844075	2.6657332886
H	0.0000000089	0.9955688029	2.6657332879
H	0.8621878859	-0.4977844091	2.6657332835

H	-0.0000000076	-2.1814211726	-1.8272090348
H	-0.8621878823	-2.6792055772	-0.419262123
H	0.8621878746	-2.6792055789	-0.4192621282
H	-1.8891661519	2.0862793954	-0.419262114
H	-2.7513540318	0.592926185	-0.4192621133
H	-1.8891661571	1.0907105896	-1.8272090251
H	1.8891661483	1.090710586	-1.8272090363
H	2.7513540305	0.5929261797	-0.4192621297
H	1.8891661535	2.0862793917	-0.4192621253

Tabelle 10.152 Standardorientierung von MeLi ( $C_{3v}$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-0.0250451088	0.1244380904	-0.3733891064
Li	0.101433392	-0.5039827759	1.5122488894
H	0.3035839908	-0.6420586712	-1.085591465
H	0.5945328543	1.0111126864	-0.5541593434
H	-1.0516647382	0.393860804	-0.6494508891

Tabelle 10.153 Standardorientierung von (MeLi)<sub>2</sub> ( $C_{2h}$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	0.9250360112	0.5736168154	0.
C	-0.9491296211	1.5516943103	0.
Li	-0.9250360112	-0.5736168154	0.
C	0.9491296211	-1.5516943103	0.
H	-0.7765933415	2.1944616275	0.8765751344
H	-0.7765933415	2.1944616275	-0.8765751344
H	-2.0437549553	1.4105176173	0.
H	2.0437549553	-1.4105176173	0.
H	0.7765933415	-2.1944616275	-0.8765751344
H	0.7765933415	-2.1944616275	0.8765751344

Tabelle 10.154 Standardorientierung von (MeLi)<sub>4</sub> ( $T_d$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	1.2001163741	-0.6928875142	0.4899454559
Li	-0.0000000044	0.0000000006	-1.4698363708
Li	0.0000000028	1.3857750206	0.489945462
Li	-1.2001163726	-0.6928875119	0.489945463
C	0.0000000065	-0.000000004	2.1911483277
C	-0.0000000042	-2.0658344528	-0.7303827751
C	-1.789065117	1.0329172276	-0.7303827659
C	1.7890651147	1.0329172242	-0.7303827766
H	-0.8618715316	-0.4976017688	2.6689548708
H	0.0000000089	0.9952035256	2.6689548701
H	0.8618715465	-0.4976017705	2.6689548656
H	-0.0000000076	-2.1845802685	-1.8279385087
H	-0.8618715429	-2.6821820344	-0.4205081771

H	0.8618715352	-2.6821820361	-0.4205081823
H	-1.8919020092	2.087493666	-0.4205081681
H	-2.7537735497	0.5946883716	-0.4205081674
H	-1.8919020144	1.0922901376	-1.827938499
H	1.8919020056	1.0922901339	-1.8279385103
H	2.7537735483	0.5946883663	-0.4205081838
H	1.8919020107	2.0874936623	-0.4205081794

Tabelle 10.155 Standardorientierung von MeLi ( $C_{3v}$ ) [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
C	-0.0250968802	0.1246953217	-0.3741609541
Li	0.1013612831	-0.5036244955	1.5111738341
H	0.3035715007	-0.6421269755	-1.0849332507
H	0.5944765829	1.0107956173	-0.5535810976
H	-1.0514732942	0.3936366173	-0.648858304

Tabelle 10.156 Standardorientierung von (MeLi)<sub>2</sub> ( $C_{2h}$ ) [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
Li	0.9270223792	0.5742511756	0.
C	-0.9472961583	1.5510733168	0.
Li	-0.9270223792	-0.5742511756	0.
C	0.9472961583	-1.5510733168	0.
H	-0.7764228206	2.1933283117	0.8763350977
H	-0.7764228206	2.1933283117	-0.8763350977
H	-2.040933165	1.4077266917	0.
H	2.040933165	-1.4077266917	0.
H	0.7764228206	-2.1933283117	-0.8763350977
H	0.7764228206	-2.1933283117	0.8763350977

Tabelle 10.157 Standardorientierung von (MeLi)<sub>4</sub> ( $T_d$ ) [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
Li	1.2025747437	-0.6943068546	0.490949081
Li	-0.0000000044	0.0000000006	-1.4728472464
Li	0.0000000028	1.3886137013	0.4909490872
Li	-1.2025747422	-0.6943068523	0.4909490882
C	0.0000000065	-0.0000000004	2.1894937981
C	-0.0000000042	-2.0642745473	-0.7298312652
C	-1.7877141992	1.0321372749	-0.7298312561
C	1.7877141969	1.0321372714	-0.7298312667
H	-0.861112537	-0.4971635631	2.6673158734
H	0.0000000089	0.9943271141	2.6673158727
H	0.8611125519	-0.4971635648	2.6673158682
H	-0.0000000076	-2.183327144	-1.8265658876
H	-0.8611125483	-2.6804907043	-0.420374989
H	0.8611125406	-2.680490706	-0.4203749941
H	-1.8908167716	2.0859906924	-0.42037498

H	-2.7519293175	0.5945000151	-0.4203749793
H	-1.8908167768	1.0916635754	-1.8265658779
H	1.890816768	1.0916635717	-1.8265658892
H	2.7519293162	0.5945000098	-0.4203749957
H	1.8908167732	2.0859906887	-0.4203749913

Tabelle 10.158 Standardorientierung von MeLi ( $C_{3v}$ ) [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
C	-0.0246463876	0.1224570054	-0.3674446679
Li	0.1008361443	-0.5010152918	1.5033446645
H	0.3021867791	-0.6386950338	-1.0832420944
H	0.5919338199	1.0076475679	-0.5540051598
H	-1.0474638233	0.3929453682	-0.6489030847

Tabelle 10.159 Standardorientierung von (MeLi)<sub>2</sub> ( $C_{2h}$ ) [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
Li	0.9235346965	0.5682123442	0.
C	-0.9396712114	1.544354047	0.
Li	-0.9235346965	-0.5682123442	0.
C	0.9396712114	-1.544354047	0.
H	-0.7753850898	2.1906138361	0.8725244234
H	-0.7753850898	2.1906138361	-0.8725244234
H	-2.0310689846	1.39616825	0.
H	2.0310689846	-1.39616825	0.
H	0.7753850898	-2.1906138361	-0.8725244234
H	0.7753850898	-2.1906138361	0.8725244234

Tabelle 10.160 Standardorientierung von (MeLi)<sub>4</sub> ( $T_d$ ) [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
Li	1.2024781285	-0.6942510738	0.4909096381
Li	-0.0000000044	0.0000000006	-1.4727289174
Li	0.0000000028	1.3885021397	0.4909096442
Li	-1.202478127	-0.6942510715	0.4909096452
C	0.0000000065	-0.000000004	2.1814851727
C	-0.0000000042	-2.0567239429	-0.7271617234
C	-1.781175184	1.0283619726	-0.7271617143
C	1.7811751816	1.0283619692	-0.7271617249
H	-0.8594610158	-0.4962100568	2.6595319059
H	0.0000000089	0.9924201017	2.6595319052
H	0.8594610307	-0.4962100585	2.6595319008
H	-0.0000000075	-2.1766240199	-1.8221732832
H	-0.8594610271	-2.672834074	-0.4186793074
H	0.8594610194	-2.6728340756	-0.4186793126
H	-1.8850116959	2.0807321178	-0.4186792985
H	-2.7444727205	0.5921019593	-0.4186792978
H	-1.885011701	1.0883120133	-1.8221732735

H	1.8850116923	1.0883120097	-1.8221732848
H	2.7444727192	0.592101954	-0.4186793141
H	1.8850116974	2.0807321142	-0.4186793097

Tabelle 10.161 Standardorientierung von MeLi ( $C_{3v}$ ) [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
C	-0.0247593203	0.1230181223	-0.3691283538
Li	0.1004947096	-0.49931884	1.4982542955
H	0.3015854963	-0.6375440205	-1.0803104055
H	0.5907157586	1.005294046	-0.5522000465
H	-1.045192133	0.3919003501	-0.6468959641

Tabelle 10.162 Standardorientierung von (MeLi)<sub>2</sub> ( $C_{2h}$ ) [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
Li	0.9206271201	0.5692410263	0.
C	-0.9401048211	1.5389133747	0.
Li	-0.9206271201	-0.5692410263	0.
C	0.9401048211	-1.5389133747	0.
H	-0.7698452121	2.1803853904	0.8705330356
H	-0.7698452121	2.1803853904	-0.8705330356
H	-2.0282051655	1.394154836	0.
H	2.0282051655	-1.394154836	0.
H	0.7698452121	-2.1803853904	-0.8705330356
H	0.7698452121	-2.1803853904	0.8705330356

Tabelle 10.163 Standardorientierung von (MeLi)<sub>4</sub> ( $T_d$ ) [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
Li	1.1992706579	-0.6923992398	0.4896001937
Li	-0.0000000044	0.0000000006	-1.4688005842
Li	0.0000000028	1.3847984716	0.4896001998
Li	-1.1992706564	-0.6923992374	0.4896002008
C	0.0000000065	-0.000000004	2.1767570702
C	-0.0000000042	-2.0522662451	-0.7255856893
C	-1.7773147045	1.0261331238	-0.7255856802
C	1.7773147021	1.0261331203	-0.7255856907
H	-0.8579307212	-0.4953265408	2.650091233
H	0.0000000089	0.9906530696	2.6500912323
H	0.857930736	-0.4953265425	2.6500912279
H	-0.0000000075	-2.1683122789	-1.8173604184
H	-0.8579307324	-2.6636388169	-0.4163654034
H	0.8579307247	-2.6636388186	-0.4163654085
H	-1.877813517	2.0748092152	-0.4163653945
H	-2.735744247	0.5888296048	-0.4163653938
H	-1.8778135221	1.0841561428	-1.8173604088
H	1.8778135134	1.0841561392	-1.81736042
H	2.7357442457	0.5888295995	-0.4163654101

H	1.8778135185	2.0748092116	-0.4163654057
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Tabelle 10.164 Standardorientierung von MeLi ( $C_{3v}$ ) [globales Minimum; M06L/6-31+G(d)].

	x	y	z
C	-0.0234780601	0.1166520553	-0.3500263501
Li	0.1014066986	-0.5038501471	1.5118509237
H	0.3011470643	-0.6346670479	-1.0913719442
H	0.5905119385	1.0095040834	-0.5628330553
H	-1.0467233943	0.3956126552	-0.657605813

Tabelle 10.165 Standardorientierung von (MeLi)<sub>2</sub> ( $C_{2h}$ ) [globales Minimum; M06L/6-31+G(d)].

	x	y	z
Li	0.946682284	0.5645295237	0.
C	-0.9085027546	1.5460356955	0.
Li	-0.946682284	-0.5645295237	0.
C	0.9085027546	-1.5460356955	0.
H	-0.7336754928	2.2045196308	0.8727757421
H	-0.7336754928	2.2045196308	-0.8727757421
H	-2.0138910574	1.4570861553	0.
H	2.0138910574	-1.4570861553	0.
H	0.7336754928	-2.2045196308	-0.8727757421
H	0.7336754928	-2.2045196308	0.8727757421

Tabelle 10.166 Standardorientierung von (MeLi)<sub>4</sub> ( $T_d$ ) [globales Minimum; M06L/6-31+G(d)].

	x	y	z
Li	1.2128964239	-0.7002660794	0.4951628893
Li	-0.0000000044	0.0000000006	-1.4854886712
Li	0.0000000028	1.4005321509	0.4951628955
Li	-1.2128964223	-0.7002660771	0.4951628965
C	0.0000000065	-0.0000000004	2.178738485
C	-0.0000000042	-2.0541343409	-0.7262461609
C	-1.7789325229	1.0270671717	-0.7262461517
C	1.7789325205	1.0270671682	-0.7262461623
H	-0.8584639271	-0.4956343874	2.6780760716
H	0.0000000089	0.9912687628	2.6780760709
H	0.858463942	-0.4956343891	2.6780760665
H	-0.0000000076	-2.1944914067	-1.8272691791
H	-0.8584639384	-2.6901257913	-0.4254034424
H	0.8584639307	-2.690125793	-0.4254034475
H	-1.9004853067	2.0885144724	-0.4254034333
H	-2.7589492427	0.6016113221	-0.4254034326
H	-1.9004853118	1.0972457067	-1.8272691694
H	1.9004853031	1.097245703	-1.8272691807
H	2.7589492413	0.6016113167	-0.4254034491
H	1.9004853082	2.0885144687	-0.4254034447

Tabelle 10.167 Standardorientierung von MeLi ( $C_{3v}$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-0.0242074921	0.1202763096	-0.360901278
Li	0.101023628	-0.5019468233	1.5061398153
H	0.3040909174	-0.6430025158	-1.088235052
H	0.5955686868	1.0131740851	-0.5558368583
H	-1.0536214716	0.3948001217	-0.6513016312

Tabelle 10.168 Standardorientierung von  $(\text{MeLi})_2$  ( $C_{2h}$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	0.9330138684	0.5827533444	0.
C	-0.9456819998	1.5370911339	0.
Li	-0.9330138684	-0.5827533444	0.
C	0.9456819998	-1.5370911339	0.
H	-0.7734958424	2.1893942847	0.8782769626
H	-0.7734958424	2.1893942847	-0.8782769626
H	-2.0483022837	1.4167449507	0.
H	2.0483022837	-1.4167449507	0.
H	0.7734958424	-2.1893942847	-0.8782769626
H	0.7734958424	-2.1893942847	0.8782769626

Tabelle 10.169 Standardorientierung von  $(\text{MeLi})_4$  ( $T_d$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	1.2159314909	-0.7020183762	0.4964019502
Li	-0.0000000044	0.0000000006	-1.4892058539
Li	0.0000000028	1.4040367444	0.4964019564
Li	-1.2159314893	-0.7020183738	0.4964019574
C	0.0000000065	-0.0000000004	2.1925581606
C	-0.0000000042	-2.067163656	-0.7308527194
C	-1.7902162408	1.0335818292	-0.7308527102
C	1.7902162384	1.0335818258	-0.7308527209
H	-0.8624492137	-0.4979352938	2.6834568661
H	0.0000000009	0.9958705755	2.6834568654
H	0.8624492288	-0.4979352955	2.683456861
H	-0.0000000076	-2.1980305308	-1.8334014079
H	-0.8624492251	-2.6959658218	-0.4250277252
H	0.8624492174	-2.6959658234	-0.4250277304
H	-1.9035502781	2.0948858471	-0.4250277162
H	-2.7659995008	0.6010799778	-0.4250277155
H	-1.9035502832	1.0990152688	-1.8334013982
H	1.9035502745	1.0990152651	-1.8334014095
H	2.7659994994	0.6010799725	-0.4250277319
H	1.9035502796	2.0948858435	-0.4250277275

Tabelle 10.170 Standardorientierung von MeLi ( $C_{3v}$ ) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
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C	-0.0243233346	0.1208518846	-0.3626283467
Li	0.100937761	-0.5015201847	1.5048596446
H	0.3039008794	-0.642685074	-1.0870083049
H	0.59516815	1.0122954732	-0.5549945972
H	-1.0528310002	0.3943680857	-0.6503904276

Tabelle 10.171 Standardorientierung von (MeLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Li	0.9343431292	0.5837029685	0.
C	-0.9447099764	1.5370026321	0.
Li	-0.9343431292	-0.5837029685	0.
C	0.9447099764	-1.5370026321	0.
H	-0.7730808579	2.1876457601	0.8775160093
H	-0.7730808579	2.1876457601	-0.8775160093
H	-2.0453820334	1.4146182607	0.
H	2.0453820334	-1.4146182607	0.
H	0.7730808579	-2.1876457601	-0.8775160093
H	0.7730808579	-2.1876457601	0.8775160093

Tabelle 10.172 Standardorientierung von (MeLi)<sub>4</sub> (T<sub>d</sub>) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Li	1.2182235451	-0.7033416943	0.4973376774
Li	-0.0000000044	0.0000000006	-1.4920130356
Li	0.0000000028	1.4066833806	0.4973376836
Li	-1.2182235435	-0.7033416919	0.4973376846
C	0.0000000065	-0.000000004	2.1919063965
C	-0.0000000042	-2.0665491669	-0.7306354647
C	-1.7896840776	1.0332745847	-0.7306354555
C	1.7896840753	1.0332745812	-0.7306354662
H	-0.8612738148	-0.4972566769	2.6816309255
H	0.000000009	0.9945133417	2.6816309248
H	0.8612738298	-0.4972566785	2.6816309204
H	-0.0000000076	-2.1967614288	-1.8315131487
H	-0.8612738261	-2.6940181028	-0.4250588845
H	0.8612738184	-2.6940181045	-0.4250588897
H	-1.9024512035	2.0928940623	-0.4250588755
H	-2.7637250272	0.6011240437	-0.4250588748
H	-1.9024512086	1.0983807178	-1.8315131389
H	1.9024511999	1.0983807141	-1.8315131503
H	2.7637250258	0.6011240384	-0.4250588912
H	1.902451205	2.0928940586	-0.4250588868

Tabelle 10.173 Standardorientierung von MeLi (C<sub>3v</sub>) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
C	-0.0243233346	0.1208518846	-0.3626283467
Li	0.100937761	-0.5015201847	1.5048596446
H	0.3039008794	-0.642685074	-1.0870083049

H	0.59516815	1.0122954732	-0.5549945972
H	-1.0528310002	0.3943680857	-0.6503904276

Tabelle 10.174 Standardorientierung von (MeLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Li	0.9343431292	0.5837029685	0.
C	-0.9447099764	1.5370026321	0.
Li	-0.9343431292	-0.5837029685	0.
C	0.9447099764	-1.5370026321	0.
H	-0.7730808579	2.1876457601	0.8775160093
H	-0.7730808579	2.1876457601	-0.8775160093
H	-2.0453820334	1.4146182607	0.
H	2.0453820334	-1.4146182607	0.
H	0.7730808579	-2.1876457601	-0.8775160093
H	0.7730808579	-2.1876457601	0.8775160093

Tabelle 10.175 Standardorientierung von (MeLi)<sub>4</sub> (T<sub>d</sub>) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Li	1.2182235451	-0.7033416943	0.4973376774
Li	-0.0000000044	0.0000000006	-1.4920130356
Li	0.0000000028	1.4066833806	0.4973376836
Li	-1.2182235435	-0.7033416919	0.4973376846
C	0.0000000065	-0.0000000004	2.1919063965
C	-0.0000000042	-2.0665491669	-0.7306354647
C	-1.7896840776	1.0332745847	-0.7306354555
C	1.7896840753	1.0332745812	-0.7306354662
H	-0.8612738148	-0.4972566769	2.6816309255
H	0.0000000009	0.9945133417	2.6816309248
H	0.8612738298	-0.4972566785	2.6816309204
H	-0.0000000076	-2.1967614288	-1.8315131487
H	-0.8612738261	-2.6940181028	-0.4250588845
H	0.8612738184	-2.6940181045	-0.4250588897
H	-1.9024512035	2.0928940623	-0.4250588755
H	-2.7637250272	0.6011240437	-0.4250588748
H	-1.9024512086	1.0983807178	-1.8315131389
H	1.9024511999	1.0983807141	-1.8315131503
H	2.7637250258	0.6011240384	-0.4250588912
H	1.902451205	2.0928940586	-0.4250588868

Tabelle 10.176 Standardorientierung von MeLi (C<sub>3v</sub>) [globales Minimum; M062X/6-31+G(d)].

	x	y	z
C	-0.0245694252	0.1220746097	-0.3662972524
Li	0.1011679844	-0.5026640719	1.5082919895
H	0.3036934137	-0.642169932	-1.0867610934
H	0.5947875007	1.0118265855	-0.5550637141
H	-1.0522317709	0.3942666095	-0.6504028234

Tabelle 10.177 Standardorientierung von (MeLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; M062X/6-31+G(d)].

	x	y	z
Li	0.9232841814	0.5708412283	0.
C	-0.9407422264	1.5405057859	0.
Li	-0.9232841814	-0.5708412283	0.
C	0.9407422264	-1.5405057859	0.
H	-0.7737312984	2.1898295164	0.8770681374
H	-0.7737312984	2.1898295164	-0.8770681374
H	-2.039129235	1.4024573337	0.
H	2.039129235	-1.4024573337	0.
H	0.7737312984	-2.1898295164	-0.8770681374
H	0.7737312984	-2.1898295164	0.8770681374

Tabelle 10.178 Standardorientierung von (MeLi)<sub>4</sub> (T<sub>d</sub>) [globales Minimum; M062X/6-31+G(d)].

	x	y	z
Li	1.1945437118	-0.6896701361	0.487670426
Li	-0.0000000044	0.0000000006	-1.4630112812
Li	0.0000000028	1.3793402643	0.4876704321
Li	-1.1945437102	-0.6896701338	0.4876704331
C	0.0000000065	-0.0000000004	2.174925912
C	-0.0000000041	-2.0505398126	-0.7249753032
C	-1.77581957	1.0252699075	-0.7249752941
C	1.7758195677	1.025269904	-0.7249753047
H	-0.8623559035	-0.497881421	2.6590617975
H	0.0000000089	0.9957628301	2.6590617968
H	0.8623559184	-0.4978814227	2.6590617924
H	-0.0000000075	-2.1750665547	-1.825168135
H	-0.8623559148	-2.672947973	-0.4169468274
H	0.8623559071	-2.6729479746	-0.4169468325
H	-1.8836628914	2.0832961136	-0.4169468184
H	-2.7460188038	0.5896518625	-0.4169468177
H	-1.8836628966	1.0875332807	-1.8251681253
H	1.8836628878	1.0875332771	-1.8251681365
H	2.7460188025	0.5896518572	-0.4169468341
H	1.883662893	2.0832961099	-0.4169468296

Tabelle 10.179 Standardorientierung von MeLi (C<sub>3v</sub>) [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
C	-0.0246250835	0.1223511538	-0.3671270498
Li	0.1010993553	-0.5023230818	1.5072688155
H	0.303534145	-0.6418675791	-1.0859681593
H	0.5944640092	1.011195825	-0.5545707407
H	-1.0516260852	0.3939842497	-0.6498560638

Tabelle 10.180 Standardorientierung von (MeLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
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Li	0.9251168345	0.5712850799	0.
C	-0.9389241828	1.5400382611	0.
Li	-0.9251168345	-0.5712850799	0.
C	0.9389241828	-1.5400382611	0.
H	-0.7737538539	2.1886976059	0.876467368
H	-0.7737538539	2.1886976059	-0.876467368
H	-2.0358959899	1.3997179499	0.
H	2.0358959899	-1.3997179499	0.
H	0.7737538539	-2.1886976059	-0.876467368
H	0.7737538539	-2.1886976059	0.876467368

Tabelle 10.181 Standardorientierung von  $(\text{MeLi})_4$  ( $T_d$ ) [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
Li	1.1968084109	-0.6909776608	0.4885949856
Li	-0.0000000044	0.0000000006	-1.4657849599
Li	0.0000000028	1.3819553137	0.4885949917
Li	-1.1968084094	-0.6909776585	0.4885949927
C	0.0000000065	-0.0000000004	2.173516255
C	-0.0000000041	-2.0492107752	-0.7245054175
C	-1.7746685899	1.0246053888	-0.7245054084
C	1.7746685876	1.0246053854	-0.724505419
H	-0.861307203	-0.4972759535	2.65739472
H	0.0000000089	0.994551895	2.6573947193
H	0.8613072178	-0.4972759552	2.6573947148
H	-0.0000000075	-2.173898464	-1.8234707619
H	-0.8613072142	-2.6711744146	-0.4169619751
H	0.8613072066	-2.6711744163	-0.4169619803
H	-1.8826512951	2.0815011331	-0.4169619662
H	-2.743958507	0.5896732846	-0.4169619655
H	-1.8826513003	1.0869492353	-1.8234707522
H	1.8826512915	1.0869492317	-1.8234707635
H	2.7439585056	0.5896732793	-0.4169619818
H	1.8826512967	2.0815011295	-0.4169619774

Tabelle 10.182 Standardorientierung von  $\text{MeLi}$  ( $C_{3v}$ ) [globales Minimum; M062X/6-311+G(d,p)].

	x	y	z
C	-0.0242139405	0.1203083494	-0.3609974164
Li	0.1005672862	-0.4996794442	1.4993363237
H	0.3021967377	-0.6385927154	-1.0840769025
H	0.5919947588	1.0080395564	-0.5547468499
H	-1.0476913325	0.3932292013	-0.6496614718

Tabelle 10.183 Standardorientierung von  $(\text{MeLi})_2$  ( $C_{2h}$ ) [globales Minimum; M062X/6-311+G(d,p)].

	x	y	z
Li	0.9200562587	0.5608143995	0.
C	-0.929667374	1.5367814276	0.
Li	-0.9200562587	-0.5608143995	0.

C	0.929667374	-1.5367814276	0.
H	-0.7747307293	2.1893976868	0.872936436
H	-0.7747307293	2.1893976868	-0.872936436
H	-2.0235927767	1.3838732283	0.
H	2.0235927767	-1.3838732283	0.
H	0.7747307293	-2.1893976868	-0.872936436
H	0.7747307293	-2.1893976868	0.872936436

Tabelle 10.184 Standardorientierung von  $(\text{MeLi})_4$  ( $T_d$ ) [globales Minimum; M062X/6-311+G(d,p)].

	x	y	z
Li	1.1917514586	-0.688058028	0.4865304934
Li	-0.0000000043	0.0000000006	-1.4595914834
Li	0.0000000028	1.3761160481	0.4865304995
Li	-1.1917514571	-0.6880580257	0.4865305005
C	0.0000000064	-0.0000000039	2.1656685995
C	-0.0000000041	-2.0418119347	-0.7218895324
C	-1.7682610061	1.0209059685	-0.7218895233
C	1.7682610037	1.0209059651	-0.7218895338
H	-0.8601482678	-0.4966068419	2.6485254331
H	0.0000000089	0.9932136719	2.6485254324
H	0.8601482826	-0.4966068436	2.648525428
H	-0.0000000075	-2.1659824945	-1.8192526441
H	-0.860148279	-2.6625893336	-0.4146363906
H	0.8601482714	-2.6625893353	-0.4146363957
H	-1.8757958645	2.0762049253	-0.4146363817
H	-2.7359441411	0.5863844114	-0.414636381
H	-1.8757958696	1.0829912506	-1.8192526345
H	1.8757958609	1.0829912469	-1.8192526457
H	2.7359441398	0.5863844061	-0.4146363972
H	1.875795866	2.0762049216	-0.4146363928

Tabelle 10.185 Standardorientierung von  $\text{MeLi}$  ( $C_{3v}$ ) [globales Minimum; MP2/6-31+G(d)].

	x	y	z
C	-0.0254782385	0.1265901381	-0.3798465351
Li	0.102260366	-0.5080916775	1.5245780487
H	0.3051945996	-0.6458027601	-1.089162971
H	0.5975736013	1.0154946425	-0.555118633
H	-1.0567157572	0.3952087029	-0.6508785775

Tabelle 10.186 Standardorientierung von  $(\text{MeLi})_2$  ( $C_{2h}$ ) [globales Minimum; MP2/6-31+G(d)].

	x	y	z
Li	0.9443703306	0.5570439596	0.
C	-0.9147812333	1.5905681983	0.
Li	-0.9443703306	-0.5570439596	0.
C	0.9147812333	-1.5905681983	0.
H	-0.7435794142	2.2337668065	0.8797292392

H	-0.7435794142	2.2337668065	-0.8797292392
H	-2.0113884883	1.437600629	0.
H	2.0113884883	-1.437600629	0.
H	0.7435794142	-2.2337668065	-0.8797292392
H	0.7435794142	-2.2337668065	0.8797292392

Tabelle 10.187 Standardorientierung von  $(\text{MeLi})_4$  ( $T_d$ ) [globales Minimum; MP2/6-31+G(d)].

	x	y	z
Li	1.2090285167	-0.6980329422	0.4935838228
Li	-0.0000000044	0.0000000006	-1.4807514717
Li	0.0000000028	1.3960658764	0.493583829
Li	-1.2090285151	-0.6980329398	0.49358383
C	0.0000000065	-0.000000004	2.2073401011
C	-0.0000000042	-2.0811002031	-0.7357800329
C	-1.8022856446	1.0405501028	-0.7357800237
C	1.8022856423	1.0405500993	-0.7357800344
H	-0.8653673131	-0.4996200592	2.6846094551
H	0.0000000089	0.9992401064	2.6846094544
H	0.865367328	-0.4996200609	2.68460945
H	-0.0000000076	-2.1979940252	-1.8369624285
H	-0.8653673245	-2.6976140816	-0.4238235095
H	0.8653673167	-2.6976140833	-0.4238235146
H	-1.9035186633	2.0982371252	-0.4238235005
H	-2.7688859853	0.5993769596	-0.4238234998
H	-1.9035186684	1.098997016	-1.8369624187
H	1.9035186597	1.0989970123	-1.83696243
H	2.768885984	0.5993769542	-0.4238235162
H	1.9035186649	2.0982371215	-0.4238235118

Tabelle 10.188 Standardorientierung von  $\text{MeLi}$  ( $C_{3v}$ ) [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
C	-0.0246820262	0.1226340793	-0.3679759954
Li	0.1017168759	-0.5053912933	1.516475283
H	0.3032788651	-0.6407633202	-1.0887109509
H	0.5941536098	1.0119868945	-0.5574142108
H	-1.0516246164	0.3948922561	-0.6526814811

Tabelle 10.189 Standardorientierung von  $(\text{MeLi})_2$  ( $C_{2h}$ ) [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
Li	-1.0917654078	-0.0082193689	0.
C	-0.0241255714	1.8176902488	0.
Li	1.0917654078	0.0082193689	0.
C	0.0241255714	-1.8176902488	0.
H	-0.4918342678	2.2985445154	-0.8757883967
H	-0.4918342678	2.2985445154	0.8757883967
H	0.9976239518	2.2444042986	0.

H	-0.9976239518	-2.2444042986	0.
H	0.4918342678	-2.2985445154	0.8757883967
H	0.4918342678	-2.2985445154	-0.8757883967

Tabelle 10.190 Standardorientierung von (MeLi)<sub>4</sub> (T<sub>d</sub>) [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
Li	1.2098151553	-0.6984871082	0.4939049666
Li	-0.0000000044	0.0000000006	-1.4817149033
Li	0.0000000028	1.3969742084	0.4939049729
Li	-1.2098151537	-0.6984871058	0.4939049739
C	0.0000000065	-0.0000000004	2.185916282
C	-0.0000000042	-2.0609016328	-0.7286387599
C	-1.7847931696	1.0304508176	-0.7286387507
C	1.7847931672	1.0304508142	-0.7286387614
H	-0.8627027196	-0.4980816555	2.6694341653
H	0.0000000089	0.9961632989	2.6694341646
H	0.8627027346	-0.4980816571	2.6694341601
H	-0.0000000076	-2.1847122272	-1.8290031565
H	-0.862702731	-2.6827938799	-0.4202155005
H	0.8627027233	-2.6827938815	-0.4202155056
H	-1.8920162888	2.0885194187	-0.4202154915
H	-2.7547190174	0.5942744643	-0.4202154908
H	-1.892016294	1.092356117	-1.8290031468
H	1.8920162852	1.0923561133	-1.8290031581
H	2.754719016	0.594274459	-0.4202155072
H	1.8920162904	2.088519415	-0.4202155028

Tabelle 10.191 Standardorientierung von MeLi (C<sub>3v</sub>) [globales Minimum; G3].

	x	y	z
C	-0.0253569004	0.125987258	-0.3780375345
Li	0.1019813947	-0.5067055812	1.5204189317
H	0.3041395032	-0.6432713042	-1.08733331
H	0.5956080754	1.0128530388	-0.5549519152
H	-1.0535300455	0.3944985872	-0.6504136759

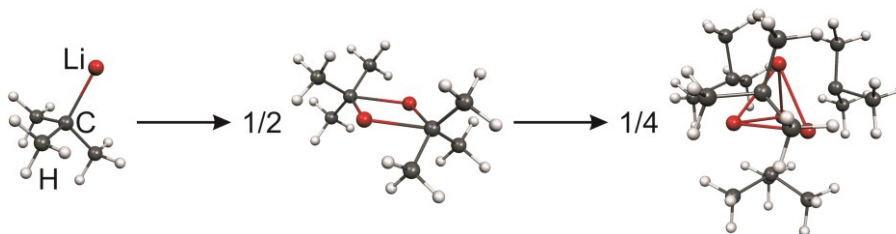
Tabelle 10.192 Standardorientierung von (MeLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; G3].

	x	y	z
Li	0.9094201407	0.5681170232	0.
C	-0.9512300192	1.5699241504	0.
Li	-0.9094201407	-0.5681170232	0.
C	0.9512300192	-1.5699241504	0.
H	-0.7846447343	2.212378824	0.878911004
H	-0.7846447343	2.212378824	-0.878911004
H	-2.0452191956	1.410560126	0.
H	2.0452191956	-1.410560126	0.
H	0.7846447343	-2.212378824	-0.878911004

H	0.7846447343	-2.212378824	0.878911004
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Tabelle 10.193 Standardorientierung von (MeLi)<sub>4</sub> (T<sub>d</sub>) [globales Minimum; G3].

	x	y	z
Li	1.1878118772	-0.6857835096	0.4849221661
Li	-0.0000000043	0.0000000006	-1.4547665013
Li	0.0000000028	1.3715670113	0.4849221722
Li	-1.1878118756	-0.6857835073	0.4849221731
C	0.0000000065	-0.0000000004	2.1917348816
C	-0.0000000042	-2.0663874611	-0.7305782931
C	-1.7895440363	1.0331937318	-0.7305782839
C	1.7895440339	1.0331937283	-0.7305782946
H	-0.8656979733	-0.4998109659	2.6659607361
H	0.0000000089	0.9996219199	2.6659607354
H	0.8656979882	-0.4998109676	2.6659607309
H	-0.0000000076	-2.1802845731	-1.8311061659
H	-0.8656979846	-2.6800955362	-0.4174272812
H	0.8656979769	-2.6800955379	-0.4174272863
H	-1.8881818279	2.0897642126	-0.4174272722
H	-2.7538798101	0.5903313268	-0.4174272715
H	-1.8881818331	1.0901422899	-1.8311061562
H	1.8881818243	1.0901422863	-1.8311061675
H	2.7538798087	0.5903313214	-0.4174272879
H	1.8881818294	2.0897642089	-0.4174272834

10.2.1.3. Aggregation von *tert*-ButyllithiumAbbildung 10.20 Von monomeren *tert*-Butyllithium (<sup>t</sup>BuLi, C<sub>3v</sub>) über das dimere Aggregat [(<sup>t</sup>BuLi)<sub>2</sub>, C<sub>2h</sub>] zum Tetramer [(<sup>t</sup>BuLi)<sub>4</sub>, T].Tabelle 10.194 Berechnete Energien der optimierten Strukturen zur Aggregation von *tert*-Butyllithium.

	Method	Basissatz	imaginäre Frequenzen	SCF [Hartree]	ZPE [Hartree]
<sup>t</sup> BuLi	SVWN	6-31+G(d)	0	-164.3650345	-164.249425
( <sup>t</sup> BuLi) <sub>2</sub>	SVWN	6-31+G(d)	0	-328.8150881	-328.581221
( <sup>t</sup> BuLi) <sub>4</sub>	SVWN	6-31+G(d)	0	-657.7350372	-657.260334
<sup>t</sup> BuLi	PBE	6-31+G(d)	0	-165.0684109	-164.952697
( <sup>t</sup> BuLi) <sub>2</sub>	PBE	6-31+G(d)	1	-330.2071229	-329.974333

	Methode	Basissatz	imaginäre		
			Frequenzen	SCF [Hartree]	ZPE [Hartree]
( <sup>t</sup> BuLi) <sub>4</sub>	PBE	6-31+G(d)	0	-660.4796477	-660.006318
<sup>t</sup> BuLi	TPSS	6-31+G(d)	0	-165.3572573	-165.239874
( <sup>t</sup> BuLi) <sub>2</sub>	TPSS	6-31+G(d)	2	-330.783081	-330.547151
( <sup>t</sup> BuLi) <sub>4</sub>	TPSS	6-31+G(d)	0	-661.6280754	-661.148341
<sup>t</sup> BuLi	PBE0	6-31+G(d)	0	-165.1039467	-164.984207
( <sup>t</sup> BuLi) <sub>2</sub>	PBE0	6-31+G(d)	0	-330.2804126	-330.039308
( <sup>t</sup> BuLi) <sub>4</sub>	PBE0	6-31+G(d)	0	-660.6287802	-660.139899
<sup>t</sup> BuLi	TPSSh	6-31+G(d)	0	-165.3430627	-165.224289
( <sup>t</sup> BuLi) <sub>2</sub>	TPSSh	6-31+G(d)	1	-330.7557167	-330.516854
( <sup>t</sup> BuLi) <sub>4</sub>	TPSSh	6-31+G(d)	0	-661.5743933	-661.088835
<sup>t</sup> BuLi	B3LYP	6-31+G(d)	0	-165.3369709	-165.218077
( <sup>t</sup> BuLi) <sub>2</sub>	B3LYP	6-31+G(d)	0	-330.7408517	-330.501801
( <sup>t</sup> BuLi) <sub>4</sub>	B3LYP	6-31+G(d)	0	-661.5339982	-661.048927
<sup>t</sup> BuLi	B3LYP	6-311+G(d,p)	0	-165.3796397	-165.261868
( <sup>t</sup> BuLi) <sub>2</sub>	B3LYP	6-311+G(d,p)	0	-330.8268972	-330.589975
( <sup>t</sup> BuLi) <sub>4</sub>	B3LYP	6-311+G(d,p)	0	-661.7030012	-661.222367
<sup>t</sup> BuLi	M052X	6-31+G(d)	0	-165.2941915	-165.172999
( <sup>t</sup> BuLi) <sub>2</sub>	M052X	6-31+G(d)	0	-330.6641097	-330.420017
( <sup>t</sup> BuLi) <sub>4</sub>	M052X	6-31+G(d)	0	-661.4162512	-660.921475
<sup>t</sup> BuLi	M052X	6-31+G(d,p)	0	-165.3058983	-165.185399
( <sup>t</sup> BuLi) <sub>2</sub>	M052X	6-31+G(d,p)	0	-330.6876839	-330.444913
( <sup>t</sup> BuLi) <sub>4</sub>	M052X	6-31+G(d,p)	0	-661.4633644	-660.971254
<sup>t</sup> BuLi	M052X	6-311+G(d,p)	0	-165.3365811	-165.21636
( <sup>t</sup> BuLi) <sub>2</sub>	M052X	6-311+G(d,p)	0	-330.7503532	-330.508042
( <sup>t</sup> BuLi) <sub>4</sub>	M052X	6-311+G(d,p)	0	-661.5870215	-661.095963
<sup>t</sup> BuLi	M052X	6-311+G(3df,3pd)	0	-165.3504692	-165.230159
( <sup>t</sup> BuLi) <sub>2</sub>	M052X	6-311+G(3df,3pd)	0	-330.779509	-330.536752
( <sup>t</sup> BuLi) <sub>4</sub>	M052X	6-311+G(3df,3pd)	0	-661.6435568	-661.151982
<sup>t</sup> BuLi	M06L	6-31+G(d)	0	-165.2993583	-165.180557
( <sup>t</sup> BuLi) <sub>2</sub>	M06L	6-31+G(d)	0	-330.6714823	-330.431582
( <sup>t</sup> BuLi) <sub>4</sub>	M06L	6-31+G(d)	0	-661.4337261	-660.948412
<sup>t</sup> BuLi	M06	6-31+G(d)	0	-165.1957734	-165.077503
( <sup>t</sup> BuLi) <sub>2</sub>	M06	6-31+G(d)	0	-330.4614844	-330.222783
( <sup>t</sup> BuLi) <sub>4</sub>	M06	6-31+G(d)	0	-661.0052131	-660.522103
<sup>t</sup> BuLi	M06	6-31+G(d,p)	0	-165.2068347	-165.089161
( <sup>t</sup> BuLi) <sub>2</sub>	M06	6-31+G(d,p)	0	-330.4836545	-330.246173
( <sup>t</sup> BuLi) <sub>4</sub>	M06	6-31+G(d,p)	0	-661.0503425	-660.569621
<sup>t</sup> BuLi	M06	6-311+G(d,p)	0	-165.2380537	-165.120605
( <sup>t</sup> BuLi) <sub>2</sub>	M06	6-311+G(d,p)	0	-330.5463353	-330.309221
( <sup>t</sup> BuLi) <sub>4</sub>	M06	6-311+G(d,p)	0	-661.1754483	-660.694836
<sup>t</sup> BuLi	M062X	6-31+G(d)	0	-165.2364498	-165.116111
( <sup>t</sup> BuLi) <sub>2</sub>	M062X	6-31+G(d)	0	-330.5472503	-330.304871
( <sup>t</sup> BuLi) <sub>4</sub>	M062X	6-31+G(d)	0	-661.1864245	-660.694562
<sup>t</sup> BuLi	M062X	6-31+G(d,p)	0	-165.2457236	-165.12606
( <sup>t</sup> BuLi) <sub>2</sub>	M062X	6-31+G(d,p)	0	-330.5659245	-330.324848
( <sup>t</sup> BuLi) <sub>4</sub>	M062X	6-31+G(d,p)	0	-661.224009	-660.734907
<sup>t</sup> BuLi	M062X	6-311+G(d,p)	0	-165.2793732	-165.159967
( <sup>t</sup> BuLi) <sub>2</sub>	M062X	6-311+G(d,p)	0	-330.6349174	-330.394264
( <sup>t</sup> BuLi) <sub>4</sub>	M062X	6-311+G(d,p)	0	-661.3604803	-660.87212
<sup>t</sup> BuLi	MP2	6-31+G(d)	0	-164.6586492	-164.536944

	Methode	Basissatz	imaginäre		
			Frequenzen	SCF [Hartree]	ZPE [Hartree]
<sup>t</sup> BuLi) <sub>2</sub>	MP2	6-31+G(d)	0	-329.3890557	-329.144815
( <sup>t</sup> BuLi) <sub>4</sub>	MP2	6-31+G(d)	0	-658.8668782	-658.373124
<sup>t</sup> BuLi	MP2	6-311+G(d,p)	0	-164.7861806	-164.666162
( <sup>t</sup> BuLi) <sub>2</sub>	MP2	6-311+G(d,p)	0	-329.6451199	-329.403504
( <sup>t</sup> BuLi) <sub>4</sub>	MP2	6-311+G(d,p)	0	-659.3796467	-658.890691
<sup>t</sup> BuLi	G3	G3	0		-165.125542
( <sup>t</sup> BuLi) <sub>2</sub>	G3	G3	1		-330.325471
( <sup>t</sup> BuLi) <sub>4</sub>	G3	G3	0		-660.738119

Tabelle 10.195 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
C	0.	0.0000001667	0.2889110575
Li	0.	0.0000001667	2.2940108876
C	0.	1.4109039876	-0.2538491124
H	0.8943233949	1.9928784639	0.0473370097
H	0.	1.3980948597	-1.3802342141
H	-0.8943233949	1.9928784639	0.0473370097
C	-1.2218785512	-0.7054517438	-0.2538491124
H	-1.2787215346	-1.7709457611	0.0473370097
H	-2.1730449295	-0.2219322028	0.0473370097
H	-1.210785521	-0.6990471798	-1.3802342141
C	1.2218785512	-0.7054517438	-0.2538491124
H	2.1730449295	-0.2219322028	0.0473370097
H	1.2787215346	-1.7709457611	0.0473370097
H	1.210785521	-0.6990471798	-1.3802342141

Tabelle 10.196 Standardorientierung von (<sup>t</sup>BuLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
Li	0.	0.	1.1050393155
C	-0.7418290888	1.5896920334	0.
Li	0.	0.	-1.1050393155
C	0.7418290888	-1.5896920334	0.
C	-0.0440010618	2.1575291484	-1.217430288
H	1.0312158722	1.8604747393	-1.2927266377
H	-0.5436938592	1.8815999805	-2.1752472576
H	-0.0243354291	3.2791304005	-1.224153639
C	-2.1775072989	2.0458912131	0.
H	-2.7348241392	1.6870027171	-0.8872481962
H	-2.7348241392	1.6870027171	0.8872481962
H	-2.26663286	3.1660117678	0.
C	-0.0440010618	2.1575291484	1.217430288
H	-0.5436938592	1.8815999805	2.1752472576
H	1.0312158722	1.8604747393	1.2927266377
H	-0.0243354291	3.2791304005	1.224153639
C	0.0440010618	-2.1575291484	1.217430288
H	0.5436938592	-1.8815999805	2.1752472576

H	-1.0312158722	-1.8604747393	1.2927266377
H	0.0243354291	-3.2791304005	1.224153639
C	2.1775072989	-2.0458912131	0.
H	2.7348241392	-1.6870027171	-0.8872481962
H	2.7348241392	-1.6870027171	0.8872481962
H	2.26663286	-3.1660117678	0.
C	0.0440010618	-2.1575291484	-1.217430288
H	-1.0312158722	-1.8604747393	-1.2927266377
H	0.5436938592	-1.8815999805	-2.1752472576
H	0.0243354291	-3.2791304005	-1.224153639

Tabelle 10.197 Standardorientierung von  $(^t\text{BuLi})_4$  (T) [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
Li	-0.8311725402	-0.8311725402	0.8311725402
Li	0.8311725402	0.8311725402	0.8311725402
Li	-0.8311725402	0.8311725402	-0.8311725402
Li	0.8311725402	-0.8311725402	-0.8311725402
C	-1.254976997	-1.254976997	-1.254976997
C	1.254976997	-1.254976997	1.254976997
C	1.254976997	1.254976997	-1.254976997
C	-1.254976997	1.254976997	1.254976997
C	-0.4687553665	1.8769437062	2.3938177549
H	-0.0361905386	1.121690493	3.0850482468
H	0.3641078321	2.5382181467	2.0587864351
H	-1.1140424732	2.5379555502	3.0306496202
C	-1.8769437062	2.3938177549	0.4687553665
H	-1.121690493	3.0850482468	0.0361905386
H	-2.5382181467	2.0587864351	-0.3641078321
H	-2.5379555502	3.0306496202	1.1140424732
C	-2.3938177549	0.4687553665	1.8769437062
H	-3.0850482468	0.0361905386	1.121690493
H	-2.0587864351	-0.3641078321	2.5382181467
H	-3.0306496202	1.1140424732	2.5379555502
C	1.8769437062	2.3938177549	-0.4687553665
H	1.121690493	3.0850482468	-0.0361905386
H	2.5382181467	2.0587864351	0.3641078321
H	2.5379555502	3.0306496202	-1.1140424732
C	2.3938177549	0.4687553665	-1.8769437062
H	3.0850482468	0.0361905386	-1.121690493
H	2.0587864351	-0.3641078321	-2.5382181467
H	3.0306496202	1.1140424732	-2.5379555502
C	0.4687553665	1.8769437062	-2.3938177549
H	0.0361905386	1.121690493	-3.0850482468
H	-0.3641078321	2.5382181467	-2.0587864351
H	1.1140424732	2.5379555502	-3.0306496202
C	-1.8769437062	-2.3938177549	-0.4687553665
H	-1.121690493	-3.0850482468	-0.0361905386
H	-2.5382181467	-2.0587864351	0.3641078321
H	-2.5379555502	-3.0306496202	-1.1140424732
C	-2.3938177549	-0.4687553665	-1.8769437062

H	-3.0850482468	-0.0361905386	-1.121690493
H	-2.0587864351	0.3641078321	-2.5382181467
H	-3.0306496202	-1.1140424732	-2.5379555502
C	-0.4687553665	-1.8769437062	-2.3938177549
H	-0.0361905386	-1.121690493	-3.0850482468
H	0.3641078321	-2.5382181467	-2.0587864351
H	-1.1140424732	-2.5379555502	-3.0306496202
C	2.3938177549	-0.4687553665	1.8769437062
H	3.0850482468	-0.0361905386	1.121690493
H	2.0587864351	0.3641078321	2.5382181467
H	3.0306496202	-1.1140424732	2.5379555502
C	0.4687553665	-1.8769437062	2.3938177549
H	0.0361905386	-1.121690493	3.0850482468
H	-0.3641078321	-2.5382181467	2.0587864351
H	1.1140424732	-2.5379555502	3.0306496202
C	1.8769437062	-2.3938177549	0.4687553665
H	1.121690493	-3.0850482468	0.0361905386
H	2.5382181467	-2.0587864351	-0.3641078321
H	2.5379555502	-3.0306496202	1.1140424732

Tabelle 10.198 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; PBE/6-31+G(d)].

	x	y	z
C	0.	0.0000001667	0.2752967943
Li	0.	0.0000001667	2.3189967164
C	0.	1.4386950979	-0.2638304575
H	0.8928843376	2.0135602546	0.0537737865
H	0.	1.4532610776	-1.3869169448
H	-0.8928843376	2.0135602546	0.0537737865
C	-1.2459463588	-0.7193472989	-0.2638304575
H	-1.2973520194	-1.7800403963	0.0537737865
H	-2.190236357	-0.2335193583	0.0537737865
H	-1.2585608672	-0.7266302888	-1.3869169448
C	1.2459463588	-0.7193472989	-0.2638304575
H	2.190236357	-0.2335193583	0.0537737865
H	1.2973520194	-1.7800403963	0.0537737865
H	1.2585608672	-0.7266302888	-1.3869169448

Tabelle 10.199 Standardorientierung von (<sup>t</sup>BuLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; PBE/6-31+G(d)].

	x	y	z
Li	0.	0.	1.1088075643
C	-0.6942108698	1.6738414182	0.
Li	0.	0.	-1.1088075643
C	0.6942108698	-1.6738414182	0.
C	-0.0160574843	2.2890546303	-1.2396652184
H	1.0725078242	2.0572167681	-1.3031802731
H	-0.4858422295	1.9627171274	-2.1973061657
H	-0.0772566215	3.4073254683	-1.2648451177

C	-2.1733815249	2.0741080362	0.
H	-2.7119296732	1.686750571	-0.8872615567
H	-2.7119296732	1.686750571	0.8872615567
H	-2.3188893588	3.186199482	0.
C	-0.0160574843	2.2890546303	1.2396652184
H	-0.4858422295	1.9627171274	2.1973061657
H	1.0725078242	2.0572167681	1.3031802731
H	-0.0772566215	3.4073254683	1.2648451177
C	0.0160574843	-2.2890546303	1.2396652184
H	0.4858422295	-1.9627171274	2.1973061657
H	-1.0725078242	-2.0572167681	1.3031802731
H	0.0772566215	-3.4073254683	1.2648451177
C	2.1733815249	-2.0741080362	0.
H	2.7119296732	-1.686750571	-0.8872615567
H	2.7119296732	-1.686750571	0.8872615567
H	2.3188893588	-3.186199482	0.
C	0.0160574843	-2.2890546303	-1.2396652184
H	-1.0725078242	-2.0572167681	-1.3031802731
H	0.4858422295	-1.9627171274	-2.1973061657
H	0.0772566215	-3.4073254683	-1.2648451177

Tabelle 10.200 Standardorientierung von  $(t\text{-BuLi})_4$  (T) [globales Minimum; PBE/6-31+G(d)].

	x	y	z
Li	-0.8505160292	-0.8505160292	0.8505160292
Li	0.8505160292	0.8505160292	0.8505160292
Li	-0.8505160292	0.8505160292	-0.8505160292
Li	0.8505160292	-0.8505160292	-0.8505160292
C	-1.3186581822	-1.3186581822	-1.3186581822
C	1.3186581822	-1.3186581822	1.3186581822
C	1.3186581822	1.3186581822	-1.3186581822
C	-1.3186581822	1.3186581822	1.3186581822
C	-0.5196171661	1.9884984169	2.458179606
H	-0.071572557	1.2547963095	3.1592544196
H	0.3004757092	2.649567062	2.0989429606
H	-1.1651503665	2.6522658245	3.0868030875
C	-1.9884984169	2.458179606	0.5196171661
H	-1.2547963095	3.1592544196	0.071572557
H	-2.649567062	2.0989429606	-0.3004757092
H	-2.6522658245	3.0868030875	1.1651503665
C	-2.458179606	0.5196171661	1.9884984169
H	-3.1592544196	0.071572557	1.2547963095
H	-2.0989429606	-0.3004757092	2.649567062
H	-3.0868030875	1.1651503665	2.6522658245
C	1.9884984169	2.458179606	-0.5196171661
H	1.2547963095	3.1592544196	-0.071572557
H	2.649567062	2.0989429606	0.3004757092
H	2.6522658245	3.0868030875	-1.1651503665
C	2.458179606	0.5196171661	-1.9884984169
H	3.1592544196	0.071572557	-1.2547963095
H	2.0989429606	-0.3004757092	-2.649567062

H	3.0868030875	1.1651503665	-2.6522658245
C	0.5196171661	1.9884984169	-2.458179606
H	0.071572557	1.2547963095	-3.1592544196
H	-0.3004757092	2.649567062	-2.0989429606
H	1.1651503665	2.6522658245	-3.0868030875
C	-1.9884984169	-2.458179606	-0.5196171661
H	-1.2547963095	-3.1592544196	-0.071572557
H	-2.649567062	-2.0989429606	0.3004757092
H	-2.6522658245	-3.0868030875	-1.1651503665
C	-2.458179606	-0.5196171661	-1.9884984169
H	-3.1592544196	-0.071572557	-1.2547963095
H	-2.0989429606	0.3004757092	-2.649567062
H	-3.0868030875	-1.1651503665	-2.6522658245
C	-0.5196171661	-1.9884984169	-2.458179606
H	-0.071572557	-1.2547963095	-3.1592544196
H	0.3004757092	-2.649567062	-2.0989429606
H	-1.1651503665	-2.6522658245	-3.0868030875
C	2.458179606	-0.5196171661	1.9884984169
H	3.1592544196	-0.071572557	1.2547963095
H	2.0989429606	0.3004757092	2.649567062
H	3.0868030875	-1.1651503665	2.6522658245
C	0.5196171661	-1.9884984169	2.458179606
H	0.071572557	-1.2547963095	3.1592544196
H	-0.3004757092	-2.649567062	2.0989429606
H	1.1651503665	-2.6522658245	3.0868030875
C	1.9884984169	-2.458179606	0.5196171661
H	1.2547963095	-3.1592544196	0.071572557
H	2.649567062	-2.0989429606	-0.3004757092
H	2.6522658245	-3.0868030875	1.1651503665

Tabelle 10.201 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
C	0.	0.0000001667	0.2888799192
Li	0.	0.0000001667	2.3278529415
C	0.	1.4398661223	-0.266609155
H	0.8890976461	2.0120647457	0.049368921
H	0.	1.4465776146	-1.3828083012
H	-0.8890976461	2.0120647457	0.049368921
C	-1.2469604956	-0.7199328111	-0.266609155
H	-1.2979502164	-1.7760132708	0.049368921
H	-2.1870478625	-0.2360509748	0.049368921
H	-1.2527728184	-0.7232885573	-1.3828083012
C	1.2469604956	-0.7199328111	-0.266609155
H	2.1870478625	-0.2360509748	0.049368921
H	1.2979502164	-1.7760132708	0.049368921
H	1.2527728184	-0.7232885573	-1.3828083012

Tabelle 10.202 Standardorientierung von (<sup>t</sup>BuLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
Li	0.	0.	1.1053404834
C	-0.6646456373	1.6931044902	0.
Li	0.	0.	-1.1053404834
C	0.6646456373	-1.6931044902	0.
C	-0.0021723889	2.3395196592	-1.2420127406
H	1.0887272811	2.1510412576	-1.292014565
H	-0.445684921	1.9847505731	-2.1967279041
H	-0.1170216485	3.4461965053	-1.2699538365
C	-2.1562239939	2.0742247213	0.
H	-2.6835775881	1.6787823724	-0.8843071867
H	-2.6835775881	1.6787823724	0.8843071867
H	-2.3157399287	3.1774496276	0.
C	-0.0021723889	2.3395196592	1.2420127406
H	-0.445684921	1.9847505731	2.1967279041
H	1.0887272811	2.1510412576	1.292014565
H	-0.1170216485	3.4461965053	1.2699538365
C	0.0021723889	-2.3395196592	1.2420127406
H	0.445684921	-1.9847505731	2.1967279041
H	-1.0887272811	-2.1510412576	1.292014565
H	0.1170216485	-3.4461965053	1.2699538365
C	2.1562239939	-2.0742247213	0.
H	2.6835775881	-1.6787823724	-0.8843071867
H	2.6835775881	-1.6787823724	0.8843071867
H	2.3157399287	-3.1774496276	0.
C	0.0021723889	-2.3395196592	-1.2420127406
H	-1.0887272811	-2.1510412576	-1.292014565
H	0.445684921	-1.9847505731	-2.1967279041
H	0.1170216485	-3.4461965053	-1.2699538365

Tabelle 10.203 Standardorientierung von (<sup>t</sup>BuLi)<sub>4</sub> (T) [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
Li	-0.8516260884	-0.8516260884	0.8516260884
Li	0.8516260884	0.8516260884	0.8516260884
Li	-0.8516260884	0.8516260884	-0.8516260884
Li	0.8516260884	-0.8516260884	-0.8516260884
C	-1.3175750625	-1.3175750625	-1.3175750625
C	1.3175750625	-1.3175750625	1.3175750625
C	1.3175750625	1.3175750625	-1.3175750625
C	-1.3175750625	1.3175750625	1.3175750625
C	-0.5251384873	1.9848247175	2.4721189677
H	-0.0913562266	1.2462717345	3.1686198784
H	0.3007848074	2.6334901157	2.1186080485
H	-1.169383804	2.6483031065	3.089670365
C	-1.9848247175	2.4721189677	0.5251384873
H	-1.2462717345	3.1686198784	0.0913562266
H	-2.6334901157	2.1186080485	-0.3007848074
H	-2.6483031065	3.089670365	1.169383804
C	-2.4721189677	0.5251384873	1.9848247175

H	-3.1686198784	0.0913562266	1.2462717345
H	-2.1186080485	-0.3007848074	2.6334901157
H	-3.089670365	1.169383804	2.6483031065
C	1.9848247175	2.4721189677	-0.5251384873
H	1.2462717345	3.1686198784	-0.0913562266
H	2.6334901157	2.1186080485	0.3007848074
H	2.6483031065	3.089670365	-1.169383804
C	2.4721189677	0.5251384873	-1.9848247175
H	3.1686198784	0.0913562266	-1.2462717345
H	2.1186080485	-0.3007848074	-2.6334901157
H	3.089670365	1.169383804	-2.6483031065
C	0.5251384873	1.9848247175	-2.4721189677
H	0.0913562266	1.2462717345	-3.1686198784
H	-0.3007848074	2.6334901157	-2.1186080485
H	1.169383804	2.6483031065	-3.089670365
C	-1.9848247175	-2.4721189677	-0.5251384873
H	-1.2462717345	-3.1686198784	-0.0913562266
H	-2.6334901157	-2.1186080485	0.3007848074
H	-2.6483031065	-3.089670365	-1.169383804
C	-2.4721189677	-0.5251384873	-1.9848247175
H	-3.1686198784	-0.0913562266	-1.2462717345
H	-2.1186080485	0.3007848074	-2.6334901157
H	-3.089670365	-1.169383804	-2.6483031065
C	-0.5251384873	-1.9848247175	-2.4721189677
H	-0.0913562266	-1.2462717345	-3.1686198784
H	0.3007848074	-2.6334901157	-2.1186080485
H	-1.169383804	-2.6483031065	-3.089670365
C	2.4721189677	-0.5251384873	1.9848247175
H	3.1686198784	-0.0913562266	1.2462717345
H	2.1186080485	0.3007848074	2.6334901157
H	3.089670365	-1.169383804	2.6483031065
C	0.5251384873	-1.9848247175	2.4721189677
H	0.0913562266	-1.2462717345	3.1686198784
H	-0.3007848074	-2.6334901157	2.1186080485
H	1.169383804	-2.6483031065	3.089670365
C	1.9848247175	-2.4721189677	0.5251384873
H	1.2462717345	-3.1686198784	0.0913562266
H	2.6334901157	-2.1186080485	-0.3007848074
H	2.6483031065	-3.089670365	1.169383804

Tabelle 10.204 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
C	0.	0.0000001667	0.2825395005
Li	0.	0.0000001667	2.3062148107
C	0.	1.4272760204	-0.2637047176
H	0.8859411829	1.9999886076	0.0496563551
H	0.	1.4373587064	-1.3769614199
H	-0.8859411829	1.9999886076	0.0496563551

C	-1.2360571475	-0.7136377602	-0.2637047176
H	-1.2890702057	-1.7672416244	0.0496563551
H	-2.1750113886	-0.2327464831	0.0496563551
H	-1.2447890097	-0.7186791032	-1.3769614199
C	1.2360571475	-0.7136377602	-0.2637047176
H	2.1750113886	-0.2327464831	0.0496563551
H	1.2890702057	-1.7672416244	0.0496563551
H	1.2447890097	-0.7186791032	-1.3769614199

Tabelle 10.205 Standardorientierung von  $({}^t\text{BuLi})_2$  ( $\text{C}_{2h}$ ) [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
Li	0.	0.	1.0982055595
C	-0.6792751466	1.6725137332	0.
Li	0.	0.	-1.0982055595
C	0.6792751466	-1.6725137332	0.
C	-0.0113425421	2.2924945678	-1.2319400982
H	1.0719491804	2.0781942578	-1.2900480273
H	-0.4679140986	1.9564545925	-2.1828581673
H	-0.091981508	3.3992284048	-1.2590239646
C	-2.1525964312	2.0615731265	0.
H	-2.6845297693	1.6736694817	-0.8808145048
H	-2.6845297693	1.6736694817	0.8808145048
H	-2.3032037635	3.162997483	0.
C	-0.0113425421	2.2924945678	1.2319400982
H	-0.4679140986	1.9564545925	2.1828581673
H	1.0719491804	2.0781942578	1.2900480273
H	-0.091981508	3.3992284048	1.2590239646
C	0.0113425421	-2.2924945678	1.2319400982
H	0.4679140986	-1.9564545925	2.1828581673
H	-1.0719491804	-2.0781942578	1.2900480273
H	0.091981508	-3.3992284048	1.2590239646
C	2.1525964312	-2.0615731265	0.
H	2.6845297693	-1.6736694817	-0.8808145048
H	2.6845297693	-1.6736694817	0.8808145048
H	2.3032037635	-3.162997483	0.
C	0.0113425421	-2.2924945678	-1.2319400982
H	-1.0719491804	-2.0781942578	-1.2900480273
H	0.4679140986	-1.9564545925	-2.1828581673
H	0.091981508	-3.3992284048	-1.2590239646

Tabelle 10.206 Standardorientierung von  $({}^t\text{BuLi})_4$  (T) [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
Li	-0.8454662186	-0.8454662186	0.8454662186
Li	0.8454662186	0.8454662186	0.8454662186
Li	-0.8454662186	0.8454662186	-0.8454662186
Li	0.8454662186	-0.8454662186	-0.8454662186
C	-1.3067099668	-1.3067099668	-1.3067099668
C	1.3067099668	-1.3067099668	1.3067099668
C	1.3067099668	1.3067099668	-1.3067099668

C	-1.3067099668	1.3067099668	1.3067099668
C	-0.518130213	1.9559974097	2.4527462318
H	-0.0892593368	1.2165085267	3.1463272005
H	0.3081270819	2.6042117702	2.1101118108
H	-1.1575393347	2.6169111964	3.0729048098
C	-1.9559974097	2.4527462318	0.518130213
H	-1.2165085267	3.1463272005	0.0892593368
H	-2.6042117702	2.1101118108	-0.3081270819
H	-2.6169111964	3.0729048098	1.1575393347
C	-2.4527462318	0.518130213	1.9559974097
H	-3.1463272005	0.0892593368	1.2165085267
H	-2.1101118108	-0.3081270819	2.6042117702
H	-3.0729048098	1.1575393347	2.6169111964
C	1.9559974097	2.4527462318	-0.518130213
H	1.2165085267	3.1463272005	-0.0892593368
H	2.6042117702	2.1101118108	0.3081270819
H	2.6169111964	3.0729048098	-1.1575393347
C	2.4527462318	0.518130213	-1.9559974097
H	3.1463272005	0.0892593368	-1.2165085267
H	2.1101118108	-0.3081270819	-2.6042117702
H	3.0729048098	1.1575393347	-2.6169111964
C	0.518130213	1.9559974097	-2.4527462318
H	0.0892593368	1.2165085267	-3.1463272005
H	-0.3081270819	2.6042117702	-2.1101118108
H	1.1575393347	2.6169111964	-3.0729048098
C	-1.9559974097	-2.4527462318	-0.518130213
H	-1.2165085267	-3.1463272005	-0.0892593368
H	-2.6042117702	-2.1101118108	0.3081270819
H	-2.6169111964	-3.0729048098	-1.1575393347
C	-2.4527462318	-0.518130213	-1.9559974097
H	-3.1463272005	-0.0892593368	-1.2165085267
H	-2.1101118108	0.3081270819	-2.6042117702
H	-3.0729048098	-1.1575393347	-2.6169111964
C	-0.518130213	-1.9559974097	-2.4527462318
H	-0.0892593368	-1.2165085267	-3.1463272005
H	0.3081270819	-2.6042117702	-2.1101118108
H	-1.1575393347	-2.6169111964	-3.0729048098
C	2.4527462318	-0.518130213	1.9559974097
H	3.1463272005	-0.0892593368	1.2165085267
H	2.1101118108	0.3081270819	2.6042117702
H	3.0729048098	-1.1575393347	2.6169111964
C	0.518130213	-1.9559974097	2.4527462318

Tabelle 10.207 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
C	0.	0.0000001667	0.2900714728
Li	0.	0.0000001667	2.3219750934
C	0.	1.4349093662	-0.2662054776

H	0.8867374977	2.0065645969	0.0481825302
H	0.	1.4406814478	-1.3792770964
H	-0.8867374977	2.0065645969	0.0481825302
C	-1.2426678189	-0.7174544331	-0.2662054776
H	-1.294367022	-1.7712192479	0.0481825302
H	-2.1811045197	-0.2353448489	0.0481825302
H	-1.2476665882	-0.7203404739	-1.3792770964
C	1.2426678189	-0.7174544331	-0.2662054776
H	2.1811045197	-0.2353448489	0.0481825302
H	1.294367022	-1.7712192479	0.0481825302
H	1.2476665882	-0.7203404739	-1.3792770964

Tabelle 10.208 Standardorientierung von (<sup>t</sup>BuLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
Li	0.	0.	1.1020993371
C	-0.6620897517	1.6907539015	0.
Li	0.	0.	-1.1020993371
C	0.6620897517	-1.6907539015	0.
C	-0.0022355693	2.3355769922	-1.2383363828
H	1.0861554283	2.1493115827	-1.2877878685
H	-0.4433160714	1.9806312299	-2.1907701378
H	-0.1187876066	3.4388227424	-1.2663363812
C	-2.1496355033	2.0695394981	0.
H	-2.6758037209	1.6749965978	-0.8819885485
H	-2.6758037209	1.6749965978	0.8819885485
H	-2.3091714755	3.1695426964	0.
C	-0.0022355693	2.3355769922	1.2383363828
H	-0.4433160714	1.9806312299	2.1907701378
H	1.0861554283	2.1493115827	1.2877878685
H	-0.1187876066	3.4388227424	1.2663363812
C	0.0022355693	-2.3355769922	1.2383363828
H	0.4433160714	-1.9806312299	2.1907701378
H	-1.0861554283	-2.1493115827	1.2877878685
H	0.1187876066	-3.4388227424	1.2663363812
C	2.1496355033	-2.0695394981	0.
H	2.6758037209	-1.6749965978	-0.8819885485
H	2.6758037209	-1.6749965978	0.8819885485
H	2.3091714755	-3.1695426964	0.
C	0.0022355693	-2.3355769922	-1.2383363828
H	-1.0861554283	-2.1493115827	-1.2877878685
H	0.4433160714	-1.9806312299	-2.1907701378
H	0.1187876066	-3.4388227424	-1.2663363812

Tabelle 10.209 Standardorientierung von (<sup>t</sup>BuLi)<sub>4</sub> (T) [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
Li	-0.8491476741	-0.8491476741	0.8491476741
Li	0.8491476741	0.8491476741	0.8491476741
Li	-0.8491476741	0.8491476741	-0.8491476741
Li	0.8491476741	-0.8491476741	-0.8491476741

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C	-1.3137331152	-1.3137331152	-1.3137331152
C	1.3137331152	-1.3137331152	1.3137331152
C	1.3137331152	1.3137331152	-1.3137331152
C	-1.3137331152	1.3137331152	1.3137331152
C	-0.5237842657	1.9776450782	2.4654877683
H	-0.0919243301	1.240521734	3.1602854588
H	0.3008192047	2.6243821003	2.114263858
H	-1.1662847233	2.6392751095	3.0811654025
C	-1.9776450782	2.4654877683	0.5237842657
H	-1.240521734	3.1602854588	0.0919243301
H	-2.6243821003	2.114263858	-0.3008192047
H	-2.6392751095	3.0811654025	1.1662847233
C	-2.4654877683	0.5237842657	1.9776450782
H	-3.1602854588	0.0919243301	1.240521734
H	-2.114263858	-0.3008192047	2.6243821003
H	-3.0811654025	1.1662847233	2.6392751095
C	1.9776450782	2.4654877683	-0.5237842657
H	1.240521734	3.1602854588	-0.0919243301
H	2.6243821003	2.114263858	0.3008192047
H	2.6392751095	3.0811654025	-1.1662847233
C	2.4654877683	0.5237842657	-1.9776450782
H	3.1602854588	0.0919243301	-1.240521734
H	2.114263858	-0.3008192047	-2.6243821003
H	3.0811654025	1.1662847233	-2.6392751095
C	0.5237842657	1.9776450782	-2.4654877683
H	0.0919243301	1.240521734	-3.1602854588
H	-0.3008192047	2.6243821003	-2.114263858
H	1.1662847233	2.6392751095	-3.0811654025
C	-1.9776450782	-2.4654877683	-0.5237842657
H	-1.240521734	-3.1602854588	-0.0919243301
H	-2.6243821003	-2.114263858	0.3008192047
H	-2.6392751095	-3.0811654025	-1.1662847233
C	-2.4654877683	-0.5237842657	-1.9776450782
H	-3.1602854588	-0.0919243301	-1.240521734
H	-2.114263858	0.3008192047	-2.6243821003
H	-3.0811654025	-1.1662847233	-2.6392751095
C	-0.5237842657	-1.9776450782	-2.4654877683
H	-0.0919243301	-1.240521734	-3.1602854588
H	0.3008192047	-2.6243821003	-2.114263858
H	-1.1662847233	-2.6392751095	-3.0811654025
C	2.4654877683	-0.5237842657	1.9776450782
H	3.1602854588	-0.0919243301	1.240521734
H	2.114263858	0.3008192047	2.6243821003
H	3.0811654025	-1.1662847233	2.6392751095
C	0.5237842657	-1.9776450782	2.4654877683
H	0.0919243301	-1.240521734	3.1602854588
H	-0.3008192047	-2.6243821003	2.114263858
H	1.1662847233	-2.6392751095	3.0811654025
C	1.9776450782	-2.4654877683	0.5237842657
H	1.240521734	-3.1602854588	0.0919243301
H	2.6243821003	-2.114263858	-0.3008192047

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H	2.6392751095	-3.0811654025	1.1662847233
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Tabelle 10.210 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
C	0.	0.0000001667	0.2773769374
Li	0.	0.0000001667	2.3120911039
C	0.	1.4381822486	-0.2657751536
H	0.8861683528	2.0087259282	0.0517083157
H	0.	1.4545538643	-1.379232816
H	-0.8861683528	2.0087259282	0.0517083157
C	-1.2455022182	-0.7190908743	-0.2657751536
H	-1.2965233623	-1.7718070197	0.0517083157
H	-2.1826917152	-0.2369184085	0.0517083157
H	-1.2596804533	-0.7272766822	-1.379232816
C	1.2455022182	-0.7190908743	-0.2657751536
H	2.1826917152	-0.2369184085	0.0517083157
H	1.2965233623	-1.7718070197	0.0517083157
H	1.2596804533	-0.7272766822	-1.379232816

Tabelle 10.211 Standardorientierung von (<sup>t</sup>BuLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
Li	0.	0.	1.0942574801
C	-0.6621573773	1.6893006656	0.
Li	0.	0.	-1.0942574801
C	0.6621573773	-1.6893006656	0.
C	0.000672607	2.3212121812	-1.2413322215
H	1.0874600517	2.1264608428	-1.2949499671
H	-0.4456516298	1.9680704768	-2.1915738295
H	-0.1034491106	3.4260901	-1.276037398
C	-2.1504655928	2.0601298686	0.
H	-2.6767783468	1.6641886342	-0.8813861337
H	-2.6767783468	1.6641886342	0.8813861337
H	-2.3182525343	3.1595177127	0.
C	0.000672607	2.3212121812	1.2413322215
H	-0.4456516298	1.9680704768	2.1915738295
H	1.0874600517	2.1264608428	1.2949499671
H	-0.1034491106	3.4260901	1.276037398
C	-0.000672607	-2.3212121812	1.2413322215
H	0.4456516298	-1.9680704768	2.1915738295
H	-1.0874600517	-2.1264608428	1.2949499671
H	0.1034491106	-3.4260901	1.276037398
C	2.1504655928	-2.0601298686	0.
H	2.6767783468	-1.6641886342	-0.8813861337
H	2.6767783468	-1.6641886342	0.8813861337
H	2.3182525343	-3.1595177127	0.
C	-0.000672607	-2.3212121812	-1.2413322215
H	-1.0874600517	-2.1264608428	-1.2949499671

H	0.4456516298	-1.9680704768	-2.1915738295
H	0.1034491106	-3.4260901	-1.276037398

Tabelle 10.212 Standardorientierung von  $(t\text{BuLi})_4$  (T) [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
Li	-0.8491401612	-0.8491401612	0.8491401612
Li	0.8491401612	0.8491401612	0.8491401612
Li	-0.8491401612	0.8491401612	-0.8491401612
Li	0.8491401612	-0.8491401612	-0.8491401612
C	-1.3185830004	-1.3185830004	-1.3185830004
C	1.3185830004	-1.3185830004	1.3185830004
C	1.3185830004	1.3185830004	-1.3185830004
C	-1.3185830004	1.3185830004	1.3185830004
C	-0.523633648	1.98427358	2.4654222763
H	-0.0921764443	1.2514631777	3.1639311024
H	0.3010704216	2.6289453527	2.1134245105
H	-1.1624002891	2.6499504075	3.0807939795
C	-1.98427358	2.4654222763	0.523633648
H	-1.2514631777	3.1639311024	0.0921764443
H	-2.6289453527	2.1134245105	-0.3010704216
H	-2.6499504075	3.0807939795	1.1624002891
C	-2.4654222763	0.523633648	1.98427358
H	-3.1639311024	0.0921764443	1.2514631777
H	-2.1134245105	-0.3010704216	2.6289453527
H	-3.0807939795	1.1624002891	2.6499504075
C	1.98427358	2.4654222763	-0.523633648
H	1.2514631777	3.1639311024	-0.0921764443
H	2.6289453527	2.1134245105	0.3010704216
H	2.6499504075	3.0807939795	-1.1624002891
C	2.4654222763	0.523633648	-1.98427358
H	3.1639311024	0.0921764443	-1.2514631777
H	2.1134245105	-0.3010704216	-2.6289453527
H	3.0807939795	1.1624002891	-2.6499504075
C	0.523633648	1.98427358	-2.4654222763
H	0.0921764443	1.2514631777	-3.1639311024
H	-0.3010704216	2.6289453527	-2.1134245105
H	1.1624002891	2.6499504075	-3.0807939795
C	-1.98427358	-2.4654222763	-0.523633648
H	-1.2514631777	-3.1639311024	-0.0921764443
H	-2.6289453527	-2.1134245105	0.3010704216
H	-2.6499504075	-3.0807939795	-1.1624002891
C	-2.4654222763	-0.523633648	-1.98427358
H	-3.1639311024	-0.0921764443	-1.2514631777
H	-2.1134245105	0.3010704216	-2.6289453527
H	-3.0807939795	-1.1624002891	-2.6499504075
C	-0.523633648	-1.98427358	-2.4654222763
H	-0.0921764443	-1.2514631777	-3.1639311024
H	0.3010704216	-2.6289453527	-2.1134245105
H	-1.1624002891	-2.6499504075	-3.0807939795
C	2.4654222763	-0.523633648	1.98427358

H	3.1639311024	-0.0921764443	1.2514631777
H	2.1134245105	0.3010704216	2.6289453527
H	3.0807939795	-1.1624002891	2.6499504075
C	0.523633648	-1.98427358	2.4654222763
H	0.0921764443	-1.2514631777	3.1639311024
H	-0.3010704216	-2.6289453527	2.1134245105
H	1.1624002891	-2.6499504075	3.0807939795
C	1.98427358	-2.4654222763	0.523633648
H	1.2514631777	-3.1639311024	0.0921764443
H	2.6289453527	-2.1134245105	-0.3010704216
H	2.6499504075	-3.0807939795	1.1624002891

Tabelle 10.213 Standardorientierung von  ${}^t\text{BuLi}$  ( $\text{C}_{3v}$ ) [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
C	0.	0.0000001667	0.2792032666
Li	0.	0.0000001667	2.3036538752
C	0.	1.4369601209	-0.2656098662
H	0.8835369611	2.0061049138	0.0510475624
H	0.	1.4525297696	-1.375872964
H	-0.8835369611	2.0061049138	0.0510475624
C	-1.2444438246	-0.7184798104	-0.2656098662
H	-1.2955691931	-1.7682176604	0.0510475624
H	-2.1791061542	-0.2378867533	0.0510475624
H	-1.2579275358	-0.7262646348	-1.375872964
C	1.2444438246	-0.7184798104	-0.2656098662
H	2.1791061542	-0.2378867533	0.0510475624
H	1.2955691931	-1.7682176604	0.0510475624
H	1.2579275358	-0.7262646348	-1.375872964

Tabelle 10.214 Standardorientierung von  $({}^t\text{BuLi})_2$  ( $\text{C}_{2h}$ ) [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
Li	0.	0.	1.0970847401
C	-0.6794177055	1.6841817246	0.
Li	0.	0.	-1.0970847401
C	0.6794177055	-1.6841817246	0.
C	-0.0091743031	2.3027584386	-1.2420162088
H	1.0708760739	2.0867403082	-1.2994123358
H	-0.465835782	1.9570833105	-2.1863132428
H	-0.0898712999	3.4061115059	-1.2781978692
C	-2.1622762645	2.0705166701	0.
H	-2.6905244459	1.6804528561	-0.8788097233
H	-2.6905244459	1.6804528561	0.8788097233
H	-2.3181081779	3.1684426826	0.
C	-0.0091743031	2.3027584386	1.2420162088
H	-0.465835782	1.9570833105	2.1863132428
H	1.0708760739	2.0867403082	1.2994123358
H	-0.0898712999	3.4061115059	1.2781978692

C	0.0091743031	-2.3027584386	1.2420162088
H	0.465835782	-1.9570833105	2.1863132428
H	-1.0708760739	-2.0867403082	1.2994123358
H	0.0898712999	-3.4061115059	1.2781978692
C	2.1622762645	-2.0705166701	0.
H	2.6905244459	-1.6804528561	-0.8788097233
H	2.6905244459	-1.6804528561	0.8788097233
H	2.3181081779	-3.1684426826	0.
C	0.0091743031	-2.3027584386	-1.2420162088
H	-1.0708760739	-2.0867403082	-1.2994123358
H	0.465835782	-1.9570833105	-2.1863132428
H	0.0898712999	-3.4061115059	-1.2781978692

Tabelle 10.215 Standardorientierung von (tBuLi)<sub>4</sub> (T) [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
Li	-0.8518806779	-0.8518806779	0.8518806779
Li	0.8518806779	0.8518806779	0.8518806779
Li	-0.8518806779	0.8518806779	-0.8518806779
Li	0.8518806779	-0.8518806779	-0.8518806779
C	-1.322453556	-1.322453556	-1.322453556
C	1.322453556	-1.322453556	1.322453556
C	1.322453556	1.322453556	-1.322453556
C	-1.322453556	1.322453556	1.322453556
C	-0.5243118327	1.995181024	2.4607077667
H	-0.0870449011	1.2690026726	3.1579171477
H	0.2933720155	2.6393734222	2.1008807669
H	-1.1607351695	2.6591161062	3.0747251244
C	-1.995181024	2.4607077667	0.5243118327
H	-1.2690026726	3.1579171477	0.0870449011
H	-2.6393734222	2.1008807669	-0.2933720155
H	-2.6591161062	3.0747251244	1.1607351695
C	-2.4607077667	0.5243118327	1.995181024
H	-3.1579171477	0.0870449011	1.2690026726
H	-2.1008807669	-0.2933720155	2.6393734222
H	-3.0747251244	1.1607351695	2.6591161062
C	1.995181024	2.4607077667	-0.5243118327
H	1.2690026726	3.1579171477	-0.0870449011
H	2.6393734222	2.1008807669	0.2933720155
H	2.6591161062	3.0747251244	-1.1607351695
C	2.4607077667	0.5243118327	-1.995181024
H	3.1579171477	0.0870449011	-1.2690026726
H	2.1008807669	-0.2933720155	-2.6393734222
H	3.0747251244	1.1607351695	-2.6591161062
C	0.5243118327	1.995181024	-2.4607077667
H	0.0870449011	1.2690026726	-3.1579171477
H	-0.2933720155	2.6393734222	-2.1008807669
H	1.1607351695	2.6591161062	-3.0747251244
C	-1.995181024	-2.4607077667	-0.5243118327
H	-1.2690026726	-3.1579171477	-0.0870449011
H	-2.6393734222	-2.1008807669	0.2933720155

H	-2.6591161062	-3.0747251244	-1.1607351695
C	-2.4607077667	-0.5243118327	-1.995181024
H	-3.1579171477	-0.0870449011	-1.2690026726
H	-2.1008807669	0.2933720155	-2.6393734222
H	-3.0747251244	-1.1607351695	-2.6591161062
C	-0.5243118327	-1.995181024	-2.4607077667
H	-0.0870449011	-1.2690026726	-3.1579171477
H	0.2933720155	-2.6393734222	-2.1008807669
H	-1.1607351695	-2.6591161062	-3.0747251244
C	2.4607077667	-0.5243118327	1.995181024
H	3.1579171477	-0.0870449011	1.2690026726
H	2.1008807669	0.2933720155	2.6393734222
H	3.0747251244	-1.1607351695	2.6591161062
C	0.5243118327	-1.995181024	2.4607077667
H	0.0870449011	-1.2690026726	3.1579171477
H	-0.2933720155	-2.6393734222	2.1008807669
H	1.1607351695	-2.6591161062	3.0747251244
C	1.995181024	-2.4607077667	0.5243118327
H	1.2690026726	-3.1579171477	0.0870449011
H	2.6393734222	-2.1008807669	-0.2933720155
H	2.6591161062	-3.0747251244	1.1607351695

Tabelle 10.216 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	0.	0.0000001667	0.2939788119
Li	0.	0.0000001667	2.3253135611
C	0.	1.425064728	-0.2645634735
H	0.8844893193	1.9949791839	0.043198127
H	0.	1.4136681004	-1.3733655651
H	-0.8844893193	1.9949791839	0.043198127
C	-1.2341421121	-0.712532114	-0.2645634735
H	-1.2854578493	-1.7634795618	0.043198127
H	-2.1699471685	-0.2314991221	0.043198127
H	-1.2242723431	-0.7068338002	-1.3733655651
C	1.2341421121	-0.712532114	-0.2645634735
H	2.1699471685	-0.2314991221	0.043198127
H	1.2854578493	-1.7634795618	0.043198127
H	1.2242723431	-0.7068338002	-1.3733655651

Tabelle 10.217 Standardorientierung von (<sup>t</sup>BuLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	0.	0.	1.1046286991
C	-0.7256571448	1.6455287592	0.
Li	0.	0.	-1.1046286991
C	0.7256571448	-1.6455287592	0.
C	-0.0371051947	2.2545580032	-1.2308128872
H	1.0346850655	2.0002036515	-1.2912786567

H	-0.5107837648	1.9425129618	-2.1762866903
H	-0.0783370128	3.358653044	-1.2373951347
C	-2.183857833	2.0928095983	0.
H	-2.7238997195	1.7257236426	-0.879365517
H	-2.7238997195	1.7257236426	0.879365517
H	-2.281266578	3.1958675393	0.
C	-0.0371051947	2.2545580032	1.2308128872
H	-0.5107837648	1.9425129618	2.1762866903
H	1.0346850655	2.0002036515	1.2912786567
H	-0.0783370128	3.358653044	1.2373951347
C	0.0371051947	-2.2545580032	1.2308128872
H	0.5107837648	-1.9425129618	2.1762866903
H	-1.0346850655	-2.0002036515	1.2912786567
H	0.0783370128	-3.358653044	1.2373951347
C	2.183857833	-2.0928095983	0.
H	2.7238997195	-1.7257236426	-0.879365517
H	2.7238997195	-1.7257236426	0.879365517
H	2.281266578	-3.1958675393	0.
C	0.0371051947	-2.2545580032	-1.2308128872
H	-1.0346850655	-2.0002036515	-1.2912786567
H	0.5107837648	-1.9425129618	-2.1762866903
H	0.0783370128	-3.358653044	-1.2373951347

Tabelle 10.218 Standardorientierung von  $(t\text{BuLi})_4$  (T) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	-0.8456168735	-0.8456168735	0.8456168735
Li	0.8456168735	0.8456168735	0.8456168735
Li	-0.8456168735	0.8456168735	-0.8456168735
Li	0.8456168735	-0.8456168735	-0.8456168735
C	-1.2949705375	-1.2949705375	-1.2949705375
C	1.2949705375	-1.2949705375	1.2949705375
C	1.2949705375	1.2949705375	-1.2949705375
C	-1.2949705375	1.2949705375	1.2949705375
C	-0.5134811272	1.9421981947	2.4515424848
H	-0.0974938691	1.1995304975	3.1434904153
H	0.3163713614	2.5833190549	2.1152140577
H	-1.1599799783	2.6015328789	3.0580166251
C	-1.9421981947	2.4515424848	0.5134811272
H	-1.1995304975	3.1434904153	0.0974938691
H	-2.5833190549	2.1152140577	-0.3163713614
H	-2.6015328789	3.0580166251	1.1599799783
C	-2.4515424848	0.5134811272	1.9421981947
H	-3.1434904153	0.0974938691	1.1995304975
H	-2.1152140577	-0.3163713614	2.5833190549
H	-3.0580166251	1.1599799783	2.6015328789
C	1.9421981947	2.4515424848	-0.5134811272
H	1.1995304975	3.1434904153	-0.0974938691
H	2.5833190549	2.1152140577	0.3163713614
H	2.6015328789	3.0580166251	-1.1599799783
C	2.4515424848	0.5134811272	-1.9421981947

H	3.1434904153	0.0974938691	-1.1995304975
H	2.1152140577	-0.3163713614	-2.5833190549
H	3.0580166251	1.1599799783	-2.6015328789
C	0.5134811272	1.9421981947	-2.4515424848
H	0.0974938691	1.1995304975	-3.1434904153
H	-0.3163713614	2.5833190549	-2.1152140577
H	1.1599799783	2.6015328789	-3.0580166251
C	-1.9421981947	-2.4515424848	-0.5134811272
H	-1.1995304975	-3.1434904153	-0.0974938691
H	-2.5833190549	-2.1152140577	0.3163713614
H	-2.6015328789	-3.0580166251	-1.1599799783
C	-2.4515424848	-0.5134811272	-1.9421981947
H	-3.1434904153	-0.0974938691	-1.1995304975
H	-2.1152140577	0.3163713614	-2.5833190549
H	-3.0580166251	-1.1599799783	-2.6015328789
C	-0.5134811272	-1.9421981947	-2.4515424848
H	-0.0974938691	-1.1995304975	-3.1434904153
H	0.3163713614	-2.5833190549	-2.1152140577
H	-1.1599799783	-2.6015328789	-3.0580166251
C	2.4515424848	-0.5134811272	1.9421981947
H	3.1434904153	-0.0974938691	1.1995304975
H	2.1152140577	0.3163713614	2.5833190549
H	3.0580166251	-1.1599799783	2.6015328789
C	0.5134811272	-1.9421981947	2.4515424848
H	0.0974938691	-1.1995304975	3.1434904153
H	-0.3163713614	-2.5833190549	2.1152140577
H	1.1599799783	-2.6015328789	3.0580166251
C	1.9421981947	-2.4515424848	0.5134811272
H	1.1995304975	-3.1434904153	0.0974938691
H	2.5833190549	-2.1152140577	-0.3163713614
H	2.6015328789	-3.0580166251	1.1599799783

Tabelle 10.219 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
C	0.	0.0000001667	0.2931075367
Li	0.	0.0000001667	2.3248480446
C	0.	1.4255430217	-0.2646701021
H	0.884460439	1.9945402218	0.0433730864
H	0.	1.4134123057	-1.3731632566
H	-0.884460439	1.9945402218	0.0433730864
C	-1.2345563267	-0.7127712608	-0.2646701021
H	-1.2850921371	-1.7632350697	0.0433730864
H	-2.1695525761	-0.231304652	0.0433730864
H	-1.2240508184	-0.7067059029	-1.3731632566
C	1.2345563267	-0.7127712608	-0.2646701021
H	2.1695525761	-0.231304652	0.0433730864
H	1.2850921371	-1.7632350697	0.0433730864
H	1.2240508184	-0.7067059029	-1.3731632566

Tabelle 10.220 Standardorientierung von (<sup>t</sup>BuLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
Li	0.	0.	1.1050441932
C	-0.7277518221	1.6445870933	0.
Li	0.	0.	-1.1050441932
C	0.7277518221	-1.6445870933	0.
C	-0.0376128339	2.2511225705	-1.2314899465
H	1.0330284797	1.992933492	-1.2919256766
H	-0.5140175306	1.9411312087	-2.1758283541
H	-0.0746844508	3.3548414618	-1.2375767169
C	-2.1857654192	2.0928211895	0.
H	-2.72516293	1.7255928191	-0.8792015561
H	-2.72516293	1.7255928191	0.8792015561
H	-2.2820335337	3.1957007064	0.
C	-0.0376128339	2.2511225705	1.2314899465
H	-0.5140175306	1.9411312087	2.1758283541
H	1.0330284797	1.992933492	1.2919256766
H	-0.0746844508	3.3548414618	1.2375767169
C	0.0376128339	-2.2511225705	1.2314899465
H	0.5140175306	-1.9411312087	2.1758283541
H	-1.0330284797	-1.992933492	1.2919256766
H	0.0746844508	-3.3548414618	1.2375767169
C	2.1857654192	-2.0928211895	0.
H	2.72516293	-1.7255928191	-0.8792015561
H	2.72516293	-1.7255928191	0.8792015561
H	2.2820335337	-3.1957007064	0.
C	0.0376128339	-2.2511225705	-1.2314899465
H	-1.0330284797	-1.992933492	-1.2919256766
H	0.5140175306	-1.9411312087	-2.1758283541
H	0.0746844508	-3.3548414618	-1.2375767169

Tabelle 10.221 Standardorientierung von (<sup>t</sup>BuLi)<sub>4</sub> (T) [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
Li	-0.8454125195	-0.8454125195	0.8454125195
Li	0.8454125195	0.8454125195	0.8454125195
Li	-0.8454125195	0.8454125195	-0.8454125195
Li	0.8454125195	-0.8454125195	-0.8454125195
C	-1.2949768712	-1.2949768712	-1.2949768712
C	1.2949768712	-1.2949768712	1.2949768712
C	1.2949768712	1.2949768712	-1.2949768712
C	-1.2949768712	1.2949768712	1.2949768712
C	-0.5120891805	1.9411550873	2.4515376775
H	-0.0967245249	1.1972153409	3.1420475262
H	0.3175314648	2.5817282379	2.1145748377
H	-1.1578414725	2.6003811717	3.0580794687
C	-1.9411550873	2.4515376775	0.5120891805
H	-1.1972153409	3.1420475262	0.0967245249
H	-2.5817282379	2.1145748377	-0.3175314648
H	-2.6003811717	3.0580794687	1.1578414725
C	-2.4515376775	0.5120891805	1.9411550873

H	-3.1420475262	0.0967245249	1.1972153409
H	-2.1145748377	-0.3175314648	2.5817282379
H	-3.0580794687	1.1578414725	2.6003811717
C	1.9411550873	2.4515376775	-0.5120891805
H	1.1972153409	3.1420475262	-0.0967245249
H	2.5817282379	2.1145748377	0.3175314648
H	2.6003811717	3.0580794687	-1.1578414725
C	2.4515376775	0.5120891805	-1.9411550873
H	3.1420475262	0.0967245249	-1.1972153409
H	2.1145748377	-0.3175314648	-2.5817282379
H	3.0580794687	1.1578414725	-2.6003811717
C	0.5120891805	1.9411550873	-2.4515376775
H	0.0967245249	1.1972153409	-3.1420475262
H	-0.3175314648	2.5817282379	-2.1145748377
H	1.1578414725	2.6003811717	-3.0580794687
C	-1.9411550873	-2.4515376775	-0.5120891805
H	-1.1972153409	-3.1420475262	-0.0967245249
H	-2.5817282379	-2.1145748377	0.3175314648
H	-2.6003811717	-3.0580794687	-1.1578414725
C	-2.4515376775	-0.5120891805	-1.9411550873
H	-3.1420475262	-0.0967245249	-1.1972153409
H	-2.1145748377	0.3175314648	-2.5817282379
H	-3.0580794687	-1.1578414725	-2.6003811717
C	-0.5120891805	-1.9411550873	-2.4515376775
H	-0.0967245249	-1.1972153409	-3.1420475262
H	0.3175314648	-2.5817282379	-2.1145748377
H	-1.1578414725	-2.6003811717	-3.0580794687
C	2.4515376775	-0.5120891805	1.9411550873
H	3.1420475262	-0.0967245249	1.1972153409
H	2.1145748377	0.3175314648	2.5817282379
H	3.0580794687	-1.1578414725	2.6003811717
C	0.5120891805	-1.9411550873	2.4515376775
H	0.0967245249	-1.1972153409	3.1420475262
H	-0.3175314648	-2.5817282379	2.1145748377
H	1.1578414725	-2.6003811717	3.0580794687
C	1.9411550873	-2.4515376775	0.5120891805
H	1.1972153409	-3.1420475262	0.0967245249
H	2.5817282379	-2.1145748377	-0.3175314648
H	2.6003811717	-3.0580794687	1.1578414725

Tabelle 10.222 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
C	0.	0.0000001667	0.2977621529
Li	0.	0.0000001667	2.3175932607
C	0.	1.4235390721	-0.2640336995
H	0.8831029443	1.9925663323	0.0420731577
H	0.	1.4072718608	-1.3703330787
H	-0.8831029443	1.9925663323	0.0420731577

C	-1.2328208554	-0.711769286	-0.2640336995
H	-1.284061446	-1.7610725001	0.0420731577
H	-2.1671643903	-0.2314933322	0.0420731577
H	-1.2187330371	-0.7036356804	-1.3703330787
C	1.2328208554	-0.711769286	-0.2640336995
H	2.1671643903	-0.2314933322	0.0420731577
H	1.284061446	-1.7610725001	0.0420731577
H	1.2187330371	-0.7036356804	-1.3703330787

Tabelle 10.223 Standardorientierung von  $({}^t\text{BuLi})_2$  ( $C_{2h}$ ) [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
Li	0.	0.	1.1103837601
C	-0.7406204028	1.6373021427	0.
Li	0.	0.	-1.1103837601
C	0.7406204028	-1.6373021427	0.
C	-0.0469387775	2.2381344054	-1.2304366237
H	1.0185409783	1.9653178792	-1.2963426852
H	-0.5319475144	1.938636904	-2.1716646785
H	-0.0681830285	3.3402534227	-1.2301459511
C	-2.192553288	2.1015327033	0.
H	-2.7349519144	1.7412879584	-0.8780758704
H	-2.7349519144	1.7412879584	0.8780758704
H	-2.273362162	3.2036270716	0.
C	-0.0469387775	2.2381344054	1.2304366237
H	-0.5319475144	1.938636904	2.1716646785
H	1.0185409783	1.9653178792	1.2963426852
H	-0.0681830285	3.3402534227	1.2301459511
C	0.0469387775	-2.2381344054	1.2304366237
H	0.5319475144	-1.938636904	2.1716646785
H	-1.0185409783	-1.9653178792	1.2963426852
H	0.0681830285	-3.3402534227	1.2301459511
C	2.192553288	-2.1015327033	0.
H	2.7349519144	-1.7412879584	-0.8780758704
H	2.7349519144	-1.7412879584	0.8780758704
H	2.273362162	-3.2036270716	0.
C	0.0469387775	-2.2381344054	-1.2304366237
H	-1.0185409783	-1.9653178792	-1.2963426852
H	0.5319475144	-1.938636904	-2.1716646785
H	0.0681830285	-3.3402534227	-1.2301459511

Tabelle 10.224 Standardorientierung von  $({}^t\text{BuLi})_4$  (T) [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
Li	-0.8491110895	-0.8491110895	0.8491110895
Li	0.8491110895	0.8491110895	0.8491110895
Li	-0.8491110895	0.8491110895	-0.8491110895
Li	0.8491110895	-0.8491110895	-0.8491110895
C	-1.2946320513	-1.2946320513	-1.2946320513
C	1.2946320513	-1.2946320513	1.2946320513
C	1.2946320513	1.2946320513	-1.2946320513

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C	-1.2946320513	1.2946320513	1.2946320513
C	-0.5131536489	1.9409717359	2.4498110298
H	-0.0959908905	1.198524626	3.1384339506
H	0.3125130296	2.5834983195	2.1120244408
H	-1.1611584391	2.5960963857	3.0551530018
C	-1.9409717359	2.4498110298	0.5131536489
H	-1.198524626	3.1384339506	0.0959908905
H	-2.5834983195	2.1120244408	-0.3125130296
H	-2.5960963857	3.0551530018	1.1611584391
C	-2.4498110298	0.5131536489	1.9409717359
H	-3.1384339506	0.0959908905	1.198524626
H	-2.1120244408	-0.3125130296	2.5834983195
H	-3.0551530018	1.1611584391	2.5960963857
C	1.9409717359	2.4498110298	-0.5131536489
H	1.198524626	3.1384339506	-0.0959908905
H	2.5834983195	2.1120244408	0.3125130296
H	2.5960963857	3.0551530018	-1.1611584391
C	2.4498110298	0.5131536489	-1.9409717359
H	3.1384339506	0.0959908905	-1.198524626
H	2.1120244408	-0.3125130296	-2.5834983195
H	3.0551530018	1.1611584391	-2.5960963857
C	0.5131536489	1.9409717359	-2.4498110298
H	0.0959908905	1.198524626	-3.1384339506
H	-0.3125130296	2.5834983195	-2.1120244408
H	1.1611584391	2.5960963857	-3.0551530018
C	-1.9409717359	-2.4498110298	-0.5131536489
H	-1.198524626	-3.1384339506	-0.0959908905
H	-2.5834983195	-2.1120244408	0.3125130296
H	-2.5960963857	-3.0551530018	-1.1611584391
C	-2.4498110298	-0.5131536489	-1.9409717359
H	-3.1384339506	-0.0959908905	-1.198524626
H	-2.1120244408	0.3125130296	-2.5834983195
H	-3.0551530018	-1.1611584391	-2.5960963857
C	-0.5131536489	-1.9409717359	-2.4498110298
H	-0.0959908905	-1.198524626	-3.1384339506
H	0.3125130296	-2.5834983195	-2.1120244408
H	-1.1611584391	-2.5960963857	-3.0551530018
C	2.4498110298	-0.5131536489	1.9409717359
H	3.1384339506	-0.0959908905	1.198524626
H	2.1120244408	0.3125130296	2.5834983195
H	3.0551530018	-1.1611584391	2.5960963857
C	0.5131536489	-1.9409717359	2.4498110298
H	0.0959908905	-1.198524626	3.1384339506
H	-0.3125130296	-2.5834983195	2.1120244408
H	1.1611584391	-2.5960963857	3.0551530018
C	1.9409717359	-2.4498110298	0.5131536489
H	1.198524626	-3.1384339506	0.0959908905
H	2.5834983195	-2.1120244408	-0.3125130296
H	2.5960963857	-3.0551530018	1.1611584391

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Tabelle 10.225 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
C	0.	0.0000001667	0.2972652667
Li	0.	0.0000001667	2.3136523851
C	0.	1.4201721289	-0.2636636882
H	0.8808996081	1.9867470379	0.0407717947
H	0.	1.4001996703	-1.3666211114
H	-0.8808996081	1.9867470379	0.0407717947
C	-1.229904997	-0.7100858144	-0.2636636882
H	-1.2801234573	-1.7562547077	0.0407717947
H	-2.1610230654	-0.2304918301	0.0407717947
H	-1.2126083405	-0.7000995851	-1.3666211114
C	1.229904997	-0.7100858144	-0.2636636882
H	2.1610230654	-0.2304918301	0.0407717947
H	1.2801234573	-1.7562547077	0.0407717947
H	1.2126083405	-0.7000995851	-1.3666211114

Tabelle 10.226 Standardorientierung von (<sup>t</sup>BuLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
Li	0.	0.	1.1111798833
C	-0.7479118239	1.6262950379	0.
Li	0.	0.	-1.1111798833
C	0.7479118239	-1.6262950379	0.
C	-0.0517802942	2.2214445879	-1.227849701
H	1.0082795241	1.9404559449	-1.2942708296
H	-0.5396573932	1.9279221239	-2.1652170633
H	-0.0636920404	3.3202112864	-1.2235496223
C	-2.1932063583	2.1003344815	0.
H	-2.736020931	1.7464564966	-0.8760718681
H	-2.736020931	1.7464564966	0.8760718681
H	-2.2624822597	3.1998197503	0.
C	-0.0517802942	2.2214445879	1.227849701
H	-0.5396573932	1.9279221239	2.1652170633
H	1.0082795241	1.9404559449	1.2942708296
H	-0.0636920404	3.3202112864	1.2235496223
C	0.0517802942	-2.2214445879	1.227849701
H	0.5396573932	-1.9279221239	2.1652170633
H	-1.0082795241	-1.9404559449	1.2942708296
H	0.0636920404	-3.3202112864	1.2235496223
C	2.1932063583	-2.1003344815	0.
H	2.736020931	-1.7464564966	-0.8760718681
H	2.736020931	-1.7464564966	0.8760718681
H	2.2624822597	-3.1998197503	0.
C	0.0517802942	-2.2214445879	-1.227849701
H	-1.0082795241	-1.9404559449	-1.2942708296
H	0.5396573932	-1.9279221239	-2.1652170633
H	0.0636920404	-3.3202112864	-1.2235496223

Tabelle 10.227 Standardorientierung von (tBuLi)<sub>4</sub> (T) [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
Li	-0.848929777	-0.848929777	0.848929777
Li	0.848929777	0.848929777	0.848929777
Li	-0.848929777	0.848929777	-0.848929777
Li	0.848929777	-0.848929777	-0.848929777
C	-1.2917369204	-1.2917369204	-1.2917369204
C	1.2917369204	-1.2917369204	1.2917369204
C	1.2917369204	1.2917369204	-1.2917369204
C	-1.2917369204	1.2917369204	1.2917369204
C	-0.5112083161	1.9351202306	2.4447850257
H	-0.0947753842	1.1933394881	3.1291353692
H	0.3109020258	2.5766882818	2.1078153863
H	-1.158848536	2.5864476663	3.0486791233
C	-1.9351202306	2.4447850257	0.5112083161
H	-1.1933394881	3.1291353692	0.0947753842
H	-2.5766882818	2.1078153863	-0.3109020258
H	-2.5864476663	3.0486791233	1.158848536
C	-2.4447850257	0.5112083161	1.9351202306
H	-3.1291353692	0.0947753842	1.1933394881
H	-2.1078153863	-0.3109020258	2.5766882818
H	-3.0486791233	1.158848536	2.5864476663
C	1.9351202306	2.4447850257	-0.5112083161
H	1.1933394881	3.1291353692	-0.0947753842
H	2.5766882818	2.1078153863	0.3109020258
H	2.5864476663	3.0486791233	-1.158848536
C	2.4447850257	0.5112083161	-1.9351202306
H	3.1291353692	0.0947753842	-1.1933394881
H	2.1078153863	-0.3109020258	-2.5766882818
H	3.0486791233	1.158848536	-2.5864476663
C	0.5112083161	1.9351202306	-2.4447850257
H	0.0947753842	1.1933394881	-3.1291353692
H	-0.3109020258	2.5766882818	-2.1078153863
H	1.158848536	2.5864476663	-3.0486791233
C	-1.9351202306	-2.4447850257	-0.5112083161
H	-1.1933394881	-3.1291353692	-0.0947753842
H	-2.5766882818	-2.1078153863	0.3109020258
H	-2.5864476663	-3.0486791233	-1.158848536
C	-2.4447850257	-0.5112083161	-1.9351202306
H	-3.1291353692	-0.0947753842	-1.1933394881
H	-2.1078153863	0.3109020258	-2.5766882818
H	-3.0486791233	-1.158848536	-2.5864476663
C	-0.5112083161	-1.9351202306	-2.4447850257
H	-0.0947753842	-1.1933394881	-3.1291353692
H	0.3109020258	-2.5766882818	-2.1078153863
H	-1.158848536	-2.5864476663	-3.0486791233
C	2.4447850257	-0.5112083161	1.9351202306
H	3.1291353692	-0.0947753842	1.1933394881
H	2.1078153863	0.3109020258	2.5766882818
H	3.0486791233	-1.158848536	2.5864476663
C	0.5112083161	-1.9351202306	2.4447850257

H	0.0947753842	-1.1933394881	3.1291353692
H	-0.3109020258	-2.5766882818	2.1078153863
H	1.158848536	-2.5864476663	3.0486791233
C	1.9351202306	-2.4447850257	0.5112083161
H	1.1933394881	-3.1291353692	0.0947753842
H	2.5766882818	-2.1078153863	-0.3109020258
H	2.5864476663	-3.0486791233	1.158848536

Tabelle 10.228 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; M06L/6-31+G(d)].

	x	y	z
C	0.	0.0000001667	0.3070765823
Li	0.	0.0000001667	2.3208090631
C	0.	1.4173290116	-0.2597066931
H	0.8865625581	1.9992643468	0.0403642278
H	0.	1.4124893367	-1.3754189685
H	-0.8865625581	1.9992643468	0.0403642278
C	-1.2274427852	-0.7086642558	-0.2597066931
H	-1.2881322898	-1.7674176208	0.0403642278
H	-2.1746948479	-0.231846226	0.0403642278
H	-1.2232515038	-0.7062444183	-1.3754189685
C	1.2274427852	-0.7086642558	-0.2597066931
H	2.1746948479	-0.231846226	0.0403642278
H	1.2881322898	-1.7674176208	0.0403642278
H	1.2232515038	-0.7062444183	-1.3754189685

Tabelle 10.229 Standardorientierung von (<sup>t</sup>BuLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; M06L/6-31+G(d)].

	x	y	z
Li	0.	0.	1.1194833655
C	-0.7026515797	1.6554178573	0.
Li	0.	0.	-1.1194833655
C	0.7026515797	-1.6554178573	0.
C	-0.028396474	2.2740097248	-1.2264344083
H	1.0541497941	2.0479915076	-1.2867964304
H	-0.4871358065	1.9454846857	-2.1801486534
H	-0.0926259857	3.382852935	-1.2568137242
C	-2.162892258	2.0806844942	0.
H	-2.7074568707	1.7086285871	-0.8812690618
H	-2.7074568707	1.7086285871	0.8812690618
H	-2.290236494	3.1869517792	0.
C	-0.028396474	2.2740097248	1.2264344083
H	-0.4871358065	1.9454846857	2.1801486534
H	1.0541497941	2.0479915076	1.2867964304
H	-0.0926259857	3.382852935	1.2568137242
C	0.028396474	-2.2740097248	1.2264344083
H	0.4871358065	-1.9454846857	2.1801486534
H	-1.0541497941	-2.0479915076	1.2867964304
H	0.0926259857	-3.382852935	1.2568137242

C	2.162892258	-2.0806844942	0.
H	2.7074568707	-1.7086285871	-0.8812690618
H	2.7074568707	-1.7086285871	0.8812690618
H	2.290236494	-3.1869517792	0.
C	0.028396474	-2.2740097248	-1.2264344083
H	-1.0541497941	-2.0479915076	-1.2867964304
H	0.4871358065	-1.9454846857	-2.1801486534
H	0.0926259857	-3.382852935	-1.2568137242

Tabelle 10.230 Standardorientierung von  $(t\text{BuLi})_4$  (T) [globales Minimum; M06L/6-31+G(d)].

	x	y	z
Li	-0.8532052294	-0.8532052294	0.8532052294
Li	0.8532052294	0.8532052294	0.8532052294
Li	-0.8532052294	0.8532052294	-0.8532052294
Li	0.8532052294	-0.8532052294	-0.8532052294
C	-1.2934693906	-1.2934693906	-1.2934693906
C	1.2934693906	-1.2934693906	1.2934693906
C	1.2934693906	1.2934693906	-1.2934693906
C	-1.2934693906	1.2934693906	1.2934693906
C	-0.5136517297	1.9109336089	2.4578950157
H	-0.0871761296	1.1510152657	3.1350930973
H	0.3201394906	2.563197256	2.1347395826
H	-1.146043219	2.5623855024	3.0976891014
C	-1.9109336089	2.4578950157	0.5136517297
H	-1.1510152657	3.1350930973	0.0871761296
H	-2.563197256	2.1347395826	-0.3201394906
H	-2.5623855024	3.0976891014	1.146043219
C	-2.4578950157	0.5136517297	1.9109336089
H	-3.1350930973	0.0871761296	1.1510152657
H	-2.1347395826	-0.3201394906	2.563197256
H	-3.0976891014	1.146043219	2.5623855024
C	1.9109336089	2.4578950157	-0.5136517297
H	1.1510152657	3.1350930973	-0.0871761296
H	2.563197256	2.1347395826	0.3201394906
H	2.5623855024	3.0976891014	-1.146043219
C	2.4578950157	0.5136517297	-1.9109336089
H	3.1350930973	0.0871761296	-1.1510152657
H	2.1347395826	-0.3201394906	-2.563197256
H	3.0976891014	1.146043219	-2.5623855024
C	0.5136517297	1.9109336089	-2.4578950157
H	0.0871761296	1.1510152657	-3.1350930973
H	-0.3201394906	2.563197256	-2.1347395826
H	1.146043219	2.5623855024	-3.0976891014
C	-1.9109336089	-2.4578950157	-0.5136517297
H	-1.1510152657	-3.1350930973	-0.0871761296
H	-2.563197256	-2.1347395826	0.3201394906
H	-2.5623855024	-3.0976891014	-1.146043219
C	-2.4578950157	-0.5136517297	-1.9109336089
H	-3.1350930973	-0.0871761296	-1.1510152657
H	-2.1347395826	0.3201394906	-2.563197256

H	-3.0976891014	-1.146043219	-2.5623855024
C	-0.5136517297	-1.9109336089	-2.4578950157
H	-0.0871761296	-1.1510152657	-3.1350930973
H	0.3201394906	-2.563197256	-2.1347395826
H	-1.146043219	-2.5623855024	-3.0976891014
C	2.4578950157	-0.5136517297	1.9109336089
H	3.1350930973	-0.0871761296	1.1510152657
H	2.1347395826	0.3201394906	2.563197256
H	3.0976891014	-1.146043219	2.5623855024
C	0.5136517297	-1.9109336089	2.4578950157
H	0.0871761296	-1.1510152657	3.1350930973
H	-0.3201394906	-2.563197256	2.1347395826
H	1.146043219	-2.5623855024	3.0976891014
C	1.9109336089	-2.4578950157	0.5136517297
H	1.1510152657	-3.1350930973	0.0871761296
H	2.563197256	-2.1347395826	-0.3201394906
H	2.5623855024	-3.0976891014	1.146043219

Tabelle 10.231 Standardorientierung von  ${}^t\text{BuLi}$  ( $C_{3v}$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	0.	0.0000001667	0.292710273
Li	0.	0.0000001667	2.3139252124
C	0.	1.4209183847	-0.2613631533
H	0.8883777957	1.9983194019	0.0459302275
H	0.	1.4199146033	-1.3778111196
H	-0.8883777957	1.9983194019	0.0459302275
C	-1.2305512735	-0.7104589424	-0.2613631533
H	-1.2864063247	-1.7685171901	0.0459302275
H	-2.1747841204	-0.2298017117	0.0459302275
H	-1.2296819733	-0.7099570516	-1.3778111196
C	1.2305512735	-0.7104589424	-0.2613631533
H	2.1747841204	-0.2298017117	0.0459302275
H	1.2864063247	-1.7685171901	0.0459302275
H	1.2296819733	-0.7099570516	-1.3778111196

Tabelle 10.232 Standardorientierung von  $({}^t\text{BuLi})_2$  ( $C_{2h}$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	0.	0.	1.1149894092
C	-0.7103626081	1.6596753221	0.
Li	0.	0.	-1.1149894092
C	0.7103626081	-1.6596753221	0.
C	-0.0328260359	2.2752094248	-1.2259158914
H	1.0491938955	2.0380221545	-1.2892269021
H	-0.5010368861	1.9575124472	-2.1800051267
H	-0.0881563137	3.3860882117	-1.2402510162
C	-2.1693834477	2.0865897892	0.
H	-2.7137869895	1.7144239667	-0.8828726607

H	-2.7137869895	1.7144239667	0.8828726607
H	-2.28666495	3.1952871004	0.
C	-0.0328260359	2.2752094248	1.2259158914
H	-0.5010368861	1.9575124472	2.1800051267
H	1.0491938955	2.0380221545	1.2892269021
H	-0.0881563137	3.3860882117	1.2402510162
C	0.0328260359	-2.2752094248	1.2259158914
H	0.5010368861	-1.9575124472	2.1800051267
H	-1.0491938955	-2.0380221545	1.2892269021
H	0.0881563137	-3.3860882117	1.2402510162
C	2.1693834477	-2.0865897892	0.
H	2.7137869895	-1.7144239667	-0.8828726607
H	2.7137869895	-1.7144239667	0.8828726607
H	2.28666495	-3.1952871004	0.
C	0.0328260359	-2.2752094248	-1.2259158914
H	-1.0491938955	-2.0380221545	-1.2892269021
H	0.5010368861	-1.9575124472	-2.1800051267
H	0.0881563137	-3.3860882117	-1.2402510162

Tabelle 10.233 Standardorientierung von (<sup>6</sup>BuLi)<sub>4</sub> (T) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	-0.8563802441	-0.8563802441	0.8563802441
Li	0.8563802441	0.8563802441	0.8563802441
Li	-0.8563802441	0.8563802441	-0.8563802441
Li	0.8563802441	-0.8563802441	-0.8563802441
C	-1.3094550288	-1.3094550288	-1.3094550288
C	1.3094550288	-1.3094550288	1.3094550288
C	1.3094550288	1.3094550288	-1.3094550288
C	-1.3094550288	1.3094550288	1.3094550288
C	-0.5272151931	1.9706188559	2.4501451782
H	-0.0783461181	1.2374917142	3.1439243829
H	0.2861968554	2.6371382881	2.1023441714
H	-1.1761446553	2.6201399058	3.0768183276
C	-1.9706188559	2.4501451782	0.5272151931
H	-1.2374917142	3.1439243829	0.0783461181
H	-2.6371382881	2.1023441714	-0.2861968554
H	-2.6201399058	3.0768183276	1.1761446553
C	-2.4501451782	0.5272151931	1.9706188559
H	-3.1439243829	0.0783461181	1.2374917142
H	-2.1023441714	-0.2861968554	2.6371382881
H	-3.0768183276	1.1761446553	2.6201399058
C	1.9706188559	2.4501451782	-0.5272151931
H	1.2374917142	3.1439243829	-0.0783461181
H	2.6371382881	2.1023441714	0.2861968554
H	2.6201399058	3.0768183276	-1.1761446553
C	2.4501451782	0.5272151931	-1.9706188559
H	3.1439243829	0.0783461181	-1.2374917142
H	2.1023441714	-0.2861968554	-2.6371382881
H	3.0768183276	1.1761446553	-2.6201399058
C	0.5272151931	1.9706188559	-2.4501451782

H	0.0783461181	1.2374917142	-3.1439243829
H	-0.2861968554	2.6371382881	-2.1023441714
H	1.1761446553	2.6201399058	-3.0768183276
C	-1.9706188559	-2.4501451782	-0.5272151931
H	-1.2374917142	-3.1439243829	-0.0783461181
H	-2.6371382881	-2.1023441714	0.2861968554
H	-2.6201399058	-3.0768183276	-1.1761446553
C	-2.4501451782	-0.5272151931	-1.9706188559
H	-3.1439243829	-0.0783461181	-1.2374917142
H	-2.1023441714	0.2861968554	-2.6371382881
H	-3.0768183276	-1.1761446553	-2.6201399058
C	-0.5272151931	-1.9706188559	-2.4501451782
H	-0.0783461181	-1.2374917142	-3.1439243829
H	0.2861968554	-2.6371382881	-2.1023441714
H	-1.1761446553	-2.6201399058	-3.0768183276
C	2.4501451782	-0.5272151931	1.9706188559
H	3.1439243829	-0.0783461181	1.2374917142
H	2.1023441714	0.2861968554	2.6371382881
H	3.0768183276	-1.1761446553	2.6201399058
C	0.5272151931	-1.9706188559	2.4501451782
H	0.0783461181	-1.2374917142	3.1439243829
H	-0.2861968554	-2.6371382881	2.1023441714
H	1.1761446553	-2.6201399058	3.0768183276
C	1.9706188559	-2.4501451782	0.5272151931
H	1.2374917142	-3.1439243829	0.0783461181
H	2.6371382881	-2.1023441714	-0.2861968554
H	2.6201399058	-3.0768183276	1.1761446553

Tabelle 10.234 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
C	0.	0.0000001667	0.2916109819
Li	0.	0.0000001667	2.3129113389
C	0.	1.421544576	-0.2617042803
H	0.8873168307	1.9971518045	0.0458565811
H	0.	1.4200829974	-1.3766183127
H	-0.8873168307	1.9971518045	0.0458565811
C	-1.2310935711	-0.710772038	-0.2617042803
H	-1.2859256382	-1.7670145688	0.0458565811
H	-2.1732424689	-0.2301367356	0.0458565811
H	-1.2298278069	-0.7100412487	-1.3766183127
C	1.2310935711	-0.710772038	-0.2617042803
H	2.1732424689	-0.2301367356	0.0458565811
H	1.2859256382	-1.7670145688	0.0458565811
H	1.2298278069	-0.7100412487	-1.3766183127

Tabelle 10.235 Standardorientierung von <sup>t</sup>BuLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
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Li	0.	0.	1.1155696235
C	-0.710795781	1.6603493715	0.
Li	0.	0.	-1.1155696235
C	0.710795781	-1.6603493715	0.
C	-0.0325637419	2.2745238596	-1.2266453826
H	1.0474850991	2.0354395348	-1.2894616705
H	-0.5020283687	1.9577931277	-2.1785395996
H	-0.0859849404	3.3838405794	-1.240648823
C	-2.1703435339	2.0863751295	0.
H	-2.7128171469	1.7137035273	-0.8816877466
H	-2.7128171469	1.7137035273	0.8816877466
H	-2.2875999206	3.1935241096	0.
C	-0.0325637419	2.2745238596	1.2266453826
H	-0.5020283687	1.9577931277	2.1785395996
H	1.0474850991	2.0354395348	1.2894616705
H	-0.0859849404	3.3838405794	1.240648823
C	0.0325637419	-2.2745238596	1.2266453826
H	0.5020283687	-1.9577931277	2.1785395996
H	-1.0474850991	-2.0354395348	1.2894616705
H	0.0859849404	-3.3838405794	1.240648823
C	2.1703435339	-2.0863751295	0.
H	2.7128171469	-1.7137035273	-0.8816877466
H	2.7128171469	-1.7137035273	0.8816877466
H	2.2875999206	-3.1935241096	0.
C	0.0325637419	-2.2745238596	-1.2266453826
H	-1.0474850991	-2.0354395348	-1.2894616705
H	0.5020283687	-1.9577931277	-2.1785395996
H	0.0859849404	-3.3838405794	-1.240648823

Tabelle 10.236 Standardorientierung von (<sup>t</sup>BuLi)<sub>4</sub> (T) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Li	-0.8561091215	-0.8561091215	0.8561091215
Li	0.8561091215	0.8561091215	0.8561091215
Li	-0.8561091215	0.8561091215	-0.8561091215
Li	0.8561091215	-0.8561091215	-0.8561091215
C	-1.309497616	-1.309497616	-1.309497616
C	1.309497616	-1.309497616	1.309497616
C	1.309497616	1.309497616	-1.309497616
C	-1.309497616	1.309497616	1.309497616
C	-0.5253777235	1.9700749062	2.4497206824
H	-0.0757660542	1.2365659404	3.1402907627
H	0.2857704586	2.6360511205	2.1005550417
H	-1.1728517385	2.6178380739	3.0767486974
C	-1.9700749062	2.4497206824	0.5253777235
H	-1.2365659404	3.1402907627	0.0757660542
H	-2.6360511205	2.1005550417	-0.2857704586
H	-2.6178380739	3.0767486974	1.1728517385
C	-2.4497206824	0.5253777235	1.9700749062
H	-3.1402907627	0.0757660542	1.2365659404
H	-2.1005550417	-0.2857704586	2.6360511205

H	-3.0767486974	1.1728517385	2.6178380739
C	1.9700749062	2.4497206824	-0.5253777235
H	1.2365659404	3.1402907627	-0.0757660542
H	2.6360511205	2.1005550417	0.2857704586
H	2.6178380739	3.0767486974	-1.1728517385
C	2.4497206824	0.5253777235	-1.9700749062
H	3.1402907627	0.0757660542	-1.2365659404
H	2.1005550417	-0.2857704586	-2.6360511205
H	3.0767486974	1.1728517385	-2.6178380739
C	0.5253777235	1.9700749062	-2.4497206824
H	0.0757660542	1.2365659404	-3.1402907627
H	-0.2857704586	2.6360511205	-2.1005550417
H	1.1728517385	2.6178380739	-3.0767486974
C	-1.9700749062	-2.4497206824	-0.5253777235
H	-1.2365659404	-3.1402907627	-0.0757660542
H	-2.6360511205	-2.1005550417	0.2857704586
H	-2.6178380739	-3.0767486974	-1.1728517385
C	-2.4497206824	-0.5253777235	-1.9700749062
H	-3.1402907627	-0.0757660542	-1.2365659404
H	-2.1005550417	0.2857704586	-2.6360511205
H	-3.0767486974	-1.1728517385	-2.6178380739
C	-0.5253777235	-1.9700749062	-2.4497206824
H	-0.0757660542	-1.2365659404	-3.1402907627
H	0.2857704586	-2.6360511205	-2.1005550417
H	-1.1728517385	-2.6178380739	-3.0767486974
C	2.4497206824	-0.5253777235	1.9700749062
H	3.1402907627	-0.0757660542	1.2365659404
H	2.1005550417	0.2857704586	2.6360511205
H	3.0767486974	-1.1728517385	2.6178380739
C	0.5253777235	-1.9700749062	2.4497206824
H	0.0757660542	-1.2365659404	3.1402907627
H	-0.2857704586	-2.6360511205	2.1005550417
H	1.1728517385	-2.6178380739	3.0767486974
C	1.9700749062	-2.4497206824	0.5253777235
H	1.2365659404	-3.1402907627	0.0757660542
H	2.6360511205	-2.1005550417	-0.2857704586
H	2.6178380739	-3.0767486974	1.1728517385

Tabelle 10.237 Standardorientierung von <sup>4</sup>BuLi (C<sub>3v</sub>) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
C	0.	0.0000001667	0.2916109819
Li	0.	0.0000001667	2.3129113389
C	0.	1.421544576	-0.2617042803
H	0.8873168307	1.9971518045	0.0458565811
H	0.	1.4200829974	-1.3766183127
H	-0.8873168307	1.9971518045	0.0458565811
C	-1.2310935711	-0.710772038	-0.2617042803
H	-1.2859256382	-1.7670145688	0.0458565811

H	-2.1732424689	-0.2301367356	0.0458565811
H	-1.2298278069	-0.7100412487	-1.3766183127
C	1.2310935711	-0.710772038	-0.2617042803
H	2.1732424689	-0.2301367356	0.0458565811
H	1.2859256382	-1.7670145688	0.0458565811
H	1.2298278069	-0.7100412487	-1.3766183127

Tabelle 10.238 Standardorientierung von  $(t\text{BuLi})_2$  ( $C_{2h}$ ) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Li	0.	0.	1.1155696235
C	-0.710795781	1.6603493715	0.
Li	0.	0.	-1.1155696235
C	0.710795781	-1.6603493715	0.
C	-0.0325637419	2.2745238596	-1.2266453826
H	1.0474850991	2.0354395348	-1.2894616705
H	-0.5020283687	1.9577931277	-2.1785395996
H	-0.0859849404	3.3838405794	-1.240648823
C	-2.1703435339	2.0863751295	0.
H	-2.7128171469	1.7137035273	-0.8816877466
H	-2.7128171469	1.7137035273	0.8816877466
H	-2.2875999206	3.1935241096	0.
C	-0.0325637419	2.2745238596	1.2266453826
H	-0.5020283687	1.9577931277	2.1785395996
H	1.0474850991	2.0354395348	1.2894616705
H	-0.0859849404	3.3838405794	1.240648823
C	0.0325637419	-2.2745238596	1.2266453826
H	0.5020283687	-1.9577931277	2.1785395996
H	-1.0474850991	-2.0354395348	1.2894616705
H	0.0859849404	-3.3838405794	1.240648823
C	2.1703435339	-2.0863751295	0.
H	2.7128171469	-1.7137035273	-0.8816877466
H	2.7128171469	-1.7137035273	0.8816877466
H	2.2875999206	-3.1935241096	0.
C	0.0325637419	-2.2745238596	-1.2266453826
H	-1.0474850991	-2.0354395348	-1.2894616705
H	0.5020283687	-1.9577931277	-2.1785395996
H	0.0859849404	-3.3838405794	-1.240648823

Tabelle 10.239 Standardorientierung von  $(t\text{BuLi})_4$  (T) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Li	-0.8561091215	-0.8561091215	0.8561091215
Li	0.8561091215	0.8561091215	0.8561091215
Li	-0.8561091215	0.8561091215	-0.8561091215
Li	0.8561091215	-0.8561091215	-0.8561091215
C	-1.309497616	-1.309497616	-1.309497616
C	1.309497616	-1.309497616	1.309497616
C	1.309497616	1.309497616	-1.309497616
C	-1.309497616	1.309497616	1.309497616
C	-0.5253777235	1.9700749062	2.4497206824

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H	-0.0757660542	1.2365659404	3.1402907627
H	0.2857704586	2.6360511205	2.1005550417
H	-1.1728517385	2.6178380739	3.0767486974
C	-1.9700749062	2.4497206824	0.5253777235
H	-1.2365659404	3.1402907627	0.0757660542
H	-2.6360511205	2.1005550417	-0.2857704586
H	-2.6178380739	3.0767486974	1.1728517385
C	-2.4497206824	0.5253777235	1.9700749062
H	-3.1402907627	0.0757660542	1.2365659404
H	-2.1005550417	-0.2857704586	2.6360511205
H	-3.0767486974	1.1728517385	2.6178380739
C	1.9700749062	2.4497206824	-0.5253777235
H	1.2365659404	3.1402907627	-0.0757660542
H	2.6360511205	2.1005550417	0.2857704586
H	2.6178380739	3.0767486974	-1.1728517385
C	2.4497206824	0.5253777235	-1.9700749062
H	3.1402907627	0.0757660542	-1.2365659404
H	2.1005550417	-0.2857704586	-2.6360511205
H	3.0767486974	1.1728517385	-2.6178380739
C	0.5253777235	1.9700749062	-2.4497206824
H	0.0757660542	1.2365659404	-3.1402907627
H	-0.2857704586	2.6360511205	-2.1005550417
H	1.1728517385	2.6178380739	-3.0767486974
C	-1.9700749062	-2.4497206824	-0.5253777235
H	-1.2365659404	-3.1402907627	-0.0757660542
H	-2.6360511205	-2.1005550417	0.2857704586
H	-2.6178380739	-3.0767486974	-1.1728517385
C	-2.4497206824	-0.5253777235	-1.9700749062
H	-3.1402907627	-0.0757660542	-1.2365659404
H	-2.1005550417	0.2857704586	-2.6360511205
H	-3.0767486974	-1.1728517385	-2.6178380739
C	-0.5253777235	-1.9700749062	-2.4497206824
H	-0.0757660542	-1.2365659404	-3.1402907627
H	0.2857704586	-2.6360511205	-2.1005550417
H	-1.1728517385	-2.6178380739	-3.0767486974
C	2.4497206824	-0.5253777235	1.9700749062
H	3.1402907627	-0.0757660542	1.2365659404
H	2.1005550417	0.2857704586	2.6360511205
H	3.0767486974	-1.1728517385	2.6178380739
C	0.5253777235	-1.9700749062	2.4497206824
H	0.0757660542	-1.2365659404	3.1402907627
H	-0.2857704586	-2.6360511205	2.1005550417
H	1.1728517385	-2.6178380739	3.0767486974
C	1.9700749062	-2.4497206824	0.5253777235
H	1.2365659404	-3.1402907627	0.0757660542
H	2.6360511205	-2.1005550417	-0.2857704586
H	2.6178380739	-3.0767486974	1.1728517385

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Tabelle 10.240 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; M062X/6-31+G(d)].

	x	y	z
C	0.	0.0000001667	0.2936276116
Li	0.	0.0000001667	2.3159142858
C	0.	1.4259417456	-0.2637599221
H	0.8857756182	1.998791818	0.0453445046
H	0.	1.4207937133	-1.3752117142
H	-0.8857756182	1.998791818	0.0453445046
C	-1.2349016317	-0.7129706228	-0.2637599221
H	-1.2881165378	-1.7664998463	0.0453445046
H	-2.173892156	-0.2322914716	0.0453445046
H	-1.2304433049	-0.7103966067	-1.3752117142
C	1.2349016317	-0.7129706228	-0.2637599221
H	2.173892156	-0.2322914716	0.0453445046
H	1.2881165378	-1.7664998463	0.0453445046
H	1.2304433049	-0.7103966067	-1.3752117142

Tabelle 10.241 Standardorientierung von (<sup>t</sup>BuLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; M062X/6-31+G(d)].

	x	y	z
Li	0.	0.	1.1019678595
C	-0.7090677577	1.6453917835	0.
Li	0.	0.	-1.1019678595
C	0.7090677577	-1.6453917835	0.
C	-0.0269652812	2.2615250218	-1.2311159655
H	1.0497140195	2.0185121815	-1.2935753631
H	-0.4957356709	1.9433096975	-2.1801377768
H	-0.0797368441	3.3679092534	-1.2419162835
C	-2.1726024642	2.0764731969	0.
H	-2.7118294453	1.7027278938	-0.88072358
H	-2.7118294453	1.7027278938	0.88072358
H	-2.2866818044	3.1805355529	0.
C	-0.0269652812	2.2615250218	1.2311159655
H	-0.4957356709	1.9433096975	2.1801377768
H	1.0497140195	2.0185121815	1.2935753631
H	-0.0797368441	3.3679092534	1.2419162835
C	0.0269652812	-2.2615250218	1.2311159655
H	0.4957356709	-1.9433096975	2.1801377768
H	-1.0497140195	-2.0185121815	1.2935753631
H	0.0797368441	-3.3679092534	1.2419162835
C	2.1726024642	-2.0764731969	0.
H	2.7118294453	-1.7027278938	-0.88072358
H	2.7118294453	-1.7027278938	0.88072358
H	2.2866818044	-3.1805355529	0.
C	0.0269652812	-2.2615250218	-1.2311159655
H	-1.0497140195	-2.0185121815	-1.2935753631
H	0.4957356709	-1.9433096975	-2.1801377768
H	0.0797368441	-3.3679092534	-1.2419162835

Tabelle 10.242 Standardorientierung von  $(t\text{-BuLi})_4$  (T) [globales Minimum; M062X/6-31+G(d)].

	x	y	z
Li	0.0000000006	1.3723190925	0.4851880686
Li	-1.1884631965	-0.6861595464	0.4851880692
Li	1.1884631965	-0.6861595471	0.4851880682
Li	-0.0000000006	-0.0000000004	-1.4555642043
C	1.8160336087	1.0484874919	-0.7413926166
C	-1.8160336087	1.048487493	-0.7413926151
C	-0.0000000009	-2.0969749861	-0.7413926157
C	0.0000000009	-0.0000000003	2.224177849
C	-1.3759120747	-0.3610209949	2.8102261587
H	-2.1525065726	0.3708906155	2.5428613179
H	-1.741559917	-1.3556275143	2.4983786224
H	-1.3553987647	-0.3975558501	3.9167176418
C	1.0006093917	-1.011064314	2.8102261577
H	0.7550525927	-2.0495706827	2.5428613168
H	2.0447878253	-0.8304213744	2.4983786208
H	1.0219928502	-0.9750318391	3.9167176408
C	0.3753026864	1.3720853081	2.8102261579
H	1.3974539831	1.6786800665	2.5428613164
H	-0.3032279052	2.186048888	2.4983786216
H	0.3334059193	1.3725876886	3.916717641
C	-1.0006093917	-2.9865280682	0.0164985247
H	-0.7550525927	-3.0806228683	1.0847333326
H	-2.0447878253	-2.6323010776	-0.049864093
H	-1.0219928502	-4.017727418	-0.3863037127
C	-0.3753026864	-2.1921448612	-2.2303564866
H	-1.3974539831	-1.8378726184	-2.430295183
H	0.3032279052	-1.6268109912	-2.8938195304
H	-0.3334059193	-3.2351875758	-2.5996606297
C	1.3759120747	-2.7698469628	-0.5963681943
H	2.1525065726	-2.2738024368	-1.1972994646
H	1.741559917	-2.8073697923	0.4453050038
H	1.3553987647	-3.8252354226	-0.9307532967
C	1.7108017964	2.5764982911	-0.5963681946
H	0.892917386	3.0010265919	-1.1972994643
H	1.5604735995	2.9119200258	0.4453050037
H	2.6350516682	3.0864274735	-0.9307532975
C	3.0867138718	0.6267108811	0.0164985229
H	3.0454239601	0.8864167069	1.0847333308
H	3.3020335159	-0.4546876637	-0.0498640953
H	3.990450434	1.1237919378	-0.3863037149
C	2.08610448	0.7710507702	-2.2303564877
H	2.2903713661	-0.2912943406	-2.4302951846
H	1.2572456907	1.0760085649	-2.8938195309
H	2.9684575843	1.3288557922	-2.5996606313
C	-3.0867138718	0.1933486706	-0.5963681926
H	-3.0454239601	-0.7272241563	-1.1972994625
H	-3.3020335159	-0.1045502345	0.4453050058
H	-3.990450434	0.7388079479	-0.9307532947
C	-2.08610448	2.3598171861	0.0164985249

H	-2.2903713661	2.1942061605	1.084733333
H	-1.2572456907	3.0869887403	-0.0498640936
H	-2.9684575843	2.8939354791	-0.3863037121
C	-1.7108017964	1.4210940897	-2.2303564861
H	-0.892917386	2.1291669577	-2.4302951834
H	-1.5604735995	0.5508024248	-2.8938195298
H	-2.6350516682	1.9063317822	-2.599660629

Tabelle 10.243 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
C	0.	0.0000001667	0.2927856649
Li	0.	0.0000001667	2.3152379988
C	0.	1.42640083	-0.2638802157
H	0.885345019	1.9982568899	0.0453685111
H	0.	1.4209982254	-1.3746333495
H	-0.885345019	1.9982568899	0.0453685111
C	-1.2352992104	-0.713200165	-0.2638802157
H	-1.2878685761	-1.7658594725	0.0453685111
H	-2.1732135951	-0.2323969174	0.0453685111
H	-1.2306204176	-0.7104988627	-1.3746333495
C	1.2352992104	-0.713200165	-0.2638802157
H	2.1732135951	-0.2323969174	0.0453685111
H	1.2878685761	-1.7658594725	0.0453685111
H	1.2306204176	-0.7104988627	-1.3746333495

Tabelle 10.244 Standardorientierung von (<sup>t</sup>BuLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
Li	0.	0.	1.1024707938
C	-0.7106573761	1.6446274581	0.
Li	0.	0.	-1.1024707938
C	0.7106573761	-1.6446274581	0.
C	-0.0271723007	2.2584495605	-1.2317877575
H	1.0481027389	2.0122314552	-1.2942123453
H	-0.4979387517	1.9418008289	-2.179435833
H	-0.0762744182	3.3640805331	-1.242765416
C	-2.1741481063	2.0761329866	0.
H	-2.7125225011	1.7022371398	-0.8801600299
H	-2.7125225011	1.7022371398	0.8801600299
H	-2.2878304071	3.1795461463	0.
C	-0.0271723007	2.2584495605	1.2317877575
H	-0.4979387517	1.9418008289	2.179435833
H	1.0481027389	2.0122314552	1.2942123453
H	-0.0762744182	3.3640805331	1.242765416
C	0.0271723007	-2.2584495605	1.2317877575
H	0.4979387517	-1.9418008289	2.179435833
H	-1.0481027389	-2.0122314552	1.2942123453
H	0.0762744182	-3.3640805331	1.242765416

C	2.1741481063	-2.0761329866	0.
H	2.7125225011	-1.7022371398	-0.8801600299
H	2.7125225011	-1.7022371398	0.8801600299
H	2.2878304071	-3.1795461463	0.
C	0.0271723007	-2.2584495605	-1.2317877575
H	-1.0481027389	-2.0122314552	-1.2942123453
H	0.4979387517	-1.9418008289	-2.179435833
H	0.0762744182	-3.3640805331	-1.242765416

Tabelle 10.245 Standardorientierung von  $({}^t\text{BuLi})_4$  (T) [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
Li	-0.8402681764	-0.8402681764	0.8402681764
Li	0.8402681764	0.8402681764	0.8402681764
Li	-0.8402681764	0.8402681764	-0.8402681764
Li	0.8402681764	-0.8402681764	-0.8402681764
C	-1.2840184261	-1.2840184261	-1.2840184261
C	1.2840184261	-1.2840184261	1.2840184261
C	1.2840184261	1.2840184261	-1.2840184261
C	-1.2840184261	1.2840184261	1.2840184261
C	-0.5006572982	1.9155952793	2.4480704214
H	-0.096307979	1.1623736503	3.1394638061
H	0.3434418537	2.5469864519	2.1201864588
H	-1.1376553966	2.583640413	3.0580690854
C	-1.9155952793	2.4480704214	0.5006572982
H	-1.1623736503	3.1394638061	0.096307979
H	-2.5469864519	2.1201864588	-0.3434418537
H	-2.583640413	3.0580690854	1.1376553966
C	-2.4480704214	0.5006572982	1.9155952793
H	-3.1394638061	0.096307979	1.1623736503
H	-2.1201864588	-0.3434418537	2.5469864519
H	-3.0580690854	1.1376553966	2.583640413
C	1.9155952793	2.4480704214	-0.5006572982
H	1.1623736503	3.1394638061	-0.096307979
H	2.5469864519	2.1201864588	0.3434418537
H	2.583640413	3.0580690854	-1.1376553966
C	2.4480704214	0.5006572982	-1.9155952793
H	3.1394638061	0.096307979	-1.1623736503
H	2.1201864588	-0.3434418537	-2.5469864519
H	3.0580690854	1.1376553966	-2.583640413
C	0.5006572982	1.9155952793	-2.4480704214
H	0.096307979	1.1623736503	-3.1394638061
H	-0.3434418537	2.5469864519	-2.1201864588
H	1.1376553966	2.583640413	-3.0580690854
C	-1.9155952793	-2.4480704214	-0.5006572982
H	-1.1623736503	-3.1394638061	-0.096307979
H	-2.5469864519	-2.1201864588	0.3434418537
H	-2.583640413	-3.0580690854	-1.1376553966
C	-2.4480704214	-0.5006572982	-1.9155952793
H	-3.1394638061	-0.096307979	-1.1623736503
H	-2.1201864588	0.3434418537	-2.5469864519

H	-3.0580690854	-1.1376553966	-2.583640413
C	-0.5006572982	-1.9155952793	-2.4480704214
H	-0.096307979	-1.1623736503	-3.1394638061
H	0.3434418537	-2.5469864519	-2.1201864588
H	-1.1376553966	-2.583640413	-3.0580690854
C	2.4480704214	-0.5006572982	1.9155952793
H	3.1394638061	-0.096307979	1.1623736503
H	2.1201864588	0.3434418537	2.5469864519
H	3.0580690854	-1.1376553966	2.583640413
C	0.5006572982	-1.9155952793	2.4480704214
H	0.096307979	-1.1623736503	3.1394638061
H	-0.3434418537	-2.5469864519	2.1201864588
H	1.1376553966	-2.583640413	3.0580690854
C	1.9155952793	-2.4480704214	0.5006572982
H	1.1623736503	-3.1394638061	0.096307979
H	2.5469864519	-2.1201864588	-0.3434418537
H	2.583640413	-3.0580690854	1.1376553966

Tabelle 10.246 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; MP2/6-31+G(d)].

	x	y	z
C	0.	0.0000001667	0.2842423122
Li	0.	0.0000001667	2.3542711704
C	0.	1.4273737418	-0.2674801232
H	0.8865694995	1.9964215805	0.0442939449
H	0.	1.4194610821	-1.3790475864
H	-0.8865694995	1.9964215805	0.0442939449
C	-1.2361417768	-0.7136866209	-0.2674801232
H	-1.2856669113	-1.766002249	0.0442939449
H	-2.1722364107	-0.2304188315	0.0442939449
H	-1.2292892124	-0.709730291	-1.3790475864
C	1.2361417768	-0.7136866209	-0.2674801232
H	2.1722364107	-0.2304188315	0.0442939449
H	1.2856669113	-1.766002249	0.0442939449
H	1.2292892124	-0.709730291	-1.3790475864

Tabelle 10.247 Standardorientierung von (<sup>t</sup>BuLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; MP2/6-31+G(d)].

	x	y	z
Li	0.	0.	1.1121428658
C	-0.7266110686	1.6709073953	0.
Li	0.	0.	-1.1121428658
C	0.7266110686	-1.6709073953	0.
C	-0.0418583989	2.2767020167	-1.232549835
H	1.0344473442	2.030263292	-1.2899276444
H	-0.513966903	1.9531277895	-2.1785112356
H	-0.0914624943	3.3841940489	-1.2501847517
C	-2.1864599935	2.1127113738	0.
H	-2.7261822665	1.7431434626	-0.8821867517

H	-2.7261822665	1.7431434626	0.8821867517
H	-2.28872056	3.2185967212	0.
C	-0.0418583989	2.2767020167	1.232549835
H	-0.513966903	1.9531277895	2.1785112356
H	1.0344473442	2.030263292	1.2899276444
H	-0.0914624943	3.3841940489	1.2501847517
C	0.0418583989	-2.2767020167	1.232549835
H	0.513966903	-1.9531277895	2.1785112356
H	-1.0344473442	-2.030263292	1.2899276444
H	0.0914624943	-3.3841940489	1.2501847517
C	2.1864599935	-2.1127113738	0.
H	2.7261822665	-1.7431434626	-0.8821867517
H	2.7261822665	-1.7431434626	0.8821867517
H	2.28872056	-3.2185967212	0.
C	0.0418583989	-2.2767020167	-1.232549835
H	-1.0344473442	-2.030263292	-1.2899276444
H	0.513966903	-1.9531277895	-2.1785112356
H	0.0914624943	-3.3841940489	-1.2501847517

Tabelle 10.248 Standardorientierung von (<sup>t</sup>BuLi)<sub>4</sub> (T) [globales Minimum; MP2/6-31+G(d)].

	x	y	z
Li	-0.850844382	-0.850844382	0.850844382
Li	0.850844382	0.850844382	0.850844382
Li	-0.850844382	0.850844382	-0.850844382
Li	0.850844382	-0.850844382	-0.850844382
C	-1.3046392279	-1.3046392279	-1.3046392279
C	1.3046392279	-1.3046392279	1.3046392279
C	1.3046392279	1.3046392279	-1.3046392279
C	-1.3046392279	1.3046392279	1.3046392279
C	-0.5181809763	1.9647637773	2.4492953722
H	-0.104340111	1.2293405582	3.1548614502
H	0.316052796	2.5988909219	2.1010855381
H	-1.1603844364	2.6402546479	3.0495419793
C	-1.9647637773	2.4492953722	0.5181809763
H	-1.2293405582	3.1548614502	0.104340111
H	-2.5988909219	2.1010855381	-0.316052796
H	-2.6402546479	3.0495419793	1.1603844364
C	-2.4492953722	0.5181809763	1.9647637773
H	-3.1548614502	0.104340111	1.2293405582
H	-2.1010855381	-0.316052796	2.5988909219
H	-3.0495419793	1.1603844364	2.6402546479
C	1.9647637773	2.4492953722	-0.5181809763
H	1.2293405582	3.1548614502	-0.104340111
H	2.5988909219	2.1010855381	0.316052796
H	2.6402546479	3.0495419793	-1.1603844364
C	2.4492953722	0.5181809763	-1.9647637773
H	3.1548614502	0.104340111	-1.2293405582
H	2.1010855381	-0.316052796	-2.5988909219
H	3.0495419793	1.1603844364	-2.6402546479
C	0.5181809763	1.9647637773	-2.4492953722

H	0.104340111	1.2293405582	-3.1548614502
H	-0.316052796	2.5988909219	-2.1010855381
H	1.1603844364	2.6402546479	-3.0495419793
C	-1.9647637773	-2.4492953722	-0.5181809763
H	-1.2293405582	-3.1548614502	-0.104340111
H	-2.5988909219	-2.1010855381	0.316052796
H	-2.6402546479	-3.0495419793	-1.1603844364
C	-2.4492953722	-0.5181809763	-1.9647637773
H	-3.1548614502	-0.104340111	-1.2293405582
H	-2.1010855381	0.316052796	-2.5988909219
H	-3.0495419793	-1.1603844364	-2.6402546479
C	-0.5181809763	-1.9647637773	-2.4492953722
H	-0.104340111	-1.2293405582	-3.1548614502
H	0.316052796	-2.5988909219	-2.1010855381
H	-1.1603844364	-2.6402546479	-3.0495419793
C	2.4492953722	-0.5181809763	1.9647637773
H	3.1548614502	-0.104340111	1.2293405582
H	2.1010855381	0.316052796	2.5988909219
H	3.0495419793	-1.1603844364	2.6402546479
C	0.5181809763	-1.9647637773	2.4492953722
H	0.104340111	-1.2293405582	3.1548614502
H	-0.316052796	-2.5988909219	2.1010855381
H	1.1603844364	-2.6402546479	3.0495419793
C	1.9647637773	-2.4492953722	0.5181809763
H	1.2293405582	-3.1548614502	0.104340111
H	2.5988909219	-2.1010855381	-0.316052796
H	2.6402546479	-3.0495419793	1.1603844364

Tabelle 10.249 Standardorientierung von <sup>t</sup>BuLi (C<sub>3v</sub>) [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
C	0.	0.0000001667	0.2999508206
Li	0.	0.0000001667	2.3536130509
C	0.	1.4252795323	-0.2660080121
H	0.8864196342	1.9973919418	0.0398395356
H	0.	1.4051277919	-1.376627672
H	-0.8864196342	1.9973919418	0.0398395356
C	-1.2343281381	-0.7126395161	-0.2660080121
H	-1.2865822015	-1.7663576425	0.0398395356
H	-2.1730018357	-0.2310337993	0.0398395356
H	-1.216876219	-0.7025636459	-1.376627672
C	1.2343281381	-0.7126395161	-0.2660080121
H	2.1730018357	-0.2310337993	0.0398395356
H	1.2865822015	-1.7663576425	0.0398395356
H	1.216876219	-0.7025636459	-1.376627672

Tabelle 10.250 Standardorientierung von (<sup>t</sup>BuLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
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Li	0.	0.	1.1191301654
C	-0.7341534714	1.6609831084	0.
Li	0.	0.	-1.1191301654
C	0.7341534714	-1.6609831084	0.
C	-0.0487733804	2.274546249	-1.2317793586
H	1.0242775514	2.0164532453	-1.2976897273
H	-0.5287447822	1.9624962719	-2.1769088191
H	-0.0872109916	3.3814656593	-1.2357369633
C	-2.1920314402	2.1191210405	0.
H	-2.7352085995	1.755590147	-0.8821196599
H	-2.7352085995	1.755590147	0.8821196599
H	-2.2794070298	3.2255115817	0.
C	-0.0487733804	2.274546249	1.2317793586
H	-0.5287447822	1.9624962719	2.1769088191
H	1.0242775514	2.0164532453	1.2976897273
H	-0.0872109916	3.3814656593	1.2357369633
C	0.0487733804	-2.274546249	1.2317793586
H	0.5287447822	-1.9624962719	2.1769088191
H	-1.0242775514	-2.0164532453	1.2976897273
H	0.0872109916	-3.3814656593	1.2357369633
C	2.1920314402	-2.1191210405	0.
H	2.7352085995	-1.755590147	-0.8821196599
H	2.7352085995	-1.755590147	0.8821196599
H	2.2794070298	-3.2255115817	0.
C	0.0487733804	-2.274546249	-1.2317793586
H	-1.0242775514	-2.0164532453	-1.2976897273
H	0.5287447822	-1.9624962719	-2.1769088191
H	0.0872109916	-3.3814656593	-1.2357369633

Tabelle 10.251 Standardorientierung von (<sup>t</sup>BuLi)<sub>4</sub> (T) [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
Li	-0.854083	-0.854083	0.854083
Li	0.854083	0.854083	0.854083
Li	-0.854083	0.854083	-0.854083
Li	0.854083	-0.854083	-0.854083
C	-1.297392	-1.297392	-1.297392
C	1.297392	-1.297392	1.297392
C	1.297392	1.297392	-1.297392
C	-1.297392	1.297392	1.297392
C	-0.516423	1.957265	2.449186
H	-0.09342	1.219048	3.146659
H	0.311307	2.600727	2.1032
H	-1.166121	2.619825	3.054288
C	-1.957265	2.449186	0.516423
H	-1.219048	3.146659	0.09342
H	-2.600727	2.1032	-0.311307
H	-2.619825	3.054288	1.166121
C	-2.449186	0.516423	1.957265
H	-3.146659	0.09342	1.219048
H	-2.1032	-0.311307	2.600727

H	-3.054288	1.166121	2.619825
C	1.957265	2.449186	-0.516423
H	1.219048	3.146659	-0.09342
H	2.600727	2.1032	0.311307
H	2.619825	3.054288	-1.166121
C	2.449186	0.516423	-1.957265
H	3.146659	0.09342	-1.219048
H	2.1032	-0.311307	-2.600727
H	3.054288	1.166121	-2.619825
C	0.516423	1.957265	-2.449186
H	0.09342	1.219048	-3.146659
H	-0.311307	2.600727	-2.1032
H	1.166121	2.619825	-3.054288
C	-1.957265	-2.449186	-0.516423
H	-1.219048	-3.146659	-0.09342
H	-2.600727	-2.1032	0.311307
H	-2.619825	-3.054288	-1.166121
C	-2.449186	-0.516423	-1.957265
H	-3.146659	-0.09342	-1.219048
H	-2.1032	0.311307	-2.600727
H	-3.054288	-1.166121	-2.619825
C	-0.516423	-1.957265	-2.449186
H	-0.09342	-1.219048	-3.146659
H	0.311307	-2.600727	-2.1032
H	-1.166121	-2.619825	-3.054288
C	2.449186	-0.516423	1.957265
H	3.146659	-0.09342	1.219048
H	2.1032	0.311307	2.600727
H	3.054288	-1.166121	2.619825
C	0.516423	-1.957265	2.449186
H	0.09342	-1.219048	3.146659
H	-0.311307	-2.600727	2.1032
H	1.166121	-2.619825	3.054288
C	1.957265	-2.449186	0.516423
H	1.219048	-3.146659	0.09342
H	2.600727	-2.1032	-0.311307
H	2.619825	-3.054288	1.166121

Tabelle 10.252 Standardorientierung von <sup>4</sup>BuLi (C<sub>3v</sub>) [globales Minimum; G3].

	x	y	z
C	0.	0.0000001667	0.282685548
Li	0.	0.0000001667	2.3564247973
C	0.	1.424899431	-0.2690469804
H	0.8850323987	1.9931205567	0.0442132337
H	0.	1.4203253966	-1.3775182733
H	-0.8850323987	1.9931205567	0.0442132337
C	-1.2339989607	-0.7124494655	-0.2690469804
H	-1.2835766912	-1.7630205688	0.0442132337

H	-2.1686090899	-0.2300994878	0.0442132337
H	-1.2300377307	-0.7101624483	-1.3775182733
C	1.2339989607	-0.7124494655	-0.2690469804
H	2.1686090899	-0.2300994878	0.0442132337
H	1.2835766912	-1.7630205688	0.0442132337
H	1.2300377307	-0.7101624483	-1.3775182733

Tabelle 10.253 Standardorientierung von (<sup>t</sup>BuLi)<sub>2</sub> (C<sub>2h</sub>) [globales Minimum; G3].

	x	y	z
Li	0.	0.	1.1028427201
C	-0.7656053268	1.6188064619	0.
Li	0.	0.	-1.1028427201
C	0.7656053268	-1.6188064619	0.
C	-0.065526418	2.1917609876	-1.2353989771
H	1.0073287631	1.9267865407	-1.2761498493
H	-0.531374401	1.840079162	-2.1753088686
H	-0.0997150695	3.2947362634	-1.3007505667
C	-2.2163931927	2.0718965528	0.
H	-2.7552880462	1.7022583251	-0.8814803098
H	-2.7552880462	1.7022583251	0.8814803098
H	-2.3204715296	3.1747085246	0.
C	-0.065526418	2.1917609876	1.2353989771
H	-0.531374401	1.840079162	2.1753088686
H	1.0073287631	1.9267865407	1.2761498493
H	-0.0997150695	3.2947362634	1.3007505667
C	0.065526418	-2.1917609876	1.2353989771
H	0.531374401	-1.840079162	2.1753088686
H	-1.0073287631	-1.9267865407	1.2761498493
H	0.0997150695	-3.2947362634	1.3007505667
C	2.2163931927	-2.0718965528	0.
H	2.7552880462	-1.7022583251	-0.8814803098
H	2.7552880462	-1.7022583251	0.8814803098
H	2.3204715296	-3.1747085246	0.
C	0.065526418	-2.1917609876	-1.2353989771
H	-1.0073287631	-1.9267865407	-1.2761498493
H	0.531374401	-1.840079162	-2.1753088686
H	0.0997150695	-3.2947362634	-1.3007505667

Tabelle 10.254 Standardorientierung von (<sup>t</sup>BuLi)<sub>4</sub> (T) [globales Minimum; G3].

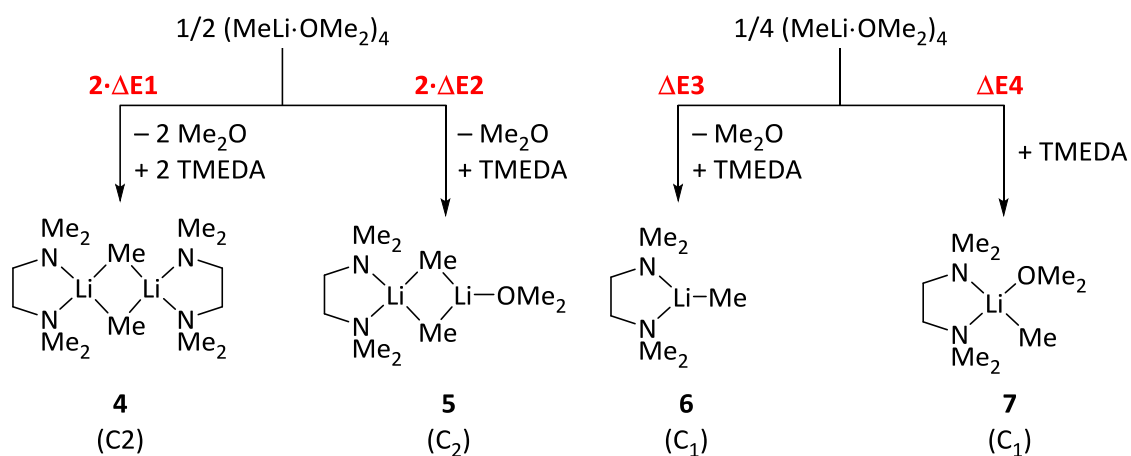
	x	y	z
Li	-0.8264757427	-0.8264757427	0.8264757427
Li	0.8264757427	0.8264757427	0.8264757427
Li	-0.8264757427	0.8264757427	-0.8264757427
Li	0.8264757427	-0.8264757427	-0.8264757427
C	-1.2818277948	-1.2818277948	-1.2818277948
C	1.2818277948	-1.2818277948	1.2818277948
C	1.2818277948	1.2818277948	-1.2818277948
C	-1.2818277948	1.2818277948	1.2818277948
C	-0.4978578167	1.9132316329	2.4403914249

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H	-0.094349042	1.1590096909	3.1295391549
H	0.3451936583	2.5421023364	2.1062900602
H	-1.1323194881	2.5845185929	3.0492244536
C	-1.9132316329	2.4403914249	0.4978578167
H	-1.1590096909	3.1295391549	0.094349042
H	-2.5421023364	2.1062900602	-0.3451936583
H	-2.5845185929	3.0492244536	1.1323194881
C	-2.4403914249	0.4978578167	1.9132316329
H	-3.1295391549	0.094349042	1.1590096909
H	-2.1062900602	-0.3451936583	2.5421023364
H	-3.0492244536	1.1323194881	2.5845185929
C	1.9132316329	2.4403914249	-0.4978578167
H	1.1590096909	3.1295391549	-0.094349042
H	2.5421023364	2.1062900602	0.3451936583
H	2.5845185929	3.0492244536	-1.1323194881
C	2.4403914249	0.4978578167	-1.9132316329
H	3.1295391549	0.094349042	-1.1590096909
H	2.1062900602	-0.3451936583	-2.5421023364
H	3.0492244536	1.1323194881	-2.5845185929
C	0.4978578167	1.9132316329	-2.4403914249
H	0.094349042	1.1590096909	-3.1295391549
H	-0.3451936583	2.5421023364	-2.1062900602
H	1.1323194881	2.5845185929	-3.0492244536
C	-1.9132316329	-2.4403914249	-0.4978578167
H	-1.1590096909	-3.1295391549	-0.094349042
H	-2.5421023364	-2.1062900602	0.3451936583
H	-2.5845185929	-3.0492244536	-1.1323194881
C	-2.4403914249	-0.4978578167	-1.9132316329
H	-3.1295391549	-0.094349042	-1.1590096909
H	-2.1062900602	0.3451936583	-2.5421023364
H	-3.0492244536	-1.1323194881	-2.5845185929
C	-0.4978578167	-1.9132316329	-2.4403914249
H	-0.094349042	-1.1590096909	-3.1295391549
H	0.3451936583	-2.5421023364	-2.1062900602
H	-1.1323194881	-2.5845185929	-3.0492244536
C	2.4403914249	-0.4978578167	1.9132316329
H	3.1295391549	-0.094349042	1.1590096909
H	2.1062900602	0.3451936583	2.5421023364
H	3.0492244536	-1.1323194881	2.5845185929
C	0.4978578167	-1.9132316329	2.4403914249
H	0.094349042	-1.1590096909	3.1295391549
H	-0.3451936583	-2.5421023364	2.1062900602
H	1.1323194881	-2.5845185929	3.0492244536
C	1.9132316329	-2.4403914249	0.4978578167
H	1.1590096909	-3.1295391549	0.094349042
H	2.5421023364	-2.1062900602	-0.3451936583
H	2.5845185929	-3.0492244536	1.1323194881

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## 10.2.1.4. Deaggregation von Methyllithium mit TMEDA



Schema 10.1 Betrachtete Wege der Deaggregation von  $(\text{MeLi} \cdot \text{Me}_2\text{O})_4$  ( $S_4$ ) mit TMEDA ( $C_2$ ) in Gegenwart von Dimethylether ( $C_2$ ). Die Punktgruppe ist in Klammern angegeben.

Tabelle 10.255 Berechnete Energien der optimierten Strukturen für die Deaggregation von Methyllithium mit TMEDA in Dimethylether.

Verbindung	Methode	Basissatz	SCF [Hartree]	ZPE [Hartree]
$(\text{MeLi} \cdot \text{OMe}_2)_4$	SVWN	6-31+G(d)	-805.5954444	-805.134965
TMEDA	SVWN	6-31+G(d)	-345.8792903	-345.66209
$\text{Me}_2\text{O}$	SWN	6-31+G(d)	-154.2235093	-154.14562
<b>4</b>	SVWN	6-31+G(d)	-786.112976	-785.605695
<b>5</b>	SVWN	6-31+G(d)	-594.4366912	-594.069023
<b>6</b>	SVWN	6-31+G(d)	-393.022329	-392.769718
<b>7</b>	SVWN	6-31+G(d)	-547.2744001	-546.942243
$(\text{MeLi} \cdot \text{OMe}_2)_4$	PBE	6-31+G(d)	-808.8279427	-808.370479
TMEDA	PBE	6-31+G(d)	-347.2756188	-347.058379
$\text{Me}_2\text{O}$	PBE	6-31+G(d)	-154.8306546	-154.7528
<b>4</b>	PBE	6-31+G(d)	-789.3030149	-788.79595
<b>5</b>	PBE	6-31+G(d)	-596.8485906	-596.48124
<b>6</b>	PBE	6-31+G(d)	-394.6292649	-394.376634
<b>7</b>	PBE	6-31+G(d)	-549.4721088	-549.140142
$(\text{MeLi} \cdot \text{OMe}_2)_4$	TPSS	6-31+G(d)	-810.1092991	-809.645387
TMEDA	TPSS	6-31+G(d)	-347.8093841	-347.588934
$\text{Me}_2\text{O}$	TPSS	6-31+G(d)	-155.053255	-154.974046
<b>4</b>	TPSS	6-31+G(d)	-790.565506	-790.05114
<b>5</b>	TPSS	6-31+G(d)	-597.8014289	-597.428662
<b>6</b>	TPSS	6-31+G(d)	-395.2622633	-395.005949
<b>7</b>	TPSS	6-31+G(d)	-550.3257942	-549.988718
$(\text{MeLi} \cdot \text{OMe}_2)_4$	PBE0	6-31+G(d)	-808.9437389	-808.47038
TMEDA	PBE0	6-31+G(d)	-347.3292722	-347.104348
$\text{Me}_2\text{O}$	PBE0	6-31+G(d)	-154.8453841	-154.764676
<b>4</b>	PBE0	6-31+G(d)	-789.4392333	-788.914471
<b>5</b>	PBE0	6-31+G(d)	-596.9455714	-596.56548
<b>6</b>	PBE0	6-31+G(d)	-394.696755	-394.435451

Verbindung	Methode	Basissatz	SCF [Hartree]	ZPE [Hartree]
<b>7</b>	PBE0	6-31+G(d)	-549.5549538	-549.21123
(MeLi·OMe <sub>2</sub> ) <sub>4</sub>	TPSSh	6-31+G(d)	-810.029176	-809.559568
TMEDA	TPSSh	6-31+G(d)	-347.7778145	-347.554591
Me <sub>2</sub> O	TPSSh	6-31+G(d)	-155.0370683	-154.956851
<b>4</b>	TPSSh	6-31+G(d)	-790.4948544	-789.974184
<b>5</b>	TPSSh	6-31+G(d)	-597.7459559	-597.368619
<b>6</b>	TPSSh	6-31+G(d)	-395.2265583	-394.967133
<b>7</b>	TPSSh	6-31+G(d)	-550.2742895	-549.933005
(MeLi·OMe <sub>2</sub> ) <sub>4</sub>	B3LYP	6-31+G(d)	-810.0220699	-809.552828
TMEDA	B3LYP	6-31+G(d)	-347.7581936	-347.534984
Me <sub>2</sub> O	B3LYP	6-31+G(d)	-155.0336966	-154.953657
<b>4</b>	B3LYP	6-31+G(d)	-790.458383	-789.937435
<b>5</b>	B3LYP	6-31+G(d)	-597.7278592	-597.350555
<b>6</b>	B3LYP	6-31+G(d)	-395.2101306	-394.950607
<b>7</b>	B3LYP	6-31+G(d)	-550.2526845	-549.911545
(MeLi·OMe <sub>2</sub> ) <sub>4</sub>	B3LYP	6-311+G(d,p)	-810.2531367	-809.788154
TMEDA	B3LYP	6-311+G(d,p)	-347.8467513	-347.625504
Me <sub>2</sub> O	B3LYP	6-311+G(d,p)	-155.0770439	-154.997766
<b>4</b>	B3LYP	6-311+G(d,p)	-790.6635023	-790.147304
<b>5</b>	B3LYP	6-311+G(d,p)	-597.8888251	-597.515139
<b>6</b>	B3LYP	6-311+G(d,p)	-395.3122291	-395.05519
<b>7</b>	B3LYP	6-311+G(d,p)	-550.3987975	-550.060853
(MeLi·OMe <sub>2</sub> ) <sub>4</sub>	M052X	6-31+G(d)	-809.8392331	-809.35865
TMEDA	M052X	6-31+G(d)	-347.687268	-347.459351
Me <sub>2</sub> O	M052X	6-31+G(d)	-154.995679	-154.913736
<b>4</b>	M052X	6-31+G(d)	-790.3079161	-789.77613
<b>5</b>	M052X	6-31+G(d)	-597.5997887	-597.214223
<b>6</b>	M052X	6-31+G(d)	-395.1253899	-394.860842
<b>7</b>	M052X	6-31+G(d)	-550.142262	-549.793608
(MeLi·OMe <sub>2</sub> ) <sub>4</sub>	M052X	6-31+G(d,p)	-809.8907727	-809.413094
TMEDA	M052X	6-31+G(d,p)	-347.7078464	-347.481162
Me <sub>2</sub> O	M052X	6-31+G(d,p)	-155.0036945	-154.922218
<b>4</b>	M052X	6-31+G(d,p)	-790.3593737	-789.830303
<b>5</b>	M052X	6-31+G(d,p)	-597.6385305	-597.255145
<b>6</b>	M052X	6-31+G(d,p)	-395.151052	-394.887867
<b>7</b>	M052X	6-31+G(d,p)	-550.1763042	-549.829542
(MeLi·OMe <sub>2</sub> ) <sub>4</sub>	M052X	6-311+G(d,p)	-810.0760732	-809.600042
TMEDA	M052X	6-311+G(d,p)	-347.7783137	-347.552023
Me <sub>2</sub> O	M052X	6-311+G(d,p)	-155.0404023	-154.959152
<b>4</b>	M052X	6-311+G(d,p)	-790.5177517	-789.990312
<b>5</b>	M052X	6-311+G(d,p)	-597.7644322	-597.382233
<b>6</b>	M052X	6-311+G(d,p)	-395.2296964	-394.96735
<b>7</b>	M052X	6-311+G(d,p)	-550.2925587	-549.946522
(MeLi·OMe <sub>2</sub> ) <sub>4</sub>	M052X	6-311+G(3df,3pd)	-810.1464689	-809.669993
TMEDA	M052X	6-311+G(3df,3pd)	-347.8100765	-347.583502
Me <sub>2</sub> O	M052X	6-311+G(3df,3pd)	-155.0553667	-154.974001
<b>4</b>	M052X	6-311+G(3df,3pd)	-790.5854366	-790.057668
<b>5</b>	M052X	6-311+G(3df,3pd)	-597.8156834	-597.433325
<b>6</b>	M052X	6-311+G(3df,3pd)	-395.2633756	-395.000877
<b>7</b>	M052X	6-311+G(3df,3pd)	-550.3400907	-549.993835
(MeLi·OMe <sub>2</sub> ) <sub>4</sub>	M06L	6-31+G(d)	-809.8663417	-809.398292

Verbindung	Methode	Basissatz	SCF [Hartree]	ZPE [Hartree]
TMEDA	M06L	6-31+G(d)	-347.6817672	-347.458728
Me <sub>2</sub> O	M06L	6-31+G(d)	-154.9969941	-154.917114
<b>4</b>	M06L	6-31+G(d)	-790.3070345	-789.78625
<b>5</b>	M06L	6-31+G(d)	-597.6039773	-597.22742
<b>6</b>	M06L	6-31+G(d)	-395.1229029	-394.863679
<b>7</b>	M06L	6-31+G(d)	-550.1419112	-549.800854
(MeLi·OMe <sub>2</sub> ) <sub>4</sub>	M06	6-31+G(d)	-809.4515834	-808.984639
TMEDA	M06	6-31+G(d)	-347.484688	-347.262609
Me <sub>2</sub> O	M06	6-31+G(d)	-154.9256711	-154.845987
<b>4</b>	M06	6-31+G(d)	-789.8510142	-789.333081
<b>5</b>	M06	6-31+G(d)	-597.2735961	-596.899181
<b>6</b>	M06	6-31+G(d)	-394.8963081	-394.63845
<b>7</b>	M06	6-31+G(d)	-549.842982	-549.503173
(MeLi·OMe <sub>2</sub> ) <sub>4</sub>	M06	6-31+G(d,p)	-809.4981239	-809.033277
TMEDA	M06	6-31+G(d,p)	-347.5030491	-347.282092
Me <sub>2</sub> O	M06	6-31+G(d,p)	-154.932601	-154.853295
<b>4</b>	M06	6-31+G(d,p)	-789.898422	-789.38224
<b>5</b>	M06	6-31+G(d,p)	-597.3087204	-596.936009
<b>6</b>	M06	6-31+G(d,p)	-394.9194758	-394.662877
<b>7</b>	M06	6-31+G(d,p)	-549.8736423	-549.535587
(MeLi·OMe <sub>2</sub> ) <sub>4</sub>	M06	6-311+G(d,p)	-809.6686434	-809.204725
TMEDA	M06	6-311+G(d,p)	-347.5705675	-347.350106
Me <sub>2</sub> O	M06	6-311+G(d,p)	-154.965705	-154.886694
<b>4</b>	M06	6-311+G(d,p)	-790.0515134	-789.537317
<b>5</b>	M06	6-311+G(d,p)	-597.4284037	-597.056591
<b>6</b>	M06	6-311+G(d,p)	-394.9948812	-394.739221
<b>7</b>	M06	6-311+G(d,p)	-549.9834329	-549.646319
(MeLi·OMe <sub>2</sub> ) <sub>4</sub>	M062X	6-31+G(d)	-809.5921556	-809.114546
TMEDA	M062X	6-31+G(d)	-347.5752752	-347.349337
Me <sub>2</sub> O	M062X	6-31+G(d)	-154.9493881	-154.868254
<b>4</b>	M062X	6-31+G(d)	-790.0549505	-789.527561
<b>5</b>	M062X	6-31+G(d)	-597.4099635	-597.027687
<b>6</b>	M062X	6-31+G(d)	-394.9963779	-394.734125
<b>7</b>	M062X	6-31+G(d)	-549.9695961	-549.623925
(MeLi·OMe <sub>2</sub> ) <sub>4</sub>	M062X	6-31+G(d,p)	-809.6325003	-809.157484
TMEDA	M062X	6-31+G(d,p)	-347.5909267	-347.366193
Me <sub>2</sub> O	M062X	6-31+G(d,p)	-154.9554086	-154.874729
<b>4</b>	M062X	6-31+G(d,p)	-790.0951256	-789.570445
<b>5</b>	M062X	6-31+G(d,p)	-597.4401272	-597.059954
<b>6</b>	M062X	6-31+G(d,p)	-395.0162823	-394.755342
<b>7</b>	M062X	6-31+G(d,p)	-549.9959015	-549.651994
(MeLi·OMe <sub>2</sub> ) <sub>4</sub>	M062X	6-311+G(d,p)	-809.8315867	-809.35776
TMEDA	M062X	6-311+G(d,p)	-347.6673395	-347.442854
Me <sub>2</sub> O	M062X	6-311+G(d,p)	-154.9948657	-154.914334
<b>4</b>	M062X	6-311+G(d,p)	-790.2667108	-789.74238
<b>5</b>	M062X	6-311+G(d,p)	-597.576206	-597.196896
<b>6</b>	M062X	6-311+G(d,p)	-395.1025898	-394.841435
<b>7</b>	M062X	6-311+G(d,p)	-550.1213799	-549.777852
(MeLi·OMe <sub>2</sub> ) <sub>4</sub>	MP2	6-31+G(d)	-807.050413	-806.569326
TMEDA	MP2	6-31+G(d)	-346.5176155	-346.289758
Me <sub>2</sub> O	MP2	6-31+G(d)	-154.5146295	-154.432852

Verbindung	Methode	Basissatz	SCF [Hartree]	ZPE [Hartree]
4	MP2	6-31+G(d)	-787.5416464	-787.01048
5	MP2	6-31+G(d)	-595.5176552	-595.133118
6	MP2	6-31+G(d)	-393.740638	-393.476352
7	MP2	6-31+G(d)	-548.2770647	-547.929243
(MeLi-OMe <sub>2</sub> ) <sub>4</sub>	MP2	6-311+G(d,p)	-807.6578597	-807.182555
TMEDA	MP2	6-311+G(d,p)	-346.7587241	-346.533301
Me <sub>2</sub> O	MP2	6-311+G(d,p)	-154.6234455	-154.542434
4	MP2	6-311+G(d,p)	-788.1070569	-787.582254
5	MP2	6-311+G(d,p)	-595.952977	-595.572902
6	MP2	6-311+G(d,p)	-394.0226722	-393.761348
7	MP2	6-311+G(d,p)	-548.6695379	-548.325276

Tabelle 10.256 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
Li	0.555257476	1.0515026445	0.8255215649
Li	-0.555257476	-1.0515026445	0.8255215649
Li	1.0515026445	-0.555257476	-0.8256930122
Li	-1.0515026445	0.555257476	-0.8256930122
C	0.7617537305	1.5890727788	-1.2556866071
C	-1.5890727788	0.7617537305	1.2555151598
C	-0.7617537305	-1.5890727788	-1.2556866071
C	1.5890727788	-0.7617537305	1.2555151598
H	0.0164035074	2.3707572459	-1.5414386823
H	1.1690839541	1.2494465526	-2.2376351031
H	1.6014509551	2.1743808275	-0.8117285233
H	-2.3707572459	0.0164035074	1.541267235
H	-2.1743808275	1.6014509551	0.8115570759
H	-1.2494465526	1.1690839541	2.2374636557
H	-0.0164035074	-2.3707572459	-1.5414386823
H	-1.1690839541	-1.2494465526	-2.2376351031
H	-1.6014509551	-2.1743808275	-0.8117285233
H	1.2494465526	-1.1690839541	2.2374636557
H	2.3707572459	-0.0164035074	1.541267235
H	2.1743808275	-1.6014509551	0.8115570759
O	2.5216324277	-1.0756854757	-1.9183497123
O	-1.0756854757	-2.5216324277	1.9181782649
O	1.0756854757	2.5216324277	1.9181782649
O	-2.5216324277	1.0756854757	-1.9183497123
C	-0.2978695806	-3.6502789834	1.6024371516
H	0.7540795967	-3.5023386458	1.9277311799
H	-0.712918581	-4.5576961862	2.0877797563
H	-0.3273518214	-3.7658836207	0.5056647526
C	-1.0983178768	-2.25155962	3.2949663521
H	-1.5803730478	-3.0833291211	3.8494850844
H	-0.0676872706	-2.1043847172	3.6850898578
H	-1.6777172402	-1.3233626071	3.4359943619
C	-3.6502789834	0.2978695806	-1.602608599
H	-4.5576961862	0.712918581	-2.0879512037

H	-3.5023386458	-0.7540795967	-1.9279026273
H	-3.7658836207	0.3273518214	-0.5058362
C	-2.25155962	1.0983178768	-3.2951377995
H	-2.1043847172	0.0676872706	-3.6852613052
H	-3.0833291211	1.5803730478	-3.8496565318
H	-1.3233626071	1.6777172402	-3.4361658092
C	3.6502789834	-0.2978695806	-1.602608599
H	3.7658836207	-0.3273518214	-0.5058362
H	4.5576961862	-0.712918581	-2.0879512037
H	3.5023386458	0.7540795967	-1.9279026273
C	2.25155962	-1.0983178768	-3.2951377995
H	2.1043847172	-0.0676872706	-3.6852613052
H	3.0833291211	-1.5803730478	-3.8496565318
H	1.3233626071	-1.6777172402	-3.4361658092
C	0.2978695806	3.6502789834	1.6024371516
H	-0.7540795967	3.5023386458	1.9277311799
H	0.712918581	4.5576961862	2.0877797563
H	0.3273518214	3.7658836207	0.5056647526
C	1.0983178768	2.25155962	3.2949663521
H	1.5803730478	3.0833291211	3.8494850844
H	0.0676872706	2.1043847172	3.6850898578
H	1.6777172402	1.3233626071	3.4359943619

Tabelle 10.257 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
C	-0.0428784033	0.7556872029	-0.0760800951
C	0.0428784033	-0.7556872029	-0.0760800951
N	-1.3766116135	1.2355594446	-0.3304670321
N	1.3766116135	-1.2355594446	-0.3304670321
C	-1.3823873043	2.6648334158	-0.459414682
C	-2.2991784298	0.814951623	0.6873080234
C	1.3823873043	-2.6648334158	-0.459414682
C	2.2991784298	-0.814951623	0.6873080234
H	0.6233194839	1.130085444	-0.8784352006
H	0.3397828562	1.1729846863	0.8959376851
H	-0.6233194839	-1.130085444	-0.8784352006
H	-0.3397828562	-1.1729846863	0.8959376851
H	-2.3986918538	3.0187401352	-0.7078133438
H	-0.6988947764	2.9756050321	-1.2694909032
H	-1.0587983578	3.1789969688	0.4839776961
H	-2.3639863147	-0.2859480333	0.7290758208
H	-3.3067471038	1.2073777302	0.4636036065
H	-1.9999299909	1.1832662611	1.704909425
H	2.3986918538	-3.0187401352	-0.7078133438
H	0.6988947764	-2.9756050321	-1.2694909032
H	1.0587983578	-3.1789969688	0.4839776961
H	3.3067471038	-1.2073777302	0.4636036065
H	1.9999299909	-1.1832662611	1.704909425
H	2.3639863147	0.2859480333	0.7290758208

Tabelle 10.258 Standardorientierung von  $\text{Me}_2\text{O}$  ( $\text{C}_{2v}$ ) [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
C	0.	1.1510962271	-0.1917853247
O	0.	0.	0.5943166093
C	0.	-1.1510962271	-0.1917853247
H	-0.9012289139	1.1990885063	-0.8442559059
H	0.9012289139	1.1990885063	-0.8442559059
H	0.	2.0209252425	0.4845063319
H	0.9012289139	-1.1990885063	-0.8442559059
H	-0.9012289139	-1.1990885063	-0.8442559059
H	0.	-2.0209252425	0.4845063319

Tabelle 10.259 Standardorientierung von  $\mathbf{4}$  ( $\text{C}_2$ ) [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
C	0.0547532266	3.6057499315	0.8968196404
N	0.2422043035	2.2848798788	1.4644467544
C	-0.7902359843	1.962638112	2.4170500857
C	1.5453257323	2.1294751461	2.0642092577
C	0.8048392353	3.7560654273	-0.4079211201
N	0.3758987674	2.7719438517	-1.3815541845
C	-0.9075348538	3.0988996509	-1.9558437749
C	1.3647368474	2.5728462361	-2.4131181213
C	-0.0547532266	-3.6057499315	0.8968196404
N	-0.2422043035	-2.2848798788	1.4644467544
C	-1.5453257323	-2.1294751461	2.0642092577
C	0.7902359843	-1.962638112	2.4170500857
C	-0.8048392353	-3.7560654273	-0.4079211201
N	-0.3758987674	-2.7719438517	-1.3815541845
C	-1.3647368474	-2.5728462361	-2.4131181213
C	0.9075348538	-3.0988996509	-1.9558437749
Li	0.1321955799	1.086219606	-0.2411379164
Li	-0.1321955799	-1.086219606	-0.2411379164
C	-1.7951611646	0.2165668877	-0.4794080342
C	1.7951611646	-0.2165668877	-0.4794080342
H	-1.0298847538	3.7433963704	0.7209357281
H	0.3652891968	4.4084915545	1.611757751
H	-0.6309132749	0.9363678908	2.7971802359
H	-1.7786074835	1.9848474459	1.9249852845
H	-0.7915669783	2.6619651488	3.2890280796
H	1.6894302084	1.0763704366	2.3643567684
H	1.6683398969	2.7896175006	2.9583305823
H	2.3432409073	2.3624668522	1.338865983
H	0.68693822	4.7978569086	-0.7983507615
H	1.888369131	3.6065159244	-0.2353422921
H	-1.2331085973	2.2813177164	-2.621507163
H	-1.6777546271	3.1902660986	-1.1706993249
H	-0.8670550219	4.0525970256	-2.537747721
H	1.0142420389	1.7917834814	-3.1100527094
H	1.5580264467	3.5065848264	-2.9954173793
H	2.3093400635	2.2160794669	-1.9647427685

H	-0.3652891968	-4.4084915545	1.611757751
H	1.0298847538	-3.7433963704	0.7209357281
H	-1.6894302084	-1.0763704366	2.3643567684
H	-2.3432409073	-2.3624668522	1.338865983
H	-1.6683398969	-2.7896175006	2.9583305823
H	0.6309132749	-0.9363678908	2.7971802359
H	0.7915669783	-2.6619651488	3.2890280796
H	1.7786074835	-1.9848474459	1.9249852845
H	-1.888369131	-3.6065159244	-0.2353422921
H	-0.68693822	-4.7978569086	-0.7983507615
H	-1.0142420389	-1.7917834814	-3.1100527094
H	-2.3093400635	-2.2160794669	-1.9647427685
H	-1.5580264467	-3.5065848264	-2.9954173793
H	1.2331085973	-2.2813177164	-2.621507163
H	0.8670550219	-4.0525970256	-2.537747721
H	1.6777546271	-3.1902660986	-1.1706993249
H	-2.0473250134	0.2939680025	-1.5637612261
H	-2.273624881	1.112790394	-0.0160972218
H	-2.4198895615	-0.6311484828	-0.1087014306
H	2.0473250134	-0.2939680025	-1.5637612261
H	2.273624881	-1.112790394	-0.0160972218
H	2.4198895615	0.6311484828	-0.1087014306

Tabelle 10.260 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
O	0.	0.	3.71556077
C	0.0119227456	1.1757431969	4.479973362
Li	0.	0.	1.8753721361
Li	0.	0.	-0.2898780161
C	-0.0027662859	1.814269047	0.869841678
H	0.0193875042	2.0212020093	3.7712274751
H	0.9162311368	1.2175941512	5.1220975981
H	-0.8904432523	1.2350660183	5.1234675108
H	-0.0524769685	2.2183587351	-0.1694867189
H	0.8823576383	2.3301420101	1.3098885119
H	-0.8888768877	2.2725705472	1.369752314
C	-0.6652997555	0.3603558351	-2.9281622571
N	-1.4411975837	0.034250221	-1.7470720156
C	-2.4491838342	1.0297688341	-1.4720407473
C	-2.0358879039	-1.2790611207	-1.8292309135
H	-0.4965999348	1.4548590077	-2.9250870747
H	-1.2273337421	0.1287365962	-3.8669896403
H	-2.9848398953	0.7616728736	-0.5449180065
H	-1.9740899086	2.0135394048	-1.3090291839
H	-3.1941130718	1.1111506479	-2.3005697335
H	-2.4970746279	-1.5365484075	-0.8600947956
H	-2.8112928231	-1.3288604846	-2.6326300543
H	-1.2686952244	-2.0461643882	-2.0306013376
C	-0.0119227456	-1.1757431969	4.479973362
C	0.0027662859	-1.814269047	0.869841678

H	-0.0193875042	-2.0212020093	3.7712274751
H	-0.9162311368	-1.2175941512	5.1220975981
H	0.8904432523	-1.2350660183	5.1234675108
H	0.0524769685	-2.2183587351	-0.1694867189
H	-0.8823576383	-2.3301420101	1.3098885119
H	0.8888768877	-2.2725705472	1.369752314
C	0.6652997555	-0.3603558351	-2.9281622571
N	1.4411975837	-0.034250221	-1.7470720156
C	2.4491838342	-1.0297688341	-1.4720407473
C	2.0358879039	1.2790611207	-1.8292309135
H	0.4965999348	-1.4548590077	-2.9250870747
H	1.2273337421	-0.1287365962	-3.8669896403
H	2.9848398953	-0.7616728736	-0.5449180065
H	1.9740899086	-2.0135394048	-1.3090291839
H	3.1941130718	-1.1111506479	-2.3005697335
H	2.4970746279	1.5365484075	-0.8600947956
H	2.8112928231	1.3288604846	-2.6326300543
H	1.2686952244	2.0461643882	-2.0306013376

Tabelle 10.261 Standardorientierung von **6** [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
N	-1.5175352535	0.050963893	-0.0347717398
C	-1.0467977839	-1.2158355975	-0.5676521196
C	0.2827999311	-1.618028461	0.0357187064
N	1.207069953	-0.5068525911	0.022967896
C	1.6955885955	-0.2006584702	-1.3041848668
C	2.3095679788	-0.6719415641	0.9372604617
C	-2.6695339226	0.5220410364	-0.7681398429
C	-1.8191629129	-0.0453469231	1.3773855122
H	-0.9525171195	-1.0996215344	-1.6645536956
H	-1.7965037358	-2.0277979604	-0.3970860752
H	0.6836765702	-2.5100624353	-0.5054197479
H	0.1432446561	-1.9302572703	1.088623748
H	2.2655288667	0.7456553556	-1.2653424702
H	0.8553303343	-0.0457533483	-2.0051677797
H	2.3400976228	-1.0203824502	-1.7042834072
H	2.8915136225	0.2663187946	0.9665465528
H	2.9839401807	-1.5095059564	0.6366567497
H	1.9311735072	-0.8730061156	1.9553297381
H	-2.9735871321	1.5131879284	-0.3908261094
H	-3.5363932686	-0.1751530613	-0.6737262032
H	-2.4173284499	0.6251341441	-1.8377811889
H	-2.197955719	0.9251770273	1.7416541197
H	-0.9099615046	-0.2909778781	1.9560703645
H	-2.5895494394	-0.8270998802	1.5847711227
Li	0.1721545596	1.2289561555	0.1520848557
C	1.2297879225	2.9200258	0.1479390511
H	1.3325860414	3.3641311926	-0.8668762467
H	2.2713969397	2.729465987	0.4980670341
H	0.8517609598	3.7413641828	0.7923905803

Tabelle 10.262 Standardorientierung von **7** [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
N	0.6453459158	1.5538132289	-0.1392958447
C	1.8924722113	0.9379379468	0.2804541583
C	2.1432783281	-0.37252907	-0.4304603199
N	1.1080826373	-1.3474562158	-0.1300740261
C	1.3537037966	-2.0017634044	1.1381453226
C	0.9714331758	-2.3207664075	-1.1852495055
C	0.2668342309	2.6033572994	0.7811041423
C	0.7089020222	2.0532643838	-1.4900501509
H	1.8089972547	0.7569861545	1.3706474915
H	2.7565859208	1.6314126371	0.1233492516
H	3.1541301652	-0.7637781683	-0.1601570992
H	2.1563428525	-0.2102115801	-1.525329381
H	0.5112181862	-2.6719078726	1.3799331843
H	1.3946716696	-1.2587744379	1.9523183354
H	2.3018117947	-2.5935397853	1.1100086509
H	0.1645459903	-3.0317625389	-0.9311546163
H	1.907519861	-2.910199229	-1.3414684292
H	0.7037009169	-1.8205567454	-2.1328724062
H	-0.689209256	3.0529400823	0.4578654641
H	1.0366210294	3.4115929586	0.8270301847
H	0.1071912263	2.1610152271	1.7811563814
H	-0.2639854185	2.4974805491	-1.7667242204
H	0.9167369157	1.2401497075	-2.206523526
H	1.4945520532	2.8398543553	-1.60732945
Li	-0.4691054175	-0.0966818041	0.3444742424
C	-0.9752771571	-0.084385584	2.3276106465
H	-0.0967791955	0.2161736502	2.9533832898
H	-1.2601382848	-1.0839553376	2.7343225895
H	-1.7900762034	0.5996218691	2.6641769576
C	-2.7230286521	0.8530783217	-0.5223644173
O	-1.9910734352	-0.3079847791	-0.8463195192
H	-2.2059361764	1.708923202	-0.9895934058
H	-2.7433445584	0.9885969633	0.5811612112
H	-3.7552045535	0.7855351019	-0.9268726492
C	-2.6226789024	-1.4540670038	-0.317708066
H	-2.6496903515	-1.3911866326	0.7914287241
H	-2.0216879132	-2.3286514652	-0.6201679027
H	-3.647954679	-1.555023577	-0.7330332929

Tabelle 10.263 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; PBE/6-31+G(d)].

	x	y	z
Li	0.5013467911	1.1317239445	0.8615040759
Li	-0.5013467911	-1.1317239445	0.8615040759
Li	1.1317239445	-0.5013467911	-0.8616755233
Li	-1.1317239445	0.5013467911	-0.8616755233
C	0.6864816838	1.6863699079	-1.2976702366

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C	-1.6863699079	0.6864816838	1.2974987893
C	-0.6864816838	-1.6863699079	-1.2976702366
C	1.6863699079	-0.6864816838	1.2974987893
H	-0.0663376498	2.4846280599	-1.5089170852
H	1.0245032884	1.3765707049	-2.3158773027
H	1.5613427715	2.2547403929	-0.900743143
H	-2.4846280599	-0.0663376498	1.5087456379
H	-2.2547403929	1.5613427715	0.9005716956
H	-1.3765707049	1.0245032884	2.3157058554
H	0.0663376498	-2.4846280599	-1.5089170852
H	-1.0245032884	-1.3765707049	-2.3158773027
H	-1.5613427715	-2.2547403929	-0.900743143
H	1.3765707049	-1.0245032884	2.3157058554
H	2.4846280599	0.0663376498	1.5087456379
H	2.2547403929	-1.5613427715	0.9005716956
O	2.7056191074	-1.0248317768	-2.0206835174
O	-1.0248317768	-2.7056191074	2.0205120701
O	1.0248317768	2.7056191074	2.0205120701
O	-2.7056191074	1.0248317768	-2.0206835174
C	-0.3479384093	-3.9339211029	1.740340124
H	0.6703447663	-3.9316023858	2.1777150999
H	-0.9214628047	-4.7923863833	2.1434580223
H	-0.2798639969	-4.0158685529	0.6450895721
C	-1.1949477209	-2.4851758704	3.4214668214
H	-1.8067840578	-3.2933776513	3.8699286155
H	-0.2145844516	-2.4392520158	3.9374804124
H	-1.7162787985	-1.5220245763	3.5314933528
C	-3.9339211029	0.3479384093	-1.7405115713
H	-4.7923863833	0.9214628047	-2.1436294696
H	-3.9316023858	-0.6703447663	-2.1778865473
H	-4.0158685529	0.2798639969	-0.6452610194
C	-2.4851758704	1.1949477209	-3.4216382688
H	-2.4392520158	0.2145844516	-3.9376518598
H	-3.2933776513	1.8067840578	-3.8701000628
H	-1.5220245763	1.7162787985	-3.5316648002
C	3.9339211029	-0.3479384093	-1.7405115713
H	4.0158685529	-0.2798639969	-0.6452610194
H	4.7923863833	-0.9214628047	-2.1436294696
H	3.9316023858	0.6703447663	-2.1778865473
C	2.4851758704	-1.1949477209	-3.4216382688
H	2.4392520158	-0.2145844516	-3.9376518598
H	3.2933776513	-1.8067840578	-3.8701000628
H	1.5220245763	-1.7162787985	-3.5316648002
C	0.3479384093	3.9339211029	1.740340124
H	-0.6703447663	3.9316023858	2.1777150999
H	0.9214628047	4.7923863833	2.1434580223
H	0.2798639969	4.0158685529	0.6450895721
C	1.1949477209	2.4851758704	3.4214668214
H	1.8067840578	3.2933776513	3.8699286155
H	0.2145844516	2.4392520158	3.9374804124
H	1.7162787985	1.5220245763	3.5314933528

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Tabelle 10.264 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; PBE/6-31+G(d)].

	x	y	z
C	-0.0567082656	0.766748672	-0.0640356974
C	0.0567082656	-0.766748672	-0.0640356974
N	-1.4272935215	1.2332987492	-0.3033926796
N	1.4272935215	-1.2332987492	-0.3033926796
C	-1.4434150045	2.6714527321	-0.5579884687
C	-2.3273946081	0.9000736386	0.799071712
C	1.4434150045	-2.6714527321	-0.5579884687
C	2.3273946081	-0.9000736386	0.799071712
H	0.577473269	1.144485854	-0.8865497947
H	0.3437585266	1.1959104006	0.8894327845
H	-0.577473269	-1.144485854	-0.8865497947
H	-0.3437585266	-1.1959104006	0.8894327845
H	-2.4730245192	2.9941115789	-0.7906828527
H	-0.8044097109	2.9038953624	-1.4271359153
H	-1.0807239557	3.2733794632	0.3130749799
H	-2.3879416686	-0.19216644	0.9326214505
H	-3.3413535521	1.2691279429	0.5679085886
H	-2.0047537754	1.3532266332	1.770786893
H	2.4730245192	-2.9941115789	-0.7906828527
H	0.8044097109	-2.9038953624	-1.4271359153
H	1.0807239557	-3.2733794632	0.3130749799
H	3.3413535521	-1.2691279429	0.5679085886
H	2.0047537754	-1.3532266332	1.770786893
H	2.3879416686	0.19216644	0.9326214505

Tabelle 10.265 Standardorientierung von Me<sub>2</sub>O (C<sub>2v</sub>) [globales Minimum; PBE/6-31+G(d)].

	x	y	z
C	0.	1.1752663203	-0.1986633484
O	0.	0.	0.596972024
C	0.	-1.1752663203	-0.1986633484
H	-0.9021992092	1.2294182809	-0.8457875095
H	0.9021992092	1.2294182809	-0.8457875095
H	0.	2.0321134184	0.4931198555
H	0.9021992092	-1.2294182809	-0.8457875095
H	-0.9021992092	-1.2294182809	-0.8457875095
H	0.	-2.0321134184	0.4931198555

Tabelle 10.266 Standardorientierung von **4** (C<sub>2</sub>) [globales Minimum; PBE/6-31+G(d)].

	x	y	z
C	0.0698859879	3.911830393	0.8166586144
N	0.2834816853	2.6320317978	1.5180814723
C	-0.7487045696	2.4125350231	2.5388683454
C	1.6146084942	2.5644315984	2.1357470022
C	0.7994900028	3.9659837386	-0.5318888527
N	0.3597939004	2.8996633772	-1.4512663672
C	-0.9422671591	3.2083748885	-2.0594165811
C	1.3607138793	2.6630079816	-2.5005742448

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C	-0.0698859879	-3.911830393	0.8166586144
N	-0.2834816853	-2.6320317978	1.5180814723
C	-1.6146084942	-2.5644315984	2.1357470022
C	0.7487045696	-2.4125350231	2.5388683454
C	-0.7994900028	-3.9659837386	-0.5318888527
N	-0.3597939004	-2.8996633772	-1.4512663672
C	-1.3607138793	-2.6630079816	-2.5005742448
C	0.9422671591	-3.2083748885	-2.0594165811
Li	0.1375036172	1.1497374889	-0.1479634371
Li	-0.1375036172	-1.1497374889	-0.1479634371
C	-1.8448421863	0.2203563878	-0.3320413479
C	1.8448421863	-0.2203563878	-0.3320413479
H	-1.0166009734	4.0264619385	0.6560071977
H	0.3915541297	4.779908681	1.4411481753
H	-0.5826751098	1.433010781	3.0177577671
H	-1.743838761	2.3931542988	2.0661859444
H	-0.7351486775	3.1983970436	3.3306564535
H	1.7590745948	1.5662831937	2.5796893734
H	1.7433045415	3.337441539	2.9303005869
H	2.402873602	2.7015631067	1.3795173661
H	0.6587561218	4.9777277423	-0.9824988717
H	1.8851479542	3.8426846107	-0.372539161
H	-1.2575896121	2.3635825281	-2.691997381
H	-1.7132606547	3.3374506576	-1.2839762278
H	-0.8996365196	4.1328100998	-2.6826717423
H	1.0156415512	1.8435209185	-3.1521455735
H	1.534260243	3.5668900969	-3.1305853946
H	2.3138009701	2.350864184	-2.0435308523
H	-0.3915541297	-4.779908681	1.4411481753
H	1.0166009734	-4.0264619385	0.6560071977
H	-1.7590745948	-1.5662831937	2.5796893734
H	-2.402873602	-2.7015631067	1.3795173661
H	-1.7433045415	-3.337441539	2.9303005869
H	0.5826751098	-1.433010781	3.0177577671
H	0.7351486775	-3.1983970436	3.3306564535
H	1.743838761	-2.3931542988	2.0661859444
H	-1.8851479542	-3.8426846107	-0.372539161
H	-0.6587561218	-4.9777277423	-0.9824988717
H	-1.0156415512	-1.8435209185	-3.1521455735
H	-2.3138009701	-2.350864184	-2.0435308523
H	-1.534260243	-3.5668900969	-3.1305853946
H	1.2575896121	-2.3635825281	-2.691997381
H	0.8996365196	-4.1328100998	-2.6826717423
H	1.7132606547	-3.3374506576	-1.2839762278
H	-2.1418165467	0.286987482	-1.4068518818
H	-2.293806331	1.1325283747	0.1310659224
H	-2.4819039305	-0.6017461745	0.0748266939
H	2.1418165467	-0.286987482	-1.4068518818
H	2.293806331	-1.1325283747	0.1310659224
H	2.4819039305	0.6017461745	0.0748266939

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Tabelle 10.267 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; PBE/6-31+G(d)].

	x	y	z
O	0.	0.	3.9466893107
C	0.0205731632	1.1929289629	4.733146138
Li	0.	0.	1.9981586994
Li	0.	0.	-0.2677493284
C	0.0039903448	1.8574100914	0.9735259756
H	0.0344708949	2.0378255525	4.028226211
H	0.9249921469	1.2234851838	5.3728595724
H	-0.8817685014	1.2542502875	5.3735841538
H	-0.0443940389	2.3175631989	-0.0422075221
H	0.9007508369	2.340982767	1.4314682536
H	-0.8682689795	2.3156490234	1.5008301297
C	-0.6800678364	0.3559660607	-3.0477881281
N	-1.4863201373	0.0210197442	-1.8576977855
C	-2.5255027517	1.0324785838	-1.6178031887
C	-2.1020300978	-1.3093432734	-1.9706287892
H	-0.5271595888	1.4496307718	-3.0496939704
H	-1.2217687833	0.1104106187	-3.9922363357
H	-3.0831170435	0.7691009762	-0.7040945794
H	-2.0584676726	2.0174899508	-1.4562299676
H	-3.2472748193	1.1047011185	-2.4646332342
H	-2.6199741126	-1.5511611341	-1.028746984
H	-2.8337863164	-1.3567760492	-2.8110967409
H	-1.3334405443	-2.0818053868	-2.1284691168
C	-0.0205731632	-1.1929289629	4.733146138
C	-0.0039903448	-1.8574100914	0.9735259756
H	-0.0344708949	-2.0378255525	4.028226211
H	-0.9249921469	-1.2234851838	5.3728595724
H	0.8817685014	-1.2542502875	5.3735841538
H	0.0443940389	-2.3175631989	-0.0422075221
H	-0.9007508369	-2.340982767	1.4314682536
H	0.8682689795	-2.3156490234	1.5008301297
C	0.6800678364	-0.3559660607	-3.0477881281
N	1.4863201373	-0.0210197442	-1.8576977855
C	2.5255027517	-1.0324785838	-1.6178031887
C	2.1020300978	1.3093432734	-1.9706287892
H	0.5271595888	-1.4496307718	-3.0496939704
H	1.2217687833	-0.1104106187	-3.9922363357
H	3.0831170435	-0.7691009762	-0.7040945794
H	2.0584676726	-2.0174899508	-1.4562299676
H	3.2472748193	-1.1047011185	-2.4646332342
H	2.6199741126	1.5511611341	-1.028746984
H	2.8337863164	1.3567760492	-2.8110967409
H	1.3334405443	2.0818053868	-2.1284691168

Tabelle 10.268 Standardorientierung von **6** [globales Minimum; PBE/6-31+G(d)].

	x	y	z
N	-1.4595479537	0.0918325943	0.0330655235
C	-1.0354832055	-1.228996942	-0.4723092207

C	0.3279811156	-1.6525409333	0.0950956914
N	1.358296543	-0.6147454118	-0.107085237
C	1.827411546	-0.565419856	-1.5017038023
C	2.5013949787	-0.8049362199	0.7985941515
C	-2.4983289772	0.6884011744	-0.820455629
C	-1.9331608347	0.024771511	1.4253066744
H	-0.9778459914	-1.1599668188	-1.5730497849
H	-1.7875903965	-2.0203336223	-0.2447974382
H	0.6261241198	-2.626284932	-0.359423944
H	0.2429858289	-1.828190871	1.1821368506
H	2.5414298989	0.2667020647	-1.613604255
H	0.9859411766	-0.3794857039	-2.1891287873
H	2.3269460496	-1.5138961432	-1.8064346276
H	3.2103100798	0.0282644482	0.6655252673
H	3.034953469	-1.7645845323	0.6098494279
H	2.1542931591	-0.7932526128	1.8452394988
H	-2.7336587799	1.6993381432	-0.4502029057
H	-3.4336294906	0.083202165	-0.8331053566
H	-2.1237693302	0.782828899	-1.853296112
H	-2.1726535311	1.0421563767	1.7751981332
H	-1.1481468978	-0.3806950573	2.0845354271
H	-2.8405889502	-0.6143269762	1.5258999448
Li	0.3353121399	1.2394573601	0.146361887
C	0.8408831959	3.195558148	0.353481158
H	0.7850808728	3.7670458891	-0.6012606491
H	1.8781495464	3.3513695702	0.7286398303
H	0.1873026187	3.7508682889	1.0645832836

Tabelle 10.269 Standardorientierung von **7** [globales Minimum; PBE/6-31+G(d)].

	x	y	z
N	0.7576574483	1.6110574392	-0.1104186452
C	2.0513666027	0.9609666357	0.1832863465
C	2.2078152804	-0.3922049163	-0.52080824
N	1.1866952439	-1.371539581	-0.0954927411
C	1.5369601259	-1.9836518212	1.1986681366
C	1.0159771266	-2.4170829219	-1.1120817934
C	0.4970085177	2.6860861145	0.8619965068
C	0.7160003093	2.1441295988	-1.4778797952
H	2.1039826478	0.8190635728	1.276894047
H	2.9069598009	1.6202670745	-0.0995617275
H	3.2381253965	-0.7792683417	-0.3394003205
H	2.1145033103	-0.2579492572	-1.6129587005
H	0.7262446091	-2.6595090496	1.5130660928
H	1.6210133269	-1.2110994531	1.9771492937
H	2.4918349612	-2.5569991269	1.1343559328
H	0.2527207605	-3.1371583034	-0.7719847119
H	1.9577146791	-2.9822847466	-1.3051327669
H	0.6732943478	-1.9682603725	-2.0599404037
H	-0.4711592385	3.1606679582	0.6307095224
H	1.2883932564	3.4712275516	0.8399614904

H	0.423702742	2.2505674543	1.8711612676
H	-0.2635865361	2.6180495769	-1.6560075466
H	0.8353579946	1.3366049087	-2.2178548006
H	1.5093711895	2.9079251079	-1.6559113463
Li	-0.5176175022	-0.069325256	0.4568654013
C	-1.112846823	-0.105615279	2.4550654877
H	-0.2833232107	0.140282775	3.1646791952
H	-1.4794856716	-1.1006007039	2.8081007288
H	-1.9265161485	0.6069336197	2.735523328
C	-3.0063267923	0.8358014731	-0.5737711019
O	-2.1566197405	-0.28881064	-0.8345975894
H	-2.4727334739	1.7308591827	-0.9297368087
H	-3.2037789619	0.9296620031	0.5114079382
H	-3.9599834644	0.735621429	-1.1307070538
C	-2.8013685388	-1.5102464981	-0.4472379586
H	-2.980903707	-1.5239872889	0.6448129318
H	-2.1206027596	-2.3317718515	-0.7187471744
H	-3.7563391084	-1.6318560672	-0.9976504213

Tabelle 10.270 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
Li	0.5016264148	1.1225668134	0.8566519311
Li	-0.5016264148	-1.1225668134	0.8566519311
Li	1.1225668134	-0.5016264148	-0.8568233785
Li	-1.1225668134	0.5016264148	-0.8568233785
C	0.6897210256	1.6762176271	-1.2910536832
C	-1.6762176271	0.6897210256	1.2908822359
C	-0.6897210256	-1.6762176271	-1.2910536832
C	1.6762176271	-0.6897210256	1.2908822359
H	-0.0564209304	2.4693977175	-1.49951095
H	1.0252423918	1.3647788406	-2.3000880263
H	1.559070633	2.2344377055	-0.8915328642
H	-2.4693977175	-0.0564209304	1.4993395026
H	-2.2344377055	1.559070633	0.8913614169
H	-1.3647788406	1.0252423918	2.299916579
H	0.0564209304	-2.4693977175	-1.49951095
H	-1.0252423918	-1.3647788406	-2.3000880263
H	-1.559070633	-2.2344377055	-0.8915328642
H	1.3647788406	-1.0252423918	2.299916579
H	2.4693977175	0.0564209304	1.4993395026
H	2.2344377055	-1.559070633	0.8913614169
O	2.6777638922	-1.007804871	-2.0091963565
O	-1.007804871	-2.6777638922	2.0090249092
O	1.007804871	2.6777638922	2.0090249092
O	-2.6777638922	1.007804871	-2.0091963565
C	-0.3399748893	-3.8911667403	1.7281075829
H	0.6686242122	-3.891687102	2.1649694361
H	-0.9099792947	-4.7440373537	2.1233676433

H	-0.2665827222	-3.9735712595	0.6417262493
C	-1.1854937414	-2.4599717319	3.3922252131
H	-1.7986121797	-3.2592913693	3.8325365501
H	-0.2166518107	-2.4202529316	3.9109098249
H	-1.6988248723	-1.5024964047	3.5050011656
C	-3.8911667403	0.3399748893	-1.7282790303
H	-4.7440373537	0.9099792947	-2.1235390907
H	-3.891687102	-0.6686242122	-2.1651408834
H	-3.9735712595	0.2665827222	-0.6418976966
C	-2.4599717319	1.1854937414	-3.3923966604
H	-2.4202529316	0.2166518107	-3.9110812723
H	-3.2592913693	1.7986121797	-3.8327079975
H	-1.5024964047	1.6988248723	-3.505172613
C	3.8911667403	-0.3399748893	-1.7282790303
H	3.9735712595	-0.2665827222	-0.6418976966
H	4.7440373537	-0.9099792947	-2.1235390907
H	3.891687102	0.6686242122	-2.1651408834
C	2.4599717319	-1.1854937414	-3.3923966604
H	2.4202529316	-0.2166518107	-3.9110812723
H	3.2592913693	-1.7986121797	-3.8327079975
H	1.5024964047	-1.6988248723	-3.505172613
C	0.3399748893	3.8911667403	1.7281075829
H	-0.6686242122	3.891687102	2.1649694361
H	0.9099792947	4.7440373537	2.1233676433
H	0.2665827222	3.9735712595	0.6417262493
C	1.1854937414	2.4599717319	3.3922252131
H	1.7986121797	3.2592913693	3.8325365501
H	0.2166518107	2.4202529316	3.9109098249
H	1.6988248723	1.5024964047	3.5050011656

Tabelle 10.271 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
C	-0.0549723079	0.7613948422	-0.0683747216
C	0.0549723079	-0.7613948422	-0.0683747216
N	-1.4142709987	1.2254928798	-0.2973984424
N	1.4142709987	-1.2254928798	-0.2973984424
C	-1.4328759658	2.6512764197	-0.5500465927
C	-2.3047270004	0.8905668706	0.7956716678
C	1.4328759658	-2.6512764197	-0.5500465927
C	2.3047270004	-0.8905668706	0.7956716678
H	0.5723521622	1.1335182753	-0.8872237732
H	0.3477028021	1.1867123175	0.8743283078
H	-0.5723521622	-1.1335182753	-0.8872237732
H	-0.3477028021	-1.1867123175	0.8743283078
H	-2.4551569812	2.9725894704	-0.7773153301
H	-0.8027872083	2.884403206	-1.4149434344
H	-1.0700497015	3.2469038701	0.3125480113
H	-2.370630868	-0.1938819485	0.9220899759
H	-3.3109315107	1.2613757999	0.5733501086
H	-1.9798994665	1.3324010037	1.7604252231

H	2.4551569812	-2.9725894704	-0.7773153301
H	0.8027872083	-2.884403206	-1.4149434344
H	1.0700497015	-3.2469038701	0.3125480113
H	3.3109315107	-1.2613757999	0.5733501086
H	1.9798994665	-1.3324010037	1.7604252231
H	2.370630868	0.1938819485	0.9220899759

Tabelle 10.272 Standardorientierung von Me<sub>2</sub>O (C<sub>2v</sub>) [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
C	0.	1.1645549262	-0.1979596386
O	0.	0.	0.5838402231
C	0.	-1.1645549262	-0.1979596386
H	-0.894434006	1.219466043	-0.8396523362
H	0.894434006	1.219466043	-0.8396523362
H	0.	2.0162420171	0.4867116995
H	0.894434006	-1.219466043	-0.8396523362
H	-0.894434006	-1.219466043	-0.8396523362
H	0.	-2.0162420171	0.4867116995

Tabelle 10.273 Standardorientierung von 4 (C<sub>2</sub>) [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
C	0.0598385595	3.8715400967	0.8130758898
N	0.2856273014	2.603614736	1.5030533467
C	-0.7315597295	2.3708967376	2.5176720713
C	1.6088237736	2.542180315	2.1077697331
C	0.785226514	3.9377484255	-0.5254628529
N	0.3660117209	2.8748599828	-1.4361665827
C	-0.925012187	3.1634309352	-2.0467123594
C	1.366621155	2.6420865997	-2.4684886279
C	-0.0598385595	-3.8715400967	0.8130758898
N	-0.2856273014	-2.603614736	1.5030533467
C	-1.6088237736	-2.542180315	2.1077697331
C	0.7315597295	-2.3708967376	2.5176720713
C	-0.785226514	-3.9377484255	-0.5254628529
N	-0.3660117209	-2.8748599828	-1.4361665827
C	-1.366621155	-2.6420865997	-2.4684886279
C	0.925012187	-3.1634309352	-2.0467123594
Li	0.1430355058	1.1408493413	-0.1474858386
Li	-0.1430355058	-1.1408493413	-0.1474858386
C	-1.8381065487	0.2281153942	-0.3316599262
C	1.8381065487	-0.2281153942	-0.3316599262
H	-1.019025262	3.9753190033	0.6516233691
H	0.3686450869	4.7327264757	1.4368246227
H	-0.5575974872	1.3984780251	2.9889200067
H	-1.7219208067	2.3454716943	2.0549926939
H	-0.7207470282	3.1467919676	3.30620378
H	1.7627072353	1.5515367917	2.5448111954
H	1.7348111436	3.306531927	2.8979519534
H	2.3880873446	2.6864019334	1.3556543419

H	0.6300561236	4.9380991621	-0.9732524989
H	1.8640991359	3.8345326067	-0.3648625411
H	-1.2275108626	2.3199472806	-2.6728250263
H	-1.6967099766	3.2875432221	-1.2830588754
H	-0.8885121959	4.0775785413	-2.668833451
H	1.0367102518	1.8229362991	-3.1142458103
H	1.5350849563	3.5369838375	-3.0963136625
H	2.3131025751	2.3425925317	-2.0092553255
H	-0.3686450869	-4.7327264757	1.4368246227
H	1.019025262	-3.9753190033	0.6516233691
H	-1.7627072353	-1.5515367917	2.5448111954
H	-2.3880873446	-2.6864019334	1.3556543419
H	-1.7348111436	-3.306531927	2.8979519534
H	0.5575974872	-1.3984780251	2.9889200067
H	0.7207470282	-3.1467919676	3.30620378
H	1.7219208067	-2.3454716943	2.0549926939
H	-1.8640991359	-3.8345326067	-0.3648625411
H	-0.6300561236	-4.9380991621	-0.9732524989
H	-1.0367102518	-1.8229362991	-3.1142458103
H	-2.3131025751	-2.3425925317	-2.0092553255
H	-1.5350849563	-3.5369838375	-3.0963136625
H	1.2275108626	-2.3199472806	-2.6728250263
H	0.8885121959	-4.0775785413	-2.668833451
H	1.6967099766	-3.2875432221	-1.2830588754
H	-2.1355998728	0.2702351219	-1.398480911
H	-2.2712170227	1.1488015168	0.1082258542
H	-2.4705469933	-0.5746281055	0.0968884329
H	2.1355998728	-0.2702351219	-1.398480911
H	2.2712170227	-1.1488015168	0.1082258542
H	2.4705469933	0.5746281055	0.0968884329

Tabelle 10.274 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
O	0.	0.	3.9137302818
C	0.0195719265	1.1809376059	4.6884512827
Li	0.	0.	1.9809618957
Li	0.	0.	-0.2698173763
C	0.0055050191	1.8510638815	0.9607269956
H	0.0332048744	2.0222345582	3.992409611
H	0.9160665525	1.2125008235	5.3235518539
H	-0.8752048469	1.2420828515	5.323811906
H	-0.031113034	2.302307255	-0.0499831853
H	0.8934318502	2.3263648113	1.4237059784
H	-0.8644249891	2.306050956	1.4762425493
C	-0.6760040152	0.3526226275	-3.0238567082
N	-1.4718148342	0.0201254159	-1.84327268
C	-2.4997695247	1.0229129888	-1.5970383199
C	-2.0816482146	-1.2990998237	-1.9513299012
H	-0.5245313869	1.437892267	-3.0291401216
H	-1.2151682646	0.1069965097	-3.9585583927

H	-3.0501325054	0.7613579313	-0.6884070072
H	-2.0371970966	2.000877131	-1.4367521987
H	-3.2192524935	1.0962192022	-2.4334601162
H	-2.5882990546	-1.5431494697	-1.0134952852
H	-2.8142473141	-1.3445349883	-2.7786647228
H	-1.3213267863	-2.066346852	-2.1165154997
C	-0.0195719265	-1.1809376059	4.6884512827
C	-0.0055050191	-1.8510638815	0.9607269956
H	-0.0332048744	-2.0222345582	3.992409611
H	-0.9160665525	-1.2125008235	5.3235518539
H	0.8752048469	-1.2420828515	5.323811906
H	0.031113034	-2.302307255	-0.0499831853
H	-0.8934318502	-2.3263648113	1.4237059784
H	0.8644249891	-2.306050956	1.4762425493
C	0.6760040152	-0.3526226275	-3.0238567082
N	1.4718148342	-0.0201254159	-1.84327268
C	2.4997695247	-1.0229129888	-1.5970383199
C	2.0816482146	1.2990998237	-1.9513299012
H	0.5245313869	-1.437892267	-3.0291401216
H	1.2151682646	-0.1069965097	-3.9585583927
H	3.0501325054	-0.7613579313	-0.6884070072
H	2.0371970966	-2.000877131	-1.4367521987
H	3.2192524935	-1.0962192022	-2.4334601162
H	2.5882990546	1.5431494697	-1.0134952852
H	2.8142473141	1.3445349883	-2.7786647228
H	1.3213267863	2.066346852	-2.1165154997

Tabelle 10.275 Standardorientierung von **6** [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
N	-1.4461026362	0.0878344438	0.0240816899
C	-1.0289064179	-1.2231663956	-0.4713214442
C	0.3242668849	-1.6446092207	0.0945347692
N	1.3435915226	-0.6141295526	-0.0976703167
C	1.8044951564	-0.5469311324	-1.4804952812
C	2.4779227551	-0.8069068973	0.7974204337
C	-2.4788255396	0.6770241139	-0.8195740879
C	-1.9035023392	0.0326257226	1.4084706237
H	-0.9709963527	-1.1621677851	-1.5639736765
H	-1.7771669081	-2.0044073689	-0.2416461323
H	0.623892596	-2.6067121637	-0.3610656905
H	0.2352255934	-1.826956721	1.1714793089
H	2.5177695041	0.27590853	-1.5840106233
H	0.9696181435	-0.3477418887	-2.1590849184
H	2.2938690081	-1.4855295881	-1.7977951821
H	3.1818158091	0.020786825	0.6723097881
H	3.0077254931	-1.7564542254	0.6019703354
H	2.1366553758	-0.8046629029	1.8372951609
H	-2.7117766006	1.6822830318	-0.457138534
H	-3.4065382168	0.0771625248	-0.8246842955
H	-2.1140668121	0.7661733221	-1.8475299939

H	-2.1466060429	1.0432015448	1.7494397038
H	-1.1174130509	-0.3571095043	2.0622191432
H	-2.7979360557	-0.6063154634	1.5219065563
Li	0.3318694081	1.2263633774	0.1456785367
C	0.8363912303	3.1739363021	0.3495403915
H	0.7810755609	3.7398328034	-0.5992924767
H	1.8664102364	3.3284329025	0.7217174601
H	0.1876346952	3.7263753659	1.0548737516

Tabelle 10.276 Standardorientierung von **7** [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
N	0.7461103592	1.5957973129	-0.1138960441
C	2.0238994572	0.955368491	0.200079615
C	2.1971158024	-0.3858231744	-0.5006347542
N	1.1791288187	-1.3589005704	-0.1019250177
C	1.5102988941	-1.9813316172	1.1775233262
C	1.0128846631	-2.3815330235	-1.123960936
C	0.4711994699	2.6669993524	0.8388241273
C	0.7183038625	2.1118694671	-1.4742427313
H	2.0566516901	0.8094213634	1.285510553
H	2.874586069	1.613885394	-0.0619123055
H	3.2149349282	-0.7691864944	-0.3000888935
H	2.1294979465	-0.2478569098	-1.5855215988
H	0.6994510469	-2.6497725055	1.4784732241
H	1.595204737	-1.2248240358	1.9599423704
H	2.4528569312	-2.5570249804	1.1146880597
H	0.2554309734	-3.1025211504	-0.8004144781
H	1.9482426065	-2.9380388001	-1.3192387668
H	0.6753821216	-1.9257616492	-2.0606863279
H	-0.4894525214	3.1326087198	0.5973841833
H	1.2522238359	3.4494440939	0.818238722
H	0.3915121367	2.2451644333	1.8441645147
H	-0.2471444649	2.5911272855	-1.6632369349
H	0.83276901	1.3045354035	-2.2027461416
H	1.51359269	2.8599816435	-1.6516288993
Li	-0.5085485684	-0.0715229844	0.4473450756
C	-1.0806850582	-0.1026746247	2.4422595177
H	-0.2565615068	0.1446342805	3.1444953223
H	-1.4422870611	-1.0911315406	2.792987811
H	-1.8900595653	0.6037670683	2.7184264796
C	-2.9744903015	0.8288854382	-0.5624428516
O	-2.1408318356	-0.2893230981	-0.8035739628
H	-2.4367181865	1.7157154808	-0.9061735502
H	-3.1890929071	0.9258485872	0.5099061351
H	-3.9127857932	0.7369595705	-1.1288159225
C	-2.7811057384	-1.49367434	-0.4214598746
H	-2.9778783911	-1.4990591782	0.6584823419
H	-2.1041401072	-2.3141235742	-0.6704248702
H	-3.7199880434	-1.6213771341	-0.9798845174

Tabelle 10.277 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
Li	0.4829704184	1.1428654926	0.8644038867
Li	-0.4829704184	-1.1428654926	0.8644038867
Li	1.1428654926	-0.4829704184	-0.864575334
Li	-1.1428654926	0.4829704184	-0.864575334
C	0.6620478682	1.7012438117	-1.2995438437
C	-1.7012438117	0.6620478682	1.2993723963
C	-0.6620478682	-1.7012438117	-1.2995438437
C	1.7012438117	-0.6620478682	1.2993723963
H	-0.0971807376	2.4860246088	-1.5029798243
H	0.9985405046	1.3994385677	-2.3132578759
H	1.5265050657	2.2734723084	-0.904044664
H	-2.4860246088	-0.0971807376	1.5028083769
H	-2.2734723084	1.5265050657	0.9038732166
H	-1.3994385677	0.9985405046	2.3130864286
H	0.0971807376	-2.4860246088	-1.5029798243
H	-0.9985405046	-1.3994385677	-2.3132578759
H	-1.5265050657	-2.2734723084	-0.904044664
H	1.3994385677	-0.9985405046	2.3130864286
H	2.4860246088	0.0971807376	1.5028083769
H	2.2734723084	-1.5265050657	0.9038732166
O	2.7197026949	-0.9870123376	-2.0212498689
O	-0.9870123376	-2.7197026949	2.0210784215
O	0.9870123376	2.7197026949	2.0210784215
O	-2.7197026949	0.9870123376	-2.0212498689
C	-0.3561326973	-3.9689196093	1.7366061046
H	0.6324785628	-4.0186886282	2.2127356931
H	-0.9813913989	-4.7985118364	2.094539446
H	-0.2496151615	-4.0263426082	0.6525054822
C	-1.2085766481	-2.5244841565	3.416688281
H	-1.8647786233	-3.3130344362	3.8104191291
H	-0.2561350555	-2.5320744082	3.9647666587
H	-1.6918228409	-1.552267579	3.5254092912
C	-3.9689196093	0.3561326973	-1.7367775519
H	-4.7985118364	0.9813913989	-2.0947108934
H	-4.0186886282	-0.6324785628	-2.2129071405
H	-4.0263426082	0.2496151615	-0.6526769296
C	-2.5244841565	1.2085766481	-3.4168597284
H	-2.5320744082	0.2561350555	-3.964938106
H	-3.3130344362	1.8647786233	-3.8105905764
H	-1.552267579	1.6918228409	-3.5255807386
C	3.9689196093	-0.3561326973	-1.7367775519
H	4.0263426082	-0.2496151615	-0.6526769296
H	4.7985118364	-0.9813913989	-2.0947108934
H	4.0186886282	0.6324785628	-2.2129071405
C	2.5244841565	-1.2085766481	-3.4168597284
H	2.5320744082	-0.2561350555	-3.964938106
H	3.3130344362	-1.8647786233	-3.8105905764
H	1.552267579	-1.6918228409	-3.5255807386
C	0.3561326973	3.9689196093	1.7366061046

H	-0.6324785628	4.0186886282	2.2127356931
H	0.9813913989	4.7985118364	2.094539446
H	0.2496151615	4.0263426082	0.6525054822
C	1.2085766481	2.5244841565	3.416688281
H	1.8647786233	3.3130344362	3.8104191291
H	0.2561350555	2.5320744082	3.9647666587
H	1.6918228409	1.552267579	3.5254092912

Tabelle 10.278 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
C	-0.0569650755	0.7652238991	-0.0927957052
C	0.0569650755	-0.7652238991	-0.0927957052
N	-1.4381130263	1.2206766255	-0.2900102736
N	1.4381130263	-1.2206766255	-0.2900102736
C	-1.4676480708	2.6501777527	-0.5898943654
C	-2.2892724491	0.9275436587	0.8615994156
C	1.4676480708	-2.6501777527	-0.5898943654
C	2.2892724491	-0.9275436587	0.8615994156
H	0.5412910495	1.1389423324	-0.9311796514
H	0.3666737608	1.1954537887	0.8372180808
H	-0.5412910495	-1.1389423324	-0.9311796514
H	-0.3666737608	-1.1954537887	0.8372180808
H	-2.5003165174	2.958392413	-0.7850588354
H	-0.8720876524	2.8484588394	-1.4869175775
H	-1.0707784079	3.2720659532	0.2380140808
H	-2.3412517907	-0.1514305691	1.0310191992
H	-3.3031506223	1.2880715857	0.6592101502
H	-1.9265752169	1.4108393487	1.7919064818
H	2.5003165174	-2.958392413	-0.7850588354
H	0.8720876524	-2.8484588394	-1.4869175775
H	1.0707784079	-3.2720659532	0.2380140808
H	3.3031506223	-1.2880715857	0.6592101502
H	1.9265752169	-1.4108393487	1.7919064818
H	2.3412517907	0.1514305691	1.0310191992

Tabelle 10.279 Standardorientierung von Me<sub>2</sub>O (C<sub>2v</sub>) [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
C	0.	1.175570196	-0.2014430052
O	0.	0.	0.5903000434
C	0.	-1.175570196	-0.2014430052
H	-0.895781954	1.2255633728	-0.8406946647
H	0.895781954	1.2255633728	-0.8406946647
H	0.	2.021617926	0.489049813
H	0.895781954	-1.2255633728	-0.8406946647
H	-0.895781954	-1.2255633728	-0.8406946647
H	0.	-2.021617926	0.489049813

Tabelle 10.280 Standardorientierung von **4** (C<sub>2</sub>) [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
C	0.0521413201	3.9410603742	0.7652154956
N	0.3032701665	2.6911220678	1.5047388005
C	-0.7090023627	2.4946026053	2.550896194
C	1.641872535	2.6798211638	2.1103922436
C	0.7823298232	3.9671624067	-0.5808863855
N	0.3684826654	2.8542208912	-1.4540598972
C	-0.9328336846	3.1191498507	-2.0846425138
C	1.3793339736	2.5997688635	-2.4898757708
C	-0.0521413201	-3.9410603742	0.7652154956
N	-0.3032701665	-2.6911220678	1.5047388005
C	-1.641872535	-2.6798211638	2.1103922436
C	0.7090023627	-2.4946026053	2.550896194
C	-0.7823298232	-3.9671624067	-0.5808863855
N	-0.3684826654	-2.8542208912	-1.4540598972
C	-1.3793339736	-2.5997688635	-2.4898757708
C	0.9328336846	-3.1191498507	-2.0846425138
Li	0.1533258814	1.1518697884	-0.0933874865
Li	-0.1533258814	-1.1518697884	-0.0933874865
C	-1.8514788039	0.244032204	-0.2377241311
C	1.8514788039	-0.244032204	-0.2377241311
H	-1.0283695401	4.0144242068	0.6011732626
H	0.3488721941	4.8273448723	1.3579806276
H	-0.5171836984	1.5446328998	3.0583965033
H	-1.7016513806	2.4449480061	2.0964669811
H	-0.6920134913	3.3057589544	3.3024038814
H	1.8028416931	1.7168294597	2.6018377477
H	1.7595360242	3.4898249037	2.8545316845
H	2.4107784169	2.7914388621	1.3426612836
H	0.6129408087	4.945953002	-1.0679395927
H	1.8615999759	3.8767198672	-0.4184866972
H	-1.2229273823	2.2518135475	-2.6824087067
H	-1.7026305625	3.2656876518	-1.3237024812
H	-0.8945988223	4.0125357414	-2.7356070128
H	1.0558407445	1.7538958341	-3.1028006061
H	1.5301318495	3.4763671399	-3.146756466
H	2.3289287832	2.3342463855	-2.0178294078
H	-0.3488721941	-4.8273448723	1.3579806276
H	1.0283695401	-4.0144242068	0.6011732626
H	-1.8028416931	-1.7168294597	2.6018377477
H	-2.4107784169	-2.7914388621	1.3426612836
H	-1.7595360242	-3.4898249037	2.8545316845
H	0.5171836984	-1.5446328998	3.0583965033
H	0.6920134913	-3.3057589544	3.3024038814
H	1.7016513806	-2.4449480061	2.0964669811
H	-1.8615999759	-3.8767198672	-0.4184866972
H	-0.6129408087	-4.945953002	-1.0679395927
H	-1.0558407445	-1.7538958341	-3.1028006061
H	-2.3289287832	-2.3342463855	-2.0178294078
H	-1.5301318495	-3.4763671399	-3.146756466

H	1.2229273823	-2.2518135475	-2.6824087067
H	0.8945988223	-4.0125357414	-2.7356070128
H	1.7026305625	-3.2656876518	-1.3237024812
H	-2.1952781591	0.2543660186	-1.2932752315
H	-2.2522028159	1.1910069745	0.182897236
H	-2.485927118	-0.5278396974	0.2463534339
H	2.1952781591	-0.2543660186	-1.2932752315
H	2.2522028159	-1.1910069745	0.182897236
H	2.485927118	0.5278396974	0.2463534339

Tabelle 10.281 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
O	0.	0.	3.9537951738
C	0.0223895892	1.1918867286	4.7396323861
Li	0.	0.	2.0038619636
Li	0.	0.	-0.2672579374
C	0.0066423505	1.8621888941	0.9728366241
H	0.0377965055	2.0284691968	4.039769303
H	0.9200849014	1.2146670068	5.372315001
H	-0.8736500904	1.2482781716	5.3725561253
H	-0.0387159423	2.3115157706	-0.0410771394
H	0.8992327953	2.3433115261	1.4256337675
H	-0.8586911107	2.3254264227	1.4932810314
C	-0.6778178533	0.3574956913	-3.0472973087
N	-1.4774052391	0.0189232604	-1.8550951572
C	-2.520175502	1.0278787285	-1.6171423848
C	-2.0959623725	-1.3098012547	-1.9755092393
H	-0.5239675166	1.4419665964	-3.0436666848
H	-1.2196675937	0.1133028547	-3.980125801
H	-3.0712446992	0.7629890213	-0.7104496321
H	-2.0565207329	2.0053992587	-1.4613681715
H	-3.2332327177	1.0924704584	-2.4592455579
H	-2.6141525132	-1.5479793683	-1.0431912088
H	-2.8174645835	-1.3476781848	-2.8124170296
H	-1.331503206	-2.073894034	-2.1337751054
C	-0.0223895892	-1.1918867286	4.7396323861
C	-0.0066423505	-1.8621888941	0.9728366241
H	-0.0377965055	-2.0284691968	4.039769303
H	-0.9200849014	-1.2146670068	5.372315001
H	0.8736500904	-1.2482781716	5.3725561253
H	0.0387159423	-2.3115157706	-0.0410771394
H	-0.8992327953	-2.3433115261	1.4256337675
H	0.8586911107	-2.3254264227	1.4932810314
C	0.6778178533	-0.3574956913	-3.0472973087
N	1.4774052391	-0.0189232604	-1.8550951572
C	2.520175502	-1.0278787285	-1.6171423848
C	2.0959623725	1.3098012547	-1.9755092393
H	0.5239675166	-1.4419665964	-3.0436666848
H	1.2196675937	-0.1133028547	-3.980125801
H	3.0712446992	-0.7629890213	-0.7104496321

H	2.0565207329	-2.0053992587	-1.4613681715
H	3.2332327177	-1.0924704584	-2.4592455579
H	2.6141525132	1.5479793683	-1.0431912088
H	2.8174645835	1.3476781848	-2.8124170296
H	1.331503206	2.073894034	-2.1337751054

Tabelle 10.282 Standardorientierung von **6** [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
N	-1.4523708991	0.0918103102	0.0422913487
C	-1.0331272987	-1.2260452118	-0.4722594942
C	0.3271384964	-1.6492086909	0.0964187123
N	1.3528324463	-0.6099805727	-0.1153985711
C	1.8285793402	-0.5838026544	-1.5085947616
C	2.4949362057	-0.7923550095	0.7942658043
C	-2.4862074694	0.6957649838	-0.8132249342
C	-1.9424010686	0.0092025973	1.4281855532
H	-0.9720428863	-1.1481393298	-1.5632398445
H	-1.7812814653	-2.0081592425	-0.2491285494
H	0.6254520946	-2.6145261195	-0.3512438398
H	0.2439634725	-1.8130994929	1.176363381
H	2.5402928268	0.2378464209	-1.6254412246
H	0.9940574723	-0.4083754231	-2.1934940896
H	2.321389209	-1.5313099105	-1.7902193537
H	3.1990788209	0.0312440771	0.6497093555
H	3.0182476429	-1.7484476173	0.6169262242
H	2.1450620619	-0.7676400451	1.830597856
H	-2.7220325741	1.6937752419	-0.4345594451
H	-3.4104539251	0.0919096167	-0.8363351024
H	-2.1038701184	0.7969908907	-1.8332483892
H	-2.1846407288	1.0156445027	1.7799920436
H	-1.168237756	-0.4012185556	2.082836744
H	-2.842211254	-0.6264996626	1.5066311855
Li	0.3360589404	1.2403646904	0.1466555418
C	0.8410734421	3.2002645199	0.3531900277
H	0.7892722383	3.7706361118	-0.5958485307
H	1.8713545164	3.360604491	0.7287753851
H	0.1904802171	3.7568890836	1.0570519671

Tabelle 10.283 Standardorientierung von **7** [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
N	0.7545801706	1.6047056506	-0.1288304294
C	2.0332376628	0.9577319774	0.2267213629
C	2.2278905691	-0.381381602	-0.4891848797
N	1.1890970492	-1.3633507708	-0.1192262973
C	1.5065214204	-2.0103803142	1.1668512608
C	1.0500219544	-2.3841513474	-1.1656402253
C	0.4592679123	2.6852822901	0.8282501413
C	0.7793014005	2.1412719469	-1.4951830673
H	2.0206257723	0.7985848921	1.3102142464

H	2.8901080966	1.6202002143	-0.0004668816
H	3.2384728565	-0.7689349016	-0.2651319581
H	2.1809760994	-0.2344735848	-1.5736246895
H	0.694336212	-2.6899986451	1.4358115862
H	1.572176348	-1.260830725	1.9571220442
H	2.4545658071	-2.5768057862	1.1070290832
H	0.2822263264	-3.104207405	-0.8665800066
H	1.9911192334	-2.9372035813	-1.3394021648
H	0.7395517863	-1.9124854533	-2.1033418547
H	-0.489763867	3.1566032648	0.5551993102
H	1.2486953379	3.4590613503	0.829262971
H	0.3513739999	2.255109425	1.8265909108
H	-0.1798105871	2.6224087276	-1.7085003167
H	0.9216739227	1.3382253539	-2.2231735941
H	1.5822464831	2.8891651654	-1.6315721839
Li	-0.5179807665	-0.0738318318	0.4209043835
C	-1.0596859101	-0.0931142242	2.4398620471
H	-0.2325330444	0.1687318055	3.1369458508
H	-1.406840791	-1.0845621239	2.803591171
H	-1.876640063	0.6051842235	2.7233785844
C	-3.036799056	0.8226556251	-0.5665738795
O	-2.202461848	-0.3169295436	-0.7956029406
H	-2.5003012658	1.6905630411	-0.9550760185
H	-3.2219731136	0.9496015546	0.5072837695
H	-3.9870053445	0.7093855182	-1.1074953179
C	-2.8512849586	-1.5176493071	-0.361328058
H	-3.0214853475	-1.4873550894	0.7216317741
H	-2.1820461416	-2.3443609263	-0.6067439454
H	-3.8019463165	-1.6459128631	-0.8981497883

Tabelle 10.284 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
Li	0.4748204778	1.1484231187	0.8638251324
Li	-0.4748204778	-1.1484231187	0.8638251324
Li	1.1484231187	-0.4748204778	-0.8639965798
Li	-1.1484231187	0.4748204778	-0.8639965798
C	0.641820588	1.704262947	-1.2977064182
C	-1.704262947	0.641820588	1.2975349708
C	-0.641820588	-1.704262947	-1.2977064182
C	1.704262947	-0.641820588	1.2975349708
H	-0.1304964759	2.467224536	-1.5246828803
H	1.006266413	1.3963029207	-2.2980299078
H	1.4834857803	2.2979374973	-0.8893858741
H	-2.467224536	-0.1304964759	1.5245114329
H	-2.2979374973	1.4834857803	0.8892144268
H	-1.3963029207	1.006266413	2.2978584605
H	0.1304964759	-2.467224536	-1.5246828803
H	-1.006266413	-1.3963029207	-2.2980299078

H	-1.4834857803	-2.2979374973	-0.8893858741
H	1.3963029207	-1.006266413	2.2978584605
H	2.467224536	0.1304964759	1.5245114329
H	2.2979374973	-1.4834857803	0.8892144268
O	2.7251319235	-0.9613919409	-2.0132074221
O	-0.9613919409	-2.7251319235	2.0130359747
O	0.9613919409	2.7251319235	2.0130359747
O	-2.7251319235	0.9613919409	-2.0132074221
C	-0.3598186437	-3.9820177755	1.7164761836
H	0.6178638641	-4.0712693397	2.2106853525
H	-1.0121002627	-4.804489075	2.0431356729
H	-0.2298344536	-4.0258460022	0.6335814053
C	-1.2143103961	-2.5405094769	3.401301737
H	-1.8993741812	-3.3162128513	3.7725028431
H	-0.2780947601	-2.5762594815	3.976864253
H	-1.6780187243	-1.5584778634	3.5143056587
C	-3.9820177755	0.3598186437	-1.7166476309
H	-4.804489075	1.0121002627	-2.0433071202
H	-4.0712693397	-0.6178638641	-2.2108567999
H	-4.0258460022	0.2298344536	-0.6337528527
C	-2.5405094769	1.2143103961	-3.4014731843
H	-2.5762594815	0.2780947601	-3.9770357003
H	-3.3162128513	1.8993741812	-3.7726742904
H	-1.5584778634	1.6780187243	-3.5144771061
C	3.9820177755	-0.3598186437	-1.7166476309
H	4.0258460022	-0.2298344536	-0.6337528527
H	4.804489075	-1.0121002627	-2.0433071202
H	4.0712693397	0.6178638641	-2.2108567999
C	2.5405094769	-1.2143103961	-3.4014731843
H	2.5762594815	-0.2780947601	-3.9770357003
H	3.3162128513	-1.8993741812	-3.7726742904
H	1.5584778634	-1.6780187243	-3.5144771061
C	0.3598186437	3.9820177755	1.7164761836
H	-0.6178638641	4.0712693397	2.2106853525
H	1.0121002627	4.804489075	2.0431356729
H	0.2298344536	4.0258460022	0.6335814053
C	1.2143103961	2.5405094769	3.401301737
H	1.8993741812	3.3162128513	3.7725028431
H	0.2780947601	2.5762594815	3.976864253
H	1.6780187243	1.5584778634	3.5143056587

Tabelle 10.285 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
C	-0.0416958948	0.7665530194	-0.1131499925
C	0.0416958948	-0.7665530194	-0.1131499925
N	-1.4109723814	1.259734549	-0.2849347535
N	1.4109723814	-1.259734549	-0.2849347535
C	-1.4176362739	2.6758407381	-0.6343749696
C	-2.2507157894	1.0145894917	0.8833487375
C	1.4176362739	-2.6758407381	-0.6343749696

C	2.2507157894	-1.0145894917	0.8833487375
H	0.5545238781	1.1240038869	-0.9600910493
H	0.4114783001	1.1885092718	0.8068420227
H	-0.5545238781	-1.1240038869	-0.9600910493
H	-0.4114783001	-1.1885092718	0.8068420227
H	-2.4467396042	3.0043414365	-0.8171844937
H	-0.8406370444	2.8352951034	-1.5514780567
H	-0.9885034124	3.3192096714	0.161393121
H	-2.3230116194	-0.0570222711	1.0885459174
H	-3.2624345563	1.3867239173	0.6890510389
H	-1.8675222704	1.5169403418	1.7961014776
H	2.4467396042	-3.0043414365	-0.8171844937
H	0.8406370444	-2.8352951034	-1.5514780567
H	0.9885034124	-3.3192096714	0.161393121
H	3.2624345563	-1.3867239173	0.6890510389
H	1.8675222704	-1.5169403418	1.7961014776
H	2.3230116194	0.0570222711	1.0885459174

Tabelle 10.286 Standardorientierung von Me<sub>2</sub>O (C<sub>2v</sub>) [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
C	0.	1.177435884	-0.1953720587
O	0.	0.	0.5879691518
C	0.	-1.177435884	-0.1953720587
H	-0.8954471911	1.2336874867	-0.835652271
H	0.8954471911	1.2336874867	-0.835652271
H	0.	2.0239054792	0.4961245247
H	0.8954471911	-1.2336874867	-0.835652271
H	-0.8954471911	-1.2336874867	-0.835652271
H	0.	-2.0239054792	0.4961245247

Tabelle 10.287 Standardorientierung von **4** (C<sub>2</sub>) [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
C	-0.3727860904	3.9482158404	0.7587275263
N	-0.0172281775	2.737237892	1.5170899463
C	-1.0190203743	2.4478620783	2.5485547929
C	1.3111306402	2.8469818745	2.1308695869
C	0.3393730028	4.0244442961	-0.5956100999
N	0.0167096558	2.8848245895	-1.4699256995
C	-1.3135252735	3.0194287836	-2.0761455395
C	1.031809941	2.7193798109	-2.5167411118
C	0.3727860904	-3.9482158404	0.7587275263
N	0.0172281775	-2.737237892	1.5170899463
C	-1.3111306402	-2.8469818745	2.1308695869
C	1.0190203743	-2.4478620783	2.5485547929
C	-0.3393730028	-4.0244442961	-0.5956100999
N	-0.0167096558	-2.8848245895	-1.4699256995
C	-1.031809941	-2.7193798109	-2.5167411118
C	1.3135252735	-3.0194287836	-2.0761455395
Li	0.0046104822	1.1615408094	-0.0910983587

Li	-0.0046104822	-1.1615408094	-0.0910983587
C	-1.8580457875	0.0067314411	-0.236199606
C	1.8580457875	-0.0067314411	-0.236199606
H	-1.4566672318	3.9375267543	0.6038159949
H	-0.1459398706	4.8653525629	1.3359242265
H	-0.74594389	1.5248476691	3.06906528
H	-1.9974168245	2.2960882073	2.0851590784
H	-1.0957840989	3.2603134467	3.2957343184
H	1.5610997347	1.9042019572	2.625062004
H	1.3515263467	3.6638681416	2.8764299041
H	2.0752047151	3.0288479334	1.3718361521
H	0.0864307683	4.986983652	-1.0803383439
H	1.4233563985	4.0289466738	-0.4411753133
H	-1.5304049902	2.1303751969	-2.673648741
H	-2.0849725732	3.0869081907	-1.3057156096
H	-1.3787258189	3.9132050436	-2.7252590158
H	0.7794468223	1.8495659931	-3.1301709394
H	1.0991416525	3.6054314498	-3.1757384981
H	2.0089034732	2.536474425	-2.0614246138
H	0.1459398706	-4.8653525629	1.3359242265
H	1.4566672318	-3.9375267543	0.6038159949
H	-1.5610997347	-1.9042019572	2.625062004
H	-2.0752047151	-3.0288479334	1.3718361521
H	-1.3515263467	-3.6638681416	2.8764299041
H	0.74594389	-1.5248476691	3.06906528
H	1.0957840989	-3.2603134467	3.2957343184
H	1.9974168245	-2.2960882073	2.0851590784
H	-1.4233563985	-4.0289466738	-0.4411753133
H	-0.0864307683	-4.986983652	-1.0803383439
H	-0.7794468223	-1.8495659931	-3.1301709394
H	-2.0089034732	-2.536474425	-2.0614246138
H	-1.0991416525	-3.6054314498	-3.1757384981
H	1.5304049902	-2.1303751969	-2.673648741
H	1.3787258189	-3.9132050436	-2.7252590158
H	2.0849725732	-3.0869081907	-1.3057156096
H	-2.1892425892	0.0301373879	-1.2941503239
H	-2.3821035486	0.8633071121	0.2340694011
H	-2.3786978243	-0.8718832274	0.1945016016
H	2.1892425892	-0.0301373879	-1.2941503239
H	2.3821035486	-0.8633071121	0.2340694011
H	2.3786978243	0.8718832274	0.1945016016

Tabelle 10.288 Standardorientierung von  $\mathbf{5}(\text{C}_2)$  [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
O	0.	0.	3.9453082153
C	0.0152813047	1.1928883046	4.7243614099
Li	0.	0.	2.0063058864
Li	0.	0.	-0.2599952827
C	-0.0027396743	1.8555377719	0.9857676
H	0.0253760656	2.0306381632	4.0246876286

H	0.9126136726	1.2270244569	5.3582064345
H	-0.8804117027	1.2496340177	5.3589010306
H	-0.0500120104	2.3111125206	-0.0227701634
H	0.8884155448	2.3305090941	1.4447734496
H	-0.8703935739	2.3042046397	1.5122210786
C	-0.6815672734	0.3507960527	-3.0401466637
N	-1.4897030757	0.0113668947	-1.8557319086
C	-2.5301263089	1.0189433103	-1.6144149216
C	-2.1000475945	-1.3195644295	-1.9700066193
H	-0.536269165	1.4361171866	-3.0436283983
H	-1.2151694575	0.1014392843	-3.9769372532
H	-3.0870042997	0.7535416288	-0.7109830372
H	-2.0701585394	1.9972044017	-1.450735269
H	-3.24266975	1.0912330676	-2.4570526221
H	-2.6224648706	-1.5592061183	-1.0399977467
H	-2.8190434634	-1.3685848444	-2.8091612608
H	-1.3348720188	-2.0845144933	-2.1205029116
C	-0.0152813047	-1.1928883046	4.7243614099
C	0.0027396743	-1.8555377719	0.9857676
H	-0.0253760656	-2.0306381632	4.0246876286
H	-0.9126136726	-1.2270244569	5.3582064345
H	0.8804117027	-1.2496340177	5.3589010306
H	0.0500120104	-2.3111125206	-0.0227701634
H	-0.8884155448	-2.3305090941	1.4447734496
H	0.8703935739	-2.3042046397	1.5122210786
C	0.6815672734	-0.3507960527	-3.0401466637
N	1.4897030757	-0.0113668947	-1.8557319086
C	2.5301263089	-1.0189433103	-1.6144149216
C	2.1000475945	1.3195644295	-1.9700066193
H	0.536269165	-1.4361171866	-3.0436283983
H	1.2151694575	-0.1014392843	-3.9769372532
H	3.0870042997	-0.7535416288	-0.7109830372
H	2.0701585394	-1.9972044017	-1.450735269
H	3.24266975	-1.0912330676	-2.4570526221
H	2.6224648706	1.5592061183	-1.0399977467
H	2.8190434634	1.3685848444	-2.8091612608
H	1.3348720188	2.0845144933	-2.1205029116

Tabelle 10.289 Standardorientierung von **6** [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
N	1.4551277916	-0.2778038914	-0.0052310256
C	0.682046045	-1.4926847773	0.3090804266
C	-0.7086497915	-1.4780973371	-0.3389695647
N	-1.4637518964	-0.2558321504	-0.0093256288
C	-1.9990551243	-0.285403789	1.3598160079
C	-2.5508381261	-0.0152602297	-0.9681940373
C	2.545442949	-0.0646681832	0.9564540782
C	1.9898428794	-0.2978330143	-1.3746889317
H	0.5814635299	-1.5485830998	1.3982373354
H	1.2165704667	-2.4084129332	-0.0043159839

H	-1.2570723933	-2.3895258406	-0.0373420529
H	-0.6086188887	-1.521534759	-1.4287393579
H	-2.4906966072	0.6675064278	1.5751842099
H	-1.1930801646	-0.4170019326	2.0875108397
H	-2.7293498808	-1.1033617307	1.4978098656
H	-3.0403985787	0.9324707814	-0.7273883231
H	-3.3069652021	-0.8207943804	-0.9520386108
H	-2.1428383717	0.0619954417	-1.9807331574
H	3.0482869883	0.8790102745	0.7274865302
H	3.290037175	-0.8806418656	0.930185279
H	2.1384044903	0.0060107108	1.9698165537
H	2.495437084	0.6504128271	-1.5779747033
H	1.1820785291	-0.408528169	-2.1039275205
H	2.7081376245	-1.1245171757	-1.5232831065
Li	0.0075519832	1.285938443	0.0072372508
C	0.0402389886	3.3113239863	0.0449408048
H	0.4508966902	3.7218031064	0.9874849798
H	-0.9578707064	3.7763754704	-0.0665061866
H	0.6588745172	3.7534467899	-0.7596969707

Tabelle 10.290 Standardorientierung von **7** [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
N	0.8279271398	1.5708827298	-0.1207122126
C	2.1097700519	0.8617458367	0.0445720382
C	2.1351890215	-0.4965592762	-0.6622353441
N	1.1192621599	-1.4288130985	-0.141309022
C	1.5451916042	-2.0405121927	1.1278620204
C	0.8223335677	-2.4750838671	-1.1245933298
C	0.7031865979	2.644408721	0.8768505078
C	0.6784829672	2.1157815465	-1.4739273234
H	2.2701583471	0.721051779	1.1180603693
H	2.9533095621	1.4745974812	-0.3272817478
H	3.1509882559	-0.9258028894	-0.5749683319
H	1.9482820445	-0.3589494185	-1.7325093681
H	0.7434993288	-2.677174544	1.5099375765
H	1.7230817893	-1.2719194882	1.8815833416
H	2.4615029205	-2.6464551824	0.9964458099
H	0.0683160431	-3.1554426101	-0.7163357113
H	1.7151121154	-3.0737776067	-1.385048583
H	0.4241640267	-2.026190977	-2.0405061987
H	-0.2556352719	3.1546466559	0.7439843096
H	1.5128368536	3.3919219253	0.7835272775
H	0.7127635757	2.2106675078	1.8795193439
H	-0.2814191004	2.6348335948	-1.5537015397
H	0.6856763341	1.3159193428	-2.2190793238
H	1.4812525807	2.8352353173	-1.7228130919
Li	-0.5084836285	-0.0541374184	0.5155144697
C	-1.0429403348	-0.1013695593	2.5227406695
H	-0.191041776	0.0748427668	3.2136931728
H	-1.4656225881	-1.0725147177	2.8557113815

H	-1.7999980769	0.6517484323	2.825724304
C	-3.0140511787	0.9676934522	-0.4467302303
O	-2.195470465	-0.1696955123	-0.717696646
H	-2.4405025532	1.8529423581	-0.730318492
H	-3.2607603339	1.0192089605	0.6211738728
H	-3.9343691881	0.9264252684	-1.0474212996
C	-2.8797454058	-1.3869550646	-0.4194421781
H	-3.1107805224	-1.4458144447	0.6516010068
H	-2.2126562603	-2.2068398087	-0.6938661236
H	-3.8033982036	-1.4590750001	-1.0120523741

Tabelle 10.291 Standardorientierung von (MeLi-OMe)<sub>2</sub> (S<sub>4</sub>) [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
Li	0.4747180134	1.1540002117	0.8718898778
Li	-0.4747180134	-1.1540002117	0.8718898778
Li	1.1540002117	-0.4747180134	-0.8720613252
Li	-1.1540002117	0.4747180134	-0.8720613252
C	0.64309393	1.7069533455	-1.2932303895
C	-1.7069533455	0.64309393	1.2930589421
C	-0.64309393	-1.7069533455	-1.2932303895
C	1.7069533455	-0.64309393	1.2930589421
H	-0.1562605194	2.3897868511	-1.6357086321
H	1.1428594461	1.4007676708	-2.2295594022
H	1.3778798461	2.3852143421	-0.8237976426
H	-2.3897868511	-0.1562605194	1.6355371847
H	-2.3852143421	1.3778798461	0.8236261952
H	-1.4007676708	1.1428594461	2.2293879548
H	0.1562605194	-2.3897868511	-1.6357086321
H	-1.1428594461	-1.4007676708	-2.2295594022
H	-1.3778798461	-2.3852143421	-0.8237976426
H	1.4007676708	-1.1428594461	2.2293879548
H	2.3897868511	0.1562605194	1.6355371847
H	2.3852143421	-1.3778798461	0.8236261952
O	2.7363861771	-0.9530593786	-2.030168216
O	-0.9530593786	-2.7363861771	2.0299967686
O	0.9530593786	2.7363861771	2.0299967686
O	-2.7363861771	0.9530593786	-2.030168216
C	-0.3684477574	-4.0011632156	1.7349906058
H	0.5935954374	-4.1145615899	2.2489926396
H	-1.0404100202	-4.8137249167	2.0370048885
H	-0.2130188979	-4.0404465645	0.6577746089
C	-1.2411236191	-2.565007385	3.4126871636
H	-1.9474870823	-3.3308386294	3.7558372837
H	-0.3248924265	-2.6241178102	4.0131785053
H	-1.690144477	-1.5793561211	3.5292394266
C	-4.0011632156	0.3684477574	-1.7351620531
H	-4.8137249167	1.0404100202	-2.0371763358
H	-4.1145615899	-0.5935954374	-2.2491640869

H	-4.0404465645	0.2130188979	-0.6579460563
C	-2.565007385	1.2411236191	-3.412858611
H	-2.6241178102	0.3248924265	-4.0133499527
H	-3.3308386294	1.9474870823	-3.7560087311
H	-1.5793561211	1.690144477	-3.529410874
C	4.0011632156	-0.3684477574	-1.7351620531
H	4.0404465645	-0.2130188979	-0.6579460563
H	4.8137249167	-1.0404100202	-2.0371763358
H	4.1145615899	0.5935954374	-2.2491640869
C	2.565007385	-1.2411236191	-3.412858611
H	2.6241178102	-0.3248924265	-4.0133499527
H	3.3308386294	-1.9474870823	-3.7560087311
H	1.5793561211	-1.690144477	-3.529410874
C	0.3684477574	4.0011632156	1.7349906058
H	-0.5935954374	4.1145615899	2.2489926396
H	1.0404100202	4.8137249167	2.0370048885
H	0.2130188979	4.0404465645	0.6577746089
C	1.2411236191	2.565007385	3.4126871636
H	1.9474870823	3.3308386294	3.7558372837
H	0.3248924265	2.6241178102	4.0131785053
H	1.690144477	1.5793561211	3.5292394266

Tabelle 10.292 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
C	-0.0665325083	0.7637029638	-0.1545893649
C	0.0665325083	-0.7637029638	-0.1545893649
N	-1.460077375	1.2077830983	-0.2304048118
N	1.460077375	-1.2077830983	-0.2304048118
C	-1.5557347392	2.5866207865	-0.6933579917
C	-2.1785196256	1.0349669097	1.0270202445
C	1.5557347392	-2.5866207865	-0.6933579917
C	2.1785196256	-1.0349669097	1.0270202445
H	0.458505556	1.1336710984	-1.0386003188
H	0.4382514663	1.2042638152	0.7248874478
H	-0.458505556	-1.1336710984	-1.0386003188
H	-0.4382514663	-1.2042638152	0.7248874478
H	-2.6068705291	2.8665804582	-0.7998786442
H	-1.0781304239	2.6856572083	-1.6707386065
H	-1.0798670614	3.3081896042	-0.0020936471
H	-2.1731980039	-0.0115539233	1.3342622625
H	-3.220471376	1.3375573653	0.8976134574
H	-1.745604517	1.6372786838	1.8489909723
H	2.6068705291	-2.8665804582	-0.7998786442
H	1.0781304239	-2.6856572083	-1.6707386065
H	1.0798670614	-3.3081896042	-0.0020936471
H	3.220471376	-1.3375573653	0.8976134574
H	1.745604517	-1.6372786838	1.8489909723
H	2.1731980039	0.0115539233	1.3342622625

Tabelle 10.293 Standardorientierung von  $\text{Me}_2\text{O}$  ( $\text{C}_{2v}$ ) [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
C	0.	1.1763424734	-0.199467849
O	0.	0.	0.5829704518
C	0.	-1.1763424734	-0.199467849
H	-0.8926644567	1.2342529101	-0.839217605
H	0.8926644567	1.2342529101	-0.839217605
H	0.	2.0227863737	0.4877853331
H	0.8926644567	-1.2342529101	-0.839217605
H	-0.8926644567	-1.2342529101	-0.839217605
H	0.	-2.0227863737	0.4877853331

Tabelle 10.294 Standardorientierung von  $\mathbf{4}$  ( $\text{C}_2$ ) [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
C	0.0791190197	3.9748476723	0.7470303422
N	0.3003269096	2.7416287738	1.5189145507
C	-0.7262182174	2.5767530975	2.5529213162
C	1.6336624008	2.7121406048	2.1296587797
C	0.796538975	3.9598546879	-0.6039862924
N	0.3474890006	2.8594984816	-1.4713525266
C	-0.9574639712	3.1420625543	-2.080424384
C	1.3389176727	2.5724985532	-2.5139470368
C	-0.0791190197	-3.9748476723	0.7470303422
N	-0.3003269096	-2.7416287738	1.5189145507
C	-1.6336624008	-2.7121406048	2.1296587797
C	0.7262182174	-2.5767530975	2.5529213162
C	-0.796538975	-3.9598546879	-0.6039862924
N	-0.3474890006	-2.8594984816	-1.4713525266
C	-1.3389176727	-2.5724985532	-2.5139470368
C	0.9574639712	-3.1420625543	-2.080424384
Li	0.1401165161	1.1552386931	-0.0761343851
Li	-0.1401165161	-1.1552386931	-0.0761343851
C	-1.8471109183	0.2237236626	-0.2100633631
C	1.8471109183	-0.2237236626	-0.2100633631
H	-0.9966735358	4.0798876127	0.5886369693
H	0.4012851603	4.866449071	1.3134135629
H	-0.5583151015	1.637801804	3.0838834888
H	-1.7138350623	2.5286026425	2.0927434175
H	-0.7125227392	3.3986261699	3.2893317708
H	1.7798470209	1.7573992181	2.6365706951
H	1.7667661102	3.5278690291	2.8613144493
H	2.4101665673	2.7960031043	1.3695968198
H	0.6570521003	4.9395904715	-1.0937061242
H	1.8711691828	3.8425078119	-0.4464480549
H	-1.2759366676	2.2820490583	-2.6701597102
H	-1.7155676457	3.3032429518	-1.3141952889
H	-0.9191741481	4.0300955908	-2.7346755858
H	0.9929174918	1.7343110759	-3.121071796
H	1.5072480354	3.4375769452	-3.1780209165
H	2.2862969121	2.2838700079	-2.0567496249

H	-0.4012851603	-4.866449071	1.3134135629
H	0.9966735358	-4.0798876127	0.5886369693
H	-1.7798470209	-1.7573992181	2.6365706951
H	-2.4101665673	-2.7960031043	1.3695968198
H	-1.7667661102	-3.5278690291	2.8613144493
H	0.5583151015	-1.637801804	3.0838834888
H	0.7125227392	-3.3986261699	3.2893317708
H	1.7138350623	-2.5286026425	2.0927434175
H	-1.8711691828	-3.8425078119	-0.4464480549
H	-0.6570521003	-4.9395904715	-1.0937061242
H	-0.9929174918	-1.7343110759	-3.121071796
H	-2.2862969121	-2.2838700079	-2.0567496249
H	-1.5072480354	-3.4375769452	-3.1780209165
H	1.2759366676	-2.2820490583	-2.6701597102
H	0.9191741481	-4.0300955908	-2.7346755858
H	1.7155676457	-3.3032429518	-1.3141952889
H	-2.1920004613	0.2656844761	-1.2592332227
H	-2.2551057259	1.144422026	0.2458998426
H	-2.4608219153	-0.5735080233	0.2468153077
H	2.1920004613	-0.2656844761	-1.2592332227
H	2.2551057259	-1.144422026	0.2458998426
H	2.4608219153	0.5735080233	0.2468153077

Tabelle 10.295 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
O	0.	0.	3.953553273
C	0.017266013	1.1925836578	4.7331921194
Li	0.	0.	2.008833029
Li	0.	0.	-0.2585830745
C	0.0032083302	1.854400749	0.9888018261
H	0.0285499522	2.0303827554	4.0374211781
H	0.9122507192	1.2263243585	5.3659012398
H	-0.8756782865	1.251626762	5.3669293058
H	-0.0452939596	2.3080646664	-0.0168686368
H	0.8915763164	2.3292123261	1.4447576437
H	-0.8594974736	2.3040249532	1.5152931932
C	-0.6781711257	0.3547406207	-3.0461974642
N	-1.4898089188	0.0182275674	-1.864452863
C	-2.5248974385	1.0311214578	-1.6249373525
C	-2.1051587441	-1.3095369828	-1.9821730799
H	-0.5251911348	1.4364707758	-3.0476506622
H	-1.2101814313	0.1122479455	-3.9823632145
H	-3.0829019049	0.7719774948	-0.7235035863
H	-2.061870705	2.0052389511	-1.4620398948
H	-3.2355333966	1.1064773036	-2.4652033455
H	-2.6314704229	-1.5484889129	-1.0572282954
H	-2.8190538251	-1.3555456388	-2.8220809827
H	-1.3449958063	-2.0767756056	-2.1286352994
C	-0.017266013	-1.1925836578	4.7331921194
C	-0.0032083302	-1.854400749	0.9888018261

H	-0.0285499522	-2.0303827554	4.0374211781
H	-0.9122507192	-1.2263243585	5.3659012398
H	0.8756782865	-1.251626762	5.3669293058
H	0.0452939596	-2.3080646664	-0.0168686368
H	-0.8915763164	-2.3292123261	1.4447576437
H	0.8594974736	-2.3040249532	1.5152931932
C	0.6781711257	-0.3547406207	-3.0461974642
N	1.4898089188	-0.0182275674	-1.864452863
C	2.5248974385	-1.0311214578	-1.6249373525
C	2.1051587441	1.3095369828	-1.9821730799
H	0.5251911348	-1.4364707758	-3.0476506622
H	1.2101814313	-0.1122479455	-3.9823632145
H	3.0829019049	-0.7719774948	-0.7235035863
H	2.061870705	-2.0052389511	-1.4620398948
H	3.2355333966	-1.1064773036	-2.4652033455
H	2.6314704229	1.5484889129	-1.0572282954
H	2.8190538251	1.3555456388	-2.8220809827
H	1.3449958063	2.0767756056	-2.1286352994

Tabelle 10.296 Standardorientierung von **6** [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
N	-1.4647847138	0.0903937106	0.053232377
C	-1.0321754586	-1.2188296169	-0.4655051388
C	0.3311289829	-1.6407435184	0.0920271209
N	1.3650212772	-0.6150230106	-0.1297290625
C	1.8370772164	-0.5930851226	-1.5213998871
C	2.5016001614	-0.7843431528	0.7852424054
C	-2.4878683431	0.7025554685	-0.8049445569
C	-1.9519527609	0.0064806612	1.4371965889
H	-0.9761088419	-1.1414109924	-1.5539886719
H	-1.7704893797	-2.0080684871	-0.2459129515
H	0.6167821992	-2.6094056161	-0.3510482953
H	0.2528487904	-1.8041576961	1.1695672798
H	2.548144463	0.2246586854	-1.6481155306
H	1.0073546189	-0.4197692867	-2.2087974509
H	2.3285859589	-1.5387908964	-1.8027132659
H	3.2080111549	0.033897393	0.6381129743
H	3.0272996588	-1.7395407084	0.6241044485
H	2.1547151354	-0.7474595573	1.8198010515
H	-2.7267839617	1.6978315071	-0.4274008737
H	-3.4134504892	0.1052604481	-0.8403886162
H	-2.1038967674	0.811742568	-1.8210898712
H	-2.1954062765	1.0079645247	1.7952059535
H	-1.1824917246	-0.4024277208	2.0942960258
H	-2.8497497724	-0.6279249292	1.5183005198
Li	0.3351456679	1.2351927044	0.144253674
C	0.8351650129	3.1914678494	0.3568808912
H	0.8625752848	3.7385642438	-0.6013129983
H	1.8292744281	3.3494759657	0.808855056
H	0.1348204788	3.7596345817	0.9929258041

Tabelle 10.297 Standardorientierung von **7** [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
N	0.772174055	1.6163923473	-0.0931619922
C	2.0673887092	0.9592209885	0.1554121978
C	2.1927218709	-0.3939247932	-0.546060344
N	1.1935251077	-1.3715207615	-0.0807487863
C	1.5795483093	-1.9684702008	1.2074262799
C	0.9897769187	-2.4236859481	-1.080568207
C	0.5412387577	2.6834528023	0.8919916243
C	0.6876298473	2.1536784121	-1.4543032474
H	2.1625761562	0.8220843251	1.2345619763
H	2.9061992079	1.6041837798	-0.1600875636
H	3.2180973359	-0.7754075041	-0.4033270207
H	2.0601211729	-0.2630393192	-1.6226498523
H	0.7922469347	-2.6428500582	1.5449670722
H	1.6783427851	-1.1981002	1.9703520979
H	2.526643734	-2.5287011882	1.1244662933
H	0.2445777694	-3.1338206897	-0.7162308782
H	1.9148207784	-2.9851975798	-1.2949890616
H	0.6232207535	-1.9890919521	-2.0131921842
H	-0.4233008999	3.1562253133	0.6973366039
H	1.323334321	3.4602228032	0.8501400732
H	0.5013642248	2.2505426521	1.8914690517
H	-0.2825137368	2.6330469426	-1.5978346946
H	0.7745895064	1.3572188408	-2.1945016868
H	1.4726628824	2.9030025711	-1.6538675652
Li	-0.519225089	-0.0687081642	0.4876044914
C	-1.1190905023	-0.1065661445	2.4851017548
H	-0.3044642186	0.1329088181	3.1962938162
H	-1.4942197195	-1.089199091	2.8290597548
H	-1.9247811461	0.6042897744	2.7495296133
C	-3.0166068403	0.8293562237	-0.6173344848
O	-2.1483842381	-0.2901035747	-0.7852468326
H	-2.4627761911	1.718569433	-0.917589355
H	-3.319887366	0.9269899019	0.4302311027
H	-3.9015431126	0.7253627886	-1.257235301
C	-2.8094803205	-1.5159710834	-0.4706529246
H	-3.093519656	-1.5380892068	0.5862912131
H	-2.1075586	-2.3244137932	-0.672614811
H	-3.6959415016	-1.643335465	-1.1042162236

Tabelle 10.298 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	0.5389346175	1.0971562978	0.8535472461
Li	-0.5389346175	-1.0971562978	0.8535472461
Li	1.0971562978	-0.5389346175	-0.8537186934
Li	-1.0971562978	0.5389346175	-0.8537186934
C	0.7440903513	1.6561149501	-1.2903642387

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C	-1.6561149501	0.7440903513	1.2901927913
C	-0.7440903513	-1.6561149501	-1.2903642387
C	1.6561149501	-0.7440903513	1.2901927913
H	0.0145187137	2.4596780389	-1.491962992
H	1.0682404994	1.3304049257	-2.2931072989
H	1.621780756	2.182942392	-0.8797806899
H	-2.4596780389	0.0145187137	1.4917915447
H	-2.182942392	1.621780756	0.8796092425
H	-1.3304049257	1.0682404994	2.2929358515
H	-0.0145187137	-2.4596780389	-1.491962992
H	-1.0682404994	-1.3304049257	-2.2931072989
H	-1.621780756	-2.182942392	-0.8797806899
H	1.3304049257	-1.0682404994	2.2929358515
H	2.4596780389	-0.0145187137	1.4917915447
H	2.182942392	-1.621780756	0.8796092425
O	2.5999660054	-1.0403064609	-2.0025086003
O	-1.0403064609	-2.5999660054	2.0023371529
O	1.0403064609	2.5999660054	2.0023371529
O	-2.5999660054	1.0403064609	-2.0025086003
C	-0.293310783	-3.780373105	1.738862121
H	0.7193315149	-3.6854244062	2.1418453372
H	-0.7924230107	-4.6457419764	2.1852264613
H	-0.2494093856	-3.8953688191	0.6580732822
C	-1.1706702334	-2.3442876518	3.3920922082
H	-1.7214767748	-3.1584319953	3.872815019
H	-0.1843109813	-2.2451421046	3.8560436473
H	-1.721785962	-1.4121675846	3.4967852535
C	-3.780373105	0.293310783	-1.7390335684
H	-4.6457419764	0.7924230107	-2.1853979086
H	-3.6854244062	-0.7193315149	-2.1420167846
H	-3.8953688191	0.2494093856	-0.6582447296
C	-2.3442876518	1.1706702334	-3.3922636555
H	-2.2451421046	0.1843109813	-3.8562150947
H	-3.1584319953	1.7214767748	-3.8729864663
H	-1.4121675846	1.721785962	-3.4969567008
C	3.780373105	-0.293310783	-1.7390335684
H	3.8953688191	-0.2494093856	-0.6582447296
H	4.6457419764	-0.7924230107	-2.1853979086
H	3.6854244062	0.7193315149	-2.1420167846
C	2.3442876518	-1.1706702334	-3.3922636555
H	2.2451421046	-0.1843109813	-3.8562150947
H	3.1584319953	-1.7214767748	-3.8729864663
H	1.4121675846	-1.721785962	-3.4969567008
C	0.293310783	3.780373105	1.738862121
H	-0.7193315149	3.6854244062	2.1418453372
H	0.7924230107	4.6457419764	2.1852264613
H	0.2494093856	3.8953688191	0.6580732822
C	1.1706702334	2.3442876518	3.3920922082
H	1.7214767748	3.1584319953	3.872815019
H	0.1843109813	2.2451421046	3.8560436473
H	1.721785962	1.4121675846	3.4967852535

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Tabelle 10.299 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-0.0481266818	0.7624561422	-0.0704035194
C	0.0481266818	-0.7624561422	-0.0704035194
N	-1.4034612536	1.2290510065	-0.3361933878
N	1.4034612536	-1.2290510065	-0.3361933878
C	-1.4068422235	2.6740431602	-0.4917507413
C	-2.316650506	0.8439588726	0.7279821129
C	1.4068422235	-2.6740431602	-0.4917507413
C	2.316650506	-0.8439588726	0.7279821129
H	0.6014348055	1.1317297954	-0.8678215748
H	0.3183820079	1.1786074483	0.8859379835
H	-0.6014348055	-1.1317297954	-0.8678215748
H	-0.3183820079	-1.1786074483	0.8859379835
H	-2.4154976677	3.0136308452	-0.7322511167
H	-0.7435685253	2.9567928423	-1.3104469488
H	-1.0736254982	3.1939062661	0.4239555082
H	-2.4002104534	-0.2410534178	0.7859479882
H	-3.3080238846	1.2468647244	0.515635672
H	-1.9887645954	1.2239571306	1.7125190239
H	2.4154976677	-3.0136308452	-0.7322511167
H	0.7435685253	-2.9567928423	-1.3104469488
H	1.0736254982	-3.1939062661	0.4239555082
H	3.3080238846	-1.2468647244	0.515635672
H	1.9887645954	-1.2239571306	1.7125190239
H	2.4002104534	0.2410534178	0.7859479882

Tabelle 10.300 Standardorientierung von Me<sub>2</sub>O (C<sub>2v</sub>) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	0.	1.1660966907	-0.1993895368
O	0.	0.	0.5925232258
C	0.	-1.1660966907	-0.1993895368
H	-0.8920228444	1.2080045477	-0.8362537517
H	0.8920228444	1.2080045477	-0.8362537517
H	0.	2.018307786	0.4770029273
H	0.8920228444	-1.2080045477	-0.8362537517
H	-0.8920228444	-1.2080045477	-0.8362537517
H	0.	-2.018307786	0.4770029273

Tabelle 10.301 Standardorientierung von **4** (C<sub>2</sub>) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	0.0463994646	3.7470147019	0.8850051235
N	0.2546867002	2.4277028224	1.4842952177
C	-0.7764312691	2.1403938591	2.4764375329
C	1.5707134057	2.3228351687	2.1091530174
C	0.7886518684	3.8843610212	-0.4420831751
N	0.369130495	2.8625733863	-1.4028070013
C	-0.9144930794	3.1990852061	-2.0148235102
C	1.378181171	2.6807067646	-2.4433407927

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C	-0.0463994646	-3.7470147019	0.8850051235
N	-0.2546867002	-2.4277028224	1.4842952177
C	-1.5707134057	-2.3228351687	2.1091530174
C	0.7764312691	-2.1403938591	2.4764375329
C	-0.7886518684	-3.8843610212	-0.4420831751
N	-0.369130495	-2.8625733863	-1.4028070013
C	-1.378181171	-2.6807067646	-2.4433407927
C	0.9144930794	-3.1990852061	-2.0148235102
Li	0.1372627074	1.1229809573	-0.2165603034
Li	-0.1372627074	-1.1229809573	-0.2165603034
C	-1.8443080678	0.2194263997	-0.4598552481
C	1.8443080678	-0.2194263997	-0.4598552481
H	-1.0255800846	3.8706384395	0.7187916244
H	0.362678864	4.5515922162	1.569424345
H	-0.6118797509	1.1412766057	2.8819965855
H	-1.7577802987	2.1548767058	2.0043135478
H	-0.7571259109	2.8656550453	3.3057651501
H	1.7174906513	1.3026971642	2.4644657867
H	1.6681500042	3.0218312187	2.9556040734
H	2.3580868371	2.5300721595	1.3868799951
H	0.634999452	4.8984294659	-0.8460700666
H	1.8611938621	3.7665461567	-0.2767704399
H	-1.2115389581	2.395373927	-2.6874460318
H	-1.6901913477	3.2893525886	-1.2560470401
H	-0.8510783662	4.14199641	-2.5815033548
H	1.0470478764	1.8990030982	-3.1273735382
H	1.5446183388	3.607486577	-3.0151236682
H	2.3163593937	2.3572031628	-1.9928640769
H	-0.362678864	-4.5515922162	1.569424345
H	1.0255800846	-3.8706384395	0.7187916244
H	-1.7174906513	-1.3026971642	2.4644657867
H	-2.3580868371	-2.5300721595	1.3868799951
H	-1.6681500042	-3.0218312187	2.9556040734
H	0.6118797509	-1.1412766057	2.8819965855
H	0.7571259109	-2.8656550453	3.3057651501
H	1.7577802987	-2.1548767058	2.0043135478
H	-1.8611938621	-3.7665461567	-0.2767704399
H	-0.634999452	-4.8984294659	-0.8460700666
H	-1.0470478764	-1.8990030982	-3.1273735382
H	-2.3163593937	-2.3572031628	-1.9928640769
H	-1.5446183388	-3.607486577	-3.0151236682
H	1.2115389581	-2.395373927	-2.6874460318
H	0.8510783662	-4.14199641	-2.5815033548
H	1.6901913477	-3.2893525886	-1.2560470401
H	-2.0805480674	0.2701627868	-1.5360729706
H	-2.3001989999	1.1250278364	-0.0253465064
H	-2.4674349394	-0.604042836	-0.0714812763
H	2.0805480674	-0.2701627868	-1.5360729706
H	2.3001989999	-1.1250278364	-0.0253465064
H	2.4674349394	0.604042836	-0.0714812763

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Tabelle 10.302 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
O	0.	0.	3.8491710754
C	-0.0015369934	1.1846894033	4.6310969421
Li	0.	0.	1.945765795
Li	0.	0.	-0.2841773344
C	-0.0018106178	1.8597552539	0.922611461
H	-0.0026260003	2.024078184	3.9395634403
H	0.8921118908	1.2212993374	5.2610245472
H	-0.8952268267	1.2188841069	5.2611075235
H	-0.005157364	2.2698739316	-0.1009943627
H	0.8674016341	2.3402788108	1.4019940196
H	-0.8905006371	2.3099620916	1.3966699493
C	-0.676157927	0.3556450542	-2.992228679
N	-1.4590715297	0.0206956236	-1.8001034548
C	-2.4860315372	1.0284455044	-1.5437230065
C	-2.0868579265	-1.2939061799	-1.9199610514
H	-0.5213797211	1.4364440718	-2.9956650924
H	-1.2252301856	0.1056318253	-3.914451166
H	-3.0266187965	0.761503083	-0.6352864374
H	-2.0190700218	1.9998940247	-1.3845319351
H	-3.2027794312	1.0983643923	-2.3769287173
H	-2.5724377814	-1.5457191422	-0.9773097628
H	-2.8331186546	-1.306198057	-2.7300829365
H	-1.3395422675	-2.0605994806	-2.1173176031
C	0.0015369934	-1.1846894033	4.6310969421
C	0.0018106178	-1.8597552539	0.922611461
H	0.0026260003	-2.024078184	3.9395634403
H	-0.8921118908	-1.2212993374	5.2610245472
H	0.8952268267	-1.2188841069	5.2611075235
H	0.005157364	-2.2698739316	-0.1009943627
H	-0.8674016341	-2.3402788108	1.4019940196
H	0.8905006371	-2.3099620916	1.3966699493
C	0.676157927	-0.3556450542	-2.992228679
N	1.4590715297	-0.0206956236	-1.8001034548
C	2.4860315372	-1.0284455044	-1.5437230065
C	2.0868579265	1.2939061799	-1.9199610514
H	0.5213797211	-1.4364440718	-2.9956650924
H	1.2252301856	-0.1056318253	-3.914451166
H	3.0266187965	-0.761503083	-0.6352864374
H	2.0190700218	-1.9998940247	-1.3845319351
H	3.2027794312	-1.0983643923	-2.3769287173
H	2.5724377814	1.5457191422	-0.9773097628
H	2.8331186546	1.306198057	-2.7300829365
H	1.3395422675	2.0605994806	-2.1173176031

Tabelle 10.303 Standardorientierung von **6** [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
N	-1.441571232	0.087902764	-0.0190550435
C	-1.0351493523	-1.2342429301	-0.4993148468

C	0.3100556404	-1.6601376069	0.0900427881
N	1.3071398192	-0.5954137341	-0.0241308841
C	1.7583276252	-0.4231445107	-1.4061626637
C	2.4549218844	-0.8490835864	0.8432417347
C	-2.5344429433	0.6244163244	-0.8273518803
C	-1.8375583786	0.0497760962	1.3893798202
H	-0.965733476	-1.1847744516	-1.5876330806
H	-1.7930769167	-1.9973538005	-0.260521233
H	0.6473318775	-2.5829535348	-0.408228234
H	0.194095596	-1.8957259423	1.1496805465
H	2.4860438588	0.3873527603	-1.4434882482
H	0.9222356976	-0.1470692406	-2.0503982507
H	2.2178793296	-1.3435288493	-1.7976533622
H	3.1437110817	-0.0072387524	0.7769735024
H	2.9844576319	-1.7712288863	0.5600731603
H	2.1204367819	-0.9368835863	1.8774926755
H	-2.7766730599	1.6283797399	-0.4798808103
H	-3.4348320902	-0.0050844176	-0.7645754581
H	-2.2202792196	0.6905807844	-1.869347203
H	-2.1378605728	1.0498760786	1.7020447365
H	-0.9982774321	-0.257342287	2.0150802606
H	-2.6747130505	-0.6453848125	1.5549857594
Li	0.3091096182	1.2262197027	0.1588131965
C	0.9068484717	3.1594580508	0.2885401249
H	0.9790524096	3.6441181652	-0.6965462295
H	1.8996653212	3.2641998836	0.751341049
H	0.2292470789	3.7884505794	0.8842530735

Tabelle 10.304 Standardorientierung von **7** [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
N	0.6871254658	1.5745866016	-0.1138877808
C	1.9599824752	0.9619312298	0.2794489277
C	2.2015714322	-0.3661818407	-0.4308530781
N	1.1483878107	-1.3411482488	-0.1239731623
C	1.4404583353	-2.0459133906	1.1271151502
C	1.004196203	-2.3039464469	-1.2111462066
C	0.3777457235	2.6843998997	0.7884525755
C	0.7193314124	2.044294607	-1.4948804245
H	1.9172617332	0.796502402	1.3582398207
H	2.8023201461	1.6447709785	0.0775102338
H	3.1913268844	-0.7563709585	-0.1485813714
H	2.2226597837	-0.2099333175	-1.5107816013
H	0.6006340668	-2.6918390119	1.3820867961
H	1.5502012372	-1.3333224835	1.9420089707
H	2.3563267639	-2.6511795071	1.0337494417
H	0.2467992614	-3.0412023018	-0.942687155
H	1.9455794075	-2.8376233184	-1.4149577688
H	0.680900437	-1.7917809306	-2.1186795762
H	-0.5811331907	3.1221390944	0.5074452735
H	1.1503699129	3.4682442996	0.7443618165

H	0.2884771416	2.3021943997	1.8044399208
H	-0.2076119123	2.5743482462	-1.7151288587
H	0.7938462823	1.2070173726	-2.1881498628
H	1.5612522046	2.7326468492	-1.6719636143
Li	-0.494385896	-0.0871377747	0.432711205
C	-1.0184918905	-0.1071963182	2.4456772256
H	-0.1777724606	0.1779330756	3.1049298716
H	-1.3300448278	-1.1023878128	2.8083293303
H	-1.839160599	0.5739840319	2.7309628686
C	-2.876327321	0.837251561	-0.5809273746
O	-2.0731884791	-0.3189507473	-0.7857649552
H	-2.3289841202	1.6866350428	-0.9846469443
H	-3.0523643554	0.9855787696	0.4879926097
H	-3.827260153	0.7318352593	-1.1130086158
C	-2.7429569931	-1.4837166137	-0.3124082095
H	-2.9469121746	-1.3895081861	0.7568892862
H	-2.0786941129	-2.3289088892	-0.4816075888
H	-3.6719576343	-1.631493622	-0.8724951752

Tabelle 10.305 Standardorientierung von  $(\text{MeLi-OMe}_2)_4$  ( $S_4$ ) [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
Li	0.5436938898	1.0983267362	0.8547596246
Li	-0.5436938898	-1.0983267362	0.8547596246
Li	1.0983267362	-0.5436938898	-0.854931072
Li	-1.0983267362	0.5436938898	-0.854931072
C	0.747092205	1.6552639566	-1.2908481399
C	-1.6552639566	0.747092205	1.2906766925
C	-0.747092205	-1.6552639566	-1.2908481399
C	1.6552639566	-0.747092205	1.2906766925
H	0.0128721466	2.4497507585	-1.5070715795
H	1.0864568005	1.324280901	-2.2859006458
H	1.6141426758	2.1918770863	-0.8724329067
H	-2.4497507585	0.0128721466	1.5069001321
H	-2.1918770863	1.6141426758	0.8722614593
H	-1.324280901	1.0864568005	2.2857291985
H	-0.0128721466	-2.4497507585	-1.5070715795
H	-1.0864568005	-1.324280901	-2.2859006458
H	-1.6141426758	-2.1918770863	-0.8724329067
H	1.324280901	-1.0864568005	2.2857291985
H	2.4497507585	-0.0128721466	1.5069001321
H	2.1918770863	-1.6141426758	0.8722614593
O	2.601371783	-1.0418932405	-2.002675059
O	-1.0418932405	-2.601371783	2.0025036117
O	1.0418932405	2.601371783	2.0025036117
O	-2.601371783	1.0418932405	-2.002675059
C	-0.2966508467	-3.7823521254	1.7324858418
H	0.7186918926	-3.6881083632	2.1292895599
H	-0.7932652842	-4.64849995	2.1802651069

H	-0.2592831453	-3.8951403214	0.6510095163
C	-1.1637052811	-2.3463469887	3.3938897522
H	-1.7136258741	-3.1594407177	3.8775682291
H	-0.1742899687	-2.2495688872	3.8522371761
H	-1.7120315583	-1.4127503725	3.5022184056
C	-3.7823521254	0.2966508467	-1.7326572891
H	-4.64849995	0.7932652842	-2.1804365543
H	-3.6881083632	-0.7186918926	-2.1294610073
H	-3.8951403214	0.2592831453	-0.6511809636
C	-2.3463469887	1.1637052811	-3.3940611995
H	-2.2495688872	0.1742899687	-3.8524086234
H	-3.1594407177	1.7136258741	-3.8777396765
H	-1.4127503725	1.7120315583	-3.5023898529
C	3.7823521254	-0.2966508467	-1.7326572891
H	3.8951403214	-0.2592831453	-0.6511809636
H	4.64849995	-0.7932652842	-2.1804365543
H	3.6881083632	0.7186918926	-2.1294610073
C	2.3463469887	-1.1637052811	-3.3940611995
H	2.2495688872	-0.1742899687	-3.8524086234
H	3.1594407177	-1.7136258741	-3.8777396765
H	1.4127503725	-1.7120315583	-3.5023898529
C	0.2966508467	3.7823521254	1.7324858418
H	-0.7186918926	3.6881083632	2.1292895599
H	0.7932652842	4.64849995	2.1802651069
H	0.2592831453	3.8951403214	0.6510095163
C	1.1637052811	2.3463469887	3.3938897522
H	1.7136258741	3.1594407177	3.8775682291
H	0.1742899687	2.2495688872	3.8522371761
H	1.7120315583	1.4127503725	3.5022184056

Tabelle 10.306 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
C	-0.0485871731	0.7623595345	-0.0703362579
C	0.0485871731	-0.7623595345	-0.0703362579
N	-1.4051386748	1.2274747801	-0.3335762166
N	1.4051386748	-1.2274747801	-0.3335762166
C	-1.4097567366	2.6717266192	-0.498780908
C	-2.3153571934	0.8483936203	0.7358308047
C	1.4097567366	-2.6717266192	-0.498780908
C	2.3153571934	-0.8483936203	0.7358308047
H	0.5994126146	1.1300987134	-0.8697972294
H	0.3200079434	1.1791249634	0.885082188
H	-0.5994126146	-1.1300987134	-0.8697972294
H	-0.3200079434	-1.1791249634	0.885082188
H	-2.4195307938	3.0094055446	-0.736730116
H	-0.750516069	2.9493092694	-1.3223188618
H	-1.0725105902	3.1977678403	0.4119143605
H	-2.3976197327	-0.2361230686	0.8016308762
H	-3.3076573354	1.248588174	0.5233679679
H	-1.9853770292	1.2355572954	1.7168243924

H	2.4195307938	-3.0094055446	-0.736730116
H	0.750516069	-2.9493092694	-1.3223188618
H	1.0725105902	-3.1977678403	0.4119143605
H	3.3076573354	-1.248588174	0.5233679679
H	1.9853770292	-1.2355572954	1.7168243924
H	2.3976197327	0.2361230686	0.8016308762

Tabelle 10.307 Standardorientierung von  $\text{Me}_2\text{O}$  ( $\text{C}_{2v}$ ) [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
C	0.	1.1666959181	-0.1991865309
O	0.	0.	0.592799501
C	0.	-1.1666959181	-0.1991865309
H	-0.8919766578	1.2090619056	-0.8363128645
H	0.8919766578	1.2090619056	-0.8363128645
H	0.	2.0193346367	0.4767800095
H	0.8919766578	-1.2090619056	-0.8363128645
H	-0.8919766578	-1.2090619056	-0.8363128645
H	0.	-2.0193346367	0.4767800095

Tabelle 10.308 Standardorientierung von  $\mathbf{4}$  ( $\text{C}_2$ ) [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
C	0.1412422088	3.7710928446	0.8940530808
N	0.2804982898	2.4377844959	1.4839022403
C	-0.7624773609	2.1888584118	2.4744308261
C	1.5924307293	2.2633009444	2.1037432234
C	0.8278446248	3.850746155	-0.4673714538
N	0.2873282165	2.8642141978	-1.4038014058
C	-1.0271050526	3.2596915308	-1.9056026568
C	1.2022406081	2.6571438858	-2.5242188137
C	-0.1412422088	-3.7710928446	0.8940530808
N	-0.2804982898	-2.4377844959	1.4839022403
C	-1.5924307293	-2.2633009444	2.1037432234
C	0.7624773609	-2.1888584118	2.4744308261
C	-0.8278446248	-3.850746155	-0.4673714538
N	-0.2873282165	-2.8642141978	-1.4038014058
C	-1.2022406081	-2.6571438858	-2.5242188137
C	1.0271050526	-3.2596915308	-1.9056026568
Li	0.105296644	1.1297085686	-0.2154811602
Li	-0.105296644	-1.1297085686	-0.2154811602
C	-1.8458719594	0.172720432	-0.4634757485
C	1.8458719594	-0.172720432	-0.4634757485
H	-0.9241770855	3.9791557833	0.7799170534
H	0.5513698507	4.5482766246	1.5592273533
H	-0.6417914291	1.1799137632	2.8713835098
H	-1.7424466367	2.2493855395	2.0023242097
H	-0.7121391705	2.9051113738	3.3100447051
H	1.7072363407	1.22522369	2.4160449718
H	1.7119271351	2.9257137999	2.9761445709
H	2.3850309701	2.4743374475	1.3883588726

H	0.7344747496	4.8741571665	-0.8672279234
H	1.8943035456	3.646099072	-0.3511717052
H	-1.392362498	2.4938341255	-2.5883450515
H	-1.7450277226	3.3326890772	-1.0900253773
H	-0.9794908676	4.2249563267	-2.4349008311
H	0.790106525	1.8918202529	-3.1825186513
H	1.352692594	3.5820370855	-3.1033624817
H	2.1622436687	2.2999160735	-2.152224596
H	-0.5513698507	-4.5482766246	1.5592273533
H	0.9241770855	-3.9791557833	0.7799170534
H	-1.7072363407	-1.22522369	2.4160449718
H	-2.3850309701	-2.4743374475	1.3883588726
H	-1.7119271351	-2.9257137999	2.9761445709
H	0.6417914291	-1.1799137632	2.8713835098
H	0.7121391705	-2.9051113738	3.3100447051
H	1.7424466367	-2.2493855395	2.0023242097
H	-1.8943035456	-3.646099072	-0.3511717052
H	-0.7344747496	-4.8741571665	-0.8672279234
H	-0.790106525	-1.8918202529	-3.1825186513
H	-2.1622436687	-2.2999160735	-2.152224596
H	-1.352692594	-3.5820370855	-3.1033624817
H	1.392362498	-2.4938341255	-2.5883450515
H	0.9794908676	-4.2249563267	-2.4349008311
H	1.7450277226	-3.3326890772	-1.0900253773
H	-2.0615939172	0.3377429696	-1.5319745374
H	-2.3672630653	0.9864254452	0.0663368469
H	-2.4208251646	-0.7298112546	-0.1976460701
H	2.0615939172	-0.3377429696	-1.5319745374
H	2.3672630653	-0.9864254452	0.0663368469
H	2.4208251646	0.7298112546	-0.1976460701

Tabelle 10.309 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
O	0.	0.	3.8489520501
C	-0.0027077787	1.1858503924	4.6303017951
Li	0.	0.	1.9475107496
Li	0.	0.	-0.2871152043
C	-0.0028819115	1.8590616711	0.9231318851
H	-0.0046226026	2.0244324847	3.9374824253
H	0.8910066094	1.2241221016	5.2602803911
H	-0.8965267487	1.2199362741	5.2603780625
H	-0.00517501	2.2663549745	-0.1008646594
H	0.8653021723	2.3400809136	1.4022361984
H	-0.8922811663	2.3085403839	1.3948918721
C	-0.6757644282	0.3562695293	-2.9921349722
N	-1.4594746814	0.0204950557	-1.8004572793
C	-2.4855937962	1.029395806	-1.5424600749
C	-2.0876675545	-1.2943623688	-1.9207418493
H	-0.5194327124	1.4369449868	-2.9937550707
H	-1.2240787501	0.1076114892	-3.9151437965

H	-3.0262521862	0.7614459895	-0.6343862751
H	-2.0169704556	1.9996951871	-1.3808652609
H	-3.202304107	1.1014567155	-2.375422147
H	-2.5728054198	-1.5462262355	-0.977930294
H	-2.8337129857	-1.306501869	-2.7309443863
H	-1.3401094979	-2.0610478444	-2.1174068843
C	0.0027077787	-1.1858503924	4.6303017951
C	0.0028819115	-1.8590616711	0.9231318851
H	0.0046226026	-2.0244324847	3.9374824253
H	-0.8910066094	-1.2241221016	5.2602803911
H	0.8965267487	-1.2199362741	5.2603780625
H	0.00517501	-2.2663549745	-0.1008646594
H	-0.8653021723	-2.3400809136	1.4022361984
H	0.8922811663	-2.3085403839	1.3948918721
C	0.6757644282	-0.3562695293	-2.9921349722
N	1.4594746814	-0.0204950557	-1.8004572793
C	2.4855937962	-1.029395806	-1.5424600749
C	2.0876675545	1.2943623688	-1.9207418493
H	0.5194327124	-1.4369449868	-2.9937550707
H	1.2240787501	-0.1076114892	-3.9151437965
H	3.0262521862	-0.7614459895	-0.6343862751
H	2.0169704556	-1.9996951871	-1.3808652609
H	3.202304107	-1.1014567155	-2.375422147
H	2.5728054198	1.5462262355	-0.977930294
H	2.8337129857	1.306501869	-2.7309443863
H	1.3401094979	2.0610478444	-2.1174068843

Tabelle 10.310 Standardorientierung von **6** [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
N	-1.4641613467	0.0789595192	-0.0072870902
C	-1.0379734418	-1.2267472683	-0.5173115105
C	0.3058541939	-1.6543442061	0.0737374601
N	1.2916897132	-0.5765333508	-0.0055084058
C	1.7651422495	-0.3727183316	-1.3763612696
C	2.4276335239	-0.8241137708	0.8791104612
C	-2.5669540788	0.613803997	-0.8043422761
C	-1.8587039427	0.0024406562	1.4004601913
H	-0.9586327086	-1.1479531576	-1.6032892376
H	-1.7901707569	-2.0033319968	-0.3051539867
H	0.655332656	-2.5616670997	-0.4441388951
H	0.1820333324	-1.9172882849	1.1261160928
H	2.4718768769	0.4567963916	-1.3866385709
H	0.9350623446	-0.1061489587	-2.032209791
H	2.2532727329	-1.2764109987	-1.7719233486
H	3.1003284773	0.0323316776	0.8391295308
H	2.9801979204	-1.7310735368	0.5908269808
H	2.0759862765	-0.9357794114	1.905411546
H	-2.8271460723	1.6056264699	-0.4356366412
H	-3.4559298542	-0.0327884592	-0.7549797938
H	-2.2540069036	0.7079168865	-1.8444513517

H	-2.180576137	0.9888129074	1.7344810072
H	-1.0126675058	-0.3006724727	2.0187659593
H	-2.6811604176	-0.7131476442	1.5514712432
Li	0.2754863295	1.2334497843	0.1709240611
C	0.9787449846	3.1345824122	0.2216798723
H	0.9874088992	3.6054893282	-0.7719916767
H	2.0165205022	3.1742859364	0.5852456889
H	0.4059041532	3.8103629816	0.8715187507

Tabelle 10.311 Standardorientierung von **7** [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
N	0.6845619666	1.5740734053	-0.1184914226
C	1.9547535541	0.9611040794	0.2842931578
C	2.2020584472	-0.3658257069	-0.4262039692
N	1.1480973992	-1.3425074564	-0.1259697334
C	1.4351920711	-2.0506719893	1.1248430365
C	1.0059263985	-2.3017055564	-1.2171372964
C	0.3672587686	2.6822388621	0.7840013806
C	0.7255999568	2.0451804234	-1.4991158564
H	1.9016437039	0.7928505181	1.3623787194
H	2.7987461509	1.6441350604	0.0902955769
H	3.190748825	-0.7544852722	-0.1384010594
H	2.2287832717	-0.2079109342	-1.5057797794
H	0.5952501443	-2.6992193399	1.3728159518
H	1.5364599931	-1.3395283608	1.9422511997
H	2.3531354134	-2.6531349512	1.0350959976
H	0.2456901652	-3.0378943393	-0.9539245916
H	1.9466309001	-2.8371796368	-1.4189384551
H	0.6869876923	-1.7857912783	-2.1240566695
H	-0.588040107	3.1220579113	0.4941579764
H	1.1412085121	3.4651862082	0.7499485207
H	0.2663165542	2.2955005228	1.7972962643
H	-0.201865327	2.5714432895	-1.7259436458
H	0.8085435289	1.2088442269	-2.1925276826
H	1.5659030573	2.7371152167	-1.6692325228
Li	-0.4936068568	-0.0890877539	0.4257582215
C	-1.0138096716	-0.1017082541	2.4429304236
H	-0.1698628689	0.1851214072	3.0964568787
H	-1.3229955921	-1.0951642709	2.810241258
H	-1.8320147316	0.5802947308	2.7306312749
C	-2.8710143073	0.8374591779	-0.5758521145
O	-2.0732692978	-0.3224374	-0.7875163246
H	-2.3256513133	1.6843750471	-0.9878915419
H	-3.0328706321	0.9880705068	0.4952659339
H	-3.8284245805	0.7339772242	-1.0965757726
C	-2.7424261216	-1.4854076217	-0.3062557413
H	-2.9300723333	-1.3906749308	0.7662412131
H	-2.0844049598	-2.3336308522	-0.4855239935
H	-3.6796597743	-1.6285099129	-0.8537428129

Tabelle 10.312 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
Li	0.5498693619	1.099742232	0.8582379573
Li	-0.5498693619	-1.099742232	0.8582379573
Li	1.099742232	-0.5498693619	-0.8584094047
Li	-1.099742232	0.5498693619	-0.8584094047
C	0.7535785005	1.652442746	-1.291304786
C	-1.652442746	0.7535785005	1.2911333386
C	-0.7535785005	-1.652442746	-1.291304786
C	1.652442746	-0.7535785005	1.2911333386
H	0.0127581612	2.4326305121	-1.5270965264
H	1.116063604	1.3217349681	-2.2760641915
H	1.6018765778	2.2074103843	-0.8635618235
H	-2.4326305121	0.0127581612	1.526925079
H	-2.2074103843	1.6018765778	0.8633903761
H	-1.3217349681	1.116063604	2.2758927441
H	-0.0127581612	-2.4326305121	-1.5270965264
H	-1.116063604	-1.3217349681	-2.2760641915
H	-1.6018765778	-2.2074103843	-0.8635618235
H	1.3217349681	-1.116063604	2.2758927441
H	2.4326305121	-0.0127581612	1.526925079
H	2.2074103843	-1.6018765778	0.8633903761
O	2.6041978491	-1.0382967155	-2.002013559
O	-1.0382967155	-2.6041978491	2.0018421116
O	1.0382967155	2.6041978491	2.0018421116
O	-2.6041978491	1.0382967155	-2.002013559
C	-0.2962853642	-3.7848562989	1.7269274067
H	0.7147881349	-3.6968207865	2.1317388857
H	-0.7983924134	-4.6516112224	2.1636917136
H	-0.2507851313	-3.8895042907	0.6462951353
C	-1.1751245739	-2.3665213042	3.3936622463
H	-1.7372313459	-3.1799569509	3.8591424189
H	-0.191541192	-2.2862109706	3.8640460833
H	-1.7148639331	-1.4304286497	3.5097403416
C	-3.7848562989	0.2962853642	-1.7270988541
H	-4.6516112224	0.7983924134	-2.163863161
H	-3.6968207865	-0.7147881349	-2.1319103331
H	-3.8895042907	0.2507851313	-0.6464665827
C	-2.3665213042	1.1751245739	-3.3938336937
H	-2.2862109706	0.191541192	-3.8642175307
H	-3.1799569509	1.7372313459	-3.8593138662
H	-1.4304286497	1.7148639331	-3.5099117889
C	3.7848562989	-0.2962853642	-1.7270988541
H	3.8895042907	-0.2507851313	-0.6464665827
H	4.6516112224	-0.7983924134	-2.163863161
H	3.6968207865	0.7147881349	-2.1319103331
C	2.3665213042	-1.1751245739	-3.3938336937
H	2.2862109706	-0.191541192	-3.8642175307
H	3.1799569509	-1.7372313459	-3.8593138662
H	1.4304286497	-1.7148639331	-3.5099117889
C	0.2962853642	3.7848562989	1.7269274067

H	-0.7147881349	3.6968207865	2.1317388857
H	0.7983924134	4.6516112224	2.1636917136
H	0.2507851313	3.8895042907	0.6462951353
C	1.1751245739	2.3665213042	3.3936622463
H	1.7372313459	3.1799569509	3.8591424189
H	0.191541192	2.2862109706	3.8640460833
H	1.7148639331	1.4304286497	3.5097403416

Tabelle 10.313 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
C	-0.0478355016	0.761403456	-0.0732122804
C	0.0478355016	-0.761403456	-0.0732122804
N	-1.4030530465	1.2279562124	-0.3352835873
N	1.4030530465	-1.2279562124	-0.3352835873
C	-1.407032073	2.67199008	-0.4928113362
C	-2.3128253086	0.843030975	0.7309084428
C	1.407032073	-2.67199008	-0.4928113362
C	2.3128253086	-0.843030975	0.7309084428
H	0.6002365694	1.1289058033	-0.8704944442
H	0.3188031027	1.1765296211	0.8812714096
H	-0.6002365694	-1.1289058033	-0.8704944442
H	-0.3188031027	-1.1765296211	0.8812714096
H	-2.4146374657	3.0114470985	-0.731002701
H	-0.7460665094	2.9542234185	-1.3114750243
H	-1.0723783352	3.1899127677	0.4212259821
H	-2.397186129	-0.2403417037	0.7888201917
H	-3.3031859004	1.2466876057	0.5233244667
H	-1.979740375	1.2224173621	1.7118398805
H	2.4146374657	-3.0114470985	-0.731002701
H	0.7460665094	-2.9542234185	-1.3114750243
H	1.0723783352	-3.1899127677	0.4212259821
H	3.3031859004	-1.2466876057	0.5233244667
H	1.979740375	-1.2224173621	1.7118398805
H	2.397186129	0.2403417037	0.7888201917

Tabelle 10.314 Standardorientierung von Me<sub>2</sub>O (C<sub>2v</sub>) [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
C	0.	1.1647772699	-0.1987123332
O	0.	0.	0.5930266186
C	0.	-1.1647772699	-0.1987123332
H	-0.89056939	1.2061167242	-0.8352271779
H	0.89056939	1.2061167242	-0.8352271779
H	0.	2.0181694516	0.4740208798
H	0.89056939	-1.2061167242	-0.8352271779
H	-0.89056939	-1.2061167242	-0.8352271779
H	0.	-2.0181694516	0.4740208798

Tabelle 10.315 Standardorientierung von **4** (C<sub>2</sub>) [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
C	-0.0287984684	3.7298374439	0.8616257101
N	0.2583560316	2.4353813676	1.4803597512
C	-0.7503074947	2.115101746	2.4855253885
C	1.5827858034	2.4105225078	2.0934406589
C	0.7403751067	3.9150180036	-0.4415500834
N	0.4269706749	2.8563441017	-1.4026467994
C	-0.8262801281	3.1300598475	-2.1024665159
C	1.5072173916	2.6909108554	-2.3713093319
C	0.0287984684	-3.7298374439	0.8616257101
N	-0.2583560316	-2.4353813676	1.4803597512
C	-1.5827858034	-2.4105225078	2.0934406589
C	0.7503074947	-2.115101746	2.4855253885
C	-0.7403751067	-3.9150180036	-0.4415500834
N	-0.4269706749	-2.8563441017	-1.4026467994
C	-1.5072173916	-2.6909108554	-2.3713093319
C	0.8262801281	-3.1300598475	-2.1024665159
Li	0.1668551931	1.1234972807	-0.2063768171
Li	-0.1668551931	-1.1234972807	-0.2063768171
C	-1.844960192	0.2709470035	-0.4265042849
C	1.844960192	-0.2709470035	-0.4265042849
H	-1.0998893572	3.7667458086	0.6596225696
H	0.2032097051	4.5588748749	1.5479322324
H	-0.5297041886	1.138188246	2.9134981562
H	-1.7314086173	2.0643641547	2.0183809984
H	-0.7651311756	2.8595535062	3.2952864567
H	1.7666736117	1.4178477404	2.5009100634
H	1.6641336069	3.155043043	2.8994968547
H	2.3546669084	2.6024617841	1.352299537
H	0.5204675916	4.9082356888	-0.8596066118
H	1.8113367869	3.8846055474	-0.2433318536
H	-1.070738733	2.2855818137	-2.7436446038
H	-1.6424454532	3.2444154742	-1.3931793646
H	-0.747157815	4.0413357283	-2.7134038974
H	1.2455404854	1.891817272	-3.062930137
H	1.6828306975	3.6134235942	-2.9436521631
H	2.4212956113	2.4008860445	-1.8560297856
H	-0.2032097051	-4.5588748749	1.5479322324
H	1.0998893572	-3.7667458086	0.6596225696
H	-1.7666736117	-1.4178477404	2.5009100634
H	-2.3546669084	-2.6024617841	1.352299537
H	-1.6641336069	-3.155043043	2.8994968547
H	0.5297041886	-1.138188246	2.9134981562
H	0.7651311756	-2.8595535062	3.2952864567
H	1.7314086173	-2.0643641547	2.0183809984
H	-1.8113367869	-3.8846055474	-0.2433318536
H	-0.5204675916	-4.9082356888	-0.8596066118
H	-1.2455404854	-1.891817272	-3.062930137
H	-2.4212956113	-2.4008860445	-1.8560297856
H	-1.6828306975	-3.6134235942	-2.9436521631

H	1.070738733	-2.2855818137	-2.7436446038
H	0.747157815	-4.0413357283	-2.7134038974
H	1.6424454532	-3.2444154742	-1.3931793646
H	-2.1277181858	0.2228721466	-1.4884756346
H	-2.2288888933	1.2428738855	-0.0811781337
H	-2.494440248	-0.4626258878	0.0744706673
H	2.1277181858	-0.2228721466	-1.4884756346
H	2.2288888933	-1.2428738855	-0.0811781337
H	2.494440248	0.4626258878	0.0744706673

Tabelle 10.316 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
O	0.	0.	3.8598426788
C	-0.0092095211	1.1848625258	4.6416540096
Li	0.	0.	1.9535419412
Li	0.	0.	-0.2833616314
C	-0.0039753709	1.859365619	0.9264790027
H	-0.016263003	2.0236412013	3.9510727796
H	0.8832049862	1.2273784304	5.2706575134
H	-0.9016030012	1.212877665	5.2715030674
H	0.0047883743	2.2682776604	-0.0946931273
H	0.8562720844	2.3415159822	1.4141767961
H	-0.894273899	2.3109000573	1.3897064415
C	-0.6746582437	0.3560220738	-2.9960516415
N	-1.4572045085	0.020630388	-1.8046387192
C	-2.4818755262	1.03036844	-1.5482456175
C	-2.0869026205	-1.292269518	-1.9284583219
H	-0.5182052489	1.4348871636	-2.9981255899
H	-1.2238189575	0.1071701264	-3.9161273748
H	-3.0279317156	0.7610662219	-0.6454992284
H	-2.0124933229	1.9977803986	-1.3807511184
H	-3.1921555329	1.105851438	-2.3841161895
H	-2.5724978142	-1.5460278402	-0.9879752026
H	-2.8313100704	-1.2992968984	-2.7378427878
H	-1.3415147153	-2.0585827896	-2.1268727768
C	0.0092095211	-1.1848625258	4.6416540096
C	0.0039753709	-1.859365619	0.9264790027
H	0.016263003	-2.0236412013	3.9510727796
H	-0.8832049862	-1.2273784304	5.2706575134
H	0.9016030012	-1.212877665	5.2715030674
H	-0.0047883743	-2.2682776604	-0.0946931273
H	-0.8562720844	-2.3415159822	1.4141767961
H	0.894273899	-2.3109000573	1.3897064415
C	0.6746582437	-0.3560220738	-2.9960516415
N	1.4572045085	-0.020630388	-1.8046387192
C	2.4818755262	-1.03036844	-1.5482456175
C	2.0869026205	1.292269518	-1.9284583219
H	0.5182052489	-1.4348871636	-2.9981255899
H	1.2238189575	-0.1071701264	-3.9161273748
H	3.0279317156	-0.7610662219	-0.6454992284

H	2.0124933229	-1.9977803986	-1.3807511184
H	3.1921555329	-1.105851438	-2.3841161895
H	2.5724978142	1.5460278402	-0.9879752026
H	2.8313100704	1.2992968984	-2.7378427878
H	1.3415147153	2.0585827896	-2.1268727768

Tabelle 10.317 Standardorientierung von **6** [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
N	-1.4840548233	0.0721234979	0.0618927452
C	-1.0282325343	-1.1858390792	-0.5350719367
C	0.3076199658	-1.6396446667	0.0487443626
N	1.2867961366	-0.5541851985	0.0460789334
C	1.7860457298	-0.2775714311	-1.3030076001
C	2.4083660018	-0.8453685374	0.9341388581
C	-2.567700583	0.6543092038	-0.7282297039
C	-1.9267319464	-0.1242532418	1.4419566794
H	-0.9282352926	-1.0250060413	-1.6082987899
H	-1.7742044471	-1.9820308429	-0.3967802632
H	0.6704096242	-2.5107018068	-0.516045306
H	0.1704145436	-1.9644646547	1.0803088326
H	2.4782487179	0.560822229	-1.257654539
H	0.9687223983	0.0127769917	-1.9618978726
H	2.2916313679	-1.1565891883	-1.7267676871
H	3.0791628689	0.0118089422	0.9489117142
H	2.9670174585	-1.732345615	0.6048062925
H	2.0427986584	-1.0146750805	1.9463046379
H	-2.8592341805	1.6071970611	-0.2906687624
H	-3.4434653817	-0.0082782388	-0.7622089342
H	-2.2208153315	0.8386980194	-1.7435853343
H	-2.2721662526	0.8262118035	1.8453959912
H	-1.1024989104	-0.4741379486	2.0621393375
H	-2.7466452344	-0.8535817399	1.50040599
Li	0.252298582	1.2429934604	0.2635768962
C	1.0308108363	3.1083483651	0.035294097
H	1.0377785895	3.4130070447	-1.0201975057
H	2.0784380707	3.1509813867	0.3641790455
H	0.5178173677	3.9135353062	0.5739348218

Tabelle 10.318 Standardorientierung von **7** [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
N	0.6832730733	1.5742828377	-0.1269372296
C	1.947637092	0.9581165591	0.2869298109
C	2.2019449307	-0.3642431302	-0.4254057222
N	1.1506815227	-1.3448163027	-0.1326887383
C	1.4333269687	-2.0507567064	1.1196202105
C	1.0211979372	-2.3051366174	-1.2233607894
C	0.3583554534	2.676787111	0.7790759246
C	0.7444329931	2.0569983012	-1.5019772617
H	1.8819974716	0.784759376	1.3617724121

H	2.7913157553	1.6415808238	0.1053128083
H	3.1880964123	-0.7510163228	-0.1336424739
H	2.233542708	-0.2038740434	-1.5026459963
H	0.5981964651	-2.7057924446	1.3605346099
H	1.5222283182	-1.3403502218	1.9371536253
H	2.355089604	-2.6447353327	1.034333486
H	0.2612030072	-3.0420267384	-0.9672068229
H	1.9644231983	-2.8369290937	-1.4134263501
H	0.7116258173	-1.792504025	-2.1336128313
H	-0.5891758461	3.1233193357	0.4795802211
H	1.1361744621	3.4539112051	0.7593318547
H	0.2426888186	2.2835720363	1.7867752992
H	-0.1776376959	2.5861898682	-1.7372525619
H	0.8375897828	1.2285596141	-2.2012510022
H	1.5868373773	2.7483020421	-1.6515884962
Li	-0.4939416337	-0.0954716782	0.4090311924
C	-1.0009939266	-0.1025365274	2.4373434515
H	-0.1544777277	0.1894660768	3.0816081213
H	-1.2995989405	-1.0944519829	2.811030703
H	-1.8184920182	0.5720196385	2.7361738506
C	-2.8805305804	0.8356238653	-0.5770099875
O	-2.0893093457	-0.3299280479	-0.7727459289
H	-2.3306013745	1.6748136024	-0.9949908373
H	-3.044315095	0.9967805375	0.4907621232
H	-3.8358678316	0.7310348051	-1.0978929706
C	-2.7661072275	-1.4843346361	-0.2848901722
H	-2.9566302476	-1.3775029129	0.7844444028
H	-2.1136522713	-2.3373950335	-0.4529155723
H	-3.7010194066	-1.6257638378	-0.8335503628

Tabelle 10.319 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
Li	0.5488736864	1.0976305997	0.8582529446
Li	-0.5488736864	-1.0976305997	0.8582529446
Li	1.0976305997	-0.5488736864	-0.858424392
Li	-1.0976305997	0.5488736864	-0.858424392
C	0.7555087132	1.648718797	-1.2879304567
C	-1.648718797	0.7555087132	1.2877590093
C	-0.7555087132	-1.648718797	-1.2879304567
C	1.648718797	-0.7555087132	1.2877590093
H	0.0110139674	2.4192460641	-1.5264974749
H	1.1250710249	1.3180327091	-2.265806102
H	1.5939872087	2.2057894547	-0.8530445683
H	-2.4192460641	0.0110139674	1.5263260275
H	-2.2057894547	1.5939872087	0.8528731209
H	-1.3180327091	1.1250710249	2.2656346546
H	-0.0110139674	-2.4192460641	-1.5264974749
H	-1.1250710249	-1.3180327091	-2.265806102

H	-1.5939872087	-2.2057894547	-0.8530445683
H	1.3180327091	-1.1250710249	2.2656346546
H	2.4192460641	-0.0110139674	1.5263260275
H	2.2057894547	-1.5939872087	0.8528731209
O	2.6007566041	-1.0519881232	-1.9973799277
O	-1.0519881232	-2.6007566041	1.9972084804
O	1.0519881232	2.6007566041	1.9972084804
O	-2.6007566041	1.0519881232	-1.9973799277
C	-0.3030171206	-3.7722239893	1.7198028134
H	0.708722587	-3.6730328171	2.1120567269
H	-0.7885559805	-4.639276068	2.1667850609
H	-0.2675503873	-3.8834250357	0.6423726076
C	-1.1644461367	-2.3563975907	3.3864904582
H	-1.7062232818	-3.1709503859	3.8665836412
H	-0.1757957003	-2.2646246044	3.836631592
H	-1.7093673044	-1.427650894	3.5097040789
C	-3.7722239893	0.3030171206	-1.7199742608
H	-4.639276068	0.7885559805	-2.1669565083
H	-3.6730328171	-0.708722587	-2.1122281743
H	-3.8834250357	0.2675503873	-0.642544055
C	-2.3563975907	1.1644461367	-3.3866619055
H	-2.2646246044	0.1757957003	-3.8368030393
H	-3.1709503859	1.7062232818	-3.8667550886
H	-1.427650894	1.7093673044	-3.5098755263
C	3.7722239893	-0.3030171206	-1.7199742608
H	3.8834250357	-0.2675503873	-0.642544055
H	4.639276068	-0.7885559805	-2.1669565083
H	3.6730328171	0.708722587	-2.1122281743
C	2.3563975907	-1.1644461367	-3.3866619055
H	2.2646246044	-0.1757957003	-3.8368030393
H	3.1709503859	-1.7062232818	-3.8667550886
H	1.427650894	-1.7093673044	-3.5098755263
C	0.3030171206	3.7722239893	1.7198028134
H	-0.708722587	3.6730328171	2.1120567269
H	0.7885559805	4.639276068	2.1667850609
H	0.2675503873	3.8834250357	0.6423726076
C	1.1644461367	2.3563975907	3.3864904582
H	1.7062232818	3.1709503859	3.8665836412
H	0.1757957003	2.2646246044	3.836631592
H	1.7093673044	1.427650894	3.5097040789

Tabelle 10.320 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
C	-0.0472432708	0.7602236369	-0.0797119917
C	0.0472432708	-0.7602236369	-0.0797119917
N	-1.398348707	1.2292567236	-0.3426726885
N	1.398348707	-1.2292567236	-0.3426726885
C	-1.3992162692	2.6731766194	-0.4742882032
C	-2.3104876912	0.8312248064	0.712888893
C	1.3992162692	-2.6731766194	-0.4742882032

C	2.3104876912	-0.8312248064	0.712888893
H	0.6020156995	1.130690265	-0.8705709004
H	0.3153060783	1.170652782	0.8745160949
H	-0.6020156995	-1.130690265	-0.8705709004
H	-0.3153060783	-1.170652782	0.8745160949
H	-2.4025247539	3.0187522421	-0.706857627
H	-0.7354619771	2.9687952738	-1.2816773673
H	-1.0670835504	3.1694092593	0.4487848139
H	-2.3930369101	-0.2495911471	0.7583338832
H	-3.2970392522	1.237150041	0.5085938715
H	-1.9802731207	1.1985909213	1.6957722216
H	2.4025247539	-3.0187522421	-0.706857627
H	0.7354619771	-2.9687952738	-1.2816773673
H	1.0670835504	-3.1694092593	0.4487848139
H	3.2970392522	-1.237150041	0.5085938715
H	1.9802731207	-1.1985909213	1.6957722216
H	2.3930369101	0.2495911471	0.7583338832

Tabelle 10.321 Standardorientierung von Me<sub>2</sub>O (C<sub>2v</sub>) [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
C	0.	1.1624237259	-0.1980258544
O	0.	0.	0.5922536772
C	0.	-1.1624237259	-0.1980258544
H	-0.8875299926	1.2014802827	-0.8334145113
H	0.8875299926	1.2014802827	-0.8334145113
H	0.	2.015672483	0.4700955384
H	0.8875299926	-1.2014802827	-0.8334145113
H	-0.8875299926	-1.2014802827	-0.8334145113
H	0.	-2.015672483	0.4700955384

Tabelle 10.322 Standardorientierung von **4** (C<sub>2</sub>) [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
C	-0.0279082019	3.721983521	0.8553577994
N	0.258419178	2.4347959699	1.4816650746
C	-0.7483731764	2.1204996277	2.4857989109
C	1.5793136512	2.4133506545	2.0946110323
C	0.7424374744	3.9016192818	-0.4447441628
N	0.4261509402	2.8483527967	-1.4057308033
C	-0.8267772413	3.122537912	-2.0988800395
C	1.5005991332	2.6852983509	-2.3762070453
C	0.0279082019	-3.721983521	0.8553577994
N	-0.258419178	-2.4347959699	1.4816650746
C	-1.5793136512	-2.4133506545	2.0946110323
C	0.7483731764	-2.1204996277	2.4857989109
C	-0.7424374744	-3.9016192818	-0.4447441628
N	-0.4261509402	-2.8483527967	-1.4057308033
C	-1.5005991332	-2.6852983509	-2.3762070453
C	0.8267772413	-3.122537912	-2.0988800395
Li	0.1669520579	1.1218047248	-0.2043166833

Li	-0.1669520579	-1.1218047248	-0.2043166833
C	-1.8404129785	0.2704050129	-0.4203341635
C	1.8404129785	-0.2704050129	-0.4203341635
H	-1.0952751045	3.7568993245	0.6508769829
H	0.2014178723	4.5526223947	1.5354032247
H	-0.5301482927	1.1480276252	2.9173256559
H	-1.7272601578	2.0717014767	2.0210912088
H	-0.7606463877	2.8664704376	3.2898273696
H	1.7622184392	1.4265040427	2.5083473816
H	1.658042182	3.1607092897	2.8938965241
H	2.3499476281	2.601897506	1.3560529079
H	0.5291063972	4.8933023024	-0.8614526403
H	1.8095315316	3.8649245938	-0.2447486608
H	-1.0698724427	2.2847327593	-2.7439662548
H	-1.6390402293	3.2311248404	-1.3890819375
H	-0.7503847478	4.0352782788	-2.7021059356
H	1.2387986869	1.8890926924	-3.066156068
H	1.6710929779	3.6061791503	-2.9465010547
H	2.4150174029	2.3993629619	-1.8659306349
H	-0.2014178723	-4.5526223947	1.5354032247
H	1.0952751045	-3.7568993245	0.6508769829
H	-1.7622184392	-1.4265040427	2.5083473816
H	-2.3499476281	-2.601897506	1.3560529079
H	-1.658042182	-3.1607092897	2.8938965241
H	0.5301482927	-1.1480276252	2.9173256559
H	0.7606463877	-2.8664704376	3.2898273696
H	1.7272601578	-2.0717014767	2.0210912088
H	-1.8095315316	-3.8649245938	-0.2447486608
H	-0.5291063972	-4.8933023024	-0.8614526403
H	-1.2387986869	-1.8890926924	-3.066156068
H	-2.4150174029	-2.3993629619	-1.8659306349
H	-1.6710929779	-3.6061791503	-2.9465010547
H	1.0698724427	-2.2847327593	-2.7439662548
H	0.7503847478	-4.0352782788	-2.7021059356
H	1.6390402293	-3.2311248404	-1.3890819375
H	-2.1196835402	0.2207615459	-1.4792891624
H	-2.2168477997	1.241499527	-0.0762451383
H	-2.4859927359	-0.4601255495	0.0819993222
H	2.1196835402	-0.2207615459	-1.4792891624
H	2.2168477997	-1.241499527	-0.0762451383
H	2.4859927359	0.4601255495	0.0819993222

Tabelle 10.323 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
O	0.	0.	3.8534157188
C	-0.012985864	1.1805112469	4.6341759057
Li	0.	0.	1.9506493292
Li	0.	0.	-0.2824890192
C	-0.0081775628	1.8541144785	0.9265128368
H	-0.0227940074	2.0199488464	3.9490230604

H	0.8760356497	1.2242902034	5.2626444323
H	-0.9021232458	1.2040510331	5.2635637889
H	0.0025977429	2.2629356405	-0.0908046038
H	0.8473116745	2.3319440119	1.4185240149
H	-0.8989327291	2.2970057276	1.3884942746
C	-0.671958896	0.3580925785	-2.9849986994
N	-1.4590369466	0.0225893244	-1.8007465743
C	-2.4824837192	1.0300777595	-1.5499195496
C	-2.0869626958	-1.2870210681	-1.9282442789
H	-0.5106234236	1.4329313259	-2.9824044185
H	-1.2177130935	0.1155804942	-3.904973894
H	-3.0320190034	0.7625530958	-0.6525855072
H	-2.0155923757	1.9954083225	-1.3838564683
H	-3.1865041632	1.1033869165	-2.3870689913
H	-2.5820201131	-1.5381606853	-0.9956972338
H	-2.8210233652	-1.2931845283	-2.7427331854
H	-1.3429852691	-2.052106411	-2.1188295648
C	0.012985864	-1.1805112469	4.6341759057
C	0.0081775628	-1.8541144785	0.9265128368
H	0.0227940074	-2.0199488464	3.9490230604
H	-0.8760356497	-1.2242902034	5.2626444323
H	0.9021232458	-1.2040510331	5.2635637889
H	-0.0025977429	-2.2629356405	-0.0908046038
H	-0.8473116745	-2.3319440119	1.4185240149
H	0.8989327291	-2.2970057276	1.3884942746
C	0.671958896	-0.3580925785	-2.9849986994
N	1.4590369466	-0.0225893244	-1.8007465743
C	2.4824837192	-1.0300777595	-1.5499195496
C	2.0869626958	1.2870210681	-1.9282442789
H	0.5106234236	-1.4329313259	-2.9824044185
H	1.2177130935	-0.1155804942	-3.904973894
H	3.0320190034	-0.7625530958	-0.6525855072
H	2.0155923757	-1.9954083225	-1.3838564683
H	3.1865041632	-1.1033869165	-2.3870689913
H	2.5820201131	1.5381606853	-0.9956972338
H	2.8210233652	1.2931845283	-2.7427331854
H	1.3429852691	2.052106411	-2.1188295648

Tabelle 10.324 Standardorientierung von **6** [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
N	-1.479913479	0.0776320567	0.0600955676
C	-1.0209301993	-1.175787844	-0.5351405239
C	0.3081391328	-1.6330178028	0.0542628114
N	1.2907284648	-0.5551732813	0.0611274804
C	1.7818827311	-0.2624962501	-1.2840668881
C	2.4137908082	-0.8679855734	0.9341210013
C	-2.5630680448	0.654303539	-0.7282224672
C	-1.9209208344	-0.1182022257	1.4371369299
H	-0.9137546461	-1.0132484875	-1.6041072235
H	-1.7657173259	-1.9698174532	-0.4034925947

H	0.6698331326	-2.5007549094	-0.510249607
H	0.1640310755	-1.9598160453	1.0808260978
H	2.4850070619	0.5620540462	-1.2305940108
H	0.9661218539	0.0495543317	-1.9296055347
H	2.2697259009	-1.139355362	-1.7245345932
H	3.0899799428	-0.01934292	0.9585613677
H	2.9615129138	-1.7503734196	0.5851714814
H	2.0555693817	-1.0542297021	1.9424268648
H	-2.8587445334	1.6029360377	-0.2921072622
H	-3.4330970024	-0.0107052075	-0.7605571675
H	-2.2190428215	0.8375885869	-1.7413041771
H	-2.2678990503	0.8286887368	1.838964391
H	-1.0989000719	-0.4663866241	2.0555232309
H	-2.7370170323	-0.8471671749	1.494399433
Li	0.2547873982	1.2395999735	0.2740921465
C	1.0146724776	3.10465586	0.0219548019
H	1.0052937589	3.3873158351	-1.0358811357
H	2.0628928275	3.1520363589	0.3353060815
H	0.5054281792	3.9116349204	0.5535484985

Tabelle 10.325 Standardorientierung von **7** [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
N	0.6783270999	1.5747933921	-0.1301435285
C	1.9366158945	0.9520954845	0.2809936404
C	2.185814609	-0.367482095	-0.4326878638
N	1.1426602909	-1.3497336409	-0.1335965862
C	1.427425292	-2.0408802183	1.1227760399
C	1.0246803161	-2.3204889131	-1.2120040098
C	0.358017351	2.6711478873	0.779828375
C	0.7434838491	2.0681257189	-1.4976966133
H	1.8709607383	0.776662031	1.352279025
H	2.7807468977	1.630172124	0.1012091834
H	3.172363272	-0.751304599	-0.1501814368
H	2.2071694713	-0.2064561273	-1.506783156
H	0.6027616001	-2.703989836	1.3633927968
H	1.5048351648	-1.325716486	1.9331069491
H	2.3542257542	-2.6218274872	1.0444070988
H	0.2691761653	-3.0566119935	-0.9537860364
H	1.9696332573	-2.847481616	-1.3878554655
H	0.7221441091	-1.8212192722	-2.1281763805
H	-0.5832984826	3.1241302225	0.4819021396
H	1.1384145861	3.4412607976	0.7637252189
H	0.2417041731	2.275216942	1.7830200226
H	-0.1794630446	2.5885908548	-1.7344899511
H	0.8526602728	1.2500622726	-2.2016033837
H	1.5773771041	2.7676363342	-1.6327794954
Li	-0.4992906209	-0.0943359535	0.4055219572
C	-1.0018631544	-0.1023586149	2.4321283295
H	-0.1526535905	0.1921446069	3.0648656563
H	-1.2925526625	-1.0939194587	2.8012143676

H	-1.8174822982	0.5676570597	2.7312860688
C	-2.8725327492	0.83635765	-0.5702412956
O	-2.0874752083	-0.3255594866	-0.7886966914
H	-2.3330051359	1.6774811661	-0.9904447013
H	-3.017166165	0.9893805077	0.4985367676
H	-3.8353064986	0.7353521452	-1.071300633
C	-2.754994277	-1.4789436049	-0.2950366331
H	-2.9264594102	-1.3772826701	0.7751175838
H	-2.1099223027	-2.3308788183	-0.4777431833
H	-3.698223668	-1.615244306	-0.8242421756

Tabelle 10.326 Standardorientierung von (MeLi-OMe)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; M06L/6-31+G(d)].

	x	y	z
Li	0.5577684439	1.0928298319	0.8681042292
Li	-0.5577684439	-1.0928298319	0.8681042292
Li	1.0928298319	-0.5577684439	-0.8682756766
Li	-1.0928298319	0.5577684439	-0.8682756766
C	0.7652033252	1.6504711277	-1.2551497566
C	-1.6504711277	0.7652033252	1.2549783092
C	-0.7652033252	-1.6504711277	-1.2551497566
C	1.6504711277	-0.7652033252	1.2549783092
H	0.0577837843	2.4862391097	-1.4415769339
H	1.0975622611	1.3792789786	-2.277953363
H	1.6548704882	2.1712720206	-0.8432752165
H	-2.4862391097	0.0577837843	1.4414054865
H	-2.1712720206	1.6548704882	0.8431037692
H	-1.3792789786	1.0975622611	2.2777819156
H	-0.0577837843	-2.4862391097	-1.4415769339
H	-1.0975622611	-1.3792789786	-2.277953363
H	-1.6548704882	-2.1712720206	-0.8432752165
H	1.3792789786	-1.0975622611	2.2777819156
H	2.4862391097	-0.0577837843	1.4414054865
H	2.1712720206	-1.6548704882	0.8431037692
O	2.4979429844	-1.0399809232	-2.2147852379
O	-1.0399809232	-2.4979429844	2.2146137905
O	1.0399809232	2.4979429844	2.2146137905
O	-2.4979429844	1.0399809232	-2.2147852379
C	-0.2422740808	-3.6648643144	2.1109285092
H	0.7910793643	-3.4612438283	2.4318975566
H	-0.663855756	-4.4752757489	2.7245143026
H	-0.24477054	-3.9631556684	1.0592077861
C	-1.0924662732	-2.0112304108	3.5427454854
H	-1.5419413975	-2.7607926296	4.2116500526
H	-0.0830049847	-1.760831335	3.9085911117
H	-1.7108898988	-1.1093371269	3.5303299982
C	-3.6648643144	0.2422740808	-2.1110999566
H	-4.4752757489	0.663855756	-2.72468575
H	-3.4612438283	-0.7910793643	-2.432069004

H	-3.9631556684	0.24477054	-1.0593792335
C	-2.0112304108	1.0924662732	-3.5429169328
H	-1.760831335	0.0830049847	-3.9087625591
H	-2.7607926296	1.5419413975	-4.2118215
H	-1.1093371269	1.7108898988	-3.5305014455
C	3.6648643144	-0.2422740808	-2.1110999566
H	3.9631556684	-0.24477054	-1.0593792335
H	4.4752757489	-0.663855756	-2.72468575
H	3.4612438283	0.7910793643	-2.432069004
C	2.0112304108	-1.0924662732	-3.5429169328
H	1.760831335	-0.0830049847	-3.9087625591
H	2.7607926296	-1.5419413975	-4.2118215
H	1.1093371269	-1.7108898988	-3.5305014455
C	0.2422740808	3.6648643144	2.1109285092
H	-0.7910793643	3.4612438283	2.4318975566
H	0.663855756	4.4752757489	2.7245143026
H	0.24477054	3.9631556684	1.0592077861
C	1.0924662732	2.0112304108	3.5427454854
H	1.5419413975	2.7607926296	4.2116500526
H	0.0830049847	1.760831335	3.9085911117
H	1.7108898988	1.1093371269	3.5303299982

Tabelle 10.327 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; M06L/6-31+G(d)].

	x	y	z
C	-0.0269789746	0.7601629142	-0.1034261875
C	0.0269789746	-0.7601629142	-0.1034261875
N	-1.3673634683	1.2726064735	-0.3526672984
N	1.3673634683	-1.2726064735	-0.3526672984
C	-1.330283001	2.7151706533	-0.4824171058
C	-2.2912449919	0.8891866725	0.6977578861
C	1.330283001	-2.7151706533	-0.4824171058
C	2.2912449919	-0.8891866725	0.6977578861
H	0.6291173288	1.127612921	-0.9046733306
H	0.3714061755	1.1658576431	0.8539385452
H	-0.6291173288	-1.127612921	-0.9046733306
H	-0.3714061755	-1.1658576431	0.8539385452
H	-2.3332049934	3.0926246934	-0.7124381326
H	-0.6596653452	2.99746029	-1.3020649358
H	-0.9766970735	3.2212341186	0.4413144488
H	-2.4002917081	-0.1996961187	0.7369342794
H	-3.2777153903	1.3188926497	0.4908539608
H	-1.9659819552	1.2403690739	1.7009568702
H	2.3332049934	-3.0926246934	-0.7124381326
H	0.6596653452	-2.99746029	-1.3020649358
H	0.9766970735	-3.2212341186	0.4413144488
H	3.2777153903	-1.3188926497	0.4908539608
H	1.9659819552	-1.2403690739	1.7009568702
H	2.4002917081	0.1996961187	0.7369342794

Tabelle 10.328 Standardorientierung von  $\text{Me}_2\text{O}$  ( $\text{C}_{2v}$ ) [globales Minimum; M06L/6-31+G(d)].

	x	y	z
C	0.	1.1605430843	0.1958706434
O	0.	0.	-0.5949461471
C	0.	-1.1605430843	0.1958706434
H	0.8945067317	1.2104520005	0.840667611
H	-0.8945067317	1.2104520005	0.840667611
H	0.	2.0168975463	-0.4833925217
H	-0.8945067317	-1.2104520005	0.840667611
H	0.8945067317	-1.2104520005	0.840667611
H	0.	-2.0168975463	-0.4833925217

Tabelle 10.329 Standardorientierung von  $\mathbf{4}$  ( $\text{C}_2$ ) [globales Minimum; M06L/6-31+G(d)].

	x	y	z
C	0.268281	3.915052	0.768507
N	0.120979	2.63221	1.464016
C	-1.020646	2.632649	2.366389
C	1.334564	2.285593	2.194656
C	0.947103	3.737493	-0.579566
N	0.225984	2.793064	-1.433926
C	-1.075828	3.300545	-1.845015
C	1.020646	2.435079	-2.600569
C	-0.268281	-3.915052	0.768507
N	-0.120979	-2.63221	1.464016
C	-1.334564	-2.285593	2.194656
C	1.020646	-2.632649	2.366389
C	-0.947103	-3.737493	-0.579566
N	-0.225984	-2.793064	-1.433926
C	-1.020646	-2.435079	-2.600569
C	1.075828	-3.300545	-1.845015
Li	-0.005453	1.13547	-0.128403
Li	0.005453	-1.13547	-0.128403
C	-1.833579	0.018587	-0.258461
C	1.833579	-0.018587	-0.258461
H	-0.731938	4.344349	0.630243
H	0.834531	4.645492	1.377822
H	-1.12486	1.639612	2.818088
H	-1.938926	2.842489	1.806687
H	-0.919104	3.377455	3.17996
H	1.246345	1.266621	2.588315
H	1.519982	2.982413	3.035915
H	2.200717	2.2989	1.525958
H	1.062001	4.725773	-1.071036
H	1.959801	3.332301	-0.437424
H	-1.54814	2.574042	-2.513489
H	-1.738418	3.421381	-0.980981
H	-0.999749	4.271181	-2.37403
H	0.494859	1.659459	-3.170091
H	1.202599	3.299453	-3.268604
H	1.982833	2.023448	-2.277399

H	-0.834531	-4.645492	1.377822
H	0.731938	-4.344349	0.630243
H	-1.246345	-1.266621	2.588315
H	-2.200717	-2.2989	1.525958
H	-1.519982	-2.982413	3.035915
H	1.12486	-1.639612	2.818088
H	0.919104	-3.377455	3.17996
H	1.938926	-2.842489	1.806687
H	-1.959801	-3.332301	-0.437424
H	-1.062001	-4.725773	-1.071036
H	-0.494859	-1.659459	-3.170091
H	-1.982833	-2.023448	-2.277399
H	-1.202599	-3.299453	-3.268604
H	1.54814	-2.574042	-2.513489
H	0.999749	-4.271181	-2.37403
H	1.738418	-3.421381	-0.980981
H	-2.19104	0.452395	-1.216908
H	-2.431025	0.547398	0.512823
H	-2.286391	-0.995716	-0.266914
H	2.19104	-0.452395	-1.216908
H	2.431025	-0.547398	0.512823
H	2.286391	0.995716	-0.266914

Tabelle 10.330 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; M06L/6-31+G(d)].

	x	y	z
O	0.	0.	3.9248068438
C	0.0259861549	1.1775905015	4.7086764164
Li	0.	0.	1.9748580164
Li	0.	0.	-0.2704289697
C	0.0007894452	1.8300707684	0.9122617636
H	0.0446177394	2.0241265837	4.0179140672
H	0.9227607606	1.1998478745	5.3460825826
H	-0.8689442042	1.2394848932	5.3460384529
H	-0.0471317675	2.2301032223	-0.1228713354
H	0.8739144215	2.3651041298	1.3388132115
H	-0.8738732258	2.3129368723	1.3965511215
C	-0.6694772616	0.3601595456	-3.0153003492
N	-1.4601863053	0.0298275472	-1.826373191
C	-2.4924795422	1.0287976202	-1.5814474668
C	-2.0665583658	-1.2922385317	-1.9327391728
H	-0.508746704	1.4466497799	-3.0115972677
H	-1.2204609517	0.1283037065	-3.9485525156
H	-3.0256153476	0.7778984289	-0.6578428818
H	-2.0324801444	2.013655209	-1.446649757
H	-3.2284142838	1.0838516262	-2.4068331292
H	-2.5767275486	-1.5340065499	-0.9947579192
H	-2.7970182563	-1.3440696249	-2.7637131417
H	-1.3008973494	-2.0582065912	-2.0914139985
C	-0.0259861549	-1.1775905015	4.7086764164
C	-0.0007894452	-1.8300707684	0.9122617636

H	-0.0446177394	-2.0241265837	4.0179140672
H	-0.9227607606	-1.1998478745	5.3460825826
H	0.8689442042	-1.2394848932	5.3460384529
H	0.0471317675	-2.2301032223	-0.1228713354
H	-0.8739144215	-2.3651041298	1.3388132115
H	0.8738732258	-2.3129368723	1.3965511215
C	0.6694772616	-0.3601595456	-3.0153003492
N	1.4601863053	-0.0298275472	-1.826373191
C	2.4924795422	-1.0287976202	-1.5814474668
C	2.0665583658	1.2922385317	-1.9327391728
H	0.508746704	-1.4466497799	-3.0115972677
H	1.2204609517	-0.1283037065	-3.9485525156
H	3.0256153476	-0.7778984289	-0.6578428818
H	2.0324801444	-2.0136555209	-1.446649757
H	3.2284142838	-1.0838516262	-2.4068331292
H	2.5767275486	1.5340065499	-0.9947579192
H	2.7970182563	1.3440696249	-2.7637131417
H	1.3008973494	2.0582065912	-2.0914139985

Tabelle 10.331 Standardorientierung von **6** [globales Minimum; M06L/6-31+G(d)].

	x	y	z
N	1.4845461259	-0.3314322426	0.0207469582
C	0.680907208	-1.5032862029	0.3822421633
C	-0.6811504546	-1.490101563	-0.2948199384
N	-1.3429821922	-0.1942229368	-0.1450050927
C	-1.8128601737	0.0219205387	1.2219499625
C	-2.4480751514	-0.0442471566	-1.0817985516
C	2.6515881303	-0.2173624294	0.8869197507
C	1.8978747217	-0.3781278393	-1.378809563
H	0.5634706675	-1.4936121219	1.4738520743
H	1.2067707875	-2.4461371028	0.1333538033
H	-1.2980022623	-2.3181423667	0.1065715411
H	-0.5709758483	-1.6823207796	-1.3703476431
H	-2.2549489023	1.0207335022	1.2963083452
H	-0.9748180656	-0.0175784352	1.9281922536
H	-2.5616356762	-0.7334344719	1.527328609
H	-2.8656377056	0.9634501063	-0.987811526
H	-3.2549770371	-0.7800813386	-0.9044551093
H	-2.0832201766	-0.1702342825	-2.1075858985
H	3.2066879956	0.6920459078	0.6349821537
H	3.3331120698	-1.0834670921	0.7919946901
H	2.3285076709	-0.1407488029	1.9308279534
H	2.5114986101	0.4999409622	-1.6061037467
H	1.0231100599	-0.3559486468	-2.0398833689
H	2.4858267482	-1.2858124697	-1.6125122609
Li	0.1279550144	1.3323381779	-0.0609257603
C	-0.2436223848	3.2719322218	0.2492750188
H	-0.2658115863	3.5404556823	1.324405724
H	-1.2452878154	3.5673729434	-0.1248504346
H	0.4434016224	4.0119172387	-0.2011531067

Tabelle 10.332 Standardorientierung von **7** [globales Minimum; M06L/6-31+G(d)].

	x	y	z
N	0.7259767721	1.5298735949	-0.150396366
C	1.969975982	0.8541226029	0.2369730625
C	2.1729069199	-0.4535381138	-0.5066883377
N	1.0882797002	-1.4062486311	-0.2313908815
C	1.3526559924	-2.1473850902	1.0014576103
C	0.9074703475	-2.328412291	-1.3428015162
C	0.4720685792	2.6459332348	0.7558206311
C	0.7605523416	1.9901938338	-1.5305116357
H	1.897659086	0.6604958945	1.3171769775
H	2.8472180173	1.513996243	0.0776313303
H	3.1570164754	-0.8834829995	-0.2402111812
H	2.203537256	-0.2719465543	-1.5885859241
H	0.4933554236	-2.7838735976	1.2378480967
H	1.4716028978	-1.454047334	1.8393915428
H	2.2577032412	-2.7793210246	0.9088707701
H	0.1042133791	-3.0349953998	-1.1064208764
H	1.8201555728	-2.9153286774	-1.5620667725
H	0.6220227909	-1.7745998791	-2.2451924424
H	-0.4744383894	3.1287224046	0.4865986322
H	1.2749374448	3.4072746459	0.7136862056
H	0.3778678797	2.2619419029	1.7768968677
H	-0.1493072177	2.5615648672	-1.7441798999
H	0.7882308553	1.1431494608	-2.2252195656
H	1.6304746826	2.6441862377	-1.7375173539
Li	-0.5148134814	-0.0981447886	0.4257811654
C	-0.8794037287	-0.0692390144	2.4410055485
H	0.0195540199	0.2047899513	3.0378832824
H	-1.1863236145	-1.0419955231	2.8806464881
H	-1.6511765051	0.641049759	2.8071908951
C	-2.8690296669	0.9556537162	-0.4369435412
O	-2.1923256421	-0.2583388837	-0.725779484
H	-2.3223782331	1.7570038902	-0.9430631903
H	-2.8786343122	1.1412491516	0.6489558458
H	-3.9001567205	0.9240930999	-0.8217228827
C	-2.8774260197	-1.3597412302	-0.1433403839
H	-2.9272192517	-1.2471234752	0.9499307383
H	-2.3068040239	-2.2598196995	-0.3898842707
H	-3.8905868503	-1.4462412838	-0.5658761844

Tabelle 10.333 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	0.5441556124	1.1069080765	0.8700208205
Li	-0.5441556124	-1.1069080765	0.8700208205
Li	1.1069080765	-0.5441556124	-0.8701922678
Li	-1.1069080765	0.5441556124	-0.8701922678
C	0.7329316967	1.6726002168	-1.2652899267

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C	-1.6726002168	0.7329316967	1.2651184794
C	-0.7329316967	-1.6726002168	-1.2652899267
C	1.6726002168	-0.7329316967	1.2651184794
H	-0.0016844277	2.4743608411	-1.4952061391
H	1.110176756	1.375012468	-2.2663238857
H	1.590273098	2.2269777102	-0.8275536546
H	-2.4743608411	-0.0016844277	1.4950346918
H	-2.2269777102	1.590273098	0.8273822073
H	-1.375012468	1.110176756	2.2661524383
H	0.0016844277	-2.4743608411	-1.4952061391
H	-1.110176756	-1.375012468	-2.2663238857
H	-1.590273098	-2.2269777102	-0.8275536546
H	1.375012468	-1.110176756	2.2661524383
H	2.4743608411	0.0016844277	1.4950346918
H	2.2269777102	-1.590273098	0.8273822073
O	2.5801550233	-1.0152677598	-2.1229158126
O	-1.0152677598	-2.5801550233	2.1227443653
O	1.0152677598	2.5801550233	2.1227443653
O	-2.5801550233	1.0152677598	-2.1229158126
C	-0.3017777361	-3.7807980898	1.9139649964
H	0.7286248305	-3.6938190016	2.2951805084
H	-0.8076174008	-4.6213505162	2.4149727681
H	-0.2750603044	-3.9616253891	0.8343508274
C	-1.1070558428	-2.233698185	3.486883308
H	-1.6511097394	-3.0107950598	4.0469884978
H	-0.1039475347	-2.1063178745	3.9272782934
H	-1.6543218322	-1.2869715155	3.549114831
C	-3.7807980898	0.3017777361	-1.9141364437
H	-4.6213505162	0.8076174008	-2.4151442154
H	-3.6938190016	-0.7286248305	-2.2953519558
H	-3.9616253891	0.2750603044	-0.8345222747
C	-2.233698185	1.1070558428	-3.4870547554
H	-2.1063178745	0.1039475347	-3.9274497408
H	-3.0107950598	1.6511097394	-4.0471599451
H	-1.2869715155	1.6543218322	-3.5492862784
C	3.7807980898	-0.3017777361	-1.9141364437
H	3.9616253891	-0.2750603044	-0.8345222747
H	4.6213505162	-0.8076174008	-2.4151442154
H	3.6938190016	0.7286248305	-2.2953519558
C	2.233698185	-1.1070558428	-3.4870547554
H	2.1063178745	-0.1039475347	-3.9274497408
H	3.0107950598	-1.6511097394	-4.0471599451
H	1.2869715155	-1.6543218322	-3.5492862784
C	0.3017777361	3.7807980898	1.9139649964
H	-0.7286248305	3.6938190016	2.2951805084
H	0.8076174008	4.6213505162	2.4149727681
H	0.2750603044	3.9616253891	0.8343508274
C	1.1070558428	2.233698185	3.486883308
H	1.6511097394	3.0107950598	4.0469884978
H	0.1039475347	2.1063178745	3.9272782934
H	1.6543218322	1.2869715155	3.549114831

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Tabelle 10.334 Standardorientierung von TMEDA ( $C_2$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-0.0510679692	0.7588523965	-0.0794656577
C	0.0510679692	-0.7588523965	-0.0794656577
N	-1.4032478895	1.2317148794	-0.328012862
N	1.4032478895	-1.2317148794	-0.328012862
C	-1.4080791223	2.670334417	-0.4904305629
C	-2.3151957444	0.8440049705	0.729179625
C	1.4080791223	-2.670334417	-0.4904305629
C	2.3151957444	-0.8440049705	0.729179625
H	0.5978703425	1.1392338178	-0.882872674
H	0.3305244879	1.1801281331	0.8797398869
H	-0.5978703425	-1.1392338178	-0.882872674
H	-0.3305244879	-1.1801281331	0.8797398869
H	-2.4222585464	3.0166390859	-0.7267292097
H	-0.7469292963	2.9571937119	-1.3179203839
H	-1.0670716599	3.200977714	0.4255676888
H	-2.4084113651	-0.2468584562	0.7866068156
H	-3.3122543509	1.2530273539	0.5232320546
H	-1.9861772617	1.2180204332	1.7242162794
H	2.4222585464	-3.0166390859	-0.7267292097
H	0.7469292963	-2.9571937119	-1.3179203839
H	1.0670716599	-3.200977714	0.4255676888
H	3.3122543509	-1.2530273539	0.5232320546
H	1.9861772617	-1.2180204332	1.7242162794
H	2.4084113651	0.2468584562	0.7866068156

Tabelle 10.335 Standardorientierung von  $Me_2O$  ( $C_{2v}$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	0.	1.1602620049	-0.1953184922
O	0.	0.	0.5886558375
C	0.	-1.1602620049	-0.1953184922
H	-0.8956199255	1.2104789705	-0.8399515125
H	0.8956199255	1.2104789705	-0.8399515125
H	0.	2.0196143367	0.4822610984
H	0.8956199255	-1.2104789705	-0.8399515125
H	-0.8956199255	-1.2104789705	-0.8399515125
H	0.	-2.0196143367	0.4822610984

Tabelle 10.336 Standardorientierung von **4** ( $C_2$ ) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	0.2699529076	3.9331809152	0.7942736785
N	0.3010916241	2.645266001	1.4876286143
C	-0.7425861633	2.555030368	2.4960801457
C	1.601910344	2.4004916828	2.0959407047
C	0.8570981223	3.8363518298	-0.6048263961
N	0.160916075	2.8467824778	-1.4221714613
C	-1.1735410039	3.2890620875	-1.7984848509
C	0.9283893083	2.5044971442	-2.6098926066

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C	-0.2699529076	-3.9331809152	0.7942736785
N	-0.3010916241	-2.645266001	1.4876286143
C	-1.601910344	-2.4004916828	2.0959407047
C	0.7425861633	-2.555030368	2.4960801457
C	-0.8570981223	-3.8363518298	-0.6048263961
N	-0.160916075	-2.8467824778	-1.4221714613
C	-0.9283893083	-2.5044971442	-2.6098926066
C	1.1735410039	-3.2890620875	-1.7984848509
Li	0.0511910748	1.1431737453	-0.1141493794
Li	-0.0511910748	-1.1431737453	-0.1141493794
C	-1.8318379294	0.1044459709	-0.3187487957
C	1.8318379294	-0.1044459709	-0.3187487957
H	-0.7759624436	4.2650464113	0.7349265588
H	0.8081237209	4.7124733209	1.3719041641
H	-0.7119896431	1.5632678196	2.9655347852
H	-1.7287233634	2.6739594919	2.029851203
H	-0.6245025894	3.3216292069	3.2890574064
H	1.6370369989	1.3802393755	2.4978741696
H	1.8073629752	3.1203692993	2.9144610131
H	2.4007412668	2.4779864018	1.3498187668
H	0.8394317544	4.8384054524	-1.0848477533
H	1.9134867242	3.5345967811	-0.5449445896
H	-1.6475218031	2.5238620684	-2.4237906972
H	-1.811231332	3.4193598999	-0.9156992007
H	-1.1436127188	4.2437260456	-2.3630301174
H	0.4150353954	1.6991367833	-3.1523435783
H	1.0487433579	3.3709757703	-3.2915848304
H	1.9198196342	2.1340860135	-2.3213441599
H	-0.8081237209	-4.7124733209	1.3719041641
H	0.7759624436	-4.2650464113	0.7349265588
H	-1.6370369989	-1.3802393755	2.4978741696
H	-2.4007412668	-2.4779864018	1.3498187668
H	-1.8073629752	-3.1203692993	2.9144610131
H	0.7119896431	-1.5632678196	2.9655347852
H	0.6245025894	-3.3216292069	3.2890574064
H	1.7287233634	-2.6739594919	2.029851203
H	-1.9134867242	-3.5345967811	-0.5449445896
H	-0.8394317544	-4.8384054524	-1.0848477533
H	-0.4150353954	-1.6991367833	-3.1523435783
H	-1.9198196342	-2.1340860135	-2.3213441599
H	-1.0487433579	-3.3709757703	-3.2915848304
H	1.6475218031	-2.5238620684	-2.4237906972
H	1.1436127188	-4.2437260456	-2.3630301174
H	1.811231332	-3.4193598999	-0.9156992007
H	-2.0929204792	0.465971213	-1.3368489552
H	-2.4109783712	0.7572001323	0.3681587469
H	-2.3559668794	-0.8718237642	-0.2462395847
H	2.0929204792	-0.465971213	-1.3368489552
H	2.4109783712	-0.7572001323	0.3681587469
H	2.3559668794	0.8718237642	-0.2462395847

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Tabelle 10.337 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
O	0.	0.	3.9140091877
C	-0.0060059294	1.1780509445	4.6902969504
Li	0.	0.	1.9796886037
Li	0.	0.	-0.272487334
C	-0.0028564846	1.8432705726	0.9404545651
H	-0.0099114718	2.0263738265	3.9986452647
H	0.8907833226	1.2259616681	5.3279837705
H	-0.9036993453	1.2170604926	5.3273466972
H	-0.0210187945	2.2589649434	-0.089170871
H	0.863554273	2.353643224	1.4096244017
H	-0.8969810831	2.2982971672	1.4169806242
C	-0.671576621	0.3568645165	-3.014646806
N	-1.4672222047	0.0276257553	-1.8321475891
C	-2.4904551527	1.0333012138	-1.5827177448
C	-2.0861987801	-1.2866547112	-1.9447313797
H	-0.5135120909	1.4452256742	-3.0197347361
H	-1.2223638055	0.1167622617	-3.9480344326
H	-3.0388914778	0.774185677	-0.6683758667
H	-2.0252159509	2.0142630053	-1.4259610652
H	-3.2135063204	1.103913084	-2.4202007742
H	-2.6010797041	-1.5302338398	-1.0076624739
H	-2.8176056453	-1.3198075197	-2.7775490509
H	-1.3315380668	-2.0640821612	-2.1101413396
C	0.0060059294	-1.1780509445	4.6902969504
C	0.0028564846	-1.8432705726	0.9404545651
H	0.0099114718	-2.0263738265	3.9986452647
H	-0.8907833226	-1.2259616681	5.3279837705
H	0.9036993453	-1.2170604926	5.3273466972
H	0.0210187945	-2.2589649434	-0.089170871
H	-0.863554273	-2.353643224	1.4096244017
H	0.8969810831	-2.2982971672	1.4169806242
C	0.671576621	-0.3568645165	-3.014646806
N	1.4672222047	-0.0276257553	-1.8321475891
C	2.4904551527	-1.0333012138	-1.5827177448
C	2.0861987801	1.2866547112	-1.9447313797
H	0.5135120909	-1.4452256742	-3.0197347361
H	1.2223638055	-0.1167622617	-3.9480344326
H	3.0388914778	-0.774185677	-0.6683758667
H	2.0252159509	-2.0142630053	-1.4259610652
H	3.2135063204	-1.103913084	-2.4202007742
H	2.6010797041	1.5302338398	-1.0076624739
H	2.8176056453	1.3198075197	-2.7775490509
H	1.3315380668	2.0640821612	-2.1101413396

Tabelle 10.338 Standardorientierung von **6** [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
N	-1.4373489636	0.0825745527	-0.0379259664
C	-1.0304318427	-1.2477989167	-0.4843291795

C	0.3090391604	-1.6621859841	0.106977678
N	1.3182231608	-0.6163420536	-0.0402886347
C	1.7569521085	-0.471067007	-1.4235798669
C	2.4612101449	-0.8507089723	0.8299902776
C	-2.5065323156	0.6189098681	-0.8675233082
C	-1.8332390837	0.0899070557	1.3656916069
H	-0.9678573887	-1.2270185116	-1.5818785479
H	-1.7960448487	-2.0100605896	-0.2307202723
H	0.6399658204	-2.6119199543	-0.3620834397
H	0.1985009445	-1.8710948721	1.18081688
H	2.5060541567	0.3274117687	-1.4854755716
H	0.9180402547	-0.1847933075	-2.072272119
H	2.1990128671	-1.4085457794	-1.8154780743
H	3.1638630857	-0.0133636352	0.7430496305
H	2.9915663831	-1.789817358	0.5761037733
H	2.1291824727	-0.9060877326	1.8743178498
H	-2.7401839778	1.6410271875	-0.5465060895
H	-3.4275882693	0.0060889525	-0.806393417
H	-2.1805721303	0.6600794146	-1.9143990952
H	-2.1261202301	1.1060328759	1.6559931391
H	-0.9949626691	-0.2071336149	2.0102760537
H	-2.6826550845	-0.5954259619	1.5572183965
Li	0.3276466416	1.2545907355	0.1411412732
C	0.8644218457	3.1741783008	0.3494905926
H	0.580359833	3.8081833805	-0.5118895164
H	1.9587832135	3.3022856198	0.4611557869
H	0.4211067107	3.6662345385	1.2361751606

Tabelle 10.339 Standardorientierung von **7** [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
N	0.7230164704	1.5885363902	-0.0525567432
C	2.0152962673	0.9637695378	0.2320150406
C	2.187195664	-0.3689422078	-0.4748294941
N	1.1487829979	-1.3332877401	-0.1043929299
C	1.4762874162	-2.0082921709	1.149151753
C	0.957172826	-2.3118130172	-1.1628036773
C	0.5056539334	2.7196987254	0.8406769971
C	0.617462049	2.0045904405	-1.4420249084
H	2.0782551214	0.8216329338	1.3209772397
H	2.8500601973	1.6395970639	-0.0527696362
H	3.1967145664	-0.7737505317	-0.2587225375
H	2.1462893449	-0.21996471	-1.5630879919
H	0.6438236049	-2.6575879937	1.4457722499
H	1.6068721856	-1.2798498087	1.9567832859
H	2.3981151824	-2.6166344954	1.0486924123
H	0.2158956692	-3.0573058098	-0.8478753616
H	1.8944901982	-2.8507853516	-1.4082751388
H	0.58388572	-1.8176474865	-2.0699332423
H	-0.4818060852	3.1578750025	0.6489185624
H	1.2739876272	3.5071182136	0.7028229391

H	0.5168677729	2.3729681505	1.8805439313
H	-0.3159462511	2.5624925676	-1.586532801
H	0.5864907149	1.1369462446	-2.1131367
H	1.458367867	2.6618270723	-1.7445543319
Li	-0.5061215483	-0.0606378492	0.5375200445
C	-1.1217916695	-0.1237363151	2.4895466998
H	-0.3104702879	0.1531206194	3.1986517667
H	-1.4512081134	-1.1273392512	2.8350551761
H	-1.9596220536	0.5536370325	2.7603244344
C	-2.8868245642	0.8291869875	-0.6324058146
O	-2.030009581	-0.2803353315	-0.8129436955
H	-2.3562760025	1.7183500008	-0.9902748158
H	-3.1353346229	0.9565477861	0.4334058991
H	-3.8105749542	0.7032692423	-1.2202598201
C	-2.6654723285	-1.4803179215	-0.4116371892
H	-2.9407952623	-1.4338110083	0.6535146943
H	-1.9501068033	-2.2969071199	-0.559987132
H	-3.5591152689	-1.6656658912	-1.0295471648

Tabelle 10.340 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Li	0.5468480341	1.1055291426	0.8745810171
Li	-0.5468480341	-1.1055291426	0.8745810171
Li	1.1055291426	-0.5468480341	-0.8747524645
Li	-1.1055291426	0.5468480341	-0.8747524645
C	0.7428161352	1.6788190918	-1.2520504211
C	-1.6788190918	0.7428161352	1.2518789737
C	-0.7428161352	-1.6788190918	-1.2520504211
C	1.6788190918	-0.7428161352	1.2518789737
H	0.0016645242	2.4671375497	-1.4982454575
H	1.1544790721	1.3919260845	-2.2401518021
H	1.5760597842	2.2444952118	-0.7864482817
H	-2.4671375497	0.0016645242	1.4980740102
H	-2.2444952118	1.5760597842	0.7862768343
H	-1.3919260845	1.1544790721	2.2399803548
H	-0.0016645242	-2.4671375497	-1.4982454575
H	-1.1544790721	-1.3919260845	-2.2401518021
H	-1.5760597842	-2.2444952118	-0.7864482817
H	1.3919260845	-1.1544790721	2.2399803548
H	2.4671375497	-0.0016645242	1.4980740102
H	2.2444952118	-1.5760597842	0.7862768343
O	2.5332069173	-1.0111524137	-2.1892422723
O	-1.0111524137	-2.5332069173	2.1890708249
O	1.0111524137	2.5332069173	2.1890708249
O	-2.5332069173	1.0111524137	-2.1892422723
C	-0.2819655847	-3.7340228627	2.0348210457
H	0.7526832737	-3.6116540168	2.3905480481
H	-0.7641969326	-4.5525557899	2.5895717099

H	-0.2691793233	-3.9766218956	0.9684326961
C	-1.0880187148	-2.1155875544	3.5352972671
H	-1.6048048425	-2.8708027441	4.1461200098
H	-0.0821534425	-1.9435300714	3.9512735424
H	-1.6533049473	-1.1790336899	3.5577325055
C	-3.7340228627	0.2819655847	-2.0349924931
H	-4.5525557899	0.7641969326	-2.5897431573
H	-3.6116540168	-0.7526832737	-2.3907194955
H	-3.9766218956	0.2691793233	-0.9686041434
C	-2.1155875544	1.0880187148	-3.5354687144
H	-1.9435300714	0.0821534425	-3.9514449898
H	-2.8708027441	1.6048048425	-4.1462914572
H	-1.1790336899	1.6533049473	-3.5579039529
C	3.7340228627	-0.2819655847	-2.0349924931
H	3.9766218956	-0.2691793233	-0.9686041434
H	4.5525557899	-0.7641969326	-2.5897431573
H	3.6116540168	0.7526832737	-2.3907194955
C	2.1155875544	-1.0880187148	-3.5354687144
H	1.9435300714	-0.0821534425	-3.9514449898
H	2.8708027441	-1.6048048425	-4.1462914572
H	1.1790336899	-1.6533049473	-3.5579039529
C	0.2819655847	3.7340228627	2.0348210457
H	-0.7526832737	3.6116540168	2.3905480481
H	0.7641969326	4.5525557899	2.5895717099
H	0.2691793233	3.9766218956	0.9684326961
C	1.0880187148	2.1155875544	3.5352972671
H	1.6048048425	2.8708027441	4.1461200098
H	0.0821534425	1.9435300714	3.9512735424
H	1.6533049473	1.1790336899	3.5577325055

Tabelle 10.341 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
C	-0.0515419969	0.7585192011	-0.0852330067
C	0.0515419969	-0.7585192011	-0.0852330067
N	-1.4060673524	1.230032	-0.3252284569
N	1.4060673524	-1.230032	-0.3252284569
C	-1.4128898511	2.6680282025	-0.4979619915
C	-2.3101533742	0.8489915983	0.7420393713
C	1.4128898511	-2.6680282025	-0.4979619915
C	2.3101533742	-0.8489915983	0.7420393713
H	0.5919970379	1.137166216	-0.8921780763
H	0.3366252009	1.1798572893	0.8700716661
H	-0.5919970379	-1.137166216	-0.8921780763
H	-0.3366252009	-1.1798572893	0.8700716661
H	-2.4277967567	3.0125675201	-0.7268266213
H	-0.7605526466	2.9495211679	-1.3323221368
H	-1.0640916533	3.2051003898	0.4097274676
H	-2.4022232955	-0.2399893506	0.8090105329
H	-3.308038655	1.2546230436	0.5412455645
H	-1.9749207622	1.2302065911	1.7307666874

H	2.4277967567	-3.0125675201	-0.7268266213
H	0.7605526466	-2.9495211679	-1.3323221368
H	1.0640916533	-3.2051003898	0.4097274676
H	3.308038655	-1.2546230436	0.5412455645
H	1.9749207622	-1.2302065911	1.7307666874
H	2.4022232955	0.2399893506	0.8090105329

Tabelle 10.342 Standardorientierung von  $\text{Me}_2\text{O}$  ( $\text{C}_{2v}$ ) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
C	0.	1.1608453611	-0.1947591933
O	0.	0.	0.5899635475
C	0.	-1.1608453611	-0.1947591933
H	-0.8940188782	1.2119963504	-0.8393128793
H	0.8940188782	1.2119963504	-0.8393128793
H	0.	2.0209241818	0.4797706781
H	0.8940188782	-1.2119963504	-0.8393128793
H	-0.8940188782	-1.2119963504	-0.8393128793
H	0.	-2.0209241818	0.4797706781

Tabelle 10.343 Standardorientierung von **4** ( $\text{C}_2$ ) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
C	0.257200343	3.878472826	0.8490673875
N	0.2960006461	2.5626341419	1.4879656653
C	-0.7458204371	2.4252091579	2.4936069741
C	1.6004474863	2.2968247889	2.0810641918
C	0.8556835112	3.8463911481	-0.5477999267
N	0.1724972989	2.8871053635	-1.412087792
C	-1.1610914861	3.3378549158	-1.7844897291
C	0.9556616239	2.5944309427	-2.6038676884
C	-0.257200343	-3.878472826	0.8490673875
N	-0.2960006461	-2.5626341419	1.4879656653
C	-1.6004474863	-2.2968247889	2.0810641918
C	0.7458204371	-2.4252091579	2.4936069741
C	-0.8556835112	-3.8463911481	-0.5477999267
N	-0.1724972989	-2.8871053635	-1.412087792
C	-0.9556616239	-2.5944309427	-2.6038676884
C	1.1610914861	-3.3378549158	-1.7844897291
Li	0.0525046444	1.1425553869	-0.1815345635
Li	-0.0525046444	-1.1425553869	-0.1815345635
C	-1.8320991279	0.1042835728	-0.4042502438
C	1.8320991279	-0.1042835728	-0.4042502438
H	-0.7907178423	4.2011957968	0.7940792474
H	0.7817968825	4.6381616461	1.4619617298
H	-0.7079182268	1.4170097438	2.9231971067
H	-1.7324991902	2.5543834464	2.0342357726
H	-0.6324709822	3.1587935822	3.3160036795
H	1.6384291593	1.2637415406	2.4445967458
H	1.81032412	2.9855930028	2.9229887935
H	2.3948159034	2.3988220763	1.3349050516

H	0.8344899854	4.8668537623	-0.983549409
H	1.9127772944	3.5504093997	-0.4921573389
H	-1.6286197052	2.5917224331	-2.4349915646
H	-1.8044305088	3.4383755062	-0.9034930182
H	-1.1306169402	4.3084782709	-2.3179346233
H	0.4493945335	1.8155051362	-3.1870207091
H	1.0870121983	3.4876262692	-3.2453962104
H	1.9408994498	2.2088861869	-2.3181882554
H	-0.7817968825	-4.6381616461	1.4619617298
H	0.7907178423	-4.2011957968	0.7940792474
H	-1.6384291593	-1.2637415406	2.4445967458
H	-2.3948159034	-2.3988220763	1.3349050516
H	-1.81032412	-2.9855930028	2.9229887935
H	0.7079182268	-1.4170097438	2.9231971067
H	0.6324709822	-3.1587935822	3.3160036795
H	1.7324991902	-2.5543834464	2.0342357726
H	-1.9127772944	-3.5504093997	-0.4921573389
H	-0.8344899854	-4.8668537623	-0.983549409
H	-0.4493945335	-1.8155051362	-3.1870207091
H	-1.9408994498	-2.2088861869	-2.3181882554
H	-1.0870121983	-3.4876262692	-3.2453962104
H	1.6286197052	-2.5917224331	-2.4349915646
H	1.1306169402	-4.3084782709	-2.3179346233
H	1.8044305088	-3.4383755062	-0.9034930182
H	-2.0884830674	0.4807329893	-1.4163437087
H	-2.4215327869	0.7362683118	0.2906777249
H	-2.3422102345	-0.8792910092	-0.354682289
H	2.0884830674	-0.4807329893	-1.4163437087
H	2.4215327869	-0.7362683118	0.2906777249
H	2.3422102345	0.8792910092	-0.354682289

Tabelle 10.344 Standardorientierung von **5** ( $C_2$ ) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
O	0.	0.	3.9101833947
C	-0.012263438	1.1791695767	4.6862869667
Li	0.	0.	1.9784846684
Li	0.	0.	-0.2758853743
C	-0.0096523898	1.8433741704	0.9384454918
H	-0.0206898443	2.0267535052	3.9955205812
H	0.8828244866	1.2335199031	5.3235893928
H	-0.9087144998	1.2150831585	5.3230105164
H	-0.0264509765	2.2529899178	-0.0918932267
H	0.8522402328	2.3572193448	1.4080478924
H	-0.9067162885	2.2934093516	1.4103095175
C	-0.6701928314	0.3590061545	-3.0127296163
N	-1.4671229408	0.0295600373	-1.8306640911
C	-2.4877008429	1.0382008216	-1.5783632025
C	-2.087953603	-1.2844552262	-1.9443052049
H	-0.5076610084	1.4456137729	-3.0153166904
H	-1.220006894	0.1232928592	-3.9462418674

H	-3.0365904957	0.7787691008	-0.66599127
H	-2.0196894843	2.0158327286	-1.4173890754
H	-3.2098361059	1.114221794	-2.4142568012
H	-2.6044089573	-1.5273196671	-1.0094681883
H	-2.8167219298	-1.317812804	-2.7775214631
H	-1.3347005217	-2.0622491961	-2.1065975405
C	0.012263438	-1.1791695767	4.6862869667
C	0.0096523898	-1.8433741704	0.9384454918
H	0.0206898443	-2.0267535052	3.9955205812
H	-0.8828244866	-1.2335199031	5.3235893928
H	0.9087144998	-1.2150831585	5.3230105164
H	0.0264509765	-2.2529899178	-0.0918932267
H	-0.8522402328	-2.3572193448	1.4080478924
H	0.9067162885	-2.2934093516	1.4103095175
C	0.6701928314	-0.3590061545	-3.0127296163
N	1.4671229408	-0.0295600373	-1.8306640911
C	2.4877008429	-1.0382008216	-1.5783632025
C	2.087953603	1.2844552262	-1.9443052049
H	0.5076610084	-1.4456137729	-3.0153166904
H	1.220006894	-0.1232928592	-3.9462418674
H	3.0365904957	-0.7787691008	-0.66599127
H	2.0196894843	-2.0158327286	-1.4173890754
H	3.2098361059	-1.114221794	-2.4142568012
H	2.6044089573	1.5273196671	-1.0094681883
H	2.8167219298	1.317812804	-2.7775214631
H	1.3347005217	2.0622491961	-2.1065975405

Tabelle 10.345 Standardorientierung von **6** [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
N	-1.4394049675	0.080862089	-0.0356761044
C	-1.0301548074	-1.2480996058	-0.4855311928
C	0.3087374895	-1.6615076339	0.1068698959
N	1.3169798759	-0.6143692979	-0.0410619976
C	1.7575457492	-0.4701505246	-1.4245506647
C	2.4589298494	-0.8431140296	0.8330850798
C	-2.5068496267	0.6202683816	-0.8666549562
C	-1.8372187387	0.0841790826	1.3680794667
H	-0.9649689668	-1.2241783366	-1.5817258234
H	-1.7936497314	-2.0120190879	-0.2361784868
H	0.6392998343	-2.6108652457	-0.3601678967
H	0.1969999474	-1.8689473198	1.1797047606
H	2.5029226108	0.3299099679	-1.4869005411
H	0.9197585697	-0.1875863933	-2.0741509606
H	2.2025015098	-1.4054662902	-1.814314358
H	3.1580398711	-0.0044747446	0.7468160839
H	2.993143797	-1.7795679087	0.5835643675
H	2.1250913142	-0.8971103921	1.8755116997
H	-2.7405823503	1.6404707559	-0.5441750493
H	-3.4275776499	0.0090264642	-0.8101092446
H	-2.178913824	0.6646945396	-1.9113787657

H	-2.1299548057	1.0981659546	1.6608461564
H	-1.0005584988	-0.2138310544	2.0121185276
H	-2.6855582277	-0.600857822	1.5571904147
Li	0.3238067932	1.2534705387	0.1413475132
C	0.8694144793	3.1706354527	0.3454350117
H	0.5773537673	3.8049995452	-0.5106216291
H	1.9645476166	3.288838757	0.442264132
H	0.4407111203	3.6607641581	1.2380195618

Tabelle 10.346 Standardorientierung von **7** [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
N	0.7223137977	1.5862093117	-0.0528922875
C	2.015182508	0.9620595267	0.2323011619
C	2.1868808423	-0.3697634114	-0.4756029381
N	1.1479721926	-1.3340940677	-0.1052262632
C	1.4722535444	-2.0068866312	1.1510851017
C	0.9557933159	-2.3139533307	-1.1631209869
C	0.4996490958	2.7139179399	0.8443677142
C	0.616691763	2.0049583558	-1.442141709
H	2.0769876796	0.8180639971	1.3199922129
H	2.8496674972	1.6368725306	-0.0505199114
H	3.1957221654	-0.7736467567	-0.2612121759
H	2.1449968286	-0.219074469	-1.5624194183
H	0.6410846704	-2.6569403577	1.4450012072
H	1.5952682052	-1.2776702682	1.9576631356
H	2.3950743796	-2.612017983	1.0565114277
H	0.2104190243	-3.0544691747	-0.850526604
H	1.8897540473	-2.8577600299	-1.4042779473
H	0.5883333949	-1.820565107	-2.0714618645
H	-0.4863365303	3.1512908327	0.6509084524
H	1.2661824928	3.5023495616	0.7138442844
H	0.5056763261	2.3627553474	1.8815700306
H	-0.3203910518	2.5537523012	-1.5879473904
H	0.5947250783	1.1397141653	-2.1146759701
H	1.4510835521	2.6695555692	-1.7414098219
Li	-0.5050855714	-0.0627983554	0.5298609261
C	-1.1238093615	-0.1140635683	2.4826310404
H	-0.3066312112	0.1574809908	3.1845415909
H	-1.4642154086	-1.1093572406	2.8354681011
H	-1.9501885914	0.5761846923	2.7491787359
C	-2.8804472855	0.829050749	-0.6242850103
O	-2.0253241795	-0.2808007664	-0.8207307639
H	-2.3571981829	1.7191820493	-0.987150222
H	-3.111464014	0.9538285341	0.4447189248
H	-3.8122306099	0.7055992708	-1.1970847014
C	-2.6571550344	-1.4835703681	-0.4179733937
H	-2.9157343544	-1.4440286982	0.6506032302
H	-1.9468383352	-2.3001994344	-0.5814545846
H	-3.5591546795	-1.664613707	-1.0223113135

Tabelle 10.347 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Li	0.5468480341	1.1055291426	0.8745810171
Li	-0.5468480341	-1.1055291426	0.8745810171
Li	1.1055291426	-0.5468480341	-0.8747524645
Li	-1.1055291426	0.5468480341	-0.8747524645
C	0.7428161352	1.6788190918	-1.2520504211
C	-1.6788190918	0.7428161352	1.2518789737
C	-0.7428161352	-1.6788190918	-1.2520504211
C	1.6788190918	-0.7428161352	1.2518789737
H	0.0016645242	2.4671375497	-1.4982454575
H	1.1544790721	1.3919260845	-2.2401518021
H	1.5760597842	2.2444952118	-0.7864482817
H	-2.4671375497	0.0016645242	1.4980740102
H	-2.2444952118	1.5760597842	0.7862768343
H	-1.3919260845	1.1544790721	2.2399803548
H	-0.0016645242	-2.4671375497	-1.4982454575
H	-1.1544790721	-1.3919260845	-2.2401518021
H	-1.5760597842	-2.2444952118	-0.7864482817
H	1.3919260845	-1.1544790721	2.2399803548
H	2.4671375497	-0.0016645242	1.4980740102
H	2.2444952118	-1.5760597842	0.7862768343
O	2.5332069173	-1.0111524137	-2.1892422723
O	-1.0111524137	-2.5332069173	2.1890708249
O	1.0111524137	2.5332069173	2.1890708249
O	-2.5332069173	1.0111524137	-2.1892422723
C	-0.2819655847	-3.7340228627	2.0348210457
H	0.7526832737	-3.6116540168	2.3905480481
H	-0.7641969326	-4.5525557899	2.5895717099
H	-0.2691793233	-3.9766218956	0.9684326961
C	-1.0880187148	-2.1155875544	3.5352972671
H	-1.6048048425	-2.8708027441	4.1461200098
H	-0.0821534425	-1.9435300714	3.9512735424
H	-1.6533049473	-1.1790336899	3.5577325055
C	-3.7340228627	0.2819655847	-2.0349924931
H	-4.5525557899	0.7641969326	-2.5897431573
H	-3.6116540168	-0.7526832737	-2.3907194955
H	-3.9766218956	0.2691793233	-0.9686041434
C	-2.1155875544	1.0880187148	-3.5354687144
H	-1.9435300714	0.0821534425	-3.9514449898
H	-2.8708027441	1.6048048425	-4.1462914572
H	-1.1790336899	1.6533049473	-3.5579039529
C	3.7340228627	-0.2819655847	-2.0349924931
H	3.9766218956	-0.2691793233	-0.9686041434
H	4.5525557899	-0.7641969326	-2.5897431573
H	3.6116540168	0.7526832737	-2.3907194955
C	2.1155875544	-1.0880187148	-3.5354687144
H	1.9435300714	-0.0821534425	-3.9514449898
H	2.8708027441	-1.6048048425	-4.1462914572
H	1.1790336899	-1.6533049473	-3.5579039529
C	0.2819655847	3.7340228627	2.0348210457

H	-0.7526832737	3.6116540168	2.3905480481
H	0.7641969326	4.5525557899	2.5895717099
H	0.2691793233	3.9766218956	0.9684326961
C	1.0880187148	2.1155875544	3.5352972671
H	1.6048048425	2.8708027441	4.1461200098
H	0.0821534425	1.9435300714	3.9512735424
H	1.6533049473	1.1790336899	3.5577325055

Tabelle 10.348 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
C	-0.0515419969	0.7585192011	-0.0852330067
C	0.0515419969	-0.7585192011	-0.0852330067
N	-1.4060673524	1.230032	-0.3252284569
N	1.4060673524	-1.230032	-0.3252284569
C	-1.4128898511	2.6680282025	-0.4979619915
C	-2.3101533742	0.8489915983	0.7420393713
C	1.4128898511	-2.6680282025	-0.4979619915
C	2.3101533742	-0.8489915983	0.7420393713
H	0.5919970379	1.137166216	-0.8921780763
H	0.3366252009	1.1798572893	0.8700716661
H	-0.5919970379	-1.137166216	-0.8921780763
H	-0.3366252009	-1.1798572893	0.8700716661
H	-2.4277967567	3.0125675201	-0.7268266213
H	-0.7605526466	2.9495211679	-1.3323221368
H	-1.0640916533	3.2051003898	0.4097274676
H	-2.4022232955	-0.2399893506	0.8090105329
H	-3.308038655	1.2546230436	0.5412455645
H	-1.9749207622	1.2302065911	1.7307666874
H	2.4277967567	-3.0125675201	-0.7268266213
H	0.7605526466	-2.9495211679	-1.3323221368
H	1.0640916533	-3.2051003898	0.4097274676
H	3.308038655	-1.2546230436	0.5412455645
H	1.9749207622	-1.2302065911	1.7307666874
H	2.4022232955	0.2399893506	0.8090105329

Tabelle 10.349 Standardorientierung von Me<sub>2</sub>O (C<sub>2v</sub>) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
C	0.	1.1608453611	-0.1947591933
O	0.	0.	0.5899635475
C	0.	-1.1608453611	-0.1947591933
H	-0.8940188782	1.2119963504	-0.8393128793
H	0.8940188782	1.2119963504	-0.8393128793
H	0.	2.0209241818	0.4797706781
H	0.8940188782	-1.2119963504	-0.8393128793
H	-0.8940188782	-1.2119963504	-0.8393128793
H	0.	-2.0209241818	0.4797706781

Tabelle 10.350 Standardorientierung von **4** (C<sub>2</sub>) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
C	0.257200343	3.878472826	0.8490673875
N	0.2960006461	2.5626341419	1.4879656653
C	-0.7458204371	2.4252091579	2.4936069741
C	1.6004474863	2.2968247889	2.0810641918
C	0.8556835112	3.8463911481	-0.5477999267
N	0.1724972989	2.8871053635	-1.412087792
C	-1.1610914861	3.3378549158	-1.7844897291
C	0.9556616239	2.5944309427	-2.6038676884
C	-0.257200343	-3.878472826	0.8490673875
N	-0.2960006461	-2.5626341419	1.4879656653
C	-1.6004474863	-2.2968247889	2.0810641918
C	0.7458204371	-2.4252091579	2.4936069741
C	-0.8556835112	-3.8463911481	-0.5477999267
N	-0.1724972989	-2.8871053635	-1.412087792
C	-0.9556616239	-2.5944309427	-2.6038676884
C	1.1610914861	-3.3378549158	-1.7844897291
Li	0.0525046444	1.1425553869	-0.1815345635
Li	-0.0525046444	-1.1425553869	-0.1815345635
C	-1.8320991279	0.1042835728	-0.4042502438
C	1.8320991279	-0.1042835728	-0.4042502438
H	-0.7907178423	4.2011957968	0.7940792474
H	0.7817968825	4.6381616461	1.4619617298
H	-0.7079182268	1.4170097438	2.9231971067
H	-1.7324991902	2.5543834464	2.0342357726
H	-0.6324709822	3.1587935822	3.3160036795
H	1.6384291593	1.2637415406	2.4445967458
H	1.81032412	2.9855930028	2.9229887935
H	2.3948159034	2.3988220763	1.3349050516
H	0.8344899854	4.8668537623	-0.983549409
H	1.9127772944	3.5504093997	-0.4921573389
H	-1.6286197052	2.5917224331	-2.4349915646
H	-1.8044305088	3.4383755062	-0.9034930182
H	-1.1306169402	4.3084782709	-2.3179346233
H	0.4493945335	1.8155051362	-3.1870207091
H	1.0870121983	3.4876262692	-3.2453962104
H	1.9408994498	2.2088861869	-2.3181882554
H	-0.7817968825	-4.6381616461	1.4619617298
H	0.7907178423	-4.2011957968	0.7940792474
H	-1.6384291593	-1.2637415406	2.4445967458
H	-2.3948159034	-2.3988220763	1.3349050516
H	-1.81032412	-2.9855930028	2.9229887935
H	0.7079182268	-1.4170097438	2.9231971067
H	0.6324709822	-3.1587935822	3.3160036795
H	1.7324991902	-2.5543834464	2.0342357726
H	-1.9127772944	-3.5504093997	-0.4921573389
H	-0.8344899854	-4.8668537623	-0.983549409
H	-0.4493945335	-1.8155051362	-3.1870207091
H	-1.9408994498	-2.2088861869	-2.3181882554
H	-1.0870121983	-3.4876262692	-3.2453962104

H	1.6286197052	-2.5917224331	-2.4349915646
H	1.1306169402	-4.3084782709	-2.3179346233
H	1.8044305088	-3.4383755062	-0.9034930182
H	-2.0884830674	0.4807329893	-1.4163437087
H	-2.4215327869	0.7362683118	0.2906777249
H	-2.3422102345	-0.8792910092	-0.354682289
H	2.0884830674	-0.4807329893	-1.4163437087
H	2.4215327869	-0.7362683118	0.2906777249
H	2.3422102345	0.8792910092	-0.354682289

Tabelle 10.351 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
O	0.	0.	3.9101833947
C	-0.012263438	1.1791695767	4.6862869667
Li	0.	0.	1.9784846684
Li	0.	0.	-0.2758853743
C	-0.0096523898	1.8433741704	0.9384454918
H	-0.0206898443	2.0267535052	3.9955205812
H	0.8828244866	1.2335199031	5.3235893928
H	-0.9087144998	1.2150831585	5.3230105164
H	-0.0264509765	2.2529899178	-0.0918932267
H	0.8522402328	2.3572193448	1.4080478924
H	-0.9067162885	2.2934093516	1.4103095175
C	-0.6701928314	0.3590061545	-3.0127296163
N	-1.4671229408	0.0295600373	-1.8306640911
C	-2.4877008429	1.0382008216	-1.5783632025
C	-2.087953603	-1.2844552262	-1.9443052049
H	-0.5076610084	1.4456137729	-3.0153166904
H	-1.220006894	0.1232928592	-3.9462418674
H	-3.0365904957	0.7787691008	-0.66599127
H	-2.0196894843	2.0158327286	-1.4173890754
H	-3.2098361059	1.114221794	-2.4142568012
H	-2.6044089573	-1.5273196671	-1.0094681883
H	-2.8167219298	-1.317812804	-2.7775214631
H	-1.3347005217	-2.0622491961	-2.1065975405
C	0.012263438	-1.1791695767	4.6862869667
C	0.0096523898	-1.8433741704	0.9384454918
H	0.0206898443	-2.0267535052	3.9955205812
H	-0.8828244866	-1.2335199031	5.3235893928
H	0.9087144998	-1.2150831585	5.3230105164
H	0.0264509765	-2.2529899178	-0.0918932267
H	-0.8522402328	-2.3572193448	1.4080478924
H	0.9067162885	-2.2934093516	1.4103095175
C	0.6701928314	-0.3590061545	-3.0127296163
N	1.4671229408	-0.0295600373	-1.8306640911
C	2.4877008429	-1.0382008216	-1.5783632025
C	2.087953603	1.2844552262	-1.9443052049
H	0.5076610084	-1.4456137729	-3.0153166904
H	1.220006894	-0.1232928592	-3.9462418674

H	3.0365904957	-0.7787691008	-0.66599127
H	2.0196894843	-2.0158327286	-1.4173890754
H	3.2098361059	-1.114221794	-2.4142568012
H	2.6044089573	1.5273196671	-1.0094681883
H	2.8167219298	1.317812804	-2.7775214631
H	1.3347005217	2.0622491961	-2.1065975405

Tabelle 10.352 Standardorientierung von **6** [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
N	-1.4394049675	0.080862089	-0.0356761044
C	-1.0301548074	-1.2480996058	-0.4855311928
C	0.3087374895	-1.6615076339	0.1068698959
N	1.3169798759	-0.6143692979	-0.0410619976
C	1.7575457492	-0.4701505246	-1.4245506647
C	2.4589298494	-0.8431140296	0.8330850798
C	-2.5068496267	0.6202683816	-0.8666549562
C	-1.8372187387	0.0841790826	1.3680794667
H	-0.9649689668	-1.2241783366	-1.5817258234
H	-1.7936497314	-2.0120190879	-0.2361784868
H	0.6392998343	-2.6108652457	-0.3601678967
H	0.1969999474	-1.8689473198	1.1797047606
H	2.5029226108	0.3299099679	-1.4869005411
H	0.9197585697	-0.1875863933	-2.0741509606
H	2.2025015098	-1.4054662902	-1.814314358
H	3.1580398711	-0.0044747446	0.7468160839
H	2.993143797	-1.7795679087	0.5835643675
H	2.1250913142	-0.8971103921	1.8755116997
H	-2.7405823503	1.6404707559	-0.5441750493
H	-3.4275776499	0.0090264642	-0.8101092446
H	-2.178913824	0.6646945396	-1.9113787657
H	-2.1299548057	1.0981659546	1.6608461564
H	-1.0005584988	-0.2138310544	2.0121185276
H	-2.6855582277	-0.600857822	1.5571904147
Li	0.3238067932	1.2534705387	0.1413475132
C	0.8694144793	3.1706354527	0.3454350117
H	0.5773537673	3.8049995452	-0.5106216291
H	1.9645476166	3.288838757	0.442264132
H	0.4407111203	3.6607641581	1.2380195618

Tabelle 10.353 Standardorientierung von **7** [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
N	0.7223137977	1.5862093117	-0.0528922875
C	2.015182508	0.9620595267	0.2323011619
C	2.1868808423	-0.3697634114	-0.4756029381
N	1.1479721926	-1.3340940677	-0.1052262632
C	1.4722535444	-2.0068866312	1.1510851017
C	0.9557933159	-2.3139533307	-1.1631209869
C	0.4996490958	2.7139179399	0.8443677142
C	0.616691763	2.0049583558	-1.442141709

H	2.0769876796	0.8180639971	1.3199922129
H	2.8496674972	1.6368725306	-0.0505199114
H	3.1957221654	-0.7736467567	-0.2612121759
H	2.1449968286	-0.219074469	-1.5624194183
H	0.6410846704	-2.6569403577	1.4450012072
H	1.5952682052	-1.2776702682	1.9576631356
H	2.3950743796	-2.612017983	1.0565114277
H	0.2104190243	-3.0544691747	-0.850526604
H	1.8897540473	-2.8577600299	-1.4042779473
H	0.5883333949	-1.820565107	-2.0714618645
H	-0.4863365303	3.1512908327	0.6509084524
H	1.2661824928	3.5023495616	0.7138442844
H	0.5056763261	2.3627553474	1.8815700306
H	-0.3203910518	2.5537523012	-1.5879473904
H	0.5947250783	1.1397141653	-2.1146759701
H	1.4510835521	2.6695555692	-1.7414098219
Li	-0.5050855714	-0.0627983554	0.5298609261
C	-1.1238093615	-0.1140635683	2.4826310404
H	-0.3066312112	0.1574809908	3.1845415909
H	-1.4642154086	-1.1093572406	2.8354681011
H	-1.9501885914	0.5761846923	2.7491787359
C	-2.8804472855	0.829050749	-0.6242850103
O	-2.0253241795	-0.2808007664	-0.8207307639
H	-2.3571981829	1.7191820493	-0.987150222
H	-3.111464014	0.9538285341	0.4447189248
H	-3.8122306099	0.7055992708	-1.1970847014
C	-2.6571550344	-1.4835703681	-0.4179733937
H	-2.9157343544	-1.4440286982	0.6506032302
H	-1.9468383352	-2.3001994344	-0.5814545846
H	-3.5591546795	-1.664613707	-1.0223113135

Tabelle 10.354 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; M062X/6-31+G(d)].

	x	y	z
Li	0.5494714644	1.0744086995	0.8467398833
Li	-0.5494714644	-1.0744086995	0.8467398833
Li	1.0744086995	-0.5494714644	-0.8469113307
Li	-1.0744086995	0.5494714644	-0.8469113307
C	0.7551187509	1.642393931	-1.2683426488
C	-1.642393931	0.7551187509	1.2681712014
C	-0.7551187509	-1.642393931	-1.2683426488
C	1.642393931	-0.7551187509	1.2681712014
H	0.0239996669	2.4436127767	-1.4942343664
H	1.1180544088	1.3324354195	-2.2667293594
H	1.6158984189	2.1861920064	-0.8335915526
H	-2.4436127767	0.0239996669	1.4940629191
H	-2.1861920064	1.6158984189	0.8334201052
H	-1.3324354195	1.1180544088	2.266557912
H	-0.0239996669	-2.4436127767	-1.4942343664

H	-1.1180544088	-1.3324354195	-2.2667293594
H	-1.6158984189	-2.1861920064	-0.8335915526
H	1.3324354195	-1.1180544088	2.266557912
H	2.4436127767	-0.0239996669	1.4940629191
H	2.1861920064	-1.6158984189	0.8334201052
O	2.5333924816	-1.0413364949	-2.0054231338
O	-1.0413364949	-2.5333924816	2.0052516864
O	1.0413364949	2.5333924816	2.0052516864
O	-2.5333924816	1.0413364949	-2.0054231338
C	-0.2758068965	-3.6974749802	1.7468105293
H	0.7479853714	-3.57406335	2.123806173
H	-0.7434678744	-4.5706143927	2.2199986177
H	-0.2535839925	-3.8314771861	0.6635151448
C	-1.1363078195	-2.2341442023	3.3843944581
H	-1.6640059392	-3.0393870981	3.9118350916
H	-0.1368166025	-2.1054143783	3.82140821
H	-1.6983566516	-1.3024608922	3.4737223959
C	-3.6974749802	0.2758068965	-1.7469819767
H	-4.5706143927	0.7434678744	-2.2201700651
H	-3.57406335	-0.7479853714	-2.1239776204
H	-3.8314771861	0.2535839925	-0.6636865922
C	-2.2341442023	1.1363078195	-3.3845659055
H	-2.1054143783	0.1368166025	-3.8215796573
H	-3.0393870981	1.6640059392	-3.9120065389
H	-1.3024608922	1.6983566516	-3.4738938433
C	3.6974749802	-0.2758068965	-1.7469819767
H	3.8314771861	-0.2535839925	-0.6636865922
H	4.5706143927	-0.7434678744	-2.2201700651
H	3.57406335	0.7479853714	-2.1239776204
C	2.2341442023	-1.1363078195	-3.3845659055
H	2.1054143783	-0.1368166025	-3.8215796573
H	3.0393870981	-1.6640059392	-3.9120065389
H	1.3024608922	-1.6983566516	-3.4738938433
C	0.2758068965	3.6974749802	1.7468105293
H	-0.7479853714	3.57406335	2.123806173
H	0.7434678744	4.5706143927	2.2199986177
H	0.2535839925	3.8314771861	0.6635151448
C	1.1363078195	2.2341442023	3.3843944581
H	1.6640059392	3.0393870981	3.9118350916
H	0.1368166025	2.1054143783	3.82140821
H	1.6983566516	1.3024608922	3.4737223959

Tabelle 10.355 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; M062X/6-31+G(d)].

	x	y	z
C	-0.0449944364	0.7627340273	-0.068876757
C	0.0449944364	-0.7627340273	-0.068876757
N	-1.3973365364	1.2377588304	-0.3317715375
N	1.3973365364	-1.2377588304	-0.3317715375
C	-1.402426243	2.682489547	-0.4806959876
C	-2.3220672945	0.8361089075	0.7151652587

C	1.402426243	-2.682489547	-0.4806959876
C	2.3220672945	-0.8361089075	0.7151652587
H	0.6082972036	1.134598705	-0.8669597793
H	0.3276341348	1.1762168035	0.8908076487
H	-0.6082972036	-1.134598705	-0.8669597793
H	-0.3276341348	-1.1762168035	0.8908076487
H	-2.4121832207	3.0232769446	-0.727940469
H	-0.7321509433	2.9720990315	-1.2952171241
H	-1.0762642313	3.202509949	0.4412622939
H	-2.4059388186	-0.252825786	0.7564563083
H	-3.3144803027	1.2415264188	0.4978155066
H	-2.0070997387	1.2011277644	1.7130656383
H	2.4121832207	-3.0232769446	-0.727940469
H	0.7321509433	-2.9720990315	-1.2952171241
H	1.0762642313	-3.202509949	0.4412622939
H	3.3144803027	-1.2415264188	0.4978155066
H	2.0070997387	-1.2011277644	1.7130656383
H	2.4059388186	0.252825786	0.7564563083

Tabelle 10.356 Standardorientierung von  $\text{Me}_2\text{O}$  ( $\text{C}_{2v}$ ) [globales Minimum; M062X/6-31+G(d)].

	x	y	z
C	0.	1.1650729209	-0.1981814672
O	0.	0.	0.5869387737
C	0.	-1.1650729209	-0.1981814672
H	-0.8938993255	1.2127058726	-0.8382856487
H	0.8938993255	1.2127058726	-0.8382856487
H	0.	2.017929709	0.4826508777
H	0.8938993255	-1.2127058726	-0.8382856487
H	-0.8938993255	-1.2127058726	-0.8382856487
H	0.	-2.017929709	0.4826508777

Tabelle 10.357 Standardorientierung von  $\mathbf{4}$  ( $\text{C}_2$ ) [globales Minimum; M062X/6-31+G(d)].

	x	y	z
C	0.2562471131	3.8569798762	0.7657370976
N	0.1808315602	2.5663279834	1.4562186347
C	-0.952382985	2.5055834593	2.3724145215
C	1.419893066	2.2708643353	2.1725386
C	0.9252400947	3.7095190049	-0.599157293
N	0.2402414195	2.7204207014	-1.4318082894
C	-1.0849637245	3.1710039369	-1.8461502418
C	1.0468787834	2.3710428031	-2.5967551293
C	-0.2562471131	-3.8569798762	0.7657370976
N	-0.1808315602	-2.5663279834	1.4562186347
C	-1.419893066	-2.2708643353	2.1725386
C	0.952382985	-2.5055834593	2.3724145215
C	-0.9252400947	-3.7095190049	-0.599157293
N	-0.2402414195	-2.7204207014	-1.4318082894
C	-1.0468787834	-2.3710428031	-2.5967551293
C	1.0849637245	-3.1710039369	-1.8461502418

Li	0.0382862884	1.1218894079	-0.1085223794
Li	-0.0382862884	-1.1218894079	-0.1085223794
C	-1.8467638291	0.0741861878	-0.2321290076
C	1.8467638291	-0.0741861878	-0.2321290076
H	-0.7611014317	4.2402335546	0.6387010154
H	0.8019667428	4.6050790903	1.3673059127
H	-0.9964439536	1.5094002167	2.8221758063
H	-1.8833039176	2.6649388049	1.8219869264
H	-0.8728311204	3.2566937644	3.1786063391
H	1.3958301993	1.2373795935	2.5293004787
H	1.5589899093	2.9529391739	3.0304084666
H	2.2782669823	2.3619575776	1.5040698498
H	0.9675534007	4.6958291574	-1.0991554421
H	1.9586119538	3.3673460935	-0.4673951806
H	-1.5193087607	2.4281522607	-2.5188441118
H	-1.7535685371	3.2542072596	-0.9850964098
H	-1.0407286944	4.1446572161	-2.3672507636
H	0.5426484505	1.5775580707	-3.155853049
H	1.2000216753	3.2365455501	-3.2660792361
H	2.0178081544	1.9904938341	-2.2694428251
H	-0.8019667428	-4.6050790903	1.3673059127
H	0.7611014317	-4.2402335546	0.6387010154
H	-1.3958301993	-1.2373795935	2.5293004787
H	-2.2782669823	-2.3619575776	1.5040698498
H	-1.5589899093	-2.9529391739	3.0304084666
H	0.9964439536	-1.5094002167	2.8221758063
H	0.8728311204	-3.2566937644	3.1786063391
H	1.8833039176	-2.6649388049	1.8219869264
H	-1.9586119538	-3.3673460935	-0.4673951806
H	-0.9675534007	-4.6958291574	-1.0991554421
H	-0.5426484505	-1.5775580707	-3.155853049
H	-2.0178081544	-1.9904938341	-2.2694428251
H	-1.2000216753	-3.2365455501	-3.2660792361
H	1.5193087607	-2.4281522607	-2.5188441118
H	1.0407286944	-4.1446572161	-2.3672507636
H	1.7535685371	-3.2542072596	-0.9850964098
H	-2.1907882236	0.506390694	-1.1913129193
H	-2.4114163141	0.6206967194	0.5465077064
H	-2.3023526036	-0.9356280921	-0.2244560776
H	2.1907882236	-0.506390694	-1.1913129193
H	2.4114163141	-0.6206967194	0.5465077064
H	2.3023526036	0.9356280921	-0.2244560776

Tabelle 10.358 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; M062X/6-31+G(d)].

	x	y	z
O	0.	0.	3.7966633551
C	0.0033413508	1.1845124384	4.5697961963
Li	0.	0.	1.9144580224
Li	0.	0.	-0.2853808011
C	-0.0041913873	1.8428398537	0.8936501026

H	0.0056636683	2.023083817	3.871386318
H	0.8991247253	1.2240275123	5.2027446403
H	-0.8922187566	1.2290941882	5.2027191371
H	-0.0127791121	2.2438040399	-0.1383708091
H	0.8643472182	2.3442455388	1.360936445
H	-0.8936610142	2.3069469546	1.361441636
C	-0.6766646352	0.3554470094	-2.9743331418
N	-1.4540828157	0.0228037639	-1.777736988
C	-2.4733481314	1.0320693545	-1.5014267709
C	-2.0765110747	-1.2952675072	-1.8805813962
H	-0.5221827374	1.4399414133	-2.9802911543
H	-1.2299116566	0.1053151723	-3.8978796201
H	-2.9963926627	0.7679401066	-0.5781548624
H	-2.0005948795	2.0061220488	-1.3531214741
H	-3.211061317	1.1040477066	-2.3200943985
H	-2.5409841665	-1.5497171505	-0.9242415242
H	-2.8420876706	-1.3168520544	-2.6764325053
H	-1.3269894303	-2.0607870049	-2.0920166963
C	-0.0033413508	-1.1845124384	4.5697961963
C	0.0041913873	-1.8428398537	0.8936501026
H	-0.0056636683	-2.023083817	3.871386318
H	-0.8991247253	-1.2240275123	5.2027446403
H	0.8922187566	-1.2290941882	5.2027191371
H	0.0127791121	-2.2438040399	-0.1383708091
H	-0.8643472182	-2.3442455388	1.360936445
H	0.8936610142	-2.3069469546	1.361441636
C	0.6766646352	-0.3554470094	-2.9743331418
N	1.4540828157	-0.0228037639	-1.777736988
C	2.4733481314	-1.0320693545	-1.5014267709
C	2.0765110747	1.2952675072	-1.8805813962
H	0.5221827374	-1.4399414133	-2.9802911543
H	1.2299116566	-0.1053151723	-3.8978796201
H	2.9963926627	-0.7679401066	-0.5781548624
H	2.0005948795	-2.0061220488	-1.3531214741
H	3.211061317	-1.1040477066	-2.3200943985
H	2.5409841665	1.5497171505	-0.9242415242
H	2.8420876706	1.3168520544	-2.6764325053
H	1.3269894303	2.0607870049	-2.0920166963

Tabelle 10.359 Standardorientierung von **6** [globales Minimum; M062X/6-31+G(d)].

	x	y	z
N	-1.4698327645	0.0676405338	0.0433885495
C	-1.0296864927	-1.2067834241	-0.5310823328
C	0.3096287527	-1.6566365149	0.0548069377
N	1.2862901726	-0.5673410465	0.0476335906
C	1.7651266912	-0.270279258	-1.3045401662
C	2.4157864766	-0.8497094523	0.9281783034
C	-2.5409088283	0.6644895657	-0.7518046747
C	-1.8947739642	-0.0854185513	1.4344987546
H	-0.9361823102	-1.0680460347	-1.6131124519

H	-1.7835673075	-1.9991812094	-0.3743559881
H	0.6757484411	-2.5355684531	-0.5058033564
H	0.1743021489	-1.9786316294	1.0929394885
H	2.4624935467	0.5696904535	-1.2592339469
H	0.9343210563	0.0337963705	-1.9485299899
H	2.2644601945	-1.1446965881	-1.7567893645
H	3.0805125474	0.0176352785	0.9450792691
H	2.9869602757	-1.7332188903	0.5948580954
H	2.0552713147	-1.0274807832	1.9453959126
H	-2.8056878154	1.6364425251	-0.3286151966
H	-3.4400602808	0.0252627409	-0.775195739
H	-2.190899008	0.8243468642	-1.774980918
H	-2.2151744321	0.8852606334	1.8221361244
H	-1.0635657681	-0.4370553623	2.0531689977
H	-2.730638381	-0.7998252021	1.5301807044
Li	0.2516442044	1.211640818	0.2622235266
C	0.9845453822	3.0751181972	0.061764976
H	0.994927637	3.4004750227	-0.9940249942
H	2.033699505	3.1453459016	0.4017019227
H	0.4456510057	3.8668674946	0.6077689659

Tabelle 10.360 Standardorientierung von **7** [globales Minimum; M062X/6-31+G(d)].

	x	y	z
N	0.6623265707	1.5685081647	-0.1158007019
C	1.9278565407	0.9616747372	0.3122235396
C	2.198373737	-0.3602590867	-0.4006376982
N	1.1350248689	-1.3387666564	-0.1379642375
C	1.3905681383	-2.0709590526	1.1051173083
C	0.9893366111	-2.2695736425	-1.2516208024
C	0.3162650021	2.6774476962	0.7734203547
C	0.7160774721	2.0205581286	-1.5014760263
H	1.8507065891	0.7869871436	1.3916705643
H	2.7740150183	1.6536159539	0.1425963968
H	3.1815310974	-0.7523384507	-0.0882804691
H	2.2587787617	-0.1944739796	-1.4811503403
H	0.5340372528	-2.7109828491	1.3321941496
H	1.4923947367	-1.3725945376	1.9379793919
H	2.3013501418	-2.69029565	1.0210556335
H	0.2109416695	-3.0005208436	-1.015564169
H	1.9244452297	-2.8194395044	-1.4580111305
H	0.688880698	-1.7266708651	-2.1526294874
H	-0.6487625876	3.0963806552	0.4727241928
H	1.0749752167	3.4793274091	0.7383715219
H	0.2167781593	2.2988923179	1.7933391274
H	-0.206208258	2.5556840504	-1.7429171538
H	0.7942049658	1.1719240369	-2.1857645178
H	1.5662332346	2.703528413	-1.6793013849
Li	-0.4769982653	-0.0894301452	0.4185215431
C	-0.9719574581	-0.0973569484	2.4190683393
H	-0.1276710341	0.2077763553	3.0723035853

H	-1.2628998551	-1.0943308635	2.8052632073
H	-1.8011818483	0.5724292176	2.7217155503
C	-2.8051680029	0.8361424827	-0.5883396923
O	-2.033110244	-0.3387281908	-0.7717498182
H	-2.2448859593	1.6637447585	-1.0283259834
H	-2.9606087565	1.0233821191	0.4820474691
H	-3.7714935352	0.7400737919	-1.1014223093
C	-2.7054386407	-1.4778767553	-0.2553295572
H	-2.9111407426	-1.3448883157	0.8134543517
H	-2.0407839959	-2.3338644254	-0.3897109981
H	-3.6372845285	-1.6481746694	-0.8112477492

Tabelle 10.361 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
Li	0.553879689	1.0747632476	0.8481299946
Li	-0.553879689	-1.0747632476	0.8481299946
Li	1.0747632476	-0.553879689	-0.848301442
Li	-1.0747632476	0.553879689	-0.848301442
C	0.7584337668	1.6417773928	-1.2678487212
C	-1.6417773928	0.7584337668	1.2676772738
C	-0.7584337668	-1.6417773928	-1.2678487212
C	1.6417773928	-0.7584337668	1.2676772738
H	0.0226411045	2.4330584751	-1.5078967061
H	1.1383417043	1.3296642994	-2.2579059419
H	1.6064584687	2.1956248839	-0.8235938334
H	-2.4330584751	0.0226411045	1.5077252587
H	-2.1956248839	1.6064584687	0.823422386
H	-1.3296642994	1.1383417043	2.2577344945
H	-0.0226411045	-2.4330584751	-1.5078967061
H	-1.1383417043	-1.3296642994	-2.2579059419
H	-1.6064584687	-2.1956248839	-0.8235938334
H	1.3296642994	-1.1383417043	2.2577344945
H	2.4330584751	-0.0226411045	1.5077252587
H	2.1956248839	-1.6064584687	0.823422386
O	2.5334726986	-1.0434921789	-2.0065223707
O	-1.0434921789	-2.5334726986	2.0063509234
O	1.0434921789	2.5334726986	2.0063509234
O	-2.5334726986	1.0434921789	-2.0065223707
C	-0.2796640618	-3.6982180645	1.7417021371
H	0.74693745	-3.5746792856	2.1100850901
H	-0.7427971702	-4.5715763425	2.2178508342
H	-0.2655949204	-3.8317650763	0.6584703373
C	-1.1265492946	-2.2325659585	3.3866380811
H	-1.6518254574	-3.035079373	3.9197104089
H	-0.1235937597	-2.1057443993	3.8154915112
H	-1.6849180964	-1.2993211876	3.4796414823
C	-3.6982180645	0.2796640618	-1.7418735845
H	-4.5715763425	0.7427971702	-2.2180222815

H	-3.5746792856	-0.74693745	-2.1102565375
H	-3.8317650763	0.2655949204	-0.6586417847
C	-2.2325659585	1.1265492946	-3.3868095285
H	-2.1057443993	0.1235937597	-3.8156629585
H	-3.035079373	1.6518254574	-3.9198818563
H	-1.2993211876	1.6849180964	-3.4798129297
C	3.6982180645	-0.2796640618	-1.7418735845
H	3.8317650763	-0.2655949204	-0.6586417847
H	4.5715763425	-0.7427971702	-2.2180222815
H	3.5746792856	0.74693745	-2.1102565375
C	2.2325659585	-1.1265492946	-3.3868095285
H	2.1057443993	-0.1235937597	-3.8156629585
H	3.035079373	-1.6518254574	-3.9198818563
H	1.2993211876	-1.6849180964	-3.4798129297
C	0.2796640618	3.6982180645	1.7417021371
H	-0.74693745	3.5746792856	2.1100850901
H	0.7427971702	4.5715763425	2.2178508342
H	0.2655949204	3.8317650763	0.6584703373
C	1.1265492946	2.2325659585	3.3866380811
H	1.6518254574	3.035079373	3.9197104089
H	0.1235937597	2.1057443993	3.8154915112
H	1.6849180964	1.2993211876	3.4796414823

Tabelle 10.362 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
C	-0.0452862927	0.762565284	-0.0696290673
C	0.0452862927	-0.762565284	-0.0696290673
N	-1.3986753176	1.2365721753	-0.3297672038
N	1.3986753176	-1.2365721753	-0.3297672038
C	-1.4047819217	2.6808378183	-0.4861434342
C	-2.3206576979	0.8393124322	0.7218128437
C	1.4047819217	-2.6808378183	-0.4861434342
C	2.3206576979	-0.8393124322	0.7218128437
H	0.6063596568	1.1329159212	-0.8692483644
H	0.3298197059	1.1761615066	0.8887439948
H	-0.6063596568	-1.1329159212	-0.8692483644
H	-0.3298197059	-1.1761615066	0.8887439948
H	-2.4150231144	3.0202518746	-0.7307265533
H	-0.7384207739	2.9666325891	-1.304434575
H	-1.0751309304	3.2057828892	0.4312350352
H	-2.4037824655	-0.248844242	0.7692372341
H	-3.3135385498	1.2424266891	0.5052955736
H	-2.0038745169	1.2094029849	1.7167355166
H	2.4150231144	-3.0202518746	-0.7307265533
H	0.7384207739	-2.9666325891	-1.304434575
H	1.0751309304	-3.2057828892	0.4312350352
H	3.3135385498	-1.2424266891	0.5052955736
H	2.0038745169	-1.2094029849	1.7167355166
H	2.4037824655	0.248844242	0.7692372341

Tabelle 10.363 Standardorientierung von  $\text{Me}_2\text{O}$  ( $\text{C}_{2v}$ ) [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
C	0.	1.1655383222	-0.1978633952
O	0.	0.	0.5875654712
C	0.	-1.1655383222	-0.1978633952
H	-0.8932975447	1.2138234366	-0.8381148526
H	0.8932975447	1.2138234366	-0.8381148526
H	0.	2.0188791104	0.4816778648
H	0.8932975447	-1.2138234366	-0.8381148526
H	-0.8932975447	-1.2138234366	-0.8381148526
H	0.	-2.0188791104	0.4816778648

Tabelle 10.364 Standardorientierung von  $\mathbf{4}$  ( $\text{C}_2$ ) [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
C	0.2609866634	3.8587206578	0.7603263945
N	0.1745239618	2.5703527546	1.4543321578
C	-0.9649711975	2.5170633798	2.3638750614
C	1.4088175322	2.2683917794	2.1770300091
C	0.9300644707	3.7016929452	-0.6032389814
N	0.2367757662	2.7158747114	-1.433456213
C	-1.0873568178	3.1728572298	-1.845442066
C	1.0395742295	2.3584330871	-2.5991510381
C	-0.2609866634	-3.8587206578	0.7603263945
N	-0.1745239618	-2.5703527546	1.4543321578
C	-1.4088175322	-2.2683917794	2.1770300091
C	0.9649711975	-2.5170633798	2.3638750614
C	-0.9300644707	-3.7016929452	-0.6032389814
N	-0.2367757662	-2.7158747114	-1.433456213
C	-1.0395742295	-2.3584330871	-2.5991510381
C	1.0873568178	-3.1728572298	-1.845442066
Li	0.033847104	1.1239511484	-0.1048806169
Li	-0.033847104	-1.1239511484	-0.1048806169
C	-1.8474749313	0.069127311	-0.220051122
C	1.8474749313	-0.069127311	-0.220051122
H	-0.7526655419	4.2497324226	0.6304875335
H	0.8120129318	4.6041883937	1.35933165
H	-1.0172350064	1.5220766752	2.8142898959
H	-1.8912677132	2.6791981011	1.8071890614
H	-0.8872330244	3.2684626966	3.1692236221
H	1.3756087926	1.2366120234	2.5366850561
H	1.549983478	2.9519339501	3.0326621158
H	2.2698025948	2.3492265184	1.5111340647
H	0.9817233801	4.6860283464	-1.1052376181
H	1.959614843	3.3498794972	-0.4688562259
H	-1.527521147	2.4304691444	-2.5141321395
H	-1.7528585181	3.2611721171	-0.9830086354
H	-1.0401510945	4.144435946	-2.3689832627
H	0.5286816246	1.5683623587	-3.1561218804
H	1.1988512097	3.2209234428	-3.2700362655
H	2.0070766647	1.9703222462	-2.2718505229

H	-0.8120129318	-4.6041883937	1.35933165
H	0.7526655419	-4.2497324226	0.6304875335
H	-1.3756087926	-1.2366120234	2.5366850561
H	-2.2698025948	-2.3492265184	1.5111340647
H	-1.549983478	-2.9519339501	3.0326621158
H	1.0172350064	-1.5220766752	2.8142898959
H	0.8872330244	-3.2684626966	3.1692236221
H	1.8912677132	-2.6791981011	1.8071890614
H	-1.959614843	-3.3498794972	-0.4688562259
H	-0.9817233801	-4.6860283464	-1.1052376181
H	-0.5286816246	-1.5683623587	-3.1561218804
H	-2.0070766647	-1.9703222462	-2.2718505229
H	-1.1988512097	-3.2209234428	-3.2700362655
H	1.527521147	-2.4304691444	-2.5141321395
H	1.0401510945	-4.144435946	-2.3689832627
H	1.7528585181	-3.2611721171	-0.9830086354
H	-2.200288481	0.5170711406	-1.1675422164
H	-2.4112288287	0.593602139	0.5726889152
H	-2.2925368763	-0.9442040959	-0.2307038168
H	2.200288481	-0.5170711406	-1.1675422164
H	2.4112288287	-0.593602139	0.5726889152
H	2.2925368763	0.9442040959	-0.2307038168

Tabelle 10.365 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
O	0.	0.	3.796393414
C	0.0025482693	1.1854851865	4.5691511464
Li	0.	0.	1.9157949622
Li	0.	0.	-0.2874749584
C	-0.0047900146	1.84217625	0.8932621457
H	0.004299689	2.0232734298	3.8702468927
H	0.8978516387	1.2266608477	5.2020316053
H	-0.892579083	1.2305178269	5.2020144509
H	-0.0130821164	2.2376514982	-0.1398327152
H	0.8628210973	2.3449164875	1.3581138106
H	-0.8941549148	2.3067134911	1.3581280298
C	-0.6761651498	0.3561096883	-2.9736488698
N	-1.4544031832	0.022496338	-1.7775871458
C	-2.4728836418	1.0327863011	-1.4997550141
C	-2.0769157945	-1.2959519127	-1.8810270965
H	-0.5199070729	1.4400577852	-2.9775509338
H	-1.2283205161	0.1080698033	-3.897856808
H	-2.9965556969	0.7674513093	-0.5777434758
H	-1.9987071349	2.005194016	-1.3480821796
H	-3.2098965426	1.1077722122	-2.3180594619
H	-2.5403299475	-1.5510702517	-0.92490178
H	-2.8422940218	-1.3178249744	-2.6763050678
H	-1.3273307427	-2.06095961	-2.0920907363
C	-0.0025482693	-1.1854851865	4.5691511464
C	0.0047900146	-1.84217625	0.8932621457

H	-0.004299689	-2.0232734298	3.8702468927
H	-0.8978516387	-1.2266608477	5.2020316053
H	0.892579083	-1.2305178269	5.2020144509
H	0.0130821164	-2.2376514982	-0.1398327152
H	-0.8628210973	-2.3449164875	1.3581138106
H	0.8941549148	-2.3067134911	1.3581280298
C	0.6761651498	-0.3561096883	-2.9736488698
N	1.4544031832	-0.022496338	-1.7775871458
C	2.4728836418	-1.0327863011	-1.4997550141
C	2.0769157945	1.2959519127	-1.8810270965
H	0.5199070729	-1.4400577852	-2.9775509338
H	1.2283205161	-0.1080698033	-3.897856808
H	2.9965556969	-0.7674513093	-0.5777434758
H	1.9987071349	-2.005194016	-1.3480821796
H	3.2098965426	-1.1077722122	-2.3180594619
H	2.5403299475	1.5510702517	-0.92490178
H	2.8422940218	1.3178249744	-2.6763050678
H	1.3273307427	2.06095961	-2.0920907363

Tabelle 10.366 Standardorientierung von **6** [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
N	-1.4759955345	0.0659329009	0.0456794795
C	-1.0307000167	-1.2038171042	-0.5361169851
C	0.3083165954	-1.6537673326	0.0499014584
N	1.28206508	-0.5617325638	0.0490987803
C	1.7678466433	-0.2604232969	-1.300180836
C	2.4075256966	-0.8385333751	0.9370938443
C	-2.5511266431	0.6616336435	-0.7456827082
C	-1.8978656873	-0.0960720524	1.4371694899
H	-0.9345885441	-1.0575521774	-1.61657627
H	-1.7819839256	-1.9994803307	-0.3864733182
H	0.6760746548	-2.5294480756	-0.5138086745
H	0.1713886265	-1.9804404281	1.0859830404
H	2.4555714227	0.5865773275	-1.2497166691
H	0.9390450479	0.0359494571	-1.949524778
H	2.2780561489	-1.129772994	-1.7486750859
H	3.0660261217	0.0328778284	0.9595044212
H	2.9866059841	-1.7174772844	0.6069769953
H	2.0417505856	-1.0197732072	1.9513204338
H	-2.8196302996	1.630209242	-0.3183571534
H	-3.4472671519	0.0190883393	-0.7708234369
H	-2.2034045821	0.827561031	-1.7681569541
H	-2.2240043182	0.8701823683	1.8294798432
H	-1.0636202561	-0.4446346836	2.052630668
H	-2.7283269219	-0.816135808	1.5314162207
Li	0.2442585991	1.2130501444	0.2620370469
C	1.002716893	3.0647072608	0.0483705866
H	1.0026037518	3.387189065	-1.0072311799
H	2.0579095438	3.1106956067	0.3705062271
H	0.4911444859	3.8675464991	0.6018105139

Tabelle 10.367 Standardorientierung von **7** [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
N	0.6601284619	1.5669996174	-0.118383914
C	1.9253634493	0.9609107762	0.3128476038
C	2.1978297544	-0.3607144714	-0.3994945485
N	1.1350883499	-1.3402651309	-0.1371522381
C	1.3891047883	-2.0713015597	1.1074138556
C	0.9895606791	-2.2715948811	-1.2508971426
C	0.3096419565	2.6747888808	0.7713066753
C	0.7154062731	2.0191947768	-1.5043111922
H	1.8442858884	0.7850957487	1.3916063344
H	2.7716533124	1.6525162952	0.1457586318
H	3.1810756788	-0.7507608171	-0.0865286974
H	2.2584043285	-0.1946078386	-1.4795555816
H	0.5334875866	-2.7125655012	1.3323828725
H	1.4847873055	-1.3719093793	1.9397052883
H	2.3012472103	-2.6881138966	1.0270363182
H	0.2094941368	-3.0004593119	-1.0159960357
H	1.923120406	-2.8237253232	-1.4554302624
H	0.6917358074	-1.7289345176	-2.1523706021
H	-0.6538351998	3.0936205979	0.4671086301
H	1.0674751656	3.4769438274	0.7411149519
H	0.2050822662	2.2934885752	1.7893212361
H	-0.2091672149	2.5480574699	-1.7486848388
H	0.8005564379	1.1713813813	-2.1880263591
H	1.5612341253	2.7071705927	-1.6800595084
Li	-0.4757530845	-0.0910417697	0.414875208
C	-0.9703983878	-0.0944531686	2.4176300271
H	-0.1230874181	0.2123726555	3.064584663
H	-1.2594838186	-1.0887690433	2.8087392988
H	-1.7964364661	0.5767606362	2.721714336
C	-2.7997740797	0.8398216443	-0.5801390407
O	-2.0306784876	-0.3361514332	-0.7757462706
H	-2.2401200933	1.6693133454	-1.0168214324
H	-2.9481011086	1.0198145183	0.4922570634
H	-3.7686021489	0.7500133162	-1.088532839
C	-2.7023686557	-1.4778367208	-0.2620140564
H	-2.8955453681	-1.3527088747	0.8098463901
H	-2.042701199	-2.33503867	-0.4102269487
H	-3.6402026376	-1.6407603466	-0.8090558755

Tabelle 10.368 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; M062X/6-311+G(d,p)].

	x	y	z
Li	0.5597801904	1.0719990459	0.8488018945
Li	-0.5597801904	-1.0719990459	0.8488018945
Li	1.0719990459	-0.5597801904	-0.8489733419
Li	-1.0719990459	0.5597801904	-0.8489733419
C	0.7658793619	1.6406982672	-1.2676421379

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C	-1.6406982672	0.7658793619	1.2674706905
C	-0.7658793619	-1.6406982672	-1.2676421379
C	1.6406982672	-0.7658793619	1.2674706905
H	0.0249523716	2.4239066753	-1.5097229873
H	1.1544288447	1.3351323508	-2.2539095259
H	1.6029936843	2.2016780466	-0.8167725601
H	-2.4239066753	0.0249523716	1.5095515399
H	-2.2016780466	1.6029936843	0.8166011127
H	-1.3351323508	1.1544288447	2.2537380785
H	-0.0249523716	-2.4239066753	-1.5097229873
H	-1.1544288447	-1.3351323508	-2.2539095259
H	-1.6029936843	-2.2016780466	-0.8167725601
H	1.3351323508	-1.1544288447	2.2537380785
H	2.4239066753	-0.0249523716	1.5095515399
H	2.2016780466	-1.6029936843	0.8166011127
O	2.5302488064	-1.0428332882	-2.0102508496
O	-1.0428332882	-2.5302488064	2.0100794022
O	1.0428332882	2.5302488064	2.0100794022
O	-2.5302488064	1.0428332882	-2.0102508496
C	-0.2753989598	-3.6923863378	1.746885512
H	0.7488299154	-3.563715271	2.1135318384
H	-0.733888326	-4.5651541319	2.2240547046
H	-0.2610240638	-3.8282354736	0.6658077453
C	-1.1359713699	-2.2347255333	3.3902089299
H	-1.6669667205	-3.0361142647	3.9152142116
H	-0.1377789896	-2.1139259443	3.8263964994
H	-1.6902866751	-1.3013260521	3.4838732203
C	-3.6923863378	0.2753989598	-1.7470569594
H	-4.5651541319	0.733888326	-2.2242261519
H	-3.563715271	-0.7488299154	-2.1137032858
H	-3.8282354736	0.2610240638	-0.6659791927
C	-2.2347255333	1.1359713699	-3.3903803773
H	-2.1139259443	0.1377789896	-3.8265679468
H	-3.0361142647	1.6669667205	-3.915385659
H	-1.3013260521	1.6902866751	-3.4840446677
C	3.6923863378	-0.2753989598	-1.7470569594
H	3.8282354736	-0.2610240638	-0.6659791927
H	4.5651541319	-0.733888326	-2.2242261519
H	3.563715271	0.7488299154	-2.1137032858
C	2.2347255333	-1.1359713699	-3.3903803773
H	2.1139259443	-0.1377789896	-3.8265679468
H	3.0361142647	-1.6669667205	-3.915385659
H	1.3013260521	-1.6902866751	-3.4840446677
C	0.2753989598	3.6923863378	1.746885512
H	-0.7488299154	3.563715271	2.1135318384
H	0.733888326	4.5651541319	2.2240547046
H	0.2610240638	3.8282354736	0.6658077453
C	1.1359713699	2.2347255333	3.3902089299
H	1.6669667205	3.0361142647	3.9152142116
H	0.1377789896	2.1139259443	3.8263964994
H	1.6902866751	1.3013260521	3.4838732203

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Tabelle 10.369 Standardorientierung von TMEDA ( $C_2$ ) [globales Minimum; M062X/6-311+G(d,p)].

	x	y	z
C	-0.0444539281	0.7622679471	-0.0702872821
C	0.0444539281	-0.7622679471	-0.0702872821
N	-1.3972827049	1.2374206488	-0.3318391069
N	1.3972827049	-1.2374206488	-0.3318391069
C	-1.4024281035	2.6824262933	-0.480120954
C	-2.3209874203	0.8346609845	0.715936192
C	1.4024281035	-2.6824262933	-0.480120954
C	2.3209874203	-0.8346609845	0.715936192
H	0.6077099273	1.1314031519	-0.8670145699
H	0.3279717823	1.1738142144	0.8867358675
H	-0.6077099273	-1.1314031519	-0.8670145699
H	-0.3279717823	-1.1738142144	0.8867358675
H	-2.4096702952	3.0234278393	-0.7267980307
H	-0.7335466537	2.9726471111	-1.292326407
H	-1.0771688138	3.1999262852	0.4401601428
H	-2.4075738605	-0.251774825	0.754390533
H	-3.310945674	1.2418670522	0.5029255288
H	-2.0034073821	1.1954639546	1.7113490864
H	2.4096702952	-3.0234278393	-0.7267980307
H	0.7335466537	-2.9726471111	-1.292326407
H	1.0771688138	-3.1999262852	0.4401601428
H	3.310945674	-1.2418670522	0.5029255288
H	2.0034073821	-1.1954639546	1.7113490864
H	2.4075738605	0.251774825	0.754390533

Tabelle 10.370 Standardorientierung von  $Me_2O$  ( $C_{2v}$ ) [globales Minimum; M062X/6-311+G(d,p)].

	x	y	z
C	0.	1.164170108	-0.197614452
O	0.	0.	0.5877917903
C	0.	-1.164170108	-0.197614452
H	-0.8915061771	1.2119819408	-0.8368602249
H	0.8915061771	1.2119819408	-0.8368602249
H	0.	2.0176423025	0.4788065067
H	0.8915061771	-1.2119819408	-0.8368602249
H	-0.8915061771	-1.2119819408	-0.8368602249
H	0.	-2.0176423025	0.4788065067

Tabelle 10.371 Standardorientierung von **4** ( $C_2$ ) [globales Minimum; M062X/6-311+G(d,p)].

	x	y	z
C	0.2481324982	3.9099972767	0.639907034
N	0.1389123959	2.6757580703	1.4234915344
C	-1.0288097296	2.6907481524	2.2991164138
C	1.3512025509	2.4288118051	2.2025083065
C	0.942426942	3.6527897082	-0.6947697033
N	0.2601375856	2.6129352139	-1.4669512657
C	-1.0506862756	3.0474810631	-1.9403455285
C	1.0844582148	2.178309894	-2.5906807983

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C	-0.2481324982	-3.9099972767	0.639907034
N	-0.1389123959	-2.6757580703	1.4234915344
C	-1.3512025509	-2.4288118051	2.2025083065
C	1.0288097296	-2.6907481524	2.2991164138
C	-0.942426942	-3.6527897082	-0.6947697033
N	-0.2601375856	-2.6129352139	-1.4669512657
C	-1.0844582148	-2.178309894	-2.5906807983
C	1.0506862756	-3.0474810631	-1.9403455285
Li	0.0332486084	1.1236164171	-0.004788511
Li	-0.0332486084	-1.1236164171	-0.004788511
C	-1.8594923777	0.0669245052	0.0391475311
C	1.8594923777	-0.0669245052	0.0391475311
H	-0.7573721682	4.2971800525	0.4632274947
H	0.7926692992	4.6902597259	1.194004117
H	-1.0853564721	1.7418693091	2.8351317439
H	-1.9367571472	2.7872666809	1.7013847485
H	-0.9835012477	3.5123018812	3.0319595332
H	1.2915990827	1.4393982832	2.6587030469
H	1.4816091934	3.188217945	2.9902396687
H	2.2271756476	2.4312972861	1.5539976384
H	1.0096217036	4.5958102305	-1.2640759632
H	1.9645825566	3.307399916	-0.5141632774
H	-1.4919432532	2.2517329624	-2.5413907705
H	-1.7250545344	3.2265901453	-1.1022203155
H	-0.9810627372	3.9623950637	-2.5514685843
H	0.5779063256	1.364205145	-3.1119494019
H	1.2667569991	2.9966225824	-3.3060153784
H	2.03865708	1.8012049683	-2.2212920006
H	-0.7926692992	-4.6902597259	1.194004117
H	0.7573721682	-4.2971800525	0.4632274947
H	-1.2915990827	-1.4393982832	2.6587030469
H	-2.2271756476	-2.4312972861	1.5539976384
H	-1.4816091934	-3.188217945	2.9902396687
H	1.0853564721	-1.7418693091	2.8351317439
H	0.9835012477	-3.5123018812	3.0319595332
H	1.9367571472	-2.7872666809	1.7013847485
H	-1.9645825566	-3.307399916	-0.5141632774
H	-1.0096217036	-4.5958102305	-1.2640759632
H	-0.5779063256	-1.364205145	-3.1119494019
H	-2.03865708	-1.8012049683	-2.2212920006
H	-1.2667569991	-2.9966225824	-3.3060153784
H	1.4919432532	-2.2517329624	-2.5413907705
H	0.9810627372	-3.9623950637	-2.5514685843
H	1.7250545344	-3.2265901453	-1.1022203155
H	-2.3272112847	0.7373412069	-0.7021650854
H	-2.3063609579	0.358055384	1.0042642434
H	-2.3156477263	-0.9152460059	-0.1782434508
H	2.3272112847	-0.7373412069	-0.7021650854
H	2.3063609579	-0.358055384	1.0042642434
H	2.3156477263	0.9152460059	-0.1782434508

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Tabelle 10.372 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; M062X/6-311+G(d,p)].

	x	y	z
O	0.	0.	3.8034935533
C	-0.0014102217	1.1850338991	4.5765404837
Li	0.	0.	1.9156881011
Li	0.	0.	-0.2856073272
C	-0.002832486	1.8439160508	0.8966969182
H	-0.0030818023	2.022036972	3.8793738152
H	0.8923418315	1.2295214704	5.2079963442
H	-0.8946095921	1.2267460143	5.208968221
H	0.0023583279	2.2425303693	-0.1327539945
H	0.8583175398	2.3427767071	1.3728406007
H	-0.8927588149	2.3100287124	1.3537126284
C	-0.6765651347	0.3545548434	-2.9793436818
N	-1.4519430183	0.0210365486	-1.7813802951
C	-2.4696006106	1.0322303537	-1.5030051003
C	-2.0763173213	-1.2965182211	-1.8865713407
H	-0.5227677938	1.4364657338	-2.9857295631
H	-1.2286796168	0.103323248	-3.8996006181
H	-2.9964850385	0.7646747662	-0.5856462923
H	-1.9948101188	2.0012478555	-1.3449762719
H	-3.2016872389	1.1116177702	-2.3222799297
H	-2.5334542195	-1.5548405698	-0.9303478755
H	-2.8446479421	-1.3137270267	-2.6759136826
H	-1.3299881057	-2.0600720697	-2.1045040919
C	0.0014102217	-1.1850338991	4.5765404837
C	0.002832486	-1.8439160508	0.8966969182
H	0.0030818023	-2.022036972	3.8793738152
H	-0.8923418315	-1.2295214704	5.2079963442
H	0.8946095921	-1.2267460143	5.208968221
H	-0.0023583279	-2.2425303693	-0.1327539945
H	-0.8583175398	-2.3427767071	1.3728406007
H	0.8927588149	-2.3100287124	1.3537126284
C	0.6765651347	-0.3545548434	-2.9793436818
N	1.4519430183	-0.0210365486	-1.7813802951
C	2.4696006106	-1.0322303537	-1.5030051003
C	2.0763173213	1.2965182211	-1.8865713407
H	0.5227677938	-1.4364657338	-2.9857295631
H	1.2286796168	-0.103323248	-3.8996006181
H	2.9964850385	-0.7646747662	-0.5856462923
H	1.9948101188	-2.0012478555	-1.3449762719
H	3.2016872389	-1.1116177702	-2.3222799297
H	2.5334542195	1.5548405698	-0.9303478755
H	2.8446479421	1.3137270267	-2.6759136826
H	1.3299881057	2.0600720697	-2.1045040919

Tabelle 10.373 Standardorientierung von **6** [globales Minimum; M062X/6-311+G(d,p)].

	x	y	z
N	-1.418308274	0.1877212416	0.3873013008
C	-0.91260083	-0.7630196857	-0.6115172874

C	0.3373543204	-1.4903518651	-0.1249883163
N	1.4174149961	-0.5449300043	0.1917632326
C	2.1639545729	-0.1785629047	-1.0194760067
C	2.3338775341	-1.1061238172	1.1821018819
C	-2.4053397658	1.0815167434	-0.2271970477
C	-2.0062440932	-0.4934516755	1.5379474511
H	-0.6742863288	-0.1879501445	-1.510824322
H	-1.6871920695	-1.4983476025	-0.8836803969
H	0.6600431817	-2.2156949554	-0.8870058249
H	0.1059274781	-2.0645499026	0.7747263045
H	2.891587772	0.5956583005	-0.7757957298
H	1.4921662734	0.2464747573	-1.7639249981
H	2.6815674453	-1.0552092307	-1.4388894926
H	3.1188047498	-0.380689762	1.4011474353
H	2.8085397084	-2.0319256083	0.8226214558
H	1.7966067289	-1.3254241912	2.1068927071
H	-2.7538142873	1.799729481	0.5161266382
H	-3.2706620728	0.5192990477	-0.6110884566
H	-1.9304042192	1.6389708776	-1.0346274506
H	-2.3983401107	0.2499231122	2.2332548235
H	-1.2573922691	-1.0836000565	2.0676259239
H	-2.8312812875	-1.1588474349	1.2388260053
Li	0.3595660745	1.2492033474	0.5028201384
C	0.5738940182	2.7838817211	-0.8058514649
H	0.2820549611	2.4457451275	-1.8187679409
H	1.5956755615	3.1759323382	-0.9273988457
H	-0.0527777684	3.6687627456	-0.6144667176

Tabelle 10.374 Standardorientierung von **7** [globales Minimum; M062X/6-311+G(d,p)].

	x	y	z
N	0.6583208512	1.5657410579	-0.1234446995
C	1.9230767868	0.9615196925	0.3126014573
C	2.2014240102	-0.3588423091	-0.3982605857
N	1.141793881	-1.3421751937	-0.1378028037
C	1.3952640949	-2.0691657334	1.1095533709
C	1.0074479272	-2.2783434854	-1.2490400287
C	0.304771103	2.6736763235	0.7652569396
C	0.721477755	2.0201266031	-1.5085680089
H	1.8390024857	0.7856560226	1.3886914676
H	2.765925595	1.6537190531	0.1481199586
H	3.1825939469	-0.7446156327	-0.0821872462
H	2.2646562502	-0.1933846903	-1.475897121
H	0.542619116	-2.7113266089	1.3340163234
H	1.4868879596	-1.3691173605	1.9391712724
H	2.3075254959	-2.6820190896	1.0314557589
H	0.2315551302	-3.0094709035	-1.0160293344
H	1.9438538075	-2.8241768773	-1.4452349135
H	0.7129439666	-1.7419865598	-2.1531624472
H	-0.6548457895	3.0935085636	0.4572484195
H	1.0628253423	3.4726425759	0.738316682

H	0.1954900809	2.2932369634	1.7810972318
H	-0.1977145998	2.5533308803	-1.7554704902
H	0.8052834403	1.1746575041	-2.1924417369
H	1.5698055965	2.7027376745	-1.6785402874
Li	-0.4764330766	-0.0984567575	0.404196048
C	-0.9642268829	-0.1047693294	2.416008473
H	-0.1129950005	0.2072441256	3.0513996946
H	-1.240176919	-1.0993686292	2.8094969317
H	-1.7898747357	0.5574560272	2.7322136199
C	-2.8089945125	0.8474505671	-0.5731972547
O	-2.0476207821	-0.333026476	-0.766278041
H	-2.2413817924	1.6730938912	-1.0018123328
H	-2.9627816365	1.0244688638	0.4967045331
H	-3.7733968165	0.7660062274	-1.0868531177
C	-2.7288477196	-1.4721635479	-0.2615412912
H	-2.923004283	-1.3509296761	0.8084938832
H	-2.0773507362	-2.3326109023	-0.4125873192
H	-3.66539134	-1.6237708542	-0.8098710057

Tabelle 10.375 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; MP2/6-31+G(d)].

	x	y	z
Li	1.114778	-0.532629	0.859808
Li	-1.114778	0.532629	0.859808
Li	-0.532629	-1.114778	-0.859808
Li	0.532629	1.114778	-0.859808
C	1.664536	-0.721433	-1.295339
C	0.721433	1.664536	1.295339
C	-1.664536	0.721433	-1.295339
C	-0.721433	-1.664536	1.295339
H	2.371389	0.061561	-1.633932
H	1.328317	-1.201526	-2.232856
H	2.312756	-1.48243	-0.821387
H	-0.061561	2.371389	1.633932
H	1.48243	2.312756	0.821387
H	1.201526	1.328317	2.232856
H	-2.371389	-0.061561	-1.633932
H	-1.328317	1.201526	-2.232856
H	-2.312756	1.48243	-0.821387
H	-1.201526	-1.328317	2.232856
H	0.061561	-2.371389	1.633932
H	-1.48243	-2.312756	0.821387
O	-1.012063	-2.691025	-1.987747
O	-2.691025	1.012063	1.987747
O	2.691025	-1.012063	1.987747
O	1.012063	2.691025	-1.987747
C	-3.872777	0.263061	1.681351
H	-3.785871	-0.760721	2.065095
H	-4.751255	0.752049	2.120052

H	-3.958827	0.246286	0.59493
C	-2.476651	1.114778	3.397647
H	-3.314297	1.643519	3.868998
H	-2.372997	0.117898	3.844224
H	-1.554868	1.680893	3.534372
C	0.263061	3.872777	-1.681351
H	0.752049	4.751255	-2.120052
H	-0.760721	3.785871	-2.065095
H	0.246286	3.958827	-0.59493
C	1.114778	2.476651	-3.397647
H	0.117898	2.372997	-3.844224
H	1.643519	3.314297	-3.868998
H	1.680893	1.554868	-3.534372
C	-0.263061	-3.872777	-1.681351
H	-0.246286	-3.958827	-0.59493
H	-0.752049	-4.751255	-2.120052
H	0.760721	-3.785871	-2.065095
C	-1.114778	-2.476651	-3.397647
H	-0.117898	-2.372997	-3.844224
H	-1.643519	-3.314297	-3.868998
H	-1.680893	-1.554868	-3.534372
C	3.872777	-0.263061	1.681351
H	3.785871	0.760721	2.065095
H	4.751255	-0.752049	2.120052
H	3.958827	-0.246286	0.59493
C	2.476651	-1.114778	3.397647
H	3.314297	-1.643519	3.868998
H	2.372997	-0.117898	3.844224
H	1.554868	-1.680893	3.534372

Tabelle 10.376 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; MP2/6-31+G(d)].

	x	y	z
C	-0.0289740511	0.7626590567	-0.0759480408
C	0.0289740511	-0.7626590567	-0.0759480408
N	-1.3784525602	1.2602013373	-0.3427850033
N	1.3784525602	-1.2602013373	-0.3427850033
C	-1.3471613053	2.7062611682	-0.533662314
C	-2.2978774161	0.9196632445	0.7383252401
C	1.3471613053	-2.7062611682	-0.533662314
C	2.2978774161	-0.9196632445	0.7383252401
H	0.6255992198	1.1188735972	-0.8795467266
H	0.3521251444	1.1751066845	0.8803167286
H	-0.6255992198	-1.1188735972	-0.8795467266
H	-0.3521251444	-1.1751066845	0.8803167286
H	-2.3531155435	3.061730115	-0.7747812243
H	-0.6827159974	2.9486278136	-1.3676243457
H	-0.99245788	3.2447707663	0.3666573585
H	-2.4067842512	-0.164046479	0.818318423
H	-3.2813179978	1.3444610814	0.517923088
H	-1.9575469981	1.3127342867	1.7168758164

H	2.3531155435	-3.061730115	-0.7747812243
H	0.6827159974	-2.9486278136	-1.3676243457
H	0.99245788	-3.2447707663	0.3666573585
H	3.2813179978	-1.3444610814	0.517923088
H	1.9575469981	-1.3127342867	1.7168758164
H	2.4067842512	0.164046479	0.818318423

Tabelle 10.377 Standardorientierung von Me<sub>2</sub>O (C<sub>2v</sub>) [globales Minimum; MP2/6-31+G(d)].

	x	y	z
C	0.	1.1736608831	0.2014379062
O	0.	0.	-0.5983873299
C	0.	-1.1736608831	0.2014379062
H	0.8944016933	1.2162120513	0.8389984529
H	-0.8944016933	1.2162120513	0.8389984529
H	0.	2.0215750317	-0.4839008769
H	-0.8944016933	-1.2162120513	0.8389984529
H	0.8944016933	-1.2162120513	0.8389984529
H	0.	-2.0215750317	-0.4839008769

Tabelle 10.378 Standardorientierung von 4 (C<sub>2</sub>) [globales Minimum; MP2/6-31+G(d)].

	x	y	z
C	3.598698	1.217535	0.880706
N	2.394117	0.621528	1.476407
C	1.812976	1.521534	2.477135
C	2.69932	-0.667904	2.107442
C	3.901362	0.605902	-0.483001
N	2.781922	0.788661	-1.415557
C	2.69932	2.173882	-1.892372
C	2.919092	-0.11457	-2.563499
C	-3.598698	-1.217535	0.880706
N	-2.394117	-0.621528	1.476407
C	-2.69932	0.667904	2.107442
C	-1.812976	-1.521534	2.477135
C	-3.901362	-0.605902	-0.483001
N	-2.781922	-0.788661	-1.415557
C	-2.919092	0.11457	-2.563499
C	-2.69932	-2.173882	-1.892372
Li	1.087128	0.323076	-0.227457
Li	-1.087128	-0.323076	-0.227457
C	-0.520638	1.785494	-0.456125
C	0.520638	-1.785494	-0.456125
H	3.425468	2.293617	0.775384
H	4.47647	1.099182	1.544605
H	0.910668	1.060634	2.888977
H	1.527995	2.463497	2.002776
H	2.515297	1.726382	3.305467
H	1.768806	-1.128888	2.447925
H	3.382467	-0.542957	2.967192
H	3.15718	-1.347146	1.386735

H	4.836365	1.042602	-0.885919
H	4.070018	-0.471709	-0.377805
H	1.86318	2.258471	-2.589619
H	2.502905	2.856083	-1.063085
H	3.630091	2.48131	-2.403022
H	2.055127	0.013685	-3.221264
H	3.839712	0.089703	-3.139416
H	2.931845	-1.149624	-2.214374
H	-4.47647	-1.099182	1.544605
H	-3.425468	-2.293617	0.775384
H	-1.768806	1.128888	2.447925
H	-3.15718	1.347146	1.386735
H	-3.382467	0.542957	2.967192
H	-0.910668	-1.060634	2.888977
H	-2.515297	-1.726382	3.305467
H	-1.527995	-2.463497	2.002776
H	-4.070018	0.471709	-0.377805
H	-4.836365	-1.042602	-0.885919
H	-2.055127	-0.013685	-3.221264
H	-2.931845	1.149624	-2.214374
H	-3.839712	-0.089703	-3.139416
H	-1.86318	-2.258471	-2.589619
H	-3.630091	-2.48131	-2.403022
H	-2.502905	-2.856083	-1.063085
H	-0.375989	2.129524	-1.497265
H	-0.04734	2.560196	0.176516
H	-1.604453	1.914771	-0.269105
H	0.375989	-2.129524	-1.497265
H	0.04734	-2.560196	0.176516
H	1.604453	-1.914771	-0.269105

Tabelle 10.379 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; MP2/6-31+G(d)].

	x	y	z
O	0.	0.	3.9049464672
C	0.0838624747	1.1873189721	4.6975767096
Li	0.	0.	1.9813168366
Li	0.	0.	-0.2693366117
C	0.0306002361	1.8611979284	0.9453074218
H	0.1420444963	2.0240441324	4.0018554331
H	0.9801173288	1.1576780761	5.3286512067
H	-0.8071287586	1.283621374	5.3294240848
H	-0.0848878898	2.2556286798	-0.0814338308
H	0.9427088062	2.3539809753	1.3295339483
H	-0.8108224639	2.3145792621	1.5036246252
C	-0.6768876651	0.3516397496	-3.0167483474
N	-1.4594344991	0.0084101994	-1.8208683953
C	-2.5141001412	1.0024689301	-1.5889814356
C	-2.0692454648	-1.321588008	-1.9435175175
H	-0.5319474559	1.4373772667	-3.0188528854
H	-1.2267452504	0.0994992187	-3.9438963254

H	-3.0592213512	0.7371256821	-0.67922687
H	-2.0648396658	1.9874794551	-1.4432374916
H	-3.2270922751	1.0475513235	-2.4313592045
H	-2.5785841806	-1.5669938675	-1.008629652
H	-2.7958744217	-1.3548897432	-2.7750061648
H	-1.3036627168	-2.0807818441	-2.1118152238
C	-0.0838624747	-1.1873189721	4.6975767096
C	-0.0306002361	-1.8611979284	0.9453074218
H	-0.1420444963	-2.0240441324	4.0018554331
H	-0.9801173288	-1.1576780761	5.3286512067
H	0.8071287586	-1.283621374	5.3294240848
H	0.0848878898	-2.2556286798	-0.0814338308
H	-0.9427088062	-2.3539809753	1.3295339483
H	0.8108224639	-2.3145792621	1.5036246252
C	0.6768876651	-0.3516397496	-3.0167483474
N	1.4594344991	-0.0084101994	-1.8208683953
C	2.5141001412	-1.0024689301	-1.5889814356
C	2.0692454648	1.321588008	-1.9435175175
H	0.5319474559	-1.4373772667	-3.0188528854
H	1.2267452504	-0.0994992187	-3.9438963254
H	3.0592213512	-0.7371256821	-0.67922687
H	2.0648396658	-1.9874794551	-1.4432374916
H	3.2270922751	-1.0475513235	-2.4313592045
H	2.5785841806	1.5669938675	-1.008629652
H	2.7958744217	1.3548897432	-2.7750061648
H	1.3036627168	2.0807818441	-2.1118152238

Tabelle 10.380 Standardorientierung von **6** [globales Minimum; MP2/6-31+G(d)].

	x	y	z
N	1.4164300699	-0.2732941291	0.0306758365
C	0.6717713475	-1.5054134159	0.3208409164
C	-0.7007203323	-1.496161564	-0.3468187026
N	-1.421104986	-0.2458394947	-0.0735251743
C	-1.8948666718	-0.1907235953	1.3169182021
C	-2.5590948833	-0.0904370465	-0.9873966212
C	2.5489407124	-0.1181191758	0.951594693
C	1.9022816101	-0.2522293456	-1.3560433357
H	0.5614802784	-1.5782344134	1.4078908463
H	1.2310703276	-2.40308225	-0.0036619027
H	-1.2776190249	-2.3780557524	-0.0099145004
H	-0.5924380761	-1.5857433644	-1.4329046599
H	-2.4278387216	0.7504041032	1.4721957488
H	-1.0502975795	-0.2164018989	2.0104326021
H	-2.5705018527	-1.0319741108	1.5497228017
H	-3.0449082735	0.8683649113	-0.7916829342
H	-3.2983682806	-0.9006062059	-0.8655062409
H	-2.1995426913	-0.0912989807	-2.0199445677
H	3.0515790398	0.8288686907	0.7415905139
H	3.2757889194	-0.9425197302	0.8524516154
H	2.1802837877	-0.0914121337	1.9804732573

H	2.4464418835	0.680021528	-1.5264855969
H	1.0632040127	-0.2859738231	-2.0559657189
H	2.5720388667	-1.1041536747	-1.5657625644
Li	0.0129380964	1.2967204233	-0.0170097477
C	0.0321140575	3.3344713028	0.0863073999
H	0.0685586302	3.7068017875	1.124495142
H	-0.8592654492	3.7943742593	-0.3733364599
H	0.9028971827	3.7774560988	-0.4267418478

Tabelle 10.381 Standardorientierung von **7** [globales Minimum; MP2/6-31+G(d)].

	x	y	z
N	0.752342687	1.5365956644	-0.1224537689
C	2.0285542535	0.8618473969	0.1595308048
C	2.1413234004	-0.4694292867	-0.5729207773
N	1.0703344329	-1.3971226229	-0.1734082448
C	1.4340621102	-2.1110474243	1.0607067653
C	0.814262672	-2.3668134494	-1.2423760106
C	0.5755516985	2.6602788324	0.8080016083
C	0.6956070985	2.0218907343	-1.5039995932
H	2.0732809855	0.6963954394	1.24158856
H	2.8868816242	1.5064781931	-0.1141774391
H	3.1378417533	-0.9103756137	-0.3851933433
H	2.0697786074	-0.3082711669	-1.6534801812
H	0.5932189467	-2.732449911	1.3769477294
H	1.627199019	-1.3980539492	1.8629379283
H	2.3241183568	-2.74698405	0.9053289319
H	0.0519198183	-3.0765468373	-0.9099117156
H	1.721305186	-2.9365701575	-1.5115883193
H	0.4433905396	-1.8456185022	-2.129906123
H	-0.3844474188	3.144824731	0.6090805613
H	1.3795057886	3.4100355393	0.6994750338
H	0.5573037414	2.2769656172	1.8298858989
H	-0.2250468022	2.5942873193	-1.6429269868
H	0.6785556774	1.186781479	-2.2076468452
H	1.5520584629	2.6775312176	-1.7444937953
Li	-0.4951502773	-0.0657836891	0.4909103092
C	-0.9538156487	-0.0867557432	2.5254367137
H	-0.0674212056	0.1522509222	3.1470012852
H	-1.3010965075	-1.0698827652	2.8982878443
H	-1.7282884279	0.6363966277	2.846721347
C	-2.9013069001	0.963241374	-0.4605592824
O	-2.1174775775	-0.2094702781	-0.7159032396
H	-2.3251291869	1.8131504543	-0.8274109472
H	-3.0813990389	1.0711654262	0.6147384308
H	-3.8531502966	0.9055563843	-1.0037564451
C	-2.8224335104	-1.3833830711	-0.2866917172
H	-3.0067283136	-1.3390059719	0.7919361415
H	-2.1826397014	-2.2356921825	-0.5167209376
H	-3.7674540466	-1.4749456805	-0.8370371809

Tabelle 10.382 Standardorientierung von (MeLi-OMe<sub>2</sub>)<sub>4</sub> (S<sub>4</sub>) [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
Li	1.1129211169	-0.543207795	0.8623042958
Li	-1.1129211169	0.543207795	0.8623042958
Li	-0.543207795	-1.1129211169	-0.8623042958
Li	0.543207795	1.1129211169	-0.8623042958
C	1.6602456721	-0.7292820245	-1.2895357427
C	0.7292820245	1.6602456721	1.2895357427
C	-1.6602456721	0.7292820245	-1.2895357427
C	-0.7292820245	-1.6602456721	1.2895357427
H	2.3811039026	0.0445481439	-1.6198389801
H	1.3338016061	-1.2004510933	-2.2352654635
H	2.302109535	-1.5001010678	-0.8223358867
H	-0.0445481439	2.3811039026	1.6198389801
H	1.5001010678	2.302109535	0.8223358867
H	1.2004510933	1.3338016061	2.2352654635
H	-2.3811039026	-0.0445481439	-1.6198389801
H	-1.3338016061	1.2004510933	-2.2352654635
H	-2.302109535	1.5001010678	-0.8223358867
H	-1.2004510933	-1.3338016061	2.2352654635
H	0.0445481439	-2.3811039026	1.6198389801
H	-1.5001010678	-2.302109535	0.8223358867
O	-1.0128122382	-2.6535239632	-1.9933150761
O	-2.6535239632	1.0128122382	1.9933150761
O	2.6535239632	-1.0128122382	1.9933150761
O	1.0128122382	2.6535239632	-1.9933150761
C	-3.8389071567	0.2785985318	1.7019502366
H	-3.7650849335	-0.7422725488	2.0962404813
H	-4.7113798071	0.7808610943	2.1380014406
H	-3.9356680656	0.2475888712	0.6163686858
C	-2.4360387977	1.1191215021	3.3945822167
H	-3.2612118278	1.6670253605	3.8664207675
H	-2.3525993447	0.1239660588	3.8495846672
H	-1.5031491429	1.6665284685	3.5339810538
C	0.2785985318	3.8389071567	-1.7019502366
H	0.7808610943	4.7113798071	-2.1380014406
H	-0.7422725488	3.7650849335	-2.0962404813
H	0.2475888712	3.9356680656	-0.6163686858
C	1.1191215021	2.4360387977	-3.3945822167
H	0.1239660588	2.3525993447	-3.8495846672
H	1.6670253605	3.2612118278	-3.8664207675
H	1.6665284685	1.5031491429	-3.5339810538
C	-0.2785985318	-3.8389071567	-1.7019502366
H	-0.2475888712	-3.9356680656	-0.6163686858
H	-0.7808610943	-4.7113798071	-2.1380014406
H	0.7422725488	-3.7650849335	-2.0962404813
C	-1.1191215021	-2.4360387977	-3.3945822167
H	-0.1239660588	-2.3525993447	-3.8495846672
H	-1.6670253605	-3.2612118278	-3.8664207675
H	-1.6665284685	-1.5031491429	-3.5339810538
C	3.8389071567	-0.2785985318	1.7019502366

H	3.7650849335	0.7422725488	2.0962404813
H	4.7113798071	-0.7808610943	2.1380014406
H	3.9356680656	-0.2475888712	0.6163686858
C	2.4360387977	-1.1191215021	3.3945822167
H	3.2612118278	-1.6670253605	3.8664207675
H	2.3525993447	-0.1239660588	3.8495846672
H	1.5031491429	-1.6665284685	3.5339810538

Tabelle 10.383 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
C	-0.0495498602	0.7625335381	-0.0785007224
C	0.0495498602	-0.7625335381	-0.0785007224
N	-1.4100087988	1.2255569166	-0.3400408812
N	1.4100087988	-1.2255569166	-0.3400408812
C	-1.4133340718	2.6738580094	-0.4999059486
C	-2.310998848	0.8478807653	0.7418848878
C	1.4133340718	-2.6738580094	-0.4999059486
C	2.310998848	-0.8478807653	0.7418848878
H	0.5959923879	1.1340986691	-0.8819636506
H	0.3216972088	1.1806996871	0.8784068617
H	-0.5959923879	-1.1340986691	-0.8819636506
H	-0.3216972088	-1.1806996871	0.8784068617
H	-2.4267586482	3.0130358479	-0.7326601406
H	-0.7540843119	2.9520905494	-1.3266062085
H	-1.0713969194	3.1975204477	0.4134668078
H	-2.3973606888	-0.2388198717	0.8075257329
H	-3.3054275028	1.2555447416	0.5397993713
H	-1.9672394409	1.2334943727	1.7217048905
H	2.4267586482	-3.0130358479	-0.7326601406
H	0.7540843119	-2.9520905494	-1.3266062085
H	1.0713969194	-3.1975204477	0.4134668078
H	3.3054275028	-1.2555447416	0.5397993713
H	1.9672394409	-1.2334943727	1.7217048905
H	2.3973606888	0.2388198717	0.8075257329

Tabelle 10.384 Standardorientierung von Me<sub>2</sub>O (C<sub>2v</sub>) [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
C	0.	1.1613170444	-0.198105269
O	0.	0.	0.603031874
C	0.	-1.1613170444	-0.198105269
H	-0.8929358065	1.2031965151	-0.8380779941
H	0.8929358065	1.2031965151	-0.8380779941
H	0.	2.019955258	0.4741128201
H	0.8929358065	-1.2031965151	-0.8380779941
H	-0.8929358065	-1.2031965151	-0.8380779941
H	0.	-2.019955258	0.4741128201

Tabelle 10.385 Standardorientierung von **4** (C<sub>2</sub>) [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
C	3.483145	1.432546	0.886821
N	2.333697	0.734063	1.475869
C	1.691614	1.57693	2.486847
C	2.751132	-0.525943	2.098097
C	3.868233	0.8274	-0.461077
N	2.751132	0.880684	-1.411131
C	2.581478	2.234231	-1.948724
C	2.981895	-0.054742	-2.515811
C	-3.483145	-1.432546	0.886821
N	-2.333697	-0.734063	1.475869
C	-2.751132	0.525943	2.098097
C	-1.691614	-1.57693	2.486847
C	-3.868233	-0.8274	-0.461077
N	-2.751132	-0.880684	-1.411131
C	-2.981895	0.054742	-2.515811
C	-2.581478	-2.234231	-1.948724
Li	1.07327	0.355897	-0.233668
Li	-1.07327	-0.355897	-0.233668
C	-0.580597	1.7599	-0.474394
C	0.580597	-1.7599	-0.474394
H	3.204944	2.482894	0.753263
H	4.356396	1.412627	1.565172
H	0.835941	1.041139	2.907441
H	1.324652	2.494826	2.022181
H	2.385687	1.832768	3.307279
H	1.8671	-1.063041	2.450474
H	3.432714	-0.344023	2.948332
H	3.253953	-1.164517	1.370085
H	4.759453	1.348115	-0.859
H	4.142505	-0.224407	-0.328602
H	1.737031	2.239565	-2.641096
H	2.351538	2.939787	-1.148013
H	3.490338	2.570269	-2.479269
H	2.134575	-0.008623	-3.204987
H	3.905685	0.18921	-3.069774
H	3.04911	-1.072682	-2.124958
H	-4.356396	-1.412627	1.565172
H	-3.204944	-2.482894	0.753263
H	-1.8671	1.063041	2.450474
H	-3.253953	1.164517	1.370085
H	-3.432714	0.344023	2.948332
H	-0.835941	-1.041139	2.907441
H	-2.385687	-1.832768	3.307279
H	-1.324652	-2.494826	2.022181
H	-4.142505	0.224407	-0.328602
H	-4.759453	-1.348115	-0.859
H	-2.134575	0.008623	-3.204987
H	-3.04911	1.072682	-2.124958
H	-3.905685	-0.18921	-3.069774

H	-1.737031	-2.239565	-2.641096
H	-3.490338	-2.570269	-2.479269
H	-2.351538	-2.939787	-1.148013
H	-0.529747	2.074041	-1.534438
H	-0.058658	2.562424	0.081748
H	-1.642955	1.907836	-0.198563
H	0.529747	-2.074041	-1.534438
H	0.058658	-2.562424	0.081748
H	1.642955	-1.907836	-0.198563

Tabelle 10.386 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
O	0.	0.	3.902603
C	0.048637	1.180537	4.694603
Li	0.	0.	1.980409
Li	0.	0.	-0.265239
C	0.	1.854372	0.9388
H	0.082679	2.02561	4.006879
H	0.944292	1.177842	5.327552
H	-0.843729	1.251419	5.328223
H	-0.142956	2.246082	-0.085874
H	0.908925	2.372763	1.296603
H	-0.833828	2.310237	1.50681
C	-0.686887	0.33375	-3.008905
N	-1.456667	-0.02997	-1.81251
C	-2.540145	0.932666	-1.590841
C	-2.029076	-1.374314	-1.943239
H	-0.568299	1.422192	-3.011766
H	-1.229816	0.064586	-3.933796
H	-3.09226	0.647814	-0.691391
H	-2.120562	1.929001	-1.433634
H	-3.240359	0.960791	-2.444005
H	-2.530049	-1.642165	-1.010144
H	-2.754412	-1.418544	-2.774756
H	-1.242852	-2.110594	-2.118803
C	-0.048637	-1.180537	4.694603
C	0.	-1.854372	0.9388
H	-0.082679	-2.02561	4.006879
H	-0.944292	-1.177842	5.327552
H	0.843729	-1.251419	5.328223
H	0.142956	-2.246082	-0.085874
H	-0.908925	-2.372763	1.296603
H	0.833828	-2.310237	1.50681
C	0.686887	-0.33375	-3.008905
N	1.456667	0.02997	-1.81251
C	2.540145	-0.932666	-1.590841
C	2.029076	1.374314	-1.943239
H	0.568299	-1.422192	-3.011766
H	1.229816	-0.064586	-3.933796
H	3.09226	-0.647814	-0.691391

H	2.120562	-1.929001	-1.433634
H	3.240359	-0.960791	-2.444005
H	2.530049	1.642165	-1.010144
H	2.754412	1.418544	-2.774756
H	1.242852	2.110594	-2.118803

Tabelle 10.387 Standardorientierung von **6** [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
N	-1.454247431	0.0926366303	0.042835902
C	-1.0331544101	-1.2061090383	-0.4977716869
C	0.3149547425	-1.6407576826	0.0765920905
N	1.3160867485	-0.5759530476	-0.0500425424
C	1.7786332418	-0.4435525543	-1.4374304888
C	2.4649192605	-0.839344267	0.8215533138
C	-2.5441052041	0.6522043173	-0.7638145165
C	-1.8965980175	-0.0348681845	1.436668273
H	-0.9605119269	-1.1047756003	-1.5851852466
H	-1.7863853787	-1.9891843752	-0.29601591
H	0.6436264956	-2.5684443615	-0.4260671105
H	0.2093695798	-1.8744226909	1.1407519304
H	2.5120000892	0.3642513817	-1.4912013029
H	0.9459787934	-0.1846089197	-2.0965651845
H	2.2384591526	-1.3793723966	-1.7984070674
H	3.1746503559	-0.0132815659	0.7354676777
H	2.9735583339	-1.7808537482	0.5533670872
H	2.1298832552	-0.9017111771	1.8603692174
H	-2.8198474587	1.6308477493	-0.3643079533
H	-3.4319598267	-0.0024406081	-0.7588535218
H	-2.205377606	0.7832477104	-1.7946894729
H	-2.2075340094	0.9464881229	1.8031950889
H	-1.0780991639	-0.3893239069	2.0684246473
H	-2.7426284986	-0.7371909797	1.5281205233
Li	0.3048605433	1.2596164453	0.1873111519
C	0.9363157798	3.1915440133	0.2470061392
H	1.4387154536	3.4989676148	-0.6870659071
H	1.6685048693	3.381762848	1.050794269
H	0.1303242366	3.9287682709	0.4026155999

Tabelle 10.388 Standardorientierung von **7** [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
N	0.6866133812	1.5729679163	-0.1122054955
C	1.9688823601	0.954351238	0.2533057678
C	2.1814728731	-0.3763569739	-0.4622926432
N	1.1404950861	-1.351686616	-0.1050301793
C	1.4774285669	-2.0197936611	1.160468634
C	1.0103291759	-2.3561453145	-1.1624556717
C	0.4042782709	2.6818924099	0.8079999759
C	0.7149839191	2.0729753535	-1.4877560691
H	1.9524713566	0.7921530295	1.336051365

H	2.8130323853	1.6328965011	0.0270079885
H	3.1869652446	-0.7659518649	-0.222844947
H	2.1511083181	-0.2242118306	-1.5455668559
H	0.6612039397	-2.6876195297	1.4444335541
H	1.5809432983	-1.2825607803	1.9572170132
H	2.4121607214	-2.599652171	1.061605369
H	0.2681105665	-3.1012394985	-0.8630166513
H	1.964184224	-2.8777451688	-1.354504466
H	0.6740667734	-1.8787156837	-2.0873298533
H	-0.5493681309	3.1425900588	0.5356148856
H	1.1935549278	3.4528582511	0.7644619971
H	0.3175958194	2.2889896909	1.822813332
H	-0.2254309354	2.5879155626	-1.7006607752
H	0.8142567259	1.250194768	-2.1990827622
H	1.5451949241	2.7843175366	-1.6455096021
Li	-0.511562557	-0.0910880311	0.4277487076
C	-1.0092454143	-0.0982837735	2.4482796668
H	-0.1381001332	0.1760602358	3.0783483333
H	-1.3295969657	-1.0822255362	2.8433843077
H	-1.8047958087	0.6043907352	2.7645389264
C	-2.921302686	0.8418234385	-0.5587355127
O	-2.0902953985	-0.2947309779	-0.7802436734
H	-2.3595039462	1.7190647624	-0.8823063796
H	-3.1640676485	0.9330034854	0.5060170567
H	-3.8406982473	0.759781831	-1.1522888868
C	-2.7733433596	-1.487228539	-0.3982930287
H	-3.0130029731	-1.4604308822	0.6704719966
H	-2.1009757829	-2.3217998087	-0.6013264069
H	-3.6885348711	-1.6042081631	-0.9924970173

### 10.2.1.5. Deprotonierung TMEDA

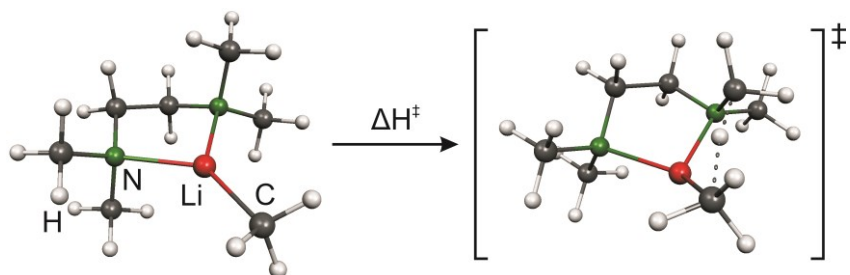


Abbildung 10.21 Deprotonierung von TMEDA mit Methyllithium.

Tabelle 10.389 Berechnete Energien der optimierten Strukturen für und Deprotonierung von TMEDA mit Methyllithium.

Verbindung	Methode	Basissatz	SCF	ZPE
TMEDA-MeLi	SVWN	6-31+G(d)	-393.0223356	-392.769742
<b>TS1</b>	SVWN	6-31+G(d)	-392.9976718	-392.748928

TMEDA·MeLi	PBE	6-31+G(d)	-394.62923	-394.376468
<b>TS1</b>	PBE	6-31+G(d)	-394.5937492	-394.345363
TMEDA·MeLi	TPSS	6-31+G(d)	-395.2621713	-395.005959
<b>TS1</b>	TPSS	6-31+G(d)	-395.2212299	-394.969508
TMEDA·MeLi	PBE0	6-31+G(d)	-394.696755	-394.435451
<b>TS1</b>	PBE0	6-31+G(d)	-394.6554585	-394.398379
TMEDA·MeLi	TPSSh	6-31+G(d)	-395.2264676	-394.967107
<b>TS1</b>	TPSSh	6-31+G(d)	-395.1835623	-394.928644
TMEDA·MeLi	B3LYP	6-31+G(d)	-395.2101185	-394.950552
<b>TS1</b>	B3LYP	6-31+G(d)	-395.1648817	-394.909765
TMEDA·MeLi	B3LYP	6-311+G(d,p)	-395.3122067	-395.055145
<b>TS1</b>	B3LYP	6-311+G(d,p)	-395.2694133	-395.016421
TMEDA·MeLi	M052X	6-31+G(d)	-395.1253805	-394.860863
<b>TS1</b>	M052X	6-31+G(d)	-395.0801496	-394.819924
TMEDA·MeLi	M052X	6-31+G(d,p)	-395.1510374	-394.88795
<b>TS1</b>	M052X	6-31+G(d,p)	-395.1072943	-394.848362
TMEDA·MeLi	M052X	6-311+G(d,p)	-395.2296964	-394.96735
<b>TS1</b>	M052X	6-311+G(d,p)	-395.1867874	-394.92855
TMEDA·MeLi	M052X	6-311+G(3df,3pd)	-395.2633756	-395.000877
<b>TS1</b>	M052X	6-311+G(3df,3pd)	-395.2202056	-394.961724
TMEDA·MeLi	M06L	6-31+G(d)	-395.1229029	-394.863679
<b>TS1</b>	M06L	6-31+G(d)	-395.0811062	-394.826234
TMEDA·MeLi	M06	6-31+G(d)	-394.8963072	-394.638507
<b>TS1</b>	M06	6-31+G(d)	-394.852008	-394.598648
TMEDA·MeLi	M06	6-31+G(d,p)	-394.9194762	-394.662898
<b>TS1</b>	M06	6-31+G(d,p)	-394.8760287	-394.623946
TMEDA·MeLi	M06	6-311+G(d,p)	-394.9948823	-394.73913
<b>TS1</b>	M06	6-311+G(d,p)	-394.9523784	-394.700896
TMEDA·MeLi	M062X	6-31+G(d)	-394.9963779	-394.734126
<b>TS1</b>	M062X	6-31+G(d)	-394.9533364	-394.695129
TMEDA·MeLi	M062X	6-31+G(d,p)	-395.0162823	-394.755342
<b>TS1</b>	M062X	6-31+G(d,p)	-394.9745655	-394.71767
TMEDA·MeLi	M062X	6-311+G(d,p)	-395.1025898	-394.841435
<b>TS1</b>	M062X	6-311+G(d,p)	-395.0606502	-394.804202
TMEDA·MeLi	MP2	6-31+G(d)	-393.740638	-393.476352
<b>TS1</b>	MP2	6-31+G(d)	-393.6913616	-393.431508
TMEDA·MeLi	MP2	6-311+G(d,p)	-394.0226722	-393.761348
<b>TS1</b>	MP2	6-311+G(d,p)	-393.9791591	-393.722169

Tabelle 10.390 Standardorientierung von TMEDA·MeLi [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
Li	-0.0361821459	1.2490017401	0.0679905462
C	0.7584418113	3.0771558487	0.0123214361
N	1.2540294471	-0.3115952372	0.0990551445
N	-1.5192272741	-0.1906090527	-0.0950334878
C	0.5112956905	-1.5498622934	0.1575550728
C	-0.8347793989	-1.4003978626	-0.5191027997
H	1.8120438371	3.0586264863	0.3778532007
H	0.8070883514	3.4993758131	-1.0156469409
H	0.2517228039	3.8517780693	0.6256875283
H	0.3725764678	-1.8114487367	1.2242725821

H	1.0683648555	-2.4015131322	-0.304666291
H	-0.7100522328	-1.3429545724	-1.6177425292
H	-1.4583718906	-2.3061730849	-0.3160679855
C	-2.7036361723	0.0341383792	-0.8906833318
H	-3.4495637666	-0.7871288621	-0.7663479963
H	-3.1775655276	0.9860388865	-0.5966224621
H	-2.4318253407	0.1018294225	-1.958352524
C	-1.8526794758	-0.2340598904	1.3126465769
H	-2.3994009586	0.6831643981	1.5916541937
H	-2.4901279958	-1.1168228797	1.5616894583
H	-0.9370493839	-0.2810614071	1.9302770171
C	1.7501904694	-0.0179159583	-1.2278416004
H	0.9283865555	-0.036531367	-1.9665800752
H	2.1700359338	1.0046385258	-1.2329700012
H	2.527663722	-0.7528955844	-1.5484652732
C	2.325419794	-0.2439443672	1.0614132918
H	3.1321623403	-0.9854479243	0.8465000459
H	2.7565435958	0.772749601	1.043242733
H	1.9352378881	-0.433089958	2.077336471

Tabelle 10.391 Standardorientierung von TS1 [Übergangszustand; SVWN/6-31+G(d)].

	x	y	z
Li	0.1012583743	0.9224603963	0.7693759252
C	-0.0585675166	2.9647019991	0.2899765743
N	1.4834754754	-0.3635619608	0.1607387095
N	-1.3940713272	-0.2523977303	0.1337132231
C	0.7043402498	-1.3710586623	-0.5246243699
C	-0.6436643327	-0.8502115651	-0.9622222772
C	-2.5389067208	0.4689793213	-0.3754199864
C	-1.8056714216	-1.2466174008	1.0995523818
C	1.6516840473	0.8300511139	-0.6824633414
C	2.7218773577	-0.9445244701	0.6212098847
H	0.7148338392	1.9285792739	-0.3480718147
H	0.3564986086	3.3919902974	1.2268294778
H	0.1260304513	3.7193520409	-0.4964700942
H	-1.1629088304	2.9091355542	0.4068969628
H	0.5967081481	-2.2524879016	0.1389282515
H	1.2479724744	-1.719580565	-1.4419536622
H	-0.4910064675	-0.0602765051	-1.7213706631
H	-1.2295859209	-1.674931191	-1.4374276602
H	-3.2435901166	-0.2059659859	-0.9167645697
H	-3.0840927122	0.9461566192	0.457835894
H	-2.2011624918	1.2634998385	-1.06330694
H	-2.3700556261	-0.7636405482	1.9161867123
H	-2.460245819	-2.0229852686	0.6350595168
H	-0.9252604905	-1.7483347451	1.5375540639
H	2.5747612313	1.3459302919	-0.3542149443
H	1.7842908036	0.5426334998	-1.754132737
H	3.3472544743	-1.2941865179	-0.2362424089
H	3.3021028603	-0.1937289207	1.1824824126

H	2.5215673984	-1.804010308	1.2920904789
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Tabelle 10.392 Standardorientierung von TMEDA-MeLi [globales Minimum; PBE/6-31+G(d)].

	x	y	z
Li	0.1231293089	1.2829943294	0.0794798234
C	0.3219014692	3.2996179477	0.2096459132
N	1.4242690215	-0.4050152096	-0.0321489154
N	-1.4676030517	-0.1372430829	-0.0169282534
C	0.5613110979	-1.5788829944	0.2045203833
C	-0.8316071706	-1.4063228067	-0.4213309256
H	1.0824109786	3.6231526664	0.9565854006
H	0.6333879137	3.7730484653	-0.7496249303
H	-0.616403379	3.8243516119	0.5017320404
H	0.4677769844	-1.707014698	1.2975025603
H	1.0223291882	-2.5168132492	-0.184754854
H	-0.7495746861	-1.4001455481	-1.5227154221
H	-1.4618353637	-2.2876577303	-0.1568844576
C	-2.5655268419	0.2285743461	-0.9248401683
H	-3.3951465857	-0.5147173168	-0.9051069642
H	-2.9633514985	1.2138539237	-0.6326580292
H	-2.1855103286	0.3069607163	-1.9570696161
C	-1.9581806889	-0.1814243543	1.3703364767
H	-2.3706082104	0.804656135	1.6390787074
H	-2.749656725	-0.9537472401	1.5083503071
H	-1.1330532927	-0.4006189677	2.0677328531
C	1.9191326248	-0.3520642211	-1.417561751
H	1.0783155942	-0.3231295467	-2.1298768219
H	2.5069910271	0.5698680771	-1.5559896088
H	2.5597108445	-1.2297183745	-1.6652902491
C	2.5568188643	-0.3698463256	0.9057069414
H	3.2376724168	-1.2424764841	0.7787259035
H	3.1314119572	0.5564931895	0.7438893967
H	2.1822305315	-0.3616882584	1.9428662599

Tabelle 10.393 Standardorientierung von TS1 [Übergangszustand; PBE/6-31+G(d)].

	x	y	z
Li	0.0629669998	0.9615972593	0.7196676771
C	0.0855365406	3.0836443835	0.3713398237
N	1.4864602817	-0.3401777821	0.1307097943
N	-1.4591893851	-0.2990498087	0.1161901769
C	0.7148283055	-1.3892082272	-0.5495284833
C	-0.6826822048	-0.9256384561	-0.982354314
C	-2.6471682413	0.3818979127	-0.4250388103
C	-1.8605853676	-1.2874332319	1.1304946163
C	1.663352277	0.8720226235	-0.741418213
C	2.7455152523	-0.9027604205	0.6352051332
H	0.7959194739	2.0142249404	-0.3198669377

H	0.3864681295	3.3648738108	1.4046562432
H	0.4672543901	3.8902102736	-0.2826292547
H	-1.0239715005	3.1456796881	0.3172787802
H	0.6422639129	-2.2614832226	0.1273412071
H	1.2457649261	-1.7375873863	-1.4703746747
H	-0.5815847865	-0.1677732265	-1.7780084887
H	-1.2350803532	-1.7929818444	-1.4131074415
H	-3.3342000786	-0.3252073391	-0.9424194376
H	-3.1999370159	0.8683416945	0.3961342882
H	-2.3331173491	1.1601701726	-1.1392370679
H	-2.4290315725	-0.7824119891	1.9295576182
H	-2.5011816899	-2.0896405268	0.6978977372
H	-0.9712943517	-1.7546701612	1.582840991
H	2.6305345978	1.3352590392	-0.4692420137
H	1.7237050321	0.5795751638	-1.815885095
H	3.3958682077	-1.2702129591	-0.1926027258
H	3.2979924301	-0.1253552047	1.1867275489
H	2.5404591398	-1.7409351756	1.3294163223

Tabelle 10.394 Standardorientierung von TMEDA-MeLi [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
Li	0.0361389245	1.3040625649	0.0175542241
C	0.1034351536	3.3400860858	0.0555272345
N	1.4428380387	-0.3038761676	-0.0105476932
N	-1.4589945069	-0.2255868276	-0.0031827517
C	0.6567594959	-1.5227143316	0.2937937972
C	-0.7393399103	-1.473188274	-0.3517023876
H	0.409569325	3.755454617	1.0397096064
H	0.8190409941	3.77620051	-0.6743500665
H	-0.8690116057	3.8270574853	-0.1720543842
H	0.5615943869	-1.5871064963	1.385966658
H	1.180335518	-2.441157753	-0.03805221
H	-0.6466893311	-1.5031207676	-1.4456043903
H	-1.3121764839	-2.3733998687	-0.0527135876
C	-2.5703941039	0.0301687201	-0.9433754033
H	-3.3399428127	-0.7648694007	-0.9038493186
H	-3.0339408832	0.9905803154	-0.6913564571
H	-2.1767139519	0.0934684255	-1.9650489031
C	-1.9781506446	-0.2582305904	1.3810016736
H	-2.4566211811	0.7025540543	1.602268642
H	-2.7151174788	-1.0723656351	1.5242492075
H	-1.1558537894	-0.4009679837	2.091933204
C	1.9664495125	-0.3179870974	-1.393380764
H	1.1415171065	-0.3965354268	-2.1112391233
H	2.4933608532	0.6242384981	-1.5819291159
H	2.662381922	-1.1631132791	-1.5603368632
C	2.5612735262	-0.1365033087	0.9411450937
H	3.2896527509	-0.9679444607	0.8777202631

H	3.0741664066	0.8068822242	0.7225006218
H	2.166384769	-0.0867678317	1.9630991937

Tabelle 10.395 Standardorientierung von **TS1** [Übergangszustand; TPSS/6-31+G(d)].

	x	y	z
Li	0.069377701	0.9625507797	0.7248829028
C	0.081657519	3.0968233698	0.3775790426
N	1.4769145748	-0.3439368658	0.1357922359
N	-1.4509492885	-0.2935181847	0.1140094877
C	0.7142195809	-1.3992370018	-0.555496531
C	-0.6820367689	-0.9287150993	-0.9928590497
C	-2.6494110729	0.3822884922	-0.4290296725
C	-1.8529332939	-1.2871633809	1.1323191199
C	1.6621350133	0.8726021104	-0.7506094607
C	2.7430583918	-0.9045376551	0.6422730119
H	0.793431534	2.0158915504	-0.3233759722
H	0.3910392988	3.3720064803	1.4060166629
H	0.4546482575	3.9028472402	-0.2744804785
H	-1.0245857049	3.1572577543	0.336815573
H	0.6369416407	-2.2654888804	0.1186563136
H	1.249756305	-1.7393372774	-1.4673854082
H	-0.578905474	-0.1730222423	-1.7814653521
H	-1.2403780035	-1.787831777	-1.4144508362
H	-3.3284713643	-0.3295694227	-0.9357231161
H	-3.1942269139	0.8662619236	0.3908114291
H	-2.3372040482	1.1514090634	-1.1443646218
H	-2.4209705986	-0.781043888	1.9227983331
H	-2.4854296157	-2.0855591717	0.6985493987
H	-0.9638117552	-1.7446340736	1.5806829811
H	2.6343383247	1.3158045886	-0.4837433828
H	1.7171322585	0.5645426995	-1.8150659362
H	3.3896409777	-1.2659180345	-0.1815272129
H	3.2843322904	-0.1261479742	1.1920145884
H	2.5365562345	-1.7396551232	1.33012095

Tabelle 10.396 Standardorientierung von (MeLi-OMe)<sub>2</sub> (S<sub>4</sub>) [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
Li	0.4816638861	1.1472361036	0.8667024818
Li	-0.4816638861	-1.1472361036	0.8667024818
Li	1.1472361036	-0.4816638861	-0.8668739292
Li	-1.1472361036	0.4816638861	-0.8668739292
C	0.6593143946	1.7067084302	-1.3024814091
C	-1.7067084302	0.6593143946	1.3023099617
C	-0.6593143946	-1.7067084302	-1.3024814091
C	1.7067084302	-0.6593143946	1.3023099617
H	-0.1039662749	2.4912972247	-1.5084024868
H	0.9992081996	1.4061683883	-2.318801363

H	1.5235227698	2.2849492774	-0.9066524506
H	-2.4912972247	-0.1039662749	1.5082310395
H	-2.2849492774	1.5235227698	0.9064810033
H	-1.4061683883	0.9992081996	2.3186299156
H	0.1039662749	-2.4912972247	-1.5084024868
H	-0.9992081996	-1.4061683883	-2.318801363
H	-1.5235227698	-2.2849492774	-0.9066524506
H	1.4061683883	-0.9992081996	2.3186299156
H	2.4912972247	0.1039662749	1.5082310395
H	2.2849492774	-1.5235227698	0.9064810033
O	2.7325208763	-0.992116119	-2.0258286059
O	-0.992116119	-2.7325208763	2.0256571586
O	0.992116119	2.7325208763	2.0256571586
O	-2.7325208763	0.992116119	-2.0258286059
C	-0.3599359644	-3.9901337937	1.7411521161
H	0.6300682949	-4.0417425974	2.2207529048
H	-0.99042454	-4.8196679514	2.0987555449
H	-0.2525565535	-4.0448448246	0.6543753526
C	-1.2150557926	-2.5388673086	3.4293547374
H	-1.8740911875	-3.3299254696	3.8212640482
H	-0.2600190702	-2.5481802375	3.9786263959
H	-1.6986948072	-1.5637496407	3.5365682776
C	-3.9901337937	0.3599359644	-1.7413235635
H	-4.8196679514	0.99042454	-2.0989269923
H	-4.0417425974	-0.6300682949	-2.2209243522
H	-4.0448448246	0.2525565535	-0.6545467999
C	-2.5388673086	1.2150557926	-3.4295261847
H	-2.5481802375	0.2600190702	-3.9787978432
H	-3.3299254696	1.8740911875	-3.8214354956
H	-1.5637496407	1.6986948072	-3.536739725
C	3.9901337937	-0.3599359644	-1.7413235635
H	4.0448448246	-0.2525565535	-0.6545467999
H	4.8196679514	-0.99042454	-2.0989269923
H	4.0417425974	0.6300682949	-2.2209243522
C	2.5388673086	-1.2150557926	-3.4295261847
H	2.5481802375	-0.2600190702	-3.9787978432
H	3.3299254696	-1.8740911875	-3.8214354956
H	1.5637496407	-1.6986948072	-3.536739725
C	0.3599359644	3.9901337937	1.7411521161
H	-0.6300682949	4.0417425974	2.2207529048
H	0.99042454	4.8196679514	2.0987555449
H	0.2525565535	4.0448448246	0.6543753526
C	1.2150557926	2.5388673086	3.4293547374
H	1.8740911875	3.3299254696	3.8212640482
H	0.2600190702	2.5481802375	3.9786263959
H	1.6986948072	1.5637496407	3.5365682776

Tabelle 10.397 Standardorientierung von TMEDA (C<sub>2</sub>) [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
C	-0.0579448493	0.7675113304	-0.0973279224

C	0.0579448493	-0.7675113304	-0.0973279224
N	-1.4468062545	1.2220380957	-0.2904357399
N	1.4468062545	-1.2220380957	-0.2904357399
C	-1.4779576225	2.6558966699	-0.5995380593
C	-2.2918717378	0.9376734076	0.8756760354
C	1.4779576225	-2.6558966699	-0.5995380593
C	2.2918717378	-0.9376734076	0.8756760354
H	0.5364633373	1.1432115796	-0.9410107323
H	0.3698972548	1.2000121078	0.8332909059
H	-0.5364633373	-1.1432115796	-0.9410107323
H	-0.3698972548	-1.2000121078	0.8332909059
H	-2.514962919	2.9624390508	-0.7894209046
H	-0.8869580934	2.8476095651	-1.5042348454
H	-1.0740978841	3.2845213547	0.224098943
H	-2.3389372722	-0.1425213988	1.0555222306
H	-3.3101323547	1.2953013433	0.6755790902
H	-1.9220717299	1.4324245374	1.8009119988
H	2.514962919	-2.9624390508	-0.7894209046
H	0.8869580934	-2.8476095651	-1.5042348454
H	1.0740978841	-3.2845213547	0.224098943
H	3.3101323547	-1.2953013433	0.6755790902
H	1.9220717299	-1.4324245374	1.8009119988
H	2.3389372722	0.1425213988	1.0555222306

Tabelle 10.398 Standardorientierung von Me<sub>2</sub>O (C<sub>2v</sub>) [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
C	0.	1.1806980297	-0.2022303093
O	0.	0.	0.5958736864
C	0.	-1.1806980297	-0.2022303093
H	-0.8985220656	1.2296023147	-0.8428385824
H	0.8985220656	1.2296023147	-0.8428385824
H	0.	2.0276783035	0.4913381309
H	0.8985220656	-1.2296023147	-0.8428385824
H	-0.8985220656	-1.2296023147	-0.8428385824
H	0.	-2.0276783035	0.4913381309

Tabelle 10.399 Standardorientierung von 4 (C<sub>2</sub>) [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
C	0.0650168993	3.9428756419	0.7971803093
N	0.2856756622	2.6653431829	1.5121311397
C	-0.7469653715	2.4633400299	2.5459664504
C	1.621536986	2.6187294513	2.1373165197
C	0.8023958392	3.9805228882	-0.5498744583
N	0.3619397013	2.8925855793	-1.4520599215
C	-0.9428567435	3.199073959	-2.0714327701
C	1.3671085741	2.6505084583	-2.5055185857
C	-0.0650168993	-3.9428756419	0.7971803093
N	-0.2856756622	-2.6653431829	1.5121311397
C	-1.621536986	-2.6187294513	2.1373165197

C	0.7469653715	-2.4633400299	2.5459664504
C	-0.8023958392	-3.9805228882	-0.5498744583
N	-0.3619397013	-2.8925855793	-1.4520599215
C	-1.3671085741	-2.6505084583	-2.5055185857
C	0.9428567435	-3.199073959	-2.0714327701
Li	0.1400789018	1.1554435418	-0.1279863673
Li	-0.1400789018	-1.1554435418	-0.1279863673
C	-1.8549212549	0.2256914634	-0.2992478915
C	1.8549212549	-0.2256914634	-0.2992478915
H	-1.0157026741	4.044441736	0.6319254992
H	0.381584991	4.8109582294	1.4115963647
H	-0.5757600514	1.4970881072	3.0354682224
H	-1.736174075	2.4399687395	2.0757147207
H	-0.7260283076	3.2600728417	3.3169393754
H	1.7629462642	1.6365176709	2.6018841427
H	1.7396786986	3.4070547153	2.9086033763
H	2.4021292038	2.7436072388	1.3797476452
H	0.6586726411	4.9764610813	-1.0170090794
H	1.8810616348	3.8567202094	-0.3867895772
H	-1.2480240913	2.3524841691	-2.695704263
H	-1.708226599	3.3342563877	-1.3000592232
H	-0.8929021953	4.1138879363	-2.6963262535
H	1.0240077143	1.8257131227	-3.1408559903
H	1.5287718621	3.5454185759	-3.1396571407
H	2.3161862013	2.3555838553	-2.0439727391
H	-0.381584991	-4.8109582294	1.4115963647
H	1.0157026741	-4.044441736	0.6319254992
H	-1.7629462642	-1.6365176709	2.6018841427
H	-2.4021292038	-2.7436072388	1.3797476452
H	-1.7396786986	-3.4070547153	2.9086033763
H	0.5757600514	-1.4970881072	3.0354682224
H	0.7260283076	-3.2600728417	3.3169393754
H	1.736174075	-2.4399687395	2.0757147207
H	-1.8810616348	-3.8567202094	-0.3867895772
H	-0.6586726411	-4.9764610813	-1.0170090794
H	-1.0240077143	-1.8257131227	-3.1408559903
H	-2.3161862013	-2.3555838553	-2.0439727391
H	-1.5287718621	-3.5454185759	-3.1396571407
H	1.2480240913	-2.3524841691	-2.695704263
H	0.8929021953	-4.1138879363	-2.6963262535
H	1.708226599	-3.3342563877	-1.3000592232
H	-2.1705472318	0.2786868123	-1.3656886419
H	-2.2899030199	1.1449783209	0.1553183701
H	-2.4894114509	-0.5830134647	0.1289537659
H	2.1705472318	-0.2786868123	-1.3656886419
H	2.2899030199	-1.1449783209	0.1553183701
H	2.4894114509	0.5830134647	0.1289537659

Tabelle 10.400 Standardorientierung von **5** (C<sub>2</sub>) [globales Minimum; TPSS/6-31+G(d)].

x	y	z
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O	0.	0.	3.9679336551
C	0.0227840192	1.1974860816	4.7594352142
Li	0.	0.	2.0112214036
Li	0.	0.	-0.2666248317
C	0.0060939161	1.8655934625	0.9778515825
H	0.0382839559	2.0344987053	4.0560392447
H	0.9232385486	1.2189128605	5.3932085705
H	-0.8759388106	1.2529694616	5.3935985693
H	-0.0435379837	2.3167811857	-0.0385136876
H	0.9018539243	2.3503809983	1.4279786732
H	-0.8598466569	2.3310640387	1.5019143109
C	-0.6794256007	0.3592708215	-3.0577359708
N	-1.4826296536	0.0189464215	-1.8602123019
C	-2.5311420452	1.0319441391	-1.6251227006
C	-2.1048208993	-1.3148232622	-1.9842238866
H	-0.5248427081	1.4463593551	-3.0517342268
H	-1.2227843358	0.115224337	-3.9932454572
H	-3.0845544363	0.7656823509	-0.717068919
H	-2.0654930555	2.0114351298	-1.4690749451
H	-3.243996465	1.0954380861	-2.4713326179
H	-2.6274346526	-1.551733749	-1.0509910181
H	-2.8251097224	-1.351732255	-2.8261241958
H	-1.3372663827	-2.0801351552	-2.1400478019
C	-0.0227840192	-1.1974860816	4.7594352142
C	-0.0060939161	-1.8655934625	0.9778515825
H	-0.0382839559	-2.0344987053	4.0560392447
H	-0.9232385486	-1.2189128605	5.3932085705
H	0.8759388106	-1.2529694616	5.3935985693
H	0.0435379837	-2.3167811857	-0.0385136876
H	-0.9018539243	-2.3503809983	1.4279786732
H	0.8598466569	-2.3310640387	1.5019143109
C	0.6794256007	-0.3592708215	-3.0577359708
N	1.4826296536	-0.0189464215	-1.8602123019
C	2.5311420452	-1.0319441391	-1.6251227006
C	2.1048208993	1.3148232622	-1.9842238866
H	0.5248427081	-1.4463593551	-3.0517342268
H	1.2227843358	-0.115224337	-3.9932454572
H	3.0845544363	-0.7656823509	-0.717068919
H	2.0654930555	-2.0114351298	-1.4690749451
H	3.243996465	-1.0954380861	-2.4713326179
H	2.6274346526	1.551733749	-1.0509910181
H	2.8251097224	1.351732255	-2.8261241958
H	1.3372663827	2.0801351552	-2.1400478019

Tabelle 10.401 Standardorientierung von **6** [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
N	-1.4569821193	0.0939186123	0.0462945257
C	-1.0359449194	-1.2290412344	-0.4732027156
C	0.3285033176	-1.6531287814	0.0969501675
N	1.3583380249	-0.609312048	-0.119603459

C	1.8385128528	-0.5927809404	-1.5182439782
C	2.5049426633	-0.7906823388	0.7950654661
C	-2.494247342	0.7012299846	-0.813818511
C	-1.9554861615	0.0050318419	1.4356386732
H	-0.9744563402	-1.1470457278	-1.5665878207
H	-1.7857876464	-2.0138922158	-0.2509656389
H	0.6269810093	-2.6221094089	-0.3498577439
H	0.2469890905	-1.8130528021	1.1803676009
H	2.5503600009	0.2317510924	-1.6385563644
H	1.0016036791	-0.423568985	-2.2060031335
H	2.3346730885	-1.5441511095	-1.7924464202
H	3.2104341077	0.0345194311	0.6462846752
H	3.0286595766	-1.7504958618	0.6207374675
H	2.1521562865	-0.7614796656	1.8330977285
H	-2.730806983	1.7005012388	-0.4313206655
H	-3.4203645814	0.0949926124	-0.8400290486
H	-2.1073588328	0.8045127901	-1.8347714933
H	-2.1967020283	1.0134244288	1.7907235253
H	-1.1821414596	-0.4118109544	2.0916082441
H	-2.859515383	-0.6306583296	1.5069075663
Li	0.3374958462	1.2459629291	0.1468961938
C	0.8429356019	3.2098501397	0.3551746356
H	0.7921003484	3.7825696757	-0.5958821935
H	1.8753981956	3.3711295255	0.7328670867
H	0.190102107	3.7679561011	1.06033063

Tabelle 10.402 Standardorientierung von **7** [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
N	0.758188167	1.6105463138	-0.1301310977
C	2.0427320822	0.9598736881	0.2254531506
C	2.2352746206	-0.3829587706	-0.4936817044
N	1.1916182318	-1.3681196928	-0.119296627
C	1.5131558283	-2.0155683645	1.1729524505
C	1.0552289394	-2.3963558086	-1.1677828164
C	0.4643865985	2.6944128224	0.8337462407
C	0.7862351472	2.1548788114	-1.5002386701
H	2.0295387364	0.8003537671	1.3115738488
H	2.9021320919	1.6234247962	-0.0033541259
H	3.2488339675	-0.7725187163	-0.2718913077
H	2.1834578372	-0.2361494708	-1.5806915721
H	0.7006325427	-2.6991477065	1.4414955213
H	1.5754523858	-1.2616851814	1.9630382965
H	2.4659375186	-2.5798873301	1.1133347558
H	0.2846979402	-3.1166463871	-0.8664960601
H	1.9994763994	-2.9509634861	-1.3382929176
H	0.746054127	-1.9245984533	-2.1089520092
H	-0.4852976904	3.1695254625	0.558913992
H	1.258530096	3.4675570753	0.8374354994
H	0.3539576192	2.2587708445	1.8323479798
H	-0.1764049186	2.6349504561	-1.7138084988

H	0.9335500981	1.3516672081	-2.2311000743
H	1.5900021926	2.9071613692	-1.6316113854
Li	-0.5214291369	-0.0731965056	0.4200226066
C	-1.0670026672	-0.092014592	2.4430716526
H	-0.237603815	0.1706019522	3.1420271464
H	-1.4145855336	-1.0858806666	2.8088406196
H	-1.8859046791	0.6077640039	2.7287555813
C	-3.0535931253	0.8247964234	-0.5679489181
O	-2.2137417529	-0.3195412732	-0.8056753348
H	-2.5194686462	1.693493246	-0.9653401437
H	-3.227422509	0.9523509175	0.510602629
H	-4.0109365341	0.7069779613	-1.1010478047
C	-2.8644896454	-1.5263129632	-0.3632563286
H	-3.0230099877	-1.4958671765	0.7242959308
H	-2.195710596	-2.3538592677	-0.6187355925
H	-3.8229639301	-1.651283306	-0.8927529126

Tabelle 10.403 Standardorientierung von TMEDA-MeLi [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
Li	0.1235272692	1.2664165477	0.0865430406
C	0.3170211435	3.276668761	0.1894340069
N	1.4126643741	-0.4063467566	-0.0144715468
N	-1.4540018287	-0.1377545965	-0.0226739655
C	0.5552333709	-1.5698359701	0.2067935048
C	-0.8224490098	-1.3935671104	-0.4255087323
H	1.2955067212	3.6082009805	0.5843725792
H	0.2149042085	3.7749179527	-0.7928607289
H	-0.4364352579	3.7598537084	0.8393605559
H	0.4517239514	-1.7050954446	1.2893733548
H	1.0159523653	-2.4974375852	-0.1808694777
H	-0.7305720509	-1.383676684	-1.5174904664
H	-1.4516567231	-2.2673133074	-0.1732240477
C	-2.5295999987	0.2383913459	-0.9320797977
H	-3.3541875299	-0.496839111	-0.9305157131
H	-2.927299916	1.2138072173	-0.6378522361
H	-2.1416000096	0.3269092243	-1.9515455367
C	-1.9530000177	-0.1877680034	1.3474700917
H	-2.3606733177	0.7901617259	1.6196441008
H	-2.7435433985	-0.9499907618	1.4706885012
H	-1.1436862859	-0.4155021261	2.0477309667
C	1.9132462562	-0.3438832975	-1.3836572192
H	1.0857741446	-0.3130097757	-2.0988610808
H	2.4964879101	0.5723422967	-1.5136594195
H	2.5522074467	-1.2115151557	-1.6287623663
C	2.5261623698	-0.372951648	0.9257757999
H	3.2018053189	-1.2385436191	0.8041661214
H	3.1002753881	0.5454409068	0.7736432171
H	2.1469551058	-0.367034714	1.9524084935

Tabelle 10.404 Standardorientierung von TS1 [Übergangszustand; PBE0/6-31+G(d)].

	x	y	z
Li	0.0587478727	0.9519569323	0.7187296764
C	0.0802547908	3.0630777423	0.3585093932
N	1.4722306516	-0.3425599989	0.1340203602
N	-1.4460337321	-0.2953910364	0.1128231655
C	0.7078957205	-1.3788328623	-0.5461827463
C	-0.6779600055	-0.9127026022	-0.9771853979
C	-2.6246092516	0.3812205913	-0.4191652439
C	-1.8386669837	-1.2747939234	1.120124679
C	1.648976438	0.863496406	-0.7268691947
C	2.720775004	-0.9009314154	0.6297910653
H	0.783455928	1.9998939374	-0.3177705955
H	0.3959007136	3.3494735181	1.377099073
H	0.4400116	3.8622836015	-0.3033821474
H	-1.0225673289	3.1142050443	0.3266560776
H	0.6302600859	-2.2481172768	0.1199691058
H	1.2370697405	-1.7219952154	-1.457910936
H	-0.5719982643	-0.1590801748	-1.7642408097
H	-1.2285511931	-1.7692352219	-1.4084187493
H	-3.3095226031	-0.3208750407	-0.9262568961
H	-3.1695932879	0.8685293876	0.3955465655
H	-2.3168865431	1.1511361642	-1.132444235
H	-2.407172051	-0.7772977145	1.9124942834
H	-2.4685448768	-2.0747956996	0.6918916516
H	-0.9549305021	-1.7331126207	1.572641013
H	2.6038990957	1.3283116234	-0.4459431856
H	1.7271679581	0.5729434237	-1.7915459603
H	3.3662342617	-1.2563859803	-0.1943192062
H	3.2690370275	-0.1350328569	1.1853094162
H	2.5209857349	-1.7404187319	1.3097747783

Tabelle 10.405 Standardorientierung von TMEDA-MeLi [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
Li	0.0967902479	1.2950092139	0.0348105285
C	0.2530747193	3.322135142	0.076770476
N	1.4252783587	-0.3696206111	0.0018766839
N	-1.4594347919	-0.161483938	-0.0150911427
C	0.5866636303	-1.5501786127	0.2831619703
C	-0.7971073023	-1.4311362339	-0.3688754363
H	0.9753624823	3.6981326579	0.8285451462
H	0.5879189392	3.7579748282	-0.8858605534
H	-0.6984122147	3.8408537186	0.3090574255
H	0.4803562921	-1.6258043462	1.3708536624
H	1.0699790667	-2.4842951917	-0.0562397725
H	-0.6982385933	-1.4571066778	-1.459599489
H	-1.4106153181	-2.3048251461	-0.0829621169
C	-2.5472172697	0.1530895132	-0.9549253711

H	-3.3510790878	-0.6034841027	-0.9271973036
H	-2.9674043793	1.1291355023	-0.6985104186
H	-2.1475554799	0.2073894615	-1.9719207337
C	-1.982575162	-0.179263642	1.3609665093
H	-2.4184015433	0.7974277503	1.5876347225
H	-2.7535211611	-0.9585311739	1.4962482718
H	-1.17349154	-0.3621740335	2.0738495112
C	1.9497307356	-0.3830839129	-1.3737729975
H	1.1275991822	-0.4094538284	-2.0946336098
H	2.5200171045	0.5337849921	-1.5451305016
H	2.6040720979	-1.2543999295	-1.5542281334
C	2.540388354	-0.2659385009	0.9564523815
H	3.2295577224	-1.1257396942	0.8846282572
H	3.0958827044	0.653826397	0.7552428471
H	2.145886206	-0.2131886013	1.9755611868

Tabelle 10.406 Standardorientierung von TS1 [Übergangszustand; TPSSh/6-31+G(d)].

	x	y	z
Li	0.0691851294	0.9577442819	0.7265820245
C	0.0778406855	3.0859014118	0.3688514115
N	1.4728106193	-0.3448960819	0.1365812685
N	-1.4460720406	-0.2928538788	0.1141152933
C	0.7116367743	-1.3934186093	-0.5533832473
C	-0.6800298941	-0.9222164013	-0.9886740238
C	-2.6385452012	0.3833925632	-0.4240158038
C	-1.845132093	-1.2827679768	1.1278323275
C	1.6566563724	0.8688350899	-0.742864825
C	2.7336915847	-0.9039775205	0.6386155547
H	0.7877058744	2.0088774699	-0.3227142014
H	0.3847218871	3.3630049641	1.3944948358
H	0.4484958832	3.8896946562	-0.2827357087
H	-1.0256713983	3.143129721	0.3275355662
H	0.6329368792	-2.2595014777	0.116343095
H	1.2454986182	-1.7320985018	-1.4630122529
H	-0.5753433234	-0.1674806416	-1.7742381156
H	-1.2368648367	-1.7776583718	-1.4122517674
H	-3.3177145314	-0.3244526424	-0.9298610313
H	-3.1815810008	0.8663813301	0.3940397287
H	-2.3280432704	1.1516261795	-1.1370184421
H	-2.4126748265	-0.7802668059	1.9173191634
H	-2.4752164341	-2.0795986605	0.6951726922
H	-0.9588573838	-1.7394958283	1.5761806443
H	2.6232751582	1.3151832553	-0.4715891568
H	1.7197963724	0.5636046621	-1.8046890378
H	3.3787785443	-1.2604286588	-0.1844989751
H	3.2746469307	-0.1307333049	1.1907208841
H	2.5299349209	-1.7405602226	1.3209070991

Tabelle 10.407 Standardorientierung von TMEDA-MeLi [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
N	-1.371221226	0.5531179299	0.0705440011
C	-0.3679028804	1.5969938852	0.345712512
C	0.9673696877	1.3184832759	-0.357802634
N	1.4831369105	-0.0300083523	-0.0618927277
C	2.0562020737	-0.1225942498	1.2889069182
C	2.4732759117	-0.461174197	-1.058450242
C	-2.4451461667	0.5553174767	1.0734127005
C	-1.9431889167	0.6728132695	-1.2786762262
H	-0.2145862312	1.6313281127	1.4296218881
H	-0.7298072908	2.5984603855	0.0479906321
H	1.693620809	2.1031457129	-0.0757742454
H	0.8361727851	1.3919456551	-1.4426972884
H	2.3688748369	-1.1534997114	1.4775532907
H	1.3109218207	0.1435974211	2.0439758716
H	2.9295733821	0.5433152264	1.4120729544
H	2.7782391077	-1.4888484375	-0.8424381785
H	3.3702546177	0.1839575197	-1.0604907062
H	2.026426423	-0.4435413792	-2.0572626278
H	-3.1271220938	-0.2756087218	0.8725006132
H	-3.0207192208	1.4984387892	1.0659342013
H	-2.021180791	0.4117394333	2.0720974029
H	-2.634327614	-0.1568915976	-1.4514168687
H	-1.1576858643	0.6156720959	-2.0377122504
H	-2.4875100092	1.6253963296	-1.4116975231
Li	-0.2552236876	-1.2608434203	0.0061181446
C	-0.6776858314	-3.2421750479	-0.0200872611
H	-1.1304384729	-3.6056521629	0.9223386825
H	0.2083434866	-3.884325021	-0.1859906831
H	-1.3943316755	-3.5238529078	-0.8156131168

Tabelle 10.408 Standardorientierung von TS1 [Übergangszustand; B3LYP/6-31+G(d)].

	x	y	z
Li	0.0691277702	0.9616245321	0.6629037696
C	0.2620623648	3.0853831465	0.4243533396
N	1.4594530592	-0.3684993261	0.1101368556
N	-1.4799648605	-0.2656287626	0.0936823434
C	0.6699436829	-1.4223693625	-0.534964877
C	-0.7218761779	-0.9535442344	-0.9777614639
C	-2.647796359	0.429567823	-0.4685834061
C	-1.9040832115	-1.1978102064	1.1487145117
C	1.6657405721	0.823028153	-0.7888431366
C	2.7002482865	-0.9307827849	0.6493698413
H	0.8884954302	2.0019158997	-0.312671244
H	0.5845315296	3.2945874895	1.4598989909
H	0.6877922199	3.8870456831	-0.1947791508
H	-0.8346699921	3.2167481124	0.3834766286
H	0.5822591039	-2.2632349017	0.1650329205
H	1.1866467826	-1.8083397608	-1.4363216946

H	-0.6168929042	-0.2430432141	-1.8027976555
H	-1.2878473878	-1.8227825232	-1.3595001652
H	-3.3534953893	-0.270939879	-0.948860729
H	-3.1763002314	0.9624578715	0.3281843843
H	-2.3183781407	1.1615363559	-1.2113893153
H	-2.4497876583	-0.6485906342	1.9227324065
H	-2.563892787	-1.9910416797	0.7540554975
H	-1.033711046	-1.6686730371	1.6131003521
H	2.6629594055	1.2283918264	-0.5746700682
H	1.6561205051	0.5147170822	-1.8500966156
H	3.3487429383	-1.3382090248	-0.1482163724
H	3.2558379661	-0.1492451671	1.1749450637
H	2.4742725288	-1.7323004766	1.366031989

Tabelle 10.409 Standardorientierung von TMEDA-MeLi [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
Li	0.0020745629	1.2873131266	-0.0430696102
C	0.0203177135	3.3173213625	-0.0648773522
N	-1.4620633872	-0.264704935	0.0413763805
N	1.4566612844	-0.2761871569	-0.0351509987
C	-0.7094031722	-1.4952628747	-0.2569367079
C	0.6970799649	-1.4774780988	0.3515859666
H	-0.932072671	3.7687101714	-0.3913096726
H	0.2259512756	3.7592958672	0.9253675592
H	0.7866651255	3.7433017844	-0.7350772203
H	-0.6389159657	-1.5844019136	-1.3436965658
H	-1.2421089427	-2.3939230045	0.0965310043
H	0.6265708043	-1.487682773	1.4419540404
H	1.2242152275	-2.4025695566	0.0641288641
C	2.573752422	-0.0222489146	0.8845633545
H	3.3204326053	-0.832628137	0.8660296821
H	3.0632623099	0.9127215119	0.6082318314
H	2.1984190696	0.0833572956	1.9043250084
C	1.9482146386	-0.3498798973	-1.4180627228
H	2.44829582	0.5856413094	-1.6731047539
H	2.6576269377	-1.1818174731	-1.5581515828
H	1.1200754793	-0.4837475628	-2.11611373
C	-1.950875559	-0.2332518071	1.4270609438
H	-1.1213761939	-0.3157448293	2.1313665672
H	-2.4479131719	0.7201783606	1.611971779
H	-2.6617095089	-1.0507488831	1.6306120526
C	-2.5802155855	-0.0745405972	-0.8921396001
H	-3.3300814907	-0.8782726728	-0.8127386452
H	-3.0656914804	0.8799841938	-0.6838776294
H	-2.2072951119	-0.0459368957	-1.9178982421

Tabelle 10.410 Standardorientierung von TS1 [Übergangszustand; B3LYP/6-311+G(d,p)].

	x	y	z
Li	0.0501552493	0.9763752585	0.6364296447
C	0.3202662622	3.0955288996	0.4912083802
N	1.4448057556	-0.3614473722	0.1027885381
N	-1.4916188587	-0.2750113955	0.0652557568
C	0.6673181935	-1.429920973	-0.5297408483
C	-0.7239726113	-0.9791582394	-0.9865649478
C	-2.6607362122	0.4004792946	-0.5160568148
C	-1.9122561262	-1.1853551953	1.1394706175
C	1.6425358873	0.825067579	-0.8038818734
C	2.6876772943	-0.9007854175	0.6565976272
H	0.9099015122	2.0102981971	-0.2823211789
H	0.7994699273	3.340667056	1.4501037673
H	0.6067210618	3.8858227161	-0.2115491954
H	-0.7692575732	3.2008231843	0.6310286737
H	0.5811118725	-2.2580264252	0.1817436444
H	1.1892474922	-1.8271085508	-1.419884688
H	-0.6191513573	-0.2867431018	-1.8235880624
H	-1.2793858052	-1.8577667664	-1.3545437833
H	-3.3638439566	-0.3122858061	-0.9754467869
H	-3.1902909743	0.9536845497	0.2623798849
H	-2.3354515154	1.1103081158	-1.2783554791
H	-2.4599738778	-0.6247699406	1.900167813
H	-2.5664884256	-1.988418345	0.7637564652
H	-1.0425681211	-1.6406596046	1.6146138552
H	2.6514728386	1.2126718617	-0.6323763157
H	1.5859441578	0.5204720701	-1.8608297255
H	3.3455966584	-1.3103164638	-0.128362503
H	3.2300882081	-0.1087443669	1.1746667191
H	2.4682210439	-1.6937118186	1.3804538152

Tabelle 10.411 Standardorientierung von TMEDA-MeLi [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	0.1070298568	1.2624643379	0.097896703
C	0.3629144372	3.273245896	0.1494756425
N	1.3777612151	-0.3936410911	0.0462512952
N	-1.4406382404	-0.1368922808	-0.0618858858
C	0.5479714138	-1.5884740755	0.2049714936
C	-0.8249697045	-1.4090128586	-0.4439506356
H	1.1837061068	3.582215238	0.8135496105
H	0.6005054788	3.6908951427	-0.8403905238
H	-0.5281719797	3.8158126026	0.498169912
H	0.4326215835	-1.7739805783	1.2745903673
H	1.0370299174	-2.4777972091	-0.223547967
H	-0.7265759159	-1.4167345464	-1.5311284377
H	-1.4674609766	-2.2622942784	-0.1740301346
C	-2.5695119086	0.1818592491	-0.9333174949

H	-3.3698221864	-0.5693114187	-0.8549248157
H	-2.9684628206	1.1578944357	-0.6583999462
H	-2.2300867809	0.2312885103	-1.9683149666
C	-1.8788665697	-0.1491386582	1.3344832373
H	-2.3319982533	0.812927586	1.5737743916
H	-2.6118737016	-0.948813539	1.520742944
H	-1.0276598249	-0.2917811929	2.0018205905
C	1.8393713598	-0.2362445638	-1.3340772358
H	0.9912910458	-0.122911683	-2.0109869299
H	2.4429449505	0.6684296615	-1.4056201726
H	2.4389619419	-1.1000322069	-1.6595763881
C	2.5241247621	-0.4225413089	0.9513954899
H	3.1923798966	-1.2699831932	0.736350376
H	3.0827020435	0.5074221299	0.8482667296
H	2.1755248538	-0.4998251068	1.9817847514

Tabelle 10.412 Standardorientierung von TS1 [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
Li	0.1209751568	0.9416480828	0.8364579785
C	-0.1093543054	2.9900193014	0.1225533907
N	1.4965609392	-0.3965729666	0.226565355
N	-1.39939425	-0.2234743448	0.167101143
C	0.7098055561	-1.317286671	-0.5894334112
C	-0.6437734764	-0.7359163266	-0.9876725778
C	-2.5883991387	0.4903678499	-0.3002006059
C	-1.7902576318	-1.3065893494	1.0686549566
C	1.7804284349	0.8575430376	-0.5363799119
C	2.7060129522	-1.0778019983	0.6781917757
H	0.7741607231	1.9448995735	-0.32196584
H	0.5609959155	3.8135349347	0.3884971815
H	-0.6295977634	3.2726857018	-0.7995620525
H	-0.8834769901	2.9505017161	0.9089024705
H	0.5759956858	-2.2504793414	-0.0356817663
H	1.253278539	-1.5657213389	-1.51707222
H	-0.4884598759	0.101373077	-1.670223419
H	-1.2271934213	-1.5068945658	-1.5161015803
H	-3.2614123061	-0.1759785523	-0.8596958968
H	-3.1286848169	0.8978236505	0.555160217
H	-2.2850244826	1.3171857731	-0.9412831751
H	-2.396748171	-0.8991266717	1.8784607661
H	-2.3783608968	-2.0737999421	0.5428122173
H	-0.9073713277	-1.7742940418	1.503426336
H	2.6510767138	1.3282413142	-0.0662149479
H	2.0503091945	0.6127684327	-1.5774158195
H	3.3331885795	-1.3769480289	-0.1755175563
H	3.2846490263	-0.4056471155	1.3106692381
H	2.4459374374	-1.9670911902	1.2607127545

Tabelle 10.413 Standardorientierung von TMEDA-MeLi [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
Li	0.1068289058	1.2596840734	0.0977052074
C	0.3635492707	3.2699449496	0.1483473195
N	1.3774361963	-0.3941487873	0.0457601471
N	-1.4407450224	-0.1375617398	-0.0612562451
C	0.5478596828	-1.5893656494	0.2045308696
C	-0.8251565364	-1.4097017532	-0.4442532078
H	1.1809936346	3.5781463102	0.8157460768
H	0.605284101	3.6857968687	-0.8405162263
H	-0.5290964957	3.8114054627	0.4925968685
H	0.4322463421	-1.7747639965	1.274207958
H	1.0361557044	-2.4788833825	-0.2244858733
H	-0.7263719317	-1.4165442413	-1.5314695996
H	-1.466948191	-2.2636013805	-0.1745567063
C	-2.5692426783	0.1835851093	-0.9329804419
H	-3.3714103948	-0.5655365704	-0.854291708
H	-2.9653774582	1.1608555875	-0.6583835984
H	-2.2296811927	0.2319470061	-1.9679615193
C	-1.8783404121	-0.1493165625	1.3357723361
H	-2.3295107307	0.8135865314	1.5750667248
H	-2.6123056859	-0.9479013206	1.5224111557
H	-1.0267295834	-0.2931768617	2.0022778693
C	1.8391286345	-0.2352850473	-1.3348472457
H	0.9906928965	-0.1239192788	-2.0115822216
H	2.4398104335	0.6713039024	-1.4056707445
H	2.4409314065	-1.0974085958	-1.6603588523
C	2.5233988825	-0.4204800406	0.9521415161
H	3.1945015979	-1.2656130097	0.737006935
H	3.0787497499	0.5115562739	0.8502835585
H	2.1740908745	-0.4995588573	1.9821316476

Tabelle 10.414 Standardorientierung von TS1 [Übergangszustand; M05-2X/6-31+G(d,p)].

	x	y	z
Li	0.1208039223	0.9425463605	0.8296676105
C	-0.1067842193	2.9892961776	0.1226582651
N	1.4958208914	-0.3952551141	0.2252052523
N	-1.400369514	-0.2239881842	0.1665012206
C	0.7090716109	-1.3163823979	-0.5909863155
C	-0.6445788313	-0.7351769349	-0.9891214209
C	-2.5903140148	0.4897303902	-0.2998325387
C	-1.789074474	-1.3074962716	1.0691296087
C	1.7826438378	0.8584427002	-0.5386421416
C	2.703472505	-1.0776472477	0.6810523816
H	0.7763683562	1.9454838517	-0.320260868
H	0.563055323	3.8162836598	0.3761712435
H	-0.6387503908	3.2647947607	-0.7943547343
H	-0.8713361822	2.9525079639	0.9178127293
H	0.5750773757	-2.2493887578	-0.0368518905
H	1.2521905526	-1.5644414951	-1.5189238694

H	-0.4885946467	0.1034940134	-1.6700783122
H	-1.2270466639	-1.5063042934	-1.5183805062
H	-3.2629278448	-0.1763449269	-0.8600813007
H	-3.1306217658	0.8957538457	0.5561079504
H	-2.287140757	1.3176974761	-0.9395662524
H	-2.3950093381	-0.9004136026	1.8793779895
H	-2.376896124	-2.0754927701	0.54419161
H	-0.9048839737	-1.773719588	1.50274187
H	2.6531083772	1.3285529615	-0.067978262
H	2.0541133106	0.6121652102	-1.5789744434
H	3.3320618179	-1.379314936	-0.1707418098
H	3.281852979	-0.4051327462	1.313214763
H	2.4405538807	-1.9652801049	1.2646871709

Tabelle 10.415 Standardorientierung von TMEDA-MeLi [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
Li	0.0357222463	1.2773217972	0.1985802181
C	0.5254438698	3.2257231939	-0.1202431674
N	1.3426747524	-0.3454420484	0.1220723156
N	-1.4901327182	-0.1598871957	0.0176843251
C	0.5432807296	-1.5687061904	0.1622024084
C	-0.8229828706	-1.3625206695	-0.4874850362
H	1.5404276045	3.4498163689	0.236261923
H	0.5262024767	3.4683395707	-1.1917205894
H	-0.1260731528	3.9696533423	0.3527427455
H	0.418013977	-1.852866243	1.207199951
H	1.0576601833	-2.4025349003	-0.3372849402
H	-0.7075449638	-1.2482179746	-1.5651174295
H	-1.4420067384	-2.2565131854	-0.3228439404
C	-2.6192197553	0.2007834471	-0.8382364488
H	-3.3803206157	-0.5913629206	-0.8574814177
H	-3.0709564371	1.119334964	-0.4685827193
H	-2.2659065506	0.3801331874	-1.8522774298
C	-1.9502791277	-0.3456538062	1.3934966491
H	-2.4535212546	0.5601898058	1.7276626166
H	-2.6495330345	-1.1897174287	1.4722036167
H	-1.1065611641	-0.527278673	2.0579951849
C	1.8450952725	-0.0699754177	-1.2260714412
H	1.0188772211	0.0518537422	-1.9253405854
H	2.3974208465	0.8674863464	-1.2116583424
H	2.4962219341	-0.8814687019	-1.5801537789
C	2.4605317576	-0.4077580384	1.0590193893
H	3.1616271619	-1.213533049	0.8011984703
H	2.9900049225	0.5431776014	1.0411443903
H	2.0865754277	-0.5753319244	2.0684050626

Tabelle 10.416 Standardorientierung von TS1 Übergangszustand; M05-2X/6-311+G(d,p)].

	x	y	z
Li	0.1242931769	0.9568976995	0.8317190832
C	-0.1163000755	2.9884542643	0.0999396391
N	1.4956765751	-0.4020447449	0.2318680609
N	-1.3987004342	-0.2175356782	0.1744365109
C	0.704973787	-1.3103249405	-0.5926038103
C	-0.6435308663	-0.7184913794	-0.9847284789
C	-2.5932902953	0.4893927667	-0.2873630517
C	-1.7778698909	-1.3082072674	1.0706527538
C	1.7897541403	0.8549638871	-0.5219688003
C	2.7007618617	-1.0932032282	0.678077254
H	0.7819467714	1.9428030455	-0.3218765718
H	0.5438514207	3.8222898782	0.3494245482
H	-0.6407049693	3.2525293423	-0.8226504091
H	-0.8859460839	2.9536376029	0.887261743
H	0.5659551674	-2.2468372408	-0.0492093516
H	1.2473420796	-1.5507547313	-1.5207814511
H	-0.4832010122	0.1257308739	-1.6553445141
H	-1.2291811589	-1.4794292722	-1.5212910387
H	-3.2593393115	-0.1794971225	-0.8488934281
H	-3.1359449296	0.8871698022	0.5692318964
H	-2.2970587479	1.320937282	-0.9233399938
H	-2.3901848114	-0.9122473427	1.879770164
H	-2.3546051646	-2.0784696423	0.5402003486
H	-0.8909811847	-1.7655977984	1.5046017306
H	2.655031947	1.321839069	-0.0431409879
H	2.0690300721	0.6141970453	-1.5591580029
H	3.3246480948	-1.3867143517	-0.177792314
H	3.2826149813	-0.4309578347	1.3155769805
H	2.4368248608	-1.985559984	1.2511264913

Tabelle 10.417 Standardorientierung von TMEDA-MeLi [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
Li	0.0384156648	1.2747636202	0.2103752821
C	0.5103994531	3.2189610734	-0.1313278
N	1.3462350879	-0.345056349	0.1359982301
N	-1.4867953752	-0.1539681035	0.0164507685
C	0.5427174228	-1.5619221474	0.1655586605
C	-0.8176042934	-1.3510941267	-0.4886272038
H	1.526141439	3.4466361817	0.2087197905
H	0.4975384297	3.438251827	-1.2040556214
H	-0.1370074898	3.9643868721	0.3359431067
H	0.4118357584	-1.8502746572	1.2053276131
H	1.0551800164	-2.3921963807	-0.3349326719
H	-0.6962272475	-1.2328497017	-1.5618843966
H	-1.4354081062	-2.2432871835	-0.3310445818
C	-2.6151889598	0.2021419521	-0.8362689736

H	-3.3703189471	-0.5913988903	-0.8537172765
H	-3.070068771	1.1154546607	-0.4668519298
H	-2.2652927588	0.3809337062	-1.8481422266
C	-1.9443443856	-0.3402658953	1.3894126025
H	-2.4482812566	0.561438002	1.7232382577
H	-2.6397819292	-1.1835113223	1.466780066
H	-1.1025605678	-0.5212113437	2.0512366639
C	1.8371197639	-0.0536361643	-1.2095667735
H	1.008112388	0.0911382565	-1.8961149995
H	2.4020356604	0.8723316573	-1.1854761396
H	2.4708197806	-0.8663681453	-1.5820930389
C	2.4701080607	-0.4300665495	1.0584523709
H	3.1602937047	-1.2338682162	0.7793105388
H	3.0058216009	0.5138528927	1.0513423893
H	2.1068478565	-0.6142705253	2.065329293

Tabelle 10.418 Standardorientierung von TS1 [Übergangszustand; M052X/6-311+G(3df,3pd)].

	x	y	z
Li	0.1288786064	0.9557062006	0.8212772024
C	-0.1190527242	2.9846233513	0.0964838061
N	1.4978820468	-0.3999584165	0.2361023745
N	-1.399547756	-0.216667417	0.1777390262
C	0.7049671659	-1.3026736969	-0.5865931709
C	-0.6408739919	-0.7106488542	-0.9777526886
C	-2.5916699534	0.4863602213	-0.2856200167
C	-1.7801771839	-1.3086738373	1.0660019007
C	1.7917668921	0.8543459465	-0.5137417299
C	2.7009200402	-1.093037921	0.6739978724
H	0.7841365962	1.9399802053	-0.3207209962
H	0.5375793475	3.8172965867	0.3434155553
H	-0.6426853862	3.2403676904	-0.8246337973
H	-0.884981323	2.9451135617	0.8821540444
H	0.564948338	-2.2369187633	-0.0461991552
H	1.2443864964	-1.5420094585	-1.5130384111
H	-0.4803739176	0.1338117667	-1.6429754974
H	-1.2221208764	-1.4681301946	-1.5173630092
H	-3.2486066562	-0.1817072391	-0.8527619901
H	-3.1404416232	0.8743871547	0.5674096984
H	-2.2972239669	1.3198039837	-0.9145448872
H	-2.3921892849	-0.9178904514	1.8734449996
H	-2.3556310113	-2.0721423708	0.5307740758
H	-0.8978244102	-1.769939151	1.4967681685
H	2.6510499032	1.3230269355	-0.034043025
H	2.0696596341	0.6158883162	-1.5481265893
H	3.3161053161	-1.3866531448	-0.184158627
H	3.2876430862	-0.4350144045	1.3058263386
H	2.439342596	-1.9836765998	1.2446235282

Tabelle 10.419 Standardorientierung von TMEDA-MeLi [globales Minimum; M06L/6-31+G(d)].

	x	y	z
Li	0.0147434273	1.3261154949	0.1497360916
C	0.5819266735	3.2352309883	-0.0231789157
N	1.3222661033	-0.3442027909	0.1104890293
N	-1.5047417746	-0.1806966168	-0.0394990877
C	0.5318197859	-1.5734806881	0.1724346615
C	-0.8254956765	-1.398869591	-0.4916430811
H	1.6090967045	3.3993107988	0.3622916526
H	0.6297557249	3.5774484813	-1.0763183861
H	-0.0252632082	4.0065921584	0.4855324825
H	0.4042292819	-1.8310612269	1.2322551654
H	1.060298182	-2.4286370659	-0.2930653873
H	-0.70934816	-1.321984125	-1.5807229553
H	-1.4444944398	-2.2989063561	-0.3066523582
C	-2.6553597632	0.1140532089	-0.8847528311
H	-3.4215926804	-0.682840782	-0.8464114923
H	-3.1143406971	1.0544994962	-0.5629919839
H	-2.3277370764	0.2329945948	-1.9232667495
C	-1.9185402507	-0.2865675538	1.356689051
H	-2.4389652643	0.6305361994	1.6521225421
H	-2.5957296564	-1.1442982722	1.5296270252
H	-1.0450726033	-0.4015164999	2.0098086364
C	1.8096763481	-0.0783205575	-1.2414748059
H	0.9709067672	0.0189964224	-1.9412235112
H	2.3513173063	0.87309225	-1.2476105432
H	2.4769557856	-0.8817507329	-1.607153828
C	2.4383193123	-0.3758066861	1.0457602356
H	3.1656172222	-1.1750648648	0.8086597017
H	2.9564269221	0.5883477473	1.0209173279
H	2.0640677036	-0.5381684307	2.0630143136

Tabelle 10.420 Standardorientierung von TS1 [globales Minimum; M06L/6-31+G(d)].

	x	y	z
Li	0.1535381255	1.0108923413	0.8824994543
C	-0.1775882882	2.9482441694	-0.0785722394
N	1.4968621191	-0.4184218842	0.2575380281
N	-1.387637487	-0.1890266402	0.2189786106
C	0.6972294358	-1.2335308728	-0.6524517617
C	-0.6404890845	-0.5973409806	-0.9854606139
C	-2.6174091515	0.4901869062	-0.1788099623
C	-1.7019898668	-1.3363694353	1.0652909389
C	1.874110176	0.8693794451	-0.404038594
C	2.6487692775	-1.1919019865	0.70240908
H	0.8186079297	1.9411652632	-0.3418689795
H	0.4120625441	3.8687584915	0.0336802923
H	-0.7499034757	3.0539467341	-1.0128731015
H	-0.9332232384	2.9781186828	0.7336432655
H	0.546924172	-2.2223199327	-0.1952666869
H	1.243443839	-1.407721851	-1.6032977352

H	-0.4879021172	0.309359758	-1.5864836554
H	-1.241704848	-1.3025747087	-1.5924903846
H	-3.2887473045	-0.1761996752	-0.751556145
H	-3.1532439162	0.8385753182	0.711213982
H	-2.371077861	1.360229527	-0.7956309907
H	-2.3178900847	-1.0070006127	1.9091233635
H	-2.2604981844	-2.1169566668	0.5151420928
H	-0.7830234595	-1.7794989551	1.4638219148
H	2.7053098782	1.2893876007	0.1841389865
H	2.2696925847	0.6640924858	-1.4199246532
H	3.3022466376	-1.4771752201	-0.1447526737
H	3.2439943891	-0.5931746226	1.3994455681
H	2.3254032591	-2.1081526788	1.2202975995

Tabelle 10.421 Standardorientierung von TMEDA-MeLi [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
Li	0.1373239004	1.2917328697	0.076259573
C	0.2955426759	3.2844681328	0.2179211278
N	1.3984024206	-0.4197825901	0.0154865096
N	-1.4290155058	-0.1361896596	-0.0708075632
C	0.5489397162	-1.5921654453	0.2121143808
C	-0.8213289236	-1.4163030804	-0.4257726602
H	1.020468781	3.6183807153	0.9845810118
H	0.6174370025	3.7690493351	-0.7235574718
H	-0.6612483455	3.7735025681	0.4859024537
H	0.4431199387	-1.7500348983	1.2950877961
H	1.0272004694	-2.5090050497	-0.1905964897
H	-0.7346922936	-1.4526614421	-1.5212977454
H	-1.4731197353	-2.2667880637	-0.1369756536
C	-2.5422823726	0.1887721945	-0.9504448848
H	-3.3675167696	-0.5456970184	-0.8656059311
H	-2.9275989152	1.1840988036	-0.698847797
H	-2.1991051739	0.2128427296	-1.9923439577
C	-1.8585534935	-0.1028171618	1.3225309315
H	-2.3015238086	0.8757670083	1.5431756533
H	-2.6051426806	-0.8917321927	1.5418233561
H	-1.0034741374	-0.2359550835	1.9990243702
C	1.8444156099	-0.2947342637	-1.3674228003
H	0.9886750584	-0.1724255163	-2.0450448384
H	2.4725307937	0.5985363084	-1.4679201824
H	2.4261971965	-1.1795858545	-1.6936719322
C	2.5420138234	-0.4334429576	0.9160072355
H	3.2075270717	-1.2995224249	0.7299123861
H	3.119334756	0.4898743441	0.7872919859
H	2.1962149408	-0.4731373069	1.9565631367

Tabelle 10.422 Standardorientierung von TS1 [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
Li	0.1284740016	0.9751759437	0.8513311125
C	-0.090112468	3.0114287588	0.0816923678
N	1.4999999546	-0.3907746164	0.2218467178
N	-1.4149219388	-0.2304615094	0.1780789686
C	0.7036690771	-1.2860794436	-0.6074459659
C	-0.6497777327	-0.7090238564	-0.9844652736
C	-2.6166851374	0.4632453466	-0.2726897798
C	-1.7792583429	-1.3277812426	1.0667844697
C	1.8227501613	0.8701001257	-0.515079633
C	2.6804570878	-1.1020466869	0.6897253493
H	0.8168247548	1.9796973042	-0.3220518596
H	0.5620911548	3.8664214086	0.3124135867
H	-0.6279029266	3.2533832574	-0.8486801917
H	-0.861792454	2.9887527991	0.8793587345
H	0.5755619446	-2.2402694102	-0.0723183157
H	1.2451353588	-1.5248903023	-1.5488783371
H	-0.5096875485	0.1483072972	-1.6581339467
H	-1.2320616651	-1.4748259721	-1.5372305815
H	-3.2895226074	-0.2123601483	-0.8356657372
H	-3.1648782332	0.8590805148	0.5913159994
H	-2.3401346963	1.3056126247	-0.917350725
H	-2.3965919301	-0.9448466581	1.8886576014
H	-2.3575445462	-2.1083593943	0.534285719
H	-0.8849473102	-1.7907315073	1.5003731171
H	2.6980631299	1.3151797184	-0.0157716831
H	2.1198661937	0.6306445977	-1.5572068926
H	3.3215702635	-1.4199553561	-0.1570193163
H	3.2746451078	-0.4469335562	1.3369194095
H	2.3925773471	-1.9927200364	1.2709500853

Tabelle 10.423 Standardorientierung von TMEDA-MeLi [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Li	0.1447756697	1.2887105858	0.0765154659
C	0.2798052709	3.2825311839	0.2230038188
N	1.4022257162	-0.4234536901	0.0104151009
N	-1.424610392	-0.1334505315	-0.067548357
C	0.5497277459	-1.5931252187	0.2135292917
C	-0.8205376466	-1.4154404181	-0.4230939601
H	0.9630843837	3.6241645842	1.0210313953
H	0.6366844867	3.7687871053	-0.7026633674
H	-0.6952223928	3.7541141973	0.4460884655
H	0.4442999836	-1.7455541557	1.2961670791
H	1.0235183045	-2.5125217441	-0.1850706468
H	-0.7341990665	-1.4523353016	-1.5174795845
H	-1.4722564938	-2.2642772507	-0.1342422322
C	-2.5346103871	0.1988820123	-0.9495548011

H	-3.3637024485	-0.529494642	-0.8679330437
H	-2.9141228819	1.1951076067	-0.6985033315
H	-2.1897453646	0.2224227462	-1.9895201888
C	-1.8553599397	-0.0988788497	1.326029436
H	-2.2915732681	0.8810933767	1.5472366709
H	-2.6057194621	-0.8824637984	1.5443900725
H	-1.0025679401	-0.2372119837	2.002298921
C	1.8456400115	-0.3044229217	-1.3745541521
H	0.9897319699	-0.1820867426	-2.04985411
H	2.4748193592	0.5858660283	-1.479865054
H	2.4236837489	-1.1904967254	-1.6992817848
C	2.5473231097	-0.4352813437	0.91017277
H	3.2109964426	-1.3017729987	0.7277437922
H	3.1253705678	0.4854752998	0.7778339468
H	2.2032829129	-0.4698414098	1.9500803876

Tabelle 10.424 Standardorientierung von TS1 [Übergangszustand; M06/6-31+G(d,p)].

	x	y	z
Li	0.1283031982	0.9742551361	0.8520106164
C	-0.0959422596	3.0041044369	0.0785765846
N	1.499917363	-0.3873878898	0.2210075982
N	-1.4136307653	-0.2307028289	0.1784123126
C	0.704484558	-1.280714192	-0.6122968877
C	-0.6485116271	-0.7024275806	-0.987528754
C	-2.6163257304	0.4660125377	-0.2671597472
C	-1.7758663599	-1.3332155351	1.0625987766
C	1.8296638312	0.8734028481	-0.5142417706
C	2.6762290786	-1.102620648	0.6952814853
H	0.8208064084	1.9759388087	-0.3196227978
H	0.5516361243	3.8695014394	0.272244196
H	-0.6598122401	3.2180260469	-0.8416909468
H	-0.8449560524	2.9928051635	0.895783846
H	0.575428655	-2.2353982622	-0.080667459
H	1.2455897698	-1.5167240156	-1.5531126363
H	-0.5078382229	0.1581638795	-1.6551983951
H	-1.2290347927	-1.4645190442	-1.5446639507
H	-3.288852454	-0.2043785226	-0.8340087682
H	-3.1637487966	0.8554708081	0.5984444894
H	-2.340654895	1.3123817824	-0.9047979632
H	-2.3905811694	-0.9557620126	1.8870361219
H	-2.3544281278	-2.1105274469	0.5284784649
H	-0.8816528455	-1.7979477232	1.4912710293
H	2.7015637527	1.3173735251	-0.0106469476
H	2.131346631	0.634118881	-1.5538604781
H	3.3197779247	-1.4235183307	-0.1467501927
H	3.2696647178	-0.4501411095	1.3434001517
H	2.3832903261	-1.9906001515	1.2754470222

Tabelle 10.425 Standardorientierung von TMEDA-MeLi [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
Li	0.1447756697	1.2887105858	0.0765154659
C	0.2798052709	3.2825311839	0.2230038188
N	1.4022257162	-0.4234536901	0.0104151009
N	-1.424610392	-0.1334505315	-0.067548357
C	0.5497277459	-1.5931252187	0.2135292917
C	-0.8205376466	-1.4154404181	-0.4230939601
H	0.9630843837	3.6241645842	1.0210313953
H	0.6366844867	3.7687871053	-0.7026633674
H	-0.6952223928	3.7541141973	0.4460884655
H	0.4442999836	-1.7455541557	1.2961670791
H	1.0235183045	-2.5125217441	-0.1850706468
H	-0.7341990665	-1.4523353016	-1.5174795845
H	-1.4722564938	-2.2642772507	-0.1342422322
C	-2.5346103871	0.1988820123	-0.9495548011
H	-3.3637024485	-0.529494642	-0.8679330437
H	-2.9141228819	1.1951076067	-0.6985033315
H	-2.1897453646	0.2224227462	-1.9895201888
C	-1.8553599397	-0.0988788497	1.326029436
H	-2.2915732681	0.8810933767	1.5472366709
H	-2.6057194621	-0.8824637984	1.5443900725
H	-1.0025679401	-0.2372119837	2.002298921
C	1.8456400115	-0.3044229217	-1.3745541521
H	0.9897319699	-0.1820867426	-2.04985411
H	2.4748193592	0.5858660283	-1.479865054
H	2.4236837489	-1.1904967254	-1.6992817848
C	2.5473231097	-0.4352813437	0.91017277
H	3.2109964426	-1.3017729987	0.7277437922
H	3.1253705678	0.4854752998	0.7778339468
H	2.2032829129	-0.4698414098	1.9500803876

Tabelle 10.426 Standardorientierung von TS1 [Übergangszustand; M06/6-31+G(d,p)].

	x	y	z
Li	0.1283031982	0.9742551361	0.8520106164
C	-0.0959422596	3.0041044369	0.0785765846
N	1.499917363	-0.3873878898	0.2210075982
N	-1.4136307653	-0.2307028289	0.1784123126
C	0.704484558	-1.280714192	-0.6122968877
C	-0.6485116271	-0.7024275806	-0.987528754
C	-2.6163257304	0.4660125377	-0.2671597472
C	-1.7758663599	-1.3332155351	1.0625987766
C	1.8296638312	0.8734028481	-0.5142417706
C	2.6762290786	-1.102620648	0.6952814853
H	0.8208064084	1.9759388087	-0.3196227978
H	0.5516361243	3.8695014394	0.272244196
H	-0.6598122401	3.2180260469	-0.8416909468
H	-0.8449560524	2.9928051635	0.895783846
H	0.575428655	-2.2353982622	-0.080667459
H	1.2455897698	-1.5167240156	-1.5531126363

H	-0.5078382229	0.1581638795	-1.6551983951
H	-1.2290347927	-1.4645190442	-1.5446639507
H	-3.288852454	-0.2043785226	-0.8340087682
H	-3.1637487966	0.8554708081	0.5984444894
H	-2.340654895	1.3123817824	-0.9047979632
H	-2.3905811694	-0.9557620126	1.8870361219
H	-2.3544281278	-2.1105274469	0.5284784649
H	-0.8816528455	-1.7979477232	1.4912710293
H	2.7015637527	1.3173735251	-0.0106469476
H	2.131346631	0.634118881	-1.5538604781
H	3.3197779247	-1.4235183307	-0.1467501927
H	3.2696647178	-0.4501411095	1.3434001517
H	2.3832903261	-1.9906001515	1.2754470222

Tabelle 10.427 Standardorientierung von TMEDA-MeLi [globales Minimum; M062X/6-31+G(d)].

	x	y	z
Li	0.0412368244	1.2460182409	0.2001857141
C	0.4869699315	3.1867965465	-0.0906322654
N	1.3437660431	-0.3598566847	0.1234027472
N	-1.4749214515	-0.161629039	0.0004194042
C	0.5460639054	-1.585498833	0.1676187582
C	-0.8230331018	-1.3819103762	-0.4831689594
H	1.4992149923	3.4376208224	0.2749634106
H	0.4876506201	3.4512500208	-1.1633493544
H	-0.1873529815	3.9141160363	0.3907085298
H	0.4221756509	-1.8670285635	1.2188590357
H	1.0637062546	-2.4264168082	-0.3281152034
H	-0.7106776458	-1.2900410408	-1.5683953917
H	-1.4519705746	-2.271901011	-0.3011039539
C	-2.5936864068	0.2170863105	-0.8602225315
H	-3.3826733392	-0.5542807892	-0.8713493101
H	-3.0202778465	1.1579282861	-0.5042368613
H	-2.2335218353	0.3728505149	-1.880501849
C	-1.9241591441	-0.3020844528	1.3852109705
H	-2.4041156749	0.6269164471	1.7041723031
H	-2.6436784631	-1.1312304548	1.4992722596
H	-1.0730994598	-0.4858768908	2.0479524236
C	1.8226551822	-0.066856332	-1.2296378162
H	0.9802453048	0.06868697	-1.9147629065
H	2.3807805753	0.8723952112	-1.214636963
H	2.4670148068	-0.8766805993	-1.613635597
C	2.4687626917	-0.4146159543	1.0519697569
H	3.1809175948	-1.2157139384	0.7892757451
H	2.9915422576	0.5450094565	1.0360311835
H	2.1012072892	-0.5900080953	2.0670787208

Tabelle 10.428 Standardorientierung von TS1 [Übergangszustand; M062X/6-31+G(d)].

	x	y	z
Li	0.1386878394	0.9499559392	0.8490656654
C	-0.1592912021	2.9544176843	0.0349173204
N	1.4973241097	-0.4114900332	0.2305160736
N	-1.3845975414	-0.2042725355	0.1799500277
C	0.7070515293	-1.2915490018	-0.6264277124
C	-0.6428161791	-0.6838825425	-0.9986020273
C	-2.58917943	0.5084564502	-0.2455310903
C	-1.737997667	-1.3053857043	1.0750190546
C	1.8145051214	0.8634082453	-0.4837971174
C	2.6815791566	-1.1266840785	0.69533991
H	0.7762723557	1.9329855083	-0.3333101545
H	0.4678944641	3.8226168667	0.2748423422
H	-0.6784657906	3.1783664416	-0.9074104232
H	-0.9471444488	2.9174973861	0.8118107577
H	0.5637855141	-2.2493969122	-0.1117440221
H	1.2525399634	-1.5090077346	-1.5644924915
H	-0.4870427441	0.1783232973	-1.6557809755
H	-1.2392995967	-1.4321186006	-1.5512477534
H	-3.2778390101	-0.1553422257	-0.7949827729
H	-3.1096352601	0.9055989559	0.6306271613
H	-2.3079444387	1.3461912661	-0.8877850629
H	-2.3416153698	-0.9197504991	1.9013798387
H	-2.3198066045	-2.0830496506	0.5510096111
H	-0.8360099118	-1.7602513892	1.4923148713
H	2.6631977096	1.3218959476	0.0434319096
H	2.1433170173	0.6448493244	-1.5170597729
H	3.3279410599	-1.4214352056	-0.1497116927
H	3.2598953924	-0.4796934555	1.3588086203
H	2.3905599619	-2.0262837441	1.2525949051

Tabelle 10.429 Standardorientierung von TMEDA-MeLi [globales Minimum; M062X/6-31+G(d,p)].

	x	y	z
Li	0.0336817752	1.2462662163	0.1996014607
C	0.5068459661	3.1786453718	-0.103009055
N	1.3387059233	-0.354827139	0.1243835419
N	-1.4808183494	-0.1642206856	0.0026754546
C	0.5446065267	-1.5831076542	0.1625860744
C	-0.8242352667	-1.3794912194	-0.4882993513
H	1.5294788044	3.4055610369	0.2463466894
H	0.4974596015	3.4386590232	-1.1756663082
H	-0.1424581534	3.9215169759	0.3859683888
H	0.4199785056	-1.8695612441	1.2120343894
H	1.0635143295	-2.4207365812	-0.3363572866
H	-0.7105559713	-1.2797651043	-1.5723449602
H	-1.4497870562	-2.2727106897	-0.3129573789
C	-2.6036060274	0.2128322039	-0.8541792209

H	-3.3890064928	-0.5614765423	-0.8666861016
H	-3.0335492987	1.1499942892	-0.4940180382
H	-2.2467014585	0.3742175933	-1.8742135476
C	-1.9256142085	-0.3129397308	1.3884979248
H	-2.4107693551	0.6110597692	1.7121810562
H	-2.6388337345	-1.1469323816	1.5016987049
H	-1.0718739675	-0.4933258047	2.0479234844
C	1.8236462969	-0.0564610234	-1.2258525587
H	0.9845781143	0.0714074381	-1.9157878757
H	2.3709240141	0.8885437845	-1.2064841227
H	2.4778617255	-0.8593805853	-1.6060524469
C	2.4586043108	-0.4041993934	1.0599082727
H	3.1777735686	-1.1993758689	0.8004022695
H	2.974359606	0.5587955532	1.0489638717
H	2.0865322716	-0.5839426077	2.0721086693

Tabelle 10.430 Standardorientierung von TS1 [Übergangszustand; M062X/6-31+G(d,p)].

	x	y	z
Li	0.1399995713	0.9531877471	0.8422272498
C	-0.1573541066	2.9536305487	0.0263956466
N	1.496264091	-0.4106907791	0.2291011837
N	-1.385191934	-0.2031025867	0.1820760922
C	0.7047861982	-1.2889509132	-0.629142344
C	-0.6448686419	-0.6797584378	-0.9989705788
C	-2.592165429	0.5085198822	-0.2397050319
C	-1.7335681201	-1.3056750004	1.077928699
C	1.8204832426	0.8628299913	-0.485702979
C	2.676400812	-1.1300262438	0.6991579039
H	0.781041142	1.933068905	-0.3367293425
H	0.4680001861	3.8253477213	0.25300937
H	-0.6856701594	3.1672153608	-0.9122203283
H	-0.9374096092	2.9210995821	0.8099861415
H	0.5606322304	-2.2470119424	-0.1159009872
H	1.2487461263	-1.5052971619	-1.5678151963
H	-0.4887090946	0.1844692612	-1.6530364601
H	-1.2411702779	-1.4262963092	-1.5532320559
H	-3.2804592929	-0.1545345943	-0.7895239108
H	-3.1117186851	0.9024271942	0.637795652
H	-2.3133637851	1.3482896038	-0.8796481622
H	-2.3358694263	-0.922198462	1.9054809878
H	-2.3143398678	-2.0846161935	0.5556917836
H	-0.8295529415	-1.7578306831	1.4925768665
H	2.6680182733	1.3194649683	0.0438687853
H	2.1531127632	0.6419126247	-1.5168150475
H	3.3243123656	-1.4287519096	-0.1427360169
H	3.2552383467	-0.4846551686	1.3628488131
H	2.3802420224	-2.0270970048	1.2567782661

Tabelle 10.431 Standardorientierung von TMEDA-MeLi [globales Minimum; M062X/6-311+G(d,p)].

	x	y	z
Li	0.2017490369	1.2806591763	0.5118734736
C	0.2564971855	2.8392955754	-0.7848338266
N	1.4594367048	-0.3800028407	0.2034977638
N	-1.4430890781	0.0258178415	0.3676364723
C	0.4971366081	-1.4391577762	-0.1324426997
C	-0.8212448827	-0.8543008358	-0.630355724
H	1.2286961437	3.3452873639	-0.8911995548
H	0.0168203183	2.4776915015	-1.8033159307
H	-0.4685420908	3.6461837305	-0.5961337467
H	0.321535023	-2.0424133219	0.760863147
H	0.9088464339	-2.1177592149	-0.8946216636
H	-0.6389063116	-0.2494037552	-1.5231630342
H	-1.5043702632	-1.6704915842	-0.9166151048
C	-2.5175733952	0.8067405421	-0.2539366535
H	-3.3090989259	0.1531021661	-0.6520428338
H	-2.9538756295	1.4754695528	0.4891892597
H	-2.0992366818	1.4202330084	-1.051986941
C	-1.9637580722	-0.7258767722	1.5067195293
H	-2.4456655121	-0.0367197599	2.2014322761
H	-2.7045980716	-1.478090606	1.1932826264
H	-1.1592637592	-1.2314250495	2.0422789556
C	2.174003528	0.0773115446	-0.9960445727
H	1.4672906783	0.4290833029	-1.7463607514
H	2.8063957772	0.9270556893	-0.7386257657
H	2.7924428565	-0.7320698826	-1.4141054719
C	2.4217355959	-0.8411966849	1.2019428426
H	3.0023558422	-1.7047097913	0.8429647425
H	3.1168640122	-0.0332689257	1.4351726719
H	1.9018259293	-1.1266381944	2.1185715143

Tabelle 10.432 Standardorientierung von TS1 [Übergangszustand; M062X/6-311+G(d,p)].

	x	y	z
Li	0.1421222488	0.9635861166	0.8453319455
C	-0.1703158708	2.9502219197	0.0152112094
N	1.4975381083	-0.4157255277	0.2366487249
N	-1.3838740772	-0.199192486	0.1865002208
C	0.7050994761	-1.282184499	-0.6323223079
C	-0.6416808442	-0.6653504678	-0.9973373016
C	-2.5943497931	0.5075847465	-0.2332718387
C	-1.7268489915	-1.3095709595	1.0745300164
C	1.82607946	0.8640204688	-0.4648575671
C	2.6779552537	-1.1417178982	0.6955222392
H	0.7851041747	1.9324742714	-0.3284684334
H	0.4404733686	3.8274199737	0.2515626114
H	-0.6787300958	3.1572913151	-0.9335438576
H	-0.9646894236	2.9092884982	0.7804514566
H	0.5577474236	-2.243767323	-0.1317345541
H	1.2488304815	-1.4882715668	-1.5704492075

H	-0.4823076816	0.2034885406	-1.6409818663
H	-1.2377540555	-1.4028812824	-1.5589213708
H	-3.2761930155	-0.1559806797	-0.7861592755
H	-3.1170014071	0.8934645815	0.6437467026
H	-2.3200533612	1.350774925	-0.8674440491
H	-2.3368076481	-0.9369173822	1.899070114
H	-2.2958941414	-2.0895919443	0.5456501445
H	-0.8224838497	-1.7537196495	1.4922003686
H	2.6688950797	1.3164450496	0.0710467907
H	2.1613810657	0.6538972519	-1.4945901497
H	3.3228177904	-1.4282785444	-0.1499308389
H	3.2572884866	-0.5069685963	1.3660791971
H	2.3835178389	-2.0448688519	1.2402058766

Tabelle 10.433 Standardorientierung von TMEDA-MeLi [globales Minimum; MP2/6-31+G(d)].

	x	y	z
Li	1.400276922	-1.3009167233	3.8612497921
C	-0.413348326	-0.6205269242	3.2189217222
N	3.4313455699	-0.8057621363	3.6026532339
N	2.1385011129	-2.9230164381	4.9839760601
C	4.2002567629	-1.6280138785	4.5458599243
C	3.5790082675	-3.0121323355	4.7124913738
H	-0.416460019	0.4633781485	3.0130484868
H	-0.7443539081	-1.1107616426	2.287314165
H	-1.2162050955	-0.7935600205	3.955942731
H	4.2156116778	-1.1032545012	5.5069530845
H	5.2533617899	-1.7356522424	4.2242710193
H	3.7082236121	-3.5960003664	3.7951416032
H	4.1098171113	-3.5579210643	5.5151749327
C	1.4865324955	-4.221663666	4.7763788214
H	1.8780800224	-4.992855366	5.4617867412
H	0.4119559437	-4.1108521614	4.9393410802
H	1.6464365163	-4.5484830542	3.7454229737
C	1.8767084398	-2.4529714068	6.3514345834
H	0.7962987061	-2.4005825267	6.5071091521
H	2.3173458377	-3.1280668567	7.1054122742
H	2.287451518	-1.4503146195	6.4966357424
C	3.6203811349	-1.2577747763	2.2167356106
H	3.2594037196	-2.2824519431	2.0956292383
H	3.0367832843	-0.6159154689	1.5524001504
H	4.6821411831	-1.2181664902	1.9175599739
C	3.8108301676	0.6076401978	3.715162142
H	4.8733714322	0.7696213221	3.4650538559
H	3.1905041246	1.1982337101	3.0369115764
H	3.6307570564	0.9526947108	4.7369133451

Tabelle 10.434 Standardorientierung von TS1 [globales Minimum; MP2/6-31+G(d)].

	x	y	z
Li	0.8110926081	-0.8411342941	0.6769394908
C	1.6795713287	-2.773091961	0.418952476
N	-1.1693855574	-0.4962813329	0.7017202658
N	1.1331179895	0.774877418	-0.5218199304
C	-1.3413701749	0.6106297649	-0.2426729602
C	-0.1714363792	0.7376321216	-1.2117506656
C	2.2174301518	0.6283525502	-1.5031665076
C	1.303840569	2.0278605874	0.2255215983
C	-1.0312768231	-1.8042967449	-0.0257021902
C	-2.2779588739	-0.4803458511	1.6609125527
H	0.3640234762	-2.3111782475	0.037776087
H	1.8534601599	-3.0228727717	1.4778296257
H	1.594363262	-3.7242491702	-0.1203278991
H	2.589182063	-2.2774024453	0.0364919053
H	-1.4717868967	1.5373126767	0.3299190626
H	-2.26092796	0.4680566004	-0.8443112922
H	-0.1586425194	-0.1277985855	-1.8807688523
H	-0.3083580241	1.6432218147	-1.8320944858
H	2.2097097394	1.4466931251	-2.2425495403
H	3.1801144968	0.6323471914	-0.9844783388
H	2.105532685	-0.3257013365	-2.0239829906
H	2.2917353502	2.033686717	0.6948102786
H	1.2233660188	2.9073821806	-0.435828013
H	0.5478035889	2.1052546652	1.0098874663
H	-1.4686871995	-2.579490395	0.6191170751
H	-1.6165122932	-1.7831141862	-0.9643314116
H	-3.2466680994	-0.6379922699	1.1557044008
H	-2.1327297152	-1.2804364525	2.3899991216
H	-2.2991879712	0.4794766311	2.191962671

Tabelle 10.435 Standardorientierung von TMEDA-MeLi [globales Minimum; MP2/6-311+G(d,p)].

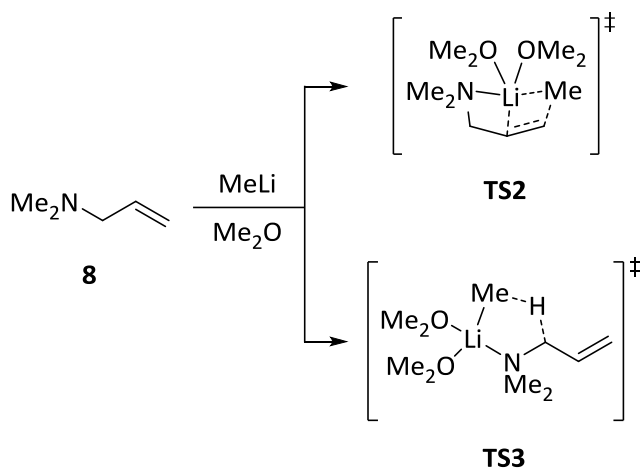
	x	y	z
Li	0.088466	1.297719	0.123042
C	0.412456	3.304755	0.08375
N	1.378439	-0.368209	0.028299
N	-1.463247	-0.135481	-0.001921
C	0.548929	-1.567338	0.189936
C	-0.826725	-1.380779	-0.449582
H	1.0755	3.650852	0.895503
H	0.896901	3.634346	-0.852242
H	-0.502638	3.914953	0.170818
H	0.439402	-1.754998	1.262768
H	1.035653	-2.458975	-0.245234
H	-0.728463	-1.330044	-1.53852
H	-1.457757	-2.259222	-0.222847
C	-2.594301	0.201425	-0.873025

H	-3.370333	-0.582342	-0.854239
H	-3.032598	1.145851	-0.542362
H	-2.240251	0.325956	-1.89955
C	-1.934202	-0.252536	1.383438
H	-2.406564	0.687156	1.679978
H	-2.664811	-1.072098	1.492614
H	-1.095899	-0.439085	2.059561
C	1.868701	-0.242933	-1.350214
H	1.032378	-0.154314	-2.048449
H	2.47044	0.665128	-1.431469
H	2.480861	-1.11422	-1.639385
C	2.519377	-0.400262	0.948152
H	3.176845	-1.264459	0.753278
H	3.096367	0.520226	0.832859
H	2.157816	-0.456027	1.978415

Tabelle 10.436 Standardorientierung von TS1 [Übergangszustand; MP2/6-311+G(d,p)].

	x	y	z
Li	0.0905284825	0.9787045414	0.7617811885
C	0.186805403	3.0644939586	0.3377014964
N	1.4524850045	-0.3849418631	0.1698839847
N	-1.4417312048	-0.2220364176	0.1264177448
C	0.6597839426	-1.4049569642	-0.5178821534
C	-0.7020896817	-0.8804916397	-0.9659881132
C	-2.6158450094	0.4655209636	-0.4243605107
C	-1.8715592217	-1.2024920242	1.1298590173
C	1.6732052846	0.8013733891	-0.7241322807
C	2.6993743768	-0.9940720152	0.6372387563
H	0.848355899	1.9636145962	-0.3183212337
H	0.5653939819	3.4029618868	1.3156025838
H	0.5057614838	3.8147348848	-0.3954178801
H	-0.9151385184	3.1133509822	0.3711660331
H	0.539466512	-2.2643214503	0.1525174092
H	1.1912010273	-1.7635037931	-1.4203911712
H	-0.5608297674	-0.1373016597	-1.7555498249
H	-1.2932296441	-1.7158493013	-1.3835173969
H	-3.3004687002	-0.2418281127	-0.9210915003
H	-3.1548456496	0.9698093127	0.3822756576
H	-2.2890191775	1.2156409547	-1.14831204
H	-2.4501509855	-0.6939822659	1.9060703084
H	-2.5009106865	-1.9884613763	0.679501971
H	-1.0025304153	-1.6706412233	1.5973829456
H	2.646567965	1.2326715199	-0.45144834
H	1.7387801365	0.475303265	-1.7789635097
H	3.3042282026	-1.3622326243	-0.2090643263
H	3.2832096136	-0.2488702597	1.181828827
H	2.4787393463	-1.8302282645	1.3123753574

## 10.2.1.6. Deprotonierung und Carbolithiierung



Schema 10.2 Berechnete Konkurrenz zwischen Carbolithiierung (**TS2**, oben) und Deprotonierung (**TS3**, unten) von Allyldimethylamin (**8**) mit Methyllithium unter Verwendung von Dimethylether zur Vervollständigung der Koordinationssphäre.

Tabelle 10.437 Berechnete Energien der optimierten Strukturen für die Konkurrenz aus Carbometallierung und Deprotonierung von **8**.

	Method	Basis	SCF [Hartree]	ZPE [Hartree]
<b>8</b>	SVWN	6-31+G(d)	-606.1101168	-605.765864
<b>TS2</b>	SVWN	6-31+G(d)	-606.1046632	-605.758992
<b>TS3</b>	SVWN	6-31+G(d)	-606.0991648	-605.758496
<b>8</b>	PBE	6-31+G(d)	-608.5505046	-608.207008
<b>TS2</b>	PBE	6-31+G(d)	-608.5363114	-608.191721
<b>TS3</b>	PBE	6-31+G(d)	-608.5305766	-608.191791
<b>8</b>	TPSS	6-31+G(d)	-609.4824882	-609.133719
<b>TS2</b>	TPSS	6-31+G(d)	-609.4635568	-609.113957
<b>TS3</b>	TPSS	6-31+G(d)	-609.4567453	-609.112891
<b>8</b>	PBEO	6-31+G(d)	-608.6312922	-608.275855
<b>TS2</b>	PBEO	6-31+G(d)	-608.6113713	-608.254609
<b>TS3</b>	PBEO	6-31+G(d)	-608.6047548	-608.253755
<b>8</b>	TPSSh	6-31+G(d)	-609.4225505	-609.069445
<b>TS2</b>	TPSSh	6-31+G(d)	-609.4017554	-609.047702
<b>TS3</b>	TPSSh	6-31+G(d)	-609.3945158	-609.046292
<b>8</b>	B3LYP	6-31+G(d)	-609.4040822	-609.051273
<b>TS2</b>	B3LYP	6-31+G(d)	-609.3801258	-609.026007
<b>TS3</b>	B3LYP	6-31+G(d)	-609.3746461	-609.026641
<b>8</b>	B3LYP	6-311+G(d,p)	-609.5699427	-609.220259
<b>TS2</b>	B3LYP	6-311+G(d,p)	-609.544991	-609.194025
<b>TS3</b>	B3LYP	6-311+G(d,p)	-609.5414493	-609.196556
<b>8</b>	M052X	6-31+G(d)	-609.278245	-608.917017
<b>TS2</b>	M052X	6-31+G(d)	-609.2558229	-608.893346
<b>TS3</b>	M052X	6-31+G(d)	-609.2453446	-608.889038
<b>8</b>	M052X	6-31+G(d,p)	-609.3149088	-608.955735
<b>TS2</b>	M052X	6-31+G(d,p)	-609.2917627	-608.931264

<b>TS3</b>	M052X	6-31+G(d,p)	-609.2828819	-608.928486
<b>8</b>	M052X	6-311+G(d,p)	-609.4479535	-609.089576
<b>TS2</b>	M052X	6-311+G(d,p)	-609.4253745	-609.066047
<b>TS3</b>	M052X	6-311+G(d,p)	-609.4157618	-609.062261
<b>8</b>	M052X	6-311+G(3df,3pd)	-609.5008887	-609.142252
<b>TS2</b>	M052X	6-311+G(3df,3pd)	-609.4782262	-609.11842
<b>TS3</b>	M052X	6-311+G(3df,3pd)	-609.4680549	-609.114049
<b>8</b>	M06L	6-31+G(d)	-609.2802185	-608.927681
<b>TS2</b>	M06L	6-31+G(d)	-609.2591275	-608.90629
<b>TS3</b>	M06L	6-31+G(d)	-609.2507825	-608.902965
<b>8</b>	M06	6-31+G(d)	-608.9583697	-608.606223
<b>TS2</b>	M06	6-31+G(d)	-608.9361868	-608.583739
<b>TS3</b>	M06	6-31+G(d)	-608.9276137	-608.580598
<b>8</b>	M06	6-31+G(d,p)	-608.9914614	-608.640883
<b>TS2</b>	M06	6-31+G(d,p)	-608.9688934	-608.618043
<b>TS3</b>	M06	6-31+G(d,p)	-608.9612185	-608.615765
<b>8</b>	M06	6-311+G(d,p)	-609.1168415	-608.768016
<b>TS2</b>	M06	6-311+G(d,p)	-609.0933064	-608.744022
<b>TS3</b>	M06	6-311+G(d,p)	-609.0856475	-608.740903
<b>8</b>	M062X	6-31+G(d)	-609.0900345	-608.731727
<b>TS2</b>	M062X	6-31+G(d)	-609.066357	-608.706979
<b>TS3</b>	M062X	6-31+G(d)	-609.0576405	-608.703855
<b>8</b>	M062X	6-31+G(d,p)	-609.1184312	-608.76198
<b>TS2</b>	M062X	6-31+G(d,p)	-609.0942431	-608.736535
<b>TS3</b>	M062X	6-31+G(d,p)	-609.0868846	-608.734866
<b>8</b>	M062X	6-311+G(d,p)	-609.2623396	-608.906309
<b>TS2</b>	M062X	6-311+G(d,p)	-609.2383849	-608.881081
<b>TS3</b>	M062X	6-311+G(d,p)	-609.2303842	-608.879025
<b>8</b>	MP2	6-31+G(d)	-607.2543722	-606.894413
<b>TS2</b>	MP2	6-31+G(d)	-607.2278896	-606.866871
<b>TS3</b>	MP2	6-31+G(d)	-607.2198042	-606.864967
<b>8</b>	MP2	6-311+G(d,p)	-607.6822358	-607.32586
<b>TS2</b>	MP2	6-311+G(d,p)	-607.6574385	-607.300049
<b>TS3</b>	MP2	6-311+G(d,p)	-607.6512606	-607.299595

Tabelle 10.438 Standardorientierung von **8** [globales Minimum; SVWN/6-31+G(d)].

	x	y	z
N	0.8173724821	-1.4039981611	-0.4176968846
C	2.0571732688	-1.1604122534	0.3122047119
C	2.7375518312	0.1096184177	-0.0614676316
C	2.8097590559	1.1544565863	0.7681790502
Li	-0.4042044064	-0.0575852752	0.4905076939
C	-0.2928795573	-0.0836632144	2.5438114639
H	2.7563778255	-2.0239759935	0.1534382757
H	1.7797420597	-1.1230918764	1.3845434273
H	3.2211595294	0.1613881251	-1.0498917744
H	3.3484818381	2.0724536716	0.5006353996
H	2.3220180319	1.1127564131	1.7532030058

H	0.6266745269	0.3786091398	2.9794267983
H	-0.337182642	-1.0954665491	3.0158864464
H	-1.1335890122	0.4740410284	3.0245207571
C	0.2044877029	-2.6189187954	0.0728876422
H	-0.7658607257	-2.7712109267	-0.4314979288
H	0.8578638902	-3.5084700788	-0.1002640051
H	0.0137861189	-2.5039233498	1.1566980665
C	1.0190786515	-1.4705394003	-1.8417677973
H	1.4179771166	-0.5135375582	-2.2232866594
H	1.7300807363	-2.2858164006	-2.12641789
H	0.053267457	-1.6717539342	-2.3403499676
C	-3.054848581	-0.6563089642	0.8910929954
H	-3.9641229632	-1.241573653	0.6376653675
H	-2.529033032	-1.0806185705	1.7617260277
H	-3.3447543516	0.3868645973	1.1374442519
C	-2.6534462587	-0.0335236906	-1.319074038
H	-3.6152965309	-0.4882526194	-1.6373842048
H	-2.8047171036	1.0504204101	-1.1254413952
H	-1.9127232313	-0.1527408543	-2.1293866508
C	0.0881880883	2.143691887	-1.4989356265
H	-0.3906792149	3.0955555803	-1.8138573513
H	1.189466602	2.2877943252	-1.4557414413
H	-0.1462453694	1.3590333743	-2.2388619889
O	-0.4018525409	1.7233086154	-0.2583476019
O	-2.1453817926	-0.6774637246	-0.1851390146
C	-0.1689046901	2.6747753016	0.7553236539
H	0.9122350343	2.926605761	0.8012129844
H	-0.754050919	3.5980731372	0.5596695458
H	-0.4660039246	2.1932084728	1.7034312869

Tabelle 10.439 Standardorientierung von **TS2** [Übergangszustand; SVWN/6-31+G(d)].

	x	y	z
C	-1.4503952767	0.2773458434	-1.792077966
N	-1.8923252938	0.3144781906	-0.4210120111
C	-2.959034555	1.2710476863	-0.2775630275
C	-2.3188297767	-1.0263768126	0.0187399641
C	-1.1691614132	-1.9266883501	0.2740677205
C	-0.5879838828	-1.9589983818	1.5185511931
Li	0.1665643269	-0.1311999347	0.4317336423
C	0.8383407259	-0.2438115174	2.3696151397
H	-0.7046765404	-0.5293325139	-1.9141744731
H	-0.9775092324	1.238225594	-2.0664413061
H	-2.6313866772	2.2674296775	-0.6275224218
H	-3.2617425066	1.3493389029	0.7828755669
H	-3.0420374461	-1.4407770839	-0.7296217193
H	-2.8814789121	-0.8772879594	0.9629857819
H	-0.7222548393	-2.4786628584	-0.5666946959
H	0.2045399671	-2.6789341625	1.7472255421
H	-1.1556213617	-1.6083923436	2.3905368973
H	1.1314449719	-0.9795619933	3.1390468815

H	0.1298631398	0.4685635	2.8419340004
H	1.7547684176	0.3206857967	2.076169197
H	-2.2973861464	0.0696971496	-2.4940868289
H	-3.8592126589	0.9817120812	-0.8752654688
C	2.2620583215	-1.977263349	-0.0572590293
H	1.7182223402	-2.8935736775	-0.3745061998
H	3.3326604486	-2.0767882092	-0.3334027538
H	2.146590722	-1.8342902764	1.0307052142
C	1.8119442156	-0.8697168918	-2.0542024805
H	1.4228117325	0.0859705257	-2.4451468086
H	2.8718121068	-0.9907359813	-2.3647976097
H	1.221389181	-1.7096659218	-2.4834249894
C	2.110598411	2.0744520976	-0.051551743
H	2.2695419113	3.0899305752	-0.4720787966
H	2.5486629233	2.0317685893	0.9688734926
H	2.6052787916	1.3157658016	-0.6781975621
C	0.0509706056	2.6328278328	0.8470091633
H	0.4837475502	2.589358137	1.8692061471
H	0.0961569239	3.6774620629	0.4720975793
H	-0.9947778835	2.287114064	0.8816832732
O	0.7423139919	1.7634488279	-0.0149509575
O	1.7051866767	-0.8352737173	-0.6599305475

Tabelle 10.440 Standardorientierung von **TS3** [Übergangszustand; SVWN/6-31+G(d)].

	x	y	z
C	1.4978214291	-2.0018602454	-1.4719847014
N	0.9256484924	-1.5233976944	-0.2338679486
C	0.6660171079	-2.6499752812	0.6336939743
C	1.7665870306	-0.5521857835	0.4735444541
C	2.2059338424	0.5520835618	-0.3480937692
C	3.327504128	1.2953567582	-0.2158770979
Li	-0.3742664645	-0.006147363	0.2410742375
C	-0.3758093666	-0.1112913705	2.3649826262
H	1.7380300728	-1.1580494581	-2.1397365399
H	0.7818969023	-2.6732581235	-1.9866089889
H	-0.0522956567	-3.346812108	0.1621271351
H	0.2507339726	-2.2980738101	1.5933459247
H	2.5980108191	-1.0468215149	1.0273246821
H	0.8613516915	-0.1989988166	1.4505916793
H	1.4931259339	0.8612356329	-1.1396887329
H	3.5126747615	2.1724569972	-0.8452537015
H	4.0919471752	1.0458347006	0.5309257742
H	-0.8008498636	0.8938127972	2.5685099017
H	0.1493863866	-0.42817918	3.2851265449
H	-1.2390505894	-0.8073688468	2.2510249568
H	2.4408167085	-2.5704553244	-1.287924925
H	1.6083637245	-3.2154985312	0.8407116975
C	-2.3918032677	-1.7530055795	-0.6013641914
H	-3.3438570765	-1.9165946611	-1.1468608327
H	-1.5487025864	-2.1686379669	-1.1776046378

H	-2.4443826942	-2.2613560811	0.3854391073
C	-3.1531144643	0.2617674064	0.3042979311
H	-4.1226251985	0.2105705451	-0.232326779
H	-3.2580692864	-0.2049142075	1.3063106103
H	-2.8356752298	1.3101733138	0.4299282252
C	0.1569205073	2.8355902053	0.6192829727
H	1.1495730731	3.01035657	0.1569836949
H	-0.4135073396	3.7852073718	0.6804271171
H	0.3094771657	2.4113282024	1.6241807566
C	-0.8168919447	2.2926561742	-1.4370554373
H	-1.413228742	1.4989489644	-1.9188727515
H	-1.382163232	3.2480687375	-1.451785086
H	0.1367668149	2.4369331862	-1.9899061398
O	-0.5737757051	1.8809991133	-0.1180255991
O	-2.1424710317	-0.3798992906	-0.4377091435

Tabelle 10.441 Standardorientierung von **8** [globales Minimum; PBE/6-31+G(d)].

	x	y	z
N	0.8967194518	-1.4668744525	-0.3926817644
C	2.1884131138	-1.281565885	0.3243923531
C	2.974250692	-0.0628463217	-0.0880014506
C	3.1869956773	0.9919704306	0.719496399
Li	-0.4309475097	0.0183392752	0.5299718708
C	-0.3425525238	-0.0282395961	2.6312738841
H	2.825316699	-2.1888044075	0.1701329266
H	1.9395714215	-1.2148935097	1.3974683917
H	3.4359448431	-0.0750276252	-1.0858662771
H	3.807202228	1.8394116794	0.4049444991
H	2.7478757331	1.037250655	1.7234485653
H	0.6038334716	0.4029034582	3.0429824053
H	-0.4049516231	-1.0406049533	3.1022771193
H	-1.1494379299	0.5537059882	3.1425665503
C	0.2595168553	-2.6988541549	0.1060677176
H	-0.7169275503	-2.8316695003	-0.3882577796
H	0.8885430782	-3.5988530722	-0.0881561635
H	0.0893082169	-2.5989193545	1.190770427
C	1.0824420063	-1.5563197604	-1.8456079381
H	1.4851331772	-0.6092274611	-2.2407911012
H	1.7750055195	-2.3820477145	-2.1354762087
H	0.1063127915	-1.7458956042	-2.3239561703
C	-3.2563240108	-0.712283447	0.870498331
H	-3.9927409164	-1.506229212	0.630568053
H	-2.6652553919	-0.9727657295	1.7604556503
H	-3.7910217462	0.2407958385	1.0561457093
C	-2.9422391016	-0.1094139264	-1.4002313914
H	-3.7258883011	-0.8205449848	-1.733608858
H	-3.3996744622	0.8913278136	-1.2594981245
H	-2.1601069617	-0.0450866683	-2.1734028557
C	0.1170158606	2.4398698039	-1.5044682146

H	-0.4629470314	3.3340323835	-1.8130680832
H	1.1924737677	2.7059739773	-1.4535162766
H	-0.0238675352	1.6422806243	-2.251147726
O	-0.3450903553	1.9400436174	-0.2548060276
O	-2.3185395434	-0.5621411473	-0.2038787479
C	-0.222849678	2.9119445009	0.7926113353
H	0.8285665322	3.2499985461	0.8865663989
H	-0.873012236	3.7858888	0.5838357241
H	-0.5291017287	2.4031800964	1.7186458478

Tabelle 10.442 Standardorientierung von **TS2** [Übergangszustand; PBE/6-31+G(d)].

	x	y	z
C	-1.9086732693	0.4032532518	-1.9084188488
N	-2.305977223	0.5374788534	-0.5096746972
C	-3.5911398449	1.2282813093	-0.4195081165
C	-2.3884083604	-0.802672513	0.1544910651
C	-1.1036394587	-1.5637224837	0.3134416951
C	-0.5285544931	-1.7975593954	1.5787809476
Li	0.5857823852	-0.2177069412	0.5342260533
C	1.022904518	-0.5189503366	2.5489477532
H	-0.9436509213	-0.1281055951	-1.9667257047
H	-1.7872985575	1.4014555248	-2.3664859003
H	-3.5176338114	2.2267929277	-0.8870910608
H	-3.8707200281	1.3602919971	0.6407905396
H	-3.1415944813	-1.4159841779	-0.4088505471
H	-2.8247492605	-0.6136058181	1.1549444104
H	-0.7587888898	-2.1724352807	-0.5350094322
H	0.1192155186	-2.6719571978	1.7090570558
H	-1.1210544439	-1.5601811436	2.4722739735
H	1.0689270104	-1.2258968229	3.3925274982
H	0.5432516367	0.4164214904	2.9046162952
H	2.0709775162	-0.2869319188	2.2478074626
H	-2.6571402483	-0.1694820453	-2.5131407469
H	-4.4180296651	0.6718237354	-0.927818233
C	2.5899094839	-2.2982476649	-0.2513251488
H	1.9009161123	-3.0829907145	-0.6225634489
H	3.6059854864	-2.4825937878	-0.6534399095
H	2.6109441651	-2.3174187378	0.8479028229
C	2.0585757642	-0.8469805183	-2.0500133727
H	1.7100395612	0.1786694591	-2.2454519452
H	3.0562763403	-0.9954673578	-2.5100754335
H	1.344296179	-1.5719392547	-2.4902115624
C	2.3835489855	2.1736764436	0.4154893758
H	2.6156155531	3.0916137982	-0.1611948445
H	2.515931509	2.3774458993	1.4964262446
H	3.0580258496	1.3595535795	0.1103319576
C	0.0746257057	2.7243200105	0.5007539741
H	0.1524429955	2.9705965823	1.5788267672
H	0.2255485485	3.646852877	-0.0952342737
H	-0.9078369223	2.2728419452	0.2818035191

O	1.0503032402	1.7363402458	0.1394366689
O	2.1304998142	-0.9975892247	-0.6314958534

Tabelle 10.443 Standardorientierung von DTS [Übergangszustand; PBE/6-31+G(d)].

	x	y	z
C	1.6048823986	-1.9627860321	-1.4990072425
N	0.9900641896	-1.4919652608	-0.2460497705
C	0.5571142806	-2.6596931439	0.5367375465
C	1.8966432052	-0.6559940654	0.5981148623
C	2.5362817241	0.4572010709	-0.0948645924
C	3.7322321309	1.0443197951	0.1966361012
Li	-0.3653514671	0.0305261151	0.2965296259
C	-0.1284407907	0.2102846424	2.5137913817
H	1.9536166383	-1.1058728915	-2.0954961752
H	0.8627191804	-2.5309569704	-2.0928791531
H	-0.1785622522	-3.2528915354	-0.0352996083
H	0.0987421926	-2.3301463145	1.4827521656
H	2.6134538746	-1.2838237145	1.1720799343
H	0.9563078882	-0.1717468807	1.5558587495
H	1.9316780468	0.9328887104	-0.8881625945
H	4.0588061132	1.958826229	-0.3091124314
H	4.4034870981	0.6332409348	0.9603752893
H	-0.8390905004	1.0579970949	2.380853394
H	0.5613569914	0.5227913083	3.3211531579
H	-0.7097726455	-0.6480206215	2.9110461596
H	2.4807095494	-2.6224811845	-1.3025850975
H	1.4192127603	-3.3238440367	0.7842564685
C	-2.6262453315	-1.6791374697	-0.9488756721
H	-3.5180093155	-1.4849492685	-1.5779482321
H	-1.7606585066	-1.9032106469	-1.5900538448
H	-2.8302197443	-2.5450186847	-0.287980359
C	-3.3381703121	-0.1397203387	0.7125773481
H	-4.266321124	0.0876942784	0.151374446
H	-3.5386133137	-0.9462131347	1.4446779726
H	-2.9946709034	0.7579593191	1.2464494661
C	0.1716826927	3.0139593749	0.2412352872
H	0.9792519958	3.3735483211	-0.4248316428
H	-0.5198158054	3.848654903	0.4708339505
H	0.6135137098	2.6191010513	1.1665911758
C	-1.1286509738	2.3103115111	-1.6193379427
H	-1.6895435386	1.4384011982	-1.9879857169
H	-1.821881786	3.1651371645	-1.4858927694
H	-0.3458864974	2.5923311294	-2.3520503231
O	-0.5468808909	1.9341137062	-0.3717508775
O	-2.2889229615	-0.5202166628	-0.1844734369

Tabelle 10.444 Standardorientierung von **8** [globales Minimum; TPSS/6-31+G(d)].

	x	y	z
N	0.9127904035	-1.4670890277	-0.4032988991
C	2.1959205932	-1.322976144	0.3525425089
C	3.0339732736	-0.1352997685	-0.0541958893
C	3.2568230379	0.9214537863	0.7442675785
Li	-0.4217546554	0.0542184478	0.4934138854
C	-0.3307327243	-0.000615045	2.604165865
H	2.7967363748	-2.2490255428	0.220165578
H	1.9174040489	-1.2360075292	1.4096813342
H	3.520208063	-0.1773362168	-1.0327091654
H	3.9075621463	1.7409810632	0.4373415834
H	2.7955848013	0.9950873572	1.7295196503
H	0.6066100448	0.4362268661	3.021509647
H	-0.3846916413	-1.0114199569	3.0724338161
H	-1.141821368	0.5701896058	3.1149303494
C	0.2346688397	-2.6917169048	0.0794126719
H	-0.7228613723	-2.8020387868	-0.4429122898
H	0.8510540457	-3.5959323537	-0.0975701312
H	0.0411192773	-2.5843618304	1.1530048596
C	1.143362097	-1.57305765	-1.8550102135
H	1.5789890046	-0.6418173572	-2.2361665863
H	1.8205432039	-2.4130608557	-2.1121648286
H	0.181283675	-1.7411692145	-2.3556459621
C	-3.2445059188	-0.7353256472	0.8981238834
H	-3.9463318934	-1.5535743014	0.6673612875
H	-2.6214608909	-0.9752715265	1.7630434559
H	-3.8074305375	0.1911142673	1.0942789581
C	-3.0154933125	-0.1165820205	-1.3872004686
H	-3.7745812866	-0.8576878359	-1.6878301708
H	-3.5026394507	0.859791661	-1.230266513
H	-2.2608856338	-0.0271984836	-2.175486499
C	0.0982639612	2.5119683621	-1.5255921606
H	-0.526507222	3.370141675	-1.8240939617
H	1.1521759927	2.8293912059	-1.471331221
H	-0.0051133601	1.710205501	-2.2639042978
O	-0.3362473427	1.9852989026	-0.2703455396
O	-2.3370242441	-0.5422703109	-0.2037027929
C	-0.2612014537	2.96506703	0.7827513929
H	0.7668224739	3.3510347269	0.8689532745
H	-0.9522436806	3.7974468683	0.5711643606
H	-0.5414023696	2.4410259834	1.7000606496

Tabelle 10.445 Standardorientierung von **TS2** [Übergangszustand; TPSS/6-31+G(d)].

	x	y	z
C	-1.7064572207	-0.0756128899	-1.919703209
N	-1.9859335811	0.237001223	-0.5079324824
C	-3.0769290471	1.2248088804	-0.4418709502
C	-2.3842249046	-1.0425464486	0.2277704701
C	-1.2273080455	-1.9228094208	0.5647360766

C	-0.6016490187	-1.8525261882	1.8287787543
Li	0.1555804679	-0.1632050951	0.4455266235
C	0.9124697057	-0.4304854841	2.4552780064
H	-0.9443311936	-0.8636067118	-1.9674763375
H	-1.3302333173	0.8193109345	-2.4342860266
H	-2.796227054	2.1335374003	-0.9929911182
H	-3.2689095286	1.4896629724	0.6066406932
H	-3.153100145	-1.5562514925	-0.3867535112
H	-2.8763124375	-0.6973320293	1.1512615687
H	-0.8523421613	-2.6157744633	-0.1918435129
H	0.0542449245	-2.6748655135	2.115903655
H	-1.1969562131	-1.4747953859	2.6645510381
H	1.0294633097	-0.9677850742	3.404669924
H	0.5304906722	0.5823020842	2.687023385
H	1.9148789155	-0.3403260807	1.9923152425
H	-2.6124328545	-0.4357983955	-2.4511130096
H	-4.0189291067	0.8363824571	-0.8808430787
C	2.2161610402	-2.2005435499	-0.5067801954
H	1.7305560472	-2.9440320666	-1.1581745623
H	3.3082410751	-2.2429677535	-0.6476147507
H	1.9622750586	-2.3953996153	0.5376477907
C	2.0086244143	-0.4931045145	-2.1518321877
H	1.6077744732	0.5167190231	-2.2770953161
H	3.095678533	-0.4912416252	-2.3347467679
H	1.5233847814	-1.1806479801	-2.8636612282
C	2.317296259	2.140334911	0.462760095
H	2.6379759288	3.0526397802	-0.0670175522
H	2.473571192	2.2644631096	1.5452187475
H	2.8852191152	1.277039209	0.1075824412
C	0.0947118591	2.9377021704	0.6355173411
H	0.2101932653	3.085389743	1.721335903
H	0.348659577	3.8729897034	0.1099957333
H	-0.9316453645	2.6440811046	0.4065329559
O	0.9352367928	1.8674555732	0.1812868559
O	1.7308877865	-0.8808715006	-0.801450504

Tabelle 10.446 Standardorientierung von **TS3** [Übergangszustand; TPSS/6-31+G(d)].

	x	y	z
C	1.6278581858	-1.9722895656	-1.4833008085
N	1.0025291311	-1.4870815168	-0.2339211503
C	0.5729881094	-2.6563043221	0.5600866808
C	1.9165442696	-0.648470046	0.6172940061
C	2.5794549786	0.4413200661	-0.0939128414
C	3.7862441396	1.0066070019	0.1881207367
Li	-0.359346108	0.028974576	0.2729976785
C	-0.1452486786	0.2337517153	2.5097587999
H	1.9687768383	-1.1217304124	-2.0826443081
H	0.891254916	-2.5479753561	-2.0658947121
H	-0.1546040421	-3.2507942103	-0.0100175595
H	0.1132304284	-2.3183324204	1.495499208

H	2.6164708201	-1.2821775975	1.1930666618
H	0.9466732133	-0.1488786369	1.5660476533
H	1.9876478873	0.9143798012	-0.8897275089
H	4.1290637079	1.9022632639	-0.3291684506
H	4.4465026768	0.59814929	0.9547005934
H	-0.8389089712	1.0859001706	2.3530181267
H	0.52531606	0.5383366672	3.3295798449
H	-0.7435563389	-0.6155479987	2.8884420278
H	2.5003467121	-2.6203766929	-1.2736085344
H	1.4349060257	-3.3074072692	0.8112977471
C	-2.6447062649	-1.6776568142	-0.9776854685
H	-3.5220562161	-1.4534810049	-1.6051347391
H	-1.778482042	-1.8942252951	-1.6088481584
H	-2.8652269701	-2.54485088	-0.3358457461
C	-3.359791098	-0.1577389029	0.7125902308
H	-4.2663937479	0.0957228021	0.1406245234
H	-3.5800425713	-0.9778372136	1.4127445428
H	-3.0075910494	0.714879421	1.2678497832
C	0.1991104271	3.0054370328	0.2191428577
H	0.9265968248	3.4412013156	-0.4815201511
H	-0.513283113	3.7780176364	0.5479030702
H	0.7216629656	2.5767948645	1.0767013096
C	-1.1958757978	2.3434019637	-1.6007549414
H	-1.7268233414	1.4680529324	-1.9852624522
H	-1.9173042669	3.1423896343	-1.3656958383
H	-0.476535834	2.7098714082	-2.350233379
O	-0.5128842109	1.9232643583	-0.4131860361
O	-2.2984696551	-0.5349607658	-0.1818162985

Tabelle 10.447 Standardorientierung von **8** [globales Minimum; PBE0/6-31+G(d)].

	x	y	z
N	0.8877634247	-1.4528650393	-0.387790274
C	2.1609301183	-1.2842512429	0.3328849731
C	2.9455054419	-0.0678672805	-0.0635287485
C	3.1061028796	0.9918908592	0.7307924478
Li	-0.4177220669	0.0289395928	0.5196778037
C	-0.3363741646	-0.0060953081	2.6108168642
H	2.7918228514	-2.183493989	0.1784076514
H	1.9109173653	-1.2232739626	1.3972731921
H	3.4420357288	-0.0851459063	-1.0348850246
H	3.7178199556	1.8402029082	0.4307893188
H	2.6275985237	1.0406334771	1.7071337859
H	0.5751111077	0.4625429505	3.0370041655
H	-0.367612345	-1.0106750142	3.0824926027
H	-1.1732757895	0.5414616185	3.0933302889
C	0.2339553331	-2.6655384481	0.0955588838
H	-0.7337140294	-2.7817286412	-0.401672715
H	0.8452293587	-3.5665311989	-0.0980627179

H	0.0599068421	-2.5730715434	1.1718935209
C	1.0796308504	-1.5336390546	-1.8269441565
H	1.5073079658	-0.6020894403	-2.2094133509
H	1.747658783	-2.367496849	-2.1152591023
H	0.1109652277	-1.6920873065	-2.3129060876
C	-3.184239554	-0.8157454995	0.8666760448
H	-3.8998932467	-1.5971982339	0.5709236601
H	-2.5790539272	-1.1409095136	1.7140594257
H	-3.7348877832	0.0918089808	1.152185286
C	-2.9397503015	-0.0024654279	-1.3201562338
H	-3.7109446643	-0.6915062957	-1.6959552654
H	-3.4091696092	0.9630541238	-1.0808535031
H	-2.1874279004	0.1498519902	-2.0980753033
C	0.1587329285	2.3719523699	-1.5280518606
H	-0.4192372172	3.2427813133	-1.8723667033
H	1.221173171	2.6489847963	-1.4657880357
H	0.0440012977	1.5588637872	-2.2494482334
O	-0.315887739	1.9125607595	-0.2866122475
O	-2.2885440595	-0.5415383577	-0.1959009191
C	-0.2192847378	2.8979408611	0.726673142
H	0.8202640272	3.2397062314	0.8321868171
H	-0.8609883293	3.758291263	0.4855703054
H	-0.5394607178	2.4235546704	1.6560393027

Tabelle 10.448 Standardorientierung von TS2 [Übergangszustand; PBE0/6-31+G(d)].

	x	y	z
C	-1.9001744544	0.3256561293	-1.9107941714
N	-2.2692484126	0.5091929712	-0.5229439175
C	-3.518161329	1.2386921645	-0.432812245
C	-2.3785998148	-0.789904168	0.1759613484
C	-1.1148331068	-1.57431415	0.331042955
C	-0.5372799846	-1.8022938733	1.5792573292
Li	0.5609336189	-0.2119437185	0.524148195
C	1.0246402754	-0.5264432145	2.5202167613
H	-0.9567061392	-0.2256822738	-1.9720714342
H	-1.7636949262	1.2991875193	-2.396724292
H	-3.4236250285	2.2115861331	-0.9301437946
H	-3.7727302245	1.4141523874	0.6187355247
H	-3.152417183	-1.3967118149	-0.3455977997
H	-2.7816057776	-0.5665385694	1.1734784993
H	-0.7747317609	-2.1736561317	-0.5150744874
H	0.1129679487	-2.6638742623	1.7073592872
H	-1.1051989172	-1.5498902182	2.473696299
H	1.0893582985	-1.2389538413	3.3487277024
H	0.5522673405	0.3937171934	2.9021212501
H	2.061463865	-0.2799251248	2.2199027012
H	-2.6659252211	-0.2404763757	-2.4807606299
H	-4.364348053	0.6980924336	-0.9033318537
C	2.5419489577	-2.2525183713	-0.2659678595
H	1.8913241816	-3.0400111744	-0.672432226

H	3.5675874208	-2.407352032	-0.6300945686
H	2.5251743868	-2.2932310024	0.8244306377
C	2.050516877	-0.7895637485	-2.0373226582
H	1.6857257747	0.2227021601	-2.2261886145
H	3.0598108084	-0.8999782512	-2.4596716237
H	1.3801630087	-1.516566891	-2.5187533848
C	2.3515699705	2.1370264317	0.4361184031
H	2.6034533376	3.0416599085	-0.1360936937
H	2.4721366003	2.341640384	1.5089245871
H	3.0166806372	1.3207494266	0.1474932278
C	0.0735904585	2.7110158852	0.4924750491
H	0.1367685477	2.9525558234	1.5633079928
H	0.2425629622	3.6264007287	-0.0930239142
H	-0.9052977166	2.282570274	0.2613651657
O	1.0308140747	1.7245038667	0.1487646804
O	2.0727726986	-0.9719816139	-0.6385774278

Tabelle 10.449 Standardorientierung von **TS3** [Übergangszustand; PBE0/6-31+G(d)].

	x	y	z
C	1.5412515536	-1.9819829502	-1.510865643
N	0.9691221211	-1.5142210024	-0.2526657374
C	0.6160833842	-2.67196607	0.5606274803
C	1.8717648603	-0.640044157	0.5308293826
C	2.4204258409	0.4834864942	-0.2107795341
C	3.590163974	1.1239806176	0.0024525076
Li	-0.3819734919	-0.0142280517	0.3286972371
C	-0.0655970913	0.1305725646	2.5405096031
H	1.82415634	-1.133812544	-2.1390846133
H	0.8065794229	-2.5909487786	-2.0557670555
H	-0.1113812453	-3.3015765196	0.0347773362
H	0.1858419211	-2.3473456108	1.5114652271
H	2.6462558577	-1.2246025063	1.0565630892
H	0.962234108	-0.1920042353	1.540270226
H	1.76483657	0.9053198564	-0.9819057412
H	3.8518273112	2.0260740903	-0.5443940319
H	4.3094097766	0.7679992302	0.737881897
H	-1.0346638524	0.6496395223	2.4093330673
H	0.5430369608	0.7860413189	3.1805530573
H	-0.2730938681	-0.7767872546	3.1273933967
H	2.4445712181	-2.5946226105	-1.3407300215
H	1.505858774	-3.2913981783	0.7816842227
C	-2.6041973385	-1.7414381748	-0.8346131567
H	-3.4372770616	-1.6134708611	-1.5403107806
H	-1.7203362728	-2.089399257	-1.371968094
H	-2.8870309163	-2.4836752201	-0.0749267549
C	-3.3518008926	0.0618536812	0.4752525601
H	-4.2091421562	0.2224842039	-0.1936985765
H	-3.6570597004	-0.587440692	1.3071995443
H	-3.0109467318	1.0210120886	0.8686811735
C	0.0626586504	2.9418197526	0.4809823197

H	0.994970941	3.2220603892	-0.025197976
H	-0.592341745	3.8202645668	0.5660291918
H	0.2984383933	2.5504397835	1.4708978414
C	-0.9342744628	2.2842850264	-1.546614572
H	-1.460707001	1.4428485219	-2.0025988704
H	-1.5903317373	3.1665745684	-1.5442185883
H	-0.0304539921	2.514456094	-2.1291315975
O	-0.6016616817	1.9076787721	-0.2280983763
O	-2.2691687403	-0.5073274689	-0.2352236394

Tabelle 10.450 Standardorientierung von **8** [globales Minimum; TPSSh/6-31+G(d)].

	x	y	z
N	0.9080521727	-1.4628065957	-0.3999648967
C	2.1843460645	-1.3168571798	0.3511823833
C	3.0166143533	-0.1290600691	-0.0557268659
C	3.2301922684	0.9278752909	0.7377551918
Li	-0.4194992817	0.0535546394	0.4943870668
C	-0.3277496959	0.0002642386	2.6000488666
H	2.7872289205	-2.2381459275	0.2200218216
H	1.9096683125	-1.2298779927	1.4065783182
H	3.5048629921	-0.1708795362	-1.0301485864
H	3.8754525311	1.7481777809	0.4308867776
H	2.7660142187	1.0012317854	1.718711091
H	0.6005191471	0.4463155322	3.0199051135
H	-0.3734722924	-1.0080184522	3.0676092557
H	-1.1454798276	0.5620332965	3.1038449206
C	0.2301153855	-2.6795420517	0.0824545063
H	-0.7264264186	-2.7888685161	-0.4363198897
H	0.8419165132	-3.5833203135	-0.0943230931
H	0.0383882889	-2.5733038531	1.153775721
C	1.1345922795	-1.5675464697	-1.8458383949
H	1.5693366247	-0.6395531144	-2.2282618529
H	1.8088473624	-2.4057730416	-2.1037324027
H	0.1745943439	-1.7344174065	-2.3450505712
C	-3.2242733332	-0.752943495	0.889182236
H	-3.9279609725	-1.5611574026	0.6428485205
H	-2.6068633908	-1.0135671681	1.7486865012
H	-3.7829666241	0.1679298748	1.1063298461
C	-2.9939074519	-0.0916649147	-1.372446698
H	-3.7542732708	-0.8212215877	-1.6872648243
H	-3.4760818518	0.8809870738	-1.1986445495
H	-2.242315781	0.0099552739	-2.1584144225
C	0.1022086171	2.4856799118	-1.5218337426
H	-0.5120920554	3.3452404991	-1.8273466217
H	1.1556851156	2.7940270483	-1.4664814432
H	-0.0039685274	1.6843380519	-2.2562449806
O	-0.3386966627	1.9733859586	-0.2716692707
O	-2.3224031783	-0.5401483805	-0.2028955042
C	-0.2607789663	2.951664092	0.7715953511

H	0.7670242145	3.3292749599	0.8608674342
H	-0.9416934911	3.7871776838	0.5544530958
H	-0.547791653	2.4393694767	1.6901835919

Tabelle 10.451 Standardorientierung von **TS2** [Übergangszustand; TPSSh/6-31+G(d)].

	x	y	z
C	-1.6966953525	-0.0744331737	-1.9110964789
N	-1.9816968753	0.2350410182	-0.5063998092
C	-3.0633492811	1.2233277289	-0.4423790235
C	-2.380750166	-1.0326681239	0.2239831693
C	-1.2279267931	-1.917207937	0.5574267756
C	-0.606656277	-1.8543373432	1.8162127126
Li	0.1579267192	-0.1617864791	0.4469776904
C	0.9089262779	-0.4277520627	2.4475918899
H	-0.936466655	-0.8602412032	-1.9590261617
H	-1.3190983015	0.8186000444	-2.422172523
H	-2.7790791503	2.1287547168	-0.9916140478
H	-3.2568086911	1.4898378243	0.6025941176
H	-3.1517567329	-1.5448393952	-0.3842486741
H	-2.867361646	-0.6918993722	1.1485827168
H	-0.8519778413	-2.6026534277	-0.2015820682
H	0.0540513768	-2.6701696923	2.099244172
H	-1.1940733496	-1.4740762511	2.6523141383
H	1.0236929834	-0.9722895493	3.3904799337
H	0.5248407246	0.5791747311	2.6898824126
H	1.9130275118	-0.3254126128	1.9966973497
H	-2.5978783587	-0.4323463047	-2.4458061132
H	-4.0038390825	0.8402776916	-0.881757127
C	2.2128347178	-2.1822534225	-0.4957245474
H	1.7412708989	-2.9350455423	-1.14200708
H	3.3032373423	-2.2144027031	-0.6301837993
H	1.9580014416	-2.3740043775	0.5463460627
C	1.9963393378	-0.4943898845	-2.1444946582
H	1.5876144147	0.5082886362	-2.2789532144
H	3.0813183448	-0.4815929156	-2.3222734113
H	1.524196598	-1.1876844288	-2.8551711251
C	2.306155917	2.1261193102	0.4477206644
H	2.6242205434	3.0348047115	-0.0839397465
H	2.4726014099	2.251315597	1.5256234876
H	2.8706807787	1.2647582426	0.0905520962
C	0.0959350597	2.9200724316	0.6417229069
H	0.2217698294	3.067320525	1.7235156398
H	0.3416695852	3.8543807119	0.1164990472
H	-0.9310975936	2.6290664049	0.4251627516
O	0.9288562758	1.8575641205	0.1806643119
O	1.7169980587	-0.8779272443	-0.8018174381

Tabelle 10.452 Standardorientierung von **TS3** [Übergangszustand; TPSSh/6-31+G(d)].

	x	y	z
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C	1.61766168	-1.9727210939	-1.47372673
N	0.996690552	-1.486525105	-0.2305364541
C	0.5661708093	-2.6474752661	0.5630351298
C	1.9062583969	-0.6496816775	0.6145427482
C	2.5620155246	0.4400326389	-0.099022952
C	3.7629573372	1.0076838745	0.1774612521
Li	-0.3576826879	0.0299104007	0.2759518728
C	-0.1406649187	0.237163044	2.5053869029
H	1.9564976346	-1.1271634811	-2.0766626574
H	0.8841178853	-2.5503792447	-2.0530103656
H	-0.1623305461	-3.2406919953	-0.0021133305
H	0.1101438403	-2.3086891789	1.4968315298
H	2.6113936999	-1.2793014029	1.1832278338
H	0.9424985573	-0.147777557	1.5667085872
H	1.9690301127	0.9070491014	-0.8935637757
H	4.1022791925	1.8989967522	-0.3440207112
H	4.4242259554	0.6044959125	0.9421864923
H	-0.8288383243	1.0899313196	2.3481438614
H	0.5277513368	0.5383442914	3.3247146993
H	-0.7422441798	-0.6068401907	2.8829588722
H	2.4890248255	-2.6173456559	-1.2639087229
H	1.4239297935	-3.2991746953	0.8137247975
C	-2.619596175	-1.6677622453	-0.9794695772
H	-3.4855440291	-1.4401033473	-1.6164992798
H	-1.7490428549	-1.8865285038	-1.5993106252
H	-2.851217688	-2.5348100002	-0.3462926888
C	-3.3455717608	-0.1584318856	0.7007903255
H	-4.2427812161	0.1019694785	0.1225964093
H	-3.5783520571	-0.9778629472	1.3932187045
H	-2.9984578203	0.7077562153	1.2641870804
C	0.2016096312	2.9914553736	0.2218751678
H	0.9245429068	3.42950793	-0.4777390292
H	-0.5070225467	3.7614949634	0.555275942
H	0.7276722442	2.5643156662	1.0747458244
C	-1.1951674961	2.3363252325	-1.5845451072
H	-1.7256130634	1.4646236864	-1.97055455
H	-1.9156611694	3.1309483804	-1.3451897044
H	-0.4832379163	2.706223155	-2.3352404148
O	-0.5085755879	1.9173247355	-0.4081625645
O	-2.2828218784	-0.5356876783	-0.1787077927

Tabelle 10.453 Standardorientierung von **TS3** [Übergangszustand; B3LYP/6-31+G(d)].

	x	y	z
N	0.9048791619	-1.4611760926	-0.3827168478
C	2.200784063	-1.3108968898	0.3280200281
C	3.0063253022	-0.0996766058	-0.0660787898
C	3.2388604277	0.9327367227	0.7504735445
Li	-0.4337119162	0.044543714	0.5431386506
C	-0.35131098	0.0068610697	2.639294815

H	2.8158078273	-2.2175608314	0.1549395491
H	1.9663997506	-1.2601182674	1.3951647124
H	3.4614941784	-0.1048146873	-1.0572771066
H	3.8670252175	1.7675840085	0.4468117517
H	2.8065899152	0.9751715364	1.747924221
H	0.5835097726	0.4465108679	3.0475758658
H	-0.4048893054	-0.9998229221	3.1061469117
H	-1.1628720864	0.5788473354	3.1378849904
C	0.2441199055	-2.6849277867	0.0982775352
H	-0.7307853901	-2.7868779641	-0.3874252306
H	0.8460330947	-3.5873917542	-0.1170245325
H	0.0864913284	-2.6068254737	1.177400956
C	1.0767596913	-1.5290610466	-1.8363633884
H	1.5000451316	-0.5947359106	-2.2157867523
H	1.7388512887	-2.3614399798	-2.1427984378
H	0.1003556272	-1.6814200738	-2.3082715469
C	-3.2445854889	-0.7911112301	0.8740952571
H	-3.9074474876	-1.6206530477	0.5863896528
H	-2.6461580064	-1.0528514325	1.7469811087
H	-3.8506513821	0.0966020161	1.1049444449
C	-2.965085435	-0.0431633049	-1.3575865715
H	-3.6779922397	-0.7909846829	-1.7364712779
H	-3.5003341118	0.8995036394	-1.1703178711
H	-2.1900201524	0.1273986912	-2.1087282235
C	0.1427174601	2.4185674446	-1.5339172256
H	-0.4960982135	3.2435312891	-1.8840709834
H	1.1846741037	2.7669342353	-1.4851989707
H	0.0755026626	1.5869909882	-2.2398141062
O	-0.2923164561	1.9431779522	-0.2714759018
O	-2.3240022115	-0.5061869137	-0.1807779137
C	-0.2555165646	2.9505794951	0.7411971159
H	0.761267189	3.3566638389	0.8394852226
H	-0.9510334234	3.7656952435	0.4920588032
H	-0.5467172478	2.4636058095	1.6725955412

Tabelle 10.454 Standardorientierung von **TS2** [Übergangszustand; B3LYP/6-31+G(d)].

	x	y	z
C	-2.01955173	0.3409171406	-1.9508668578
N	-2.3384864033	0.6222719012	-0.5567253937
C	-3.5859239202	1.3738801162	-0.4669045824
C	-2.42660847	-0.6350197653	0.2433941502
C	-1.166519841	-1.4400225518	0.3953186567
C	-0.6073484222	-1.6999034137	1.6603921511
Li	0.6217220013	-0.2482423486	0.530533723
C	1.0161094478	-0.5605080631	2.5644955729
H	-1.0759784684	-0.2100228296	-2.0082484642
H	-1.9087825857	1.2793233287	-2.50794852
H	-3.5023817312	2.3100437098	-1.0323506488
H	-3.7959078243	1.622139306	0.5800034211
H	-3.2368126784	-1.2572653663	-0.2005276512

H	-2.7796407398	-0.3328896321	1.2389119466
H	-0.8968820349	-2.1112065091	-0.4219020775
H	-0.0449952668	-2.6209803356	1.7967532607
H	-1.1767059332	-1.4170808192	2.5452989451
H	1.0264515857	-1.2280600447	3.4309946935
H	0.640206913	0.4227311168	2.8897135389
H	2.0631420423	-0.4418809123	2.2260886061
H	-2.8035076417	-0.2658956152	-2.4511574276
H	-4.455694263	0.8121028512	-0.8655539939
C	2.5508398111	-2.4089129155	-0.2656731666
H	1.8973189009	-3.1798480124	-0.6976411358
H	3.5804686936	-2.5659082032	-0.617199507
H	2.5181984391	-2.4695969121	0.8230755997
C	2.0932533135	-0.8900372146	-2.0307852242
H	1.7377501463	0.1287907591	-2.1975814937
H	3.1078259565	-0.9989496685	-2.4405507378
H	1.4223925637	-1.6014808422	-2.5332248767
C	2.4894578125	2.0765216943	0.4427536974
H	2.7791031517	2.9226257087	-0.1971044102
H	2.5853568929	2.3683728281	1.4975304514
H	3.1382428843	1.2221495852	0.2411960159
C	0.2006890242	2.7123705299	0.3697599566
H	0.2300867709	3.0434152248	1.4177914646
H	0.418917367	3.5678493279	-0.2858630777
H	-0.777879248	2.2860717861	0.1333791384
O	1.155436701	1.6703700119	0.1505784047
O	2.097395783	-1.1055949511	-0.6237031478

Tabelle 10.455 Standardorientierung von **TS3** [Übergangszustand; B3LYP/6-31+G(d)].

	x	y	z
C	1.5894301116	-1.9494583035	-1.4786951995
N	0.9850379297	-1.4738219252	-0.2251186874
C	0.5314590599	-2.6359419696	0.5502195075
C	1.9015141642	-0.6544302377	0.6257914318
C	2.5748667494	0.4390376761	-0.0648099488
C	3.7793871003	0.9840596847	0.2285348682
Li	-0.3745334513	0.0442507738	0.3100555583
C	-0.0876901966	0.2952718275	2.5282978307
H	1.9336429006	-1.1037086501	-2.0781956611
H	0.847835995	-2.5132915997	-2.0619468559
H	-0.2075871961	-3.2093598091	-0.0219315081
H	0.0791737565	-2.3092347684	1.4896876469
H	2.5982437556	-1.2952273347	1.1924573615
H	0.9573676732	-0.129727412	1.5821092383
H	1.9941743132	0.9288589001	-0.853794511
H	4.135226255	1.8796739289	-0.2743097797
H	4.4309722626	0.5572876854	0.9892008307
H	-0.8392234583	1.0877553957	2.3491679354
H	0.5940431506	0.6973999807	3.2912657401
H	-0.6118104044	-0.5584397266	2.9877945913

H	2.4561147258	-2.6072340773	-1.2871922878
H	1.3747542924	-3.3095271917	0.7936097398
C	-2.6137539377	-1.5790786924	-1.0381640907
H	-3.4486565158	-1.2407402061	-1.6687911262
H	-1.7298346257	-1.7474751137	-1.6560614993
H	-2.8958340385	-2.5171892923	-0.5400251167
C	-3.3469936952	-0.2782498148	0.8089005233
H	-4.2070239206	0.1199250478	0.2519241063
H	-3.6548937267	-1.1766882296	1.3611921827
H	-2.9812275697	0.4700504497	1.5131219274
C	0.1722448501	3.0110246073	0.1721389578
H	0.917937508	3.4293715798	-0.5165336955
H	-0.5498795309	3.7907392096	0.4516920929
H	0.6732228732	2.6268599051	1.0603514663
C	-1.1703566326	2.2696815524	-1.6423847156
H	-1.6821840329	1.3784031523	-2.0104810282
H	-1.9090932745	3.0627545237	-1.4568080349
H	-0.4487536061	2.6189967556	-2.3946652671
O	-0.5075131014	1.9100074451	-0.437409388
O	-2.2737585121	-0.5819867269	-0.0809081355

Tabelle 10.456 Standardorientierung von **8** [globales Minimum; B3LYP/6-311+G(d,p)].

	x	y	z
N	0.8993936756	-1.4470722955	-0.3881482799
C	2.1906125463	-1.2912998523	0.3279500851
C	2.9925010248	-0.0803137797	-0.0648161503
C	3.2379027823	0.9396974964	0.7544052607
Li	-0.4557785513	0.0542335644	0.5350115141
C	-0.3661047298	-0.000389803	2.6423333321
H	2.8092409731	-2.1931509428	0.1598954984
H	1.9530618935	-1.2383280469	1.3918002454
H	3.4322818277	-0.0760587715	-1.0599565327
H	3.8625779934	1.7728509315	0.4493282184
H	2.8218171673	0.9718223729	1.756171786
H	0.5793573958	0.4072212549	3.0497823568
H	-0.4478978519	-1.0020353027	3.1075141207
H	-1.1542299475	0.5921337789	3.146912502
C	0.2369897645	-2.6677675501	0.0967154762
H	-0.7343881491	-2.771957265	-0.3897470948
H	0.8375662375	-3.5692565612	-0.1113212651
H	0.0752882449	-2.5838343324	1.1721584486
C	1.0787566182	-1.5217398856	-1.8401301317
H	1.5015412838	-0.5916445529	-2.2229259857
H	1.7415658746	-2.3525142306	-2.1387211291
H	0.108176349	-1.6778981131	-2.3166974612
C	-3.259790422	-0.7796901297	0.8726658436
H	-3.8818179767	-1.644371394	0.6087356669
H	-2.6653848329	-0.9837600752	1.7609037991
H	-3.9054290646	0.086433491	1.0623202956

C	-2.9763026852	-0.0980871282	-1.3803973668
H	-3.6532759717	-0.882823163	-1.7424498151
H	-3.5497862643	0.8264031133	-1.2356355309
H	-2.2019078368	0.0766368429	-2.1276778986
C	0.1294232951	2.4240445037	-1.5280257523
H	-0.4983001139	3.2654204928	-1.8495634432
H	1.1779071784	2.7469025264	-1.5131193668
H	0.0193099967	1.6051430758	-2.2395060127
O	-0.2736706407	1.9480005815	-0.2556087486
O	-2.3356649125	-0.493962538	-0.179629451
C	-0.1801998216	2.9460202021	0.7631213735
H	0.8456435171	3.3275415944	0.8314233491
H	-0.8626242808	3.7772664559	0.5451840698
H	-0.4513965861	2.4599924345	1.6984431746

Tabelle 10.457 Standardorientierung von **TS2** [Übergangszustand; B3LYP/6-311+G(d,p)].

	x	y	z
C	-2.0690720073	0.3247454481	-1.9601983279
N	-2.3518156279	0.6299866207	-0.5639342096
C	-3.5911682363	1.3907638082	-0.4535052192
C	-2.4270647443	-0.6135817366	0.2576675733
C	-1.1688103791	-1.4208701628	0.3979298833
C	-0.6154316733	-1.6963398692	1.6614353888
Li	0.6395297505	-0.2585121746	0.5292733499
C	1.0146463296	-0.5962658703	2.5648586728
H	-1.1343549319	-0.2340585253	-2.0331500244
H	-1.9649234642	1.2503400445	-2.5343938973
H	-3.5189785836	2.3145490126	-1.0353848016
H	-3.7721210399	1.6578935041	0.5912817966
H	-3.2469085837	-1.23749729	-0.1586244272
H	-2.7580151337	-0.2974211535	1.2534138165
H	-0.9173702212	-2.0996877992	-0.4143787312
H	-0.0732149625	-2.626931587	1.792303974
H	-1.186242421	-1.4189874646	2.5436437212
H	1.0195619432	-1.2502710848	3.4371243659
H	0.6727476859	0.3993032338	2.8777408927
H	2.05335742	-0.5154415582	2.2025679332
H	-2.8675627197	-0.2818734436	-2.4302400027
H	-4.4724318384	0.8295351406	-0.8180362242
C	2.5709530103	-2.4184119054	-0.2783039819
H	1.9277499845	-3.18219962	-0.7312883462
H	3.6021212471	-2.5634305995	-0.622048015
H	2.5300400206	-2.5061694917	0.8058649195
C	2.1284316613	-0.8612559752	-2.0135115438
H	1.7709900957	0.1568665463	-2.1628742912
H	3.1462083426	-0.955184654	-2.41164155
H	1.4697583805	-1.5610931668	-2.5418344475
C	2.4934785082	2.0779651902	0.4584363757
H	2.7870418692	2.903275865	-0.2018901918
H	2.5807392747	2.4010924716	1.5020831532

H	3.1470367689	1.2231648601	0.2897638338
C	0.2027805978	2.7041000798	0.3377985711
H	0.2152773313	3.0702237679	1.3716528689
H	0.4262718119	3.5365048281	-0.3408369705
H	-0.7699937301	2.2693226758	0.102099968
O	1.163750922	1.6585674943	0.1675054769
O	2.1137663424	-1.1100754593	-0.6119203323

Tabelle 10.458 Standardorientierung von **TS3** [Übergangszustand; B3LYP/6-311+G(d,p)].

	x	y	z
C	1.5883500598	-1.9616103659	-1.4854520199
N	0.9824353492	-1.4858938272	-0.2334078479
C	0.5247413833	-2.6458291862	0.5416304684
C	1.8982169105	-0.6680168671	0.6166288159
C	2.5604726923	0.4307177112	-0.0690650578
C	3.7528427983	0.9885070795	0.2269408652
Li	-0.3667900694	0.0506498088	0.3173604151
C	-0.0772799123	0.290163734	2.5334982468
H	1.9388447379	-1.1188324817	-2.0807609193
H	0.8494483953	-2.5198185513	-2.0723514616
H	-0.2082149171	-3.2209081136	-0.0313388242
H	0.0677189969	-2.3186156991	1.4757030231
H	2.5978519597	-1.3044587181	1.1787962529
H	0.9594267162	-0.1460599784	1.5787210375
H	1.9786526457	0.9114937044	-0.8591301922
H	4.0982935189	1.8841797734	-0.276166018
H	4.40506355	0.5703300991	0.9875287305
H	-0.8648413104	1.0387945387	2.3399789783
H	0.6012870178	0.7520786275	3.260040054
H	-0.5532364048	-0.5613349711	3.0384843702
H	2.4487278674	-2.6229278477	-1.2933740863
H	1.364456341	-3.3169746918	0.7911014321
C	-2.6041119819	-1.5787645775	-1.0315898179
H	-3.4335803378	-1.2477319521	-1.6687271225
H	-1.720046373	-1.753424384	-1.6430791445
H	-2.8885303917	-2.5113678905	-0.5302189642
C	-3.348949246	-0.2650733375	0.7999988754
H	-4.2051872264	0.1258024012	0.23711457
H	-3.6590178404	-1.1562493535	1.3577168552
H	-2.9925244013	0.4879559121	1.5002204359
C	0.1698381839	3.0264250787	0.1871123772
H	0.9273101671	3.4333539481	-0.4913341307
H	-0.5501397617	3.8115646354	0.4461848221
H	0.6547300163	2.6540358445	1.0863247114
C	-1.153832596	2.2716058138	-1.6351890852
H	-1.6680825688	1.3829269723	-1.9988634555
H	-1.887426359	3.0696843832	-1.4672357815
H	-0.4260629223	2.6071105662	-2.3840398909
O	-0.5050303848	1.921268518	-0.4200853658
O	-2.2697763023	-0.5741573556	-0.0803891516

Tabelle 10.459 Standardorientierung von **8** [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
N	0.865112	-1.447864	-0.364656
C	2.147263	-1.28092	0.341964
C	2.885459	-0.027401	-0.045963
C	2.916689	1.054894	0.730415
Li	-0.397112	0.015404	0.492583
C	-0.370148	0.02885	2.588065
H	2.78819	-2.159755	0.153074
H	1.913433	-1.242637	1.407157
H	3.430023	-0.03107	-0.986537
H	3.473166	1.940591	0.443701
H	2.377291	1.077431	1.671507
H	0.473784	0.571754	3.049363
H	-0.346711	-0.97269	3.054536
H	-1.274628	0.507782	3.005671
C	0.223001	-2.671923	0.116962
H	-0.742416	-2.789086	-0.37601
H	0.844059	-3.557607	-0.090929
H	0.062251	-2.587083	1.192201
C	1.05054	-1.531926	-1.807933
H	1.494035	-0.611112	-2.186443
H	1.701358	-2.376559	-2.087424
H	0.077945	-1.671282	-2.2838
C	-3.042495	-0.97864	0.829419
H	-3.87039	-1.589274	0.453767
H	-2.430419	-1.54085	1.528714
H	-3.431151	-0.093696	1.340526
C	-2.891748	0.217896	-1.186037
H	-3.767146	-0.31301	-1.574578
H	-3.208818	1.156258	-0.720686
H	-2.20681	0.435731	-2.002832
C	0.218673	2.250626	-1.578279
H	-0.32105	3.125157	-1.957617
H	1.281014	2.493353	-1.476086
H	0.1043	1.42327	-2.276369
O	-0.31724	1.840729	-0.336478
O	-2.201153	-0.592031	-0.253227
C	-0.226163	2.86568	0.647789
H	0.817244	3.170812	0.774635
H	-0.826232	3.728972	0.341313
H	-0.596035	2.441035	1.577221

Tabelle 10.460 Standardorientierung von **TS2** [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	-1.5825264082	-0.0111654798	-1.849947949
N	-1.9270469434	0.2368704353	-0.4545617134

C	-3.0128766482	1.2080220015	-0.4011363669
C	-2.3516547791	-1.0433512321	0.1940745047
C	-1.2091774682	-1.940365113	0.5327520756
C	-0.6129415421	-1.8663153451	1.7865450065
Li	0.1465359411	-0.1572504096	0.451000028
C	0.8842778288	-0.3598479737	2.420788259
H	-0.8380582117	-0.8062272626	-1.9036319602
H	-1.1659976742	0.8941326228	-2.2977186294
H	-2.7266722765	2.1219539983	-0.9267004269
H	-3.2388754924	1.4549859258	0.6379819647
H	-3.0943891634	-1.5308715718	-0.4604492518
H	-2.8679847592	-0.7544205504	1.1156243734
H	-0.808296038	-2.6001872246	-0.2294276339
H	0.077232307	-2.6469245777	2.0821086263
H	-1.2022489787	-1.4728325294	2.6095011666
H	0.9874708075	-0.8993310872	3.3624626403
H	0.4670094305	0.6321760561	2.6462198465
H	1.8876056215	-0.2291297628	1.9907271163
H	-2.4642890132	-0.3239619753	-2.4338388205
H	-3.9289237652	0.817102128	-0.872908328
C	2.1531753633	-2.1409778351	-0.4500525675
H	1.6809607328	-2.897982286	-1.083906695
H	3.2378153896	-2.164653259	-0.5967739936
H	1.9149031834	-2.3287527675	0.5933867153
C	1.9358851967	-0.467716555	-2.0939530227
H	1.5241334014	0.528931396	-2.2383125479
H	3.0186252618	-0.4491188527	-2.2588501436
H	1.4780871234	-1.1646668522	-2.8040888613
C	2.2675384003	2.052959739	0.332202997
H	2.565106232	2.9670702414	-0.1927841543
H	2.4603471581	2.1629790123	1.4031402366
H	2.8275628808	1.202340148	-0.0467490138
C	0.0827875022	2.8259320201	0.639779623
H	0.2767625592	2.9436747886	1.7105754619
H	0.2904193688	3.7709659596	0.1267854854
H	-0.9522242841	2.5369396289	0.4862980436
O	0.890452949	1.7890196616	0.1048501567
O	1.6491428063	-0.8507142607	-0.7618652477

Tabelle 10.461 Standardorientierung von **TS3** [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	1.6121857365	-1.9503278388	-1.5264154502
N	0.9717504462	-1.5133400496	-0.2857343048
C	0.657462945	-2.700935282	0.5080004976
C	1.8243452764	-0.6212516072	0.5392686859
C	2.3788763804	0.5133971292	-0.191505349
C	3.5313981947	1.1624474446	0.0635657072
Li	-0.3817744961	-0.0159295582	0.224738383
C	-0.2963749801	0.0194021329	2.4314879799
H	1.8629255173	-1.0915663031	-2.1466913133

H	0.9309635875	-2.6000386595	-2.0845827521
H	-0.0265427173	-3.3530338895	-0.0398683312
H	0.1999772109	-2.4072567281	1.4512669246
H	2.5943093755	-1.1906554508	1.0791548756
H	0.8494650509	-0.2168894345	1.5169962085
H	1.7464475682	0.9206609751	-0.9838488869
H	3.8052287708	2.0597391181	-0.4778511805
H	4.2185722442	0.8120311709	0.8261488662
H	-0.9096359152	0.9293774913	2.3608458365
H	0.3050000297	0.1175409011	3.3407052232
H	-0.981356452	-0.8244190063	2.5958977206
H	2.5389209721	-2.5044242036	-1.3153857463
H	1.5733676172	-3.2716431634	0.7300310527
C	-2.565001873	-1.7853675383	-0.6303165699
H	-3.5160999007	-1.8289290407	-1.1691712099
H	-1.7650813816	-2.1684866748	-1.2591365357
H	-2.6336865924	-2.3816698176	0.2846459449
C	-3.2508952764	0.1840971025	0.4693057638
H	-4.2005231931	0.1854275601	-0.0741040869
H	-3.3669397462	-0.3415702252	1.4208374044
H	-2.9243008873	1.2041463219	0.6558364435
C	0.1843130366	2.9044580355	0.4158980898
H	1.0241081033	3.2462292166	-0.1939937506
H	-0.4813099692	3.7436319249	0.6394350302
H	0.5636288899	2.4625800109	1.3327632282
C	-0.9873426552	2.3183735338	-1.5483164812
H	-1.5638676412	1.5030309495	-1.9797169544
H	-1.6189337891	3.2069486934	-1.4495129104
H	-0.1321559508	2.5534321162	-2.1900631816
O	-0.5428087333	1.8892856673	-0.271933086
O	-2.2425668033	-0.4379040245	-0.3193947853

Tabelle 10.462 Standardorientierung von **8** [globales Minimum; M05-2X/6-31+G(d,p)].

	x	y	z
N	0.8646793484	-1.4397931588	-0.3698569217
C	2.1433562441	-1.2767420867	0.3445539094
C	2.8868489448	-0.0250349724	-0.0385980333
C	2.919549131	1.0548244162	0.7409136158
Li	-0.4016927573	0.0183332632	0.4884099576
C	-0.3667809563	0.0314243891	2.5868613182
H	2.7836712579	-2.156638224	0.1586327085
H	1.9021748345	-1.2364022671	1.4082415807
H	3.4342310907	-0.0274567206	-0.9776011873
H	3.4803170669	1.9386190998	0.4570786436
H	2.3756829184	1.0742636653	1.6796932722
H	0.4770511566	0.5730533085	3.0481696576
H	-0.3459167214	-0.9688061527	3.0547145082
H	-1.2704515894	0.5126149778	3.0019389155
C	0.2158997972	-2.6625043905	0.1080194034

H	-0.7480599689	-2.7744140305	-0.388942746
H	0.8347925836	-3.5500696188	-0.0975235769
H	0.0509449081	-2.5760928105	1.1826371245
C	1.056592329	-1.5217796772	-1.8128369064
H	1.5041890604	-0.6013653258	-2.1874182439
H	1.7062351018	-2.3676392564	-2.0908411125
H	0.085731466	-1.6578776104	-2.2931526898
C	-3.0425448231	-0.9846105787	0.8367735685
H	-3.8650114347	-1.6048843224	0.4649059788
H	-2.4243838943	-1.5360035739	1.5397377738
H	-3.4389846182	-0.1000732686	1.343006549
C	-2.8999276346	0.2075359049	-1.1838921782
H	-3.772203555	-0.3293832706	-1.5712370752
H	-3.2222208765	1.1454625536	-0.7209954989
H	-2.2162386561	0.4279729593	-2.0012293148
C	0.218155452	2.2419689701	-1.5823698338
H	-0.2996719084	3.1308309287	-1.9589273831
H	1.2865137802	2.4571587636	-1.4798350766
H	0.0828279988	1.4196260334	-2.2830221723
O	-0.3271974302	1.8415742506	-0.3406662713
O	-2.2041190806	-0.5961335795	-0.2484700982
C	-0.2186263014	2.8645852766	0.6452647686
H	0.8293742754	3.1554622735	0.7683498812
H	-0.8086204437	3.7360825609	0.3424674729
H	-0.5892010954	2.4421203012	1.5757447121

Tabelle 10.463 Standardorientierung von **TS2** [Übergangszustand; M05-2X/6-31+G(d,p)].

	x	y	z
C	-1.5802231596	-0.0123545254	-1.8453267338
N	-1.9274711527	0.2369288815	-0.4502619149
C	-3.0173901473	1.2042674087	-0.3984846248
C	-2.3483194906	-1.0444183099	0.2004282339
C	-1.2043412088	-1.9384871792	0.5406395169
C	-0.6095881443	-1.8615699834	1.7962083667
Li	0.1468174446	-0.1547213559	0.4488345703
C	0.8854944631	-0.3616286007	2.4219971761
H	-0.8322931489	-0.8045177709	-1.8952101017
H	-1.1669304628	0.8937428964	-2.2944325933
H	-2.7352506237	2.1183309666	-0.9260094426
H	-3.2442390668	1.452136389	0.6401547174
H	-3.0888385096	-1.5351755672	-0.4541851882
H	-2.8655267699	-0.7557348512	1.1216438054
H	-0.805554561	-2.6035362377	-0.217421396
H	0.0781185122	-2.6432399205	2.0948715197
H	-1.2021439421	-1.4672900833	2.6164338443
H	0.9832160424	-0.8845584414	3.372562773
H	0.4797084932	0.6389501568	2.6272169141
H	1.8874458404	-0.2542098017	1.984115487
H	-2.4599314277	-0.3303535912	-2.4292310715
H	-3.9316826797	0.8087905055	-0.8696415409

C	2.1441313605	-2.145938083	-0.4649177972
H	1.6659496339	-2.8916558949	-1.1078122242
H	3.2287404071	-2.1772025369	-0.6108718716
H	1.9028465119	-2.3439961136	0.5761725586
C	1.9413951218	-0.4497595989	-2.0900367526
H	1.5364803733	0.5517150199	-2.2210427654
H	3.024354658	-0.4370234417	-2.2545303886
H	1.4787717918	-1.1345920383	-2.8089068203
C	2.2694808513	2.0445059254	0.3460005715
H	2.5784353721	2.953693072	-0.1810989099
H	2.447068574	2.1603953431	1.419056251
H	2.8303611235	1.1879276973	-0.0185553613
C	0.0806823278	2.8266518548	0.6178871052
H	0.2556414425	2.9464535913	1.6919423228
H	0.3017295275	3.7694858805	0.106335656
H	-0.9523957324	2.5404207414	0.4461643268
O	0.8938494639	1.7841115377	0.1004903451
O	1.6510548911	-0.8472529412	-0.762031563

Tabelle 10.464 Standardorientierung von **TS3** [Übergangszustand; M05-2X/6-31+G(d,p)].

	x	y	z
C	1.6122299078	-1.9507816659	-1.5292054078
N	0.9715896416	-1.514705258	-0.2879112468
C	0.6536232012	-2.7026547448	0.5046485519
C	1.8247954361	-0.6248602922	0.53928031
C	2.3750835697	0.5132149279	-0.1898995572
C	3.525962066	1.1649337328	0.0640618557
Li	-0.377794596	-0.0157162254	0.2279816023
C	-0.2919272437	0.018778607	2.4335905629
H	1.8680574102	-1.0910494751	-2.1459514893
H	0.9292614008	-2.5957867917	-2.0904975907
H	-0.028345285	-3.3544686685	-0.0459130624
H	0.1928848337	-2.4076495253	1.4459453608
H	2.5981340695	-1.1944965831	1.074201024
H	0.8507185763	-0.2219777049	1.516839984
H	1.7393398313	0.9210544915	-0.9794630213
H	3.7946235768	2.0637648144	-0.4768233458
H	4.2148143937	0.8136064808	0.8243786541
H	-0.9115358086	0.923768635	2.358552874
H	0.3154130141	0.1304087709	3.3365698654
H	-0.9707936726	-0.8265010067	2.6123127587
H	2.5361485295	-2.5095198642	-1.3180752537
H	1.568498629	-3.2734808422	0.7300376533
C	-2.5622590037	-1.783921355	-0.631403603
H	-3.5103593088	-1.8260198912	-1.1758126349
H	-1.758977291	-2.1700460137	-1.2545038748
H	-2.6377759083	-2.378911993	0.2841203909
C	-3.2455419389	0.1897513617	0.4666370402
H	-4.1949618039	0.1926653688	-0.0773060565
H	-3.3632148529	-0.3337678043	1.4193368074

H	-2.9151521574	1.2091263041	0.6513192224
C	0.1792883704	2.9074709948	0.4199919463
H	1.0243119408	3.2417626315	-0.1871520778
H	-0.484662552	3.7505755492	0.6339831501
H	0.5518102056	2.4700504851	1.3420920454
C	-0.9880618308	2.3104310483	-1.5461335887
H	-1.5655482884	1.4925361357	-1.9719117541
H	-1.6178405427	3.2012479998	-1.4554309717
H	-0.1308833379	2.5390032637	-2.1878100828
O	-0.5473917539	1.889156542	-0.2649670912
O	-2.2375134276	-0.4363934399	-0.3204229495

Tabelle 10.465 Standardorientierung von **8** [globales Minimum; M05-2X/6-311+G(d,p)].

	x	y	z
N	0.8657661138	-1.4254551334	-0.3812402769
C	2.131409357	-1.2658175256	0.3552751738
C	2.8839669213	-0.0187025061	-0.0166630262
C	2.9072807434	1.0565364835	0.7614260679
Li	-0.4186605783	0.0260306778	0.4808367481
C	-0.3665891741	0.0260582806	2.5867648578
H	2.7699991972	-2.1466349333	0.180150767
H	1.8721825394	-1.2227405173	1.4129897294
H	3.4457030161	-0.0232280175	-0.945213195
H	3.4759647773	1.9371222762	0.4891304083
H	2.3495685525	1.0747415777	1.6903754532
H	0.4726861424	0.562993614	3.0564705615
H	-0.3473933175	-0.9733940792	3.0515671027
H	-1.268598539	0.5034526349	3.0041887336
C	0.210371505	-2.6494484768	0.0814947797
H	-0.7444038344	-2.7606208772	-0.4298224259
H	0.8333473011	-3.5331556021	-0.1184930815
H	0.0299892456	-2.5676486589	1.1525580801
C	1.0863395158	-1.5047120807	-1.8194042171
H	1.5389050107	-0.5842490897	-2.1834042069
H	1.7426358814	-2.3477800276	-2.0829056184
H	0.1274976133	-1.6433797541	-2.3195863589
C	-3.0486459801	-1.0052988747	0.8502935112
H	-3.8460852431	-1.6520828295	0.4738158319
H	-2.4141222263	-1.5352264805	1.5530124268
H	-3.4784348212	-0.1387049436	1.357183612
C	-2.941183496	0.2123229948	-1.1553786007
H	-3.7991004049	-0.342634036	-1.5450657319
H	-3.2875249176	1.1341521894	-0.6811439725
H	-2.26827427	0.4607890473	-1.9715212067
C	0.2250939846	2.217543652	-1.6009261947
H	-0.2592960962	3.1243921343	-1.9744609001
H	1.3002583554	2.3903089985	-1.506267243
H	0.0521336201	1.4017437958	-2.2987027603
O	-0.3252073656	1.8430764832	-0.3538862974

O	-2.2225761426	-0.58177683	-0.2304909085
C	-0.180512711	2.8715549586	0.6210404925
H	0.8733062062	3.1419542777	0.7241843342
H	-0.756675027	3.7507662274	0.3198476472
H	-0.5441564545	2.4669599701	1.5606689035

Tabelle 10.466 Standardorientierung von **TS2** [Übergangszustand; M05-2X/6-311+G(d,p)].

	x	y	z
C	-1.5779518874	-0.0564977279	-1.8532773656
N	-1.9153184832	0.2298884745	-0.4638388163
C	-2.9991571345	1.2029494758	-0.4302214434
C	-2.3404893477	-1.033112799	0.2183671023
C	-1.2042550982	-1.932303057	0.5633868664
C	-0.6046925327	-1.849093544	1.8136740731
Li	0.1498356087	-0.1477104682	0.4389186103
C	0.9165116636	-0.3718979343	2.4104733314
H	-0.8335113838	-0.8505609943	-1.8877067605
H	-1.1673518898	0.8353878014	-2.3288959653
H	-2.7139074069	2.103308571	-0.9763597571
H	-3.2241966034	1.4728960886	0.601820136
H	-3.0915116968	-1.52741447	-0.4179247985
H	-2.8442994776	-0.7219569162	1.1376841251
H	-0.8246428142	-2.619105799	-0.1820779982
H	0.0685480181	-2.6381329874	2.1199045431
H	-1.1879146673	-1.4392770966	2.6308843003
H	1.0221389449	-0.8838010242	3.3639220776
H	0.5280667236	0.6347402092	2.6082078737
H	1.9087272533	-0.2865871365	1.9519131144
H	-2.462500272	-0.385888237	-2.4198627376
H	-3.9137924268	0.8012894958	-0.8912214295
C	2.1051776988	-2.1521472195	-0.4922342219
H	1.6402838032	-2.881615129	-1.1603634284
H	3.1911341911	-2.1836446965	-0.6146614929
H	1.8402112087	-2.3709673804	0.5373849657
C	1.9437670125	-0.4231635451	-2.0862294023
H	1.5459874902	0.5808587201	-2.2066817396
H	3.0286090386	-0.4119147837	-2.2259595759
H	1.4953828263	-1.0903308247	-2.8279102284
C	2.2591886715	2.050516701	0.3747576188
H	2.5686157816	2.9681082129	-0.1338636884
H	2.4295467929	2.1467103932	1.4492542886
H	2.8247279568	1.2038328871	-0.0010106038
C	0.071499895	2.8353231908	0.629677091
H	0.2342674388	2.9486715209	1.7048452029
H	0.3041156298	3.7783788663	0.1271551519
H	-0.9599534978	2.5576664051	0.443922451
O	0.8860594458	1.792526196	0.1176372166
O	1.6226975263	-0.8466384392	-0.7743416867

Tabelle 10.467 Standardorientierung von **TS3** [Übergangszustand; M05-2X/6-311+G(d,p)].

	x	y	z
C	1.55508887	-1.9933940144	-1.5240935783
N	0.9395823073	-1.5261522286	-0.2829693
C	0.6112773356	-2.6924543653	0.5358519016
C	1.8230470444	-0.6378710473	0.5094532208
C	2.3406367677	0.4979570533	-0.2402094217
C	3.4848370072	1.1653979019	-0.0214265545
Li	-0.3824975463	-0.0107031358	0.2826781625
C	-0.1767806831	0.0929419543	2.4962963859
H	1.820679726	-1.1486775081	-2.1550150663
H	0.8562960475	-2.6342495019	-2.0677959184
H	-0.0803542452	-3.3462001432	0.0030589068
H	0.1595811732	-2.3724680487	1.4718189506
H	2.6124111514	-1.2051808805	1.0179744685
H	0.8987353402	-0.2140537494	1.523319293
H	1.6823592017	0.8866321638	-1.0184858571
H	3.7294626942	2.0586427347	-0.5793915931
H	4.1952940735	0.8318365793	0.7246057353
H	-1.0745350808	0.6986650262	2.3082014546
H	0.4329679783	0.6622627278	3.20309043
H	-0.5021424725	-0.8124474692	3.0169569706
H	2.4689269748	-2.5655808158	-1.3135432352
H	1.5192052569	-3.2685989396	0.7673093729
C	-2.5347154873	-1.7788377029	-0.7367882319
H	-3.4206497994	-1.7620862551	-1.376155621
H	-1.6792740463	-2.1445358822	-1.2967332588
H	-2.7169205135	-2.4275755156	0.1236272473
C	-3.2887078357	0.1362608119	0.4146918951
H	-4.1869197591	0.1691405448	-0.2068235403
H	-3.4920513813	-0.4269524355	1.3282465961
H	-2.97484444	1.1442256354	0.6693436472
C	0.1457964917	2.9051672721	0.5250401307
H	1.0558563894	3.1726779592	-0.0141606313
H	-0.4898493216	3.7849742114	0.6517818883
H	0.41143346	2.4847559778	1.489361843
C	-0.9212201054	2.3175538101	-1.4962776924
H	-1.4836395026	1.5081985866	-1.9541684271
H	-1.539120341	3.2181287414	-1.4508580618
H	-0.0230676051	2.5277306329	-2.0834782647
O	-0.5699963933	1.8986173383	-0.1881990722
O	-2.2201407313	-0.4631490242	-0.3068481749

Tabelle 10.468 Standardorientierung von **8** [globales Minimum; M052X/6-311+G(3df,3pd)].

	x	y	z
N	0.8647581467	-1.4299445538	-0.3815126843
C	2.1265718824	-1.2544233883	0.3516122856
C	2.865809298	-0.0036051959	-0.02190931
C	2.9112238482	1.057115417	0.7679582555

Li	-0.4214159288	0.0219639582	0.4737061352
C	-0.3777058801	0.0240077831	2.5751148657
H	2.7709445278	-2.1274105838	0.177550146
H	1.8701444915	-1.2113938196	1.4068277641
H	3.3972851527	0.0067164118	-0.9642653848
H	3.4684212748	1.9397415637	0.4918763719
H	2.3819720447	1.0627549862	1.7098818496
H	0.4619428503	0.5585395868	3.037289592
H	-0.3669057828	-0.970795143	3.0402308635
H	-1.2767798204	0.5096460734	2.9785244108
C	0.2216164753	-2.6523282934	0.0926488072
H	-0.7269173315	-2.7814297024	-0.4195808669
H	0.8535706039	-3.5282166813	-0.095561091
H	0.0379428824	-2.5610949191	1.1592239146
C	1.083876162	-1.5220247409	-1.8160068059
H	1.529423575	-0.6061436666	-2.1903121771
H	1.7433805977	-2.3616120077	-2.068984008
H	0.1286585254	-1.6721920908	-2.3126820563
C	-3.044425967	-1.0009824955	0.8396540919
H	-3.8560014038	-1.6284058521	0.4697953195
H	-2.4149385509	-1.5451749459	1.5314650283
H	-3.452124087	-0.1322861314	1.3545218449
C	-2.9443547789	0.2156499307	-1.1581048742
H	-3.8079235737	-0.3285202052	-1.5417200176
H	-3.280374592	1.1341707512	-0.6768693262
H	-2.2799564228	0.464306105	-1.977440537
C	0.2220164181	2.2203388544	-1.5922074255
H	-0.2707546432	3.1213212144	-1.9598688175
H	1.292967218	2.4040515812	-1.5038521434
H	0.054527757	1.4071300843	-2.2898471802
O	-0.315396737	1.8400174938	-0.3457884161
O	-2.2261339466	-0.5870123991	-0.2460343036
C	-0.1667270673	2.8630832889	0.628446631
H	0.8843631662	3.1347758741	0.724216515
H	-0.7428534175	3.7403444253	0.332803125
H	-0.522761967	2.4591304325	1.5678986084

Tabelle 10.469 Standardorientierung von **TS2** [Übergangszustand; M052X/6-311+G(3df,3pd)].

	x	y	z
C	-1.5901082373	-0.0698322854	-1.8451350142
N	-1.9072066759	0.2601520181	-0.4641028811
C	-2.9668552304	1.2548928928	-0.4475176978
C	-2.3523297081	-0.9729769556	0.2528849039
C	-1.2375298851	-1.8898750061	0.6089231605
C	-0.627646542	-1.7953172525	1.8510556294
Li	0.1505330073	-0.1501451187	0.4362235956
C	0.919473234	-0.3518369957	2.4041908529
H	-0.8670567031	-0.8797763477	-1.86604726
H	-1.1670355057	0.7967803667	-2.3484144268
H	-2.6657861566	2.1336759723	-1.0136018786

H	-3.1811766104	1.5512893034	0.5760340731
H	-3.119648976	-1.461351046	-0.3627900532
H	-2.8373577738	-0.6282080481	1.1664758295
H	-0.8794638285	-2.5977665692	-0.1228258495
H	0.0258850539	-2.5922961407	2.1672984733
H	-1.1956039139	-1.3599625598	2.6613794974
H	1.0178357786	-0.8446354062	3.3640121148
H	0.5518367256	0.6629954742	2.5761663912
H	1.9048131391	-0.3023043156	1.9345609257
H	-2.4858116048	-0.3933787372	-2.3910983798
H	-3.8887469759	0.862815838	-0.8946929755
C	2.0398024669	-2.2101941185	-0.4767485399
H	1.5524670418	-2.9277573514	-1.1367599675
H	3.1208179947	-2.2806171429	-0.5989637049
H	1.7676604546	-2.411896623	0.5514724778
C	1.9251126976	-0.5096924307	-2.0918882826
H	1.562397751	0.5019007472	-2.2321635739
H	3.0050836032	-0.5397381893	-2.2419754897
H	1.4486420552	-1.1744001229	-2.8134885016
C	2.2989252256	2.0166088026	0.3324200742
H	2.6218830608	2.9306827931	-0.1673334975
H	2.4748959597	2.1018090412	1.4040001885
H	2.8494780807	1.1669917691	-0.0508502421
C	0.1357880743	2.8404576773	0.6000644161
H	0.3037003078	2.9427019322	1.6724968106
H	0.3888976681	3.7793799959	0.1065470764
H	-0.900438918	2.5917447317	0.4162841906
O	0.9239331291	1.786555175	0.0796168704
O	1.6039457359	-0.8956447677	-0.7727713358

Tabelle 10.470 Standardorientierung von von **TS3** [Übergangszustand; M052X/6-311+G(3df,3pd)].

	x	y	z
C	1.5499324986	-1.9881618337	-1.5262433729
N	0.9330864972	-1.519355205	-0.290352778
C	0.6024973555	-2.6818187112	0.5270201886
C	1.8135569748	-0.6340764492	0.5011848821
C	2.3348208148	0.5002932927	-0.2404089831
C	3.4715098395	1.169444158	-0.011513958
Li	-0.3842347484	-0.0036301293	0.2834442003
C	-0.1839419149	0.0966544469	2.4902159839
H	1.8190544742	-1.1477145903	-2.155890536
H	0.8541702705	-2.6272593266	-2.0692774967
H	-0.0838834347	-3.3353227062	-0.0061374259
H	0.1489462435	-2.3620601199	1.4585321199
H	2.5945209565	-1.2006407022	1.0163342981
H	0.8921333557	-0.21150194	1.5128116964
H	1.6860058227	0.8854440499	-1.0236021666
H	3.7176155568	2.0597644487	-0.5671574559
H	4.1739789368	0.8398210267	0.7392483944
H	-1.0636058735	0.7233271655	2.3066749256

H	0.4371157314	0.6404123824	3.2016621801
H	-0.5289855364	-0.8080105058	2.9915695124
H	2.4588080371	-2.5608499932	-1.3116762173
H	1.5082438481	-3.2544474091	0.7610531091
C	-2.5338866879	-1.777068231	-0.7328441694
H	-3.4260844467	-1.7606423531	-1.3581042749
H	-1.6869878072	-2.1344934966	-1.3054137043
H	-2.7022880712	-2.4326792364	0.1213356497
C	-3.2837981338	0.1113195603	0.4467892955
H	-4.1904047507	0.1381135932	-0.1570828885
H	-3.4654782379	-0.4619731781	1.3550454953
H	-2.9821772506	1.1183418436	0.7073255305
C	0.1466915857	2.9042127091	0.5164903894
H	1.0612881405	3.162534042	-0.0134827612
H	-0.4819717822	3.7870908954	0.6293567453
H	0.3994381329	2.4914107681	1.4843082695
C	-0.8921034915	2.3166245946	-1.5081643766
H	-1.4509606897	1.513990634	-1.9752265831
H	-1.501769163	3.2196324862	-1.4760680898
H	0.0144716179	2.5193597048	-2.0791815046
O	-0.5657504998	1.9013521862	-0.1969777651
O	-2.2235261705	-0.4668388713	-0.2963093582

Tabelle 10.471 Standardorientierung von **8** [globales Minimum; M06L/6-31+G(d)].

	x	y	z
N	0.854475603	-1.4432672901	-0.3821117248
C	2.1216378543	-1.2405640869	0.3481481899
C	2.8252037445	0.0284813825	-0.0145129279
C	2.8842299647	1.0858238326	0.7965660543
Li	-0.4262412503	0.0245606432	0.485845052
C	-0.3517185703	0.0213075561	2.5433489755
H	2.7913622536	-2.1095235315	0.1713549842
H	1.8616711698	-1.2227666239	1.4145580283
H	3.3255774883	0.0668947373	-0.9864499325
H	3.4210365865	1.9928901421	0.5191450658
H	2.3867516389	1.0767034411	1.7677169759
H	0.5107503264	0.5470078985	3.0070967082
H	-0.3207430054	-0.9854615404	3.015226631
H	-1.2329856862	0.4983194777	3.0248178274
C	0.2192675733	-2.6613684569	0.11316095
H	-0.7346180013	-2.8119030424	-0.4040422417
H	0.8557074983	-3.5532048634	-0.0475252563
H	0.0253445639	-2.5479686383	1.1867483992
C	1.0631268204	-1.5418354311	-1.8178828807
H	1.5202002402	-0.6226156308	-2.200850822
H	1.7174737701	-2.39324441	-2.092125226
H	0.0952914827	-1.6803868094	-2.3155471537
C	-3.0563525301	-1.0249017249	0.8300922809
H	-3.9035429582	-1.6364562641	0.4810743224

H	-2.4169398949	-1.5979630391	1.5052962914
H	-3.4336274377	-0.1462020341	1.3733686745
C	-2.9733691938	0.1799010278	-1.176153759
H	-3.864674273	-0.3489007145	-1.549063204
H	-3.2867683418	1.1235481702	-0.7021889829
H	-2.3095356112	0.4047092992	-2.0159321968
C	0.2595056282	2.2587736712	-1.5976041927
H	-0.2001322536	3.183621351	-1.9816250786
H	1.3457217247	2.4148066752	-1.4932367592
H	0.0812010233	1.446198824	-2.3089700892
O	-0.3162104178	1.8814761703	-0.3686699649
O	-2.2522398309	-0.6282567097	-0.2723511321
C	-0.1376018634	2.8773065835	0.6281470449
H	0.9328642151	3.0982026834	0.7626228256
H	-0.6655435721	3.8010696868	0.3434766398
H	-0.5385914779	2.464996588	1.5577306042

Tabelle 10.472 Standardorientierung von **TS2** [Übergangszustand; M06L/6-31+G(d)].

	x	y	z
C	-1.5636807057	-0.0137495242	-1.8282534992
N	-1.9280467068	0.2396528178	-0.4424607296
C	-3.0326456167	1.1837682797	-0.4040263481
C	-2.3286086779	-1.0586215758	0.2198898262
C	-1.1839819607	-1.9340936008	0.5582815357
C	-0.5603040076	-1.8426381904	1.8075744235
Li	0.1302034416	-0.1322073049	0.4468284751
C	0.9033184064	-0.35574365	2.3898963276
H	-0.7938168897	-0.7953806715	-1.8649947866
H	-1.1626473092	0.898371937	-2.2902354036
H	-2.7626741507	2.1138651614	-0.9212558268
H	-3.2837854357	1.4213187047	0.6369999279
H	-3.0767173085	-1.5495923445	-0.437398226
H	-2.8570346916	-0.7567521843	1.1381099778
H	-0.7579882208	-2.5670782156	-0.2225863832
H	0.1304449012	-2.63268213	2.1001993792
H	-1.164153635	-1.4881783486	2.6455948801
H	1.0285599757	-0.8195460682	3.3731330882
H	0.5382764989	0.6748352256	2.5627208517
H	1.9035964659	-0.2918435963	1.9226280301
H	-2.4287799369	-0.361557336	-2.4290521431
H	-3.9415698801	0.7809645269	-0.8939180348
C	2.0828766706	-2.1700169613	-0.4876866309
H	1.555910174	-2.8928167957	-1.1299481094
H	3.1680875149	-2.2704531052	-0.6434051168
H	1.8380208071	-2.3631289832	0.5598483746
C	1.9494358509	-0.4692097064	-2.0988886196
H	1.5935385745	0.5569771881	-2.2264229939
H	3.0333942379	-0.5111745611	-2.2909546963
H	1.4377711567	-1.1284311325	-2.8188116802
C	2.2562710071	2.0623484373	0.4137370454

H	2.6097030204	3.0007632671	-0.0421119482
H	2.3792984107	2.1160891937	1.506415228
H	2.8357897963	1.2183446252	0.0320692902
C	0.0695989172	2.8535589834	0.5830769097
H	0.1489912246	2.9110477203	1.6807608239
H	0.3465694821	3.8289403725	0.1533100902
H	-0.9567195595	2.6029090587	0.3060688605
O	0.9004038331	1.8276899346	0.0738751753
O	1.6627483251	-0.8472584476	-0.7694603449

Tabelle 10.473 Standardorientierung von **TS3** [Übergangszustand; M06L/6-31+G(d)].

	x	y	z
C	1.5591744636	-1.8980922059	-1.5782911492
N	0.9550947115	-1.4953544057	-0.3109085255
C	0.6720345199	-2.6980611896	0.4649255147
C	1.822059468	-0.6020211906	0.5107092126
C	2.3610931967	0.5316238256	-0.2156265563
C	3.50107131	1.2143067536	0.0293489711
Li	-0.4211430203	-0.0326105492	0.2605332701
C	-0.2851483163	-0.0047232919	2.4349768897
H	1.7919422653	-1.0186884379	-2.1862867579
H	0.8609982762	-2.5362993309	-2.1393189731
H	-0.010621519	-3.3578750412	-0.0861345358
H	0.2175758545	-2.4312009864	1.424426781
H	2.6004388436	-1.1836824918	1.0368453127
H	0.8726801087	-0.2262051907	1.5040843465
H	1.7135601283	0.9279037478	-1.0112716035
H	3.7485664364	2.1248277918	-0.5123308864
H	4.2099865245	0.8891495466	0.7904998948
H	-1.0403117068	0.7952092247	2.3079628541
H	0.2978732814	0.2794458483	3.3212686264
H	-0.8391966804	-0.9182020855	2.7140071062
H	2.4980207301	-2.46182489	-1.4210187883
H	1.600147838	-3.2666337055	0.6727325291
C	-2.602226639	-1.8314242598	-0.5293556386
H	-3.561474944	-1.9316550502	-1.0586171874
H	-1.7980778149	-2.2429112108	-1.1448582485
H	-2.6552978284	-2.3824309555	0.4226619465
C	-3.3076686061	0.1858883655	0.4455007912
H	-4.2683452772	0.1470207497	-0.0893384098
H	-3.4206557615	-0.2801453691	1.4355216712
H	-2.9909917022	1.2248118725	0.5675379026
C	0.1425761423	2.9006960826	0.4978277877
H	1.108780003	3.1067802345	0.0158630261
H	-0.448497555	3.8265823475	0.5615058998
H	0.3229835363	2.4949979471	1.4959248934
C	-0.7907788756	2.2908511261	-1.5724065704
H	-1.3465687712	1.4807169448	-2.0535418912
H	-1.3766184901	3.2211988108	-1.628049906
H	0.1679643296	2.443400941	-2.0934341173

O	-0.5783069317	1.9120495319	-0.2271754748
O	-2.2966435283	-0.4668208541	-0.3074130076

Tabelle 10.474 Standardorientierung von **8** [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
N	0.8666033332	-1.4424586353	-0.3662238931
C	2.1528709994	-1.2501705231	0.3239352461
C	2.85414567	0.0229928744	-0.0381582342
C	2.9339876482	1.0676441519	0.7854350923
Li	-0.4242470351	0.0022029649	0.5446629101
C	-0.3671325719	0.0095917401	2.6127686954
H	2.8164606194	-2.1167081025	0.1082779632
H	1.9354946093	-1.250014699	1.4016029956
H	3.3432929326	0.0695659926	-1.0157474051
H	3.4753940522	1.9733802641	0.5116012302
H	2.4541420415	1.0486649901	1.7662148216
H	0.5264381346	0.5022989346	3.0559761347
H	-0.3799658519	-0.9987479767	3.0826126887
H	-1.2275567239	0.5344409241	3.0831325139
C	0.2569212681	-2.6818462888	0.1053346274
H	-0.7261245945	-2.8094993371	-0.3651359859
H	0.8866762292	-3.5621266151	-0.1343546641
H	0.1167304926	-2.6267093078	1.1923032834
C	1.025962709	-1.4925697427	-1.8095464363
H	1.4324851078	-0.5465271136	-2.1885057848
H	1.7039579963	-2.3129297391	-2.1243847109
H	0.0473085667	-1.6600963911	-2.2791411924
C	-3.1253411453	-0.8945891702	0.840919269
H	-3.9655690697	-1.5244185228	0.5053046072
H	-2.5467639522	-1.4016342762	1.6186294015
H	-3.5143089267	0.0474617495	1.2592600573
C	-2.8809184893	0.0859861856	-1.2680949754
H	-3.7585525486	-0.4625493898	-1.6482623596
H	-3.2024668301	1.0800840327	-0.9157905312
H	-2.1590000104	0.2127224185	-2.0824773272
C	0.1773808235	2.2467448788	-1.5715959828
H	-0.334834572	3.1571578805	-1.9255461253
H	1.263134197	2.4387142522	-1.5307544404
H	-0.0138388895	1.4309455399	-2.2786498062
O	-0.3101807269	1.8520950977	-0.3158680445
O	-2.2480684437	-0.6338502711	-0.2398672625
C	-0.1366627325	2.8546962482	0.6685767345
H	0.9287039124	3.1244020595	0.7580323558
H	-0.7174465411	3.7535647827	0.4045599575
H	-0.4821466879	2.4318971396	1.6176635762

Tabelle 10.475 Standardorientierung von **TS2** [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
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C	-1.6287074068	0.3168140331	-1.8308885983
N	-1.9739170555	0.3303599159	-0.4202956372
C	-3.0863356423	1.2387183924	-0.2068240652
C	-2.3279181634	-1.0495978757	0.0402402601
C	-1.1437954951	-1.9123241832	0.2936766909
C	-0.5829733781	-1.962472891	1.5644084763
Li	0.1850575533	-0.1410594854	0.4089933504
C	0.6912744689	-0.3714798892	2.4311732822
H	-0.8540037349	-0.4396083689	-2.0178453786
H	-1.2381233409	1.2977742729	-2.1380440295
H	-2.8457728411	2.2384617972	-0.5956331623
H	-3.3016763891	1.3246290809	0.8668775849
H	-3.0383857945	-1.4862341801	-0.6945189074
H	-2.8850895235	-0.9132360934	0.9821396103
H	-0.6826344661	-2.4482919336	-0.5403753322
H	0.1725643327	-2.7166577373	1.782651227
H	-1.2193631364	-1.728782767	2.4213518439
H	0.8789469699	-1.005614276	3.3071251788
H	0.0363370102	0.4570510029	2.7617386027
H	1.6668146514	0.0635549083	2.1292530843
H	-2.5029413068	0.0669118252	-2.4683866228
H	-4.0080251373	0.8924707096	-0.7188499329
C	2.4286789187	-2.0681719102	-0.1453672055
H	1.8741322119	-2.9595001329	-0.4826984997
H	3.482070963	-2.1598531269	-0.4554572885
H	2.3645396969	-1.9908091512	0.9443857063
C	1.8950922968	-0.8744063837	-2.0859958782
H	1.4772375607	0.0830754928	-2.4182410487
H	2.9311460144	-0.9642031588	-2.4527696218
H	1.2970975815	-1.7007561052	-2.5079613597
C	2.2590513858	2.132378415	0.10210081
H	2.4598495512	3.0869790768	-0.4113117211
H	2.5968798177	2.2089643142	1.1488604667
H	2.8031136505	1.3210083859	-0.3898107243
C	0.1067224106	2.7999312032	0.6974311574
H	0.4189223092	2.9048139825	1.7495277138
H	0.2045516735	3.7748454737	0.1922414831
H	-0.9343130785	2.4649247431	0.6624448595
O	0.8844389258	1.8202864359	0.0438590911
O	1.8591099358	-0.8916028119	-0.6800584661

Tabelle 10.476 Standardorientierung von **TS3** [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	1.5691117404	-1.7455144713	-1.6361471728
N	0.9882733625	-1.4436295454	-0.3328528023
C	0.6875570556	-2.6998550438	0.3422087792
C	1.8701351543	-0.6427495488	0.5559318028
C	2.4205257871	0.5553770149	-0.0533490994
C	3.5690240463	1.1854563512	0.2637561958
Li	-0.4114979615	-0.0197096241	0.2902566897

C	-0.2541757387	-0.0950561471	2.4651982353
H	1.7982321187	-0.8223903312	-2.1807150594
H	0.8573641578	-2.3336865536	-2.2363077367
H	-0.0203901363	-3.298349496	-0.2487671105
H	0.2559149196	-2.5066159939	1.3315050956
H	2.6444698055	-1.2784576247	1.0258289313
H	0.9206654478	-0.3067380319	1.5522210694
H	1.7781377654	1.0437754497	-0.8002309264
H	3.8371108147	2.143486172	-0.1791428992
H	4.2680978608	0.7642717742	0.9877649974
H	-0.748345446	0.8941832803	2.5226011751
H	0.3105661143	-0.2068780635	3.4013085434
H	-1.0551458023	-0.8600387554	2.4988077735
H	2.5084817955	-2.3237462551	-1.5345945919
H	1.6072161823	-3.3034683793	0.4832271734
C	-2.6703653568	-1.8085393792	-0.3901952458
H	-3.648260677	-1.8977884116	-0.8888318906
H	-1.8996265175	-2.2697882776	-1.0162746963
H	-2.7107880443	-2.3261933921	0.582408226
C	-3.2935135879	0.2633642916	0.5157631228
H	-4.2652523823	0.2341133122	-0.0017329677
H	-3.4034108249	-0.1583965059	1.5273943978
H	-2.9460757469	1.2984669164	0.5921141329
C	0.0511433877	2.9791691327	0.3075100548
H	0.9984445231	3.240286875	-0.1892464357
H	-0.6261240042	3.8472893831	0.2868506326
H	0.262469681	2.6884016531	1.340634767
C	-0.7957832223	2.0929498817	-1.7006873948
H	-1.2815560728	1.1957612726	-2.0996076643
H	-1.4570241756	2.9621533931	-1.8468648325
H	0.1509934474	2.270217924	-2.2375623233
O	-0.5592127373	1.871097806	-0.3281525563
O	-2.321338733	-0.4516330523	-0.2227413899

Tabelle 10.477 Standardorientierung von **8** [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
N	0.8642473265	-1.4345114699	-0.3672957017
C	2.1486726858	-1.2415140841	0.3267105324
C	2.8492144866	0.0320161667	-0.0335778831
C	2.9366533615	1.0721821441	0.7945002339
Li	-0.4291009725	0.0040292376	0.5427368143
C	-0.367237672	0.0087799627	2.6119557939
H	2.8139346168	-2.1056513954	0.1130030146
H	1.9283122099	-1.2399930178	1.4027512726
H	3.3305720757	0.0834987108	-1.0133351955
H	3.4769931906	1.9765817862	0.5202880012
H	2.4626515666	1.0469193635	1.7766231812
H	0.5323212973	0.4910599401	3.0502843986

H	-0.3899358354	-0.9985981579	3.0794085912
H	-1.2198548014	0.5426928244	3.0822392287
C	0.2520304533	-2.6735622389	0.1043103332
H	-0.7298160225	-2.7992437399	-0.3661916997
H	0.8798346068	-3.5540361166	-0.1329433194
H	0.1099421334	-2.616227994	1.1897670503
C	1.0256229062	-1.4838030427	-1.81115973
H	1.4291611368	-0.537779761	-2.1898222986
H	1.7048142011	-2.3012409807	-2.1258686487
H	0.0491659723	-1.6533888652	-2.2815170662
C	-3.1256007858	-0.899632266	0.8409633591
H	-3.9619869486	-1.5346172045	0.510140261
H	-2.5454895893	-1.3976491429	1.6219888595
H	-3.5192714256	0.0410618992	1.2547283723
C	-2.8823697966	0.0777204057	-1.2718374602
H	-3.7566683804	-0.472080093	-1.6537440291
H	-3.2076091184	1.0701677478	-0.922202231
H	-2.1613752863	0.2077114259	-2.0850467075
C	0.1732357207	2.2363913746	-1.5738455347
H	-0.3249041803	3.1534466271	-1.9262446573
H	1.2607806549	2.4116768963	-1.5380147234
H	-0.0318787208	1.4253738926	-2.2809258779
O	-0.31572992	1.8482535981	-0.3155031665
O	-2.2483292313	-0.6397355421	-0.2413763657
C	-0.1224127293	2.8479178766	0.6700509415
H	0.9458089296	3.1026684759	0.7540959513
H	-0.6914800344	3.7542739517	0.4123079583
H	-0.4659530817	2.428649805	1.620297147

Tabelle 10.478 Standardorientierung von TS2 [Übergangszustand; M06/6-31+G(d,p)].

	x	y	z
C	-1.6300174914	0.3237298693	-1.8270429068
N	-1.9745484678	0.3291972683	-0.4153737171
C	-3.0903062774	1.2330507192	-0.1950978165
C	-2.3229879043	-1.0551707963	0.0395926653
C	-1.1356322044	-1.9126484936	0.2939768203
C	-0.5777912131	-1.9597213192	1.5670244229
Li	0.1830161448	-0.1378298761	0.4031618235
C	0.6895479459	-0.3661903346	2.4287137002
H	-0.8533646204	-0.4279090129	-2.017724783
H	-1.2433376015	1.3060938806	-2.1300240149
H	-2.8544875525	2.235110802	-0.5770569031
H	-3.3049554992	1.3116102256	0.8778533355
H	-3.0275940476	-1.4930903024	-0.6980255708
H	-2.8827727798	-0.9254339565	0.9794793486
H	-0.6747461834	-2.4509707651	-0.5365970035
H	0.1778164369	-2.71106858	1.7881448595
H	-1.217999111	-1.7272736694	2.4197135787
H	0.8694073947	-0.9863217278	3.3138300286
H	0.0402346116	0.4720726742	2.7397859854

H	1.666987156	0.0508497569	2.1151158008
H	-2.5021550341	0.0734457058	-2.4647067427
H	-4.0103455236	0.8882205712	-0.7079695899
C	2.4243288671	-2.0713243086	-0.1475782089
H	1.8650149388	-2.9582056629	-0.4847363499
H	3.4754643789	-2.1698127433	-0.4582548323
H	2.3623311329	-1.9975054815	0.9414778743
C	1.8933633328	-0.8702596374	-2.0862812733
H	1.4777179341	0.0872840783	-2.4173686764
H	2.9264947825	-0.9622076275	-2.4565582712
H	1.2929113094	-1.6930163571	-2.5084944564
C	2.2644790305	2.1226304798	0.1164727336
H	2.4798407085	3.0757621323	-0.3907256451
H	2.5869237769	2.1945199139	1.1671308525
H	2.8113429927	1.3099715777	-0.367607623
C	0.1056195594	2.8053486861	0.6763909699
H	0.398669832	2.9088738716	1.7328435698
H	0.2192364444	3.7786365332	0.1744588321
H	-0.9364097115	2.4795401862	0.6238017182
O	0.8878151719	1.8187156748	0.0365951101
O	1.8605413404	-0.889412955	-0.679192645

Tabelle 10.479 Standardorientierung von **TS3** [Übergangszustand; M06/6-31+G(d,p)].

	x	y	z
C	1.5661098272	-1.7465503835	-1.6391007146
N	0.9877243829	-1.4454337455	-0.3337037796
C	0.6862720273	-2.7021110587	0.3414863286
C	1.8706606816	-0.644757084	0.554462146
C	2.4147472261	0.5558685023	-0.0535164391
C	3.5576603018	1.195060957	0.2658810323
Li	-0.4057718	-0.0205152187	0.2886632113
C	-0.2518539092	-0.096613589	2.4650306697
H	1.7959323631	-0.8243443911	-2.1822575087
H	0.8536811378	-2.3317977257	-2.2387251162
H	-0.0201475597	-3.3004396254	-0.2489585656
H	0.2539987121	-2.5089352268	1.329155683
H	2.6468169589	-1.277813597	1.0220439146
H	0.916468821	-0.3091026142	1.5548873743
H	1.7720322677	1.0391577698	-0.8016632901
H	3.8179048749	2.1526281817	-0.1787207072
H	4.2562349762	0.7792865014	0.9910880005
H	-0.7389018699	0.8944297265	2.521031736
H	0.311365367	-0.2131969141	3.3993792778
H	-1.0557186182	-0.8564714768	2.4943169946
H	2.5035695212	-2.3258064076	-1.5405398449
H	1.6044812007	-3.3050401975	0.4838908111
C	-2.6653548969	-1.8097753028	-0.3898517604
H	-3.6392324431	-1.9008623401	-0.8929613072
H	-1.8928504711	-2.2758629516	-1.008244986
H	-2.7123574068	-2.3239602215	0.5829493896

C	-3.2867968884	0.2667254629	0.5113342628
H	-4.2582273236	0.2374293183	-0.0037936793
H	-3.3968097551	-0.150268645	1.5236573284
H	-2.9389914577	1.300690019	0.5848975597
C	0.0510329052	2.9797757529	0.312293595
H	1.0042145735	3.2295343662	-0.176261634
H	-0.6169946318	3.852981188	0.2809892244
H	0.2518559972	2.6955144054	1.3482087195
C	-0.7952988015	2.089008962	-1.69651315
H	-1.2864967017	1.1948458098	-2.0925792963
H	-1.4488366972	2.9610719068	-1.8496172177
H	0.1523361322	2.2564895338	-2.2324758359
O	-0.5637138367	1.871686255	-0.3212819628
O	-2.3146971872	-0.4519269021	-0.2255934636

Tabelle 10.480 Standardorientierung von **8** [globales Minimum; M06/6-31+G(d,p)].

	x	y	z
N	0.8642473265	-1.4345114699	-0.3672957017
C	2.1486726858	-1.2415140841	0.3267105324
C	2.8492144866	0.0320161667	-0.0335778831
C	2.9366533615	1.0721821441	0.7945002339
Li	-0.4291009725	0.0040292376	0.5427368143
C	-0.367237672	0.0087799627	2.6119557939
H	2.8139346168	-2.1056513954	0.1130030146
H	1.9283122099	-1.2399930178	1.4027512726
H	3.3305720757	0.0834987108	-1.0133351955
H	3.4769931906	1.9765817862	0.5202880012
H	2.4626515666	1.0469193635	1.7766231812
H	0.5323212973	0.4910599401	3.0502843986
H	-0.3899358354	-0.9985981579	3.0794085912
H	-1.2198548014	0.5426928244	3.0822392287
C	0.2520304533	-2.6735622389	0.1043103332
H	-0.7298160225	-2.7992437399	-0.3661916997
H	0.8798346068	-3.5540361166	-0.1329433194
H	0.1099421334	-2.616227994	1.1897670503
C	1.0256229062	-1.4838030427	-1.81115973
H	1.4291611368	-0.537779761	-2.1898222986
H	1.7048142011	-2.3012409807	-2.1258686487
H	0.0491659723	-1.6533888652	-2.2815170662
C	-3.1256007858	-0.899632266	0.8409633591
H	-3.9619869486	-1.5346172045	0.510140261
H	-2.5454895893	-1.3976491429	1.6219888595
H	-3.5192714256	0.0410618992	1.2547283723
C	-2.8823697966	0.0777204057	-1.2718374602
H	-3.7566683804	-0.472080093	-1.6537440291
H	-3.2076091184	1.0701677478	-0.922202231
H	-2.1613752863	0.2077114259	-2.0850467075
C	0.1732357207	2.2363913746	-1.5738455347
H	-0.3249041803	3.1534466271	-1.9262446573

H	1.2607806549	2.4116768963	-1.5380147234
H	-0.0318787208	1.4253738926	-2.2809258779
O	-0.31572992	1.8482535981	-0.3155031665
O	-2.2483292313	-0.6397355421	-0.2413763657
C	-0.1224127293	2.8479178766	0.6700509415
H	0.9458089296	3.1026684759	0.7540959513
H	-0.6914800344	3.7542739517	0.4123079583
H	-0.4659530817	2.428649805	1.620297147

Tabelle 10.481 Standardorientierung von TS2 [Übergangszustand; M06/6-31+G(d,p)].

	x	y	z
C	-1.6300174914	0.3237298693	-1.8270429068
N	-1.9745484678	0.3291972683	-0.4153737171
C	-3.0903062774	1.2330507192	-0.1950978165
C	-2.3229879043	-1.0551707963	0.0395926653
C	-1.1356322044	-1.9126484936	0.2939768203
C	-0.5777912131	-1.9597213192	1.5670244229
Li	0.1830161448	-0.1378298761	0.4031618235
C	0.6895479459	-0.3661903346	2.4287137002
H	-0.8533646204	-0.4279090129	-2.017724783
H	-1.2433376015	1.3060938806	-2.1300240149
H	-2.8544875525	2.235110802	-0.5770569031
H	-3.3049554992	1.3116102256	0.8778533355
H	-3.0275940476	-1.4930903024	-0.6980255708
H	-2.8827727798	-0.9254339565	0.9794793486
H	-0.6747461834	-2.4509707651	-0.5365970035
H	0.1778164369	-2.71106858	1.7881448595
H	-1.217999111	-1.7272736694	2.4197135787
H	0.8694073947	-0.9863217278	3.3138300286
H	0.0402346116	0.4720726742	2.7397859854
H	1.666987156	0.0508497569	2.1151158008
H	-2.5021550341	0.0734457058	-2.4647067427
H	-4.0103455236	0.8882205712	-0.7079695899
C	2.4243288671	-2.0713243086	-0.1475782089
H	1.8650149388	-2.9582056629	-0.4847363499
H	3.4754643789	-2.1698127433	-0.4582548323
H	2.3623311329	-1.9975054815	0.9414778743
C	1.8933633328	-0.8702596374	-2.0862812733
H	1.4777179341	0.0872840783	-2.4173686764
H	2.9264947825	-0.9622076275	-2.4565582712
H	1.2929113094	-1.6930163571	-2.5084944564
C	2.2644790305	2.1226304798	0.1164727336
H	2.4798407085	3.0757621323	-0.3907256451
H	2.5869237769	2.1945199139	1.1671308525
H	2.8113429927	1.3099715777	-0.367607623
C	0.1056195594	2.8053486861	0.6763909699
H	0.398669832	2.9088738716	1.7328435698
H	0.2192364444	3.7786365332	0.1744588321
H	-0.9364097115	2.4795401862	0.6238017182
O	0.8878151719	1.8187156748	0.0365951101

O	1.8605413404	-0.889412955	-0.679192645
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Tabelle 10.482 Standardorientierung von **TS3** [Übergangszustand; M06/6-31+G(d,p)].

	x	y	z
C	1.5661098272	-1.7465503835	-1.6391007146
N	0.9877243829	-1.4454337455	-0.3337037796
C	0.6862720273	-2.7021110587	0.3414863286
C	1.8706606816	-0.644757084	0.554462146
C	2.4147472261	0.5558685023	-0.0535164391
C	3.5576603018	1.195060957	0.2658810323
Li	-0.4057718	-0.0205152187	0.2886632113
C	-0.2518539092	-0.096613589	2.4650306697
H	1.7959323631	-0.8243443911	-2.1822575087
H	0.8536811378	-2.3317977257	-2.2387251162
H	-0.0201475597	-3.3004396254	-0.2489585656
H	0.2539987121	-2.5089352268	1.329155683
H	2.6468169589	-1.277813597	1.0220439146
H	0.916468821	-0.3091026142	1.5548873743
H	1.7720322677	1.0391577698	-0.8016632901
H	3.8179048749	2.1526281817	-0.1787207072
H	4.2562349762	0.7792865014	0.9910880005
H	-0.7389018699	0.8944297265	2.521031736
H	0.311365367	-0.2131969141	3.3993792778
H	-1.0557186182	-0.8564714768	2.4943169946
H	2.5035695212	-2.3258064076	-1.5405398449
H	1.6044812007	-3.3050401975	0.4838908111
C	-2.6653548969	-1.8097753028	-0.3898517604
H	-3.6392324431	-1.9008623401	-0.8929613072
H	-1.8928504711	-2.2758629516	-1.008244986
H	-2.7123574068	-2.3239602215	0.5829493896
C	-3.2867968884	0.2667254629	0.5113342628
H	-4.2582273236	0.2374293183	-0.0037936793
H	-3.3968097551	-0.150268645	1.5236573284
H	-2.9389914577	1.300690019	0.5848975597
C	0.0510329052	2.9797757529	0.312293595
H	1.0042145735	3.2295343662	-0.176261634
H	-0.6169946318	3.852981188	0.2809892244
H	0.2518559972	2.6955144054	1.3482087195
C	-0.7952988015	2.089008962	-1.69651315
H	-1.2864967017	1.1948458098	-2.0925792963
H	-1.4488366972	2.9610719068	-1.8496172177
H	0.1523361322	2.2564895338	-2.2324758359
O	-0.5637138367	1.871686255	-0.3212819628
O	-2.3146971872	-0.4519269021	-0.2255934636

Tabelle 10.483 Standardorientierung von **8** [globales Minimum; M062X/6-31+G(d)].

	x	y	z
N	0.8488700082	-1.4239137288	-0.3677476382

C	2.1165817243	-1.2442846748	0.3617582496
C	2.8363436283	0.0272976256	-0.0015497417
C	2.8383424771	1.1030083051	0.7854212561
Li	-0.401155565	0.0162713736	0.4718908768
C	-0.3986480549	0.0379196087	2.5444162363
H	2.7775093448	-2.1130784029	0.1757574133
H	1.8636005184	-1.2222195121	1.4268866506
H	3.3922941355	0.0436891666	-0.9394230689
H	3.3831135801	2.0043634162	0.5137730547
H	2.2869647238	1.1077491739	1.7239159245
H	0.4373896367	0.5756852568	3.0344338509
H	-0.3871520891	-0.9666061469	3.0149259326
H	-1.3092942605	0.5170195679	2.958657853
C	0.1937757198	-2.6435609917	0.1048224081
H	-0.7657894673	-2.7590155462	-0.4074245707
H	0.814230927	-3.5364767075	-0.0891124877
H	0.0143167664	-2.5558692882	1.1804925769
C	1.0529069461	-1.4999701696	-1.8084264969
H	1.5220477618	-0.5829670254	-2.1741953789
H	1.6931631739	-2.3562054982	-2.0888955362
H	0.0824740096	-1.6154968514	-2.3019644525
C	-2.9704068221	-1.0688058803	0.8059255259
H	-3.8307603293	-1.6304336894	0.4166025026
H	-2.3389194989	-1.7088872083	1.4220090428
H	-3.3155640779	-0.2300569426	1.422271057
C	-2.8847248526	0.3074458044	-1.0910158224
H	-3.7949444854	-0.1648466679	-1.4849746492
H	-3.1550213783	1.2106771327	-0.5279816639
H	-2.2316652282	0.5854482822	-1.9200279192
C	0.2359715502	2.1299187134	-1.6172673183
H	-0.2609797259	3.0212988766	-2.0252733717
H	1.3151659463	2.3189002582	-1.5361535098
H	0.0684288101	1.2839598889	-2.2877913745
O	-0.3042850152	1.7917887448	-0.3612610282
O	-2.1753255737	-0.5978347829	-0.2726085528
C	-0.1695866009	2.8371324369	0.588655498
H	0.886508246	3.1199414103	0.6929638676
H	-0.7510583856	3.712215846	0.2673664931
H	-0.5377532237	2.4486078263	1.5388473112

Tabelle 10.484 Standardorientierung von **TS2** [Übergangszustand; M062X/6-31+G(d)].

	x	y	z
C	-1.5247909771	-0.0569284889	-1.8470585221
N	-1.8940061891	0.2137280055	-0.4617826221
C	-2.9644297054	1.2024762116	-0.4359597829
C	-2.3387248952	-1.052855012	0.2048660103
C	-1.2071705123	-1.952409538	0.5701644406
C	-0.6055188296	-1.8495820841	1.8168429765
Li	0.1154083167	-0.1395144089	0.46202874
C	0.9210192165	-0.3449560173	2.3926944503

H	-0.78883267	-0.8657117302	-1.8769328217
H	-1.0839718273	0.838763003	-2.2986356042
H	-2.6568445222	2.108118501	-0.9698795594
H	-3.202198918	1.4673180401	0.5993163529
H	-3.0824703644	-1.5449453876	-0.4501695632
H	-2.8649026792	-0.7404065396	1.1171103981
H	-0.8011071048	-2.6224452224	-0.1848758576
H	0.0892076451	-2.6232357726	2.1309162238
H	-1.186951081	-1.4295934346	2.6364947812
H	1.0384811214	-0.8587533615	3.3512441893
H	0.562023405	0.6761737791	2.6123150034
H	1.9206828167	-0.2634694834	1.9315845086
H	-2.4001667676	-0.3642418491	-2.4484515471
H	-3.8831496993	0.82066833	-0.9164895686
C	2.066569412	-2.125895015	-0.4796011778
H	1.6013477775	-2.8622224254	-1.1488543654
H	3.1571582739	-2.1554260871	-0.6064296974
H	1.8078960645	-2.3491313453	0.5561131827
C	1.8945683601	-0.383554364	-2.055507467
H	1.4892360503	0.625087671	-2.1593565858
H	2.9839201128	-0.3622042539	-2.2002577639
H	1.4481615224	-1.0420654706	-2.8139678038
C	2.2454248039	2.0084897469	0.3394599223
H	2.5584493668	2.9173414516	-0.1931697706
H	2.4376165234	2.1248904276	1.4136092245
H	2.801867648	1.1460684214	-0.0288788853
C	0.0647348161	2.7919004725	0.637732329
H	0.2542213244	2.913647398	1.712756899
H	0.2711282947	3.7409138443	0.1240948795
H	-0.973871562	2.5024044977	0.4824354044
O	0.871112323	1.7576907792	0.1081211854
O	1.5785271089	-0.8268422892	-0.7544951361

Tabelle 10.485 Standardorientierung von TS3 [Übergangszustand; M062X/6-31+G(d)].

	x	y	z
C	1.5921171319	-1.931997187	-1.5327639528
N	0.9606635666	-1.5051085015	-0.2843681538
C	0.65756794	-2.6945533902	0.5102909452
C	1.8013547084	-0.5933500366	0.5368468805
C	2.3676690633	0.528917256	-0.2100520168
C	3.5235061184	1.1715901156	0.0412238206
Li	-0.3861576251	-0.0236190447	0.2008081496
C	-0.3648752393	0.0074992614	2.3827895006
H	1.8286455279	-1.0677494018	-2.1562925276
H	0.9094006523	-2.5873971625	-2.0878173647
H	-0.0234575892	-3.35501186	-0.0374085613
H	0.1963275342	-2.406474009	1.4572302975
H	2.5735750741	-1.1552002847	1.0883405787
H	0.8200605066	-0.1968249486	1.4968880438
H	1.7399582701	0.932322432	-1.0132870679

H	3.8087834681	2.0632271177	-0.5088498723
H	4.2071627453	0.8254758495	0.812956447
H	-0.9733884311	0.9260548322	2.3253772165
H	0.1978573824	0.0670679907	3.3231734741
H	-1.0670858715	-0.8361400719	2.4966953865
H	2.5287838874	-2.481075398	-1.3364174672
H	1.579837933	-3.2608723678	0.7324715878
C	-2.5148252441	-1.7924682823	-0.5689370812
H	-3.487964914	-1.8968970133	-1.0656172672
H	-1.7276125265	-2.1935517437	-1.2091321285
H	-2.5292231562	-2.3385933017	0.3839575552
C	-3.2054916772	0.2274745929	0.4297560648
H	-4.1736392087	0.2002971666	-0.0867082006
H	-3.29429245	-0.250128102	1.4134211433
H	-2.8773040136	1.2601230573	0.5596191797
C	0.2053849476	2.8438213768	0.4443481164
H	1.0404267198	3.2088501556	-0.1655544116
H	-0.4566233328	3.6787689797	0.7084318638
H	0.5994708751	2.3696341019	1.3436763337
C	-0.9883311607	2.3071110494	-1.521523478
H	-1.5735907779	1.4973850924	-1.9614419735
H	-1.6199720978	3.1975294748	-1.4012780676
H	-0.140690269	2.5541764343	-2.1749488085
O	-0.5295516499	1.8556646665	-0.2636708329
O	-2.218428818	-0.4253798959	-0.352946351

Tabelle 10.486 Standardorientierung von **8** [Übergangszustand; M062X/6-31+G(d,p)].

	x	y	z
N	0.8490649805	-1.4209991347	-0.3699195983
C	2.1158288215	-1.2430807213	0.3621092033
C	2.8358786417	0.0288503786	0.0012180386
C	2.8365678705	1.1030483253	0.7899761287
Li	-0.4012049828	0.0161247555	0.4699663369
C	-0.3953251139	0.0379906181	2.5443564328
H	2.7772626095	-2.1109519582	0.1763789037
H	1.8603413409	-1.220366855	1.4263691841
H	3.3923350242	0.0475646864	-0.9357998137
H	3.3811024223	2.0040555556	0.5191692346
H	2.2825209523	1.10373644	1.7265440505
H	0.4395102186	0.5748983313	3.0349249949
H	-0.3850988586	-0.9655494037	3.014475367
H	-1.3055458138	0.517266351	2.9564761392
C	0.1900314719	-2.6393754016	0.1021136666
H	-0.7695768397	-2.7505810343	-0.4100692075
H	0.8074513553	-3.5337842373	-0.0911739546
H	0.0102976498	-2.5498876155	1.1772708296
C	1.0541833893	-1.4957890781	-1.8109548369
H	1.5250840135	-0.579516341	-2.1750734401
H	1.6925457338	-2.3524168608	-2.0922400099

H	0.0842704563	-1.6088133326	-2.30510888
C	-2.9694689813	-1.0695417926	0.8096288463
H	-3.8300465489	-1.6318510692	0.4231066385
H	-2.3374919702	-1.7070117192	1.4275370958
H	-3.3134367708	-0.2295280809	1.424393941
C	-2.883263834	0.3036750291	-1.0913101756
H	-3.793362901	-0.1677980684	-1.4851601704
H	-3.1527536461	1.2079950831	-0.5302856595
H	-2.2300321643	0.5809462276	-1.9200612097
C	0.2357696772	2.1249192663	-1.6185980331
H	-0.2529521482	3.0199273486	-2.027327724
H	1.3161049406	2.3048770022	-1.5362474294
H	0.063055593	1.2807818085	-2.289800069
O	-0.3088659107	1.7903416968	-0.3627025055
O	-2.1742700923	-0.601191635	-0.2709022089
C	-0.1700503472	2.8357473679	0.5878434345
H	0.886618032	3.115302294	0.6911914527
H	-0.7490478651	3.7124470775	0.268091532
H	-0.537065406	2.4473476959	1.5382924746

Tabelle 10.487 Standardorientierung von TS2 [Übergangszustand; M062X/6-31+G(d,p)].

	x	y	z
C	-1.5218547989	-0.0523249473	-1.8423753865
N	-1.8943216851	0.2136745323	-0.4565136576
C	-2.968741969	1.1986829923	-0.4283988308
C	-2.3351643249	-1.0567137383	0.2072760505
C	-1.2014314868	-1.9524732135	0.573817596
C	-0.6018135421	-1.8463743471	1.822309228
Li	0.1141546893	-0.1383678191	0.4585764364
C	0.9176260722	-0.343620255	2.3919423448
H	-0.7833888461	-0.858436428	-1.8719105979
H	-1.0827684376	0.8452798583	-2.2908477329
H	-2.6656405875	2.1060526734	-0.9610059494
H	-3.2067041997	1.4609917324	0.6069414467
H	-3.0745354934	-1.5509863371	-0.4503091326
H	-2.8644432786	-0.7481178823	1.1186355744
H	-0.7959275358	-2.6255333052	-0.1775024106
H	0.0919742152	-2.619224931	2.1389925656
H	-1.18728922	-1.4276802766	2.6391554745
H	1.0338799672	-0.8427531571	3.3568811082
H	0.5619793296	0.6813029062	2.5938115157
H	1.9141049203	-0.2761296352	1.9243479203
H	-2.3944666711	-0.3610902013	-2.4459218687
H	-3.8858928652	0.8145884998	-0.9088313899
C	2.0614167091	-2.1297328584	-0.4859483005
H	1.5923209493	-2.859807992	-1.1587578699
H	3.1513833147	-2.1650110322	-0.6127917188
H	1.8011535799	-2.3578550009	0.5480438934
C	1.8969956329	-0.3758847999	-2.0526091151
H	1.4962050568	0.6350933636	-2.1487996764

H	2.9857362275	-0.3588709387	-2.1992847644
H	1.4464148927	-1.0269086103	-2.8144925488
C	2.2476273855	2.0033254914	0.3447896666
H	2.5692492265	2.9100837383	-0.1853766813
H	2.4294110471	2.1196185263	1.4204144049
H	2.8044290534	1.1383825733	-0.0162104989
C	0.0646753994	2.7932534169	0.6211350875
H	0.238412505	2.9102999941	1.6990765454
H	0.2831134963	3.742920159	0.1146954203
H	-0.972544969	2.5092892358	0.4495064031
O	0.8740834193	1.7561517051	0.0998015381
O	1.5802368214	-0.8258026922	-0.7531150893

Tabelle 10.488 Standardorientierung von **TS3** [Übergangszustand; M062X/6-31+G(d,p)].

	x	y	z
C	1.5892198345	-1.9308740959	-1.5363828973
N	0.9594114401	-1.5058828975	-0.286036966
C	0.6540856006	-2.6965014921	0.5067739714
C	1.8017730231	-0.5969240451	0.5366141796
C	2.36251333	0.5294290186	-0.20791639
C	3.5148163622	1.1779559732	0.0434376805
Li	-0.3825605858	-0.0225826653	0.2045158746
C	-0.3622380741	0.0052181211	2.3860293259
H	1.8297320529	-1.0656573568	-2.1561700287
H	0.9043155423	-2.5809806837	-2.0939320167
H	-0.0252533968	-3.3561693503	-0.0429421083
H	0.1907749417	-2.4087764391	1.4523406948
H	2.5770752867	-1.1586964238	1.0829752792
H	0.8204042555	-0.2019159352	1.4993466523
H	1.7320862255	0.9313773536	-1.0094129711
H	3.793392878	2.0709497294	-0.5063143596
H	4.1997336461	0.8333132332	0.8136854037
H	-0.9727940741	0.9212679211	2.324992303
H	0.2034401401	0.0720201775	3.3229035857
H	-1.061740323	-0.8385071671	2.5072765086
H	2.5231185936	-2.4845187031	-1.3422920295
H	1.5751905399	-3.2629626367	0.7306510879
C	-2.5112457408	-1.7904282963	-0.5698466312
H	-3.4821799859	-1.8949452254	-1.0698593731
H	-1.7216962738	-2.1922513812	-1.2063393942
H	-2.5293249334	-2.3368188223	0.3825319837
C	-3.2008416079	0.230440577	0.4315452755
H	-4.1693456987	0.2049378111	-0.0834023183
H	-3.2889617216	-0.2471212956	1.4149547585
H	-2.8705707387	1.2620530029	0.5619422549
C	0.201373932	2.8484177062	0.446838453
H	1.0436060436	3.2017755222	-0.1594582339
H	-0.4566161761	3.6900096041	0.697827224
H	0.585969054	2.380602177	1.353326981
C	-0.9826224085	2.2976628023	-1.5231262405

H	-1.5703575516	1.4866914005	-1.9567303053
H	-1.6088692785	3.1931829239	-1.4174825686
H	-0.1300046232	2.5319083572	-2.1742377011
O	-0.5344693424	1.8569507717	-0.2567895922
O	-2.2142921873	-0.4230502712	-0.3525503522

Tabelle 10.489 Standardorientierung von **8** [globales Minimum; M062X/6-311+G(d,p)].

	x	y	z
N	0.8611062037	-1.4170746597	-0.3722463858
C	2.116883834	-1.240460658	0.3792252208
C	2.8448110514	0.0276672354	0.0228377639
C	2.8145201916	1.1102057609	0.7923714309
Li	-0.4139738835	0.0112237697	0.4624639986
C	-0.4226419949	0.0357517053	2.5432706548
H	2.7771609935	-2.1082125815	0.2060512721
H	1.8466536714	-1.2123315826	1.4373613871
H	3.4314845566	0.033631631	-0.8932204917
H	3.3649429985	2.0073426823	0.5277846388
H	2.2304438145	1.1212876564	1.7083335239
H	0.4143557739	0.5481304549	3.0508231676
H	-0.4443609282	-0.9675586249	3.0081078578
H	-1.3252226457	0.5332703432	2.944403637
C	0.1986458968	-2.6397380316	0.083773695
H	-0.7547852284	-2.7473088551	-0.4367172688
H	0.8174130366	-3.529806272	-0.1118200466
H	0.0102880253	-2.5605632288	1.1562673492
C	1.0926769941	-1.486912878	-1.8098354284
H	1.5627823105	-0.5680164217	-2.1623678439
H	1.7409513883	-2.3368891336	-2.0792873273
H	0.1347620619	-1.6063707971	-2.3213868684
C	-2.9653460192	-1.1083738623	0.8007794543
H	-3.8358256358	-1.6458444373	0.4070777921
H	-2.3261739473	-1.7788044341	1.3707921401
H	-3.2883972824	-0.3005058838	1.4639156081
C	-2.9205029603	0.3559657425	-1.0294340917
H	-3.8424274582	-0.0926554423	-1.4166840649
H	-3.169267598	1.2307476021	-0.4181982126
H	-2.2930159406	0.6712043693	-1.8615935242
C	0.2342747656	2.0933997517	-1.6452078082
H	-0.248316616	2.9883463695	-2.0559943308
H	1.316045718	2.2593305255	-1.5837348392
H	0.0384917239	1.2451871377	-2.3016435891
O	-0.2919525836	1.7827273045	-0.3756926524
O	-2.1928137395	-0.589282054	-0.2731750057
C	-0.1390285422	2.8447492556	0.5533803848
H	0.9143378894	3.1378683126	0.6230561625
H	-0.7351829173	3.7083641804	0.2366533802
H	-0.4768319785	2.4701170477	1.51820826

Tabelle 10.490 Standardorientierung von **TS2** [Übergangszustand; M062X/6-311+G(d,p)].

	x	y	z
C	-1.5194918577	-0.1027241687	-1.8593326865
N	-1.878732817	0.2055623239	-0.4785029944
C	-2.9446139477	1.1998479142	-0.4721039228
C	-2.3274325586	-1.0439092374	0.2210349931
C	-1.2019348321	-1.944556597	0.5976730988
C	-0.5973763877	-1.8284237361	1.8420487122
Li	0.1185923645	-0.1304055538	0.4468293899
C	0.9424383389	-0.3530265474	2.3841925115
H	-0.789593732	-0.9141593616	-1.8728403053
H	-1.0787589729	0.7766371942	-2.3364414404
H	-2.6339560959	2.0911957194	-1.023296477
H	-3.181185695	1.486492846	0.5551538843
H	-3.0762536521	-1.5435551669	-0.416975393
H	-2.8437134769	-0.7091756851	1.1278475656
H	-0.8142753142	-2.6410510186	-0.1380268542
H	0.0794272327	-2.6100063787	2.1670582001
H	-1.1752855617	-1.3960593324	2.6545103117
H	1.0774175621	-0.8511545822	3.3446561057
H	0.5929064517	0.6705343566	2.5892950513
H	1.9235858463	-0.2939124526	1.8897512524
H	-2.3989077279	-0.4195079587	-2.4443045356
H	-3.8628393086	0.812879437	-0.9427996218
C	2.0301580652	-2.1350065624	-0.5088304411
H	1.5602957348	-2.8502297185	-1.193470193
H	3.1185458972	-2.1772442731	-0.6290573123
H	1.7614307976	-2.3760367764	0.5179710657
C	1.892920085	-0.3558139794	-2.0502965197
H	1.4971856026	0.6558383727	-2.1367114475
H	2.9810532291	-0.3405161005	-2.1851107063
H	1.4485740541	-0.9922950807	-2.8248245009
C	2.2384632357	2.0182131703	0.3620004161
H	2.5497317404	2.9382517111	-0.1466703408
H	2.4283975202	2.1070227582	1.4365406163
H	2.7975490162	1.1688699343	-0.025335719
C	0.0556582098	2.7982634135	0.6608350401
H	0.235949116	2.9037702473	1.7367058887
H	0.2688548953	3.7523406585	0.1650827895
H	-0.9807266006	2.5165546576	0.4927847973
O	0.8644939044	1.769435572	0.123372052
O	1.5611036388	-0.8236490186	-0.7612653306

Tabelle 10.491 Standardorientierung von **TS3** [Übergangszustand; M062X/6-311+G(d,p)].

	x	y	z
C	1.6020359574	-1.9423023637	-1.5342835026
N	0.9593447245	-1.5126954407	-0.2920360796
C	0.6522219031	-2.7009234378	0.5041567377
C	1.7951765567	-0.5987081028	0.5317766124
C	2.3612406225	0.5231388141	-0.2122657395

C	3.5056474461	1.1740174063	0.0505341769
Li	-0.3803961013	-0.0170582066	0.1907955087
C	-0.3760302246	0.0109973192	2.3733989065
H	1.8438241522	-1.0815782284	-2.156621431
H	0.9268544612	-2.5985037676	-2.0927136771
H	-0.0208806868	-3.3634685822	-0.0456300931
H	0.1838023191	-2.4116649232	1.4445035867
H	2.5631947777	-1.1547556391	1.0882326782
H	0.8111061658	-0.2013543242	1.4890582743
H	1.7434271431	0.9160540259	-1.0244738526
H	3.7904492235	2.0614717973	-0.5012597022
H	4.1792347866	0.8361086481	0.8311316202
H	-0.988798534	0.9217771588	2.2982177785
H	0.1883444818	0.0931096894	3.3077269482
H	-1.0688718443	-0.8337213844	2.5039379551
H	2.5348106203	-2.4889387467	-1.3281946609
H	1.5719400809	-3.2625554704	0.7344852353
C	-2.5046278786	-1.8001256777	-0.5595760768
H	-3.4763781114	-1.9135910137	-1.051678786
H	-1.7183828314	-2.2024493305	-1.1964094964
H	-2.5135517616	-2.3383409114	0.3951600715
C	-3.2017948356	0.2230497105	0.4288284355
H	-4.1719870372	0.1818836905	-0.0776320122
H	-3.277459435	-0.2423525098	1.416679343
H	-2.8833741622	1.257922543	0.5454951584
C	0.2246180787	2.8465175493	0.4413642527
H	1.0592344828	3.2030027491	-0.1698355748
H	-0.4257718601	3.6858737695	0.7103238886
H	0.6187419383	2.3684323176	1.3360149038
C	-0.9999067368	2.3297114208	-1.5116578168
H	-1.5969083445	1.52920747	-1.9473539947
H	-1.6220820636	3.2214501735	-1.375474681
H	-0.1644061137	2.5759180066	-2.176920872
O	-0.523017386	1.8659266145	-0.2648166358
O	-2.2145759733	-0.4298838131	-0.3537003869

Tabelle 10.492 Standardorientierung von **8** [globales Minimum; MP2/6-31+G(d)].

	x	y	z
N	0.8569522916	-1.4459320664	-0.3468897004
C	2.1682885053	-1.2825954302	0.3191614353
C	2.878577057	-0.017836587	-0.069661466
C	2.9726617315	1.0417263739	0.7512882071
Li	-0.3924521683	0.0243805493	0.5289621884
C	-0.3475240806	0.0262064798	2.6279103263
H	2.8107437436	-2.1567095634	0.0909669715
H	1.9715513985	-1.2717269511	1.3961105572
H	3.3687222591	0.016067195	-1.0431625684
H	3.5216063024	1.934353229	0.4609022086
H	2.4993178601	1.0369949329	1.7298448571

H	0.5114798491	0.569107373	3.0691195507
H	-0.3187341903	-0.9798640406	3.0910903404
H	-1.2439274556	0.510601532	3.0642123702
C	0.2331267852	-2.6817233804	0.1490335838
H	-0.7502842253	-2.7957381761	-0.3145854863
H	0.8486649951	-3.5679896563	-0.0876661202
H	0.1089230324	-2.6056380412	1.2320442818
C	1.0044506296	-1.5329031085	-1.8010062974
H	1.4249193067	-0.6047302503	-2.1947997429
H	1.6600915742	-2.371852203	-2.0986907084
H	0.0173224084	-1.6880239657	-2.2476679729
C	-3.0920139118	-0.9511476785	0.8137326287
H	-3.9029175665	-1.5840627284	0.4299655812
H	-2.4984492325	-1.4824734288	1.5553652684
H	-3.5101293455	-0.0477202261	1.273309121
C	-2.8711282199	0.1605220523	-1.2581691333
H	-3.7236206834	-0.4030350474	-1.6595790123
H	-3.2221194634	1.1173541964	-0.8520089489
H	-2.1485034158	0.3468973188	-2.0533069235
C	0.2040444158	2.2868375495	-1.5733299206
H	-0.3239224044	3.1791013164	-1.9352973095
H	1.273246191	2.5109522569	-1.4723996297
H	0.0679496813	1.4695460762	-2.2829836294
O	-0.3386523904	1.8580777679	-0.3283739173
O	-2.2013198839	-0.5996184834	-0.2548465071
C	-0.2305239871	2.8822630102	0.671054477
H	0.8207648705	3.1627520072	0.8102384643
H	-0.8099888815	3.7633073849	0.365745095
H	-0.6202283821	2.4540814112	1.5930664807

Tabelle 10.493 Standardorientierung von **TS2** [Übergangszustand; MP2/6-31+G(d)].

	x	y	z
C	-1.5827296412	-0.0238091296	-1.8561834321
N	-1.9141805698	0.2156214753	-0.4487639148
C	-2.9884075627	1.2092201977	-0.3769744873
C	-2.3637525837	-1.0748236885	0.1863288004
C	-1.2320796891	-1.9771649364	0.5249565966
C	-0.6167227315	-1.8835020263	1.7778088917
Li	0.1105339543	-0.1249276925	0.4460947219
C	0.8310548147	-0.3663478357	2.4189343633
H	-0.8463748851	-0.828537755	-1.9191595373
H	-1.1583746883	0.8847250034	-2.2973905278
H	-2.6855345841	2.1267628873	-0.8922463066
H	-3.2036030205	1.442254084	0.670488458
H	-3.108063042	-1.5499153936	-0.4823015018
H	-2.8888106359	-0.7848534565	1.1076820789
H	-0.8175560356	-2.6250472228	-0.2463135299
H	0.0723703093	-2.6739654749	2.0683098822
H	-1.2223479622	-1.5192483282	2.6092758828
H	0.9512263404	-0.9146196801	3.3575113441

H	0.3710528137	0.6104034018	2.6472614383
H	1.8290266134	-0.2026931673	1.978305596
H	-2.4737667701	-0.3201476948	-2.4403255055
H	-3.9159435006	0.840645953	-0.8509806544
C	2.1771628599	-2.120961416	-0.4230794401
H	1.7141092964	-2.905687175	-1.0345010533
H	3.262941084	-2.1232086486	-0.5841733769
H	1.952359481	-2.2844297988	0.6292909555
C	1.926312801	-0.4806333888	-2.1088597236
H	1.4925138752	0.5062250713	-2.2727930879
H	3.012183631	-0.4428706793	-2.2684684381
H	1.486984762	-1.2042365278	-2.8080424235
C	2.2867091667	2.065273996	0.2980562737
H	2.5759829907	2.9776019707	-0.2401426801
H	2.5092530484	2.179484391	1.3652962525
H	2.8251858607	1.2053667971	-0.0959356581
C	0.1088359929	2.8650598785	0.6669211857
H	0.3226268807	2.970438453	1.7377961816
H	0.3271697488	3.8117757531	0.1556930418
H	-0.9344031583	2.5935298197	0.5227956403
O	0.8914076072	1.8065925098	0.1065396536
O	1.6353011285	-0.8400595261	-0.7595649597

Tabelle 10.494 Standardorientierung von **TS3** [Übergangszustand; MP2/6-31+G(d)].

	x	y	z
C	1.5393334306	-1.9710596091	-1.5271279846
N	0.9400064706	-1.5016803274	-0.2707917829
C	0.6088843129	-2.6759115057	0.5479453694
C	1.8451782265	-0.6243161007	0.5214458912
C	2.3725105344	0.5028269011	-0.2376749395
C	3.5575088064	1.1365427611	-0.0485903558
Li	-0.3991367558	-0.0315815896	0.3308599309
C	-0.116294417	0.0942559259	2.5425187326
H	1.7979307137	-1.1210741944	-2.1613327124
H	0.8242040849	-2.6096118105	-2.061954915
H	-0.0967711807	-3.3203287621	0.0130059473
H	0.1667966813	-2.354839081	1.4924836866
H	2.6388498452	-1.2131388861	1.0181376049
H	0.9336955316	-0.2061261086	1.5460093962
H	1.6979867255	0.9308889275	-0.9874628252
H	3.8094720793	2.042368693	-0.5931028099
H	4.290733981	0.7687367402	0.6659380786
H	-1.0450539326	0.6707520831	2.3734778252
H	0.5037848621	0.7026730838	3.2160296657
H	-0.3950905432	-0.8150112414	3.0949270507
H	2.4584871257	-2.5505915576	-1.3333276701
H	1.5151562818	-3.2677666117	0.7705381897
C	-2.5878725556	-1.7551729347	-0.8019459341
H	-3.4670880182	-1.6780306867	-1.4532308705
H	-1.7279232873	-2.1016372501	-1.3739819576

H	-2.7990980351	-2.4531060582	0.0175342383
C	-3.322588903	0.1228015424	0.4483686495
H	-4.2097856393	0.2101316847	-0.1907823259
H	-3.5597555399	-0.484793808	1.3297247549
H	-2.9838351808	1.1109350825	0.7577849378
C	0.06928529	2.9361624809	0.5368502441
H	1.0114058325	3.1928371824	0.0410985754
H	-0.5821371746	3.8174962191	0.5845056931
H	0.2740417798	2.5565839257	1.5359924386
C	-0.877056873	2.2499145557	-1.5270001638
H	-1.389458341	1.4022093776	-1.9829770865
H	-1.5229436326	3.1367045644	-1.5548194804
H	0.0540735878	2.4646812272	-2.0668514495
O	-0.5980485066	1.8823996272	-0.1745683706
O	-2.2433396675	-0.4655254619	-0.2883662666

Tabelle 10.495 Standardorientierung von **8** [globales Minimum; MP2/6-311+G(d,p)].

	x	y	z
N	0.8560873279	-1.4336506286	-0.3760399104
C	2.145906489	-1.2772136831	0.3299023829
C	2.8664889927	-0.0082287669	-0.0334250901
C	2.9157238303	1.0516192314	0.79053125
Li	-0.3957302699	0.032883778	0.4983886085
C	-0.341496152	0.0233635064	2.5926220085
H	2.7921139682	-2.1500756592	0.1137098442
H	1.9161090742	-1.2691168596	1.3998859803
H	3.3908172171	0.0292323079	-0.9880818832
H	3.4661661041	1.9486368859	0.5183267804
H	2.4004053351	1.0336971386	1.747334118
H	0.5117184917	0.5395005165	3.0752272215
H	-0.347057293	-0.9833729771	3.0574850646
H	-1.2366681374	0.5199726281	3.0201379914
C	0.2197464999	-2.6699012382	0.0972448619
H	-0.7466211363	-2.7891486286	-0.399357345
H	0.8486877508	-3.5513589686	-0.1182377735
H	0.059873907	-2.5934312862	1.1756774807
C	1.05714676	-1.5226820607	-1.8219962451
H	1.4953134542	-0.597101648	-2.202538985
H	1.7217369803	-2.3636908263	-2.0904165149
H	0.0888785692	-1.6779569222	-2.3079326332
C	-3.0727345686	-0.9665051252	0.8503865238
H	-3.8564583719	-1.6341207419	0.4687339389
H	-2.4552703219	-1.4743920511	1.5893456637
H	-3.5323509227	-0.0886662877	1.3200508083
C	-2.9186404825	0.1823010855	-1.187301089
H	-3.7566217228	-0.4022381777	-1.5894579228
H	-3.3015419334	1.1167397847	-0.7576697002
H	-2.2217603861	0.4168173779	-1.9928040177
C	0.22421105	2.241081505	-1.5872285473

H	-0.2781575221	3.140180476	-1.9686338003
H	1.2989571495	2.4400636949	-1.4907302038
H	0.0708227939	1.4185339774	-2.287898562
O	-0.3285953702	1.8520463972	-0.3423809487
O	-2.2109716482	-0.5683207212	-0.2147697274
C	-0.193180022	2.8890636814	0.6286547137
H	0.8615840751	3.1685802728	0.741161475
H	-0.7724862658	3.7692139551	0.3203026917
H	-0.5651882936	2.4874540574	1.5704904916

Tabelle 10.496 Standardorientierung von **TS2** [Übergangszustand; MP2/6-311+G(d,p)].

	x	y	z
C	-1.600505	-0.032369	-1.870018
N	-1.881296	0.274693	-0.466332
C	-2.908229	1.31553	-0.41213
C	-2.380967	-0.966814	0.219284
C	-1.285985	-1.911002	0.57426
C	-0.663094	-1.806599	1.821711
Li	0.13429	-0.111531	0.430023
C	0.844446	-0.319263	2.420731
H	-0.906969	-0.875239	-1.922971
H	-1.146676	0.83582	-2.359473
H	-2.576078	2.199998	-0.965677
H	-3.095111	1.596374	0.628835
H	-3.157409	-1.426667	-0.421232
H	-2.872839	-0.621969	1.139123
H	-0.894809	-2.585306	-0.184433
H	0.004046	-2.607119	2.132904
H	-1.249531	-1.388818	2.640702
H	0.948024	-0.842373	3.375386
H	0.413184	0.676418	2.622369
H	1.849258	-0.195046	1.981875
H	-2.522363	-0.306779	-2.414342
H	-3.858421	0.969603	-0.856151
C	2.068412	-2.216397	-0.374869
H	1.570607	-2.995057	-0.96648
H	3.152714	-2.274677	-0.535507
H	1.840908	-2.351064	0.681555
C	1.88137	-0.621308	-2.091462
H	1.501077	0.382469	-2.284797
H	2.965414	-0.645346	-2.26535
H	1.396893	-1.336602	-2.76925
C	2.340385	1.999636	0.251966
H	2.654683	2.887897	-0.312051
H	2.574178	2.13693	1.314134
H	2.860503	1.117757	-0.118413
C	0.206014	2.866343	0.610141
H	0.432964	2.997357	1.675639
H	0.446618	3.792707	0.072042
H	-0.849118	2.631384	0.487077

O	0.945515	1.775456	0.075219
O	1.588656	-0.926387	-0.737587

Tabelle 10.497 Standardorientierung von **TS3** [Übergangszustand; MP2/6-311+G(d,p)].

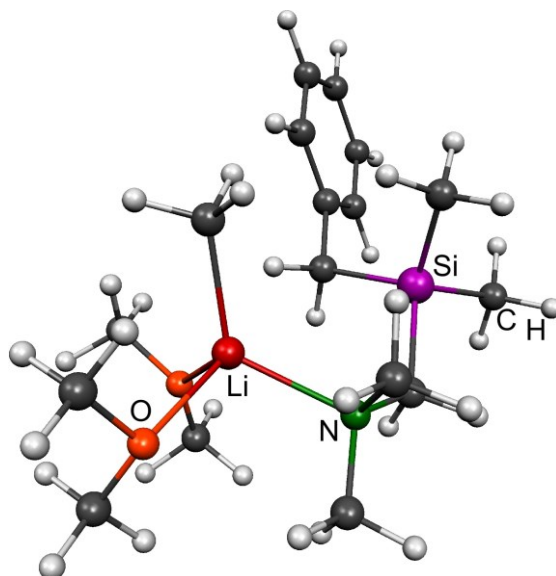
	x	y	z
C	1.428365	-2.101013	-1.472328
N	0.850405	-1.567295	-0.233648
C	0.482353	-2.701742	0.620917
C	1.793354	-0.707357	0.52926
C	2.383618	0.364254	-0.266536
C	3.581288	0.968644	-0.063699
Li	-0.392041	0.028458	0.289747
C	-0.141805	0.185843	2.488102
H	1.718029	-1.284822	-2.136885
H	0.68891	-2.730349	-1.984127
H	-0.256591	-3.332002	0.115231
H	0.068753	-2.336262	1.562659
H	2.552042	-1.312073	1.056485
H	0.902746	-0.205498	1.517703
H	1.748855	0.779532	-1.056623
H	3.879602	1.834984	-0.646003
H	4.273178	0.606897	0.692888
H	-1.012567	0.838358	2.291005
H	0.507824	0.749399	3.172301
H	-0.512695	-0.687237	3.044645
H	2.324276	-2.708407	-1.258809
H	1.368186	-3.321412	0.847779
C	-2.657885	-1.65993	-0.667052
H	-3.547651	-1.608628	-1.306784
H	-1.827222	-2.093885	-1.222821
H	-2.877802	-2.277814	0.212425
C	-3.292921	0.317518	0.439974
H	-4.194831	0.391661	-0.180279
H	-3.527637	-0.217406	1.367862
H	-2.921589	1.314457	0.675682
C	0.264259	2.939783	0.416015
H	1.231503	3.098769	-0.072405
H	-0.309767	3.874775	0.423879
H	0.427911	2.587197	1.433149
C	-0.715076	2.273284	-1.619713
H	-1.296463	1.463261	-2.062281
H	-1.283195	3.210225	-1.680387
H	0.231904	2.392631	-2.161938
O	-0.47756	1.924859	-0.26256
O	-2.258157	-0.351904	-0.275901

## 10.2.2. Details zu Kapitel 4.4

## 10.2.2.1. Monomeres Methyllithiummodell

Tabelle 10.498 Berechnete Energien der optimierten Strukturen des monomeren Substitutionsmodells mit Methyllithium

Verbindung	SCF [Hartree]	ZPE [Hartree]
<b>Ed1-1</b>	-1171.051347	-1170.550286
<b>Ed1-2</b>	-1171.051448	-1170.54948
<b>TS7</b>	-1171.024211	-1170.527818
<b>TS8</b>	-1171.038522	-1170.535233
<b>TS9</b>	-1171.034805	-1170.531585
<b>Int1</b>	-1171.042163	-1170.537254
<b>Int2</b>	-1171.035316	-1170.531424
<b>TS14</b>	-1171.027485	-1170.523892
<b>TS12</b>	-1171.027469	-1170.524555
<b>TS13</b>	-1171.024882	-1170.521184
<b>Int3</b>	-1171.035769	-1170.533121
<b>TS10</b>	-1171.035834	-1170.533364
<b>Pr1</b>	-1171.069556	-1170.56741
<b>Int1 + DME</b>	-1325.975929	-1325.389924
<b>TS15</b>	-1325.975195	-1325.390934
<b>Int4</b>	-1325.975939	-1325.390547
<b>TS16</b>	-1325.972287	-1325.38672

Abbildung 10.22 Molekel Darstellung von **Ed1** (Konformer 1).Tabelle 10.499 Standardorientierung von **Ed1** [Konformer 1; lokales Minimum; M06/6-31+G(d)].

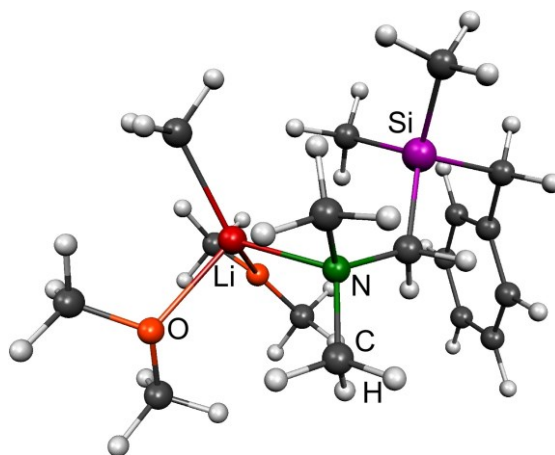
	x	y	z
C	1.0021192487	-1.0172351385	2.2165449138
H	1.3705525685	-2.0027826659	2.5768312407

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H	-0.1025989737	-1.1287059954	2.2158570374
H	1.2071637823	-0.3290431037	3.0665528074
Li	1.9110591578	-0.3784047953	0.470166271
N	1.8799647249	1.6817460315	-0.1203962557
C	0.6450528426	2.1950336757	-0.7275084271
H	0.6234181082	1.861104822	-1.7807601521
H	0.6874858776	3.307658541	-0.7758255195
O	3.9707496841	-0.735126045	0.5397262966
Si	-1.0700072263	1.6848701779	-0.0491207745
C	-1.3962949362	-0.1112372195	-0.5638014781
H	-0.6360975774	-0.7276579718	-0.0604148691
H	-1.2184281214	-0.1803083612	-1.6506304477
C	-2.7769543134	-0.5785067825	-0.2212353132
C	-3.8426751402	-0.4075143041	-1.1128342
C	-3.043584617	-1.1721956578	1.0189395219
C	-5.1323562072	-0.8111619314	-0.778636597
H	-3.6525810707	0.0473670672	-2.0876138106
C	-4.3322638866	-1.5752226452	1.3561939778
H	-2.2222618227	-1.3207955423	1.7231759335
C	-5.3840310211	-1.3960624188	0.4603097845
H	-5.9442509782	-0.6706681295	-1.4917629579
H	-4.5138270163	-2.0372008845	2.3260692617
H	-6.3918042518	-1.7140054826	0.7237569682
C	-2.2491621246	2.8181210136	-0.983987
H	-2.1371267482	2.7111657006	-2.0729742614
H	-3.2938516942	2.5884408587	-0.7333515239
H	-2.0702379218	3.8726475813	-0.7314427548
C	-1.3179722351	1.9066332696	1.7947352121
H	-2.3819021504	1.768261529	2.0349804978
H	-0.7465391919	1.1678176837	2.3743782666
H	-1.0317135598	2.915290931	2.1242409001
C	4.5804310973	-1.3601162739	-0.5623335119
H	4.2263619919	-2.3996128147	-0.6742942458
H	4.3116093922	-0.7939290784	-1.4612272188
H	5.6773631596	-1.366022466	-0.4524415835
C	4.3019179133	-1.3725905306	1.7601995735
H	3.9871192248	-2.4286192408	1.7430079722
H	5.3881397	-1.314243594	1.9372689014
H	3.7529041443	-0.8630479689	2.5569234301
C	2.0985628964	2.295806689	1.1878123306
H	2.1559822563	3.4004674422	1.104225058
H	1.291095061	2.0276114852	1.8757282641
H	3.0403441624	1.928904571	1.6162323281
C	3.0192482189	1.9894117342	-0.9771615109
H	3.9406118529	1.6014567475	-0.5230761008
H	2.8883060761	1.5198760495	-1.9622984227
H	3.12970247	3.0816415472	-1.1326717202
C	1.5262508505	-1.3751493108	-2.5424940895
H	1.8272842111	-0.3417403094	-2.7534815188
H	2.2315876474	-2.0663739835	-3.0363854247
H	0.5169651042	-1.5468802044	-2.9526314361

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C	1.1082353286	-2.8439607963	-0.7621338368
H	0.0775048906	-3.0249393592	-1.1091430724
H	1.7741436783	-3.6157762254	-1.1838502846
H	1.132444028	-2.8677679792	0.3337038483
O	1.5410734354	-1.5529239381	-1.1509872772

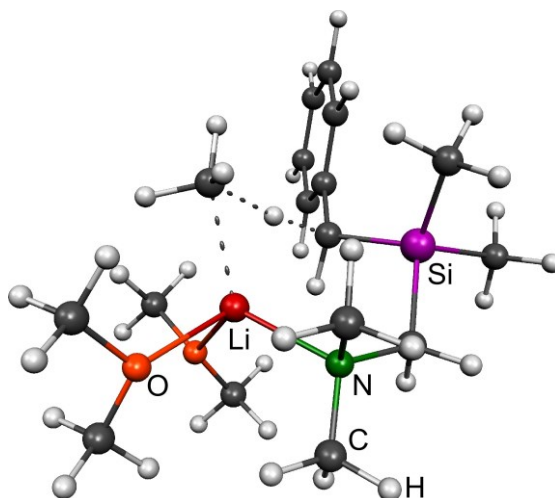
Abbildung 10.23 Molekel Darstellung von **Ed1** (Konformer 2).Tabelle 10.500 Standardorientierung von **Ed1** [Konformer 2; lokales Minimum; M06/6-31+G(d)].

	x	y	z
C	-3.0048234434	1.3768714307	-1.7852504886
H	-3.4687073935	0.8974878974	-2.6746139854
H	-2.3728919804	2.1850371102	-2.2113225692
H	-3.8446872909	1.9272275809	-1.3037447694
Li	-2.1988677607	0.1142171015	-0.354057295
N	-1.2338934442	1.0030925252	1.3343287217
C	0.2180054398	1.1451502838	1.215861201
H	0.661177377	0.1385429063	1.3031791636
H	0.6136338851	1.7161202512	2.0912424284
O	-3.728085204	-1.0266414691	0.4814342871
Si	1.0290811277	1.9142668377	-0.3305499288
C	2.8927910648	1.6812711401	0.0361345938
H	3.1353232348	2.2234723702	0.9636335064
H	3.4379873828	2.186227261	-0.7770370271
C	3.2994127625	0.2451033027	0.1332938399
C	3.6087393569	-0.4950121201	-1.0154071123
C	3.3333887261	-0.4196224916	1.3657902314
C	3.9267937832	-1.8478021451	-0.9381810286
H	3.6001544191	0.0046511427	-1.985901243
C	3.6500592215	-1.7730957544	1.4482973383
H	3.1123134536	0.1402861821	2.276896408
C	3.9450609342	-2.4967695446	0.2950553813
H	4.1695723781	-2.3970009216	-1.8475029096
H	3.6758003485	-2.2625074518	2.4215571061
H	4.199845576	-3.5536985124	0.3577109452

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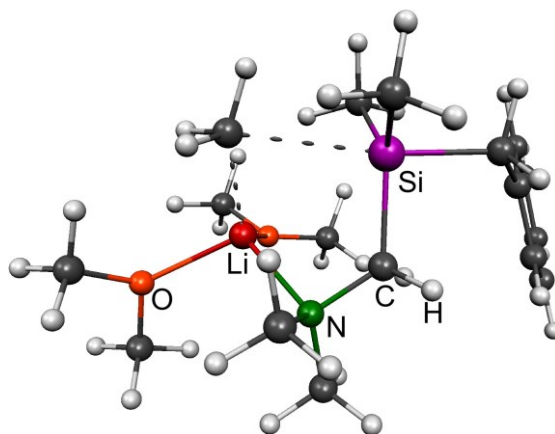
C	0.7181135012	3.7629684403	-0.4763941104
H	0.7456330123	4.2627285482	0.5019529931
H	1.4904700365	4.2235927183	-1.1087880904
H	-0.2540009793	3.9749179832	-0.9410934252
C	0.6227022532	1.0525892627	-1.9398510724
H	1.1736966288	1.5325390838	-2.762486648
H	0.9061318016	-0.008311754	-1.9118990953
H	-0.4540308922	1.1152227628	-2.1577534574
C	-3.4757765011	-2.3390764798	0.9143711865
H	-3.3194721442	-3.0172764456	0.0571885744
H	-2.5671505133	-2.3236167341	1.5264716021
H	-4.3133425608	-2.7212737891	1.5211837697
C	-4.9188289422	-0.9360524348	-0.2786233789
H	-4.8641122814	-1.5915741347	-1.1638184019
H	-5.7863751156	-1.2274128322	0.3354615642
H	-5.011727626	0.1000407707	-0.6147454945
C	-1.8978836219	2.3034268629	1.3367839383
H	-1.503097024	2.9544174272	2.1441450895
H	-1.7709356155	2.7982463632	0.3679044077
H	-2.9759510376	2.1646100943	1.4892253956
C	-1.5587682057	0.296878363	2.5670467808
H	-2.6434224891	0.1394255871	2.6333431874
H	-1.0607364637	-0.6827297004	2.580531824
H	-1.2230381497	0.8609556099	3.4609765977
C	-0.029835856	-2.290932373	-0.2649551286
H	0.1385656234	-1.9210582832	0.7536217924
H	-0.3401171549	-3.3494431479	-0.2188645496
H	0.9182639	-2.2192895442	-0.8263942275
C	-1.3606673419	-1.9224575219	-2.162772084
H	-0.4648848959	-1.9312266929	-2.8050608729
H	-1.7984172026	-2.9354619253	-2.1441719966
H	-2.0844813559	-1.1995456277	-2.5587907998
O	-1.0326857411	-1.5009803697	-0.8541256649

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Abbildung 10.24 Molekel Darstellung von **TS7**.Tabelle 10.501 Standardorientierung von **TS7** [Übergangszustand; M06/6-31+G(d)].

	x	y	z
C	0.3748776067	-0.7201718286	2.1263663933
H	0.918804282	-1.6751295862	2.2607910302
H	-0.5796349667	-0.8580199951	2.6571366553
H	0.9253049291	0.0549299026	2.6942856647
Li	1.4559778553	-0.4370314162	0.2689113966
N	1.9662094102	1.5530131287	-0.3687161232
C	0.8448644334	2.2584955139	-1.0191630228
H	0.7629012048	1.8682687895	-2.049024464
H	1.0919405902	3.3381157311	-1.124776972
O	3.4494167806	-1.0146236846	0.8136749063
Si	-0.9065006877	2.0024740546	-0.2780339055
C	-1.1045716545	0.1663448192	-0.2090211771
H	-0.3217102229	-0.265870124	0.8635223083
H	-0.6811472625	-0.2345507153	-1.1474530029
C	-2.4438228163	-0.3961527852	0.0187012317
C	-3.0341328087	-1.3107172763	-0.8764725347
C	-3.1900266573	-0.0791446981	1.172497358
C	-4.2841028093	-1.8718122228	-0.6397654637
H	-2.4972350184	-1.566597652	-1.7938153678
C	-4.4426285297	-0.6345348959	1.4080978362
H	-2.7622239041	0.6085683751	1.9046764417
C	-5.0041748566	-1.537768606	0.5061870004
H	-4.7048906862	-2.5708453241	-1.363441855
H	-4.9859403854	-0.3622500101	2.3134456579
H	-5.9849548436	-1.9725406347	0.6930536687
C	-2.0558088537	2.8858312024	-1.4865625194
H	-1.9245307506	2.5140127928	-2.5125105203
H	-3.1014734972	2.697574559	-1.2032516906
H	-1.9008693029	3.9747579695	-1.4928454583
C	-1.1095399443	2.8677391209	1.3909533967

H	-2.1767073977	3.0445868726	1.5885514117
H	-0.7141018616	2.277436125	2.2291906314
H	-0.6121017494	3.8491731539	1.3934979465
C	4.2205870821	-1.7587719962	-0.1017777207
H	3.9939592671	-2.8351178612	-0.022762449
H	3.9687120364	-1.4184145849	-1.1113529185
H	5.2962978078	-1.6020129	0.0809506623
C	3.7548503177	-1.3552746226	2.1509797107
H	3.5488077953	-2.4223041499	2.3374073467
H	4.815247895	-1.149293097	2.3679157523
H	3.1157362856	-0.7544572326	2.8047933039
C	2.2935964831	2.1947711515	0.9028680624
H	2.5663722438	3.2589415656	0.7551570506
H	1.439080245	2.1483131212	1.5862955905
H	3.14214755	1.6784505683	1.3708827538
C	3.1476785297	1.5911884056	-1.2234492416
H	3.9867158394	1.0871554506	-0.7255249666
H	2.9428036106	1.0812065563	-2.1751446239
H	3.4485503937	2.6326073367	-1.4532080811
C	1.1058328361	-1.7466486508	-2.4798222901
H	1.6347092935	-0.8358377964	-2.7849602302
H	1.5003347849	-2.604226198	-3.0482422718
H	0.0331775718	-1.6297988332	-2.7040424868
C	0.6226481304	-3.046644285	-0.5851904737
H	-0.464997632	-2.8778736101	-0.6232900592
H	0.8830464782	-3.9521688724	-1.1556559634
H	0.9244427944	-3.1689480091	0.4603615093
O	1.3227277355	-1.9261651119	-1.0996488244

Abbildung 10.25 Molekel Darstellung von **TS8**.Tabelle 10.502 Standardorientierung von **TS8** [Übergangszustand; M06/6-31+G(d)].

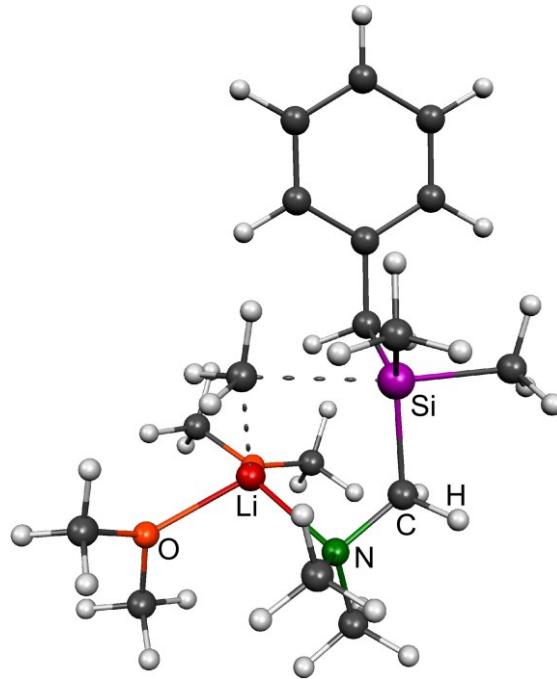
	x	y	z
C	-1.9594564052	1.611721758	-1.5357478693
H	-2.5399551128	0.8422157507	-2.1034538039

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H	-1.4763492952	2.1877095427	-2.3412586045
H	-2.7232198253	2.2995221036	-1.1156095978
Li	-1.9354576359	-0.0285151947	-0.2831950049
N	-1.249409228	0.5132812515	1.5301846292
C	0.1165316241	0.8471197828	1.1068122013
H	0.7156384057	-0.0753687753	1.1589586178
H	0.5789349674	1.523943359	1.8613072445
O	-3.8359153234	-0.6466338982	-0.0204921599
Si	0.556565956	1.6262022275	-0.6013468046
C	2.5026708249	1.7454855921	-0.1625156845
H	2.5985291248	2.4204278722	0.7034410753
H	2.9460966957	2.2738735671	-1.0235304256
C	3.2320240302	0.4738631511	0.0920801407
C	3.8594176249	-0.237413255	-0.9436621173
C	3.2956625889	-0.093028156	1.3765492314
C	4.4758498895	-1.4653230838	-0.7207977303
H	3.8706874346	0.1940176297	-1.9463537161
C	3.9117735464	-1.3194884055	1.6066335913
H	2.8583189538	0.4508829065	2.216110589
C	4.4977910532	-2.0230858668	0.555893257
H	4.9537826958	-1.9852825372	-1.5511926338
H	3.9438502378	-1.7234489106	2.6187627203
H	4.9838913362	-2.9813351928	0.7338751631
C	0.2869231633	3.4932354782	-0.7438897933
H	0.8311222047	4.0096560105	0.0605472805
H	0.714542804	3.8419754647	-1.6964967521
H	-0.7623134963	3.8039878149	-0.7200681365
C	0.7308153702	0.5698888033	-2.1696095024
H	0.8418569034	1.2673977754	-3.0146335864
H	1.6269401417	-0.0640333486	-2.1451700535
H	-0.1476549389	-0.0478154914	-2.3835179604
C	-4.1320964293	-1.6752221076	0.8943902879
H	-4.9390340771	-2.3199781607	0.5094402925
H	-3.2216486006	-2.2699180622	1.0276831885
H	-4.4457898846	-1.257959084	1.8664844768
C	-4.9419493832	0.1973689914	-0.2704200958
H	-5.7776600056	-0.3797644521	-0.696759436
H	-5.2781278952	0.6813082827	0.6610425264
H	-4.6153863669	0.9611873878	-0.9835709346
C	-1.984450585	1.7235968388	1.8767061268
H	-1.5239579756	2.2347755756	2.7462742392
H	-1.9911721376	2.4070623434	1.0216353117
H	-3.0238267768	1.4696956526	2.1314879309
C	-1.2260521559	-0.3833809769	2.6762368776
H	-2.2526670534	-0.6084961418	2.9984698483
H	-0.7314349854	-1.3275714552	2.4114466007
H	-0.6837328571	0.0628319133	3.5337801168
C	0.1143225748	-2.4323548398	-0.6323760356
H	0.5760735638	-1.940163253	0.2302679011
H	0.080584266	-3.5192426397	-0.4570862319
H	0.727381372	-2.2250906416	-1.5231724472

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C	-1.8474447572	-2.4901047003	-1.9056783936
H	-1.3034415267	-2.2596565615	-2.8359351963
H	-1.9197441421	-3.5841989202	-1.7938609427
H	-2.8533328976	-2.0601916184	-1.9565379438
O	-1.1958986003	-1.9195640959	-0.7896058723

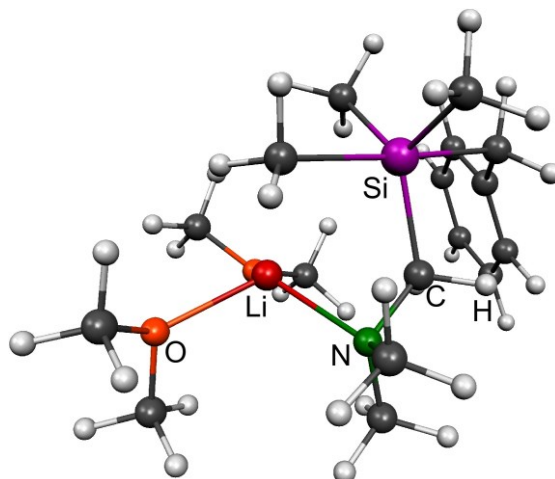
Abbildung 10.26 Molekel Darstellung von **TS9**.Tabelle 10.503 Standardorientierung von **TS9** [Übergangszustand; M06/6-31+G(d)].

	x	y	z
C	-0.2054134489	-0.457011293	-1.5443556932
H	-0.4945638837	-1.5130070117	-1.31256667
H	0.8289058362	-0.5673883601	-1.9008394554
H	-0.7803049622	-0.1862389601	-2.4541331896
Li	-1.7317105553	-0.3730767406	-0.1742469264
N	-2.2535744907	1.5476699274	0.1205596805
C	-0.9474699854	2.0354280298	0.593240325
H	-0.8732207527	1.8081452933	1.6723013606
H	-0.9316110008	3.1456269055	0.5364887929
O	-3.332262871	-1.3268174551	-0.9697384113
Si	0.7531786933	1.4296849089	-0.1145723527
C	1.5056696611	-0.0685342152	0.8659205014
H	0.803809757	-0.9116820273	0.8337496151
H	1.5828537964	0.2787928089	1.9102417279
C	2.8519688377	-0.5061505296	0.382362667
C	4.020917395	0.1477898852	0.7955618324
C	2.989744351	-1.5783857968	-0.5096827065

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C	5.2712952509	-0.2376190881	0.3215341507
H	3.9436821301	0.9705453926	1.5080005664
C	4.2383702905	-1.9673774211	-0.9854597119
H	2.0963109919	-2.1134716769	-0.8363847831
C	5.3882483578	-1.2961581654	-0.5764502544
H	6.1617489905	0.2907217321	0.6617126677
H	4.3125196542	-2.8044064443	-1.6795250562
H	6.3661697805	-1.59922803	-0.9480755521
C	1.7154331676	2.8105555304	0.8826447579
H	1.5954746031	2.7329182508	1.9762426028
H	2.794993578	2.7600489517	0.6708507464
H	1.3895688095	3.8214016826	0.5891385232
C	1.3413625254	1.9986488037	-1.8266386191
H	2.3429277875	1.57152658	-1.9959949779
H	0.711102414	1.6978174762	-2.6700138396
H	1.456531687	3.0919606242	-1.8301437538
C	-4.5555039237	-1.3027693388	-0.2713704386
H	-5.0983251663	-2.2527680962	-0.4026563367
H	-4.3266771592	-1.1581476097	0.7900276674
H	-5.1950064399	-0.4770207234	-0.6270064124
C	-3.5046470222	-1.5254632479	-2.358756259
H	-4.0225440854	-2.4786022846	-2.5491358826
H	-4.0920777175	-0.7028986192	-2.7984291971
H	-2.5083683175	-1.5473842229	-2.8115963615
C	-2.5334629158	2.0862370423	-1.2053752661
H	-2.6040977693	3.1920853443	-1.1815070122
H	-1.7343902983	1.7995686402	-1.8972475784
H	-3.4864449199	1.6854636381	-1.5808880195
C	-3.3153485138	1.9426666373	1.0342103467
H	-4.2882495023	1.5981405258	0.6555300455
H	-3.1525164184	1.4944427696	2.0237730818
H	-3.3610081589	3.0429258502	1.1576049582
C	-1.2664996024	-1.0672664162	2.8248926366
H	-1.4339882893	0.0117048503	2.909642701
H	-1.8280604928	-1.5878501028	3.6166111038
H	-0.1913118826	-1.2723508084	2.9448770188
C	-1.4913893577	-2.8549806835	1.3297173863
H	-0.4117169265	-3.0768480179	1.3292579053
H	-1.9846787617	-3.4558990361	2.1100209526
H	-1.9154079977	-3.1047264754	0.351953928
O	-1.7185087562	-1.4759521834	1.5504524667

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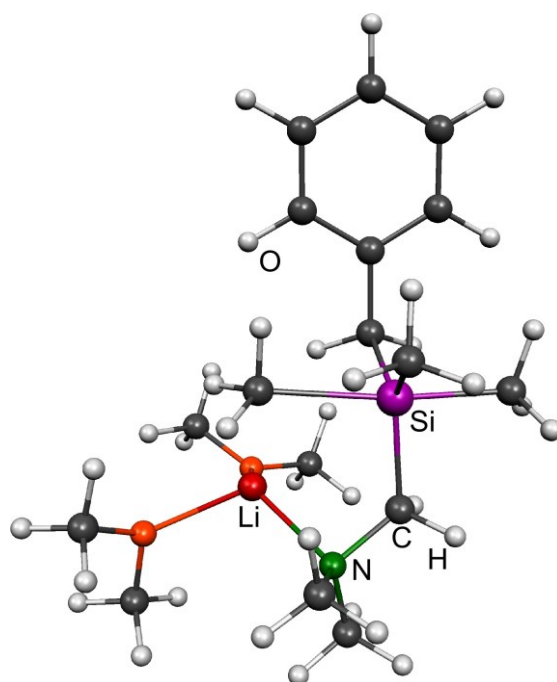
Abbildung 10.27 Molekel Darstellung von **Int1**.Tabelle 10.504 Standardorientierung von **Int1** [lokales Minimum; M06/6-31+G(d)].

	x	y	z
C	-1.7730631859	1.5474240381	-1.4154065051
H	-2.0985331942	0.640067731	-1.9710312671
H	-1.6497144535	2.2819602357	-2.2254545265
H	-2.6442885395	1.9034039583	-0.8336446114
Li	-1.7992317604	-0.2892315507	-0.2516319887
N	-1.4238572314	0.4695312151	1.5626465532
C	-0.0843682651	0.9015393043	1.1020279895
H	0.5776584774	0.0252470183	1.1554781417
H	0.3347711168	1.6171743554	1.8401540771
O	-3.64751772	-1.0543373516	-0.3867877394
Si	0.2361949917	1.7283094083	-0.6437810246
C	2.2609820979	1.8762491061	-0.0205423044
H	2.2644755448	2.5044466715	0.8844685307
H	2.718331761	2.467303203	-0.8306873446
C	3.0201756454	0.6329976451	0.2144807468
C	3.6780607957	-0.0536389367	-0.8259712136
C	3.0879536787	0.0330207106	1.489290938
C	4.3165562677	-1.2723328263	-0.6192191439
H	3.6942213116	0.3944642066	-1.8209036813
C	3.7254919364	-1.1849380867	1.7018433917
H	2.6352541038	0.5516646194	2.3374016412
C	4.3363218538	-1.8606390125	0.6453542635
H	4.8163355934	-1.7631386238	-1.4553380676
H	3.7576130792	-1.6048602958	2.7081355074
H	4.8424117614	-2.8110839325	0.8098756192
C	0.0774290673	3.6288127641	-0.6268767804
H	0.5604989539	4.0526894623	0.2646459503
H	0.607266535	4.0386625012	-1.5008083562
H	-0.9581580995	3.9916610475	-0.668622166
C	0.822346327	0.8676510382	-2.2652641393

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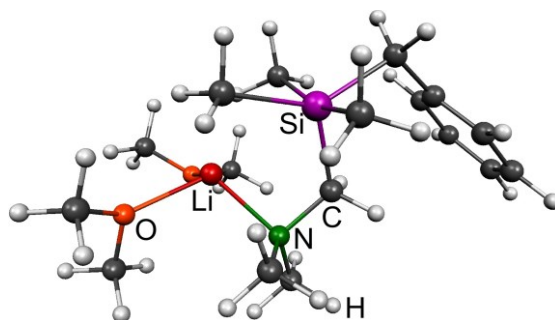
H	1.5455447215	1.5314218278	-2.763752527
H	1.3686371285	-0.0630372391	-2.0538127169
H	0.0220508163	0.6447752594	-2.9828968483
C	-3.9156693412	-2.0564117247	0.5711581594
H	-4.699314737	-2.7396848336	0.2085700624
H	-2.9882958786	-2.6169254802	0.7305422275
H	-4.244197464	-1.607853613	1.5235417754
C	-4.7854982051	-0.2627565344	-0.6681381472
H	-5.6002099413	-0.8898948164	-1.0614846878
H	-5.1334079081	0.2537165134	0.24113776
H	-4.4933557415	0.4796141248	-1.4171611275
C	-2.2186771702	1.6254913259	1.9573928811
H	-1.7859536803	2.1162671462	2.8517068885
H	-2.2453154072	2.3617984129	1.1483377312
H	-3.2481535893	1.3185021119	2.1945015434
C	-1.3086693886	-0.4316146763	2.7027564035
H	-2.3069914272	-0.718482363	3.0643402339
H	-0.7692997098	-1.345079504	2.4173928248
H	-0.7591884606	0.042258005	3.5396776753
C	0.5260092441	-2.3616522585	-0.2798836749
H	0.6460051527	-2.0609957525	0.7653139173
H	0.602700213	-3.4569756035	-0.3546424949
H	1.3274032346	-1.8940775361	-0.8733663866
C	-1.0117828103	-2.3590459901	-2.0481790461
H	-0.2776342481	-1.9225483282	-2.7428798215
H	-0.9676789056	-3.4573773037	-2.1128656357
H	-2.0189614674	-2.0221567736	-2.316623074
O	-0.7554564798	-1.9343250196	-0.7211973855

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Abbildung 10.28 Molekel Darstellung von **Int2**.Tabelle 10.505 Standardorientierung von **Int2** [lokales Minimum; M06/6-31+G(d)].

	x	y	z
C	-0.0864272912	-0.4398776919	-1.3874231516
H	-0.3439380238	-1.4413092352	-0.9675719234
H	0.8898540418	-0.6311633646	-1.8553846525
H	-0.769793557	-0.2686880676	-2.2434487713
Li	-1.7438102985	-0.3989626722	-0.1160788311
N	-2.3342824985	1.5055436365	-0.0626559563
C	-1.0356923242	2.0356438174	0.4036953125
H	-0.9907343802	1.8982885899	1.498946139
H	-1.0227961645	3.1360105676	0.2566392573
O	-3.19843652	-1.5579577181	-0.9123626239
Si	0.6872422958	1.3711008994	-0.2336380968
C	1.5349378327	0.03717	0.9366022164
H	0.8692574085	-0.8325393345	1.0340202307
H	1.6275333594	0.5119135315	1.9266463007
C	2.8789088208	-0.4059345228	0.4602632706
C	4.0368586877	0.3238859191	0.7668528153
C	3.0321039579	-1.5559975194	-0.3276684848
C	5.2850051996	-0.0633219221	0.2894773512
H	3.9509130435	1.210093505	1.3971927349
C	4.2788678542	-1.9476573166	-0.8060401656
H	2.1512821934	-2.1549873984	-0.567373205
C	5.4152255018	-1.2005270136	-0.5048977173
H	6.164758365	0.5268250457	0.5458522079
H	4.3629182599	-2.847121489	-1.416044453

H	6.3919700171	-1.5049637527	-0.8784715903
C	1.5696242002	2.8786195527	0.7115961389
H	1.4046373021	2.8806011702	1.803219538
H	2.6598196212	2.8470610234	0.5526230356
H	1.2328625025	3.8569203289	0.3300859269
C	1.3408538172	1.9360183237	-1.9397249495
H	2.3682060708	1.5490968775	-2.0436677285
H	0.7711274138	1.5780142803	-2.8065900864
H	1.4093911565	3.0319946295	-1.9809666728
C	-4.4662422126	-1.4995495583	-0.2977863733
H	-4.9795977664	-2.4715143719	-0.3714901353
H	-4.3095257819	-1.2508492232	0.7574636131
H	-5.0958099603	-0.7270683388	-0.7701553617
C	-3.2744732618	-1.906131163	-2.2809868556
H	-3.7475140612	-2.8933023049	-2.3996677535
H	-3.8572871323	-1.1571208188	-2.8408081515
H	-2.2510890729	-1.9363473116	-2.66833162
C	-2.593276782	1.9680348145	-1.421327202
H	-2.6911801004	3.0711816804	-1.4545750856
H	-1.7678961766	1.6788601777	-2.0805415316
H	-3.526328134	1.5268970345	-1.8020249388
C	-3.4189002324	1.9453849406	0.8041032326
H	-4.3831737979	1.5766895375	0.425202253
H	-3.2759917197	1.5552353955	1.8208510928
H	-3.4693946493	3.050301573	0.8632953297
C	-1.2899117834	-0.8037211845	2.915205326
H	-1.4959630805	0.2712977658	2.8931678687
H	-1.8444030059	-1.2659619162	3.7466700993
H	-0.2099670949	-0.9572347624	3.0631271614
C	-1.4464402181	-2.7401844894	1.6072700943
H	-0.3620130389	-2.9321362202	1.6502924651
H	-1.9408178209	-3.2691338916	2.4370880769
H	-1.8454328153	-3.1008697968	0.6537011351
O	-1.7110031658	-1.3513772475	1.6804768447

Abbildung 10.29 Molekel Darstellung von **TS14**.Tabelle 10.506 Standardorientierung von **TS14** [Übergangszustand; M06/6-31+G(d)].

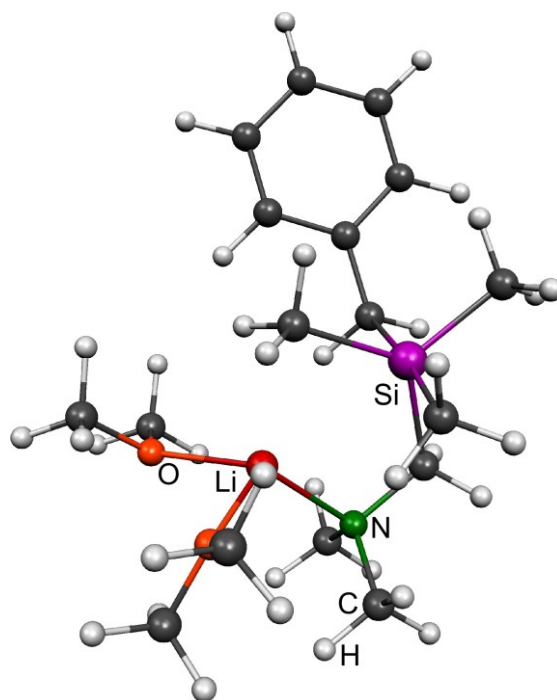
x	y	z
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C	1.1948790083	-1.7390400174	-1.6914365566
H	2.0082230384	-1.0333947807	-1.9593476313
H	0.8990741986	-2.1581206869	-2.6683881216
H	1.6232557222	-2.5864761898	-1.1338832593
Li	1.8651709323	0.0940648982	-0.2089094944
N	0.7740104161	-0.3089448234	1.4435805964
C	-0.5526611544	-0.3454290444	0.7702579788
H	-0.9187697093	0.692727258	0.7168475052
H	-1.269918089	-0.8875737176	1.4204392267
O	3.7851630048	-0.5310240578	0.1649363524
Si	-0.6034360761	-1.0644494838	-1.0463625227
C	-2.5022173574	-0.7911303517	-1.7080790457
H	-2.9380852068	-1.778974066	-1.9100755572
H	-2.4780091049	-0.2310113401	-2.653054928
C	-3.3100795631	-0.0660229233	-0.6952571628
C	-3.4290075769	1.3342411665	-0.7065630969
C	-3.9456155083	-0.7488967698	0.3563372623
C	-4.1034083999	2.0178963471	0.3006325929
H	-2.9848606498	1.8943201764	-1.5316757666
C	-4.6204818926	-0.0698517735	1.3646684
H	-3.8981838847	-1.8394072647	0.3793669175
C	-4.6967043928	1.3224377815	1.3525991043
H	-4.176810612	3.1051153066	0.2561227826
H	-5.0988633563	-0.6345238271	2.1653733046
H	-5.2275015663	1.8555563624	2.1403429959
C	-1.0507887554	-2.9473460788	-0.6228673237
H	-1.9951163778	-3.010334351	-0.0587134222
H	-1.2003548096	-3.521349505	-1.5530617637
H	-0.2839951996	-3.4832576931	-0.0402328812
C	-0.1381713769	0.6544317204	-2.0263642508
H	-0.2065584869	0.4244872256	-3.1033364333
H	-0.857919327	1.4644190065	-1.826732122
H	0.8735007747	1.0795942575	-1.8912278112
C	4.4001456852	0.0599624929	1.2915548293
H	5.4616175139	0.2718738744	1.0853118974
H	3.8751570269	0.9972427134	1.5024945729
H	4.3342998946	-0.6070564783	2.1668329043
C	4.3923768339	-1.7610478555	-0.1823686107
H	5.46280176	-1.6128352839	-0.3934368844
H	4.283262524	-2.4906175065	0.636059353
H	3.8888210802	-2.1402767832	-1.0761212608
C	1.1508236212	-1.6480895008	1.8871080681
H	0.4042842647	-2.059151107	2.5943196177
H	1.2141999842	-2.3307447516	1.0334657316
H	2.127619604	-1.6173813821	2.3916333807
C	0.7353934432	0.567789302	2.6079758798
H	1.7179679423	0.5922666598	3.1018468334
H	0.4727888991	1.589540021	2.3066318915
H	-0.0195976206	0.2276434775	3.3427951113
C	1.468137856	3.096092258	-0.1709541277
H	0.6915542518	2.7493879723	0.5186243798

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H	1.9455092279	4.0024500735	0.2313812737
H	1.0014789266	3.3217010424	-1.1417745569
C	3.4074746681	2.3736180899	-1.2713737238
H	2.9453009396	2.5134928871	-2.2618795502
H	3.9449373571	3.2926526844	-0.9902007057
H	4.1101354926	1.534187293	-1.3109568949
O	2.4238671623	2.0584800469	-0.3044222778

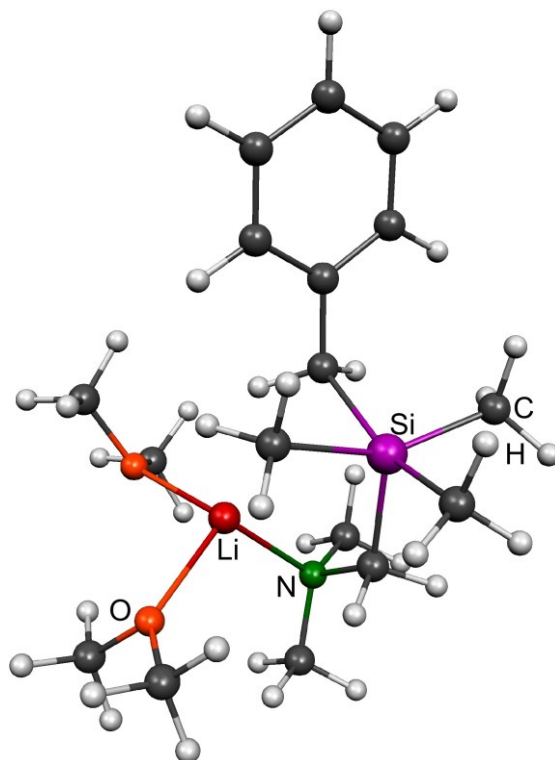
Abbildung 10.30 Molekel Darstellung von **TS12**.Tabelle 10.507 Standardorientierung von **TS12** [Übergangszustand; M06/6-31+G(d)].

	x	y	z
C	-1.732520323	0.6113188202	-1.055436453
H	-1.9912775271	1.438588449	-1.7371659057
H	-1.0664528381	-0.0765878335	-1.6121165864
Li	1.6794132236	-0.2955418471	0.1390968309
N	1.8780826804	1.1735165053	-1.3054402586
C	0.6953057762	2.0860024831	-1.1027947738
H	0.1385905484	2.1392962447	-2.0497578233
H	1.0714046178	3.1031462287	-0.9049943654
O	3.3259638997	-0.5316297857	1.2488539346
Si	-0.4602752299	1.5508954755	0.3891461314
C	-0.2928461869	-0.210618948	1.2548395643
H	0.5350282915	-0.3503311897	1.9749975153
H	-1.2043409308	-0.2294358561	1.872051004
H	-0.3854388995	-1.09937022	0.6122107385
C	-1.8537091996	2.7592070417	0.8855715664

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H	-2.7105433719	2.1991507299	1.2879801371
H	-1.5410222327	3.4956074694	1.6371764461
H	-2.223082643	3.2996644378	0.0011442337
C	4.4904462915	-0.9912155103	0.5943494689
H	4.9377252159	-1.8328567143	1.1474537185
H	4.1984678873	-1.3312987905	-0.4053585369
H	5.2337382486	-0.1824922512	0.5095487658
C	3.6050556434	-0.030948053	2.5444324607
H	4.0975859482	-0.8051289556	3.1529701308
H	4.2559295027	0.8551819435	2.4815047658
H	2.6560555368	0.2560338132	3.0066396854
C	3.1305059561	1.8825155614	-1.0558900696
H	3.2490891221	2.7408405321	-1.7451337501
H	3.1536055934	2.2632524738	-0.027081536
H	3.9849274744	1.2045831147	-1.2012810948
C	1.8992897798	0.6685686827	-2.6740555101
H	2.7091142407	-0.0674938812	-2.7977276632
H	0.9413512632	0.1876798583	-2.9102715608
H	2.053898353	1.4856384195	-3.4052398222
C	0.8925163287	-2.671604854	-1.6162228769
H	0.9504175979	-1.9001384079	-2.3881549514
H	1.2951578892	-3.6163720512	-2.012235443
H	-0.1609163415	-2.8178712948	-1.330105743
C	1.6477599667	-3.2029638804	0.5302563554
H	0.6187223481	-3.3841570218	0.8795747584
H	2.0834237278	-4.1495752357	0.1752470846
H	2.2460280015	-2.8079901028	1.3574827779
O	1.6592797535	-2.2377386095	-0.5070925614
C	-2.9537034008	-0.0926090643	-0.6225889275
C	-2.9828355574	-1.4775408266	-0.3715039972
C	-4.1614975283	0.5995114948	-0.4043043837
C	-4.1237590127	-2.1254137361	0.0888492215
H	-2.0784002978	-2.0640535139	-0.554593939
C	-5.3059672541	-0.0416154859	0.05498626
H	-4.1952463891	1.6703476325	-0.6124881774
C	-5.2996479346	-1.4120063374	0.3134418882
H	-4.0969807184	-3.2014931849	0.2654939746
H	-6.2182719806	0.5361025101	0.2069158316
H	-6.1965100258	-1.9156643879	0.6713423568
C	0.8520427456	2.3137400028	1.7179652401
H	0.4976764496	2.1498660795	2.7516774417
H	1.8714850136	1.8869386696	1.6643250894
H	0.9636039068	3.4039681572	1.586475332

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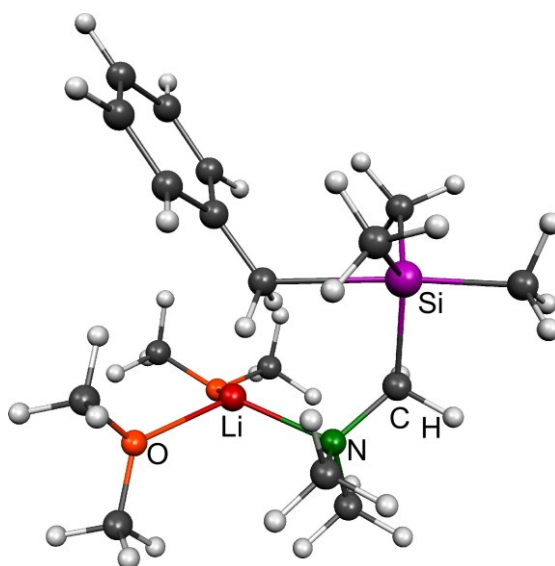
Abbildung 10.31 Molekel Darstellung von **TS13**.Tabelle 10.508 Standardorientierung von **TS13** [Übergangszustand; M06/6-31+G(d)].

	x	y	z
C	1.2452170697	-0.0077194489	0.8124636397
H	1.3221933113	0.3547628071	1.8480309276
H	0.5414726179	-0.857242508	0.8133703235
Li	-1.4525002877	-0.3797504526	-0.1522982181
N	-1.9892157637	1.1096196987	1.1782056444
C	-1.2554958722	2.018246976	0.2627998016
H	-1.2159499246	3.0368037566	0.7047738957
H	-1.8688996804	2.1198279642	-0.6494495997
O	-3.1048782285	-0.6135682595	-1.3340784647
Si	0.5374336893	1.5961105386	-0.3928674884
C	0.1793738479	0.1693035019	-1.7951277382
H	-0.5781120754	0.4739694533	-2.5330730352
H	1.1241655153	0.1256237705	-2.3592362163
H	-0.0044063443	-0.88949619	-1.5254800389
C	1.7418799884	2.7681073736	0.6038771068
H	2.7682732856	2.7055637318	0.2106161856
H	1.425161726	3.8153221814	0.48839894
H	1.792723324	2.5421128442	1.6798983057
C	-4.1827768403	-1.3817693645	-0.8410329537
H	-4.5028865932	-2.123645049	-1.5893288818
H	-3.8354642482	-1.8995235064	0.058519324

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H	-5.0392616748	-0.7347123459	-0.5900937912
C	-3.4709610892	0.1265436856	-2.4822842865
H	-3.7751210982	-0.5497476576	-3.2956059228
H	-4.3040887334	0.8106241145	-2.2517080278
H	-2.6016479198	0.7094777281	-2.8004944338
C	-3.4060062757	1.4527370046	1.2188026282
H	-3.5630036444	2.4844725935	1.5897238113
H	-3.8388542199	1.3806675988	0.2128595863
H	-3.9453672442	0.7590631463	1.8817807839
C	-1.4493721981	1.2232287719	2.5285926115
H	-1.9935972699	0.5596932324	3.2151966478
H	-0.3899254534	0.9534359838	2.542116923
H	-1.5461001596	2.2602774603	2.9054325837
C	-1.5473433327	-2.3432292352	2.0658541235
H	-2.2280548443	-1.556833845	2.410673326
H	-1.9438340791	-3.3270948952	2.3604951364
H	-0.5558422938	-2.19476581	2.5231630992
C	-0.6929065915	-3.2852079327	0.0907899706
H	0.3435258547	-3.2442624843	0.4623396145
H	-1.131253053	-4.2649489292	0.3342354527
H	-0.6970125738	-3.1453202742	-0.9956335371
O	-1.4705970596	-2.2454824763	0.6570166253
C	2.5840478955	-0.4853677539	0.3761757969
C	2.7522330539	-1.5016094001	-0.5810373341
C	3.7602599823	0.0855159321	0.8951263457
C	4.0120727415	-1.9116035567	-1.0065596055
H	1.8707126488	-1.9825398758	-1.008615943
C	5.0213234631	-0.3188181089	0.472165776
H	3.6756213511	0.863947504	1.654722003
C	5.160943288	-1.3206446857	-0.4868033165
H	4.0948026821	-2.7032623073	-1.7518893047
H	5.906213629	0.1511347396	0.9018197907
H	6.1481221986	-1.6387412356	-0.8190014324
C	0.476943792	2.9073291542	-1.8685780734
H	1.4572817893	2.9543996475	-2.3707270976
H	-0.2715252206	2.6895473028	-2.6473916061
H	0.2755111422	3.9203933905	-1.4856983834

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Abbildung 10.32 Molekel Darstellung von **Int3**.Tabelle 10.509 Standardorientierung von **Int3** [lokales Minimum; M06/6-31+G(d)].

	x	y	z
C	0.5552335015	0.3566506032	-0.0097191799
H	0.1030477437	0.1237597448	0.963956778
H	-0.017548127	0.0470995308	-0.8924176371
Li	-1.2181558159	-1.0085696476	0.1708282634
N	-2.4648560396	0.5598833729	-0.2489658349
C	-1.988352409	1.8486844939	0.3106151036
H	-2.0120954045	1.7540865965	1.4122547137
H	-2.7512194727	2.6165051626	0.0659607045
O	-1.2352921854	-2.5270512787	-1.1037735055
Si	-0.2322877193	2.6789661307	-0.0202384102
C	0.5961413624	2.7527844884	-1.7327255796
H	0.5181434822	3.7535550352	-2.1804359889
H	1.6610420573	2.5019390649	-1.6229980103
H	0.1813122122	2.0297812561	-2.4496185948
C	0.8649685694	2.8205482697	1.5283298165
H	1.8917445088	2.4917072076	1.316578115
H	0.8989402188	3.849247465	1.9143646021
H	0.4844284884	2.173210237	2.334583217
C	-2.4083718973	-3.1556828208	-1.5700566606
H	-2.2279454748	-4.2259812083	-1.7538108593
H	-3.1730705184	-3.0498947958	-0.7926095208
H	-2.7626889276	-2.6881988688	-2.5034406428
C	-0.1544480538	-2.6236553725	-2.0202913509
H	0.0260902614	-3.6766611367	-2.2834286095
H	-0.3743319978	-2.0498454826	-2.9353914775
H	0.7351375176	-2.2056397045	-1.5343364709
C	-2.5909673998	0.6800540683	-1.6992924694
H	-3.2889390966	1.4942291139	-1.974913354

H	-1.6170129385	0.9034448813	-2.148834639
H	-2.9714024755	-0.2588660532	-2.1280613763
C	-3.7772482796	0.2340182161	0.3047867687
H	-4.1488590932	-0.7112943658	-0.1191603913
H	-3.7110670249	0.121512945	1.3952886442
H	-4.5205432902	1.0255837762	0.0889218451
C	-1.2993120281	-1.0905038313	3.0849376461
H	-2.1482699971	-0.4086353524	2.9670646178
H	-1.4531712681	-1.7088489029	3.9819335719
H	-0.3752116156	-0.5012251345	3.2039649814
C	-0.1379596606	-2.8100644387	1.9936338891
H	0.8177917459	-2.2631359983	2.032957468
H	-0.2331709265	-3.4564743297	2.8787989838
H	-0.1679913816	-3.4220508192	1.0870922037
O	-1.2331205997	-1.9053474265	1.9297208736
C	1.9534541735	0.0012465288	-0.0860798396
C	2.6172268979	-0.1744744245	-1.3243193552
C	2.7574032591	-0.1436292448	1.070390542
C	3.9723152817	-0.471805013	-1.3973268007
H	2.0435482808	-0.0549734785	-2.2479224297
C	4.1119390471	-0.4390784912	0.9941115
H	2.2940685495	-0.0032199856	2.0512977624
C	4.740457589	-0.6096811038	-0.2404956742
H	4.4384955814	-0.5937815041	-2.3760258568
H	4.6886551812	-0.5361386844	1.9149522647
H	5.8029711771	-0.8395956223	-0.2994865038
C	-0.9901651706	4.4715380657	0.0126733749
H	-0.1876654459	5.2241358397	-0.0472273448
H	-1.6699009521	4.6521413199	-0.8369786633
H	-1.5551116608	4.6779887268	0.9374136405

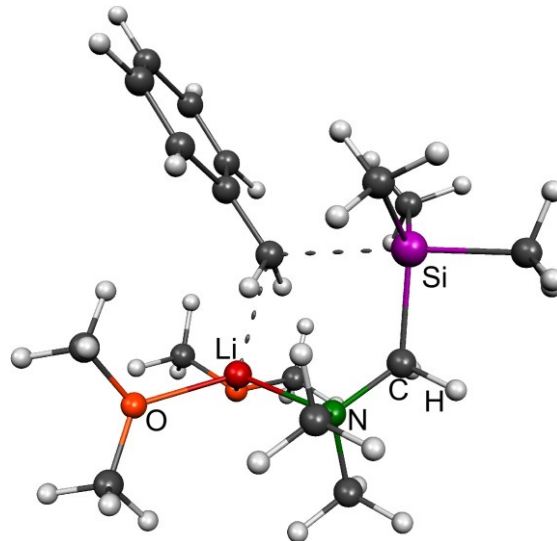
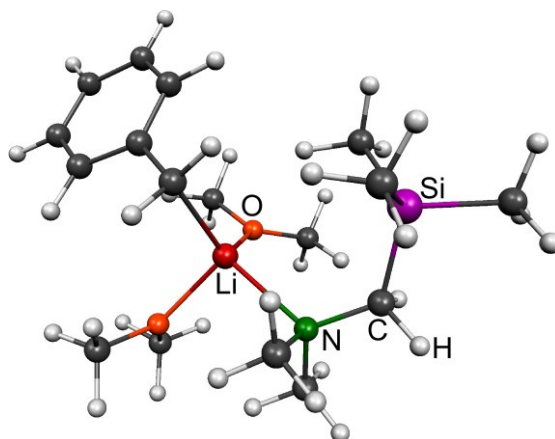
Abbildung 10.33 Molekel Darstellung von **TS10**.

Tabelle 10.510 Standardorientierung von **TS10** [Übergangszustand; M06/6-31+G(d)].

	x	y	z
C	0.6153009485	0.1707599943	-0.0232416866
H	0.1283334639	-0.0283027042	0.9402374786
H	0.0394088931	-0.077272889	-0.9218831067
Li	-1.2591483821	-1.0400318677	0.1195181845
N	-2.3739147986	0.5941132776	-0.4017725942
C	-1.8614220609	1.8653957729	0.1667801955
H	-2.0005812695	1.8114707003	1.2624666213
H	-2.5407788024	2.675173483	-0.1715651308
O	-1.3299874576	-2.6214029687	-1.0382016119
Si	-0.0362436405	2.5802250687	-0.0000001258
C	0.8995983184	2.6474622349	-1.6520416219
H	0.9549181842	3.6736168401	-2.0423227538
H	1.9221598765	2.2716370629	-1.5064097915
H	0.4447609236	2.0174552311	-2.4297087346
C	0.9734047618	2.5751199234	1.6123246346
H	1.9757136524	2.1560020454	1.449829132
H	1.0789552088	3.5866351098	2.0299506627
H	0.4857951409	1.9494680624	2.376593639
C	-2.5194059368	-3.2020869563	-1.5255563466
H	-2.3962555576	-4.2884724892	-1.6527314812
H	-3.3067980817	-3.0149294737	-0.7872290315
H	-2.80679077	-2.7601372969	-2.4937835315
C	-0.2185708709	-2.8322174897	-1.8985555813
H	-0.0916173388	-3.9072815475	-2.0946288158
H	-0.3654987363	-2.3004717827	-2.8527511477
H	0.6728538579	-2.4379321269	-1.3965621051
C	-2.3859925711	0.6839677835	-1.8598809838
H	-3.0219939844	1.5221729773	-2.2045624797
H	-1.3715921381	0.8500904335	-2.239242702
H	-2.7778838225	-0.2468673691	-2.2964520118
C	-3.7414591524	0.3640864848	0.0589375498
H	-4.1423057244	-0.5638211743	-0.376457826
H	-3.7620830442	0.2698746998	1.1529154283
H	-4.4139050689	1.1968286003	-0.2242100281
C	-1.4958245931	-0.8922948008	3.0433831431
H	-2.2529306378	-0.1330433038	2.8185454371
H	-1.7750163636	-1.4221787097	3.9664836125
H	-0.5208508161	-0.3986533698	3.1882974767
C	-0.4551983435	-2.7911524583	2.1438018816
H	0.5474533189	-2.3374759121	2.2007095544
H	-0.6589263623	-3.3578291494	3.064667303
H	-0.499175635	-3.4635241831	1.281715484
O	-1.4478854416	-1.7926393911	1.9528277805
C	1.9864740259	-0.2705961458	-0.0809940455
C	2.6532648049	-0.4794038186	-1.313580275
C	2.7659800149	-0.4759316957	1.0837298891
C	3.9868127203	-0.8627772773	-1.3737220738
H	2.0977712695	-0.3181201551	-2.2422490142
C	4.0993931341	-0.8583902487	1.019405033

H	2.3006018287	-0.3161898108	2.0607934026
C	4.730667401	-1.0595803163	-0.2092849327
H	4.45551373	-1.0072935952	-2.3482019711
H	4.6575787694	-1.0013873263	1.9457244607
H	5.77653595	-1.3580434904	-0.2579664089
C	-0.6738999607	4.4151685644	0.0770467926
H	0.1807629595	5.1092843989	0.113581016
H	-1.2774701164	4.6881041733	-0.8041244287
H	-1.2865266774	4.6144453716	0.9724635867

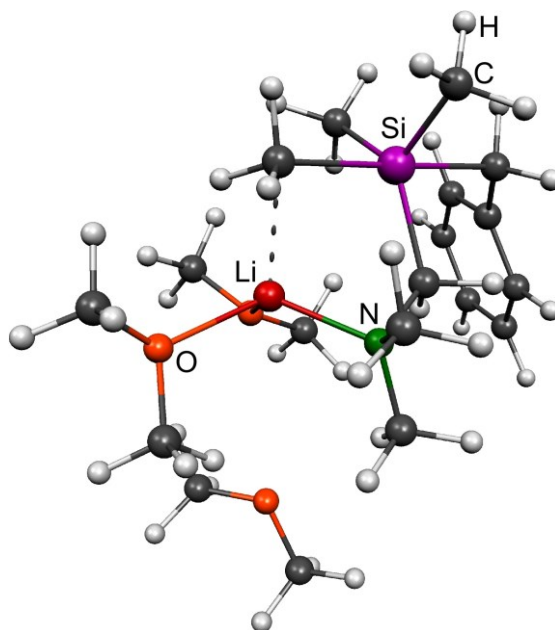
Abbildung 10.34 Molekel Darstellung von **Pr1**.Tabelle 10.511 Standardorientierung von **Pr1** [globales Minimum; M06/6-31+G(d)].

	x	y	z
C	-0.685378292	-0.6257014346	-1.7572340436
H	0.068748303	-1.3951321532	-1.9758419956
H	-0.8013827084	0.0527891259	-2.6172061031
Li	-0.1837404278	0.6406266294	-0.1171976846
N	1.8136069399	1.5377352536	-0.1076201611
C	2.9531107222	0.7335115143	0.3581245329
H	2.9379275843	0.7310673237	1.4625791685
H	3.9054082313	1.245399629	0.0876322172
O	-1.2972396205	2.3581523171	-0.2126550177
Si	3.1068436783	-1.1105970644	-0.1192690816
C	3.2154316999	-1.4201861683	-1.9690625837
H	3.578191918	-2.4428525411	-2.1456769946
H	2.244060711	-1.3261087127	-2.4718224584
H	3.9241311446	-0.7325186126	-2.452118555
C	1.7246868932	-2.1040116595	0.6720227645
H	0.730034186	-1.7195573504	0.4049917053
H	1.7661605733	-3.1512811426	0.3402860928
H	1.8179367743	-2.1016259542	1.7680121614
C	-1.8329006593	3.0266376434	0.9051742625
H	-2.9267741465	2.8952477606	0.947396738
H	-1.3792930573	2.588602343	1.8009980605

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H	-1.6003808572	4.1045552325	0.86507642
C	-1.7664094559	2.8996875953	-1.4279389191
H	-2.8676784592	2.8949967203	-1.4574796734
H	-1.4059759807	3.9355096846	-1.5523715082
H	-1.3846780309	2.2717847091	-2.2393665416
C	1.942776003	1.8021514436	-1.5396037232
H	2.9084357057	2.2966978878	-1.7696060204
H	1.8711540106	0.870289426	-2.1100235815
H	1.1301682202	2.4623065116	-1.8692394856
C	1.7923496937	2.812522444	0.6038402249
H	0.9629530116	3.4308086965	0.2356358523
H	1.6466874327	2.6431775449	1.679655485
H	2.7401921904	3.3701174659	0.4662046877
C	0.1534162764	0.1587464691	2.9358610223
H	1.1710290504	0.4133451269	2.6185953702
H	-0.1863289447	0.8862296455	3.6942313267
H	0.1598771322	-0.8471989773	3.3862570628
C	-1.9999438949	-0.2251481991	2.1036331373
H	-2.0002048758	-1.2725585403	2.4393096813
H	-2.4285527835	0.4168275048	2.8921328946
H	-2.5946261735	-0.1470962976	1.1867605754
O	-0.6768377408	0.1952056305	1.8033848243
C	-1.9276351233	-1.1621652866	-1.2641931989
C	-3.1553713922	-0.447171256	-1.3395182777
C	-2.0021459706	-2.4122389344	-0.5893175424
C	-4.3298502312	-0.9206537208	-0.7687578755
H	-3.1718850698	0.4986347595	-1.887467549
C	-3.1773093194	-2.88076149	-0.0205685121
H	-1.0990970458	-3.0257541225	-0.535523671
C	-4.3613083211	-2.1393453813	-0.0852689069
H	-5.2442412856	-0.33249309	-0.8690466622
H	-3.1749050815	-3.8521995553	0.4776193058
H	-5.2848620615	-2.5142808392	0.3530854144
C	4.7484532988	-1.6065098457	0.6637082799
H	4.9386841681	-2.6796799522	0.5251807401
H	5.5916437622	-1.0616309094	0.2166021175
H	4.757423696	-1.4082008476	1.7450012016

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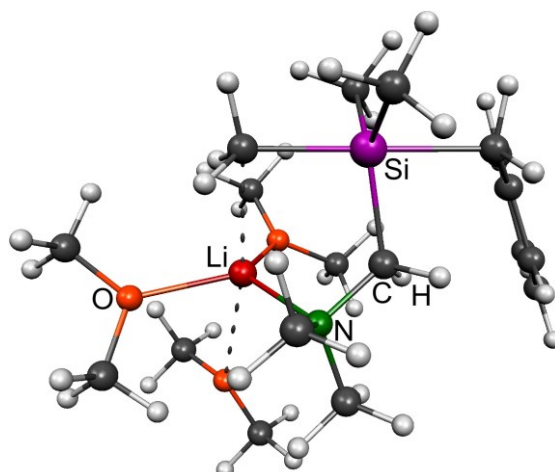
Abbildung 10.35 Molekel Darstellung von **Int1** + DME.Tabelle 10.512 Standardorientierung von **Int1** + DME [lokales Minimum; M06/6-31+G(d)].

	x	y	z
C	-0.43808	-2.883224	0.82946
H	-0.939504	-2.367089	1.677196
H	-0.003576	-3.769588	1.315333
H	-1.23251	-3.276995	0.167001
Li	-1.358837	-0.957096	0.327945
N	-0.888618	-0.906361	-1.607297
C	0.552736	-0.866611	-1.26847
H	0.788519	0.164753	-0.966886
H	1.137749	-1.029293	-2.197651
O	-3.327965	-1.137446	0.685165
Si	1.376424	-2.049067	0.058854
C	3.216357	-1.162273	-0.56126
H	3.337914	-1.401311	-1.629785
H	3.965684	-1.748963	-0.006136
C	3.405401	0.28214	-0.330578
C	3.864995	0.791894	0.90111
C	3.086865	1.242559	-1.313916
C	3.958076	2.15796	1.147953
H	4.168338	0.089094	1.678723
C	3.177648	2.609044	-1.072198
H	2.768682	0.896832	-2.299964
C	3.602789	3.085078	0.16845
H	4.325144	2.502544	2.115649
H	2.92619	3.311571	-1.868087
H	3.682425	4.154854	0.357993

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C	1.923156	-3.721603	-0.67594
H	2.782028	-4.107592	-0.1062
H	1.14191	-4.49343	-0.669707
H	2.267139	-3.585383	-1.711708
C	1.853551	-1.665626	1.889179
H	2.865355	-2.051863	2.082319
H	1.905803	-0.580611	2.06752
H	1.177335	-2.102452	2.635933
C	-4.109929	-0.32909	-0.171449
H	-5.033793	-0.010041	0.33797
H	-3.515862	0.55367	-0.437622
H	-4.379613	-0.882166	-1.086627
C	-3.987404	-2.333421	1.045909
H	-4.932565	-2.108852	1.564503
H	-4.200175	-2.944362	0.153453
H	-3.321851	-2.893073	1.710564
C	-1.186812	-2.100939	-2.387262
H	-0.683123	-2.063784	-3.373639
H	-0.835776	-2.995569	-1.863888
H	-2.270429	-2.188508	-2.554811
C	-1.260349	0.270421	-2.385711
H	-2.325222	0.225432	-2.660644
H	-1.10255	1.182415	-1.795205
H	-0.661313	0.342051	-3.31495
C	-0.00781	1.671603	1.148278
H	-0.101167	1.902258	0.083046
H	-0.253666	2.574876	1.728964
H	1.024916	1.36032	1.373194
C	-1.019328	0.402536	2.84354
H	-0.047344	0.077771	3.245981
H	-1.342016	1.318717	3.365233
H	-1.765055	-0.383921	3.005726
O	-0.934683	0.6366	1.451317
O	-2.657409	2.70468	-0.461735
C	-3.163037	3.018741	0.809635
H	-2.674244	3.917751	1.223812
H	-4.252297	3.198121	0.773816
H	-2.956838	2.161617	1.462337
C	-2.857226	3.743228	-1.385511
H	-2.341099	4.664923	-1.067602
H	-2.444957	3.416622	-2.346119
H	-3.930818	3.966236	-1.511042

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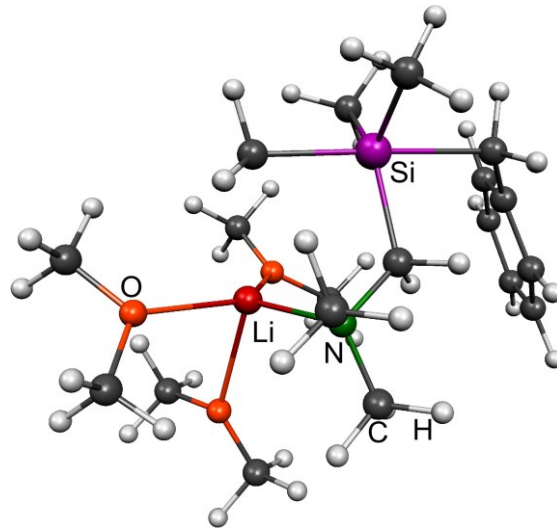
Abbildung 10.36 Molekel Darstellung von **TS15**.Tabelle 10.513 Standardorientierung von **TS15** [Übergangszustand; M06/6-31+G(d)].

	x	y	z
C	-0.85741	2.375364	-1.044021
H	-1.246253	1.576391	-1.708751
H	-0.685025	3.21547	-1.736169
H	-1.684112	2.697293	-0.386976
Li	-1.61748	0.255236	-0.162069
N	-0.86705	0.743169	1.665899
C	0.534306	0.910936	1.208694
H	0.92795	-0.095543	1.003324
H	1.134717	1.277997	2.066499
O	-3.570858	0.648868	-0.338058
Si	1.051486	2.035663	-0.304149
C	3.078274	1.543589	0.340403
H	3.186988	1.958009	1.355045
H	3.691196	2.154239	-0.340347
C	3.486567	0.132844	0.300118
C	3.97834	-0.474046	-0.876235
C	3.355118	-0.720615	1.418865
C	4.270161	-1.832526	-0.943955
H	4.148064	0.151329	-1.75433
C	3.643502	-2.079067	1.355072
H	3.023966	-0.291923	2.367536
C	4.092605	-2.657916	0.166813
H	4.655064	-2.25017	-1.875535
H	3.531536	-2.69225	2.250712
H	4.328788	-3.720207	0.117151
C	1.349286	3.849296	0.207924
H	1.621987	3.898426	1.272966
H	2.198446	4.265069	-0.354237
H	0.481355	4.503654	0.045702
C	1.593084	1.534018	-2.088168
H	2.497406	2.099914	-2.356409

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H	1.874107	0.471375	-2.133602
H	0.833939	1.722139	-2.859862
C	-4.442282	0.41109	0.746782
H	-5.236837	-0.297172	0.458958
H	-3.851745	-0.026465	1.557171
H	-4.900932	1.354169	1.083536
C	-4.235782	1.232115	-1.438742
H	-5.012326	0.550298	-1.824101
H	-4.701945	2.186374	-1.149084
H	-3.490035	1.428553	-2.215515
C	-1.333599	1.977503	2.288779
H	-0.729689	2.214526	3.186852
H	-1.242369	2.815183	1.591648
H	-2.385086	1.881547	2.595853
C	-0.931377	-0.322268	2.659845
H	-1.968806	-0.476	2.996462
H	-0.558911	-1.261923	2.22972
H	-0.307354	-0.08703	3.54442
C	0.312293	-1.961748	-0.929004
H	0.212797	-2.015855	0.16042
H	0.121547	-2.959052	-1.359265
H	1.337748	-1.64271	-1.178775
C	-0.677137	-0.991664	-2.817833
H	0.309005	-0.726505	-3.226594
H	-0.990535	-1.96928	-3.221204
H	-1.40224	-0.225957	-3.117803
O	-0.644388	-1.030554	-1.407531
O	-2.689663	-2.153068	0.407602
C	-3.227794	-2.541437	-0.831825
H	-2.533782	-3.203541	-1.378549
H	-4.186115	-3.07204	-0.69563
H	-3.396699	-1.63498	-1.42372
C	-2.474763	-3.26619	1.240824
H	-1.738573	-3.959399	0.798535
H	-2.092818	-2.901883	2.199558
H	-3.414497	-3.816868	1.415267

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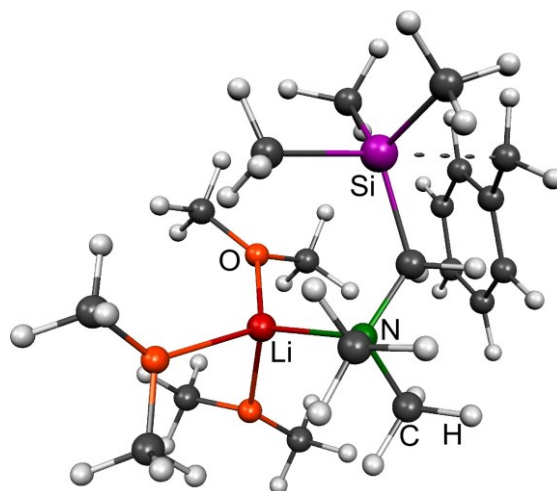
Abbildung 10.37 Molekel Darstellung von **Int4**.Tabelle 10.514 Standardorientierung von **Int4** [lokales Minimum; M06/6-31+G(d)].

	x	y	z
C	-0.923078	2.283141	-1.048013
H	-1.277154	1.414722	-1.638744
H	-0.823995	3.088809	-1.794594
H	-1.744515	2.589289	-0.379276
Li	-1.699263	0.016368	-0.0738
N	-0.849055	0.652923	1.687886
C	0.530476	0.895973	1.191809
H	0.970038	-0.090201	0.982567
H	1.127025	1.296146	2.037214
O	-3.633849	0.607663	-0.293568
Si	0.977689	2.034934	-0.330243
C	3.047972	1.604317	0.319732
H	3.145127	2.036977	1.327696
H	3.631678	2.225637	-0.376211
C	3.494801	0.208235	0.293649
C	3.995609	-0.400386	-0.87936
C	3.392174	-0.638242	1.422331
C	4.319926	-1.751891	-0.934623
H	4.146488	0.219759	-1.764622
C	3.712473	-1.98974	1.370225
H	3.056888	-0.208116	2.369078
C	4.168036	-2.570853	0.185037
H	4.710418	-2.169361	-1.86409
H	3.621463	-2.595817	2.273225
H	4.430124	-3.627481	0.145002
C	1.235	3.856423	0.175459
H	1.475007	3.919543	1.247714
H	2.091655	4.284841	-0.365038
H	0.358275	4.491171	-0.016721

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C	1.555301	1.546439	-2.106711
H	2.432823	2.153901	-2.372653
H	1.88663	0.49827	-2.145881
H	0.791779	1.696148	-2.882995
C	-4.562912	0.353095	0.736805
H	-5.337681	-0.354905	0.397126
H	-4.018268	-0.091074	1.575025
H	-5.04496	1.289161	1.059831
C	-4.241302	1.207421	-1.418986
H	-5.003818	0.535373	-1.847895
H	-4.714684	2.161721	-1.141527
H	-3.45644	1.40738	-2.155291
C	-1.380145	1.873909	2.288038
H	-0.761622	2.184326	3.153076
H	-1.376457	2.691311	1.56208
H	-2.409582	1.713759	2.640238
C	-0.800241	-0.369373	2.728774
H	-1.808848	-0.571824	3.122299
H	-0.378438	-1.301237	2.326984
H	-0.156627	-0.051946	3.572607
C	0.399746	-2.00375	-0.921876
H	0.314352	-2.051733	0.16944
H	0.227441	-3.008347	-1.344064
H	1.416568	-1.664808	-1.180435
C	-0.606185	-1.047765	-2.807778
H	0.375397	-0.756231	-3.209002
H	-0.893711	-2.030147	-3.219653
H	-1.346772	-0.296459	-3.106586
O	-0.579442	-1.095365	-1.397594
O	-2.680443	-2.064032	0.356649
C	-3.206328	-2.510118	-0.871792
H	-2.503383	-3.191988	-1.379595
H	-4.163881	-3.03537	-0.717367
H	-3.374295	-1.632779	-1.506168
C	-2.453547	-3.144245	1.233248
H	-1.68965	-3.829023	0.828078
H	-2.104273	-2.738108	2.186586
H	-3.383379	-3.711592	1.402431

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Abbildung 10.38 Molekel Darstellung von **TS16**.Tabelle 10.515 Standardorientierung von **TS16** [Übergangszustand; M06/6-31+G(d)].

	x	y	z
C	0.5903997247	2.8556108001	0.9622278532
Li	1.7323349997	-0.101487755	0.0146195323
N	0.8301593098	0.7297151361	-1.6099401637
C	-0.5760852401	1.0101634953	-1.1917997068
O	3.6102019743	0.686324092	0.2472827112
Si	-1.099729887	2.1872651479	0.2401117848
C	-3.3849387797	1.073770127	-0.6240916923
C	-3.4206836671	-0.3384913536	-0.4521414675
C	-3.8475059564	-0.9565762296	0.7625846265
C	-2.9289620845	-1.2494802748	-1.4380870013
C	-3.7234479952	-2.3181139829	0.9904900314
C	-2.8011148121	-2.6111036464	-1.2001135549
C	-3.171090515	-3.1733448119	0.0272667105
C	-1.818396827	3.8116217445	-0.4101917011
C	-1.8286059929	1.5887986191	1.8870151982
C	4.5056117908	0.3024614413	-0.7800703991
C	4.0422422767	1.8739364433	0.8872341564
C	1.4698308236	1.9261952897	-2.1474310549
C	0.7812768495	-0.2651289099	-2.6821325933
C	-0.3159196286	-1.6225616798	1.416570966
C	0.9626550553	-0.3811436891	2.9508618463
O	0.6915882503	-0.6320139022	1.5897388252
O	2.435224494	-2.0969262665	-0.2730240573
C	3.1080968798	-2.497377585	0.904299322
C	1.840265057	-3.2052653449	-0.9249005086
H	1.2645855698	2.0243335179	1.2328996168
H	0.3734082015	3.394849349	1.8981264619
H	1.1515213906	3.5539195191	0.3230811936
H	-1.0242758864	0.032963966	-0.9730468359
H	-1.1255997192	1.3788931807	-2.0821013369

H	-3.4034054623	1.4337805285	-1.66035901
H	-4.0458049329	1.6515560474	0.0332278856
H	-4.3031807564	-0.3247703542	1.5287976504
H	-2.6614604364	-0.8519199199	-2.4212039481
H	-4.0760710146	-2.7302348155	1.9386237775
H	-2.4244333581	-3.2555241289	-1.998946014
H	-3.0935035873	-4.2457259108	0.2032044771
H	-1.2634766099	4.1255733784	-1.3086758754
H	-2.8802704927	3.7491075436	-0.6728603969
H	-1.6881084693	4.6056632776	0.3404422172
H	-2.7262358513	2.1894301078	2.0943452138
H	-2.1592831006	0.5438054646	1.8586918995
H	-1.1324222739	1.7252862141	2.7286133753
H	5.5006153275	0.0845772945	-0.3605591927
H	4.1041392284	-0.6004239292	-1.2512293179
H	4.601925379	1.1036673161	-1.5299529215
H	5.0553505904	1.7378690239	1.2960606503
H	4.0447714244	2.7152502373	0.176691749
H	3.3433387474	2.0997886524	1.6968979296
H	0.8768971805	2.34993003	-2.9815902217
H	1.5691874092	2.6920809066	-1.374033312
H	2.4702537622	1.6802476478	-2.5330759548
H	1.797731944	-0.5587926552	-2.9870612539
H	0.2296287973	-1.1524353251	-2.3436877488
H	0.250241644	0.1302234514	-3.5696387207
H	-0.5445611175	-1.7032724423	0.3462532411
H	0.0328585455	-2.5951368946	1.8026848584
H	-1.2421655319	-1.3349481088	1.9329915983
H	0.0555176246	-0.0350735735	3.4681813042
H	1.3380363352	-1.291803272	3.4474633696
H	1.7264228261	0.4035316503	3.0035899192
H	2.4084879791	-2.9668837196	1.6145740143
H	3.9095990996	-3.2142072071	0.6651984882
H	3.5442589921	-1.6027365215	1.3618694723
H	1.0487081541	-3.6506334748	-0.3014348634
H	1.4022180606	-2.8512289972	-1.8610663708
H	2.6003743323	-3.9700589594	-1.147064731

### 10.2.2.2. Dimeres Methyllithiummodell

Tabelle 10.516 Berechnete Energien der optimierten Strukturen des dimeren Substitutionsmodells mit Methyllithium (R = Me).

	R'	Methode	Basissatz	SCF [Hartree]	ZPE [Hartree]
<b>Ed2-1</b>	Me	M06	6-31+G(d)	-1373.429978	-1372.811222
<b>Ed2-2</b>	Me	M06	6-31+G(d)	-1373.429326	-1372.810304
<b>Ed2-3</b>	Me	M06	6-31+G(d)	-1373.424312	-1372.805529
<b>Ed2-4</b>	Me	M06	6-31+G(d)	-1373.421908	-1372.803172

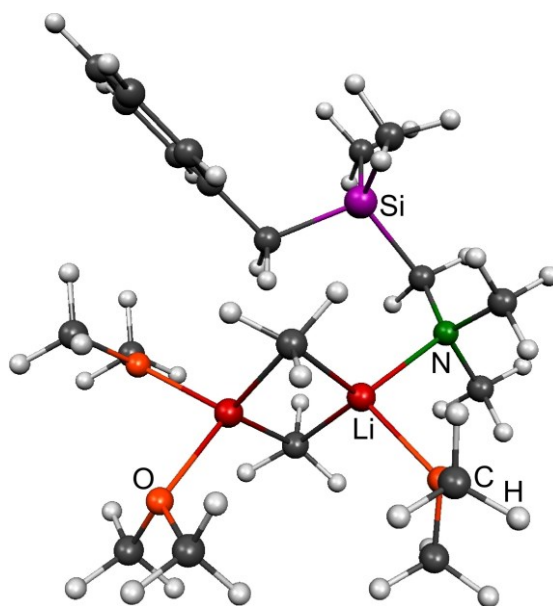
<b>TS17</b>	Me	M06	6-31+G(d)	-1373.393655	-1372.778727
<b>TS18</b>	Me	M06	6-31+G(d)	-1373.399675	-1372.778621
<b>TS19</b>	Me	M06	6-31+G(d)	-1373.398027	-1372.776889
<b>Int5</b>	Me	M06	6-31+G(d)	-1373.401554	-1372.780076
<b>Int6</b>	Me	M06	6-31+G(d)	-1373.399723	-1372.778287
<b>Pr2</b>	Me	M06	6-31+G(d)	-1373.439903	-1372.819875
<b>Ed2-1</b>	Me	M052X	6-31+G(d)	-1374.033638	-1373.398777
<b>TS17</b>	Me	M052X	6-31+G(d)	-1373.995168	-1373.364666
<b>TS18</b>	Me	M052X	6-31+G(d)	-1374.004994	-1373.367791
<b>TS19</b>	Me	M052X	6-31+G(d)	-1374.00213	-1373.365715
<b>Ed2-1</b>	OMe	M052X	6-31+G(d)	-1449.318862	-1448.676389
<b>TS17</b>	OMe	M052X	6-31+G(d)	-1449.281855	-1448.644492
<b>TS18</b>	OMe	M052X	6-31+G(d)	-1449.291202	-1448.646536
<b>TS19</b>	OMe	M052X	6-31+G(d)	-1449.289199	-1448.645861

Tabelle 10.517 Berechnete Energien des dimeren Substitutionsmodells mit Methyllithium (R, R' = Me) in Abhängigkeit des Lösungsmittels, berechnet mit der PCM-Methode auf M06/6-31+G(d)-Niveau. [Die M06/6-31+G(d)-Struktur wurde verwendet.]

Verbindung	Solvens	ZPE [Hartree]
<b>Ed2-1</b>	THF	-1372.8
<b>TS17</b>	THF	-1372.8
<b>TS18</b>	THF	-1372.8
<b>TS19</b>	THF	-1372.8
<b>Ed2-1</b>	Toluol	-1372.8
<b>TS17</b>	Toluol	-1372.8
<b>TS18</b>	Toluol	-1372.8
<b>TS19</b>	Toluol	-1372.8
<b>Ed2-1</b>	Wasser	-1372.8
<b>TS17</b>	Wasser	-1372.8
<b>TS18</b>	Wasser	-1372.8
<b>TS19</b>	Wasser	-1372.8

Tabelle 10.518 Berechnete Energien des dimeren Substitutionsmodells mit Methyllithium (R, R' = Me) in Abhängigkeit unterschiedlicher Basissätze und Funktionale. [Die M06/6-31+G(d)-Struktur wurde verwendet.]

Verbindung	Methode	Basissatz	ZPE [Hartree]
<b>Ed2-1</b>	M06	6-31+G(d,p)	-1372.8736
<b>TS17</b>	M06	6-31+G(d,p)	-1372.8414
<b>TS18</b>	M06	6-31+G(d,p)	-1372.8409
<b>TS19</b>	M06	6-31+G(d,p)	-1372.8393
<b>Ed2-1</b>	M062X	6-31+G(d)	-1373.0458
<b>TS17</b>	M062X	6-31+G(d)	-1373.0123
<b>TS18</b>	M062X	6-31+G(d)	-1373.0137
<b>TS19</b>	M062X	6-31+G(d)	-1373.0123
<b>Ed2-1</b>	M062X	6-31+G(d,p)	-1373.0999
<b>TS17</b>	M062X	6-31+G(d,p)	-1373.0671
<b>TS18</b>	M062X	6-31+G(d,p)	-1373.0676
<b>TS19</b>	M062X	6-31+G(d,p)	-1373.0664

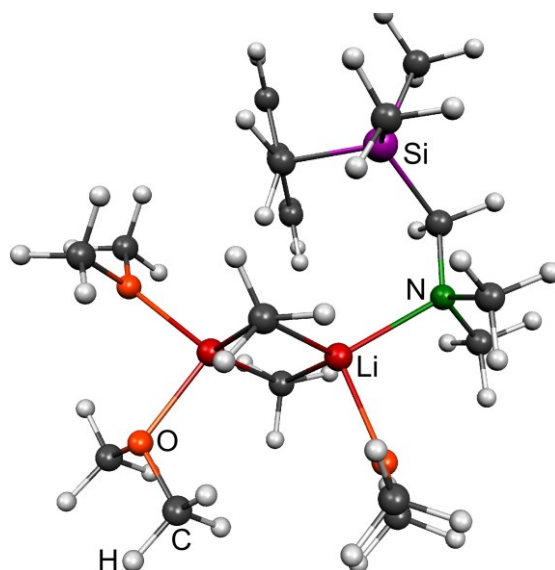
Abbildung 10.39 Molekel Darstellung von **Ed2** (Konformer 1).Tabelle 10.519 Standardorientierung von **Ed2** (R, R' = Me) [Konformer 1; lokales Minimum; M06/6-31+G(d)].

	x	y	z
C	-0.9654146211	0.4946153406	1.6740659206
Li	-1.1161046999	1.6229521964	-0.1935363408
C	-1.8883693759	0.5150771985	-1.8991055635
H	-0.6546801889	-0.497388029	2.0727823972
H	-1.7207488369	0.8596522895	2.4010365479
H	-0.0792082977	1.1331092963	1.8775642479
H	-1.9512138567	1.5350966512	-2.3400585579
H	-2.8552574876	0.0605514858	-2.2056718939
H	-1.1359546782	-0.0018508094	-2.5329223638
Li	-1.8896649831	-0.5464307045	-0.0117466207
N	-1.3749022161	-2.6636704928	-0.3617359326
C	-0.069911591	-2.9618237599	-0.9650453948
H	-0.0716509575	-2.5390952879	-1.984673262
H	0.0336960072	-4.0638855881	-1.1005854352
O	0.508089189	2.6872298675	-0.7138303621
O	-2.3465056757	3.2110396308	0.1579739886
O	-3.834873841	-0.862827974	0.7311098422
Si	1.5474540932	-2.3022577161	-0.1998392595
C	2.9023985634	-3.1392497142	-1.2039718316
H	3.8917952112	-2.7681845745	-0.901774259
H	2.786512595	-2.939360184	-2.2790408036
C	1.0242911871	2.72780144	-2.0238359751
H	0.9906385661	3.7572206016	-2.4216182324
H	2.0679666513	2.370262058	-2.0402751609
H	0.3983485535	2.0756873029	-2.643059214
C	1.2333593714	3.4932382498	0.1870651304

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H	0.7663540358	3.386114513	1.17237288
H	2.2845568744	3.1663383919	0.2448795325
H	1.1975274456	4.551951672	-0.1243397271
C	-3.6451339167	2.725635785	0.4211846235
H	-4.2761858941	3.521085546	0.8503362693
H	-4.110781781	2.3457648985	-0.5042281799
H	-3.5405794786	1.9001551899	1.1347755832
C	-2.3492412891	4.2247599862	-0.8197214836
H	-2.9588138133	5.0822751459	-0.4910312562
H	-1.3125829432	4.5482860664	-0.9623238576
H	-2.744953279	3.845744888	-1.7772790086
C	-2.4312681571	-3.0952411249	-1.2729458533
H	-3.4128638667	-2.914929897	-0.8155642551
H	-2.3712940501	-2.5243797323	-2.2085841986
H	-2.3465497491	-4.1757849384	-1.5077340622
C	-1.5264490795	-3.3575879133	0.9098031997
H	-1.3704110907	-4.4510110285	0.7996575721
H	-0.8104447789	-2.9751060399	1.646154218
H	-2.5393489972	-3.192029168	1.298952426
C	-4.0963335508	-0.9545130955	2.1131450708
H	-4.6307283327	-0.0578176852	2.4697286828
H	-4.7081637014	-1.8452364938	2.3363816817
H	-3.1333673909	-1.0200403957	2.6296341453
C	-5.0093628279	-0.7152179694	-0.0301247187
H	-4.7123180047	-0.5947610807	-1.0773594367
H	-5.6599394176	-1.6004544403	0.0739379489
H	-5.5735066323	0.1773326535	0.2900031696
C	1.8064222792	-2.7133083949	1.6163949952
H	1.6132994596	-3.7767897501	1.8167080737
H	1.1699580963	-2.1140056235	2.2820993
C	1.6141898053	-0.4386726251	-0.5009551662
H	1.5099613971	-0.2880492835	-1.5882472641
H	0.7156798439	-0.0051654968	-0.031702039
H	2.8977921438	-4.2290154017	-1.0628650753
H	2.8511818917	-2.507703089	1.8900980598
C	2.8509237906	0.2225760552	0.014068222
C	3.9514901742	0.4590032823	-0.8192099453
C	2.9479072491	0.6158939714	1.3561032901
C	5.1028707728	1.0770659659	-0.3367777646
H	3.8954772222	0.1583109461	-1.8682995866
C	4.0984299053	1.2286430805	1.84276306
H	2.0944317964	0.4519103916	2.0177057772
C	5.1819824678	1.4664533439	0.9983093969
H	5.941910451	1.2557840817	-1.0087785629
H	4.1458844492	1.5293489218	2.8891352233
H	6.0805017898	1.9507301166	1.3780964285

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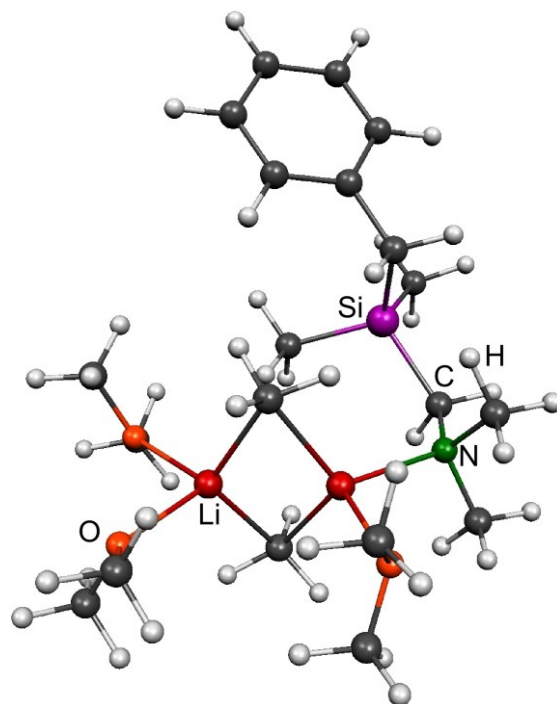
Abbildung 10.40 Molekel Darstellung von **Ed2** (Konformer 2).Tabelle 10.520 Standardorientierung von **Ed2** (R, R' = Me) [Konformer 2; lokales Minimum; M06/6-31+G(d)].

	x	y	z
C	-1.7100655566	-0.2574168893	1.7485069215
Li	-1.5195788091	1.3204971812	0.2587653955
C	-1.4520718596	0.6911202247	-1.8150865766
H	-1.520034942	-1.3432873132	1.901183215
H	-2.74178985	-0.1174113111	2.1360351779
H	-1.068802412	0.2104753649	2.5239822052
H	-0.8912308286	1.6312285376	-2.0083547373
H	-2.4665053763	0.8966751263	-2.2209446335
H	-1.0077211567	-0.0147166728	-2.5503139793
Li	-1.4998347701	-0.9267337343	-0.3327314546
N	-0.1298884816	-2.6833273411	-0.6007860527
C	1.3178359462	-2.5773049055	-0.3742894075
H	1.7407321914	-1.942180449	-1.1711793194
H	1.7882830585	-3.5774637524	-0.5207886606
O	-0.1402965922	2.7860779721	0.6826772913
O	-3.1245551386	2.5952177129	0.4322441512
O	-3.2664114965	-1.9424744588	-0.751578363
Si	2.0296642569	-1.8413393111	1.2335138851
C	3.8621353941	-2.2612782723	1.127680282
H	4.4226720097	-1.789347738	1.9472215216
H	4.299375694	-1.9064598772	0.1835785409
C	0.6292258472	3.6081480061	-0.1657814818
H	0.3235109739	4.6644466422	-0.0621483093
H	1.7023802758	3.5190326445	0.0689922177
H	0.4599061048	3.2738264852	-1.1945540788
C	-0.0421330261	3.168209232	2.0343252847
H	-0.6530029814	2.4731448278	2.6203574662
H	1.0050640035	3.1180264568	2.3774014126

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H	-0.4194096467	4.1958940847	2.1768267505
C	-4.3538728659	1.9211326821	0.290459172
H	-5.1884812525	2.5627643529	0.6172781918
H	-4.5165149579	1.6222383818	-0.75930761
H	-4.306532267	1.0271848884	0.9213015483
C	-3.059992774	3.7515640273	-0.3705651456
H	-3.8880426075	4.4383909398	-0.1306361225
H	-2.1065003167	4.2449259787	-0.1557509245
H	-3.1018339618	3.4896870271	-1.440901747
C	-0.3672169031	-3.0488465409	-1.9950018543
H	-1.4441505541	-3.1700716346	-2.1704648786
H	0.0095947125	-2.2583470724	-2.6571924854
H	0.1403177092	-3.9996175898	-2.2559775302
C	-0.6994797401	-3.7128219902	0.2610498673
H	-0.1831283768	-4.6853837784	0.1235652253
H	-0.618011948	-3.4208290237	1.3145223674
H	-1.7612574595	-3.8474881361	0.0199174571
C	-4.1491091908	-2.2176904854	0.3132196616
H	-4.8303490425	-1.3673293206	0.4839807453
H	-4.7474592938	-3.1185809154	0.0982928412
H	-3.5489407064	-2.371913629	1.2158752614
C	-3.9526787232	-1.659938769	-1.9507289123
H	-3.2088254768	-1.4080952251	-2.7131106118
H	-4.5440360581	-2.5329669469	-2.2729605019
H	-4.6265735803	-0.7970970174	-1.8200405832
C	1.3260037871	-2.5342024837	2.8331177168
H	1.3128360973	-3.6329360218	2.841508768
H	0.3079243716	-2.1683182922	3.0280585178
C	1.8314983798	0.0430705651	1.2511211621
H	0.7524740777	0.2641719766	1.2094957494
H	4.0286972846	-3.3456261237	1.1915446399
H	1.9583253762	-2.2066959916	3.6712778508
C	2.5641740936	0.7192570907	0.1370864569
C	2.0084998165	0.7731167179	-1.1481683124
C	3.8294992045	1.2861453291	0.3302793135
C	2.6916111149	1.3734593455	-2.2009397685
H	1.0022503686	0.3776332424	-1.3097571456
C	4.516013508	1.8896518485	-0.7212864277
H	4.2796847615	1.2548019926	1.3250108961
C	3.9504975684	1.9358755056	-1.9939478249
H	2.2246516299	1.4129455656	-3.1857221572
H	5.4978901792	2.3279522234	-0.5441428121
H	4.4852439381	2.4093906016	-2.8162489111
H	2.1914492459	0.3950002328	2.2324151928

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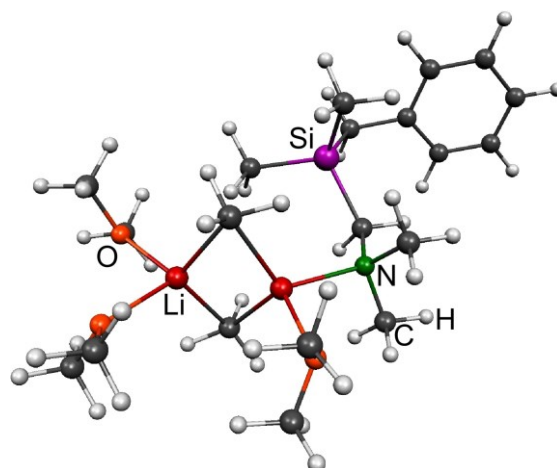
Abbildung 10.41 Molekel Darstellung von **Ed2** (Konformer 3).Tabelle 10.521 Standardorientierung von **Ed2** (R, R' = Me) [Konformer 3; lokales Minimum; M06/6-31+G(d)].

	x	y	z
C	0.9086682026	0.4637759497	-1.4180691622
Li	2.0504573286	1.2184871595	0.2745043515
C	2.5342765655	-0.2362659263	1.8105523208
H	0.4147056253	-0.4331491614	-1.8521051573
H	1.4505959048	0.8966358837	-2.2855051492
H	0.0626586472	1.1626046253	-1.2489332271
H	3.1549358368	0.5768843111	2.24520224
H	3.159025917	-1.1369341653	1.9829276165
H	1.6936546126	-0.3463988964	2.5300185765
Li	1.7042304813	-1.0507539372	-0.0192018649
N	0.476853088	-2.790370559	0.4143876165
C	-0.6943012022	-2.6081519806	1.2814167825
H	-0.3228437619	-2.3809938529	2.2959225956
H	-1.2391502449	-3.5756793446	1.3767698559
O	1.1664569697	2.787655289	1.1823825174
O	3.62452964	2.3803028824	-0.4020550376
O	3.1666113226	-2.047754848	-1.1707607638
Si	-1.9719301191	-1.2229938533	0.9682132756
C	-3.4268094004	-1.7268672522	2.0541748724
H	-4.1886725128	-0.9364273517	2.0899095455
H	-3.0912669512	-1.9104867048	3.0852003771
C	0.8858350906	2.9204966623	2.5567015919
H	1.1916403592	3.9163774549	2.918415196

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H	-0.1898589138	2.7806136492	2.7517945805
H	1.4506347307	2.1423624543	3.0818420152
C	0.429881828	3.6807463217	0.3804667473
H	0.7346903484	3.5174635387	-0.658924097
H	-0.6522084653	3.4886571831	0.4767172315
H	0.6385911138	4.7249539206	0.6656940212
C	4.2293107411	2.129727895	-1.6471682819
H	4.7818347003	3.0169986274	-1.9974737071
H	4.9313220341	1.2795461477	-1.5822619499
H	3.4313793272	1.8874549873	-2.3564780784
C	4.5689228054	2.6842990322	0.5986787951
H	5.1735243746	3.5596295942	0.3101046899
H	4.0170875923	2.9099372639	1.5169244273
H	5.2359761022	1.8250671793	0.7816718963
C	1.4250376231	-3.6892561275	1.0697433494
H	2.2859550458	-3.8620300265	0.4110344543
H	1.7812744464	-3.2371044851	2.0042843414
H	0.9570795272	-4.667016246	1.303009322
C	0.0847060665	-3.3719460392	-0.86330162
H	-0.4403290192	-4.3394144906	-0.7233481815
H	-0.5789347473	-2.6931646359	-1.4107910302
H	0.9787849306	-3.549297312	-1.4750710085
C	3.1807185798	-1.6943664506	-2.5373025627
H	3.56577388	-0.6708270948	-2.6727236262
H	3.8059257908	-2.3992431619	-3.1095541941
H	2.1504912018	-1.7262468101	-2.9048034652
C	4.4551903168	-1.9801080166	-0.6011764612
H	4.3828208384	-2.317745425	0.4370592989
H	5.1575351797	-2.6241339751	-1.1554926741
H	4.8298818933	-0.9420205373	-0.6044848847
C	-2.5589536351	-1.073458328	-0.8343859004
H	-2.9698152123	-2.0461960135	-1.1494791014
H	-1.6872053929	-0.8553598195	-1.4699552518
C	-1.3076547001	0.4166833126	1.5824806251
H	-1.0309331341	0.3314994997	2.6439292878
H	-0.4145100257	0.7308563462	1.0239001962
H	-2.0741606701	1.2005192723	1.4896267181
C	-3.5800823469	0.0128356267	-0.9867333993
C	-4.9406550839	-0.2288814173	-0.7661219459
C	-3.1874563517	1.3139693042	-1.323593351
C	-5.8784649159	0.7948857581	-0.8699132838
H	-5.2674373703	-1.2396292049	-0.513192985
C	-4.1220269449	2.3396979058	-1.4266095317
H	-2.1301706866	1.5118590404	-1.5149472987
C	-5.4730738745	2.0863316148	-1.1981288587
H	-6.9328694403	0.580552144	-0.6979892278
H	-3.793066041	3.3431382482	-1.6963564171
H	-6.2054987341	2.8879310864	-1.2824315576
H	-3.9104677114	-2.6458707209	1.6934759657

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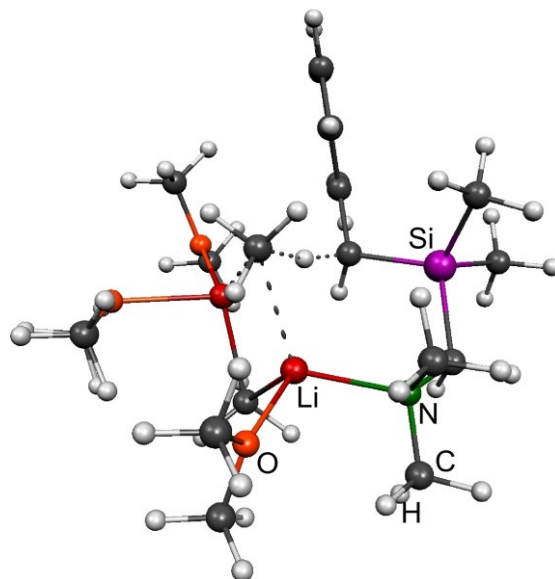
Abbildung 10.42 Molekel Darstellung von **Ed2** (Konformer 4).Tabelle 10.522 Standardorientierung von **Ed2** (R, R' = Me) [Konformer 4; lokales Minimum; M06/6-31+G(d)].

	x	y	z
C	1.8318412211	0.038166712	1.7117814724
Li	2.9425598696	-0.6041508416	-0.0427549866
C	2.2470046963	0.1389199585	-1.9500617957
H	1.0511740721	0.7402658024	2.0787038283
H	2.6802018952	0.2296156965	2.4037515641
H	1.4467604506	-0.9557884626	2.0230913205
H	3.2547814896	-0.07270118	-2.3710525837
H	1.9355086421	1.0461639812	-2.5086855268
H	1.5983454401	-0.6615280253	-2.3662265884
Li	1.3660161337	1.0740829002	-0.1837919016
N	-0.636879461	1.6920042701	-0.5667752228
C	-1.5725703418	0.6253844844	-0.9512178125
H	-1.2497246705	0.2407405705	-1.9347225916
H	-2.5826491542	1.0650525948	-1.1123888092
O	3.1168032947	-2.608641131	-0.2247512565
O	4.9830346182	-0.3901191077	0.3227906711
O	2.2440650989	2.9877658068	0.0661756527
Si	-1.7632853493	-0.946574927	0.1123744414
C	-3.3782590376	-1.7390219931	-0.52761372
H	-3.4252837205	-2.7474460778	-0.0854899391
H	-3.2692765038	-1.8816799985	-1.6149477887
C	-4.6213397723	-0.9676719753	-0.2154007024
C	-5.1630417506	-0.0606761993	-1.1340499335
C	-5.2647949683	-1.1090536473	1.0205229313
C	-6.2994788589	0.6830552535	-0.8286218488
H	-4.6878007071	0.0537249135	-2.1104162474
C	-6.4007890728	-0.3679540215	1.330390952
H	-4.8658379236	-1.8179655271	1.7485606901
C	-6.9238883546	0.5348998618	0.407193303
H	-6.7026871054	1.3781918053	-1.5643555396
H	-6.8836210504	-0.5004972728	2.2980777907

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H	-7.8148295325	1.113238569	0.6469319879
C	2.7705643752	-3.3882673922	-1.3456271385
H	3.522125463	-4.1774849716	-1.5137425762
H	1.7818939546	-3.8559529472	-1.2068554988
H	2.7326705114	-2.7181026153	-2.2112912471
C	3.1426033647	-3.3487755006	0.9730919921
H	3.4344509333	-2.6647054268	1.7770807949
H	2.1451679794	-3.7624840837	1.1965398628
H	3.8708617073	-4.1737500619	0.906635423
C	5.5533058135	0.4548617761	1.2908872902
H	6.4958000577	0.0298803222	1.6738944873
H	5.763054031	1.4549190266	0.871156171
H	4.8324700057	0.5471518428	2.1099800483
C	5.8246173988	-0.5777834541	-0.7905654937
H	6.7948370452	-0.9989272781	-0.4797074771
H	5.3253361083	-1.2761393254	-1.4698635959
H	5.9969510349	0.3759039149	-1.3173620741
C	-0.5094261602	2.6418779667	-1.6707455513
H	0.1951012986	3.437775704	-1.3948164643
H	-0.1240389257	2.1268015398	-2.5598246869
H	-1.4872885752	3.0995962253	-1.9219824396
C	-1.1220644888	2.4010697107	0.6118511534
H	-2.1479772611	2.7923965095	0.4557387724
H	-1.1310593057	1.7393705356	1.4851845212
H	-0.4584908614	3.2486883196	0.8273034714
C	2.610720041	3.2822203685	1.396342836
H	3.4208416167	2.6168717291	1.7356004603
H	2.9345117551	4.332486195	1.4830022038
H	1.736044025	3.1125759757	2.0321438373
C	3.3189310583	3.1813927723	-0.8267175028
H	2.9591766969	2.9662001054	-1.8372996266
H	3.6849534548	4.2199106241	-0.7702682122
H	4.1465484147	2.4883360984	-0.5959169757
C	-1.9049778854	-0.6866463553	1.9660030631
H	-2.6859066403	0.0387794605	2.2320481056
H	-2.164833129	-1.6440293397	2.442260486
H	-0.9492005955	-0.3587058927	2.3989593994
C	-0.3900114656	-2.1623958425	-0.2791686989
H	-0.4056209231	-2.4320641782	-1.3456578965
H	0.5968874423	-1.7344639284	-0.0525967669
H	-0.5122799574	-3.083561922	0.3106097331

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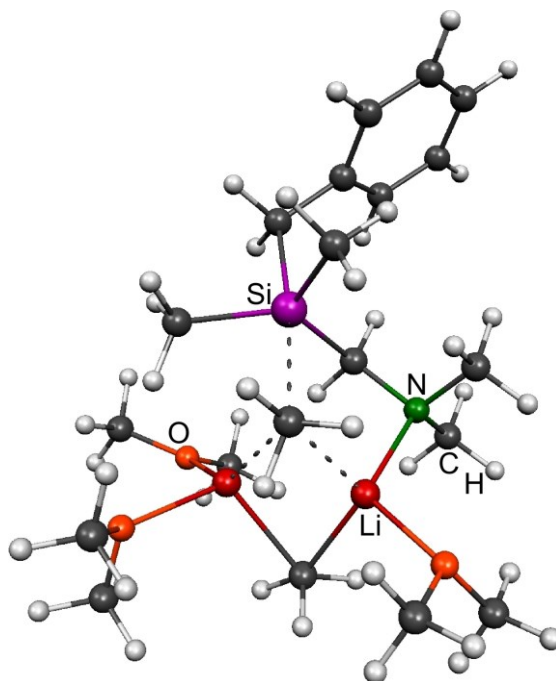
Abbildung 10.43 Molekel Darstellung von **TS17**.Tabelle 10.523 Standardorientierung von **TS17** (R, R' = Me) [Übergangszustand; M06/6-31+G(d)].

	x	y	z
C	-0.587769381	0.4110041799	1.6967756792
Li	-0.0725234925	1.5981031927	-0.312711318
C	-1.4897171057	1.1799545016	-1.8599672616
H	-0.4719700329	-0.381509699	2.452788405
H	-1.6489504682	0.7173417361	1.7221801648
H	-0.0086165115	1.2718151771	2.0746854402
H	-0.6252909543	1.4998446809	-2.4811603361
H	-2.2270661791	1.9988341227	-1.9892460927
H	-1.9013710439	0.3416236203	-2.4649072064
Li	-1.9009440186	-0.124297452	-0.2415251325
N	-2.2613080897	-2.2114507329	-0.3677145077
C	-1.1206525439	-2.9066260623	-0.9897559705
H	-1.0366780691	-2.5364938141	-2.0264005528
H	-1.3493080505	-3.9935868266	-1.0729622244
O	1.6700807712	2.4654795424	-0.7393064533
O	-0.8064092142	3.5233619558	0.4389144759
O	-3.844254832	0.4469437553	0.3859822825
Si	0.6365763125	-2.6822576058	-0.2567007357
C	1.6950455064	-3.7404853934	-1.4133841186
H	2.7546647088	-3.6487050075	-1.1335621834
H	1.6025612283	-3.4063010627	-2.4569635645
C	2.2299981411	2.6701155534	-2.0154411993
H	2.3210945723	3.7492857885	-2.23029618
H	3.2257812146	2.2049728336	-2.0806176553
H	1.5618353888	2.2073490619	-2.7503449208
C	2.4906107605	2.9675998758	0.2973308964
H	1.9923615182	2.755828475	1.2483963024

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H	3.4725520073	2.4694168934	0.2850888576
H	2.6191804479	4.0582243033	0.1876968004
C	-2.0441716568	3.5177552647	1.1141093661
H	-2.2988372354	4.5322392647	1.4619983114
H	-2.8468610484	3.1450368214	0.4536922039
H	-1.9490356485	2.8519113788	1.9779288108
C	-0.808593656	4.4529438524	-0.6228887304
H	-1.0176303434	5.467812358	-0.2472423864
H	0.1852689821	4.4331483845	-1.0804352931
H	-1.5618202514	4.1814487071	-1.3807050459
C	-3.4570037808	-2.3952689967	-1.1849033889
H	-4.313411176	-1.8895166776	-0.716985109
H	-3.2983358661	-1.9647928362	-2.1825306049
H	-3.7038204035	-3.468839896	-1.3040496378
C	-2.5151123917	-2.7367483678	0.9684855383
H	-2.6660127802	-3.8350926301	0.9506918876
H	-1.6743539435	-2.5150714768	1.6351910151
H	-3.419778732	-2.274405404	1.3850266087
C	-4.4602709542	0.3651595226	1.6493726746
H	-4.8222448596	1.3558690562	1.9722018029
H	-5.3140982626	-0.3341336854	1.6248988993
H	-3.7140212825	0.0058077267	2.3665153855
C	-4.7197199226	0.9545267937	-0.5985103422
H	-4.1765865552	0.9739907792	-1.5485116051
H	-5.6141552348	0.3155126082	-0.6904866253
H	-5.0394360277	1.978313419	-0.3420751087
C	0.8115302836	-3.4759525717	1.4518237405
H	0.3224772045	-4.4615380192	1.4730420946
H	0.4015814207	-2.8733679542	2.273376584
C	1.058147751	-0.88762311	-0.306707191
H	0.9051758412	-0.5739067849	-1.3578051264
H	0.111843207	-0.2057442007	0.6385102877
H	1.4279748441	-4.8070488736	-1.3710175204
H	1.8783610573	-3.6334619236	1.6666529568
C	2.4322706066	-0.5849821339	0.1278450162
C	3.4563355275	-0.2439714677	-0.7811534895
C	2.7967422635	-0.6133208706	1.4911126105
C	4.746809902	0.0592906419	-0.3622707476
H	3.2191865877	-0.2427422962	-1.8483687052
C	4.0885527836	-0.3141759339	1.9134589962
H	2.0364004241	-0.8668880465	2.2320669328
C	5.0782031881	0.0310351949	0.9935769828
H	5.5082038892	0.3080553696	-1.103726058
H	4.3241299604	-0.3476691523	2.9778283611
H	6.0898176978	0.2619895728	1.3244769575

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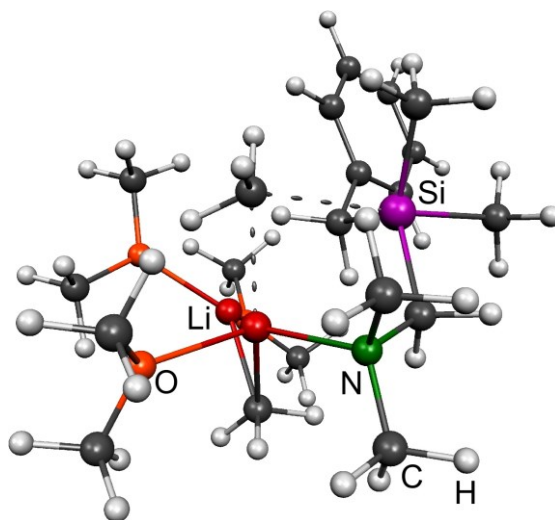
Abbildung 10.44 Molekel Darstellung von **TS18**.Tabelle 10.524 Standardorientierung von **TS18** (R, R' = Me) [Übergangszustand; M06/6-31+G(d)].

	x	y	z
C	-1.2946518289	0.4640093906	-1.7727202454
Li	-2.3698173524	-0.7053593782	0.1674990539
C	-3.2017169711	0.9590736379	1.1986252282
H	-2.3960531748	0.4967981189	-1.6110458852
H	-1.1996555672	-0.0212051126	-2.758118829
H	-1.0200700169	1.5197145973	-1.9816366544
H	-3.9583029996	1.5279666119	0.6150435128
H	-2.8764802091	1.6672943335	1.990617823
H	-3.8123600564	0.2217697335	1.7586620421
Li	-1.498347283	1.630556485	0.0759798474
N	0.3796897553	1.4785137217	0.8837757193
C	0.6845866012	0.0487756108	0.6814158708
H	-0.0946461353	-0.5354802397	1.2012534543
H	1.6303222571	-0.1743649161	1.2117374795
O	-1.9468162295	-2.0907029542	1.684295924
O	-3.7292996259	-1.9103595238	-0.7374224372
O	-1.9523901842	3.5604895461	-0.3554259976
Si	0.8154429098	-0.7125720745	-1.0872834395
C	2.4788104572	-1.7759269217	-0.684634313
H	2.6634134353	-2.3643027761	-1.5997629441
H	2.1944079697	-2.4995524218	0.0998961902
C	3.7066213957	-1.0458092739	-0.2778257962
C	4.0401718548	-0.8624590289	1.074804156
C	4.5723682955	-0.4727617946	-1.22430417

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C	5.1460995928	-0.1123996271	1.463939143
H	3.4200729781	-1.335587178	1.8394758595
C	5.6792402239	0.2783619213	-0.842295794
H	4.3711732084	-0.6295371924	-2.2854609154
C	5.9697744675	0.4752768024	0.5067096935
H	5.3707376433	0.0053684983	2.5242637484
H	6.3261798416	0.708440363	-1.6070287179
H	6.8364397062	1.0627662839	0.8065289668
C	1.5361815576	0.243072309	-2.5609251509
H	2.4946167188	0.7046113913	-2.288212869
H	1.7556631134	-0.4986815353	-3.3460482893
H	0.8908875237	1.0113379646	-2.9982118763
C	-0.191043141	-2.2768888437	-1.5328500555
H	-0.2470641525	-2.3118956197	-2.6323455979
H	0.301456992	-3.2032681181	-1.2034336661
H	-1.2292779399	-2.2888851268	-1.177780206
C	-2.1544484978	4.408771769	0.7530083712
H	-3.1422796473	4.231130456	1.2078825795
H	-1.3752847517	4.1850748297	1.4899803894
H	-2.0739488815	5.4653208606	0.4514994477
C	-2.9109436895	3.7831518578	-1.3698584718
H	-3.9292039801	3.6030128587	-0.9884042716
H	-2.8397615818	4.8166206859	-1.7439785787
H	-2.6982325238	3.0817680311	-2.1834236138
C	-4.1227789655	-1.6473875643	-2.0698598917
H	-4.7078191146	-2.4907347901	-2.4685809107
H	-4.7280917885	-0.7272262358	-2.1199921606
H	-3.2151320557	-1.5140119385	-2.6659674103
C	-4.8432067411	-2.1466501439	0.1011354556
H	-4.4587512351	-2.3584585744	1.1038052962
H	-5.4954836913	-1.2593124105	0.1409358486
H	-5.4214533396	-3.0096127063	-0.2647537835
C	-1.4102192071	-3.380201924	1.4778448809
H	-1.7177121697	-3.7126887391	0.481540006
H	-0.3083175921	-3.3565277275	1.5308229046
H	-1.7929579461	-4.0829869661	2.2351341575
C	-1.7300819869	-1.6314017412	3.003612187
H	-2.1558535236	-0.6250921377	3.0710448479
H	-2.2266670471	-2.2972317159	3.7271395516
H	-0.6513007158	-1.5962817817	3.2330922774
C	1.3696704435	2.3119435536	0.2054119239
H	2.4024233102	2.0493826421	0.5105714237
H	1.2868249589	2.191224672	-0.8799958011
H	1.1900310141	3.368473254	0.4453368495
C	0.4058814191	1.7731059555	2.3122181295
H	0.1829324745	2.8355545236	2.4871407609
H	-0.3518420623	1.1731744575	2.8320134405
H	1.3982624839	1.5520300265	2.7542013017

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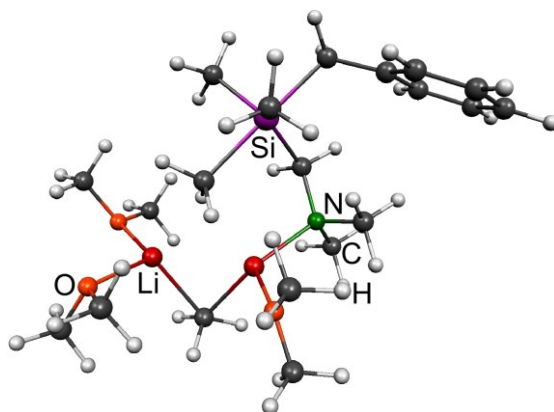
Abbildung 10.45 Molekel Darstellung von **TS19**.Tabelle 10.525 Standardorientierung von **TS19** (R, R' = Me) [Übergangszustand; M06/6-31+G(d)].

	x	y	z
C	1.1395285669	-0.4601596264	-1.6667966463
H	1.892434903	-0.9915936264	-2.2822206199
H	1.4842027139	0.600913316	-1.6475636912
H	0.2375505098	-0.4222787365	-2.3038642274
Li	0.1096569244	1.7686957306	0.6456568327
C	1.6068277395	1.2172771683	1.9545016962
O	-1.4770562879	2.610750621	1.4748681065
O	0.3395291902	2.8826887706	-1.0174595998
C	-1.8366424499	2.2612149419	2.7971323941
C	-2.5922613616	3.0297763867	0.7123657009
C	-0.300103259	2.7232477508	-2.2692559673
C	1.6188624225	3.4718053592	-1.1449072251
H	1.6996636225	2.2723941994	2.2951063016
H	2.6163264013	0.806173621	2.1503064824
H	0.9862110909	0.7321482043	2.7380038669
H	-2.2596764002	3.1327441613	3.3204190874
H	-2.5787012751	1.4464625265	2.7948143257
H	-0.9271912506	1.9333697382	3.311165294
H	-2.2168337999	3.3594433653	-0.2618722122
H	-3.3083847189	2.2020103853	0.5763389523
H	-3.0967057406	3.8746959624	1.2066736678
H	-0.4834666038	3.7063587948	-2.7317008257
H	0.3104413379	2.0994061999	-2.940096351
H	-1.2566087071	2.2167242781	-2.094248895
H	1.5377517093	4.4665851789	-1.61070607
H	2.0386445475	3.5669609752	-0.1380143513
H	2.2810031965	2.8316737785	-1.7521288642
Li	2.1699743607	-0.0075357202	0.1910954607
N	2.6170462464	-1.9325646258	0.7771930112

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C	1.2484784802	-2.3820828962	1.0490982178
C	-1.3981553468	-3.2581297903	0.8538709372
C	3.4421850864	-2.0065471727	1.9746007472
C	3.2141083409	-2.748353504	-0.2682459365
C	-0.3418425207	-3.0417325551	-1.798872831
C	-1.2520092572	-0.459385235	0.1378072614
C	-2.7307760626	-0.5225742077	-0.0525419426
C	-3.6156543412	-0.7208763516	1.0142833988
C	-3.2785364451	-0.3675167175	-1.3331812669
C	-4.9930658167	-0.7464903732	0.8148463864
C	-4.6548622571	-0.3885187625	-1.5382197766
C	-5.5216705936	-0.5739230283	-0.4628099823
Si	-0.2250607341	-2.0864827779	-0.1659515332
H	0.9146437238	-1.9002758071	1.9846963335
H	1.2534392633	-3.4731088287	1.2689886832
H	-2.4029295351	-3.316793213	0.4078392675
H	-1.5304002745	-2.9384412038	1.9010844935
H	-0.9989626549	-4.2844112093	0.8806137702
H	4.4516229836	-1.6281688962	1.7528838661
H	3.0083769106	-1.3877523198	2.7703845058
H	3.5330696835	-3.0464625322	2.34888286
H	3.2957794001	-3.8084856927	0.0488409654
H	2.6030413105	-2.700435797	-1.1754302206
H	4.223839767	-2.3810892276	-0.5024352332
H	-0.1761320424	-4.107559199	-1.5799024803
H	0.3404940946	-2.7318765007	-2.5962264192
H	-1.3733487111	-2.9611853446	-2.1762265575
H	-1.0144343793	-0.2051738077	1.1858531961
H	-0.8429638295	0.3148685252	-0.5241690337
H	-3.2108623289	-0.8667519698	2.018015755
H	-2.6032833598	-0.2288195637	-2.1816186781
H	-5.6582994372	-0.9028317326	1.6637134427
H	-5.0531796662	-0.2621041326	-2.5446492544
H	-6.5990922953	-0.5901069376	-0.6200015527
O	3.9491843188	0.8385550688	-0.4682190435
C	4.5622413733	0.4984555421	-1.6915597637
C	4.7618501294	1.6816190377	0.3150007482
H	4.7939440195	1.4066312985	-2.2737092929
H	5.4970198564	-0.0604529148	-1.5185792775
H	3.8567235131	-0.1198600685	-2.2557949412
H	4.2070440062	1.9273958781	1.2256680174
H	5.7060006421	1.1783278339	0.5816799217
H	4.9984113575	2.6099910076	-0.2327913914

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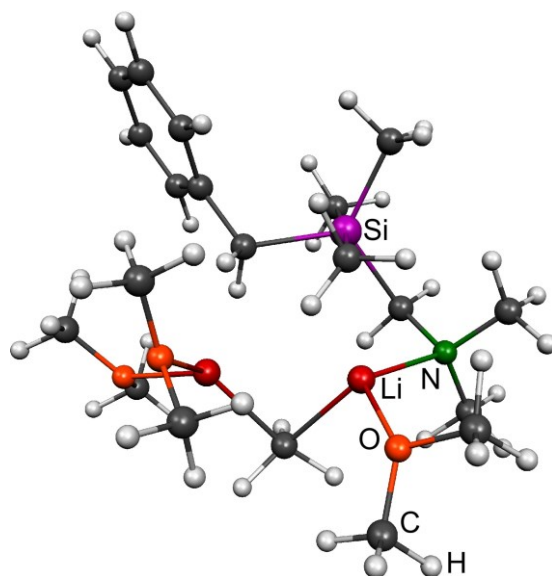
Abbildung 10.46 Molekel Darstellung von **Int5**.Tabelle 10.526 Standardorientierung von **Int5** (R, R' = Me) [lokales Minimum; M06/6-31+G(d)].

	x	y	z
C	-1.0730110506	-0.8210371843	-0.7914379728
Li	-3.3046275176	-0.2081648986	0.3146707479
C	-2.9829518272	1.2458537359	1.7800567136
H	-1.2809915629	0.2533191408	-0.9645793957
H	-1.5582058079	-1.1673058186	0.1385436772
H	-1.5560834714	-1.3437049974	-1.634539723
H	-3.4984195184	2.159816543	1.4159624658
H	-2.3413692948	1.6079829578	2.609861829
H	-3.7766852313	0.6919598844	2.3241080646
Li	-1.099037748	1.1085650048	0.7974581796
N	0.7321827296	0.5693448431	1.4760939121
C	1.0495294447	-0.8327771722	1.1238854989
H	0.2922586505	-1.4654367927	1.6228122131
H	2.022361291	-1.0928772914	1.5819159237
O	-3.9020591156	-2.0093234137	0.8665855616
O	-4.609390071	0.4256647138	-1.0300802823
O	-0.9157488293	2.8080637198	-0.2768058329
Si	0.9836886437	-1.4049110424	-0.7520507929
C	2.9727202683	-2.02284008	-0.6970817066
H	3.1369671938	-2.4787194378	-1.687702769
H	2.9962704333	-2.8385650273	0.044822263
C	4.0178650105	-1.0273350363	-0.3883488841
C	4.5517240054	-0.8945151173	0.9082059609
C	4.5032903577	-0.1262243115	-1.3558804768
C	5.4738830126	0.0962715453	1.2306825266
H	4.2395860161	-1.6037819972	1.6781353178
C	5.4223088184	0.8680998404	-1.038721911
H	4.1505198103	-0.219746377	-2.3843935408
C	5.9098383119	0.9985919612	0.2619987943
H	5.8631058273	0.1575055616	2.2477898691
H	5.7720223739	1.5438196486	-1.8202763202
H	6.6336471408	1.7742027752	0.5092476695
C	-3.217377217	-2.5494576573	1.9821653033

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H	-3.8077243401	-3.3579732738	2.4392902969
H	-2.233662282	-2.9452266155	1.6798390042
H	-3.0761923009	-1.7398070101	2.7056226631
C	-4.0912840188	-2.9672144253	-0.1582637984
H	-4.6178363559	-2.470263169	-0.9794848396
H	-3.1223115977	-3.3448494911	-0.5223822638
H	-4.6960344555	-3.8092470637	0.2117196663
C	-4.0950596691	1.4302744647	-1.8839346785
H	-4.8163120989	1.6592616118	-2.683284857
H	-3.8695651823	2.3473039503	-1.3142913087
H	-3.1709249528	1.0427328705	-2.3265722662
C	-5.8417211695	0.801103641	-0.4444956664
H	-6.6010977004	0.9683393487	-1.2236157234
H	-6.1612824236	-0.0209020649	0.2046426884
H	-5.7257045657	1.7156999717	0.1581399919
C	0.6984986365	0.7257834278	2.9279542405
H	0.4540724719	1.7659525826	3.1943340437
H	-0.0716879064	0.0699657548	3.3559990234
H	1.6735945169	0.4682838737	3.3858336805
C	1.7429693361	1.4742008479	0.9288052291
H	2.7543874172	1.2403650205	1.3093959726
H	1.7723722894	1.3904451981	-0.1644047939
H	1.4953973858	2.5127504554	1.1949536976
C	-0.2400100749	3.0290197768	-1.4967578899
H	-0.862613842	3.6353147716	-2.1748810747
H	0.7171413736	3.5478645439	-1.325606448
H	-0.040873976	2.0536233633	-1.9540526369
C	-1.2040141268	4.0097025688	0.4045369523
H	-1.7158301435	3.7492105097	1.3373884155
H	-0.2764664638	4.5611435495	0.6305045277
H	-1.8633276002	4.6516906571	-0.2022699051
C	1.2785038631	-0.3880530518	-2.3639602304
H	1.935724176	0.478969856	-2.1976241339
H	1.7974260094	-1.0253393834	-3.0956974876
H	0.3473933299	-0.0325257086	-2.8296580297
C	0.3713260536	-3.2130695607	-0.9655499884
H	1.1712027204	-3.964252717	-0.9413384952
H	-0.3544571702	-3.4653581654	-0.1752733017
H	-0.1584132396	-3.3115571386	-1.92543816

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Abbildung 10.47 Molekel Darstellung von **Int6**.Tabelle 10.527 Standardorientierung von **Int6** (R, R' = Me) [lokales Minimum; M06/6-31+G(d)].

	x	y	z
C	1.052702466	-0.6579051385	-1.5594000066
H	1.9433965061	-1.0983858368	-2.0427065176
H	1.3027281746	0.4026917165	-1.330430758
H	0.3057947558	-0.5630993608	-2.3678859424
Li	0.0365683315	1.7643717318	0.6865242263
C	1.5505518031	1.2607656233	2.0067109006
O	-1.5509509108	2.6316740028	1.4727837355
O	0.3577789052	2.8169731425	-0.9978505687
C	-1.9676753667	2.2539483195	2.7710924653
C	-2.6384761165	3.0298222107	0.6591460167
C	-0.2495668292	2.6615713821	-2.2662168901
C	1.6453557627	3.3946918267	-1.0957210738
H	1.5642880055	2.3328672284	2.30374457
H	2.5666040303	0.9206119221	2.2897992785
H	0.9076369328	0.7731766369	2.7695796564
H	-2.436277665	3.1078926876	3.2842343364
H	-2.687921644	1.4218641627	2.7199738406
H	-1.0770243821	1.940088255	3.3254037164
H	-2.2237889587	3.3687840865	-0.2960614821
H	-3.3301284449	2.1880226142	0.488215528
H	-3.1815144322	3.8636412079	1.1305878286
H	-0.3842934085	3.6429042027	-2.7478006333
H	0.3619708212	2.0114770444	-2.9115027669
H	-1.2279035143	2.191732054	-2.1153312302
H	1.5840510738	4.3883352157	-1.5663640185
H	2.0425324207	3.4873771029	-0.0797087166
H	2.3158703034	2.7461746848	-1.6848060149

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Li	2.223411705	0.0343941677	0.3438376144
N	2.6819333689	-1.8963801638	0.8031448803
C	1.298393681	-2.3587504851	1.0166770581
C	-1.3206200604	-3.1666757027	0.8014107912
C	3.4550262552	-1.9369065988	2.0386111185
C	3.3403507249	-2.7327610801	-0.1883783117
C	-0.3003948151	-3.1397668611	-1.8297861562
C	-1.2586630214	-0.4252359369	0.0624580553
C	-2.7299679323	-0.5101376881	-0.1465347299
C	-3.6313775225	-0.7312947383	0.9032609899
C	-3.2636339196	-0.3480226114	-1.4335137119
C	-5.0049033534	-0.7703535408	0.6821253586
C	-4.6360271057	-0.381018237	-1.6601467191
C	-5.517890816	-0.5876649309	-0.6006725469
Si	-0.1167330734	-2.0197979681	-0.2858202534
H	0.929361756	-1.8847214744	1.9428902813
H	1.3026343156	-3.4489752241	1.2295608526
H	-2.3158747593	-3.2618221099	0.3376131481
H	-1.4831448921	-2.7959626504	1.8291452381
H	-0.9176996181	-4.1889209704	0.893882876
H	4.4694238504	-1.5476863271	1.8580410156
H	2.9761596072	-1.3142065424	2.805017272
H	3.5413404749	-2.9687829221	2.4336023107
H	3.4505433662	-3.7729587966	0.1793562003
H	2.7533597818	-2.7618882059	-1.1122101921
H	4.3431246585	-2.3401034666	-0.4133878575
H	-0.2637339978	-4.1959732826	-1.5261313244
H	0.4316892264	-2.973319971	-2.6306158819
H	-1.3045091977	-2.9763257975	-2.254403653
H	-1.0382941621	-0.2076850045	1.1232245326
H	-0.8781267475	0.3945240834	-0.56499816
H	-3.2410527407	-0.8871005036	1.9110588889
H	-2.577832536	-0.1970759162	-2.2718235716
H	-5.6803330643	-0.945379133	1.519421464
H	-5.019882805	-0.2491851346	-2.6716508483
H	-6.592623012	-0.6142428549	-0.7742066025
O	3.9107617115	0.934212852	-0.388513228
C	4.5401422997	0.5701161236	-1.597376034
C	4.692854778	1.8270857974	0.3723793476
H	4.7495023182	1.4644165921	-2.2083699534
H	5.4876359569	0.0419235829	-1.4019778252
H	3.8554011865	-0.0869848149	-2.1439884927
H	4.1290066446	2.0737742103	1.2774946066
H	5.6541228807	1.3649405112	0.649991587
H	4.8933549847	2.7489589996	-0.1998629134

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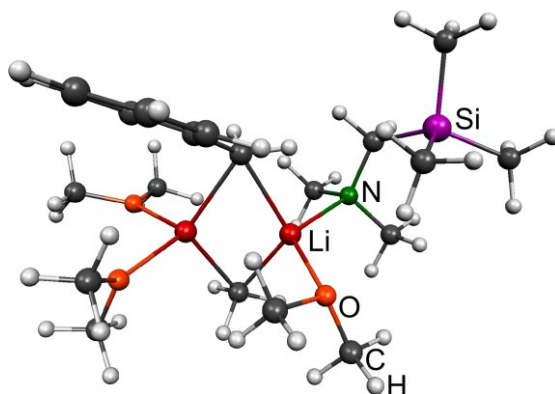


Abbildung 10.48 Molekel Darstellung von Pr2.

Tabelle 10.528 Standardorientierung von Pr2 (R, R' = Me) [globales Minimum; M06/6-31+G(d)].

	x	y	z
C	5.7270759627	0.5296369532	0.2201841352
Li	-1.6643339785	-1.0249236382	-0.1328795097
C	-0.6057191033	-2.8157968353	0.532459
H	6.2829413519	0.0381523978	-0.5909197537
H	5.715954668	-0.1535528812	1.0797074579
H	6.2984971128	1.4202800083	0.5179230341
H	-1.1511588447	-3.0005560072	1.4824443241
H	0.3708512977	-3.3203864286	0.7027228716
H	-1.1062135423	-3.4778465886	-0.2045965117
Li	0.6740942399	-1.1060373894	0.3582144533
N	2.5477800152	-1.5132538327	-0.6669288784
C	3.1642138511	-0.3605435137	-1.3362424235
H	2.3870937748	0.1221040797	-1.9513954862
H	3.9385687694	-0.7198092651	-2.05473114
O	-2.9620293235	-1.6427214746	-1.6273668068
O	-3.1795912771	-0.7116416458	1.1762022685
O	0.9392137517	-0.7155759975	2.3939717325
Si	4.0004656673	1.0386005979	-0.344359543
C	-0.2201079092	0.5928566103	-0.8074888194
H	0.7760677929	0.9379259836	-0.4840741899
H	-0.1428888836	0.2015152596	-1.8371197384
C	-1.2117220374	1.6443425435	-0.6984295892
C	-2.3718252471	1.6662580238	-1.5132675452
C	-1.1266021817	2.6853740058	0.2611416245
C	-3.3696841602	2.6192501505	-1.3624507361
H	-2.4654196342	0.905648509	-2.2932476837
C	-2.1219169496	3.6445616302	0.405156555
H	-0.2334615266	2.7476520916	0.8888798296
C	-3.2668698074	3.6212990879	-0.3942081395
H	-4.2401807807	2.5877845339	-2.0211445446
H	-1.9981327386	4.4306987937	1.1516250927
H	-4.0442095612	4.3752421545	-0.2819036556
C	-2.4088907707	-2.2804289583	-2.7550999936

H	-3.046096615	-3.1177201881	-3.0828937587
H	-2.2939555811	-1.5670843215	-3.5890126293
H	-1.4267220497	-2.6669525043	-2.4625475616
C	-4.2717238639	-1.1794801189	-1.8567037242
H	-4.5830366802	-0.6181469867	-0.9694407917
H	-4.3079650398	-0.5090247507	-2.732092365
H	-4.9567962401	-2.0264873125	-2.0266854945
C	-3.6917759416	0.4948139462	1.7033147399
H	-4.7456761836	0.6300812769	1.4066021146
H	-3.6290029653	0.4901415293	2.8048102225
H	-3.0940829941	1.3196330849	1.3011656233
C	-3.8422341697	-1.846756125	1.683258896
H	-4.9253688544	-1.7875601248	1.4801049009
H	-3.4218309524	-2.7293361396	1.1903487436
H	-3.6880461213	-1.9319799697	2.7725171268
C	2.0789083687	-2.4596037666	-1.6797350352
H	1.5589001	-3.3009162481	-1.2034650749
H	1.3739741174	-1.9561062921	-2.3532792924
H	2.9228289585	-2.8475082566	-2.2844558792
C	3.4960936727	-2.1829156639	0.2110898192
H	4.4199500404	-2.477220966	-0.3276734022
H	3.7776782278	-1.5245219059	1.0439039536
H	3.0388943851	-3.091114239	0.6265469458
C	1.1936068151	-1.8193868776	3.2353139376
H	1.4047832009	-1.4794180791	4.2621603864
H	0.3366359211	-2.5110360833	3.2429924284
H	2.0711380322	-2.3439936827	2.8430047356
C	-0.1684153169	0.0376892486	2.8477990892
H	-0.3213625775	0.8654258918	2.1452465767
H	-1.0779657822	-0.5876033663	2.8674422677
H	0.0274030087	0.4379393765	3.8556648311
C	4.1653881347	2.4197835517	-1.610293705
H	4.7119945636	2.0878870232	-2.5042293657
H	3.1729741115	2.7660536304	-1.9329692653
H	4.7016641359	3.2833528751	-1.1941169238
C	3.0033276684	1.6478763391	1.1254656783
H	3.6198649906	2.3233368074	1.7357622411
H	2.1243097599	2.2154307036	0.788856108
H	2.6460717177	0.8356257259	1.7731112113

Tabelle 10.529 Standardorientierung von **Ed2** ( $R, R' = \text{Me}$ ) [Konformer 1; globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	1.9699471838	0.0136132347	1.7863068671
Li	2.9503362493	-0.7168085121	-0.0395514694
C	2.2715080598	0.1596416151	-1.9179702838
H	0.9404774586	0.2265435415	2.1250456909
H	2.611801966	0.6082604897	2.4531963402
H	2.1390554676	-1.0317518701	2.0993098156

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H	3.1076714533	-0.4245977853	-2.3402660996
H	2.3370957363	1.1245238338	-2.4446009029
H	1.3620821859	-0.3224510638	-2.3182403052
Li	1.4632492365	1.0628082956	-0.0958420777
N	-0.5902218353	1.641301798	-0.4833571403
C	-1.5633525303	0.611961146	-0.877746108
H	-1.2401208147	0.2096671496	-1.8450575913
H	-2.5479169004	1.0844208099	-1.0578683822
O	2.9650398991	-2.6979862074	-0.3068116828
O	4.9357753213	-0.6948445438	0.3099991263
O	2.1513378742	3.0050212338	0.2039903224
Si	-1.8283375676	-0.9465499026	0.1945507441
C	-3.3129933448	-1.8053592062	-0.5990438609
H	-3.4822184314	-2.7784110245	-0.1304972278
H	-3.1535916096	-1.9692157388	-1.6685408659
C	2.5158565013	-3.3998207846	-1.4539579822
H	3.3333046335	-3.9982402427	-1.8725663471
H	1.6823713718	-4.0584368159	-1.1915096568
H	2.193207539	-2.6562639217	-2.1788083464
C	3.3899708886	-3.5729811037	0.7267258204
H	3.6962709011	-2.9539599924	1.566589604
H	2.5681219262	-4.2288119184	1.0282736055
H	4.2393067766	-4.1750066388	0.3846698952
C	5.4829443188	0.3686198149	1.0692822409
H	6.49311853	0.1120595947	1.40484384
H	5.522642884	1.2843928565	0.4695502818
H	4.8297829832	0.5182180597	1.9245950608
C	5.7085385707	-0.9771889282	-0.845277027
H	6.7282885443	-1.2544236382	-0.5588715269
H	5.2274204138	-1.8085935447	-1.3553865872
H	5.7345139031	-0.1075234446	-1.5092993437
C	-0.4407646335	2.5865703232	-1.594090523
H	0.2379398674	3.3870922586	-1.3003756175
H	-0.0269182256	2.0667890627	-2.4589768367
H	-1.4128269482	3.0256710773	-1.8702492974
C	-1.0678382346	2.368663818	0.6909473666
H	-2.0670626529	2.7995582396	0.5134040712
H	-1.1208804237	1.7030178311	1.5503652049
H	-0.3740008661	3.1789949447	0.9165635686
C	2.5325168027	3.3217863224	1.5340418733
H	3.5135445127	2.8949459814	1.7616859362
H	2.5630016148	4.4087608462	1.6645559137
H	1.7949318086	2.8818116304	2.200240552
C	3.0901994667	3.4962815413	-0.7390745372
H	2.7073072951	3.2727649569	-1.7310041481
H	3.2135746856	4.5777984369	-0.6188285382
H	4.0557846895	2.9983227346	-0.6092921978
C	-2.2213259759	-0.6487007048	2.0157637242
H	-3.0076764049	0.1017373642	2.1340235274
H	-1.3450808113	-0.3318066449	2.5849219414
C	-0.2998658513	-2.0481762833	0.0034708647

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H	-0.1762311218	-2.2494349506	-1.0654686822
H	0.570156533	-1.4711155363	0.3273255163
H	-4.2232837097	-1.2115303718	-0.4800221642
H	-2.5785700382	-1.5848301784	2.4537577314
C	-0.4071814558	-3.3280911015	0.7795277697
C	-0.9008242475	-4.4978244973	0.1889849854
C	-0.0333739731	-3.3781361775	2.1292190551
C	-1.0105579623	-5.6815594871	0.9163640262
H	-1.196636086	-4.4775719738	-0.855450049
C	-0.1439067388	-4.5587045171	2.8591301351
H	0.3586725408	-2.4823755973	2.5991554969
C	-0.6315240883	-5.7179801903	2.2565338797
H	-1.3905899495	-6.5748628651	0.43467255
H	0.1556969199	-4.573667502	3.9005339179
H	-0.7146125213	-6.6367260155	2.824118933

Tabelle 10.530 Standardorientierung von **TS17** (R, R' = Me) [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	-0.7079777183	0.2924902431	1.6960396889
Li	-0.5986188286	1.4524550803	-0.3696250765
C	-1.862400168	0.5297336773	-1.8567416917
H	-0.2613244961	-0.355695484	2.4571264738
H	-1.7953175542	0.173366439	1.7812519133
H	-0.4823467461	1.323308079	1.9980417176
H	-1.1590116188	1.115381882	-2.4750561211
H	-2.8380623288	1.0153349306	-2.0127544335
H	-1.924125087	-0.4280819322	-2.4051589963
Li	-1.801233812	-0.720993558	-0.1276234001
N	-1.4558576772	-2.7883792121	-0.2159387547
C	-0.1589829076	-3.1219371563	-0.8320018836
H	-0.2081416172	-2.8096237979	-1.8818244888
H	-0.0244352205	-4.2194474857	-0.8399206815
O	0.7647083549	2.7809914308	-0.8768802103
O	-1.8528358192	3.0708027818	0.2530815538
O	-3.7911112731	-0.8606181011	0.5170067557
Si	1.4301291102	-2.2810847714	-0.164666523
C	2.7819004316	-3.0114885843	-1.2793832841
H	3.737748406	-2.5277973141	-1.0586827842
H	2.5590893758	-2.8378082823	-2.3360159235
C	1.2860032619	3.097695443	-2.1558766525
H	1.0329658343	4.1311087893	-2.4206282893
H	2.37125119	2.9759753639	-2.1610649721
H	0.8344399207	2.4142318749	-2.8721317459
C	1.3892284906	3.5319418092	0.159002813
H	0.9128396754	3.249757466	1.0943969115
H	2.4548243246	3.2951474421	0.2019212163
H	1.2417894371	4.6031713384	-0.0185773482
C	-3.0509524233	2.7010971181	0.9171193362
H	-3.6274932661	3.5954109	1.1761428447
H	-3.647298867	2.0449822844	0.2752533023

H	-2.7724234877	2.1722857955	1.8246675895
C	-2.1368881725	3.9012536732	-0.8645722203
H	-2.651545418	4.8090383772	-0.5333871689
H	-1.1870186549	4.1624892472	-1.3219379464
H	-2.7579418269	3.36618252	-1.588571729
C	-2.5297764196	-3.4092472111	-0.9942602474
H	-3.4930903484	-3.1975062507	-0.5284918725
H	-2.5275882705	-3.0045780377	-2.0076112576
H	-2.3940453594	-4.5001883911	-1.0515321246
C	-1.5149280392	-3.2965437887	1.1538215229
H	-1.3187201112	-4.3799704169	1.1854425878
H	-0.776715631	-2.7903529555	1.7723434966
H	-2.5078281863	-3.1103244319	1.566691418
C	-4.3713822696	-0.8431117477	1.8102716758
H	-4.8824102385	0.109420949	1.9861990195
H	-5.0902854662	-1.6625353153	1.9151617767
H	-3.5701546604	-0.9638557873	2.5357716979
C	-4.7719385445	-0.709930835	-0.5000841453
H	-4.2588310124	-0.7448533353	-1.4570349538
H	-5.5084479842	-1.517810666	-0.4352127267
H	-5.2812584225	0.2534699425	-0.3964765078
C	1.8760353364	-2.8229135507	1.5987325641
H	1.7375599429	-3.9015712897	1.7202509075
H	1.2988730725	-2.3106131832	2.3709220395
C	1.2336197057	-0.4484210857	-0.3358868204
H	0.9943264442	-0.2485309628	-1.3898122865
H	0.1335561353	-0.0927727931	0.6096859086
H	2.9039166137	-4.0882545515	-1.1268586591
H	2.931302047	-2.5978399905	1.77677652
C	2.4552429697	0.2825303606	0.0708852583
C	3.3736723072	0.7996144985	-0.8667046379
C	2.7658542257	0.4944956169	1.4300520409
C	4.5156759243	1.4927747826	-0.4779426923
H	3.1823420736	0.6285194999	-1.9216971677
C	3.9111943561	1.1829054713	1.8233255503
H	2.0846182527	0.1196849734	2.1851852238
C	4.7962352595	1.6945791687	0.8749970008
H	5.1985952497	1.8663247929	-1.2338149646
H	4.1105349837	1.3243193938	2.8799216164
H	5.68768756	2.2280873805	1.1813337877

Tabelle 10.531 Standardorientierung von **TS18** (R, R' = Me) [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	-1.1573118721	0.5032929615	-1.7129391455
Li	-2.1724947306	-0.8237139272	0.1627628574
C	-3.0994850695	0.7356146797	1.3313099833
H	-2.2408380096	0.4550964555	-1.4918615959
H	-1.0699154611	0.0327316529	-2.6981600315
H	-0.9453518752	1.5687281429	-1.8946416558
H	-3.9473268713	1.2258125394	0.8211384847

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H	-2.7702438078	1.4607648171	2.095594476
H	-3.5618813285	-0.0732742644	1.9166106267
Li	-1.5531132447	1.5905191494	0.1369269768
N	0.3016200626	1.6748223713	0.9163998569
C	0.7701118436	0.2826328589	0.765178004
H	0.123869542	-0.353284643	1.3831862855
H	1.7774551214	0.212549559	1.1972889642
O	-1.8152198966	-2.2849918989	1.4831583183
O	-3.6135370212	-1.8633329488	-0.7941302843
O	-2.281854787	3.3856917782	-0.3429262306
Si	0.8386380101	-0.5640421848	-0.9751744251
C	2.4974876561	-1.64598938	-0.4732290572
H	2.6387743566	-2.3464794247	-1.3050602065
H	2.2088966704	-2.2480368743	0.3987522154
C	3.7804313511	-0.9420475617	-0.1885987313
C	4.1743308157	-0.6185634465	1.1206523855
C	4.6531641044	-0.5609123037	-1.2221772582
C	5.3529823	0.07575893	1.3832986618
H	3.5515674029	-0.9379552996	1.950376696
C	5.8327602036	0.1312791252	-0.9668258703
H	4.3988487177	-0.821509318	-2.2438326635
C	6.1895228484	0.4643965595	0.3395562089
H	5.6226687914	0.3033796649	2.4085485285
H	6.4800456894	0.4063744235	-1.7918892281
H	7.1083649252	1.0018018792	0.5400185109
C	1.6547865192	0.3241522863	-2.4533902954
H	2.5758938945	0.8137374274	-2.1298827902
H	1.9411819624	-0.4440422563	-3.1808657927
H	1.0274408694	1.0545615354	-2.9630928712
C	-0.0851730334	-2.2075489031	-1.3740828591
H	0.1687626753	-2.4291290689	-2.4182969093
H	0.2832536622	-3.0422673994	-0.7740194704
H	-1.1740292686	-2.1844621143	-1.3212682903
C	-2.6043445491	4.2052105531	0.7716879505
H	-3.5338676211	3.8662902746	1.2375996716
H	-1.7887622829	4.118408189	1.4859372017
H	-2.7036731259	5.2473280726	0.4537105581
C	-3.2967042084	3.4403648113	-1.3369724968
H	-4.2453334457	3.0787543495	-0.9282939832
H	-3.4157195675	4.4687376482	-1.6907906208
H	-2.9808256729	2.8006668074	-2.157249896
C	-3.9671379901	-1.6290503821	-2.1512437079
H	-4.5729646615	-2.459296034	-2.5256429415
H	-4.5280630978	-0.6938098629	-2.2412059547
H	-3.0451882173	-1.5560904219	-2.7221160499
C	-4.764867029	-2.0177524168	0.0274602945
H	-4.4149952146	-2.2259385754	1.0354795955
H	-5.3549027879	-1.0972636683	0.0312131162
H	-5.3729613275	-2.8504595892	-0.3387334762
C	-1.765098614	-3.6813295841	1.2288504109
H	-2.0610244053	-3.8335118769	0.1946021153

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H	-0.7507969945	-4.0599220219	1.3844258436
H	-2.4568247136	-4.2062621073	1.8959177962
C	-1.497246251	-1.9788244965	2.8344060923
H	-1.6136982995	-0.904551749	2.9536227222
H	-2.1840089155	-2.5008632122	3.5080755525
H	-0.468200876	-2.2770806137	3.0574037531
C	1.1723486716	2.5773324069	0.1612581144
H	2.2238361869	2.4633790402	0.4657999612
H	1.0928163714	2.3606165871	-0.9021283246
H	0.8610182593	3.6104652187	0.3303023578
C	0.3497018357	2.0369185381	2.3330883423
H	0.0364921918	3.0747091617	2.4671515514
H	-0.3269431099	1.3931947851	2.8966056916
H	1.3672287435	1.9269545887	2.7376853802

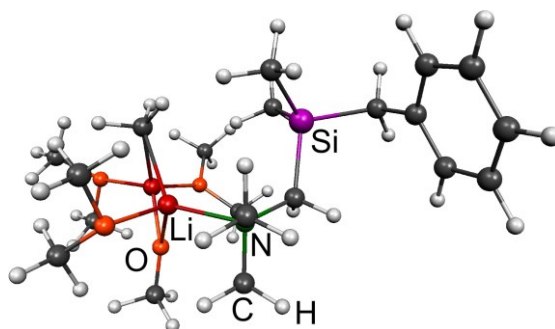
Tabelle 10.532 Standardorientierung von **TS19** (R, R' = Me) [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	1.1065664314	-0.4744267979	-1.6939303734
H	1.8461783	-1.0025935685	-2.3128312445
H	1.4415537593	0.5814357003	-1.6736339678
H	0.189791654	-0.4525459665	-2.2966762553
Li	0.1378628555	1.8099704455	0.6675569685
C	1.6620087686	1.1765547913	1.9309392075
O	-1.3408816517	2.6396989301	1.6429771954
O	0.2093110731	2.8919865771	-0.964949369
C	-1.6623991675	2.1763812736	2.9492733245
C	-2.495100757	3.1012385891	0.9485094257
C	-0.5165253161	2.7090746935	-2.1769211304
C	1.4774816105	3.4985223322	-1.194993362
H	1.7106654095	2.2068084045	2.3275768959
H	2.6871663678	0.8005058882	2.0572266532
H	1.0745767183	0.612610754	2.673146766
H	-2.0878040076	2.994428361	3.5373986982
H	-2.3818831726	1.354336199	2.8928039643
H	-0.738267483	1.83390543	3.4076873093
H	-2.1521479641	3.5370178952	0.0137211543
H	-3.1783056135	2.2704019274	0.7505756246
H	-3.002088943	3.8673403992	1.5422143224
H	-0.7184890442	3.681796128	-2.635622708
H	0.0507360753	2.0772684716	-2.8639983993
H	-1.4552907659	2.2180041435	-1.9268426
H	1.3398241777	4.47895523	-1.6602830534
H	1.9604160208	3.6101325601	-0.2267757333
H	2.0902956358	2.8584133638	-1.8348376264
Li	2.1654091486	-0.0102801495	0.1300622904
N	2.6639773308	-1.915385591	0.7173102682
C	1.2894480934	-2.2807966153	1.0854292342
C	-1.3715463047	-3.1354315975	0.9773571273
C	3.5470677817	-2.0147262512	1.8773777983
C	3.1386640301	-2.8260120322	-0.3200909188

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C	-0.3758141407	-3.0377299271	-1.7135346148
C	-1.2479106235	-0.3812365198	0.1379501345
C	-2.712763326	-0.4835913093	-0.1635526673
C	-3.6670615526	-0.6934630479	0.8393553271
C	-3.1684228529	-0.3703567527	-1.4842284707
C	-5.0242677967	-0.7782179769	0.538736435
C	-4.5245824655	-0.4519458034	-1.7903151178
C	-5.4619624738	-0.6536659014	-0.7786630639
Si	-0.2033881459	-2.0098590485	-0.1205720631
H	1.0174654615	-1.7162285949	1.9848979798
H	1.2589664688	-3.3460874363	1.3748871842
H	-2.3727556508	-3.2186732267	0.5430974137
H	-1.4926640405	-2.7565076116	2.0003688752
H	-0.967481579	-4.1509791989	1.0557118416
H	4.5594386327	-1.713469633	1.5940679572
H	3.1935990832	-1.353516918	2.6684300415
H	3.5828474452	-3.0438486605	2.2681815702
H	3.1513764261	-3.864454253	0.048825041
H	2.4805939521	-2.767867474	-1.1841985598
H	4.1527643683	-2.5543024306	-0.6209597865
H	-0.3090930609	-4.0979428448	-1.4521131792
H	0.3436185268	-2.8114723924	-2.4983751434
H	-1.3834837653	-2.8739537834	-2.112065659
H	-1.0962583611	-0.1315987522	1.1947529831
H	-0.8117921251	0.3946690916	-0.4912168622
H	-3.3358818034	-0.8071581431	1.8661962472
H	-2.4427101909	-0.2271981689	-2.2793920142
H	-5.7405357261	-0.9448038218	1.3348173462
H	-4.8487003799	-0.3625907974	-2.8206253402
H	-6.5170694688	-0.7188212298	-1.0141550425
O	3.8512115405	0.9364706936	-0.5525039909
C	4.64519531	0.2923731127	-1.535214178
C	4.6083141147	1.8486506846	0.2246319267
H	5.0935259758	1.0338430416	-2.2046319691
H	5.440210225	-0.292627454	-1.0602312019
H	3.9889530294	-0.3624940016	-2.102137258
H	3.9261022911	2.3176463457	0.9282309831
H	5.3967054192	1.3223482186	0.7733497771
H	5.0634402079	2.6065450067	-0.4222383683

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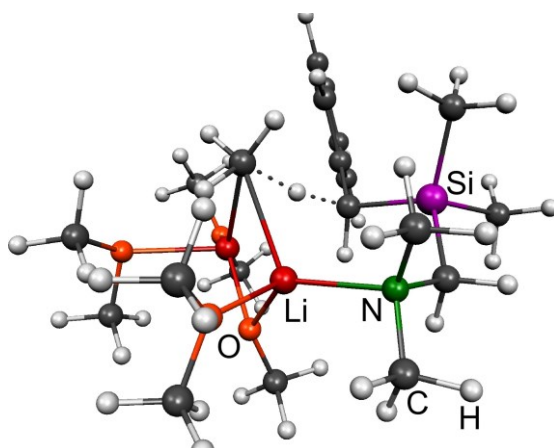
Abbildung 10.49 Molekel Darstellung von **Ed2** (R = Me; R' = OMe; Konformer 1).Tabelle 10.533 Standardorientierung von **Ed2** (R = Me; R' = OMe) [Konformer 1; globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-1.0578090715	0.4331877631	1.7054454203
Li	-1.1835721119	1.5900623864	-0.1545146686
H	-0.615759504	-0.5154333042	2.058066438
H	-1.857432117	0.657042322	2.4274567798
H	-0.2742229857	1.1832286217	1.9173048
Li	-1.8863005582	-0.6628198124	-0.0340300955
N	-1.3231425264	-2.7173539663	-0.445963866
C	-0.008481488	-3.0125463898	-1.0340454084
H	0.0028595388	-2.5810930048	-2.0423520835
H	0.1017266626	-4.1053203416	-1.1695836884
O	0.4092493424	2.6121822658	-0.772062364
O	-2.2294853353	3.2728759467	0.2071017719
O	-3.8395045206	-1.0886363617	0.4964386882
Si	1.5801297145	-2.317146953	-0.2339826779
C	2.9873674054	-3.1092475648	-1.2154137211
H	3.9468977332	-2.6821569115	-0.9122268797
H	2.8678967616	-2.9402594567	-2.2893420992
C	0.9270388191	2.5402710707	-2.0874707255
H	0.8314440339	3.5120216536	-2.5860866442
H	1.9814534927	2.2471929513	-2.0643173155
H	0.3424116494	1.7928903	-2.6185288919
C	1.1061245078	3.5457338269	0.0360091266
H	0.656076528	3.5128502302	1.0256121863
H	2.1636170009	3.2730597364	0.1022927045
H	1.0050850124	4.5544282324	-0.3793255134
C	-3.2058607214	3.252752759	1.2323986455
H	-3.6193756269	4.2560505625	1.3800003518
H	-4.0149271013	2.5606418463	0.9773485531
H	-2.7125569349	2.9130323451	2.1395760398
C	-2.7739566006	3.6611373792	-1.0447059983
H	-3.2153648087	4.660616591	-0.9711801489
H	-1.9531611974	3.6696528047	-1.7591603747
H	-3.5263220741	2.9380296156	-1.3733394419
C	-2.36135677	-3.1298406522	-1.3945488302
H	-3.3432031757	-2.9789946191	-0.9471334726

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H	-2.2859259753	-2.5253185677	-2.2996896667
H	-2.2494435769	-4.1922909558	-1.6643182757
C	-1.5019708724	-3.4586293345	0.8006627217
H	-1.3757193151	-4.5424400054	0.6420603493
H	-0.7784892538	-3.1264004191	1.5426885672
H	-2.5064100024	-3.2760628039	1.1841225491
C	-4.227160327	-0.8509192868	1.8397869892
H	-4.2745405468	0.2230283517	2.0398337345
H	-5.2031200454	-1.3081418341	2.0349068685
H	-3.4697470191	-1.2937554052	2.482344623
C	-4.7351469429	-0.486883899	-0.425755355
H	-4.3819086161	-0.724840309	-1.4253087428
H	-5.7470762029	-0.87846774	-0.2750244157
H	-4.7325719151	0.5997173739	-0.3044212729
C	1.831865352	-2.7082548732	1.5940650549
H	1.6802131371	-3.7716216263	1.7983264587
H	1.1664301802	-2.128688625	2.2371330878
C	1.5774711085	-0.4484386886	-0.5305117491
H	1.4874399959	-0.2883105944	-1.6099821632
H	0.6736547025	-0.0444168376	-0.066391309
H	3.0304362282	-4.1884543392	-1.0456731932
H	2.8595159241	-2.4542441625	1.8684026536
C	2.7969432504	0.235514664	0.012925184
C	3.923740947	0.4620997595	-0.7867826176
C	2.8432084101	0.6512790441	1.3503718449
C	5.0565542668	1.0919043144	-0.2742151277
H	3.9066760305	0.1450171672	-1.8251029549
C	3.9747542135	1.2771030076	1.8664601062
H	1.9742311233	0.4917582058	1.9798424823
C	5.0872810982	1.5037506198	1.0564498975
H	5.9136375379	1.261364043	-0.9154717024
H	3.9850216215	1.5938336195	2.9028485895
H	5.9658312839	1.9943348959	1.4572582173
O	-1.9043979273	0.5130627103	-1.4400820338
C	-2.0436727258	0.4501142632	-2.8099772983
H	-1.2235021134	-0.109944455	-3.2987078329
H	-2.9804453962	-0.0476857584	-3.1247614479
H	-2.0618240306	1.4486029583	-3.2850476467

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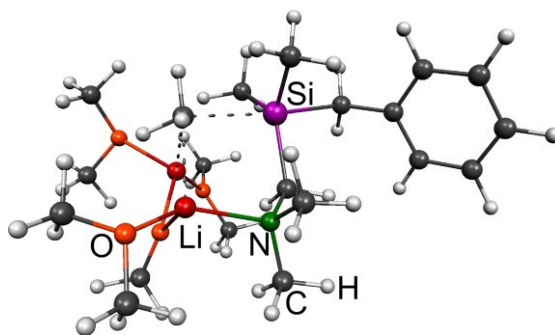
Abbildung 10.50 Molekel Darstellung von **TS17** (R = Me; R' = OMe).Tabelle 10.534 Standardorientierung von **TS17** (R = Me; R' = OMe) [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	-0.6164748151	0.4225855705	1.7044723538
Li	-0.1138391353	1.6055958606	-0.2622698819
H	-0.6146773353	-0.4420783781	2.3775596396
H	-1.6213069954	0.862652643	1.7414043988
H	0.0652073484	1.1593158587	2.147401918
Li	-1.9360627053	-0.117425769	-0.1339723813
N	-2.2866290279	-2.1405507041	-0.4272964579
C	-1.146585889	-2.8035748186	-1.0866667953
H	-1.0497491254	-2.3643829174	-2.0868493989
H	-1.3769324254	-3.8740373901	-1.2387135167
O	1.5552928419	2.4636622392	-0.7907684072
O	-0.8204164633	3.479770871	0.4287388695
O	-3.7726424196	0.5416766578	0.4816743756
Si	0.6047051629	-2.5973671847	-0.3264823114
C	1.6803357335	-3.6624115532	-1.4724087724
H	2.734069585	-3.5299150037	-1.2108928588
H	1.5590842991	-3.3630392951	-2.5175098858
C	2.0955717162	2.6217278809	-2.0897281193
H	2.1464870017	3.6853172929	-2.3497712106
H	3.0962100337	2.1860457542	-2.1397460656
H	1.433894232	2.1041348728	-2.7822369573
C	2.4101863821	2.9792979145	0.2227115423
H	1.8965026409	2.8511659954	1.1723012034
H	3.3511280853	2.4241225393	0.2355472801
H	2.5937798959	4.0447292639	0.0481649164
C	-1.8416227012	3.592164449	1.4048018156
H	-2.0929540269	4.6459445032	1.5662160215
H	-2.7344190341	3.0450741174	1.0840142267
H	-1.4636564047	3.1605756959	2.3280923251
C	-1.2044993045	4.1205794623	-0.7808324463
H	-1.3866805302	5.1846158778	-0.5960624945
H	-0.3813973414	4.0044661429	-1.4819903941

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H	-2.0965186982	3.6419731914	-1.1928921307
C	-3.4582336158	-2.1931192484	-1.3040681704
H	-4.3130462909	-1.7328540107	-0.8049455304
H	-3.2504385464	-1.6427069395	-2.2232071826
H	-3.7134803892	-3.2321365912	-1.5633122676
C	-2.6050286462	-2.8123053858	0.830728781
H	-2.8167124958	-3.8810741194	0.6680600132
H	-1.7705271254	-2.7248959345	1.5231254601
H	-3.4854559966	-2.3494221025	1.2795526637
C	-4.5189499112	0.3382146468	1.6667299063
H	-4.8724471865	1.2961132758	2.0624475611
H	-5.3807576635	-0.3107115697	1.4745833898
H	-3.8581413352	-0.1300758496	2.3936331619
C	-4.5116455531	1.2261108897	-0.5212530869
H	-3.8193658029	1.3992398423	-1.3417680022
H	-5.3652919357	0.6207831074	-0.8446452339
H	-4.8766666882	2.1823088473	-0.1311311813
C	0.7789760187	-3.3623045041	1.4011859011
H	0.3141707824	-4.3519838519	1.4430764459
H	0.3520764041	-2.7422274846	2.192186521
C	1.0226579068	-0.7964269425	-0.3623579944
H	0.8738253812	-0.449314364	-1.3945533004
H	0.0794048217	-0.1570408899	0.6006058067
H	1.4416918991	-4.7272959168	-1.3908156722
H	1.8436689808	-3.4828961921	1.6207215354
C	2.4013182378	-0.5088601371	0.0897956189
C	3.4505516468	-0.2323595197	-0.8118510193
C	2.7348971618	-0.4912528749	1.4598330391
C	4.7402139565	0.0579858199	-0.3784433128
H	3.2367425866	-0.2691391173	-1.8756866092
C	4.0262953425	-0.2058895044	1.8973238362
H	1.9568862399	-0.6938882643	2.1874902168
C	5.0419309673	0.0777821282	0.9847822272
H	5.5181760388	0.2579302672	-1.1079181093
H	4.2389999622	-0.2007070488	2.9607610271
H	6.0459734127	0.2988555571	1.3256941298
O	-1.4860890676	1.1110837813	-1.38359274
C	-1.4285477302	1.0425273009	-2.7660000655
H	-0.65984257	0.3369829849	-3.1286467804
H	-2.384671326	0.7140615579	-3.2126384686
H	-1.1991320019	2.021467756	-3.2240081154

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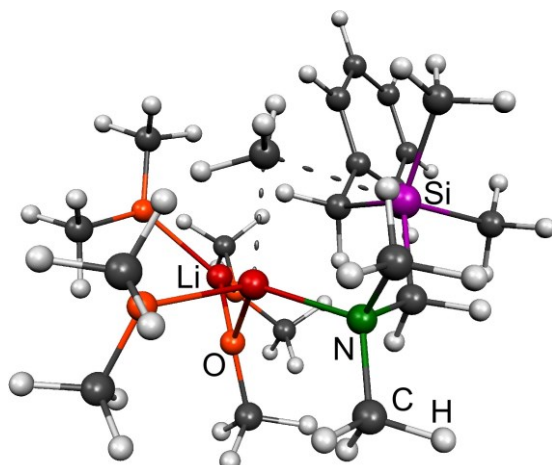
Abbildung 10.51 Molekel Darstellung von **TS18** (R = Me; R' = OMe).Tabelle 10.535 Standardorientierung von **TS18** (R = Me; R' = OMe) [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	-1.1692308241	0.4634727844	-1.7151786638
Li	-2.1550231381	-0.8352025501	0.1058914643
H	-2.255216018	0.4353110937	-1.5086549133
H	-1.0707218367	-0.0532493827	-2.6757044367
H	-0.9514788248	1.519441874	-1.9449147807
Li	-1.4968692657	1.6317255412	0.0869090733
N	0.3503255639	1.7197140587	0.8716177141
C	0.7475590056	0.3013343422	0.7862983379
H	0.023966475	-0.2747844802	1.3750562912
H	1.7189656586	0.1862309426	1.2858359755
O	-2.0196565968	-2.3001051951	1.4569800034
O	-3.6741470391	-1.7406098997	-0.8845151333
O	-2.3652778227	3.3745854042	-0.4032749923
Si	0.8561982546	-0.5937884946	-0.9263105271
C	2.5249003297	-1.6386239964	-0.3979122301
H	2.6812944381	-2.363557159	-1.2056309113
H	2.2515078823	-2.2162701382	0.4944908691
C	3.792234467	-0.8961498295	-0.1390756702
C	4.1772611989	-0.5151375917	1.1571413585
C	4.657518072	-0.5349121222	-1.1859636803
C	5.3378930658	0.2181318995	1.3932791668
H	3.5630514994	-0.8189340191	1.998757871
C	5.8191957165	0.19584686	-0.957056063
H	4.4121307873	-0.8422459023	-2.1967767217
C	6.1653284443	0.5881473248	0.3356101755
H	5.6009702029	0.4906964159	2.4092189359
H	6.4607561352	0.4546395967	-1.7917883861
H	7.0698967173	1.1561553695	0.5155480779
C	1.6415644102	0.2316306774	-2.4553604934
H	2.57882605	0.7171338739	-2.1768564351
H	1.8937518173	-0.5674990298	-3.1622685408
H	1.0100673861	0.9528786665	-2.971635076
C	-0.0656778353	-2.2594571734	-1.2219458218
H	0.3097146463	-2.634548437	-2.1817540063
H	0.204567013	-3.0023877992	-0.4676838417

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H	-1.1523396822	-2.2196639791	-1.3080910721
C	-2.5444231432	4.1758596191	0.7547675025
H	-3.1424743838	3.6443402374	1.5010382293
H	-1.5561800145	4.3870908251	1.1569630792
H	-3.0360869002	5.1167119277	0.4893489189
C	-3.6048235742	3.1037091754	-1.0465565777
H	-4.2473942201	2.5087639156	-0.3903147391
H	-4.1010125193	4.0429169488	-1.3095183313
H	-3.3791249944	2.5403797714	-1.9489758441
C	-3.9344031448	-1.6155702361	-2.2755359225
H	-4.6750566041	-2.3596026797	-2.5835347802
H	-4.3026383846	-0.6115552094	-2.5070044206
H	-2.9974848105	-1.7841222247	-2.8003778925
C	-4.8433308917	-1.5138371545	-0.1070098502
H	-4.5731738289	-1.678752616	0.9329394614
H	-5.1869638069	-0.4828446243	-0.2322779371
H	-5.6318968334	-2.2110285759	-0.4069295265
C	-2.1183047223	-3.6942327988	1.21043
H	-2.4609357724	-3.8169659417	0.1864908429
H	-1.1433730395	-4.1741943154	1.3364963541
H	-2.8379437747	-4.1455655355	1.9012934601
C	-1.5723314709	-2.020977208	2.7759052283
H	-1.5786768155	-0.9400302134	2.8897653119
H	-2.2490427781	-2.4762430313	3.5060259785
H	-0.5601416672	-2.4113302135	2.9225744152
C	1.3139185926	2.5544580307	0.1548809349
H	2.3383764213	2.3915461226	0.5227234609
H	1.2835710507	2.3179427243	-0.9072288503
H	1.0521996706	3.6070964388	0.284117372
C	0.3080834538	2.1132660351	2.2794501881
H	0.0516096981	3.1713706157	2.3669839188
H	-0.4540598681	1.5246769523	2.7930840881
H	1.2797145614	1.9506375275	2.7706207018
O	-2.642317846	0.6213132678	1.0729282022
C	-3.5039786839	0.8306901741	2.1338408424
H	-3.0489842441	1.4373570375	2.9369411412
H	-4.427736131	1.3572269423	1.8324012857
H	-3.8323933038	-0.1110724772	2.6078822368

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Abbildung 10.52 Molekel Darstellung von **TS19** (R = Me; R' = OMe).Tabelle 10.536 Standardorientierung von **TS19** (R = Me; R' = OMe) [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	1.1912501417	-0.4021272867	-1.735554476
H	1.9348562907	-0.9226853245	-2.3582082481
H	1.5115617725	0.6579941721	-1.7286975857
H	0.2631515546	-0.4069264395	-2.3222143628
Li	0.0874613249	1.8984258135	0.7488009097
O	-1.430611246	2.6053693066	1.740946697
O	0.2067582276	2.9686395079	-0.8642400665
C	-1.8189601946	1.9765199224	2.9563217022
C	-2.5417221902	3.188049092	1.067819762
C	-0.5437420365	2.8224676388	-2.0655282131
C	1.5054384233	3.504413779	-1.1082284423
H	-2.1896327349	2.7269216379	3.660295979
H	-2.5994300231	1.2353347643	2.7651615137
H	-0.9371137324	1.4901411908	3.3670865553
H	-2.1472905943	3.7326397692	0.2136183688
H	-3.2326302407	2.4081856339	0.7343028874
H	-3.0580742482	3.8826361624	1.7366055667
H	-0.6893288862	3.8015186475	-2.5323221313
H	-0.0248551455	2.149700796	-2.7523643278
H	-1.5086881334	2.394522034	-1.7989756614
H	1.4155878368	4.5133749805	-1.5213422636
H	2.0241331746	3.5304484638	-0.1529126855
H	2.0544906292	2.8597512593	-1.7983097965
Li	2.1803930593	-0.0023544586	0.1311022341
N	2.6814285853	-1.9042143865	0.708016937
C	1.310037712	-2.241824688	1.1032214087
C	-1.3625984782	-3.1186479044	0.9930025976
C	3.5813638772	-1.9862841366	1.8537923912
C	3.128795857	-2.8291649504	-0.3268773684
C	-0.3383224272	-2.9994140646	-1.7066833724
C	-1.1921289232	-0.3548071208	0.1350119716

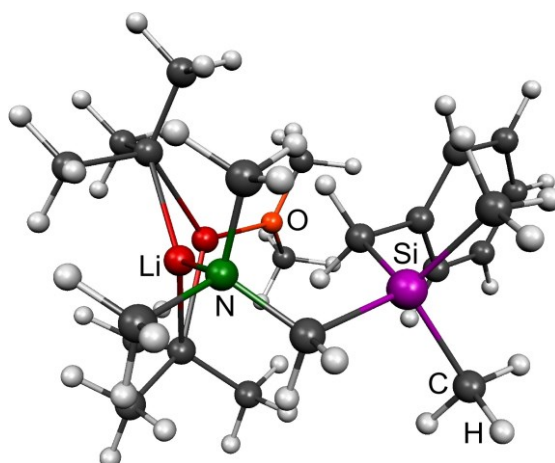
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C	-2.643554217	-0.4157283379	-0.234204777
C	-3.6440930617	-0.6670674328	0.7130288635
C	-3.0400091154	-0.2234833462	-1.5651432619
C	-4.988397192	-0.7098738825	0.3509170042
C	-4.3826981296	-0.2642340633	-1.9325349679
C	-5.3665811715	-0.5032227817	-0.974463704
Si	-0.1908077904	-2.0047691375	-0.09568185
H	1.0492247052	-1.6347169829	1.9787585555
H	1.2714932633	-3.2943300232	1.4375370029
H	-2.3668285069	-3.1869685598	0.5639995322
H	-1.4696962837	-2.7433734776	2.0186553381
H	-0.9683890354	-4.1384720616	1.0616375786
H	4.5942629089	-1.7154728637	1.5436203099
H	3.2558489156	-1.2912838985	2.6278772156
H	3.6050994815	-3.0023504685	2.2797356013
H	3.1277243751	-3.8665983848	0.0466257832
H	2.464272254	-2.758546601	-1.1848901337
H	4.1435370357	-2.5753316124	-0.6407410718
H	-0.270841163	-4.0647868294	-1.4667266048
H	0.3923192344	-2.7511739441	-2.473521063
H	-1.3401956039	-2.8285804089	-2.116404723
H	-1.0770105901	-0.1238038256	1.2001293506
H	-0.6957869955	0.4056782706	-0.4657044587
H	-3.3599759305	-0.8490060747	1.7440300407
H	-2.277991452	-0.0507545927	-2.319065
H	-5.7408684655	-0.9091321024	1.1050287745
H	-4.6600030476	-0.1134868959	-2.9693255826
H	-6.4113719594	-0.5357270628	-1.2578462885
O	3.8905758451	0.9233241352	-0.4542893231
C	4.7789618586	0.3154358141	-1.3731635318
C	4.5608900687	1.7172003548	0.508077892
H	5.3414511618	1.0791076031	-1.9208034253
H	5.4820317507	-0.3424501087	-0.8498617251
H	4.1747977716	-0.264770697	-2.0665679683
H	3.7912316941	2.138087779	1.1498040052
H	5.2469379951	1.1027066813	1.1021375846
H	5.128320076	2.5137968001	0.0139435992
O	1.5379884771	1.160983482	1.4588908743
C	1.8450112101	1.1609422936	2.8141106158
H	1.5063015756	2.0796075148	3.3226755691
H	1.3851352742	0.3136603343	3.3536198852
H	2.9299039267	1.0899998542	3.0015891238

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10.2.2.3. Dimeres *tert*-ButyllithiummodellTabelle 10.537 Berechnete Energien der optimierten Strukturen des dimeren Substitutionsmodells mit *tert*-Butyllithium.

Verbindung	SCF [Hartree]	ZPE [Hartree]
<b>Ed3-1</b>	-1299.831151	-1299.189507
<b>Ed3-2</b>	-1299.826658	-1299.1855
<b>TS20</b>	-1299.795549	-1299.157653
<b>TS21</b>	-1299.776773	-1299.131656
<b>TS22</b>	-1299.775493	-1299.132277
<b>Int7</b>	-1299.776284	-1299.133833
<b>Pr3</b>	-1299.850377	-1299.209242

Abbildung 10.53 Molekel Darstellung von **Ed3** (Konformer 1).Tabelle 10.538 Standardorientierung von **Ed3** [Konformer 1; lokales Minimum; M05-2X/6-31+G(d)].

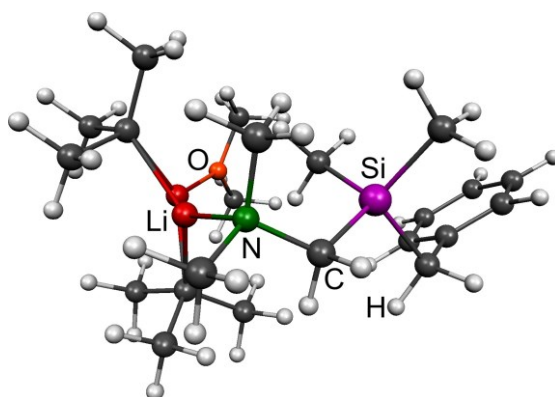
	x	y	z
C	-1.3640729887	2.1420875406	-1.2622559606
Li	0.067067246	2.112166227	0.3705276086
Li	-1.8417537118	0.8792218338	0.4948623328
O	1.9954357221	2.0857760804	0.0724974536
C	2.7794108454	2.7569772433	-0.9047137647
C	2.8139470399	1.4984164333	1.0818202008
C	-2.8636853382	2.0602953122	-1.5684660804
C	-0.63735485	1.6644294576	-2.5200686565
C	-1.0625370917	3.6402964003	-1.0951491257
H	3.3664653838	3.5510336236	-0.4337322741
H	3.4489332462	2.0441990036	-1.3942769925
H	2.1012321322	3.187583001	-1.6369167857
H	2.1561505465	0.9532424498	1.7541433955
H	3.5283918225	0.8074380882	0.6278050138

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H	3.3428141281	2.2816427724	1.6332102705
H	-3.1675046771	1.048809701	-1.8626060282
H	-3.4967119671	2.3648431733	-0.722296543
H	-3.1454346635	2.7203074396	-2.4138844408
H	0.4553017077	1.7139420955	-2.4250509178
H	-0.884653473	0.6227802663	-2.7623949695
H	-0.9061557625	2.2686950603	-3.4105081869
H	-1.6573751925	4.0906648557	-0.2920629833
H	-0.0066038376	3.8699319401	-0.8746443313
H	-1.2935356567	4.2066749934	-2.0188650206
C	-0.8894593422	1.7502569576	2.2834341568
C	-0.4585204643	0.7882753289	3.3886762414
C	-0.1786681297	3.0854907504	2.5569410783
C	-2.3856948175	2.0348567612	2.480082057
H	-0.9743959732	-0.1763787784	3.3303696855
H	0.61695499	0.5746187973	3.3603379249
H	-0.6695509798	1.1975373435	4.3981484641
H	0.9152988713	2.997672091	2.5315715009
H	-0.4610846394	3.8763110415	1.8472943786
H	-0.429860794	3.4800752201	3.5613757139
H	-2.7705109229	2.7697172327	1.7587403953
H	-3.0101004384	1.1319792587	2.3957906663
H	-2.6015341336	2.4456669829	3.4858457544
N	-2.8874672537	-0.9874115249	0.434999423
C	-2.4689864644	-1.7685888953	-0.7444768581
Si	-0.6553725925	-2.3764390718	-0.8231893077
C	0.4890148044	-1.0040219154	-0.1848838338
C	-4.3237641042	-0.6950336094	0.3304544227
C	-2.6692633022	-1.7669014205	1.6559744221
C	-0.3066889938	-2.7121073254	-2.644314109
C	-0.3859245937	-3.9813326471	0.1353127615
H	-2.6242756597	-1.146229965	-1.6316149671
H	-3.1290570598	-2.6479883145	-0.8597884421
H	0.2824571953	-0.8014151073	0.8720705109
H	-4.6406511892	-0.0815126458	1.1755752414
H	-4.5251086321	-0.1521758667	-0.5913877627
H	-4.910881669	-1.6252498136	0.3282463572
H	-3.1628537277	-2.7485785632	1.5899390688
H	-1.6039018124	-1.9180118971	1.8231286286
H	-3.073039624	-1.2279963018	2.5133971913
H	-0.3978936582	-1.8014957471	-3.2416318709
H	0.7059473733	-3.1015993941	-2.7738547316
H	-1.0064329512	-3.4516163441	-3.0435269303
H	-0.4532220397	-3.8547953328	1.2175411729
H	-1.1219948438	-4.7325802874	-0.1642276012
H	0.6069982593	-4.3771078169	-0.0941316237
H	0.2343356535	-0.095238349	-0.7401767191
C	1.9369742242	-1.3487920371	-0.3845665695
C	2.650429886	-2.0642232697	0.5838374105
C	2.607313843	-0.9652377807	-1.5521316726
C	3.9959701232	-2.3743203201	0.4000114311

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H	2.1471324434	-2.3638012026	1.4977464485
C	3.9523195893	-1.2751389833	-1.7403861203
H	2.0667780446	-0.4077532296	-2.3105034683
C	4.654857097	-1.9787199612	-0.7629060865
H	4.5307467622	-2.9209648968	1.1675710886
H	4.4526206031	-0.9645937885	-2.6502393878
H	5.7015999832	-2.2164866239	-0.9060993482

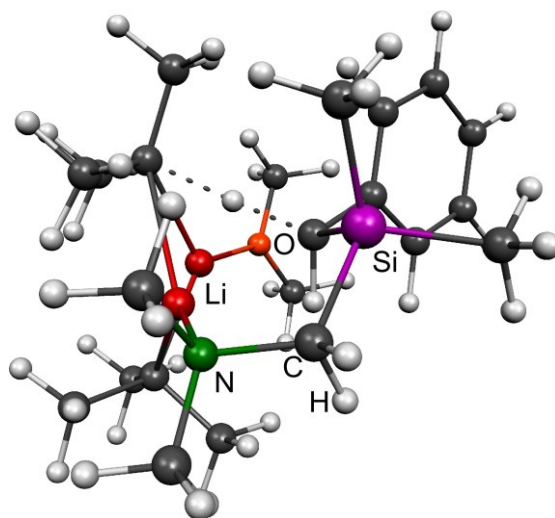
Abbildung 10.54 Molekel Darstellung von **Ed3** (Konformer 2).Tabelle 10.539 Standardorientierung von **Ed3** [Konformer 2; lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	1.7987938624	0.6427573585	2.0587451551
Li	1.9761018251	1.6184575368	0.1373218727
Li	2.1624285245	-0.6363884355	0.2798239991
O	0.7958682049	3.0854605323	-0.3849733922
C	0.1143803772	4.062715857	0.3887106853
C	0.3812877728	3.1085527152	-1.7470992109
C	2.3410804042	-0.5148055099	2.9039610935
C	0.39805101	0.9489161847	2.590144175
C	2.6941486892	1.8462068368	2.3976596734
H	0.277571033	5.056586419	-0.0375318556
H	-0.95756573	3.8425824188	0.4096451549
H	0.5149051922	4.0257436436	1.3982911946
H	0.9021737325	2.3022297615	-2.2571840118
H	-0.6984964086	2.9488591441	-1.8121356171
H	0.6437716029	4.068852189	-2.1998485181
H	1.6853501318	-1.3925285757	2.8672610238
H	3.3465304009	-0.8380425698	2.6000323137
H	2.4159869638	-0.2376592492	3.975237327
H	-0.0764744245	1.7960270362	2.0784060949
H	-0.2759094368	0.0915799768	2.4704103604
H	0.4078192761	1.1967837773	3.6716196191
H	3.7484401682	1.6488192291	2.1714498075
H	2.4258691388	2.7778518682	1.8712544188
H	2.6413909378	2.1003243829	3.474685699
C	3.2572734139	0.5430754653	-1.2319807239

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C	3.0383002986	0.1703284349	-2.6963656857
C	3.9135211708	1.9331032669	-1.2211197181
C	4.3147083129	-0.4164907831	-0.666971074
H	2.6381995974	-0.8425436406	-2.816054585
H	2.3386879429	0.8481674099	-3.2004908583
H	3.9823536789	0.207314989	-3.2779000019
H	3.283474133	2.7045919088	-1.6829518034
H	4.1686853705	2.2819694907	-0.2095322238
H	4.866323536	1.9367712875	-1.7863943885
H	4.573817058	-0.1873639755	0.3764578754
H	4.0004267962	-1.4709817232	-0.7046328707
H	5.2621425922	-0.3736479531	-1.2390716739
N	1.466236618	-2.6342323352	0.0427965658
C	0.0897417054	-2.7294825352	0.5655847634
Si	-1.2726489608	-1.7387731218	-0.3457572881
C	-0.6509618076	-0.0614592184	-0.9224782709
C	2.3379112707	-3.526337802	0.8193941384
C	1.5062802999	-3.0629272136	-1.3572918504
C	-2.6676017758	-1.494013159	0.9348214802
C	-1.9857353388	-2.7146851188	-1.7973576972
C	-3.6319200457	-0.4367224985	0.4708698179
C	-3.4363501086	0.9060720176	0.8174503235
C	-4.7155616037	-0.7548721114	-0.3547649691
C	-4.2908894475	1.898610267	0.3457708733
C	-5.5717674795	0.2366824825	-0.8294740951
C	-5.3616862666	1.5694993099	-0.4839944105
H	0.1019742292	-2.3792939114	1.6022771931
H	-0.2223909229	-3.7895792629	0.5960780931
H	0.2527333976	-0.1320823364	-1.5357503302
H	-0.4261498321	0.5785256779	-0.065091973
H	-1.4323289515	0.4248598428	-1.513613431
H	3.3680167738	-3.4337543263	0.4711948633
H	2.2993139495	-3.2569537367	1.8733605803
H	2.0195095357	-4.5735583704	0.7100189288
H	1.0756777815	-4.0692694061	-1.4737014479
H	0.9506741354	-2.365953241	-1.9831790131
H	2.5392518889	-3.0804793118	-1.7058019036
H	-2.2231757124	-1.2056538018	1.8910524222
H	-3.1815269367	-2.4480334639	1.0868568817
H	-1.2714564053	-2.8319452227	-2.61455057
H	-2.3049945638	-3.7114867278	-1.4806373678
H	-2.858998702	-2.1903342589	-2.1945688382
H	-2.6073352988	1.169120965	1.4665780577
H	-4.8938142596	-1.7916461162	-0.6205159232
H	-4.1265649377	2.9302450408	0.6348273125
H	-6.4071830355	-0.0345827864	-1.4637979213
H	-6.0290293428	2.3406890859	-0.8482143249

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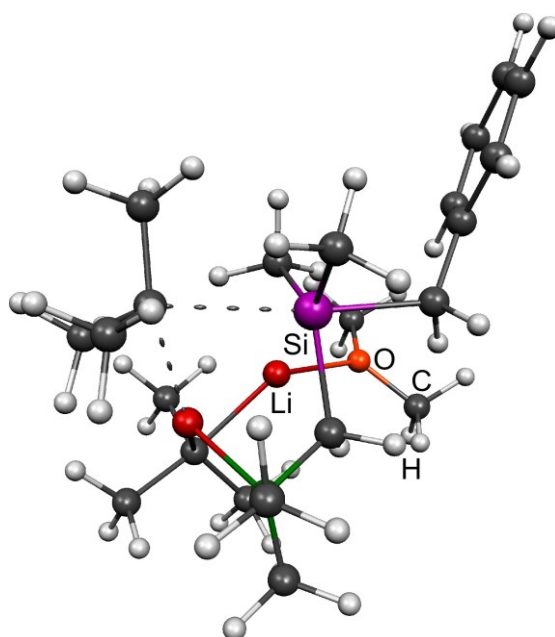
Abbildung 10.55 Molekel Darstellung von **TS20**.Tabelle 10.540 Standardorientierung von **TS20** [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	-0.7897668734	-1.9582130295	-1.3081578521
Li	-1.2437935572	-1.4179787818	0.7397451204
Li	0.9924640653	-1.3419908831	-0.2528297173
O	-2.8402711677	-0.5508368499	1.4126641937
C	-3.8669041956	0.0850231386	0.6612852848
C	-3.0308841179	-0.3521986081	2.813219135
C	0.1499016889	-3.0109557813	-1.9140954147
C	-0.8414258438	-0.7624724036	-2.2661285485
C	-2.1801689875	-2.6091691326	-1.3410579077
H	-4.819698193	-0.4276448091	0.8220403572
H	-3.9515693669	1.1309825893	0.9650032073
H	-3.5940521745	0.0325209819	-0.3896845011
H	-2.193171542	-0.814449453	3.3267745962
H	-3.043561602	0.7161977878	3.0379570982
H	-3.9688958995	-0.8204515889	3.1265362016
H	1.2062103454	-2.7086674512	-1.9543751017
H	0.1131420302	-3.9517914677	-1.3533422826
H	-0.1280064448	-3.2487748464	-2.9597343219
H	-1.585897948	-0.0197471097	-1.9513791
H	0.1135001161	-0.222838198	-2.3379935261
H	-1.1059115894	-1.065954324	-3.2987902215
H	-2.2237889482	-3.5328222271	-0.7523044036
H	-2.9797174795	-1.9567818466	-0.9715948248
H	-2.4667194219	-2.8851587906	-2.3748014104
C	0.3674515757	-2.1534988198	2.1347487312
C	0.6821768781	-1.7815014948	3.5809329192
C	-0.7276506152	-3.2290342014	2.1362047117
C	1.6310465014	-2.7874085941	1.554770156
H	1.4892490495	-1.0431381081	3.6365144635

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H	-0.1817746843	-1.3611607398	4.1037650825
H	1.014973696	-2.6637576332	4.1537916765
H	-1.6782460887	-2.8801760668	2.5585125459
H	-0.9266220272	-3.6182739937	1.1303167066
H	-0.4255928044	-4.0963155141	2.7474219747
H	1.4743831709	-3.235209153	0.5628256775
H	2.4483324478	-2.0596861456	1.4895436626
H	2.004009514	-3.6066077179	2.1914551059
N	2.8845140664	-0.6575052229	-1.1145929613
C	2.8589009883	0.7991164601	-0.8637752693
Si	2.203421638	1.3670729816	0.8464260458
C	0.4909266473	0.6131450751	1.0221420816
C	3.0324206049	-0.8985353274	-2.5567908196
C	4.0576413609	-1.2400677033	-0.4533797084
C	2.1339112441	3.2515028881	0.6978935166
C	3.3855563177	0.9812010718	2.2750029315
H	2.1574025726	1.2454365075	-1.5786560267
H	3.8467312814	1.2373255664	-1.0882012373
H	0.3713578829	-0.7099937237	1.529144838
H	3.145511426	-1.9667765185	-2.7459282147
H	2.1526859811	-0.5427443025	-3.0913797496
H	3.9196313678	-0.3762898811	-2.9429789617
H	4.9839608842	-0.8517238635	-0.902189256
H	4.0623844488	-0.9868508262	0.6039560212
H	4.0423788611	-2.3261446449	-0.557486339
H	1.4845539296	3.5555731683	-0.127702024
H	1.7268858945	3.6887128575	1.6133007842
H	3.1279544794	3.6759779889	0.5291392784
H	3.3956877031	-0.0715048029	2.563280986
H	4.4060356098	1.2815379219	2.0185325573
H	3.0842321796	1.5608877754	3.1522414657
H	0.056920261	0.6540452749	0.0093860689
C	-0.3383390478	1.4980265499	1.89001944
C	-0.1108011375	1.6074823293	3.2735740098
C	-1.3562864682	2.307364155	1.3509607406
C	-0.8517716314	2.478762989	4.0695823629
H	0.6592594524	0.9977609293	3.7290446698
C	-2.0997115408	3.1768832727	2.1425311473
H	-1.5501258418	2.2564490228	0.2835814207
C	-1.8540574902	3.2713216641	3.5134529115
H	-0.6424750497	2.5364083968	5.1316744788
H	-2.8676104481	3.7918708767	1.6857829743
H	-2.4268459338	3.9518235606	4.1311236528

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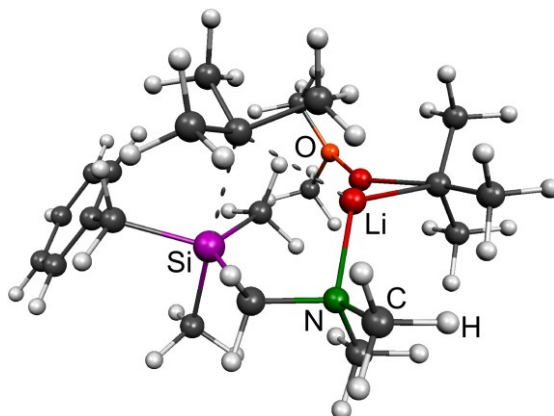
Abbildung 10.56 Molekel Darstellung von **TS21**.Tabelle 10.541 Standardorientierung von **TS21** [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	-3.3117376231	0.8038935498	-0.04504197
Li	-1.3561332806	1.4016331539	-0.1723119102
Li	-2.1545144577	-1.1238044864	0.4377627345
O	-0.5290152344	2.8480560395	-1.2027980518
C	-0.4230784842	2.8753227728	-2.6246645338
C	-0.35473768	4.140230427	-0.6266719273
C	-4.4901126988	-0.1355384794	0.2327496877
C	-3.6029708857	1.454370842	-1.410183637
C	-3.403882372	1.9398534758	0.9895773132
H	-1.1587131579	3.5670022899	-3.0433276985
H	0.5862119246	3.1792214041	-2.9123093003
H	-0.6191592721	1.8691612706	-2.9882484659
H	-0.3308991394	4.0172875685	0.4545989623
H	0.5897516377	4.5745820073	-0.9634618144
H	-1.1857610717	4.791579327	-0.909191046
H	-4.5091387831	-1.0064235685	-0.4362075975
H	-4.5030839392	-0.5048670275	1.2624927547
H	-5.4544676544	0.3853142586	0.0857919133
H	-2.8823688051	2.2356644765	-1.6858987935
H	-3.6212646982	0.7320629932	-2.2316010793
H	-4.5909696805	1.9527602784	-1.4048626368
H	-3.3260592253	1.5752567714	2.018034401
H	-2.6278664137	2.7201034101	0.8714468692
H	-4.3609723194	2.4877684144	0.9086781706
C	-0.7935189113	-1.9249317441	2.1050507294

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C	0.1865973032	-1.5614833571	3.2339543699
C	-2.1536883747	-1.393137359	2.6136372296
C	-0.971489334	-3.4505507236	2.1496465307
H	1.2267499456	-1.8142563595	3.0160377841
H	0.1526688392	-0.4990155206	3.4869802736
H	-0.0844658117	-2.1044693567	4.1553445394
H	-2.250002097	-0.301571004	2.5860739278
H	-3.0134573809	-1.8261050563	2.0791534929
H	-2.3164905431	-1.6925303294	3.6618149903
H	-1.7769774453	-3.7919850934	1.4921722488
H	-0.0714974624	-4.0103271081	1.8836537383
H	-1.2434815029	-3.7730374014	3.1705372512
N	-1.6691519245	-2.2833825579	-1.1599781707
C	-0.5457916884	-1.3432924381	-1.3042947641
Si	0.6274567164	-0.9471349605	0.2175905639
C	0.3772383488	0.7099988704	1.1844967772
C	-2.5559886232	-2.21306563	-2.3217957489
C	-1.1267094347	-3.6394910445	-1.0749909447
C	1.8758651031	-0.039702005	-1.1318093248
C	1.9064089266	-2.2893368326	0.6426611414
C	3.040372076	0.7207453617	-0.5864409134
C	2.9891493198	2.1117974513	-0.4036194306
C	4.2376248867	0.0790039421	-0.2307591482
C	4.0567114369	2.8220299551	0.1380879996
C	5.310132058	0.7831832372	0.3095632753
C	5.2260982944	2.1603277161	0.5068325594
H	-0.9513307205	-0.3976024716	-1.6880363688
H	0.1369333707	-1.7043404839	-2.0919048961
H	-0.5449290514	0.8010950796	1.7664159906
H	0.5474008667	1.5886480207	0.5555109466
H	1.1966502912	0.7502287805	1.9072100616
H	-3.3666590512	-2.9348757842	-2.2055254491
H	-2.9853354725	-1.2162573789	-2.3988575252
H	-2.0109143227	-2.4399868221	-3.2505744461
H	-0.6461771566	-3.9158042603	-2.0262355869
H	-0.3867049116	-3.6901144463	-0.2818112149
H	-1.9256447697	-4.351198267	-0.8632456364
H	1.2668711949	0.6381064901	-1.7439932223
H	2.2393739674	-0.8267042304	-1.8015617101
H	1.5529357101	-3.0982228973	1.2739048687
H	2.2642538695	-2.7082575242	-0.30297071
H	2.7637613872	-1.8216784011	1.1331323914
H	2.0917963961	2.6424581067	-0.7048669648
H	4.3305487315	-0.988768251	-0.3941130783
H	3.9790077421	3.8962661509	0.2644022983
H	6.2187473109	0.2534576818	0.5715345724
H	6.0602232116	2.7085450868	0.9268933577

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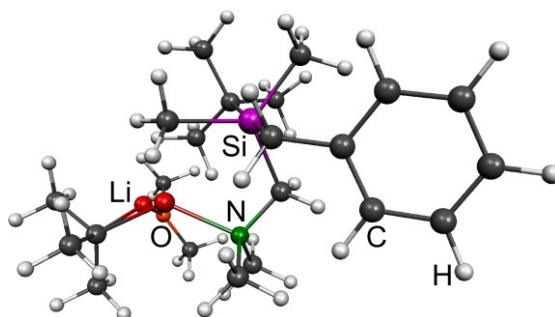
Abbildung 10.57 Molekel Darstellung von **TS22**.Tabelle 10.542 Standardorientierung von **TS22** [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	0.4175708759	-0.8745367913	2.1632810301
Li	1.9015592159	1.8101810799	-0.8196949062
Li	2.0819166225	-0.704775223	0.2374927424
O	1.063952661	3.5376779797	-0.9588622789
C	0.525825938	4.0666435162	0.25261665
C	0.2552905573	3.8658520663	-2.0871982036
C	0.0680251779	-2.1069416824	3.0084196612
C	-0.2081783946	0.3487048778	2.843473358
C	1.9324948955	-0.6901810532	2.3895948428
H	0.4744654834	5.1558126079	0.1887195988
H	-0.4704286693	3.6541219484	0.4345070598
H	1.1969603232	3.7804720285	1.0607856645
H	0.730732379	3.434277362	-2.9655736636
H	-0.7484430258	3.4509333674	-1.9666000394
H	0.2010012729	4.9511912457	-2.1974135854
H	-0.9593317596	-2.4582325111	2.878588532
H	0.7256155541	-2.9530503335	2.7792810806
H	0.2025950378	-1.900456206	4.0855513181
H	0.0274592808	1.2882099275	2.3251003781
H	-1.2950273072	0.2905769596	2.9238808328
H	0.169768007	0.4633733335	3.8758884513
H	2.5335075694	-1.5358146404	2.0198503614
H	2.3345564206	0.2435032295	1.9637396087
H	2.1671640483	-0.6280529912	3.4666029099
C	3.5758292483	0.7373109244	-0.5808715645
C	3.75883586	1.0612746514	-2.0736172625
C	4.0889002636	1.953833601	0.2107470891
C	4.5233251239	-0.4183341267	-0.2586993506
H	3.5009275696	0.2112677215	-2.7122464656
H	3.1563752427	1.9185265388	-2.4338742294
H	4.8010828107	1.3472768834	-2.3061700824
H	3.5262174439	2.8855480585	0.0265553634

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H	4.0646505979	1.7763097109	1.2905659599
H	5.1336254102	2.1982512666	-0.0572190675
H	4.5008994669	-0.6979829733	0.8020982978
H	4.3020049156	-1.3175079408	-0.8433628566
H	5.5726100201	-0.1512051681	-0.4830158112
N	1.7023262977	-2.5332564429	-0.5790968445
C	0.2886737131	-2.7780428734	-0.1898935362
Si	-0.7758496259	-1.1635591279	-0.0087929655
C	-0.1373833727	0.5961444172	-0.5105708425
C	2.5322864702	-3.6752778335	-0.1859654289
C	1.802068278	-2.3615854906	-2.030751627
C	-2.4314753041	-1.2672018712	0.991860041
C	-1.6704544389	-1.3869766549	-1.7643445194
C	-3.4509971314	-0.267949765	0.5163141936
C	-3.3330381058	1.0913934794	0.8392441463
C	-4.5459571713	-0.6543399864	-0.265234939
C	-4.2679721233	2.0247268931	0.397153551
C	-5.4799768383	0.2747424587	-0.716062082
C	-5.3463228484	1.6224046257	-0.3884766029
H	0.29589684	-3.2716523907	0.7800396841
H	-0.1657549469	-3.4739485591	-0.9137272633
H	0.4199847962	0.5221090198	-1.4556291696
H	0.4300285119	1.09087531	0.2825122836
H	-1.0296210038	1.1949860333	-0.7181662385
H	3.5673714335	-3.5098750512	-0.4909273507
H	2.5013661804	-3.7938248066	0.8975028632
H	2.1679557097	-4.6024610945	-0.6518214407
H	1.4048201159	-3.2400898207	-2.5601637801
H	1.2332808901	-1.4883974351	-2.348067471
H	2.8458287729	-2.2203941168	-2.3151115151
H	-2.2891311511	-1.1662359215	2.0634630259
H	-2.8076888128	-2.2798772812	0.8100242296
H	-0.945788386	-1.4973794629	-2.5802365083
H	-2.2871963731	-2.2948650493	-1.7765183852
H	-2.3290959524	-0.5532231776	-2.0281622391
H	-2.4996024257	1.4176307307	1.4516996847
H	-4.6604227398	-1.7001375248	-0.527929305
H	-4.1581689326	3.0674777995	0.6737265838
H	-6.3160477558	-0.0563187707	-1.3208283887
H	-6.0753447065	2.3458134957	-0.7327102673

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Abbildung 10.58 Molekel Darstellung von **Int7**.Tabelle 10.543 Standardorientierung von **Int7** [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-3.0941020727	-1.7061497817	1.3018683661
Li	-3.5124877878	-0.1289691656	0.1076352166
C	-0.4576779504	2.2579834992	0.3065046213
Li	-1.1454661332	-0.9413522184	0.8287399823
N	-0.203969273	-1.1671789296	-0.9359642549
C	0.7995707026	-0.0576956361	-1.0581722413
H	0.3900569053	0.6589404835	-1.770702327
H	1.7221865531	-0.4509744941	-1.5031433537
O	-4.6855197998	0.4714573267	-1.2658841825
Si	1.1505477642	0.89261152	0.6176422304
C	2.7708292688	-0.4102493843	1.1691274242
H	2.3772130274	-1.4215622788	1.3124049083
H	3.0473073492	-0.0480710576	2.1671136623
C	3.9890083607	-0.4871606915	0.3199074214
C	5.0860736995	0.3745291833	0.506994989
C	4.1091867991	-1.427783113	-0.7192981032
C	6.2105660845	0.3239229576	-0.3099940945
H	5.0527226104	1.0936304286	1.3180176375
C	5.2321187872	-1.4851526902	-1.5404129506
H	3.3107761825	-2.1455991127	-0.8705352739
C	6.2927081362	-0.6022906592	-1.3495650608
H	7.0325263246	1.0072461047	-0.1277382656
H	5.2820681647	-2.2308363995	-2.3263644909
H	7.1690297779	-0.6443445147	-1.9847648878
C	-4.7057210246	-0.107987768	-2.5692123689
H	-5.7377664413	-0.2144767513	-2.9103247083
H	-4.1459098114	0.5203006855	-3.2665298738
H	-4.2411976079	-1.0888897	-2.4987462868
C	-5.2993806992	1.7596374597	-1.242651618
H	-5.2721446535	2.1182428385	-0.2160688412
H	-4.7493744722	2.4488020512	-1.8875742575
H	-6.3361448196	1.6789389222	-1.5763406586
C	-0.9763626029	-1.2994622654	-2.1717271615
H	-1.7042952385	-2.1085937087	-2.0674716039
H	-1.5078388766	-0.3697142113	-2.3835975985
H	-0.3200136073	-1.5184187505	-3.0263226843

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C	0.4564745725	-2.4545728104	-0.6922845854
H	1.1247504229	-2.7185124826	-1.5239121261
H	1.0498371863	-2.4088085045	0.2188540499
H	-0.2981463962	-3.2387048743	-0.5901026112
C	0.2760407088	0.1481550618	2.2187224913
H	0.4479422102	-0.9264956239	2.3565504081
H	0.8225958883	0.6155389163	3.0438530028
H	-0.7783335124	0.378351008	2.4196239815
C	2.4231139884	2.3321558359	0.6891008065
H	3.2170097948	2.1312403976	-0.0339050756
H	2.0430616339	3.3351600967	0.5105025787
H	2.8919683272	2.3203056184	1.6781235583
C	-2.2107286541	-2.5764715913	2.2015877072
H	-1.4475245221	-3.1337666963	1.6389006531
H	-1.6943601306	-1.9958423926	2.9749636949
H	-2.8051381271	-3.3399047063	2.7340043002
C	-3.8862706419	-2.6544455641	0.3911247068
H	-4.6053293476	-2.1335154273	-0.2608501172
H	-3.227356477	-3.2395249182	-0.2597883594
H	-4.4884559319	-3.3739590028	0.9765505025
C	-4.1010896923	-0.9954955741	2.2206059572
H	-3.602444107	-0.3735581121	2.9714031389
H	-4.8172558839	-0.3387280831	1.6879502245
H	-4.7440399456	-1.7129838523	2.760896345
C	-0.2559174648	3.1200085755	-0.9495848835
H	0.7356461238	3.5716700324	-1.0013078261
H	-0.395510974	2.5460631323	-1.8721008096
H	-0.9890259001	3.9428394032	-0.9786366289
C	-1.8516007706	1.6358029461	0.1416579783
H	-1.8590183202	0.9143123467	-0.6886626372
H	-2.1809251923	1.1514474369	1.0736032263
H	-2.6019937716	2.4098730053	-0.0940842726
C	-0.5570934464	3.1986946662	1.5159303098
H	-0.7608445433	2.6554898542	2.4443712083
H	0.3608763805	3.7686888985	1.6698849087
H	-1.3715741105	3.9298788055	1.3832788829

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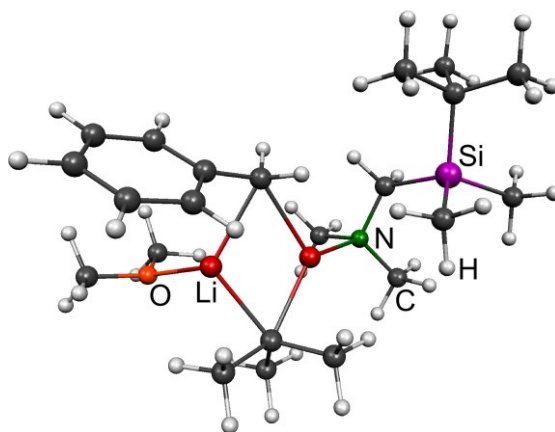


Abbildung 10.59 Molekel Darstellung von Pr3.

Tabelle 10.544 Standardorientierung von Pr3 [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	5.9727024745	-0.238800733	-0.1560303015
Li	-1.5239777066	-0.6866694963	-0.4329595557
C	-0.5429874007	-2.0111281828	0.965843536
H	6.5968225475	-0.2201056466	-1.0537098049
H	5.8861994266	-1.2779297324	0.1666828251
H	6.5006979164	0.3084154595	0.6290902965
Li	0.8029754602	-0.9272662034	-0.3087940481
N	2.4943849283	-1.586047698	-1.3126385857
C	3.3067596875	-0.4504479828	-1.7885455219
H	2.6284672689	0.2453152478	-2.2920049868
H	4.0198463682	-0.8026834319	-2.5560311992
O	-2.8504897478	-1.5344118524	-1.540380271
Si	4.2873845906	0.5581636405	-0.4851452946
C	-0.056323795	0.8266651651	-1.3408946824
H	0.686546933	1.2442511476	-0.6508892604
H	0.3032391012	0.9031768478	-2.3682254112
C	-1.3605334688	1.434452301	-1.1473579749
C	-2.2334701437	1.7389802808	-2.2246450894
C	-1.8892907231	1.6492505466	0.1525750237
C	-3.509560196	2.2400288584	-2.0159607886
H	-1.8692808854	1.6020983686	-3.2381315189
C	-3.1761317854	2.1461563348	0.3551294069
H	-1.2546869893	1.4438492672	1.0118083272
C	-4.0041962753	2.4478193138	-0.7232058179
H	-4.1297103579	2.4810669354	-2.873243057
H	-3.5270636236	2.3037872373	1.3691094846
H	-5.000011706	2.842512047	-0.5664707367
C	-2.4265419115	-1.986672047	-2.8162142906
H	-3.0209827951	-2.8515274146	-3.1253563628
H	-2.5261512068	-1.1842085169	-3.5531744913
H	-1.3811883184	-2.2747055566	-2.7236055188
C	-4.2283444455	-1.1798919545	-1.5215705849

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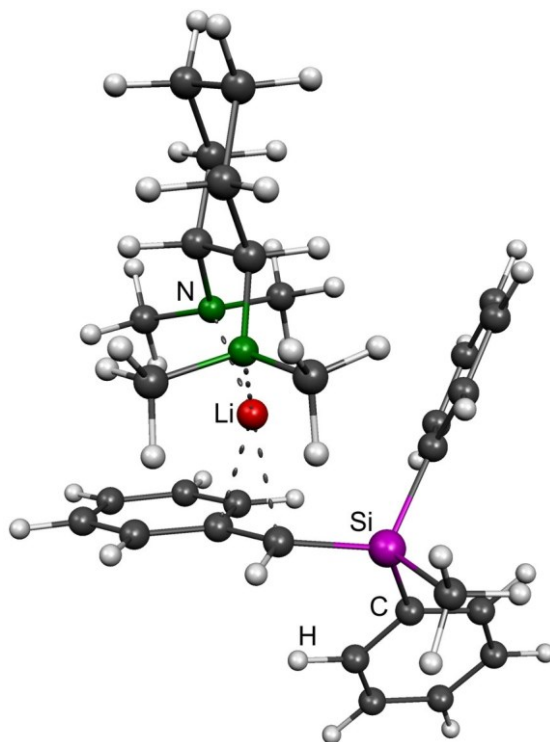
H	-4.4409948323	-0.7556515693	-0.5428743242
H	-4.4350121231	-0.4296522512	-2.2875856372
H	-4.8403796826	-2.0712473757	-1.686781164
C	1.8370515292	-2.2191756699	-2.4636884826
H	1.2115894596	-3.0463668781	-2.1216103146
H	1.207986684	-1.4836392544	-2.9665071375
H	2.5795555699	-2.605034412	-3.1778924922
C	3.3320502348	-2.58056574	-0.6419616828
H	4.1552407173	-2.9101995563	-1.2938219851
H	3.753591931	-2.163099397	0.2717602017
H	2.7270051296	-3.4464858185	-0.3720139642
C	4.5663259856	2.2917874446	-1.2332926836
C	3.3232252888	0.6896728532	1.1347846181
H	3.8126404407	1.4102283947	1.7966375826
H	2.2984893388	1.0366605127	0.9802097899
H	3.2808114126	-0.2629419777	1.667123143
C	-1.8458500902	-1.7754036442	1.7428226528
H	-1.8968257395	-0.77391376	2.1867736687
H	-2.7432851736	-1.909601669	1.1221570751
H	-1.95069218	-2.4966559144	2.5774767074
C	0.592491427	-1.8547834789	1.9846100386
H	1.5851025554	-2.068624808	1.5594932763
H	0.6319593228	-0.845637013	2.4144453608
H	0.4789772278	-2.5570841798	2.8343173046
C	-0.5574315661	-3.4725545129	0.5120925176
H	-1.3783805457	-3.6757822241	-0.1856276464
H	0.3745994886	-3.7666754297	0.0115227086
H	-0.682971807	-4.1672467284	1.3677607298
C	5.6236902928	3.0392921871	-0.4076208835
H	6.5999456574	2.5501820357	-0.4607367616
H	5.7427628222	4.0592772225	-0.7921205538
H	5.3390220217	3.1184371556	0.6462415411
C	3.2603432385	3.0979830676	-1.2164464528
H	3.4239363342	4.0799803133	-1.6765975673
H	2.4568993676	2.6051424856	-1.7708791137
H	2.9043268558	3.2676763356	-0.1964532794
C	5.0657222645	2.1683940162	-2.6804521218
H	4.3157425977	1.7129922914	-3.3329294609
H	5.2890230612	3.1635001824	-3.0835497923
H	5.9823758318	1.5740981845	-2.74801546

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## 10.2.3. Details zu Kapitel 5.3

Tabelle 10.545 Absolute Energien der optimierten Strukturen.

Struktur	Methode/Basis	SCF [Hartree]	ZPE [Hartree]
<i>(R,R,R)</i> - <b>91</b>	M05-2X/6-31+G(d)	-1574.34487104	-1573.685321
<i>(S,R,R)</i> - <b>91</b>	M05-2X/6-31+G(d)	-1574.34701148	-1573.687243

Abbildung 10.60 Molekel Darstellung von *(R,R,R)*-**91** [lokales Minimum; M052X/6-31+G(d)].Tabelle 10.546 Standardorientierung von *(R,R,R)*-**91** [lokales Minimum; M052X/6-31+G(d)].

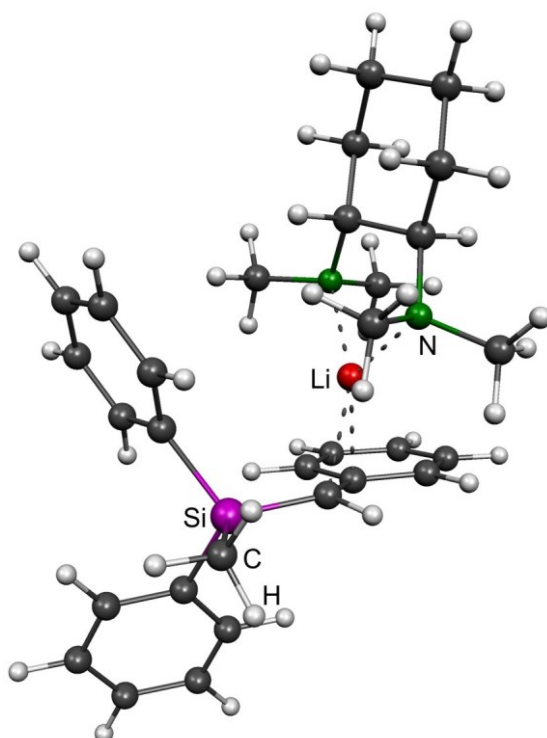
	x	y	z
C	1.8847424449	0.6063199316	-6.3874275618
C	0.5502914537	0.9948370897	-5.7520387279
C	3.042253804	1.3328200484	-5.6979506692
C	0.5736553638	0.6984303861	-4.2514716263
C	3.066383247	1.0347474818	-4.1908636234
C	5.4904661325	1.0933634193	-3.890923742
C	4.2557573268	3.0980670869	-3.4957551901
C	1.7239617898	1.4466111561	-3.5629361187
C	3.9923582818	-2.833502745	-2.148637889
C	1.462580807	-0.0312868706	-1.6001324012
C	0.8459774703	2.2783292567	-1.4499593839

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C	4.800332078	-1.8540014662	-1.5713629206
C	2.9790658492	-3.4272285955	-1.3970480248
C	7.4563804506	-0.2969254122	-0.3143553399
C	4.6307617217	-1.4404400508	-0.2401915347
C	5.1529227442	1.621839733	0.0833816111
C	3.7557643254	3.6688459898	0.440462252
C	2.7928927022	-3.0403935215	-0.0710543355
C	4.022236284	2.2879858019	0.6739603899
C	2.6686220758	4.3212264527	1.0065953443
C	3.6133392613	-2.0648396697	0.4961341682
C	3.0630018976	1.6180413659	1.4877485747
C	1.7636994264	3.6419396432	1.8264342531
C	1.9820897847	2.2813643164	2.0551820665
C	5.9116215634	-0.4500647676	2.3206118202
C	6.1568115664	-1.7534892813	2.7762385559
C	5.8529815653	0.5767425916	3.2713496601
C	6.3416194254	-2.0246580709	4.1303561888
C	6.0324602308	0.3140030141	4.6293169643
C	6.2774105679	-0.9877275038	5.0604446111
H	1.884399052	0.8356653722	-7.4556330607
H	2.0276063871	-0.4763946501	-6.2926354592
H	-0.2721732986	0.4553000778	-6.227514535
H	3.9916494349	1.0404112393	-6.1528882202
H	0.3679182649	2.0636909848	-5.9130669127
H	2.9256731908	2.4111719397	-5.8536850551
H	5.8057796965	1.4896521177	-4.8650656257
H	4.42513934	3.4904501367	-4.5066727187
H	0.6982925972	-0.3797920592	-4.1069063988
H	3.1802735007	-0.0496567827	-4.0597918612
H	-0.3767448819	0.9794746063	-3.7897142456
H	5.4266437043	0.0071000847	-3.9589465706
H	1.5784772228	2.5127869287	-3.7694166848
H	3.3386270968	3.529725273	-3.0937802438
H	6.2475772289	1.3518827132	-3.1487117112
H	5.0828042009	3.4236317741	-2.8615757158
H	4.161023285	-3.1433597457	-3.1744357032
H	2.1145309319	-0.7649770829	-2.0770772876
H	5.5991318429	-1.4178687276	-2.1626134492
H	0.4170600576	-0.3196114633	-1.769114006
H	-0.2037407325	2.0891737359	-1.7159422825
H	7.4529387157	-0.0813750364	-1.3862974129
H	1.1124936802	3.2944291346	-1.7433605445
H	2.3497911157	-4.1925422996	-1.8361367773
H	7.8112554681	-1.320650001	-0.1711989999
H	1.654656584	-0.0569335123	-0.5263356687
H	5.8986586799	2.2894390706	-0.3516314593
H	0.9568738172	2.2055782302	-0.3689369838
H	8.1708070571	0.3788730363	0.1621376757
H	4.4588998599	4.2326365961	-0.1666929025
H	2.5308416937	5.3802413426	0.8137788814
H	2.0161882656	-3.5058886191	0.5249439697

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H	3.4683650713	-1.7985051887	1.5384427084
H	6.2019277646	-2.5717611454	2.0628168971
H	3.2148659071	0.5691343247	1.7199355665
H	0.9245615345	4.1560132808	2.2777022418
H	5.6574502174	1.5916526184	2.9400848697
H	1.3033439272	1.7258340978	2.6941019106
H	6.5338132123	-3.0392354193	4.4603669382
H	5.9773138186	1.1227267147	5.3488644143
H	6.4167596696	-1.1947470203	6.1151986923
Li	3.7275014467	1.4151337072	-1.4799266717
Si	5.7508038275	-0.0551688073	0.4714591071
N	4.2020857225	1.6338301985	-3.4584236048
N	1.7536131797	1.3220014141	-2.0904124709

Abbildung 10.61 Molekel Darstellung von (*S,R,R*)-**91** [globales Minimum; M052X/6-31+G(d)].Tabelle 10.547 Standardorientierung von (*S,R,R*)-**91** [globales Minimum; M052X/6-31+G(d)].

	x	y	z
C	-5.4277127975	0.3190670275	-3.3001869456
C	-4.5680551488	1.3806424211	-3.0142295194
C	-0.9310054102	-3.9370858493	-2.9945600623
C	-5.2240169179	-0.8893003182	-2.6252056371
C	-0.6469885447	-5.1990177508	-2.4777414858
C	-3.5383020113	1.2436522222	-2.0898737132

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C	-1.2598627047	-2.8890043536	-2.1346824832
C	-4.2008928495	-1.0368942393	-1.6994235496
C	-3.2843369657	0.0169951272	-1.4059066165
C	-0.693890621	-5.4091654623	-1.0998736938
C	-1.3151982904	-3.0785591786	-0.7481273588
C	-2.2405995387	-0.0997536715	-0.4280870317
C	-1.0276996034	-4.35755397	-0.2491565571
C	-6.5839448681	1.295675483	0.0941438048
C	-3.043091771	3.6324462101	0.9374360677
C	-3.8237834643	-3.3328252788	1.4274400269
C	-6.2488856717	-0.6104821125	1.500680204
C	-2.9089501195	-2.3075232167	1.7068415672
C	-0.0817935237	-1.22969224	1.35178488
C	-4.7093434389	-3.8076003298	2.3956586897
C	-4.9681705634	2.8727638369	2.2356746889
C	-5.8356423102	1.6135844824	2.4282185816
C	-2.6849778605	2.0662372297	2.7101281204
C	-7.2431723521	2.0223961436	2.8901231313
C	-2.9153072724	-1.7830331755	3.0093475822
C	-4.6955562793	-3.2682992152	3.6804280691
C	-4.9300009709	3.6946949763	3.5326600234
C	-6.337447582	4.0907714291	3.9821189941
C	-3.7918748668	-2.2514506361	3.9878615091
C	-7.1952824104	2.8419135974	4.180704365
H	-6.2229203842	0.4241799761	-4.026939512
H	-0.899224599	-3.7691287485	-4.0647728819
H	-4.6950407353	2.3300316003	-3.5239305412
H	-0.3907977088	-6.0149704426	-3.1433471408
H	-5.8713719546	-1.7356805165	-2.8292881605
H	-1.4819329577	-1.9081196515	-2.5423283685
H	-2.8660871363	2.0788722893	-1.9132849122
H	-4.0611851718	-1.9986430494	-1.2172811623
H	-0.4721048853	-6.3886293522	-0.6919735789
H	-6.3692317195	0.6972623632	-0.7915878844
H	-6.2907108123	2.3238072843	-0.1215627698
H	-1.5164264825	0.7171676271	-0.4348599197
H	-3.7120408092	3.9242834387	0.1267468043
H	-7.6646390955	1.2647369264	0.2839204869
H	-3.8326703085	-3.7855131244	0.4410289694
H	-2.1015646558	3.295399516	0.5007717584
H	-6.0811555007	-1.2156397765	0.6088872021
H	-1.0681754868	-4.5373142019	0.8214576665
H	0.7081466836	-0.984473254	0.6375438514
H	-2.8376844359	4.5082182641	1.5684423665
H	-7.3153039718	-0.6622131992	1.7594067748
H	-5.4493847813	3.4912080211	1.4700285815
H	-5.4019034211	-4.6043481925	2.1499365516
H	-7.7175485842	2.6282647051	2.1106098061
H	-5.6590458279	-1.0308367055	2.3148287611
H	0.2462059007	-2.0920429612	1.9375602407
H	-1.8175065701	1.6381980547	2.2050864579

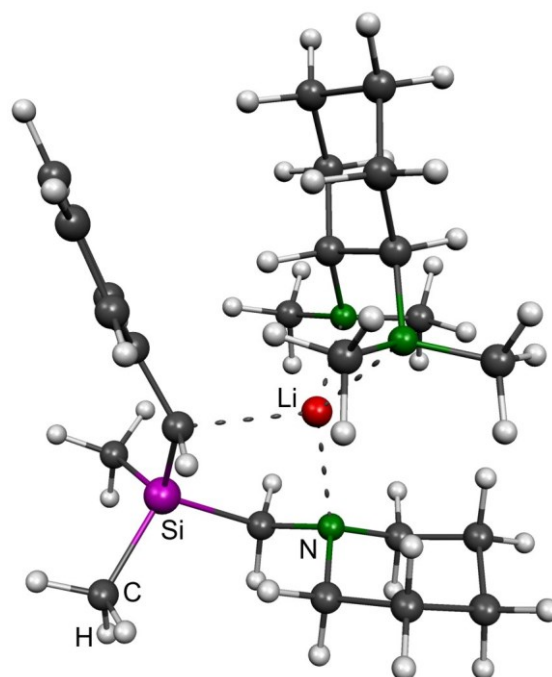
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H	-0.1978302274	-0.3797049418	2.030131839
H	-7.8604978088	1.1312423335	3.0269905684
H	-6.8004594082	4.7332422053	3.2241638675
H	-5.3811660241	1.0096985578	3.2242259967
H	-4.3086956244	4.5833662218	3.3895249299
H	-2.3478149063	2.8806615112	3.3642647712
H	-3.1386609318	1.2857201425	3.3219517516
H	-2.2028975602	-1.0075240342	3.273355423
H	-5.375013127	-3.6422847019	4.4371628506
H	-4.4671837861	3.1012677861	4.3281596801
H	-8.2079740313	3.1158927675	4.4860181245
H	-6.2833688806	4.6725775141	4.9053679723
H	-3.7603974486	-1.837202154	4.9895695789
H	-6.7701815335	2.2341726689	4.987997535
Li	-3.8882300776	0.8304671746	0.5652512944
Si	-1.6784836441	-1.6183794505	0.4097340791
N	-5.8109866594	0.7605213527	1.2221724961
N	-3.6349561795	2.5272289677	1.6917921435

#### 10.2.4. Details zu Kapitel 5.4

Tabelle 10.548 Absolute Energien der optimierten Strukturen.

Struktur	Methode/Basis	SCF [Hartree]	ZPE [Hartree]
<i>(S,R,R)</i> - <b>94b</b>	M05-2X/6-31+G(d)	-1441.55796	-1440.86416
<i>(R,R,R)</i> - <b>94b</b>	M05-2X/6-31+G(d)	-1441.55797	-1440.86414
<i>(S,R,R)</i> - <b>94b'</b>	M05-2X/6-31+G(d)	-1441.55596	-1440.86213
<i>(R,R,R)</i> - <b>94b'</b>	M05-2X/6-31+G(d)	-1441.55385	-1440.86024

Abbildung 10.62 Molekel Darstellung von *(S,R,R)*-**94b** [lokales Minimum; M05-2X/6-31+G(d)].Tabelle 10.549 Standardorientierung von *(S,R,R)*-**94b** [lokales Minimum ;M05-2X/6-31+G(d)].

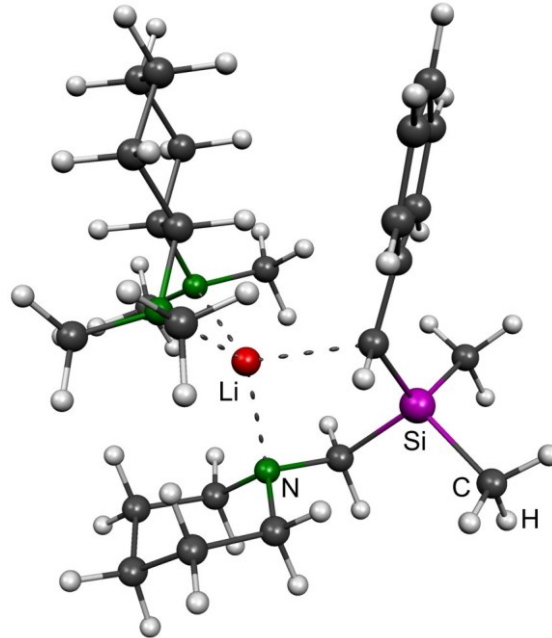
	x	y	z
C	3.4550418977	-1.2564222588	1.1560407163
C	2.832462665	1.0755688653	1.0669971347
C	3.4123660639	-2.6092470016	0.4553432928
C	4.1121397107	-2.524376352	-0.9009273813
C	2.9600421781	3.537384981	-0.7887175876
C	3.5141866374	-0.0783970331	-0.9295955288
C	1.3135901881	3.572267642	1.7422605011
C	3.5110829315	-1.3825497263	-1.7194977682
C	0.4064345722	1.739959426	-0.7178363534
C	-0.9763766449	2.1640011556	-0.7404870289
C	-1.6814948214	2.6699598834	0.3867748456
C	-1.7629491611	2.0522600892	-1.9224401156
C	-3.0407667842	2.9563740575	0.3526941362
C	-3.1239671608	2.3296796475	-1.9503801072
C	-3.7946760259	2.7712017566	-0.8080857983
N	2.8058244417	-0.215494309	0.3497657579
Si	1.7705781584	2.4819451787	0.2573057194
H	4.5029866911	-0.9709255342	1.3549446244
H	2.9427053371	-1.303980115	2.1193400189
H	3.8786564624	1.39535401	1.2213810655
H	2.4149687893	0.9020194905	2.0647188607
H	3.8813832878	-3.3656870871	1.0900395944
H	2.365487011	-2.8974067096	0.3126784511

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H	5.1798087663	-2.3333702662	-0.7433586023
H	4.030103437	-3.4714117303	-1.440590261
H	3.8613154358	3.8038736093	-0.2272039451
H	3.2691926806	3.0303671492	-1.7064592555
H	2.4566448121	4.4626174338	-1.0829517418
H	4.5533565668	0.243527035	-0.7391932181
H	3.0294478859	0.7094382255	-1.5071450486
H	2.2334682684	3.9663187406	2.1859880059
H	0.7747760609	3.028868293	2.5227796689
H	0.7001136016	4.4219330701	1.4333152029
H	4.0611043871	-1.2399336642	-2.6530545868
H	2.477899722	-1.6264747318	-1.9843061169
H	0.761740332	1.5004035177	-1.7277626592
H	-1.1396883381	2.8512429972	1.3058485046
H	-1.2683191066	1.7588324992	-2.8435798878
H	-3.5176190869	3.3384145992	1.2497419058
H	-3.6644098961	2.2189287303	-2.8850477131
H	-4.8537862803	2.9948366793	-0.830421181
C	-0.0995933488	-2.2418129084	2.254044509
C	-0.5097835006	0.0699888718	2.6590656022
C	0.0430310077	-3.3437298595	-1.4136275307
C	-1.7338762173	-1.0112692475	0.8481065786
C	-2.9985722159	-1.176594851	1.7066295247
C	-1.6731877159	-2.1073453535	-0.2277531219
C	-0.5830449747	-1.2068208691	-2.2515139066
C	-4.2631001233	-1.1867115889	0.846718387
C	-2.9596334306	-2.1151496913	-1.0670636571
C	-4.1940958971	-2.3074670048	-0.1867493556
Li	0.714267863	-0.3920070847	0.0307105934
N	-0.469214265	-0.9718611342	1.6315063559
N	-0.4224716952	-2.0107105921	-1.0324353861
H	0.799876306	-2.0814699859	2.8505130031
H	0.1324607372	-2.9921991766	1.5005177061
H	-0.8788252677	-2.6328430896	2.9217334775
H	0.5007845487	0.2436607453	3.032644071
H	-1.1430905669	-0.2069170748	3.5122915006
H	-0.8875112331	0.9910038937	2.2197137382
H	0.2515121407	-3.944451204	-0.5271705958
H	0.9639490609	-3.2576106955	-1.9921977369
H	-0.6962074355	-3.8756144256	-2.030487618
H	-1.7989855592	-0.037632113	0.3449571301
H	-2.9450526221	-2.1122778213	2.2763791723
H	-3.0591616244	-0.3574071639	2.4254104468
H	-1.6297948675	-3.0726927589	0.2891866461
H	0.4019238539	-1.0197497481	-2.6845992214
H	-1.0340441294	-0.2475211348	-2.0099215023
H	-1.1972995986	-1.7155229844	-3.0064453809
H	-5.1430447777	-1.3015059361	1.4848024908
H	-4.3550067279	-0.2227221426	0.3336776257
H	-2.8993772449	-2.9060292644	-1.8209539298
H	-3.0606760472	-1.1619791731	-1.5947691785

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H	-4.1438035368	-3.2774869569	0.3229764719
H	-5.0930346022	-2.3162317982	-0.8079165138

Abbildung 10.63 Molekel Darstellung von *(R,R,R)*-**94b** [globales Minimum; M05-2X/6-31+G(d)].Tabelle 10.550 Standardorientierung von *(R,R,R)*-**94b** [globales Minimum; M05-2X/6-31+G(d)].

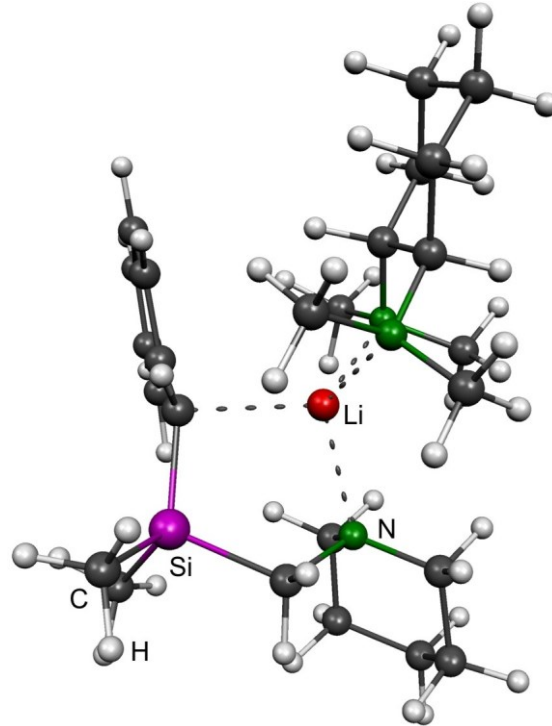
	x	y	z
C	6.8545972829	-3.3386133582	-5.143137397
C	7.9544971264	-4.1364183299	-4.4474559479
C	5.5095643695	-3.5782398167	-4.4558258213
C	8.0329450094	-3.7267224303	-2.9770539271
C	5.563334299	-3.1922547176	-2.9688988374
C	3.2058575088	-2.5910908881	-2.8889306257
C	6.6937833896	-3.9567829477	-2.2612967411
C	3.8380232337	-4.7532102261	-2.1127793528
C	7.6356439673	-2.5535814871	-0.4564554167
C	7.0888486835	-4.8315419963	-0.0297325449
Li	4.9657232699	-2.3887706752	-0.5118884789
N	4.2728088818	-3.3637895997	-2.2470956727
N	6.722315498	-3.6485215628	-0.8050264547
H	6.7851366031	-3.6145870166	-6.1984181116
H	7.0946744223	-2.2701908954	-5.0998888939
H	8.9198724524	-3.9655649829	-4.9300415891
H	7.7387349606	-5.2090059933	-4.526749674
H	4.737336736	-2.9914590122	-4.9567907451
H	5.239893636	-4.6362156552	-4.5592668588
H	8.2960825105	-2.6655781552	-2.931831209

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H	8.8216094309	-4.2858153896	-2.4639764696
H	5.7890352137	-2.1195988577	-2.9116946077
H	2.8368153057	-3.0730407247	-3.8039410438
H	3.5800524455	-1.6002096982	-3.1350832278
H	2.3660772037	-2.4873485417	-2.1989883498
H	6.4727587535	-5.026958833	-2.3437060018
H	3.7042671574	-5.2521377301	-3.0817253549
H	4.5435227551	-5.3266454968	-1.5138704555
H	2.8759114366	-4.7669642294	-1.5971547257
H	7.4237376449	-1.6813268622	-1.0713440711
H	8.6911669168	-2.8322502603	-0.5756952986
H	7.4719417153	-2.2849705727	0.5887837737
H	8.0838671397	-5.2119887946	-0.3044974901
H	6.3573189334	-5.6270840845	-0.1780734421
H	7.1065185949	-4.5769890468	1.03065206
C	7.1181766727	0.9378231947	-4.4886698998
C	5.7268603346	0.8115792072	-4.4814258345
C	7.7861320516	0.792303874	-3.2721656854
C	5.039746114	0.5174974207	-3.3115095428
C	7.1016700111	0.4876259744	-2.100399509
C	5.6928828422	0.2940117674	-2.0657671401
C	4.9538736928	-0.1423463408	-0.8995926504
C	1.9905094679	-2.9757935963	0.9325495237
C	6.9683386725	1.0835797901	1.2456698663
C	2.8741673011	-1.8555186579	1.4707186543
C	3.635049449	-4.6147507805	1.8534486879
C	2.1534828155	-4.2507217657	1.7590052553
C	4.0085359054	1.6834063454	1.4547553004
C	5.1007698092	-1.1350367831	2.025697009
C	4.4358894284	-3.4287489961	2.3772029948
N	4.2877059232	-2.2545015741	1.5083957723
Si	5.2531004274	0.3859198883	0.8306369383
H	7.6553903218	1.1736922331	-5.39861814
H	5.165562738	0.9650224093	-5.397531114
H	8.8624902994	0.9249829196	-3.2292382673
H	3.9551086587	0.4820439025	-3.3359927893
H	7.6674742481	0.4059396945	-1.1810164126
H	3.8750933964	-0.1486586169	-1.1013157765
H	2.2767603504	-3.1753751754	-0.1043237154
H	0.9492100189	-2.6439760161	0.9263744994
H	7.1933179512	1.9651960582	0.6408466814
H	7.7703981356	0.3558367135	1.0957811213
H	6.9838033124	1.3844280083	2.298046492
H	2.7835043569	-0.9701772681	0.8398975499
H	2.5465788097	-1.5724185161	2.4866708443
H	4.0142350391	-4.8837973469	0.8616211516
H	3.7844334698	-5.4761972973	2.509688483
H	1.5785525263	-5.0708360409	1.3213194338
H	1.7596950587	-4.081492433	2.767705564
H	4.1720278372	2.6279326311	0.9285215563
H	2.9739054481	1.3819653225	1.2693249073

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H	4.1212642419	1.8664074682	2.5282426776
H	6.1152820648	-1.5157530939	2.1875812853
H	4.7262098587	-0.8308863665	3.0195345173
H	5.4980999058	-3.6746785479	2.4319158157
H	4.1043565454	-3.1759907403	3.399692899

Abbildung 10.64 Molekel Darstellung von *(S,R,R)*-**94b'** [lokales Minimum; M05-2X/6-31+G(d)].Tabelle 10.551 Standardorientierung von *(S,R,R)*-**94b'** [lokales Minimum; M05-2X/6-31+G(d)].

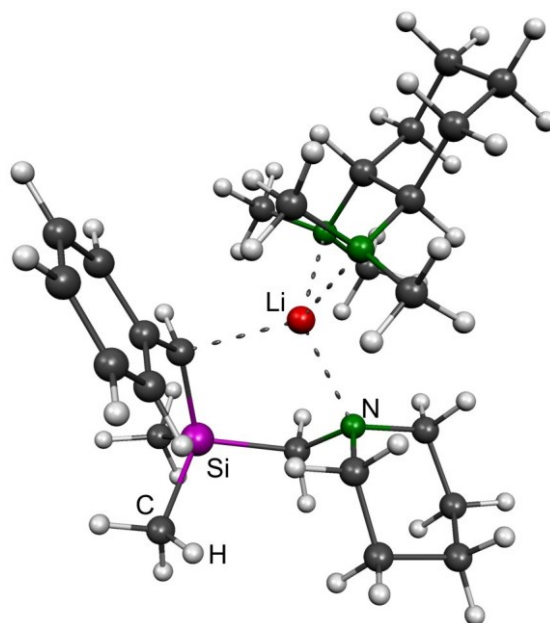
	x	y	z
C	-0.360389	4.007864	-1.454984
C	0.923411	4.506464	-1.222287
C	-3.941794	-2.291966	-2.225204
C	-3.835299	-0.8077	-1.864195
C	-2.407773	-0.48994	-1.413442
C	-0.919562	3.034057	-0.637259
C	1.620672	4.012965	-0.115065
C	-3.460353	-3.157545	-1.057573
C	-2.059108	-2.724707	-0.611236
C	-0.22413	2.48108	0.473038
C	1.066935	3.039577	0.704144
C	-3.867732	1.900862	0.880561
C	-2.664155	-0.962882	0.982119
C	-0.7281	1.426698	1.313961

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C	-2.786771	0.678262	3.45113
N	-1.949267	-1.2964	-0.269902
Si	-2.441118	0.86437	1.593097
H	-0.942307	4.390154	-2.28749
H	1.35245	5.268296	-1.860561
H	-3.312038	-2.490115	-3.101813
H	-4.965997	-2.553584	-2.501646
H	-4.088556	-0.180652	-2.723509
H	-4.544244	-0.560624	-1.068413
H	-1.729251	-0.693453	-2.250068
H	-2.291396	0.564038	-1.160273
H	-1.927289	2.696667	-0.848691
H	2.608634	4.398492	0.116206
H	-3.432899	-4.212529	-1.344793
H	-4.160653	-3.074126	-0.221695
H	-1.353063	-2.924876	-1.426111
H	-1.737193	-3.304679	0.256319
H	1.629116	2.689704	1.566152
H	-3.971055	1.844244	-0.205131
H	-3.729938	2.952091	1.147034
H	-4.810486	1.559734	1.320216
H	-3.729366	-1.233077	0.943458
H	-2.222865	-1.589107	1.769403
H	-0.138285	1.314558	2.224976
H	-3.707096	0.116092	3.638707
H	-2.884257	1.659872	3.921507
H	-1.963929	0.154002	3.947455
C	1.250303	0.853025	-2.169347
C	1.206276	-1.532699	-2.157011
C	3.884174	-0.246405	-1.332752
C	5.13686	-0.246875	-0.456384
C	2.591455	-0.32105	-0.501768
C	5.164325	-1.491115	0.42707
C	2.632582	-1.524869	0.45516
C	3.913074	-1.521008	1.303568
C	1.007418	-3.0075	1.495393
C	1.452683	-0.915576	2.537865
N	1.353967	-0.341894	-1.320408
N	1.37857	-1.614726	1.249224
H	1.92133	0.798072	-3.03699
H	0.225629	0.945862	-2.530633
H	1.479103	1.745188	-1.588063
H	2.035337	-1.665957	-2.864142
H	0.291448	-1.427199	-2.741047
H	1.109415	-2.432161	-1.549514
H	3.865275	0.652915	-1.950981
H	3.935923	-1.106104	-2.010201
H	6.028558	-0.197753	-1.086065
H	5.141928	0.647321	0.177473
H	2.519851	0.594371	0.100964
H	5.202034	-2.387614	-0.203168

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H	6.058168	-1.501958	1.055509
H	2.672493	-2.430772	-0.159013
H	3.928895	-0.638603	1.950073
H	3.919815	-2.399767	1.955434
H	0.854333	-3.528571	0.5494
H	0.071545	-3.034201	2.056334
H	1.77044	-3.545161	2.07738
H	1.788354	0.110058	2.392576
H	0.452665	-0.877181	2.97143
H	2.122472	-1.421935	3.245375
Li	-0.073435	-0.404703	0.195951

Abbildung 10.65 Molekel Darstellung von *(S,R,R)*-**94b'** [lokales Minimum; M05-2X/6-31+G(d)].Tabelle 10.552 Standardorientierung von *(S,R,R)*-**94b'** [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	1.75638	3.600711	-1.840342
C	0.981493	4.696231	-1.456714
C	2.412485	-3.733426	-2.114497
C	2.954237	-2.310817	-1.953286
C	1.83747	-1.396258	-1.444522
C	1.939075	2.511542	-0.994841
C	0.418958	4.677466	-0.175921
C	1.773749	-4.204717	-0.80593
C	0.73594	-3.191046	-0.308712
C	1.350735	2.443817	0.297882
C	0.604112	3.596837	0.672497
C	4.390894	0.436655	0.34054

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C	2.208681	-1.696588	0.957236
C	1.438745	1.303104	1.176043
C	3.337883	-0.065112	3.155896
N	1.247661	-1.817064	-0.161456
Si	2.807276	0.105638	1.339847
Li	-0.05846	-0.080103	0.287619
C	-1.624368	0.41865	2.79221
C	-1.571687	-1.814708	1.949907
C	-4.197426	-0.89084	1.354027
C	-5.466579	-0.492099	0.602069
C	-2.970469	-0.120214	0.840999
C	-5.281013	-0.75448	-0.890355
C	-2.779404	-0.339876	-0.669465
C	-4.074898	0.024138	-1.41728
C	-1.264311	-0.007937	-2.543737
C	-1.659758	1.827645	-1.085723
N	-1.723828	-0.40547	1.586763
N	-1.57139	0.361407	-1.161803
H	2.23141	3.592341	-2.816125
H	0.84036	5.541496	-2.118196
H	1.652946	-3.735884	-2.90657
H	3.202323	-4.420884	-2.426614
H	3.322363	-1.926114	-2.908489
H	3.799762	-2.302161	-1.259672
H	1.033936	-1.398418	-2.18666
H	2.180521	-0.367072	-1.343175
H	2.559256	1.6916	-1.336742
H	-0.166736	5.524069	0.167778
H	1.285644	-5.17419	-0.940828
H	2.548174	-4.342923	-0.046148
H	-0.098682	-3.155994	-1.021713
H	0.336195	-3.510534	0.655119
H	0.160891	3.617666	1.664277
H	4.300158	0.255161	-0.732324
H	4.696669	1.477672	0.474647
H	5.193309	-0.205132	0.718084
H	3.067949	-2.373493	0.847285
H	1.68421	-2.026341	1.862976
H	0.99469	1.506695	2.153691
H	3.983894	-0.934826	3.312759
H	3.880121	0.826488	3.480443
H	2.461526	-0.173922	3.802989
H	-2.458941	0.240708	3.485774
H	-0.691114	0.186217	3.305837
H	-1.600488	1.473226	2.515733
H	-2.271645	-2.125934	2.736803
H	-0.556076	-1.971736	2.316194
H	-1.720178	-2.447999	1.075172
H	-4.315047	-0.716819	2.427425
H	-4.04286	-1.96612	1.216772
H	-6.321536	-1.050735	0.990695

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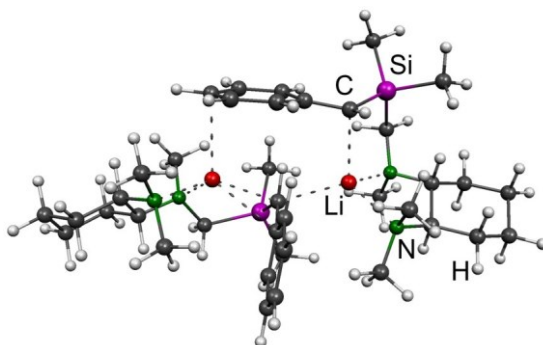
H	-5.676345	0.571668	0.762437
H	-3.175161	0.944394	0.992217
H	-5.128959	-1.828207	-1.053035
H	-6.176828	-0.470671	-1.447958
H	-2.585964	-1.40976	-0.830774
H	-4.274512	1.093454	-1.295111
H	-3.951441	-0.160173	-2.486536
H	-1.238236	-1.095547	-2.640821
H	-0.286091	0.397183	-2.805505
H	-1.994701	0.392234	-3.259024
H	-1.792603	2.156119	-0.056352
H	-0.719311	2.253038	-1.434072
H	-2.471974	2.227347	-1.705777

### 10.2.5. Details zu Kapitel 5.5

Tabelle 10.553 Absolute Energien der optimierten Strukturen auf M05-2X/6-31+G(d)-Niveau.

Struktur	SCF [Hartree]	ZPE [Hartree]
<b>95</b>	-2300.76796028	-2299.764666
<i>(S<sub>N</sub>,S)</i> - <b>98</b>	-1150.36785032	-1149.867474
<i>(S<sub>N</sub>)</i> - <b>TS1</b>	-1150.32559251	-1149.825624
<i>(S<sub>N</sub>,R)</i> - <b>98</b>	-1150.36847774	-1149.867774
<i>(R<sub>N</sub>,S)</i> - <b>98</b>	-1150.36764769	-1149.867054
<i>(R<sub>N</sub>,R)</i> - <b>98</b>	-1150.36628172	-1149.866022
<i>(S<sub>N</sub>,S)</i> - <b>96a</b>	-1383.99902511	-1383.357222
<i>(S<sub>N</sub>)</i> - <b>TS2</b>	-1383.97650058	-1383.336341
<i>(S<sub>N</sub>,R)</i> - <b>96a</b>	-1384.00515563	-1383.362459
<i>(R<sub>N</sub>,S)</i> - <b>96a</b>	-1384.00220796	-1383.360052
<i>(R<sub>N</sub>)</i> - <b>TS2</b>	-1383.97412223	-1383.332574
<i>(R<sub>N</sub>,R)</i> - <b>96a</b>	-1384.00516538	-1383.362716
pro- <i>(S)</i> - <i>(S<sub>N</sub>,R,R)</i> - <b>99</b>	-1230.13814684	-1229.560924
pro- <i>(R)</i> - <i>(S<sub>N</sub>,R,R)</i> - <b>99</b>	-1230.13631048	-1229.559620
pro- <i>(S)</i> - <i>(R<sub>N</sub>,R,R)</i> - <b>99</b>	-1230.13644496	-1229.559379
pro- <i>(R)</i> - <i>(R<sub>N</sub>,R,R)</i> - <b>99</b>	-1230.13491121	-1229.557506
<i>(S<sub>N</sub>,S,R,R)</i> - <b>TS3</b>	-1230.12066652	-1229.547035
<i>(S<sub>N</sub>,R,R,R)</i> - <b>TS3</b>	-1230.11294266	-1229.540478
<i>(R<sub>N</sub>,S,R,R)</i> - <b>TS3</b>	-1230.11389087	-1229.541284
<i>(R<sub>N</sub>,R,R,R)</i> - <b>TS3</b>	-1230.12036927	-1229.547057
<i>(S,R,R)</i> - <b>94b''</b>	-1441.55702178	-1440.862887

<i>(R,R,R)</i> - <b>94b''</b>	-1441.55683847	-1440.862546
<i>(S,R,R)</i> - <b>98</b>	-1305.38677300	-1304.802694
<i>(R,R,R)</i> - <b>98</b>	-1305.38810700	-1304.803659

Abbildung 10.66 Molekel Darstellung von **95** [globales Minimum; M05-2X/6-31+G(d)].Tabelle 10.554 Standardorientierung von **95** [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.1615478802	3.4202672802	-4.0096579023
C	2.3666734313	0.8097491334	-3.7349572436
C	1.1400365291	0.1416434711	-3.7307540863
C	0.0971502269	3.6735267694	-3.3070002525
C	-1.4480978224	6.220733743	-2.9842946412
C	-3.4998175711	0.5861030222	-2.5552230097
C	-1.8982707876	7.4738772659	-2.2310959394
C	2.7748680939	1.4308544198	-2.5493221637
C	0.3467310451	0.0965298937	-2.5892298879
C	-2.998198192	-0.6917653217	-2.3775604174
C	-1.6918912464	4.9419741022	-2.1646832114
C	1.2050650724	-3.4615684234	-2.0381578552
C	-3.926290765	1.3636832136	-1.4661348632
C	1.9924685936	1.3884081731	-1.4044544541
C	-1.1633105053	7.5807778007	-0.8964112156
C	0.737282373	0.7137041288	-1.3636629179
C	-2.8491091092	-1.2874742331	-1.0879915615
C	-0.990070831	5.0563320732	-0.8000836658
C	-2.16858315	-2.5252035411	-0.901900263
C	2.8697113805	-1.9753659414	-1.176258553
C	2.7494088465	-5.0465874975	-0.2456793851
C	-1.4275512775	6.3288665092	-0.0603830994
C	-3.9043720181	0.7574250598	-0.1998498565
C	-0.0873097525	0.6529319747	-0.1819695588
C	-3.394055175	-0.515747918	-0.0152316223
C	-2.1446426042	-5.4438218114	-0.0157604589
C	2.0706225349	-3.7602087851	0.2530856464
C	-2.3922581872	3.7734228373	0.75090098

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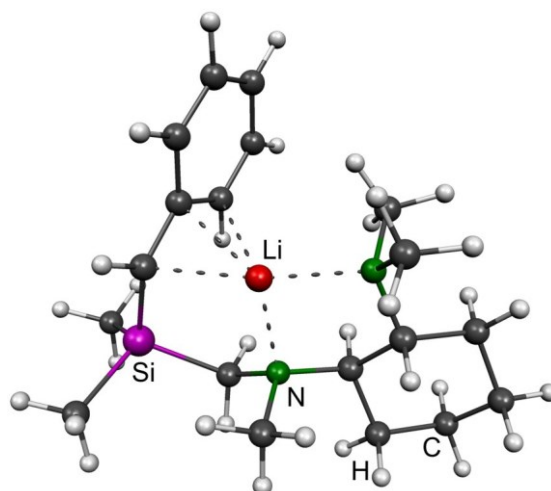
C	3.1473765991	-5.9641864237	0.9102907536
C	-0.0033004547	3.5266301131	0.8673540098
C	0.8481107703	-4.1033728545	1.1191996952
C	-4.1270293791	-3.6418143953	1.3664642072
C	1.9103760884	-6.3286965632	1.7287077507
C	-1.2413778847	-3.1469349554	1.9772394071
C	1.2456966075	-5.0577855375	2.2571064625
C	1.8415889234	1.5736967343	2.1957372765
C	-1.1555068783	1.2108424683	2.6481608171
C	0.864595557	-2.187657749	2.6519013908
H	-2.020299298	4.1495944153	-4.8180293858
H	2.9828871704	0.8438232624	-4.6242214461
H	0.7919218942	-0.3552571081	-4.6309987778
H	0.2825654902	4.4034433495	-4.105451743
H	-1.9200414581	2.4316524172	-4.4017709386
H	-1.963865869	6.1556035196	-3.9450947076
H	0.3316181544	2.6797357802	-3.6871645189
H	-3.5876972284	0.9758635095	-3.5629893144
H	-0.3778660074	6.3130904823	-3.1969961369
H	-3.2084010732	3.4287433793	-3.7020885933
H	-1.7165175646	8.3595483845	-2.8449048005
H	-2.6845679148	-1.2643278689	-3.2451017917
H	0.773941003	3.8674769274	-2.4768763088
H	-0.5993849098	-0.4321177746	-2.6188775783
H	3.7254677696	1.9530048791	-2.5164568812
H	0.8110987681	-2.6925726968	-2.7032208854
H	-2.9782104287	7.4271581816	-2.0474692737
H	1.9863929534	-4.0170864328	-2.57384223
H	-2.771484337	4.8530175736	-1.9835583941
H	0.3897865175	-4.140268364	-1.7863527724
H	-4.3716192141	2.3412030592	-1.6127821297
H	-1.9144236111	-3.0337878274	-1.8333567267
H	-0.0877444764	7.6854640064	-1.0805735557
H	2.6062447061	-1.3180186938	-2.0024498977
H	0.0814054549	5.1578132365	-0.9946595761
H	3.737440983	-2.5814329362	-1.4755482013
H	2.0571310048	-5.5966462932	-0.8913629032
H	-1.4834392501	8.4709471875	-0.3492829324
H	3.6224354847	-4.7915090489	-0.8529640425
H	-1.3950077566	-5.5435559839	-0.805163949
H	2.3631021295	1.8618372933	-0.5023554588
H	-3.0871588917	-5.8304608676	-0.4142923435
H	-1.0572580015	0.1679403742	-0.3008773946
H	-3.2424342393	4.0322231257	0.117454028
H	-2.4992903664	6.2829120113	0.1583762254
H	3.1441738194	-1.35307802	-0.3227467771
H	3.6335486884	-6.8624946985	0.5213859931
H	-4.3021869004	1.2911998964	0.6573434047
H	0.1380075103	-4.6290509269	0.4766448856
H	-0.9032003502	6.3827138743	0.8982859704
H	0.9118482903	3.7461508032	0.3068182003

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H	-4.9108302983	-3.6965552091	0.6064403064
H	1.2047879924	-6.8795033168	1.0952807831
H	-1.8495814607	-6.0843542569	0.8217683637
H	-3.3700707001	-0.927340446	0.9876253467
H	2.7952578202	-3.2355504937	0.8855573547
H	-2.549233666	2.7634757936	1.1221728314
H	-2.3662055019	4.4556922353	1.611803157
H	3.8748591577	-5.4579948268	1.5558876902
H	-4.3181519457	-2.7571786396	1.9773565854
H	2.589833127	2.2132171429	1.72065823
H	-0.0041133272	4.1899792872	1.7494343401
H	2.1760812123	-6.9856853919	2.5608207323
H	-4.2191994024	-4.5199320953	2.0135867482
H	-2.0615836743	0.7998535848	2.1976895501
H	0.3628698684	-5.3066156102	2.8516050385
H	2.2287274838	0.551676535	2.1933847703
H	-1.6453051094	-2.1941528052	2.3435579462
H	1.9166450036	-2.0522004544	2.3962880371
H	-1.2970771145	-3.8416067758	2.8321270179
H	1.9530886601	-4.5534340517	2.9246798007
H	-0.7674829145	0.4706090337	3.3516050079
H	0.423567698	-1.2002097801	2.7746937823
H	1.746600611	1.8964845205	3.2371800914
H	-1.4287379251	2.0956274624	3.2312226405
H	0.7962392224	-2.7183857768	3.6109725438
N	-1.3015807635	3.6894417654	-2.8567277449
N	1.715329537	-2.808669	-0.8271978325
N	-1.1478645547	3.8099867486	-0.0201989184
N	0.1538145634	-2.882744282	1.5778198366
Li	-1.3872811489	2.1853602385	-1.3467372791
Li	-0.0031380423	-1.7098118288	-0.1560995451
Si	-2.4173026668	-3.6403038201	0.5321345212
Si	0.1443784119	1.6552008894	1.3330916141

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Abbildung 10.67 Molekel Darstellung von  $(S_N,S,R,R)$ -**98** [lokales Minimum; M05-2X/6-31+G(d)].Tabelle 10.555 Standardorientierung von  $(S_N,S,R,R)$ -**98** [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.5076532771	3.5465288908	-3.7466432931
C	2.0684160145	0.8087164624	-3.8016158726
C	0.9802277436	-0.0681941717	-3.6698602162
C	-0.1356936822	3.8410628669	-3.7223121215
C	-1.2080029608	6.4073900536	-2.983543456
C	-1.5271077328	7.6776456713	-2.1915804408
C	2.3536535888	1.6519816925	-2.7324256729
C	0.2161894717	-0.1025735071	-2.5170731887
C	-1.5540799946	5.1494319577	-2.1738135681
C	1.5832260438	1.6383091002	-1.5708285993
C	-0.7572991393	7.6861251088	-0.8708093017
C	0.4905583499	0.7356392922	-1.3884698452
C	-0.7933350657	5.1529543348	-0.8320191655
C	-1.0963877783	6.4392160469	-0.0526403657
C	-0.3423873743	0.7464358441	-0.2265135557
C	-2.401169148	3.8201478677	0.476417621
C	-0.0634832499	3.5807640152	0.9570998202
C	1.6953256098	1.4453853358	2.1418695321
C	-1.2944545203	1.206210223	2.6297298636
H	-2.6721584847	4.2944552638	-4.5348416238
H	2.670977408	0.819335906	-4.7006672144
H	0.7335095225	-0.7427863187	-4.4830811392
H	-0.2201208691	4.4838631613	-4.6080934092
H	-2.3356324796	2.5809042303	-4.2249796975
H	-1.7529997835	6.4007304557	-3.9320131042
H	0.0522970666	2.8161494806	-4.0468743431
H	-0.1401183247	6.4077868207	-3.2245795056
H	-3.4082957494	3.4747931045	-3.1348284673
H	-1.278050321	8.5588057115	-2.7877755855
H	0.7239551976	4.1560688493	-3.131765336

H	-0.6084547641	-0.8042617885	-2.4413018786
H	3.1934445928	2.3368584304	-2.7946371915
H	-2.602896232	7.7236009194	-1.9852697163
H	-2.6245805209	5.1995119575	-1.9468148968
H	0.3187151333	7.708047737	-1.0791975385
H	0.2799726721	5.1390874593	-1.0612935674
H	-0.9899921648	8.5863747161	-0.2968840153
H	1.8735432256	2.2874791614	-0.7511946261
H	-1.0788918624	-0.0529426058	-0.1705032668
H	-3.1538449396	4.0871409702	-0.2665123384
H	-2.162430467	6.4655171469	0.200024253
H	-0.5409555252	6.4280215016	0.8892174399
H	0.9255767405	3.8739300993	0.5903111219
H	-2.5831533844	2.7909647846	0.7859402486
H	-2.5268471664	4.468063093	1.3547156704
H	2.5184723046	1.6210789165	1.4452545616
H	-0.2408547317	4.1639992685	1.8760187396
H	-2.2802366123	1.0253052386	2.1950196599
H	1.7945077781	0.4229625484	2.5152008534
H	-0.9852125537	0.2875846146	3.1358461393
H	1.8137969632	2.1286226052	2.9892138209
H	-1.3914617649	1.9872485676	3.3894202005
N	-1.3562673625	3.8708323764	-2.9029272305
N	-1.0543363703	3.9092453842	-0.0868132648
Li	-0.8933132646	2.4460916071	-1.4507818158
Si	-0.0025058048	1.6665015405	1.3177898894

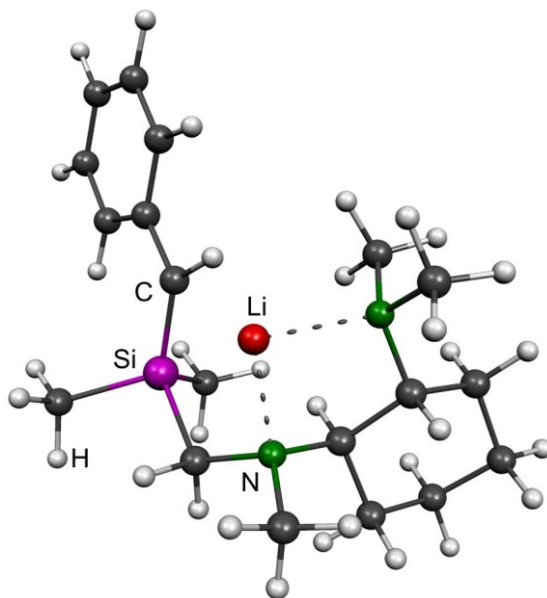


Abbildung 10.68 Molekel Darstellung von  $(S_M, R, R)$ -**TS34** [Übergangszustand; M05-2X/6-31+G(d)].

Tabelle 10.556 Standardorientierung von  $(S_N, R, R)$ -TS34 [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	4.0446502584	0.074519829	-4.0251861378
C	3.2375563986	-0.0310027454	-2.9027279824
C	-0.5420597858	-1.6604760542	-1.8712276097
C	4.2092379862	1.2979141875	-4.6788262245
C	2.5356667588	1.0765517686	-2.356276001
C	1.6921288219	0.910592533	-1.1918313283
C	-0.4766997537	-3.1484101743	0.0025234095
C	-3.1745930824	-1.5208819518	-0.8104408373
C	3.5366553361	2.40613985	-4.1650180557
C	2.7255570117	2.3033031002	-3.0412806787
C	-0.5959174158	3.04270668	-1.6863057728
C	-1.9796211529	-1.2332847505	0.1094224689
C	-4.4800370842	-0.9717081471	-0.2341675178
C	-1.8736157717	0.2710831992	0.4226201674
C	1.7508992299	3.8081648195	0.0490324761
C	-4.3572358732	0.5363575587	-0.0228807569
C	-0.1544080198	1.8816344487	1.15440592
C	-3.2066710982	0.8292145546	0.9392173189
C	-1.0127621361	0.2660563925	2.7407553174
H	4.5567212042	-0.8086491994	-4.3926287486
H	3.1468431408	-0.9950728818	-2.4081275643
H	0.4808395393	-1.9223192021	-2.1443181137
H	-1.2254191326	-2.3406852652	-2.3927007934
H	-0.7059425235	-0.6359687374	-2.2042355423
H	4.8409265052	1.3838009758	-5.5538200399
H	1.6650374752	-0.1584250807	-0.9939573738
H	0.4885289906	-3.4945687928	-0.3700103922
H	-1.2539058044	-3.8149142831	-0.3950480547
H	-3.0092900245	-1.0446604482	-1.7813389237
H	-3.2530167935	-2.5974359949	-0.9880604963
H	-1.2735959555	2.2827600352	-2.0851323854
H	-0.1175393974	3.519177371	-2.5455928107
H	-0.4754062105	-3.2203870808	1.0912144574
H	-5.3059533475	-1.2020342688	-0.9110447682
H	3.642802348	3.3720504814	-4.6474482856
H	-1.6343314477	0.7837427784	-0.5150584551
H	2.2087751351	4.3472685255	-0.7816759176
H	-4.1731389842	1.0267906937	-0.9855424639
H	-1.1912739508	3.8055154566	-1.1731247187
H	-2.1569636565	-1.7550696282	1.0568830371
H	-4.703379737	-1.457472233	0.7230618892
H	2.5541011086	3.4811934962	0.7139022532
H	-5.2875375623	0.9482952594	0.3749646002
H	1.1136144645	4.5150058719	0.5915211614
H	-3.105680739	1.9043816137	1.1095060104
H	0.6176886165	1.9978631721	1.9226283697
H	-1.48632155	-0.7093848372	2.8643577956
H	-0.9047349089	2.6627323768	1.3593645652
H	-3.4459924041	0.3688273941	1.9037552232

H	-0.0712491987	0.2591226315	3.2914953298
H	-1.6590436864	1.0337638944	3.1831639278
N	-0.6801451907	-1.7555509075	-0.4064538952
N	-0.7293011263	0.5308857761	1.3293777503
Li	0.6499099315	-0.3507216888	0.2937141433
Si	0.7285081394	2.3101393025	-0.5203156029

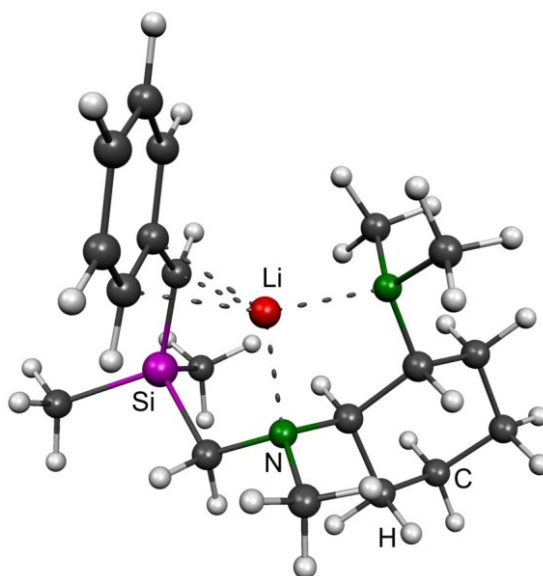


Abbildung 10.69 Molekel Darstellung von  $(S_N,R,R,R)$ -**98** [globales Minimum; M05-2X/6-31+G(d)].

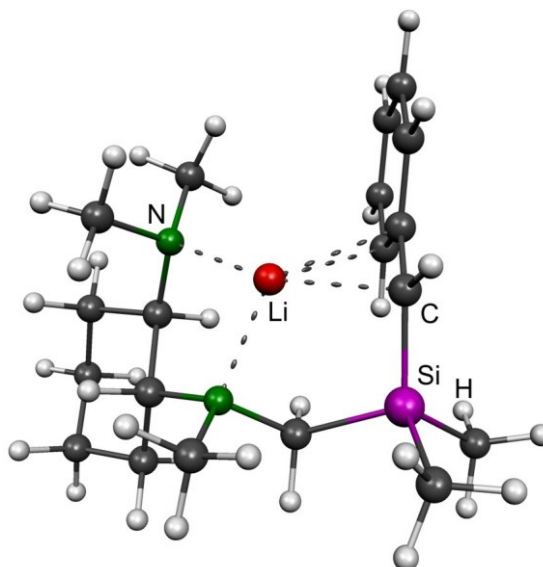
Tabelle 10.557 Standardorientierung von  $(S_N,R,R,R)$ -**98** [globales Minimum ;M05-2X/6-31+G(d)].

	x	y	z
C	-2.2777464274	0.2814241867	-2.4637510474
C	-2.331497618	-1.0928031974	-2.3301735578
C	0.9120825525	-3.3197452966	-2.034923152
C	-2.3341589379	1.1312951167	-1.3469062713
C	-2.4601196123	-1.7366502602	-1.0563311018
C	-2.3755348331	-3.151380753	-0.9137981565
C	2.1355141907	-1.4901279955	-1.0942982706
C	2.7623071108	-4.579291682	-0.2697327231
C	-2.4554806749	0.5458089211	-0.092725633
C	-2.5093533826	-0.8417333055	0.0601298206
C	-2.3912359538	-5.9908662886	0.1336189714
C	1.8178093522	-3.493403722	0.2667879796
C	3.3624455675	-5.4176360145	0.8590793788
C	0.7052203234	-4.1154211113	1.1370511489
C	-4.4101146642	-4.0571821455	1.367151906
C	2.2446108679	-6.0628600848	1.676029949
C	-1.5373536028	-3.6400688667	2.0362262712
C	1.3250106416	-4.9821100964	2.2444004325

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C	0.3274235777	-2.2697267009	2.7299433722
H	-2.1951056359	0.7089046617	-3.457572858
H	-2.2987857318	-1.7200716177	-3.2154382481
H	0.3143012754	-2.6510404983	-2.6567594578
H	1.8060089798	-3.619940241	-2.596833441
H	0.3027482135	-4.1956769356	-1.8169731722
H	-2.2957201582	2.2065896407	-1.4620187482
H	-2.3203320537	-3.7046401567	-1.8503048455
H	1.6528976766	-0.8506562496	-1.8350139539
H	3.1042125212	-1.8178669453	-1.4972945593
H	2.207947493	-5.2488596855	-0.9346971684
H	3.5525408838	-4.1140631741	-0.866557436
H	-1.4847884984	-6.1329287199	-0.4614555186
H	-3.2313622048	-6.3713328292	-0.45395577
H	2.3085375598	-0.9004833708	-0.1929213727
H	4.0269581789	-6.1784069706	0.4424641374
H	-2.5215992584	1.1709340655	0.7916618622
H	0.1016323851	-4.7632722859	0.4916552101
H	-5.1634349814	-4.479300108	0.6974038669
H	1.6682930385	-6.7399239673	1.0347873738
H	-2.3103881132	-6.6064601487	1.0342725536
H	-2.6608473189	-1.2497921131	1.0558677608
H	2.411818878	-2.8375992075	0.9127301026
H	3.9708907498	-4.7822200529	1.5133193945
H	-4.6833737601	-3.014835487	1.5537876919
H	2.6585470571	-6.664997978	2.4884676178
H	-4.4556457061	-4.5983759295	2.3177272086
H	0.5313379145	-5.4318850509	2.8456380671
H	-2.0746091199	-2.8422930822	2.560198645
H	1.323615786	-1.9038070334	2.4762252387
H	-1.4227440486	-4.445987415	2.7787126243
H	1.9156914473	-4.3462810016	2.9133731052
H	-0.3197116863	-1.4039932784	2.8797307074
H	0.383779018	-2.8233884179	3.6756755702
N	1.251391438	-2.6162571448	-0.7896998592
N	-0.2257007281	-3.0788013944	1.6409397918
Li	-0.5984849607	-2.1522680284	-0.1049674665
Si	-2.6906150071	-4.1677325522	0.5690860292

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Abbildung 10.70 Molekel Darstellung von  $(R_N,S,R,R)$ -**98** [lokales Minimum; M05-2X/6-31+G(d)].Tabelle 10.558 Standardorientierung von  $(R_N,S,R,R)$ -**98** [lokales Minimum ;M05-2X/6-31+G(d)].

	x	y	z
C	-2.9967497987	0.044064005	-1.9656180987
C	-3.715286505	-1.0913306764	-1.6504874301
C	-1.3746303011	1.843022638	-1.3614360173
C	-2.2297275491	0.7642272842	-0.9920392102
C	-3.7322189781	-1.6145131	-0.3450122125
C	-2.2712927015	0.2059345865	0.3250621084
C	-3.0078582508	-0.9421700564	0.6297877752
C	0.0431930334	4.5297206985	-1.3911646339
N	1.0637747238	-1.0944596368	-1.3988912029
N	1.2122662027	0.8889359351	0.6592122793
Si	-0.4327953059	3.032886086	-0.3357470483
Li	-0.2211988672	0.1905212891	-0.6021555526
H	0.5224626162	4.2120250194	-2.3213827926
H	-0.8462755555	5.1074799964	-1.6538477744
H	0.7337064042	5.1917508718	-0.8609874395
C	-1.2880932672	3.6873946943	1.230223207
H	-0.5752234279	4.173005832	1.9036194145
H	-2.0293845175	4.4325067155	0.9283327714
H	-1.8228132138	2.9169285288	1.7892105125
H	-3.0092606648	0.4227345117	-2.9824285672
H	-4.2824546468	-1.5863936031	-2.4318392265
H	-4.3031025197	-2.5026244192	-0.1073742204
H	-3.0127368089	-1.3021301567	1.6534759639
H	-1.7580161712	0.7208922093	1.1318618262
C	0.7753683563	-2.3929438075	-0.7830485994
H	0.9553651797	-2.3512159305	0.2917866134
H	-0.2801547977	-2.6255920721	-0.9387413202

H	1.3778248178	-3.2034015213	-1.2131184503
C	0.8543247429	-1.1721611195	-2.8461638326
H	-0.1793944582	-1.4667250054	-3.0352278222
H	1.0128772377	-0.188589737	-3.2895477124
H	1.518671347	-1.9013861357	-3.3290844321
C	0.9208667079	0.9368353795	2.0916090575
H	0.7107832024	-0.0678672616	2.4638693409
H	1.7495411188	1.3678677347	2.6702743443
H	0.0437154598	1.5598152449	2.260700506
C	1.294440106	2.2701687217	0.1186837461
H	1.8010118246	2.2277291341	-0.8516784417
H	1.9107096302	2.9095025317	0.7719202685
C	2.3955025468	0.037480608	0.3914559406
H	2.3075949605	-0.8144523148	1.0772557879
C	2.3826946846	-0.5233850686	-1.0453134146
H	2.5249854499	0.3216230735	-1.7297835897
C	3.5584813216	-1.4927270612	-1.2369731125
H	3.544506983	-1.8961756425	-2.2530163123
H	3.444684829	-2.3396330238	-0.5510006676
C	3.7442860923	0.7166865322	0.6724592879
H	3.7513006395	1.1148036639	1.6903506493
H	3.8686554091	1.5679415103	-0.0042463104
C	4.8971623888	-0.8097280169	-0.9515635816
H	5.0510690489	0.0084253535	-1.6646379382
H	5.7160429199	-1.5186569773	-1.0958549044
C	4.9121485822	-0.250745675	0.4705482248
H	5.8573651949	0.2587509549	0.6729733471
H	4.8344702454	-1.0779790652	1.1858627848
H	-1.4223347015	2.1165847403	-2.4145248884

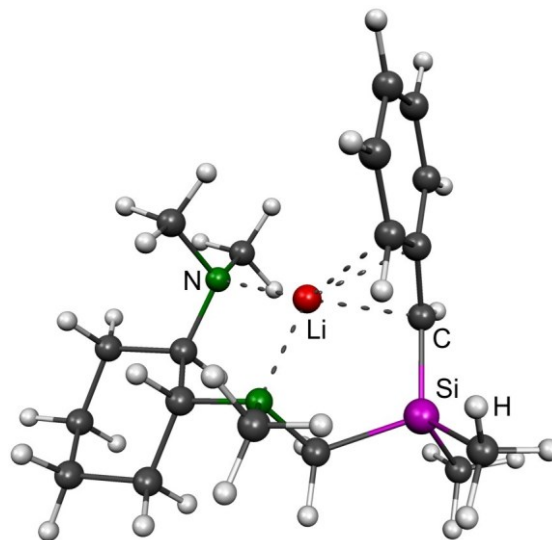


Abbildung 10.71 Molekel Darstellung von  $(R_n,R,R,R)$ -**98** [lokales Minimum; M05-2X/6-31+G(d)].

Tabelle 10.559 Standardorientierung von  $(R_M, R, R, R)$ -98 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.3434981904	2.5418736592	-0.8751120991
C	-1.9761518227	3.6819802964	-1.5689167145
C	-1.9780031951	0.8567294722	0.9415289467
C	-1.6129115978	2.0650129811	0.2563440315
C	-0.8504088308	4.4309289295	-1.1984932538
C	-0.463692368	2.8393469449	0.59423975
C	-0.1097306256	3.9912488299	-0.1048461067
C	-0.9858550371	1.4019226588	3.9504985337
N	1.2016623664	0.3133983689	-1.5788262483
N	0.7816823726	-1.0929936425	0.8493789438
Si	-1.2149755383	0.2262154382	2.474251126
Li	-0.3601273769	0.1941260022	-0.271240073
H	-0.3982472059	2.2887680997	3.7034887073
H	-1.9640058054	1.7442841902	4.2980510833
H	-0.4922656197	0.8879343292	4.7817716843
C	-2.2298108088	-1.2358979775	3.1319571317
H	-1.6307853521	-1.8967345816	3.765251895
H	-3.0522487414	-0.849293332	3.7401937802
H	-2.6690539738	-1.829586825	2.3268311163
H	-3.2298313615	1.9932343829	-1.1779156205
H	-2.5814647533	4.0033271714	-2.4101430969
H	-0.5764614642	5.3296627477	-1.7360515742
H	0.7575631429	4.5563420554	0.2223116805
H	0.1196327247	2.5674094664	1.4675623712
H	-2.9518836472	0.4481952813	0.6786657551
C	1.0353853418	-0.7779216837	-2.5412851623
H	0.9038038443	-1.7310961025	-2.0289125411
H	0.1365176209	-0.5822908976	-3.1290743992
H	1.8792281575	-0.8611854621	-3.2377854694
C	1.2616934576	1.590530485	-2.2990651488
H	0.2892899416	1.7930834747	-2.7506602297
H	1.4681608508	2.3968188555	-1.5976141869
H	2.0233049329	1.5848148562	-3.0894895319
C	0.3085783731	-2.4591877561	1.0623261165
H	0.3713221948	-3.0267966816	0.131986272
H	0.8904855608	-2.9817608957	1.8359685096
H	-0.7321005091	-2.4346972516	1.3794969472
C	0.6205614542	-0.3101052196	2.0984549428
H	1.1888310458	0.6205417669	1.9949323818
H	1.0622847547	-0.843968958	2.9556305019
C	2.142596152	-1.0803901328	0.2664823081
H	2.2081521762	-1.9709111062	-0.3693504345
C	2.3434809019	0.1436141818	-0.6468885169
H	2.3299194644	1.0421508069	-0.015021616
C	3.7167839135	0.0634429961	-1.331125632
H	3.8691554374	0.9412795735	-1.9631270053
H	3.7481612063	-0.8167532049	-1.9832149286
C	3.2832811504	-1.185713831	1.2874086504
H	3.1210678904	-2.0610767908	1.9228150037

H	3.2752336953	-0.3089114965	1.9417274115
C	4.8471340211	-0.0475059182	-0.305241859
H	4.8668744754	0.8562198115	0.314797252
H	5.8098602157	-0.103375877	-0.819050149
C	4.641999575	-1.2686244754	0.5899885548
H	5.4400085236	-1.3380494566	1.3331749156
H	4.6910638891	-2.1787185572	-0.019493707

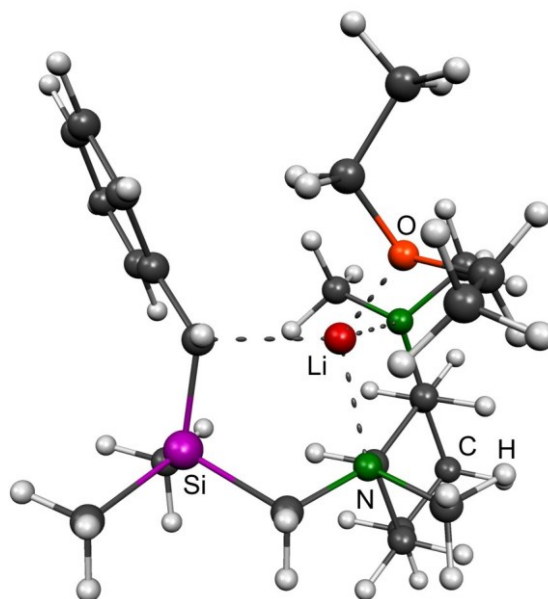


Abbildung 10.72 Molekel Darstellung von  $(S_N,S,R,R)$ -**96a** [lokales Minimum; M05-2X/6-31+G(d)].

Tabelle 10.560 Standardorientierung von  $(S_N,S,R,R)$ -**96a** [lokales Minimum; M05-2X/6-31+G(d)].

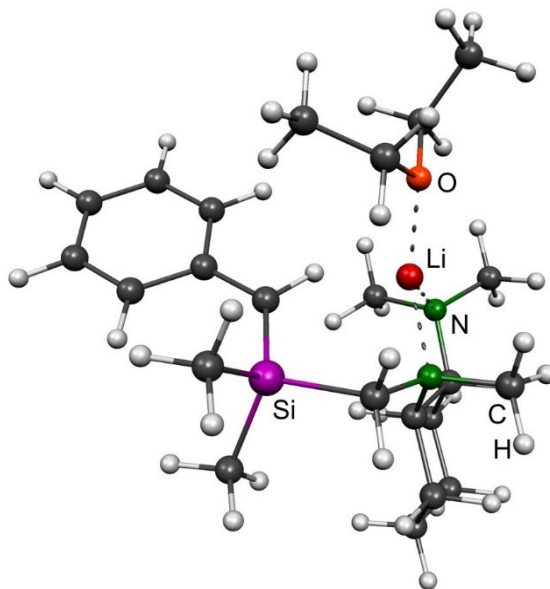
	x	y	z
C	-5.0043491035	0.3686313058	-0.8382016576
C	-3.9641161713	0.2813308895	0.0789852202
C	0.2225080475	0.7441588992	-2.1414720508
C	-4.921418439	-0.2597994088	-2.081414038
C	-2.7625884277	-0.426892561	-0.190045744
C	-1.6666124455	-0.4484300522	0.761179021
C	1.2253232271	2.8173783849	-1.4994210404
C	3.0601369844	0.2765681936	-2.2345832646
C	-3.7637214367	-0.9854193352	-2.3680911582
C	-2.717722141	-1.0653196467	-1.4570266276
C	-0.1335752962	-3.0540612427	-0.2650318428
C	2.386649768	0.7511383609	-0.9371298833
C	4.4253179049	-0.3591886314	-1.9722605837
C	2.266888959	-0.4125100953	0.0652684295
C	-1.2505740736	-3.0619653716	2.510991672
C	4.2713919147	-1.5373396596	-1.0120497031

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C	0.9592122719	-1.1373564551	2.0108932857
C	3.6415281128	-1.0603990835	0.2966424454
C	2.455985254	0.7435728398	2.225012193
N	1.0776626992	1.4077219233	-1.1500960849
N	1.5839893295	0.0061640595	1.3107702257
Li	-0.0660063938	1.0288998722	0.5457711928
Si	-0.6079144222	-1.8827920175	1.1606528266
O	-0.6174689677	2.8247521452	1.1051922403
C	0.0512776989	3.6506341872	2.0563918127
C	-2.0262189931	3.0574349688	0.9425778952
H	-5.8990401481	0.9217226106	-0.5708181213
H	-4.0774075106	0.7507650761	1.0519358095
H	-0.7933040557	1.1348005682	-2.0572626287
H	0.5762866057	0.8994097333	-3.1696733346
H	0.1672099586	-0.3237795229	-1.9370074052
H	-5.7333448175	-0.1980429041	-2.7950332155
H	-1.9449686184	0.0503262619	1.7021755694
H	0.235267568	3.2652874419	-1.591434229
H	1.760510308	2.9612158395	-2.4492270974
H	1.7611313068	3.341672163	-0.7062013665
H	2.4234523631	-0.4715261458	-2.7177453518
H	3.1520846066	1.1166794502	-2.9292166056
H	-3.6713524596	-1.4988815572	-3.3196694448
H	-1.8369651898	-1.6357876809	-1.725868234
H	0.1984385179	-2.5698266373	-1.1857514634
H	-0.9991015118	-3.6735531495	-0.516863028
H	0.664345579	-3.7243380317	0.0721858036
H	3.0343417484	1.5129784125	-0.486768119
H	4.871518136	-0.6835022148	-2.9155919166
H	5.1043168058	0.3812601794	-1.5328201042
H	1.6178908675	-1.1667517127	-0.3862662199
H	-2.154110002	-3.5689836037	2.1616171496
H	-1.5141097492	-2.5096701471	3.4175767543
H	-0.5137071651	-3.8268635264	2.7780200752
H	3.6350751954	-2.3022010004	-1.4723910057
H	5.2399227378	-2.0025264317	-0.812459812
H	0.5756492839	-0.7484181761	2.9630328436
H	1.7055765817	-1.9015201901	2.2831144991
H	3.5407436318	-1.8910733048	0.9997956163
H	4.3181590217	-0.3298617773	0.7540328844
H	2.9709149254	1.552374394	1.7016295259
H	1.8433984962	1.1839454079	3.0141372902
H	3.2055804648	0.0997851929	2.7033545586
H	1.0973204353	3.3488892196	1.9998025525
H	-0.0101399235	4.6960693667	1.7414485261
H	-2.337298427	2.348620436	0.1765927771
H	-2.547013823	2.7873293753	1.865106513
C	-2.3511338865	4.4809968537	0.523045856
H	-3.4049772297	4.532245074	0.2421771108
H	-2.1851928609	5.2050840847	1.3234402681
H	-1.7530033847	4.7730784221	-0.3431999382

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C	-0.4722856673	3.4717633212	3.4731733547
H	0.1863291842	3.9867687165	4.1760445388
H	-1.4757409267	3.8826287676	3.5953185329
H	-0.4989641636	2.4110824166	3.7347378508

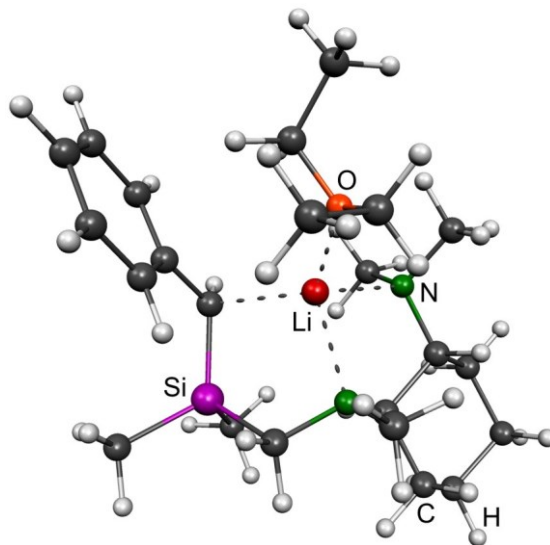
Abbildung 10.73 Molekel Darstellung von  $(S_N, R, R)$ -**TS2** [Übergangszustand; M05-2X/6-31+G(d)].Tabelle 10.561 Standardorientierung von  $(S_N, R, R)$ -**TS2** [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	-4.5057999392	-1.4840243004	-0.4333788397
C	-3.2721738159	-0.8916702116	-0.199413193
C	-0.0816069113	0.0877184311	-2.3016108281
C	-4.8944494362	-2.6361783656	0.2524999186
C	-2.33422858	-1.4157658257	0.735717882
C	-1.0707764351	-0.7865739987	0.9645038944
C	1.0927510914	2.1388967254	-2.6858076092
C	2.6504263995	-0.67926346	-2.5595459988
C	-3.9971091272	-3.1746517169	1.1802576188
C	-2.7612202743	-2.5916389494	1.4153409682
C	0.9932644289	-2.9513060679	2.0100417359
C	2.2544522817	0.3656911973	-1.5061137027
C	4.0433165621	-1.2486682496	-2.2883772008
C	2.3179430381	-0.2469001119	-0.0957475908
C	-0.4367703471	-1.2307953636	4.0214608945
C	4.0805556453	-1.8861259169	-0.901194851
C	1.560332379	0.081078514	2.2271748445
C	3.7043278326	-0.8533783925	0.16148816
C	2.8592079202	1.808011197	1.1674362887
N	0.9355261387	1.011158534	-1.7640885281

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N	1.8935447261	0.7286171859	0.9395427881
Li	0.2154203901	1.4167164673	0.129506919
Si	0.1559826807	-1.246791359	2.2115789157
O	-1.025439734	2.7735328158	0.6154905776
C	-1.4790254844	2.7446968695	1.9882318278
C	-1.9406517509	3.3442343257	-0.3272828996
H	-5.176167913	-1.0373843837	-1.1611772617
H	-3.0054758001	0.0087611049	-0.7489424463
H	-1.0470916122	0.598597922	-2.3020462409
H	0.1426220521	-0.2183838614	-3.3303148065
H	-0.1784122677	-0.7896709504	-1.6612155333
H	-5.8570640132	-3.0975144394	0.0723513584
H	-0.9581434308	0.0842802725	0.3261020771
H	0.1162943805	2.5822934627	-2.885788526
H	1.5237284627	1.8306999817	-3.6480853907
H	1.735257662	2.899866083	-2.2393792453
H	1.9335538638	-1.5055459698	-2.5408998499
H	2.6062698795	-0.2335931011	-3.5577949933
H	-4.2669897751	-4.0705829507	1.7299826095
H	-2.0966758313	-3.0533051379	2.1385831909
H	1.4743130408	-3.0652877443	1.0346573827
H	0.2520263783	-3.7504789864	2.0961931267
H	1.7464547925	-3.1122598652	2.7887453116
H	2.9952024787	1.1717023502	-1.5579248716
H	4.2984680953	-1.9812497006	-3.0578498907
H	4.791750973	-0.449091627	-2.344053224
H	1.571976702	-1.0483156565	-0.0619678613
H	-1.236635611	-1.958827276	4.1773395826
H	-0.83851631	-0.2462878721	4.2799371655
H	0.3748678423	-1.4699255405	4.7163778148
H	3.3742724058	-2.7232964004	-0.8662303062
H	5.0719810736	-2.2938059779	-0.6893390634
H	1.2253340664	0.8778217429	2.9015547706
H	2.4635354085	-0.3387145052	2.6990592186
H	3.7208203123	-1.3095667246	1.1540397371
H	4.4590469289	-0.0580782619	0.1537372778
H	3.1583378431	2.2751844567	0.2274139833
H	2.3861041457	2.5713503188	1.7885247783
H	3.7573871743	1.458881232	1.691640095
H	-0.7201358306	2.1609554881	2.5091749065
H	-1.4557242655	3.7664335218	2.3763745782
H	-1.4388208476	3.2543415481	-1.2909478207
H	-2.8492401472	2.7386974843	-0.3606743489
C	-2.2542751299	4.8021147887	-0.0361026438
H	-2.84169454	5.2175136419	-0.8574628644
H	-2.8360628639	4.9179292319	0.879329946
H	-1.3325531653	5.3793030326	0.0585649525
C	-2.8371732652	2.0950205817	2.1761228007
H	-3.0186760051	1.9859955996	3.2479533842
H	-3.6501978664	2.6966035152	1.7649697673
H	-2.8489113199	1.0978879085	1.732035211

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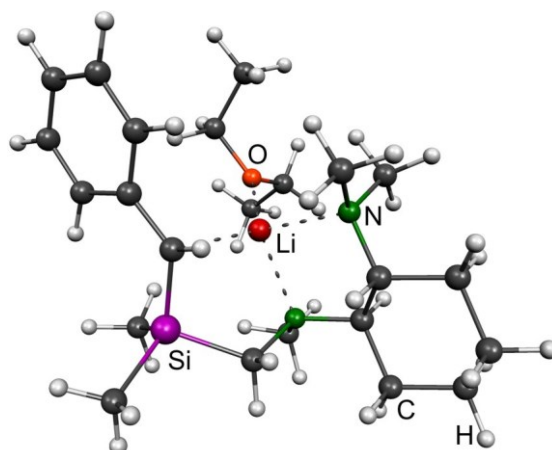
Abbildung 10.74 Molekel Darstellung von  $(S_N,R,R,R)$ -**96a** [lokales Minimum; M05-2X/6-31+G(d)].Tabelle 10.562 Standardorientierung von  $(S_N,R,R,R)$ - **96a** [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-4.9886408902	-0.3895665664	0.7638352403
C	-3.8232908871	-0.9643033577	0.27989452
C	0.4698376787	-0.4252265408	-2.4123248132
C	-5.010080002	0.280145559	1.992986238
C	-2.5900792616	-0.9019016189	0.9866399166
C	-1.3689572111	-1.4531024524	0.4460593976
C	0.7292382287	1.9439990971	-2.2912479577
C	3.2866720592	-0.0046373845	-2.165282051
C	-3.8221222013	0.3387894004	2.7236833704
C	-2.6500552793	-0.228580361	2.2369721006
C	0.9071473572	-3.4989045731	0.5168926427
C	2.3271274648	0.54923504	-1.0991010923
C	4.7230801501	-0.1056156172	-1.6538237686
C	2.3967860772	-0.2949956409	0.186870975
C	-0.6465828506	-3.0829981845	3.0913186063
C	4.764199496	-0.9999001763	-0.416643817
C	1.1094588909	-0.8452967769	2.1964982131
C	3.8528559265	-0.422087179	0.6653509944
C	1.9923669039	1.3819448503	1.9391314388
N	0.9305347744	0.6867426014	-1.5745736756
N	1.47182415	0.2132095374	1.2278664777
Li	-0.3014787763	0.4844680073	0.1292761386
Si	-0.0806934081	-2.2040606198	1.5050744733
O	-1.2536113862	2.2192828222	0.0856939594
C	-0.9280021263	3.3720761627	0.8593381607
C	-2.6281198527	2.1131472329	-0.3323529166

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H	-5.8997235577	-0.4713434105	0.1799345003
H	-3.841155039	-1.4856870785	-0.6725331353
H	-0.6114697294	-0.3437598702	-2.5337814822
H	0.9365355391	-0.4214340382	-3.4067357996
H	0.6684952899	-1.3767267764	-1.9215435747
H	-5.9231819615	0.7195267869	2.3742992939
H	-1.5183993593	-1.9925928079	-0.4915067052
H	-0.3197337012	2.0255468797	-2.5784354852
H	1.3445156044	2.0106955355	-3.2004250375
H	0.9632670861	2.7849542886	-1.6374130262
H	2.9615848537	-1.0088882349	-2.4552759862
H	3.2382478173	0.6202299442	-3.0619261645
H	-3.8057926945	0.8384857824	3.6872968801
H	-1.7450441337	-0.1464112742	2.8324872994
H	1.0228279592	-3.2360969547	-0.5379902032
H	0.3733425151	-4.4526792081	0.554545036
H	1.9034829663	-3.659367723	0.9413334619
H	2.659602665	1.5635673741	-0.8486954041
H	5.3703990651	-0.5000568985	-2.440986741
H	5.1004439176	0.8908667933	-1.3952824345
H	2.0395578163	-1.2977201677	-0.0627139446
H	-1.2394108712	-3.9636406909	2.8306648716
H	-1.2730579818	-2.4399780688	3.7135785312
H	0.2087058817	-3.4128784489	3.6899129877
H	4.4303967833	-2.0092291753	-0.6844763546
H	5.7848182699	-1.0887318998	-0.0362178562
H	0.5466137266	-0.357044409	3.0006924674
H	2.0042473999	-1.2696083612	2.6813833827
H	3.8889568629	-1.0380403409	1.5672962878
H	4.2355270729	0.5681918069	0.9358560549
H	2.3345424216	2.1445958943	1.2361114505
H	1.1889864955	1.8085161981	2.5423626697
H	2.8195662335	1.1287546894	2.6147364142
H	0.1508738956	3.3175527423	1.0034652954
H	-1.1364064719	4.2721222075	0.27400463
H	-2.6497375439	1.2248907007	-0.9620426999
H	-3.2604136174	1.9083627496	0.5329506611
C	-3.1133092398	3.3267397169	-1.1086108154
H	-4.0833029611	3.0906114641	-1.5507141175
H	-3.2497033966	4.2036284803	-0.4729388259
H	-2.4201193872	3.5818644452	-1.9140346046
C	-1.6418056037	3.416403078	2.2009445398
H	-1.2747903625	4.2659564065	2.7818620526
H	-2.7211122725	3.5260307136	2.0834111158
H	-1.4591753374	2.4971694086	2.7595254526

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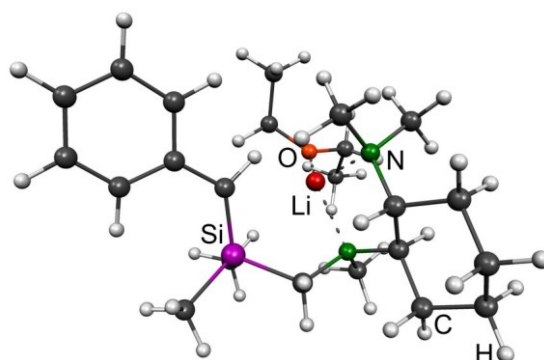
Abbildung 10.75 Molekel Darstellung von  $(R_N,S,R,R)$ -**96a** [lokales Minimum; M05-2X/6-31+G(d)].Tabelle 10.563 Standardorientierung von  $(R_N,S,R,R)$ -**96a** [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-0.2381174591	3.5756825161	-1.1958924631
C	-0.5268984359	4.5755999801	-2.113730633
C	-0.9248019426	1.8463972417	0.4645712222
C	-1.239075008	2.9599183755	-0.3928846484
C	-1.8330494368	5.043454102	-2.2858473343
C	-2.5473701257	3.4923986865	-0.556692078
C	-2.831061421	4.4929843292	-1.4780262592
C	-1.8487089212	1.7140762773	3.5303496894
N	1.059899673	-0.8056176401	-1.0964074574
N	-1.1125414823	-1.4931343833	0.6530105364
O	-1.9002486469	0.0134913046	-2.4541396262
Si	-1.9293965682	1.0423072584	1.7517678567
Li	-0.8600882285	0.051080429	-0.7806451703
H	-0.816200205	1.7475753708	3.889460622
H	-2.2383721771	2.7352971699	3.5606406658
H	-2.4360506189	1.1053880448	4.22570137
C	-3.7870320161	0.8764117738	1.365131032
H	-4.2318316903	0.0758985899	1.9645797873
H	-4.3082778341	1.8008037342	1.6285454394
H	-3.9805270794	0.6767304586	0.3073094719
H	0.7884801749	3.2377299511	-1.0855121637
H	0.280008663	5.0004677164	-2.7025211005
H	-2.0580993012	5.8266709402	-2.998644452
H	-3.8510508538	4.8539638485	-1.5619884342
H	-3.353730139	3.0990655482	0.0492817302
C	-0.8786407767	1.3932761457	-4.1938913175
H	-0.7516073391	0.544359457	-4.871143592
H	-1.0315330275	2.2938616437	-4.7920741793
H	0.0357658313	1.5328119474	-3.615220346
C	-3.9503705804	-1.2650044186	-2.8211447779
H	-4.4848566768	-0.4339679666	-3.2829929657

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H	-4.3307360392	-2.1941122827	-3.252384385
H	-4.1693506571	-1.259694553	-1.7528994598
C	1.0242653567	-1.5457236592	-2.3595040101
H	0.3759635827	-2.4177181887	-2.2725435501
H	0.6179184065	-0.8962303855	-3.1355111351
H	2.0207683017	-1.8824090459	-2.6745270241
C	2.0473167647	0.2701457073	-1.2052938562
H	1.7539042604	0.9426435229	-2.012912255
H	2.0710363537	0.8448803233	-0.280047435
H	3.056424296	-0.10691666	-1.4224740542
C	-2.3785875585	-2.2172718726	0.5546040922
H	-2.4080657546	-2.7972632635	-0.370233731
H	-2.5386982045	-2.9001149037	1.4012573276
H	-3.1997579184	-1.5033141681	0.543551525
C	-1.1029955148	-0.6939614085	1.9055170182
H	-0.0647519173	-0.4456832882	2.1508283977
H	-1.486656696	-1.2894594274	2.7487396892
C	0.0370254738	-2.4159243145	0.5149319903
H	-0.2261427909	-3.1039790241	-0.2992363347
C	1.3097095416	-1.661926768	0.0866252547
H	1.5722124354	-0.9721104363	0.8966516274
C	2.4785809056	-2.6443765101	-0.0927777963
H	3.3787934594	-2.0981085432	-0.3869849532
H	2.2457097583	-3.3425858684	-0.9042686081
C	0.3130509636	-3.2661767675	1.7660752586
H	-0.5918914192	-3.8134426818	2.0424681417
H	0.5539406077	-2.6054724722	2.6042025698
C	2.7370680605	-3.4576095939	1.1756834563
H	3.0149610185	-2.7868318252	1.9968404666
H	3.5783223061	-4.1368715703	1.0173362225
C	1.478543867	-4.2333976105	1.5583293844
H	1.6449689908	-4.8159172115	2.4677902733
H	1.2357158488	-4.9459688745	0.7609292794
C	-2.0578432374	1.2033364253	-3.2584987354
H	-2.1366730935	2.0355592213	-2.5646628174
H	-2.9957865522	1.1267941833	-3.8137764199
C	-2.4504077745	-1.1603193398	-3.0497574136
H	-1.9379089459	-2.0049309612	-2.5877069416
H	-2.2121548798	-1.169665194	-4.1187019259
H	0.149420864	1.7446829388	0.6562073417

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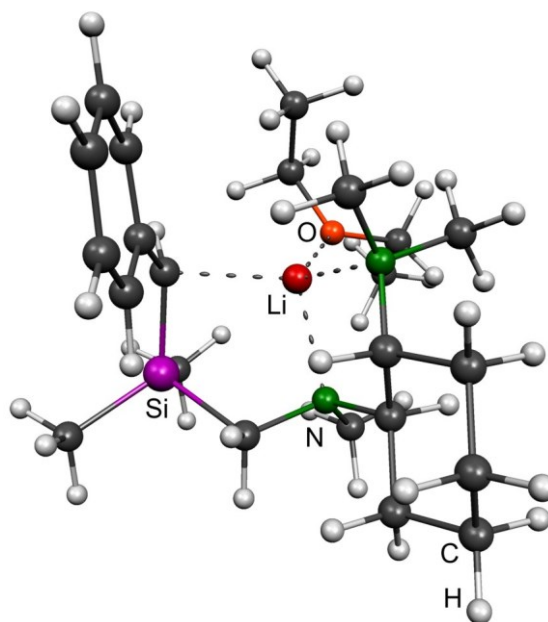
Abbildung 10.76 Molekel Darstellung von  $(R_M, R, R)$ -**TS2** [Übergangszustand [globales Minimum; M05-2X/6-31+G(d)].Tabelle 10.564 Standardorientierung von  $(R_M, R, R)$ -**TS2** [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	-2.9558613237	2.9568481614	-0.3039877123
C	-3.6082749038	4.1796252806	-0.2429092976
C	-1.7938987336	1.0159687128	0.7275680438
C	-2.4708325384	2.2804833823	0.8520262636
C	-3.82582845	4.8204280698	0.9783715573
C	-2.7254718735	2.9520055951	2.0788994361
C	-3.3724495973	4.1791126064	2.133058992
C	-0.5011021311	0.9375594349	3.5955428752
N	0.2760228539	-0.0212929249	-2.1414663587
N	0.5577325506	-1.6038227471	0.2227241007
O	-2.5552060829	-1.7753889499	-1.1279341024
Si	-1.0704149713	-0.0053571965	2.0507819364
Li	-0.9836542969	-0.7348377676	-0.6970098689
H	-0.0672150909	1.9051051133	3.3340706726
H	-1.3174635548	1.108381921	4.3002278004
H	0.2590920027	0.3448862598	4.1146213896
C	-2.1404915472	-1.4599699526	2.6746013892
H	-1.6076988994	-2.1142091771	3.373327791
H	-3.0129569433	-1.0493015116	3.1921212485
H	-2.5181998599	-2.0647534508	1.8439826658
H	-2.7964386568	2.4977820735	-1.2759785117
H	-3.9499812435	4.6407006561	-1.1643319333
H	-4.3332532861	5.7754343892	1.0291256149
H	-3.5355539408	4.6392169438	3.1024122613
H	-2.4203538137	2.4904087427	3.008212111
H	-1.9293411201	0.6721260417	-0.2988056283
C	-4.167638571	-0.3573144643	-2.2873483242
H	-4.1808100483	-0.9761337504	-3.1875894192
H	-5.1425552615	0.1235948529	-2.1872576114
H	-3.4199517698	0.427980753	-2.4101489571
C	-2.9695008027	-4.1779261729	-0.8985410937
H	-4.0056593705	-4.0620469662	-0.5788262026
H	-2.8872431145	-5.1262104326	-1.4346741286
H	-2.340179976	-4.2236235456	-0.0095493594

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C	0.1142414983	-0.8092311568	-3.3648391346
H	0.4306411148	-1.8402012295	-3.199174313
H	-0.9427981833	-0.8157323941	-3.6397954184
H	0.6850403643	-0.3997088395	-4.2078793275
C	-0.0420100409	1.3863420217	-2.4141189396
H	-1.0379987313	1.4431035416	-2.8569948066
H	-0.0585087619	1.9445791781	-1.4772866611
H	0.6677656587	1.843410031	-3.1160783536
C	0.3646157907	-2.9940091576	0.631068084
H	0.2404568399	-3.6295243624	-0.2489384815
H	1.2070270399	-3.3742726056	1.2246173159
H	-0.5323987334	-3.06169566	1.2445827395
C	0.6149928324	-0.7365502134	1.4316124199
H	1.1898852721	0.1622093776	1.1958898021
H	1.1553697711	-1.2560638108	2.2390049361
C	1.7136164028	-1.4638760047	-0.6925404418
H	1.6389536617	-2.3027642711	-1.397700949
C	1.6114505566	-0.1606878558	-1.507855413
H	1.6828595959	0.6762580407	-0.8045619643
C	2.7845710666	-0.0559426292	-2.4936066135
H	2.7073650986	0.8728986285	-3.064647555
H	2.7343874144	-0.8821937034	-3.2116646556
C	3.0816770039	-1.5596869113	0.0006378317
H	3.1492284823	-2.5019938482	0.5502014549
H	3.1704478987	-0.7545904765	0.7359630894
C	4.1304308405	-0.1300564658	-1.7712184861
H	4.2235709188	0.7116901003	-1.07570524
H	4.9457599852	-0.0417317163	-2.4932690497
C	4.2345758973	-1.4429191086	-0.997399644
H	5.1894912212	-1.5049031577	-0.4699813225
H	4.2028853429	-2.2821536199	-1.702574235
C	-3.8654105886	-1.1717338088	-1.0426262423
H	-3.8363004231	-0.5360664874	-0.1583458288
H	-4.6050832567	-1.9604051106	-0.8894041634
C	-2.5285569672	-3.0365718366	-1.8010900658
H	-1.4957126724	-3.182368595	-2.1211486656
H	-3.1515770646	-2.9800557131	-2.6987653124

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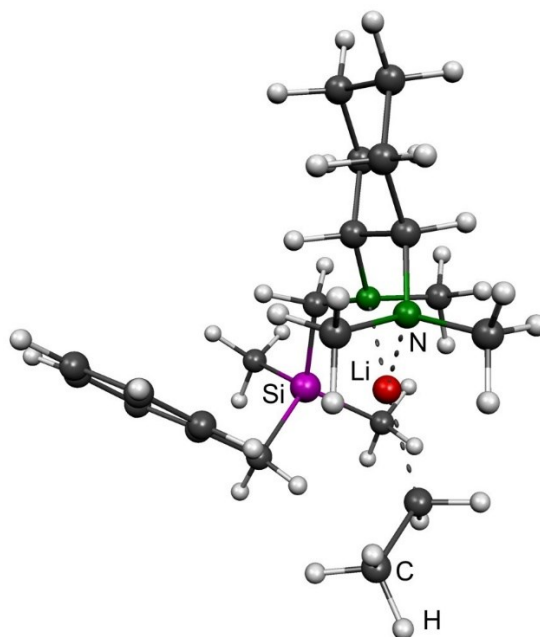
Abbildung 10.77 Molekel Darstellung von  $(R,R,R,R)$ -**96a** [globales Minimum; M05-2X/6-31+G(d)].Tabelle 10.565 Standardorientierung von  $(R,R,R,R)$ -**96a** [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.0558909579	2.8863374638	-0.7993534414
C	-1.6016662627	4.0549466584	-1.3915632772
C	-1.7995500209	0.9753759362	0.7937586585
C	-1.3534020283	2.2370336909	0.2548012536
C	-0.4216199983	4.6732262356	-0.9639164434
C	-0.1856284863	2.9187993828	0.6976117009
C	0.2646738054	4.0927677502	0.1033000794
C	-1.1463142961	1.2980088657	3.9274408712
N	0.9631618474	-0.0525849825	-1.6234271223
N	0.8112819074	-1.2718787777	0.9835064718
O	-1.8308432914	-1.9667565001	-1.0396944159
Si	-1.2283820259	0.2292774582	2.3566910809
Li	-0.626113075	-0.5251317066	-0.348550017
H	-0.531347479	2.1898455158	3.7840654374
H	-2.151319266	1.6352000761	4.1945621284
H	-0.7396600949	0.7345409506	4.7732838709
C	-2.3616370976	-1.244137755	2.7524251058
H	-1.9685053633	-1.8669855171	3.5609851726
H	-3.3359609636	-0.862538759	3.0720206829
H	-2.5259784508	-1.873158334	1.8723274244
H	-2.98491164	2.4429982718	-1.1456050642
H	-2.1799653149	4.4978636377	-2.1959868469
H	-0.0705906299	5.5879783411	-1.4242652356
H	1.1623008261	4.5659456596	0.4885559348
H	0.368176216	2.5262405069	1.5428921734

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H	-2.8321357419	0.7348268857	0.5337228167
C	-3.0009055615	-0.4811632855	-2.5513312374
H	-2.5141088944	-0.9206774713	-3.4257285295
H	-3.9853152813	-0.1152707913	-2.8525303609
H	-2.412023509	0.3709475522	-2.2060657642
C	-2.1613921623	-4.3567470114	-0.6552314479
H	-3.2501505391	-4.2909177744	-0.6878571725
H	-1.8712508214	-5.3456002525	-1.0178050559
H	-1.8439885074	-4.2575533231	0.383522361
C	1.0921899414	-1.1097939295	-2.6268846559
H	1.3687532445	-2.0559879266	-2.1619705872
H	0.1274370346	-1.2408846577	-3.1211734682
H	1.8380349842	-0.8677723092	-3.3954715177
C	0.7224723692	1.2209749097	-2.3158436424
H	-0.2166649912	1.1524952042	-2.8669000366
H	0.6303936679	2.0303192652	-1.5939361316
H	1.5203858165	1.4552776142	-3.0334072256
C	0.6029658808	-2.6421637948	1.445136836
H	0.6962930536	-3.3391166537	0.6097230925
H	1.3213853625	-2.9333950704	2.2252241332
H	-0.3986832624	-2.7305994457	1.8621268011
C	0.6041162769	-0.3384275413	2.1204696126
H	1.1361485267	0.5897871993	1.8984097214
H	1.0598882833	-0.7406926761	3.0393329625
C	2.1247263139	-1.1314701045	0.3116235114
H	2.2689253243	-2.0564279419	-0.2605549511
C	2.1175449744	0.0366150752	-0.6946463881
H	1.9603255352	0.9651988729	-0.1325268769
C	3.4768398288	0.1269523256	-1.4077985482
H	3.4727663245	0.9699118831	-2.1026097384
H	3.6363838457	-0.7811668008	-2.0004543311
C	3.3149330797	-1.012598196	1.2775668481
H	3.3093403207	-1.8615092766	1.9667613665
H	3.2045480935	-0.1095325366	1.8843733677
C	4.6353370471	0.2604076965	-0.4193012093
H	4.5234857455	1.1852690761	0.1580625705
H	5.5809251469	0.3333195786	-0.9623821311
C	4.6474915041	-0.9332293062	0.5330295122
H	5.4693681135	-0.8501932181	1.2485513247
H	4.811941587	-1.8536040577	-0.0402380184
C	-3.1331550385	-1.5034865391	-1.4387308365
H	-3.5971954115	-1.0665849753	-0.5560698823
H	-3.7334017579	-2.3592200351	-1.7570849584
C	-1.5111006659	-3.2773924795	-1.5057442296
H	-0.4262404132	-3.3573689855	-1.4557082503
H	-1.8054395278	-3.3673378405	-2.5576568381

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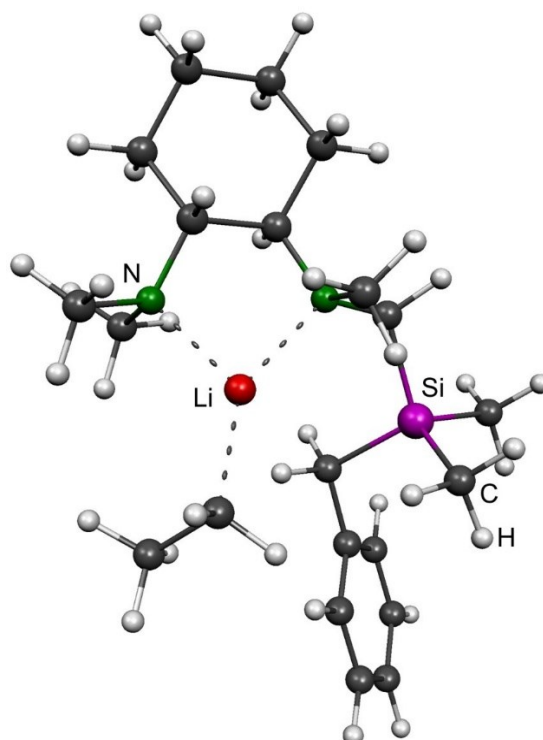
Abbildung 10.78 Molekel Darstellung von pro-(*S*)-(*S<sub>N</sub>*,*R*,*R*)-99 [globales Minimum; M05-2X/6-31+G(d)].Tabelle 10.566 Standardorientierung von pro-(*S*)-(*S<sub>N</sub>*,*R*,*R*)-99 [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.7993555854	-0.6053233332	-0.015358767
C	-1.9076872036	0.4570275024	-0.6867983612
C	-2.793062527	1.5219163372	-1.3520707142
C	-3.746258521	0.8976618721	-2.3737855223
C	-4.6222962824	-0.1646243759	-1.711014717
C	-3.7469863455	-1.2305211909	-1.0499041504
N	-1.9890152726	-1.5777152121	0.7435809997
N	-0.8927635518	0.9967491324	0.2526007659
C	-2.7074417951	-2.1514920086	1.8805930175
C	-1.4240203872	-2.652311953	-0.0756861427
C	-1.4755858326	1.7773860528	1.3491695916
C	0.1269244351	1.8000303261	-0.4427485575
Si	1.8275703707	2.0839069852	0.3929304307
C	2.6219677314	3.3874465976	-0.7267369374
C	1.7782452029	2.7519209451	2.1555726106
C	2.8595902901	0.4860456558	0.3824949514
H	-3.427598561	-0.0961943257	0.7236290574
H	-1.3298499346	-0.0434253632	-1.4740262411
H	-2.1662188847	2.2756238723	-1.8340003816
H	-3.386271382	2.033244309	-0.5856214733
H	-4.3642075597	1.6749223178	-2.8298645213
H	-3.1650452548	0.4360755428	-3.1804864314
H	-5.2863804376	-0.6283050064	-2.4444596871
H	-5.2596328441	0.3089655466	-0.9551599188

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H	-4.3664301832	-1.9912699766	-0.5659792004
H	-3.1622589921	-1.7345949849	-1.8265014216
H	-2.0177706538	-2.7747536158	2.4510811725
H	-3.0584028603	-1.3532949216	2.5361548843
H	-3.5654593646	-2.7639648365	1.5680927
H	-0.6687229163	-3.1777621204	0.5131329832
H	-0.9409262891	-2.2371557371	-0.9600931685
H	-2.1840585637	-3.3787437308	-0.3931277455
H	-1.9079155439	2.7254393862	1.0022087233
H	-0.6977200429	2.0013815385	2.0766130257
H	-2.2492463378	1.2038839885	1.8610070595
H	-0.27391997	2.7892806658	-0.720472649
H	0.3774471372	1.2941795685	-1.3825962213
H	3.6802540504	3.5178092975	-0.4853289327
H	2.128230509	4.3541278531	-0.5927196822
H	2.5456779393	3.1167584465	-1.7826967766
H	1.4425345307	1.9878196205	2.8600149132
H	2.7911419696	3.0471842474	2.4455807784
H	1.1371032084	3.632690292	2.2463309519
H	2.5545916885	-0.1100345505	1.2472516675
H	3.9069060114	0.7760069725	0.5218033368
C	0.8560695548	-1.168626028	2.9747573866
C	1.6595546573	-2.4792423833	2.8618554279
Li	-0.2992975819	-0.6102317123	1.3762473252
H	2.4848916909	-2.3884648385	2.1431902376
H	1.0342939577	-3.3078401266	2.5002708781
H	2.1143726285	-2.8288124612	3.8016099158
C	2.6892894553	-0.3012495517	-0.8856253111
C	1.92593561	-1.4745611285	-0.8946309366
C	3.2547893225	0.1273024173	-2.093519807
C	1.723880435	-2.1886613323	-2.0747740711
H	1.52100348	-1.8390489373	0.045044961
C	3.0510863524	-0.5821466401	-3.2743940898
H	3.8700618201	1.0207999095	-2.1028220959
C	2.2790470702	-1.742932175	-3.2723189749
H	1.1481409278	-3.107247765	-2.055402076
H	3.5028962232	-0.2332333626	-4.1954792695
H	2.1269269744	-2.3007407338	-4.1881665888
H	0.1007187156	-1.3068326369	3.7695361775
H	1.5261664319	-0.392419593	3.3785413617

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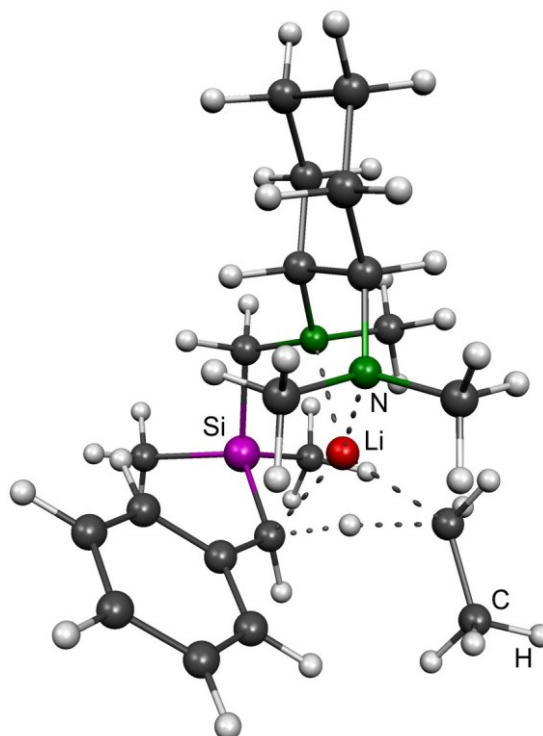
Abbildung 10.79 Molekel Darstellung von pro-(*R*)-(*S<sub>N</sub>*,*R*,*R*)-99 [lokales Minimum; M05-2X/6-31+G(d)].Tabelle 10.567 Standardorientierung von pro-(*R*)-(*S<sub>N</sub>*,*R*,*R*)-99 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	3.4699948	0.4334544176	-0.1907017249
C	2.6946825596	-0.8939036796	-0.1022072305
C	3.6388414219	-2.0047119218	0.379977608
C	4.8228508555	-2.165185169	-0.5773476019
C	5.5844369313	-0.8467104017	-0.7174809437
C	4.6430115758	0.2723418464	-1.1697660078
N	2.5676130102	1.5596789955	-0.4783351801
N	1.438284206	-0.7580864521	0.6714421457
C	3.1348635794	2.8585233028	-0.1208766109
C	2.0601699645	1.5959961066	-1.8520100277
C	1.6684193158	-0.5655948117	2.1082180807
C	0.535555277	-1.9084159361	0.4640056561
Si	-1.3445772148	-1.5620260477	0.5921513738
C	-2.1553081099	-3.2486243646	0.3392463405
C	-1.8950468071	-0.8370900276	2.2385382308
C	-1.8065225183	-0.3975348478	-0.8373537022
H	3.8970180941	0.6419179648	0.7975687317
H	2.3786114932	-1.1544472636	-1.1186295852
H	3.0888667147	-2.9455929916	0.4664980965
H	4.0211716654	-1.7571689234	1.3762181453
H	5.4881587031	-2.9550382514	-0.2205667816

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H	4.4549625931	-2.4773688137	-1.5617184389
H	6.4076109664	-0.9538211524	-1.4279160689
H	6.0283735242	-0.5804599952	0.2488395587
H	5.1867175102	1.2171367551	-1.2539686302
H	4.2561784326	0.0305485338	-2.1658823119
H	2.3522740024	3.6139267239	-0.2008691897
H	3.4771736927	2.835351187	0.914724416
H	3.9739254666	3.1460450063	-0.7696024437
H	1.2616810861	2.3386585264	-1.9067148802
H	1.6397204181	0.6274014046	-2.1282436332
H	2.8368056172	1.8646453034	-2.580149881
H	2.1081615441	-1.4526738035	2.5822624853
H	0.7168152295	-0.3554729247	2.595298747
H	2.3274332472	0.2882732666	2.2792214828
H	0.8158589584	-2.7524545566	1.1142706654
H	0.6686462322	-2.2636162355	-0.5644897291
H	-3.2433964115	-3.1508537616	0.3413537588
H	-1.8770024954	-3.9375680483	1.1415172807
H	-1.8604414134	-3.6998988265	-0.6123801862
H	-1.5371555884	0.1874058594	2.3628269898
H	-2.9879222748	-0.8120268231	2.2658436433
H	-1.5506796556	-1.4455360369	3.0794882923
H	-1.4331806485	-0.8245267295	-1.7746431088
H	-1.3086301553	0.5641563719	-0.6712594335
C	-0.5618766026	2.6721795746	0.922634449
C	-1.020595787	3.5285282904	-0.2759399575
Li	0.8028740143	1.2180847296	0.4530750091
H	-1.524494279	2.9260324862	-1.0441564541
H	-0.1662703796	4.003608436	-0.7777730287
H	-1.7147081449	4.3466454657	-0.0269536815
C	-3.2969161788	-0.1965263015	-0.9033903228
C	-4.112726093	-1.0720662593	-1.6288918491
C	-3.9041514778	0.8543024371	-0.2057731415
C	-5.495517813	-0.9075815509	-1.6557862851
H	-3.6566950945	-1.887549761	-2.1813716744
C	-5.2868296863	1.0193393705	-0.2303707325
H	-3.2823439353	1.5488623265	0.3487574689
C	-6.0896180614	0.1388884844	-0.9533530104
H	-6.1074417724	-1.5946614138	-2.228357953
H	-5.7356292245	1.8430583175	0.3117740677
H	-7.1645137146	0.2704902618	-0.974720929
H	-0.0711117774	3.3457124102	1.6458580257
H	-1.4581594979	2.3202384111	1.4580059819

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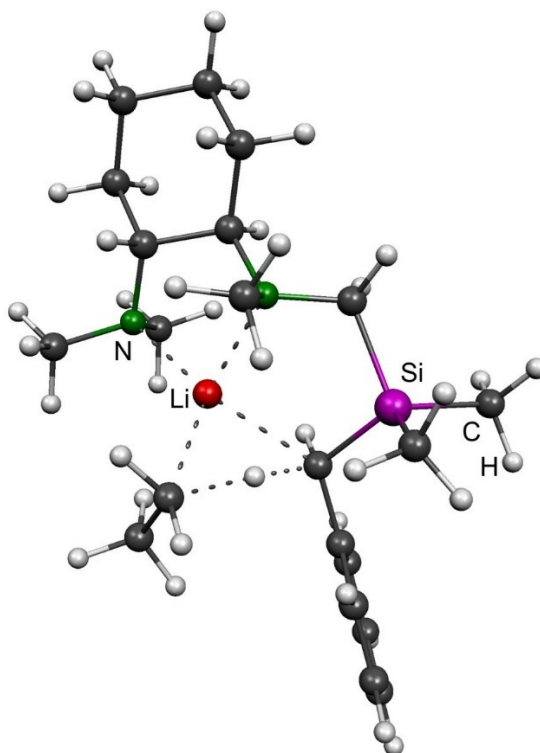
Abbildung 10.80 Molekel Darstellung von  $(S_N,S,R,R)$ -**TS38** [Übergangszustand; M05-2X/6-31+G(d)].Tabelle 10.568 Standardorientierung von  $(S_N,S,R,R)$ -**TS38** [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	-2.610965589	0.3173154388	-0.0398128274
C	-1.8929506025	-1.0451915259	0.006786813
C	-2.8675136632	-2.168778313	-0.3748932047
C	-4.0974207336	-2.1819467666	0.5336553041
C	-4.8125621788	-0.8330005325	0.4672167047
C	-3.8528429605	0.2897196815	0.8648760879
N	-1.6747476622	1.4272464768	0.2477700491
N	-0.6454782103	-1.0250615291	-0.7882005866
C	-2.1244176923	2.692431789	-0.3343533702
C	-1.4078598744	1.620938171	1.6772482954
C	-0.8797693282	-1.0492629151	-2.2356961962
C	0.2865375753	-2.1130516391	-0.4308519993
Si	2.1257739615	-1.7180776008	-0.8482816214
C	3.130823146	-2.9815841159	0.1499240121
C	2.5229380538	-2.0527286345	-2.6701209368
C	2.4139692741	0.0903323904	-0.5249847157
H	-2.9562950585	0.477736953	-1.0672285949
H	-1.5769273448	-1.2124118856	1.0435016469
H	-2.3469770801	-3.1296159566	-0.3353223169
H	-3.2023681947	-2.023616019	-1.4075995225
H	-4.7713376027	-2.9901667731	0.2392231121

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H	-3.7914431833	-2.3797782671	1.5676741364
H	-5.6857629138	-0.8261033726	1.1241611318
H	-5.1768045869	-0.6648643313	-0.5529978989
H	-4.3588204928	1.2585210418	0.8265395709
H	-3.5434969692	0.127919337	1.9027564314
H	-1.3435356463	3.4423822423	-0.1952184916
H	-2.2893802359	2.570213077	-1.4049825099
H	-3.0477392616	3.0629645507	0.1326224252
H	-0.5588232644	2.2964333381	1.7904047073
H	-1.1383206643	0.675771744	2.1465768523
H	-2.2692525743	2.051321634	2.2049265734
H	-1.2596880802	-2.022189024	-2.5751016902
H	0.0587117079	-0.8487137254	-2.7477666549
H	-1.5827048433	-0.2681574786	-2.5269831682
H	-0.0206992321	-3.0679059727	-0.8886890438
H	0.2349242763	-2.2627740855	0.6517762888
H	4.198349214	-2.8317810504	-0.0315336984
H	2.8802951078	-4.0009128113	-0.1604913708
H	2.9664317968	-2.9059593831	1.2269252448
H	2.2237863651	-1.2226990646	-3.3137393017
H	3.6019054581	-2.1883848059	-2.7882602732
H	2.0337879437	-2.9631980695	-3.027761077
H	1.6599915057	0.8028898844	-1.3821282182
H	3.3662552856	0.4148139864	-0.959311481
C	0.8980739943	1.7862517503	-2.3660780611
C	1.7533251409	3.0543781834	-2.4309712062
Li	0.1636139518	0.8636252108	-0.5321646973
H	2.8092710604	2.824264548	-2.236218149
H	1.444987241	3.7807622222	-1.6712864731
H	1.7212916693	3.569965648	-3.3991389782
C	2.2141462703	0.6999554242	0.8120959164
C	1.8111689195	-0.0109939624	1.9616467545
C	2.3692336714	2.0971016862	0.9600937668
C	1.6257646441	0.6209785681	3.1879728426
H	1.6910742663	-1.0860500268	1.90760843
C	2.1892675189	2.7290531281	2.1888010707
H	2.6726432647	2.6763367089	0.0960913514
C	1.8181217157	1.9966046833	3.3152286742
H	1.3442238282	0.0313018296	4.053386797
H	2.344486194	3.7993917709	2.2645423894
H	1.6857593414	2.4851667558	4.2727266545
H	-0.1674253493	2.0594849699	-2.4446909483
H	1.0986393298	1.1727234942	-3.2557750216

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Abbildung 10.81 Molekel Darstellung von  $(S_N, R, R, R)$ -**TS38** [Übergangszustand; M05-2X/6-31+G(d)].Tabelle 10.569 Standardorientierung von  $(S_N, R, R, R)$ -**TS38** [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	3.1720475312	0.5806801972	-0.2879983347
C	2.6158307211	-0.840256136	-0.0765141051
C	3.688540982	-1.7379191243	0.5556570646
C	4.9514973024	-1.7901391066	-0.3055044286
C	5.5025424281	-0.380648004	-0.5199769924
C	4.4374780002	0.5147965379	-1.1571613013
N	2.1285402109	1.5057424835	-0.7919590622
N	1.3312065606	-0.813621247	0.6517650776
C	2.4708613419	2.90574472	-0.5275208774
C	1.8234854235	1.3345569876	-2.2159868989
C	1.4825447359	-0.588824796	2.0938186564
C	0.5003253191	-2.0113435746	0.4152315777
Si	-1.3798750143	-1.6941994083	0.6696460161
C	-2.263722336	-3.1593649704	-0.1356166447
C	-1.8618208428	-1.6827167447	2.5021232923
C	-1.6774918815	-0.054687763	-0.1678089664
H	3.4624207509	0.9769308225	0.6918810198
H	2.386174451	-1.251416498	-1.0659468055
H	3.2785599322	-2.7409671728	0.7033299015
H	3.9550958459	-1.3475550806	1.5437113951
H	5.7016988042	-2.4277012912	0.1682630303

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H	4.716459458	-2.239421999	-1.277420237
H	6.3925719773	-0.4074397873	-1.1531504474
H	5.8078453749	0.0408998172	0.4447525843
H	4.8335085381	1.5207893277	-1.3191285236
H	4.1824736062	0.1046695349	-2.1404443219
H	1.634045347	3.5393051478	-0.8222428209
H	2.6393765787	3.0453392735	0.5407149953
H	3.363372033	3.2299680524	-1.0789434794
H	0.9385673175	1.9260348858	-2.4588363931
H	1.6032015374	0.2886490412	-2.4345246421
H	2.6440337392	1.6667064709	-2.8644026177
H	1.8735045788	-1.4754696646	2.6107404381
H	0.5113530642	-0.3376769489	2.5174519255
H	2.1497331726	0.2540315343	2.2808474783
H	0.867504343	-2.8749260374	0.9925522623
H	0.591127698	-2.2796222704	-0.6434292649
H	-3.3424926322	-2.9807881332	-0.1253140425
H	-2.0705108499	-4.0962142002	0.3951675003
H	-1.9597051376	-3.2837746342	-1.1783296505
H	-1.6527681514	-0.7219218185	2.9779475769
H	-2.9330578285	-1.8774891068	2.6006792825
H	-1.3296544362	-2.4657543486	3.0505793161
H	-1.1801255992	-0.0816566258	-1.1522757346
H	-1.199271319	0.9070855266	0.6669385548
C	-0.7072641701	2.2225576115	1.3652822068
C	-1.1297536293	3.2105976176	0.26988503
Li	0.3882508246	0.922929979	0.1517462135
H	-2.2072915767	3.1428951566	0.0986238244
H	-0.6710233763	2.9665647511	-0.7052006154
H	-0.889672308	4.2620740056	0.4706808637
C	-3.1014554368	0.3299400012	-0.3436038468
C	-3.6837907677	0.5006340826	-1.6112848765
C	-3.9178062063	0.578202312	0.7748461238
C	-5.0114863788	0.8899920378	-1.7565372376
H	-3.0781534533	0.3214252561	-2.4940431717
C	-5.2482200501	0.9625395209	0.6312206332
H	-3.4904784065	0.4891566565	1.7673296942
C	-5.8080309233	1.120997196	-0.6351753916
H	-5.4272942882	1.010910721	-2.7505028451
H	-5.8474263686	1.148610881	1.515344797
H	-6.8422524797	1.4224272379	-0.7468781703
H	0.2975305188	2.474148215	1.7499104519
H	-1.3784646597	2.2907119017	2.2253366634

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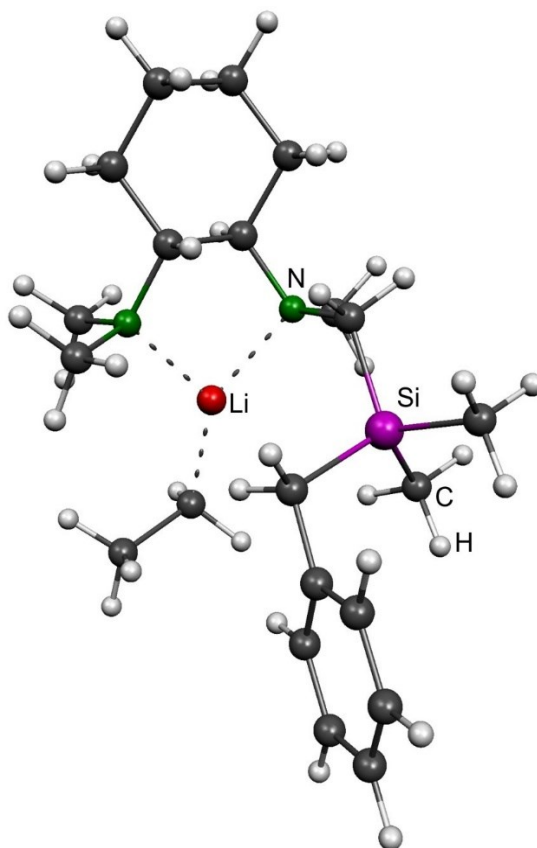


Abbildung 10.82 Molekel Darstellung von pro-(*S*)-(*R<sub>N</sub>,R,R*)-99 [lokales Minimum; M05-2X/6-31+G(d)].

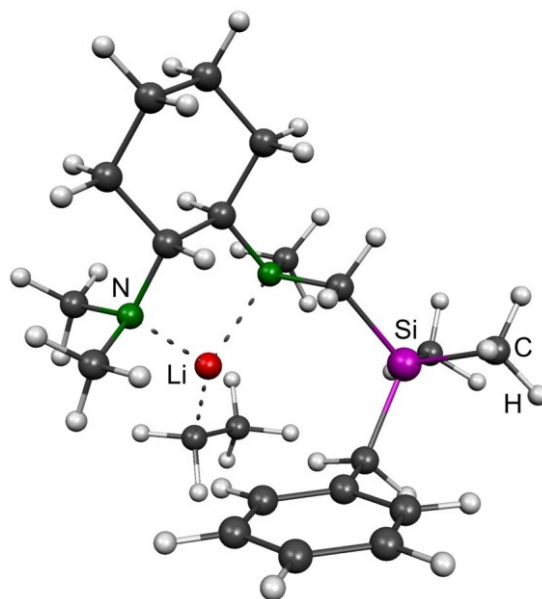
Tabelle 10.570 Standardorientierung von pro-(*S*)-(*R<sub>N</sub>,R,R*)-99 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.8949101252	0.107653927	-0.9034407966
C	-2.9346009412	-0.412772298	0.5461999861
C	-3.7319186805	-1.7234028005	0.6241529897
C	-5.1469318315	-1.5547497077	0.0675864282
C	-5.0893108989	-1.0688350817	-1.3799521379
C	-4.3198433658	0.2503834198	-1.4588473957
N	-2.0783616948	1.3337738977	-0.9993907914
N	-1.569946491	-0.4875882843	1.1255790617
C	-1.5041911042	1.530663252	-2.3295460472
C	-2.7667417046	2.5578740117	-0.5762236309
C	-1.6159323325	-0.4477309968	2.5896991474
C	-0.7965724545	-1.6642972405	0.6790294793
Si	1.1170419076	-1.5188646939	0.679106705
C	1.8686585356	-0.8704084885	2.2759807349
C	1.7235383419	-3.2761401926	0.3507704312
C	1.6109638826	-0.4009733141	-0.7815527139
H	-2.375722551	-0.6432388698	-1.5108171973
H	-3.4679917917	0.3341113303	1.1471551823

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H	-3.7681453495	-2.0725847302	1.6593939115
H	-3.2199748029	-2.4966677358	0.042494872
H	-5.6878763118	-2.5017208066	0.1350067662
H	-5.6989686617	-0.8261566007	0.672721031
H	-6.0964062981	-0.9380499155	-1.7830782463
H	-4.5918067077	-1.8255796513	-1.9977984736
H	-4.2768991689	0.6118052859	-2.4901660783
H	-4.8620956536	1.0027188362	-0.8761637745
H	-0.8161614956	2.3763549551	-2.2930518973
H	-0.9397622418	0.6443367949	-2.6224688174
H	-2.2696868993	1.7345228565	-3.0918204538
H	-2.024305077	3.3494477868	-0.4665740333
H	-3.2430746906	2.4118536162	0.3945518738
H	-3.5285000941	2.8795449898	-1.2986166873
H	-2.1439323002	0.4491417785	2.916935938
H	-0.6018381891	-0.4017009831	2.9809457158
H	-2.111463622	-1.3322317203	3.0142727794
H	-1.0384685549	-1.8677412102	-0.3695805789
H	-1.0999481288	-2.5633556644	1.2394245165
H	2.9579877721	-0.9159156169	2.1931437278
H	1.5699000523	-1.4738229068	3.1373167523
H	1.5916516795	0.1720059966	2.4501451908
H	1.3097240428	-3.6793980151	-0.5779217003
H	2.8128040124	-3.2935932759	0.2697054897
H	1.4358128249	-3.9439972172	1.1672906472
H	1.1906900504	-0.8230822607	-1.7010633905
H	1.1904957041	0.600399243	-0.6361989896
C	0.6174694346	2.7535931143	1.0219110016
C	1.1081544391	3.593254404	-0.1760049193
Li	-0.6836916667	1.2593039213	0.4925953843
H	1.6276048482	2.9797014022	-0.925395804
H	0.2686209826	4.0652557783	-0.7050003814
H	1.7996336794	4.4121691897	0.0780787279
C	3.1099167921	-0.2977284373	-0.8842580481
C	3.8516448691	-1.2303782194	-1.6172489612
C	3.7964228522	0.7202964582	-0.2118723325
C	5.2413290977	-1.1528857252	-1.6762956671
H	3.3331721818	-2.0208814271	-2.150641477
C	5.1854606395	0.7982416987	-0.2691706405
H	3.2314190653	1.4559072649	0.3507093534
C	5.9149269432	-0.1383295593	-0.9996727373
H	5.7960741991	-1.8825363315	-2.25435407
H	5.6971064554	1.597452986	0.253546626
H	6.9951290765	-0.0743948093	-1.04636746
H	0.1169112997	3.4367511361	1.7280018715
H	1.5007247598	2.4009762661	1.5797562481

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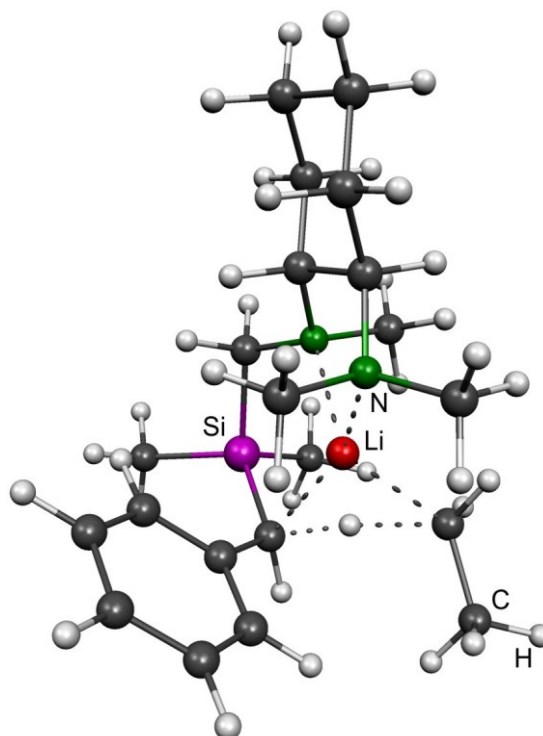
Abbildung 10.83 Molekel Darstellung von pro-(*R*)-(*R<sub>N</sub>*,*R*,*R*)-99 [lokales Minimum; M05-2X/6-31+G(d)].Tabelle 10.571 Standardorientierung von pro-(*R*)-(*R<sub>N</sub>*,*R*,*R*)-99 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.4272040037	0.7403541857	-0.0467298562
C	-2.3722608587	-0.779156088	-0.2870904558
C	-3.017084769	-1.1254801331	-1.6377055219
C	-4.4651201074	-0.6381631401	-1.7053228826
C	-4.5153763105	0.8732071942	-1.4874905738
C	-3.8806265645	1.2314675741	-0.142998017
N	-1.7493442281	1.1058580563	1.2146888031
N	-1.000534902	-1.3164808107	-0.0961609605
C	-1.393241149	2.5229295002	1.2620411259
C	-2.4957806562	0.7562547286	2.4285930136
C	-1.0380485897	-2.7198800878	0.3218123332
C	-0.136109477	-1.1480333982	-1.2752968873
Si	1.7233438907	-1.6175439898	-1.2309141668
C	2.0713045265	-3.4271831951	-0.8133131795
C	2.2148696763	-1.3630474276	-3.0403632115
C	2.7566550293	-0.5266723698	-0.0706991631
H	-1.8496200955	1.2256962656	-0.8429514701
H	-2.9834609074	-1.2518754316	0.4897191055
H	-2.9656704247	-2.2055333783	-1.8029981881
H	-2.4562377145	-0.6469183283	-2.4465784654
H	-4.9021722571	-0.9031390342	-2.6711198955
H	-5.0628439079	-1.1377715266	-0.934051021
H	-5.5461444481	1.2343100042	-1.5206136526
H	-3.9731864138	1.3742992995	-2.2977710879
H	-3.9172942454	2.3116631586	0.0205650751
H	-4.4708739501	0.7642750587	0.6527799132

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H	-0.7564642655	2.6952076719	2.1319558647
H	-0.8328027117	2.7917988995	0.3669300419
H	-2.2737656425	3.1748331072	1.347036923
H	-1.8386727063	0.8944445332	3.287560812
H	-2.7924997443	-0.2931612804	2.4094386342
H	-3.3909403958	1.3777398917	2.5615889221
H	-1.7101035105	-2.8292818151	1.1738872622
H	-0.0473500742	-3.0271350167	0.6480896203
H	-1.3697165936	-3.3886020272	-0.4863105167
H	-0.1514873097	-0.0937270295	-1.5766684411
H	-0.5322810666	-1.7188098615	-2.1321452699
H	3.0637841471	-3.685806429	-1.194182155
H	1.3490605478	-4.0978868743	-1.2861171627
H	2.0697137034	-3.6175767935	0.2613679761
H	1.9534847883	-0.3672179756	-3.4048797968
H	3.2904718556	-1.5035432983	-3.1768358235
H	1.7043020476	-2.0994723149	-3.6678356979
H	2.4293108134	-0.7074207115	0.9586836053
H	3.7870899584	-0.892838135	-0.1517004201
C	0.9092944413	-0.7362730802	3.1125088824
C	1.356071274	-2.2067590848	3.2355983075
Li	-0.2014485267	-0.2351940543	1.4508153467
H	2.0250705235	-2.4983927719	2.4135064161
H	0.4988849704	-2.8906632016	3.187598211
H	1.8954698463	-2.4545341494	4.1630881044
C	2.7028200374	0.9459850369	-0.3817526126
C	2.0545080229	1.8358154136	0.4821226838
C	3.3122457834	1.4677377057	-1.5308560341
C	2.0064134425	3.2005717636	0.1979498027
H	1.6244534518	1.452557576	1.4034648291
C	3.2618171381	2.8285237188	-1.8177171791
H	3.8454352067	0.7997615394	-2.198193131
C	2.6031207236	3.7036563945	-0.954790874
H	1.5166893223	3.8746319328	0.8914921466
H	3.746390846	3.2076665077	-2.7097028099
H	2.57090453	4.7645287217	-1.1708631396
H	0.278864169	-0.5100076994	3.9901045398
H	1.7991997139	-0.0999754963	3.2572134889

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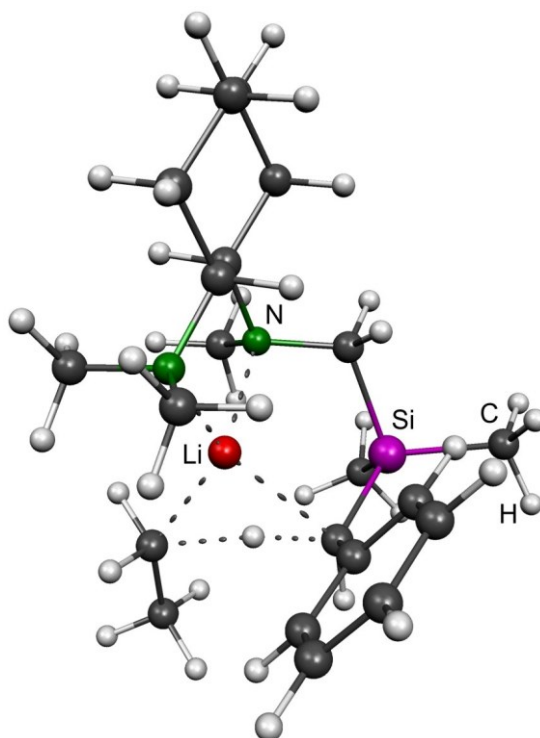
Abbildung 10.84 Molekel Darstellung von  $(R_N,S,R,R)$ -**TS38** [Übergangszustand; M05-2X/6-31+G(d)].Tabelle 10.572 Standardorientierung von  $(R_N,S,R,R)$ -**TS38** [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	-2.7827026756	0.3220413654	-0.8630534946
C	-2.8450590413	-0.3911501759	0.5012373866
C	-3.7172188515	-1.6512622486	0.4005995488
C	-5.1259245388	-1.3208721722	-0.0955657024
C	-5.0569066708	-0.6232496047	-1.4533677978
C	-4.2028595682	0.6420333483	-1.3531561528
N	-1.8746446812	1.4923875306	-0.8207683017
N	-1.488939085	-0.6251277256	1.0475825721
C	-1.4022196994	1.8729014722	-2.1535751588
C	-2.4446115426	2.6667968095	-0.1503489313
C	-1.5150081398	-0.7480534488	2.5058358003
C	-0.7789415815	-1.7780323357	0.4490234138
Si	1.1421467129	-1.6776470231	0.530614301
C	1.8053386488	-1.937346782	2.2847184825
C	1.7507116037	-3.1264613001	-0.5226414114
C	1.575566253	0.0021793388	-0.1583270173
H	-2.3297075405	-0.3729305849	-1.5800389379
H	-3.335250861	0.2916961709	1.205727565
H	-3.7601998943	-2.1453278736	1.3749479655
H	-3.2558683909	-2.3572849916	-0.2970736339
H	-5.7210915841	-2.2346793449	-0.1629353047

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H	-5.6276959941	-0.6637854041	0.624366681
H	-6.0587668836	-0.3685355829	-1.8071362701
H	-4.6196901231	-1.3059210622	-2.1911930427
H	-4.1570739657	1.1498887843	-2.3202819955
H	-4.6836889866	1.329741692	-0.6490400346
H	-0.643638452	2.6504454545	-2.0526980286
H	-0.9453822797	1.0111851276	-2.6418376189
H	-2.2090396259	2.2583049482	-2.7911397901
H	-1.6530478167	3.4022410997	0.0014208474
H	-2.8383750908	2.3918059285	0.828833193
H	-3.2453472207	3.1344452825	-0.7369209829
H	-1.9991649502	0.1279522197	2.9404000182
H	-0.4948404853	-0.7899268284	2.881528469
H	-2.04284097	-1.6531370977	2.83820346
H	-0.9948258308	-1.7977808811	-0.6250583576
H	-1.1556693118	-2.728751588	0.8580827071
H	2.8662640455	-2.1961571494	2.2341669633
H	1.2837756973	-2.7598930745	2.7831393618
H	1.7130553081	-1.0401968329	2.9010320721
H	1.3262541085	-3.0938613976	-1.5298091283
H	2.8382128355	-3.0687741069	-0.6212539511
H	1.5016602012	-4.0928501159	-0.0745798488
H	1.0601299559	0.1194253487	-1.1260937466
H	1.2350901721	0.9807924203	0.7325177302
C	0.8730023337	2.2248190645	1.599585095
C	1.4156796521	3.3632321954	0.7258994522
Li	-0.375905183	0.9598514248	0.4524174534
H	2.3807985045	3.0821323616	0.2924352423
H	0.7517395716	3.5716531541	-0.1249825062
H	1.5589696089	4.316075986	1.2508573242
C	3.0345827362	0.2219797888	-0.3521634108
C	3.6114485268	0.3452829743	-1.6278491802
C	3.8949704608	0.3424213858	0.7539970237
C	4.9744082149	0.5719957232	-1.7923432782
H	2.9730810057	0.258641366	-2.5013870215
C	5.2598418356	0.5623978335	0.5911702449
H	3.4770352368	0.2873304825	1.7527378858
C	5.8126125857	0.6782005194	-0.6830573981
H	5.3843355212	0.6626696919	-2.7919384381
H	5.8926457671	0.6554105859	1.4664858529
H	6.8739442675	0.8530170758	-0.8094067625
H	-0.0901300013	2.5230784591	2.0539403075
H	1.5436276061	2.0514631289	2.4486947957

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Abbildung 10.85 Molekel Darstellung von  $(R_N,R,R,R)$ -**TS38** [Übergangszustand; M05-2X/6-31+G(d)].Tabelle 10.573 Standardorientierung von  $(R_N,R,R,R)$ -**TS38** [Übergangszustand; M05-2X/6-31+G(d)].

	x	y	z
C	-2.161231545	0.8183155014	0.0203508333
C	-2.288877776	-0.711838557	0.1356029607
C	-3.1988103831	-1.2667993056	-0.9693869572
C	-4.5816975016	-0.6149495262	-0.9314517256
C	-4.4481872207	0.8999793255	-1.0770885498
C	-3.556433273	1.4626410883	0.0311294497
N	-1.2372300947	1.353526479	1.0453318161
N	-0.9556649273	-1.356198669	0.2217736218
C	-0.8351818859	2.7340582276	0.7682092603
C	-1.7328826506	1.2607489963	2.421548984
C	-1.0097394131	-2.5678600731	1.0402017869
C	-0.3390944726	-1.6588825127	-1.0862912381
Si	1.5616322517	-1.9609406532	-1.0416769497
C	2.0261569999	-3.6362067295	-0.2890441127
C	2.0539047793	-2.0811581609	-2.8724985593
C	2.329008473	-0.6294837818	0.0053700643
H	-1.6859622186	1.0440485752	-0.9436832519
H	-2.7871970608	-0.9231090494	1.0878817206
H	-3.2806573399	-2.3522377194	-0.8611571232
H	-2.750704113	-1.0746096967	-1.9489830355
H	-5.2089488847	-1.0246401693	-1.7269634004

H	-5.0763261068	-0.8466416495	0.0191195665
H	-5.429772082	1.3790263964	-1.0439586563
H	-4.0105709323	1.1326252778	-2.0549624366
H	-3.4654124264	2.5468020799	-0.0700216306
H	-4.0365639481	1.2663208463	0.9962895102
H	-0.0131298934	3.0014967542	1.4336683401
H	-0.473115245	2.8136234721	-0.2561107636
H	-1.6548856904	3.4484334036	0.9240220655
H	-0.9263177048	1.5471773399	3.0975996785
H	-2.0150983339	0.2362038196	2.6636825464
H	-2.5893206011	1.9224477976	2.6046578206
H	-1.4420814075	-2.3368729232	2.0144780075
H	-0.0006968793	-2.9394425861	1.2060095046
H	-1.6014621335	-3.3632051652	0.5627176644
H	-0.4813710311	-0.7920968858	-1.7400121289
H	-0.8462612648	-2.5048494627	-1.5788928126

Tabelle 10.574 Standardorientierung von (*S,R,R*)-**94b** mit Li-N<sub>pip</sub>-Bindung fixiert auf 2.0 Å [Minimum; M05-2X/6-31+G(d)].

	X	Y	z
C	3.508514287	-1.0986473262	1.1546919055
C	2.8204621416	1.2098284773	1.0207522027
C	3.525089703	-2.4656429246	0.4814368189
C	4.2300371384	-2.3787178406	-0.8718222671
C	2.8683291549	3.6372403316	-0.8826054911
C	3.5261078109	0.0381541989	-0.9550619083
C	1.2288891339	3.675417663	1.654298492
C	3.5833259452	-1.2817452124	-1.7162392166
C	0.3768393968	1.7562122017	-0.7601060419
C	-1.0243415682	2.1127702629	-0.7733805987
C	-1.7396084158	2.6062673788	0.3530714645
C	-1.8184588424	1.9397867438	-1.9428373357
C	-3.1104888587	2.831618329	0.3293930791
C	-3.190728932	2.1559791137	-1.9599795813
C	-3.8677588365	2.5913972553	-0.8190838141
N	2.8177381951	-0.0981813048	0.3274936296
Si	1.7148122373	2.569540279	0.1904587436
H	4.5425512571	-0.7650493934	1.3485160964
H	2.9966536337	-1.1476829655	2.1180473873
H	3.8607713743	1.5540680183	1.1571445189
H	2.4175979008	1.0458128204	2.02574539
H	4.0203600555	-3.1886527431	1.134864452
H	2.4924913101	-2.8000211741	0.3380045179
H	5.287303909	-2.1379310443	-0.712475391
H	4.1925006765	-3.3391952077	-1.3922298148
H	3.7633293715	3.9424945364	-0.3308920955
H	3.1888900984	3.1200229894	-1.7907044589
H	2.3364366798	4.5405488025	-1.1942758028
H	4.5492781216	0.4072056468	-0.7666936618
H	3.0118016204	0.792424198	-1.551662855

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H	2.1359916045	4.1173974239	2.0787128857
H	0.7202170438	3.1299063039	2.4533109252
H	0.5779379096	4.4913846477	1.3314908589
H	4.1308276946	-1.1335996402	-2.650405502
H	2.5641689545	-1.5779274998	-1.9802481049
H	0.7325077922	1.5129163715	-1.7687166014
H	-1.1969712516	2.827875303	1.2628889003
H	-1.3217973634	1.6489842482	-2.8637242432
H	-3.5943574712	3.2084190571	1.2249127276
H	-3.7361152544	2.001426552	-2.8855249758
H	-4.9359651068	2.7674628932	-0.8333219516
C	0.0776537592	-2.2008093533	2.3072436131
C	-0.3941246905	0.1051408366	2.6746799566
C	0.2292683795	-3.3709789167	-1.3466003286
C	-1.5898833824	-1.0394701936	0.8847353405
C	-2.8469626703	-1.2171707603	1.7525422129
C	-1.5051564849	-2.1568768065	-0.166882735
C	-0.4575728668	-1.2652395818	-2.2142581269
C	-4.1146167496	-1.2834777747	0.8998326455
C	-2.7961669137	-2.2201897043	-0.9973054909
C	-4.0195694615	-2.4274239955	-0.1054417864
Li	0.8526443984	-0.347402434	0.0512777641
N	-0.3235196192	-0.950978044	1.6632040659
N	-0.2636872459	-2.0429538718	-0.9832728891
H	0.9675050813	-2.0073997304	2.9082177291
H	0.335746478	-2.9551075356	1.5661769066
H	-0.6951305312	-2.6040085399	2.9750784973
H	0.60949562	0.3063367943	3.0530744397
H	-1.0267377405	-0.1721803293	3.5281524473
H	-0.7888666613	1.01101233	2.2187269781
H	0.4583002862	-3.9521815841	-0.4520939646
H	1.1434916102	-3.2738617554	-1.9341893401
H	-0.5019566339	-3.9302077079	-1.94870698
H	-1.6813955831	-0.0795737369	0.361000251
H	-2.7666566448	-2.1356143422	2.3467129122
H	-2.9279834721	-0.3810585631	2.4493901891
H	-1.4311483299	-3.1092132853	0.3703867601
H	0.5171858545	-1.0552347887	-2.6595319483
H	-0.9357791641	-0.3165620985	-1.9845529906
H	-1.0619250628	-1.8052092219	-2.9554531276
H	-4.9877943723	-1.4060868635	1.5458032812
H	-4.2352441295	-0.3355606621	0.3633919319
H	-2.7174913065	-3.0256598047	-1.7338784523
H	-2.9279802138	-1.2822585508	-1.5450834479
H	-3.9383915743	-3.3827445954	0.4276353764
H	-4.9212239633	-2.4773114492	-0.7207592229

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Tabelle 10.575 Standardorientierung von *(R,R,R)*-**94b** mit Li-N<sub>pip</sub>-Bindung fixiert auf 2.0 Å [Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	4.0643953421	-1.639099748	-0.3544992819
C	3.946859582	-2.1898130141	1.0641404769
C	2.8064997552	-1.971747483	-1.1580339554
C	2.7136645412	-1.5946834253	1.7428650032
C	1.5455734978	-1.4013984043	-0.4881898105
C	0.3813530129	-1.1181262557	-2.6044504487
C	1.4335829359	-1.9139210388	0.9561539497
C	-0.0954878779	-3.0625877065	-1.3137657956
C	0.3679172243	-0.1836363357	2.3623926221
C	-0.3567922779	-2.4474520141	2.5041798592
Li	-0.8764457953	-0.368745726	-0.0113712282
N	0.2874723219	-1.6533239434	-1.2432642279
N	0.1853004055	-1.4289192785	1.6073757741
H	4.9437937614	-2.049675382	-0.8573151185
H	4.1881438776	-0.5509016596	-0.3155791735
H	4.8398652373	-1.9508248036	1.6468227075
H	3.865550042	-3.2832659712	1.0304907776
H	2.9019119176	-1.5601399338	-2.1645098684
H	2.7219440914	-3.0611084567	-1.2529113955
H	2.8471305391	-0.5102259267	1.8017556791
H	2.6179848734	-1.9732296253	2.7653256624
H	1.6517724924	-0.3101815519	-0.4551197847
H	0.9854764282	-1.7578091394	-3.2613693204
H	0.8249295357	-0.1261104061	-2.5687996724
H	-0.618214007	-1.0394780167	-3.0363212965
H	1.3529856426	-3.0061330853	0.9159879686
H	0.6713097809	-3.6876834998	-1.7901509037
H	-0.3083620181	-3.4587160914	-0.32224769
H	-1.0069664939	-3.1463323192	-1.9087188867
H	0.8279831674	0.5717844798	1.7284008701
H	0.9810775486	-0.3221954377	3.2627499845
H	-0.6126664324	0.17918227	2.6753206265
H	0.3550839857	-2.7189304412	3.2977852922
H	-0.6170476802	-3.3477687154	1.9457253402
H	-1.2612757345	-2.0671785864	2.9803336133
C	3.9307552446	2.6018227853	-0.5576024184
C	3.2611749147	2.302668018	-1.7466770944
C	3.1650714708	2.7163567919	0.6033765315
C	1.8886181037	2.0951187792	-1.7641951305
C	1.791441109	2.4991034474	0.5911436175
C	1.0841616387	2.1392869261	-0.5895297208
C	-0.319645164	1.7900647386	-0.6294954065
C	-3.5108927919	-1.1645923644	-1.8272480099
C	-1.1736344746	3.5577883513	1.8830883121
C	-3.4701620477	0.1293210983	-1.0213510471
C	-3.5942326564	-2.4216484284	0.3270251894
C	-4.2260223959	-2.2732538996	-1.0566533467
C	-2.7455791102	3.7585611551	-0.6997062123

C	-2.8535734553	1.2184717825	1.0292293526
C	-3.5830108961	-1.078098481	1.0451905877
N	-2.8300312936	-0.0646438222	0.2903334907
Si	-1.6627393962	2.581650786	0.3313943359
H	5.0001195353	2.7706585659	-0.5430165152
H	3.8136599967	2.2498995631	-2.6793366503
H	3.6429239251	2.9873882507	1.539441429
H	1.3982001206	1.9186221617	-2.7163969786
H	1.2439287001	2.6217492252	1.517061312
H	-0.6524172509	1.6216430002	-1.6612445299
H	-2.4845317569	-1.4756193367	-2.0396448335
H	-3.999864378	-0.9755948988	-2.7862044085
H	-0.4805866557	4.3662261425	1.6386251032
H	-0.7073339698	2.931205808	2.6481473867
H	-2.0721286857	4.0046052966	2.3203974276
H	-2.9129053753	0.893849401	-1.5648363144
H	-4.4950309226	0.510797714	-0.8717454355
H	-2.5632067555	-2.7770406801	0.227912498
H	-4.1392826395	-3.1529587866	0.9296346647
H	-4.1823016246	-3.2160442524	-1.6078521281
H	-5.2845536413	-2.0128582089	-0.943243154
H	-2.1641675157	4.6431288498	-0.9739533638
H	-3.0875426084	3.2927995579	-1.6280904559
H	-3.6272176505	4.0889082435	-0.141030879
H	-2.5353535976	1.0100370042	2.0562407499
H	-3.8933320202	1.5833285204	1.0999934462
H	-3.1235995955	-1.1706209986	2.0309742383
H	-4.6184361564	-0.727641584	1.1969742612

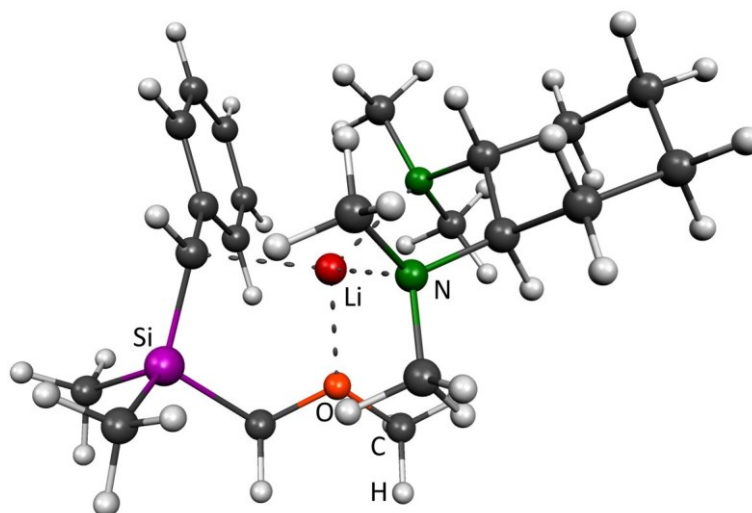
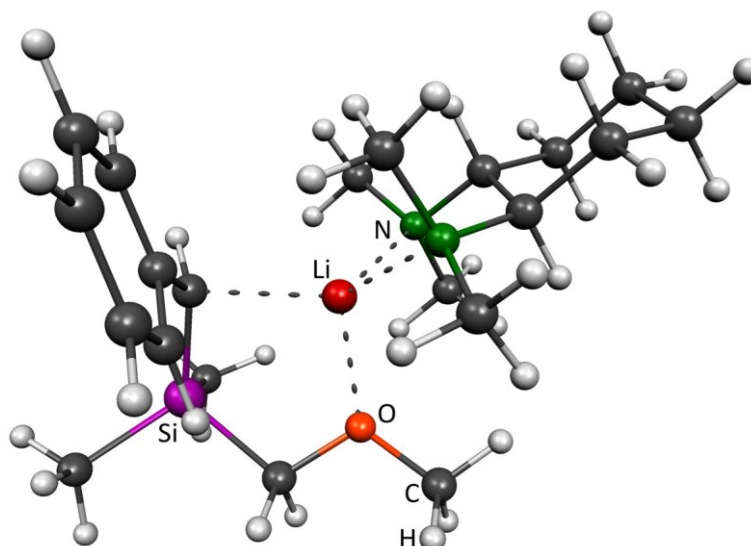


Abbildung 10.86 Molekel Darstellung von *(S,R,R)*-**101** [lokales Minimum; M05-2X/6-31+G(d)].

Tabelle 10.576 Standardorientierung von  $(S,R,R)$ -**101** [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.8326060203	0.397617871	-0.0862878523
C	-2.6796100139	1.2989668316	2.8609181476
C	-3.4993588742	3.2212665579	0.6204918046
C	-0.5042338457	2.18199125	0.9140456909
C	0.02542182	2.8687546983	-0.2412594647
C	-0.4977937669	2.6854144244	-1.5516022893
C	1.1316276867	3.7583848163	-0.1533625797
C	0.0408199244	3.3251293156	-2.6640103803
C	1.6667896262	4.3898784736	-1.2649837627
C	1.1360228064	4.1808145302	-2.5435626328
Si	-2.2848644643	1.8383874935	1.0860042612
H	-3.6334685491	-0.1990220879	0.3721627525
H	-3.2217046834	0.7891658172	-1.0360385198
H	-3.7296125008	1.0107542751	2.9628242948
H	-2.062450743	0.4562721745	3.1825680755
H	-2.4926799308	2.1269905641	3.5502288949
H	-4.534291318	2.8659336606	0.5811724918
H	-3.2421970389	3.6404478266	-0.3561015222
H	-3.4453504895	4.0315302855	1.3521077299
H	-0.0196011642	2.4592795786	1.8518746412
H	-1.3484048093	2.0240763091	-1.6914637416
H	1.5593708633	3.9469513207	0.8265060277
H	-0.403960422	3.1521587139	-3.6387956668
H	2.5086273918	5.0623906291	-1.1362935183
H	1.5521411806	4.6804259568	-3.4091565993
C	1.2858198523	-0.7524191228	-2.2236383596
C	2.6449468909	0.9476737656	-1.2484934813
C	-0.3658106568	-2.143286168	1.9412330385
C	2.6140962568	-1.2432290963	-0.2048615555
C	3.5412792397	-2.1148754721	-1.0674316644
C	1.7082143469	-2.136424448	0.6606205276
C	1.3303108632	-0.5740197621	2.5381050949
C	4.3936504601	-3.0483394638	-0.2067906289
C	2.5699551224	-3.0830724044	1.5124448942
C	3.4940833397	-3.940637316	0.6466744284
Li	0.0852441881	0.2146507786	0.1668222521
N	1.8340682287	-0.241955079	-0.9640730094
N	0.7396550345	-1.3339493798	1.4327754607
H	0.5613435954	-0.0296037485	-2.6037651089
H	0.7783116095	-1.7035728089	-2.061131412
H	2.0608260906	-0.8977724908	-2.9878234529
H	2.0489793015	1.6655977614	-1.8097887485
H	3.5418884569	0.6992897279	-1.8338770266
H	2.94228916	1.4215638554	-0.3131052093
H	-0.7922948324	-2.736681205	1.1319658021
H	-1.1450703109	-1.4810601072	2.3190881213
H	-0.0575255979	-2.8169207086	2.7528381548
H	3.2522249101	-0.6666446802	0.4737931649
H	2.9402117506	-2.7261464816	-1.749307187

H	4.1780991216	-1.4760889073	-1.6848549671
H	1.1036836111	-2.7517475496	-0.0192542855
H	0.5677080919	0.0926996411	2.9415951739
H	2.1494781121	0.0493767472	2.1788861306
H	1.6958378869	-1.2229075693	3.3452604748
H	5.0440940896	-3.653057851	-0.8434150253
H	5.0443123416	-2.4563677617	0.4472093079
H	1.9271906796	-3.7182757561	2.1274534566
H	3.1866385037	-2.4893856445	2.1959402194
H	2.8941170566	-4.5831930425	-0.0086322579
H	4.0927828909	-4.5999759062	1.2798292011
O	-1.7226863424	-0.477568705	-0.3724411979
C	-2.1091823569	-1.5679724261	-1.186851066
H	-2.4385418877	-1.214692016	-2.1696799403
H	-1.2493269588	-2.225669333	-1.3067233971
H	-2.9254105649	-2.1233869121	-0.7136423252

Abbildung 10.87 Molekel Darstellung von *(R,R,R)*-**101** [globales Minimum; M05-2X/6-31+G(d)].Tabelle 10.577 Standardorientierung von *(R,R,R)*-**101** [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-4.3940741487	-2.9404504811	0.8534220294
C	-4.2417128294	-3.03049484	-0.6637624581
C	-3.033482913	-2.6703916799	1.4960739499
C	-3.6338998495	-1.7370819605	-1.2080934242
C	-2.3992225336	-1.3778247588	0.9586136518
C	-1.3080599273	-0.2985657504	2.8505402419
C	-2.2651221015	-1.4366768803	-0.5739940758
C	-0.2303461379	-2.1692471442	1.827331004
C	-2.4157542721	0.993924095	-1.0046362973

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C	-1.1708643921	-0.3863440093	-2.4883986646
Li	-0.0232785339	0.1913251655	0.252633247
N	-1.1121185879	-1.0237228749	1.5944637365
N	-1.5998495911	-0.2246527139	-1.098126238
H	-4.8195895966	-3.8632969447	1.2551599225
H	-5.0897388619	-2.1305806752	1.1016349922
H	-5.2082318477	-3.2155981886	-1.1387400168
H	-3.5937994074	-3.8791798965	-0.9135132638
H	-3.1272914312	-2.6063091363	2.5839257437
H	-2.3773106139	-3.519797671	1.279061988
H	-4.3220232481	-0.9146930733	-0.9876908328
H	-3.5347716463	-1.7916242307	-2.295015426
H	-3.0865579717	-0.5585193411	1.1944017348
H	-1.835150703	-0.9036421612	3.6027880496
H	-1.8712550964	0.6162594382	2.662271453
H	-0.334362247	-0.0120034527	3.2484758751
H	-1.5937348543	-2.2721550461	-0.8157005751
H	-0.5879281871	-2.8136882007	2.6415551798
H	-0.1388971804	-2.7683297175	0.9209553279
H	0.7626499591	-1.7992293414	2.0832052811
H	-2.6774184641	1.2060032587	0.0324865158
H	-3.3323262389	0.9269588907	-1.6042235653
H	-1.8276508803	1.833339604	-1.371931768
H	-2.0151739175	-0.3879782822	-3.1908962577
H	-0.6207634737	-1.3209866278	-2.6034036373
H	-0.5138980642	0.4452729854	-2.7477816328
C	-0.8141848184	4.3182291021	-2.1327050061
C	-1.2802921024	4.4698605404	-0.8207914397
C	0.2318769785	3.4216442656	-2.3534267993
C	-0.7337791736	3.7425231946	0.2243999666
C	0.7835981903	2.6864968072	-1.3088155728
C	0.3214854914	2.8059341531	0.0322617707
C	0.8452775195	2.0119900167	1.1138823097
C	3.9484670413	2.6516720656	0.769498484
C	2.9192341284	0.6793635058	2.8949503516
C	2.8689711565	-0.0037876597	-0.0874678396
Si	2.5649990457	1.4206802005	1.1858455417
H	-1.2395437745	4.891645132	-2.9463977453
H	-2.080714263	5.172489591	-0.6131636113
H	0.6282475309	3.2922288593	-3.3556432533
H	-1.1114513141	3.8870752391	1.2319725318
H	1.5949333754	1.9973653165	-1.526574049
H	0.4188192879	2.2515653288	2.0889039115
H	4.0354180537	3.4006709266	1.560732503
H	3.7221580092	3.1797222517	-0.1607688718
H	4.9196642466	2.1584249818	0.6586328635
H	2.7368902116	1.4206587265	3.6776788317
H	2.2805753285	-0.1846763422	3.0985444712
H	3.960758718	0.3558584531	2.9749326283
H	3.2080840369	0.3815304708	-1.0583032147
H	3.6421234857	-0.6937271938	0.2780061925

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O	1.6512915029	-0.7498610765	-0.2896841387
C	1.8437552156	-1.8590698433	-1.1465669606
H	0.8973616842	-2.3923010941	-1.2288159353
H	2.1620121836	-1.5249285975	-2.1396552594
H	2.6029201243	-2.5302342487	-0.7324783412

Tabelle 10.578 In Analogie zu **Fehler! Verweisquelle konnte nicht gefunden werden.** weiterführende Informationen zur Deprotonierung von (*R,R*)-**72** mit *iso*-Propyllithium (**E2**, **TS4**) und *tert*-Butyllithium (**E3**, **TS5**).

Struktur	Methode/Basis	SCF [Hartree]	ZPE [Hartree]	ZPE [kJ/mol]
pro-( <i>S</i> )-(S <sub>N</sub> , <i>R,R</i> )- <b>E2</b>	M05-2X/6-31+G(d)	-1269.442986	-1268.836731	0
pro-( <i>R</i> )-(S <sub>N</sub> , <i>R,R</i> )- <b>E2</b>	M05-2X/6-31+G(d)	-1269.439876	-1268.834562	6
pro-( <i>S</i> )-(R <sub>N</sub> , <i>R,R</i> )- <b>E2</b>	M05-2X/6-31+G(d)	-1269.440733	-1268.835235	4
pro-( <i>R</i> )-(R <sub>N</sub> , <i>R,R</i> )- <b>E2</b>	M05-2X/6-31+G(d)	-1269.441026	-1268.834588	6
(S <sub>N</sub> , <i>S,R,R</i> )- <b>TS4</b>	M05-2X/6-31+G(d)	-1269.425504	-1268.823848	34
(S <sub>N</sub> , <i>R,R,R</i> )- <b>TS4</b>	M05-2X/6-31+G(d)	-1269.419057	-1268.818010	49
(R <sub>N</sub> , <i>S,R,R</i> )- <b>TS4</b>	M05-2X/6-31+G(d)	-1269.420207	-1268.818870	47
(R <sub>N</sub> , <i>R,R,R</i> )- <b>TS4</b>	M05-2X/6-31+G(d)	-1269.425462	-1268.823110	36
pro-( <i>S</i> )-(S <sub>N</sub> , <i>R,R</i> )- <b>E3</b>	M05-2X/6-31+G(d)	-1308.751612	-1308.116677	1
pro-( <i>R</i> )-(S <sub>N</sub> , <i>R,R</i> )- <b>E3</b>	M05-2X/6-31+G(d)	-1308.749674	-1308.115624	4
pro-( <i>S</i> )-(R <sub>N</sub> , <i>R,R</i> )- <b>E3</b>	M05-2X/6-31+G(d)	-1308.751345	-1308.117202	0
pro-( <i>R</i> )-(R <sub>N</sub> , <i>R,R</i> )- <b>E3</b>	M05-2X/6-31+G(d)	-1308.751973	-1308.117222	0
(S <sub>N</sub> , <i>S,R,R</i> )- <b>TS5</b>	M05-2X/6-31+G(d)	-1308.730073	-1308.100158	45
(S <sub>N</sub> , <i>R,R,R</i> )- <b>TS5</b>	M05-2X/6-31+G(d)	-1308.727013	-1308.096988	53
(R <sub>N</sub> , <i>S,R,R</i> )- <b>TS5</b>	M05-2X/6-31+G(d)	-1308.728455	-1308.098584	49
(R <sub>N</sub> , <i>R,R,R</i> )- <b>TS5</b>	M05-2X/6-31+G(d)	-1308.729782	-1308.099700	46

Tabelle 10.579 Standardorientierung von pro-(*S*)-(S<sub>N</sub>,*R,R*)-**E2** [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.7908014692	-0.6585241327	0.2462967782
C	-2.0528976428	0.3730965094	-0.6285034023
C	-3.0652284618	1.3880228941	-1.1822694944
C	-4.1667797445	0.6995061186	-1.990822735
C	-4.8899089197	-0.3356545469	-1.1307034912
C	-3.8881964902	-1.3504379347	-0.5776500971
N	-1.8480747116	-1.5835604741	0.9064614798
N	-0.9010674451	0.9816247568	0.0837853526
C	-2.3961280333	-2.144213677	2.142678019
C	-1.3722002372	-2.6664644668	0.0436073263
C	-1.3089745708	1.9242663566	1.1336011193
C	0.0244870761	1.6365715624	-0.8523751366
Si	1.7579480842	2.1877393946	-0.2597607405
C	2.4391804329	3.0790773168	-1.7844161011

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C	1.7791722871	3.412035593	1.1757332116
C	2.8253871736	0.682350821	0.1896629765
H	-3.2893434085	-0.1157902975	1.0571890995
H	-1.6147712332	-0.1653222118	-1.4770630389
H	-2.5501079637	2.1274201383	-1.7998496214
H	-3.5286383979	1.9276894115	-0.3488173506
H	-4.870724253	1.4441467552	-2.3702310563
H	-3.7255175548	0.2020609414	-2.8622819606
H	-5.6599279574	-0.8492680264	-1.7114192837
H	-5.3972456773	0.1707202935	-0.3012827855
H	-4.3976987185	-2.0956135452	0.0396714014
H	-3.4318741076	-1.8835904281	-1.4185792811
H	-1.6232267505	-2.7365802424	2.6335575884
H	-2.6759275219	-1.3368985037	2.8201360095
H	-3.2705446883	-2.7845999263	1.9599364063
H	-0.5560295491	-3.1813016495	0.5546820897
H	-0.9854377979	-2.2663469931	-0.8940525367
H	-2.156431592	-3.4028623937	-0.1758378026
H	-1.6748260414	2.8734032142	0.7191522689
H	-0.457334392	2.1282777072	1.7800794447
H	-2.0920625069	1.487325686	1.754748472
H	-0.4440650031	2.5206384571	-1.3175992435
H	0.2386337619	0.9336441386	-1.6661241823
H	3.5073845764	3.2830390365	-1.6705505556
H	1.931507775	4.0394533731	-1.9127484813
H	2.2990815135	2.499711481	-2.6997831474
H	1.6292634063	2.9199814192	2.138105252
H	2.7564579785	3.9030853545	1.2038802298
H	1.0200902268	4.1896783826	1.0553446691
H	2.4951090366	0.321057146	1.168752565
H	3.8580588122	1.0334866764	0.2947108084
C	0.8258630554	-0.6321678678	3.141188351
C	1.7545916129	-1.8491705757	3.2310130819
C	1.5021943359	0.5388320647	3.858808727
Li	-0.1858694782	-0.4620933529	1.3536754834
H	2.6734971028	-1.6981556939	2.6461188829
H	1.2875842871	-2.7662886208	2.8442702482
H	2.0897399929	-2.0748400329	4.2613161052
H	0.8390987103	1.4085360364	3.9521622628
H	2.4016330814	0.8810586806	3.3272451293
H	1.841886189	0.2881004185	4.8819247698
C	2.7370578755	-0.4210014928	-0.8278953435
C	2.0659990877	-1.612013143	-0.5281783282
C	3.305448782	-0.2868576581	-2.101543711
C	1.949812691	-2.6273964968	-1.4765595322
H	1.6758824321	-1.7526294462	0.4765244261
C	3.1892785034	-1.2984437578	-3.0507358068
H	3.8550045608	0.6161083145	-2.3441408843
C	2.503795754	-2.4734981544	-2.7448122834
H	1.4415878327	-3.5491667302	-1.2172525656
H	3.6424987903	-1.1736206001	-4.0270494292

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H	2.4191000386	-3.2646476314	-3.4795959333
H	-0.0704257771	-0.879555596	3.7428130476

Tabelle 10.580 Standardorientierung von pro-(R)-(S<sub>N</sub>,R,R)-E2 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-3.3828827026	-0.7344545943	0.0381361731
C	-2.7364573275	0.6081879622	-0.3513096002
C	-3.7532202964	1.7432211364	-0.162457804
C	-5.0033743149	1.507160634	-1.0133032503
C	-5.6418888104	0.1631159089	-0.6629505244
C	-4.6282087719	-0.9711011108	-0.8306847297
N	-2.3981413071	-1.8306988384	0.0201662846
N	-1.4352764721	0.8190742233	0.3267936868
C	-2.8245821291	-2.9902732217	0.8035242962
C	-1.9863351225	-2.2555548357	-1.3181928471
C	-1.5796195455	1.1699991765	1.7462434964
C	-0.6172094553	1.8366063186	-0.3569222619
Si	1.2806468775	1.7529787751	-0.1123275671
C	1.9516318947	3.0692789745	-1.2870813456
C	1.8637993372	2.1337917572	1.6370237731
C	1.8633680615	0.0246966185	-0.6503531492
H	-3.7177900694	-0.6591936994	1.0795210994
H	-2.5013473172	0.5568291697	-1.4201315087
H	-3.2904267177	2.6994037411	-0.4212277589
H	-4.0497497385	1.7991779616	0.8904822304
H	-5.7168925829	2.3208679792	-0.8631833124
H	-4.7295689654	1.513024785	-2.0748349062
H	-6.5167366109	-0.0211269048	-1.2910410663
H	-5.9926444651	0.1882764215	0.3752861393
H	-5.0836920175	-1.9304150626	-0.5713321563
H	-4.3316210739	-1.0269916537	-1.8840435944
H	-1.9906129533	-3.6887362225	0.8791421757
H	-3.0842788021	-2.6724355352	1.813741157
H	-3.6825098124	-3.5090881302	0.3540409322
H	-1.1297018167	-2.9260585043	-1.2211084069
H	-1.677939468	-1.3948304188	-1.9137737232
H	-2.781153357	-2.7898969297	-1.8550817468
H	-1.9908558972	2.1789577853	1.8822011533
H	-0.6033792668	1.1245622438	2.2273052075
H	-2.2274902153	0.4518509305	2.252206968
H	-0.9785463562	2.8540708578	-0.1334580451
H	-0.7422499276	1.6995797657	-1.4373264914
H	3.0434650594	3.0860492424	-1.2543652722
H	1.5881672097	4.0616386858	-1.0058163083
H	1.6526521495	2.8790594456	-2.3215810778
H	1.6658174495	1.310027806	2.3251579194
H	2.9441104257	2.3030967961	1.6246976089
H	1.3865134711	3.0388525084	2.0233161411
H	1.3200902096	-0.2657593869	-1.5571357501
H	1.6037896142	-0.6895553129	0.1411298906

C	0.4654140844	-2.1053259072	2.1351101538
C	1.2360467701	-3.2519244808	1.465680725
C	1.3928412561	-1.4391004648	3.1534474432
Li	-0.6823665481	-1.0600487053	0.7887927274
H	2.0600575861	-2.875686676	0.8426033243
H	0.6013172796	-3.8588135408	0.8051422015
H	1.7006868009	-3.9513983723	2.1869167178
H	0.8776725854	-0.6789893497	3.754544225
H	2.2341185071	-0.9329350151	2.6596058021
H	1.8518408455	-2.152356157	3.8646521367
C	3.3468634865	0.0167057289	-0.9055684393
C	3.8618427068	0.2998208237	-2.1757483401
C	4.2503394203	-0.2323978991	0.1335700229
C	5.2351042662	0.3375235806	-2.4021658105
H	3.1763706834	0.4907308496	-2.9952906866
C	5.6247906178	-0.193613682	-0.0891215863
H	3.8693621864	-0.4720179545	1.1200515932
C	6.1245233101	0.0935201933	-1.3574447657
H	5.6097860528	0.5541958228	-3.3955929067
H	6.3046886511	-0.3969091397	0.7295392527
H	7.1931350716	0.1195020318	-1.5316480253
H	-0.347962823	-2.575478035	2.7204172267

Tabelle 10.581 Standardorientierung von pro-(S)-(R<sub>N</sub>,R,R)-E2 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.8067229571	-0.4440219498	-0.9996796054
C	-2.8383389808	-0.5035318446	0.5399503784
C	-3.5922048301	-1.7560795121	1.0117444271
C	-5.0086299417	-1.8128136535	0.436826694
C	-4.9575163814	-1.7833793206	-1.0899592782
C	-4.2330598834	-0.5231530427	-1.5647204609
N	-2.0305961099	0.7226790569	-1.4704220129
N	-1.4767224075	-0.357747867	1.1108095214
C	-1.477751897	0.5262414644	-2.8094707805
C	-2.7655817807	1.9931934503	-1.4304378723
C	-1.5279433331	0.1387859815	2.4885855828
C	-0.6646999243	-1.5863505548	1.0420185618
Si	1.2406231524	-1.3846037825	1.0605085354
C	1.9495562836	-0.6390855357	2.6372701969
C	1.8908597973	-3.1443796044	0.8562671332
C	1.7376903561	-0.3232853462	-0.4409332814
H	-2.2602454071	-1.3264227744	-1.3533971214
H	-3.3984707938	0.372070172	0.8900744225
H	-3.621669495	-1.7778262734	2.1043109933
H	-3.0505527595	-2.6504148498	0.6871621583
H	-5.5164143973	-2.7142934287	0.788089208
H	-5.5899705266	-0.9560419311	0.7968163955
H	-5.9656346228	-1.8142283742	-1.5101781634
H	-4.4305598769	-2.6734307984	-1.4533969814
H	-4.1986237594	-0.4867145597	-2.6572391861

H	-4.8039112681	0.3496874009	-1.2307907031
H	-0.8118470778	1.3590625149	-3.0411954734
H	-0.8967746894	-0.3967088624	-2.8389233158
H	-2.2564646165	0.4788670776	-3.5836851971
H	-2.0579313418	2.8075724416	-1.5879213815
H	-3.2199294161	2.1405279331	-0.4499576381
H	-3.5478731662	2.0441043213	-2.1990790015
H	-2.0779336471	1.0802445858	2.5186590946
H	-0.5166968702	0.3362688725	2.8381945074
H	-1.9987257951	-0.5817095538	3.1726392676
H	-0.8581842789	-2.0816255353	0.0842408082
H	-0.9674505086	-2.30392215	1.8222772139
H	3.0346209252	-0.774768219	2.6364655811
H	1.5493654886	-1.1347010043	3.526037331
H	1.7492541897	0.4317570491	2.7112403577
H	1.520264621	-3.6095786815	-0.0614548727
H	2.9823373518	-3.144745962	0.8136515019
H	1.5839911808	-3.7689094585	1.6998439571
H	1.1784247801	-0.6618354995	-1.3206070277
H	1.469319017	0.7240371872	-0.2493059615
C	0.1897485174	2.9802513997	0.3973179022
C	0.9438238602	3.5373290181	-0.8180111854
C	1.0896072078	3.1367706282	1.6263931884
Li	-0.6636101642	1.1519369579	-0.0034150025
H	1.8223583844	2.92302907	-1.0648530099
H	0.3230484221	3.5663165918	-1.7241643415
H	1.3294921633	4.5641296169	-0.6677877724
H	1.9845139104	2.5014407514	1.5518816386
H	0.5803328759	2.8539887333	2.5564656246
H	1.4698621041	4.1666251363	1.76948742
C	3.2187141574	-0.4283630911	-0.6950923609
C	3.7404272649	-1.4278797907	-1.5240328418
C	4.1125387014	0.4502382239	-0.073120485
C	5.1129954321	-1.5505672569	-1.7231133477
H	3.0615544539	-2.1147971922	-2.0192564536
C	5.4861425053	0.3288646143	-0.2689084035
H	3.7237359753	1.2422767805	0.557521094
C	5.9935150658	-0.6732371868	-1.093163001
H	5.4940956183	-2.3291070699	-2.3733206292
H	6.1589208459	1.0247837804	0.217633465
H	7.0613048208	-0.7650239821	-1.2488797156
H	-0.679663915	3.6434938479	0.5615865648

Tabelle 10.582 Standardorientierung von pro-(R)-(R<sub>N</sub>,R,R)-E2 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	2.2733653184	-0.9393415835	-0.6322581602
C	2.4699943289	0.40679623	0.0869588031
C	3.2721800073	1.3710100447	-0.7992764209

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C	4.6318765763	0.7795671657	-1.173823642
C	4.4385986354	-0.5499784374	-1.9010345985
C	3.6413650231	-1.5198597523	-1.0273499996
N	1.4320728396	-1.8559267991	0.1665644406
N	1.1847926322	0.9529299859	0.5940215834
C	0.9441364945	-2.9852291918	-0.6239465062
C	2.0705027813	-2.366412861	1.3850052647
C	1.4034371326	1.7750938622	1.7864612327
C	0.4243973912	1.7025697122	-0.4204939558
Si	-1.3696865138	2.2957177626	-0.0828937021
C	-1.6005177351	3.3495305936	1.4657515673
C	-1.6874812635	3.4064983885	-1.5815473291
C	-2.6166208818	0.8660464231	-0.004648272
H	1.704884489	-0.748630596	-1.5513177416
H	3.0793564185	0.2121975101	0.976147264
H	3.3979879669	2.3263318479	-0.2816173195
H	2.7175183006	1.572915292	-1.7209232735
H	5.1848977694	1.4840421605	-1.7997979391
H	5.2285993638	0.6166059216	-0.2687826139
H	5.4035983257	-0.9914599707	-2.161495329
H	3.9018467229	-0.3744794971	-2.8405703114
H	3.5040713749	-2.4715741796	-1.5467326932
H	4.2203418518	-1.7266652414	-0.120566144
H	0.1677225968	-3.5033873469	-0.0574273071
H	0.5092391045	-2.6204225999	-1.5538393966
H	1.7378026606	-3.7080797201	-0.8567735491
H	1.3222125091	-2.913149713	1.9600145903
H	2.4252582417	-1.5455858684	2.0094723008
H	2.9092294958	-3.0401571827	1.1670497689
H	1.9755023954	1.2076006247	2.5215763992
H	0.4459421422	2.0222163945	2.2369657722
H	1.9387991809	2.7082689716	1.5562289496
H	0.3425497194	1.0869123458	-1.3246278612
H	0.9687489715	2.6145629235	-0.7180120092
H	-2.5466172832	3.8917526947	1.3753474529
H	-0.8037907895	4.0889022557	1.5814688592
H	-1.653352774	2.7429129162	2.3718435448
H	-1.4552778006	2.9052496507	-2.5239533951
H	-2.7316251096	3.7288017877	-1.6157162772
H	-1.066646689	4.3045968266	-1.5140552034
H	-2.4088104064	0.288809942	0.9030471364
H	-3.6021715058	1.328944947	0.1251040175
C	-1.0918094489	-1.1164199601	2.7719862835
C	-2.1163940556	-2.2426174447	2.5905100738
C	-1.7318476914	-0.024758571	3.6356279267
Li	0.0364147175	-0.6571422495	1.1046182774
H	-2.9752703689	-1.9119691582	1.9885147986
H	-1.6939203863	-3.1177084934	2.0770147959
H	-2.5437209867	-2.6093581414	3.5431589243
H	-2.5565107565	0.4798017162	3.1113545306
H	-1.0138476531	0.7544805743	3.9214689632

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H	-2.1723425667	-0.410824863	4.5745993488
C	-2.6204458021	-0.0398041426	-1.2062510863
C	-2.1814364948	-1.3642110529	-1.1006845039
C	-3.0794575093	0.4055224523	-2.4532791408
C	-2.1963330764	-2.2134582808	-2.2071442845
H	-1.8712902795	-1.739904372	-0.1295927272
C	-3.0880829957	-0.4379847988	-3.5600904209
H	-3.4506894837	1.4196068491	-2.5503152261
C	-2.6428152537	-1.7542051466	-3.4430281608
H	-1.8778880553	-3.2435987749	-2.0959206537
H	-3.4542562787	-0.071472862	-4.5117941919
H	-2.660567174	-2.4162661259	-4.3000229702
H	-0.2686039102	-1.5390974445	3.3799559663

Tabelle 10.583 Standardorientierung von  $(S_N, S, R, R)$ -TS4 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.6635138285	-0.8132184915	-0.0542676649
C	-2.2739989605	0.6243567354	-0.4487145109
C	-3.4540279007	1.5765263066	-0.204449862
C	-4.7068983164	1.1341941401	-0.9612573478
C	-5.0927982579	-0.2859999168	-0.5509295349
C	-3.9284650452	-1.2421472815	-0.8147414858
N	-1.5211514052	-1.7486678756	-0.1983931203
N	-1.0151366126	1.0403505306	0.2061526334
C	-1.6741713318	-2.9205948404	0.669292663
C	-1.3083635641	-2.2060361078	-1.5761820523
C	-1.1713707623	1.3498683613	1.6321939917
C	-0.3605569156	2.1801594455	-0.4620824735
Si	1.5061288202	2.3799235925	-0.0160663598
C	2.22955342	3.3106281587	-1.4970729794
C	1.7146957408	3.4595511893	1.525145032
C	2.2862007636	0.7141990521	0.3009961823
H	-2.9074259098	-0.8097155465	1.0138038399
H	-2.0605163534	0.6248371788	-1.5248507601
H	-3.1666973935	2.5910646754	-0.4929860542
H	-3.6849634898	1.5973878845	0.8660652245
H	-5.527032377	1.8287863909	-0.7642888556
H	-4.516054105	1.1608151195	-2.040505184
H	-5.9781632691	-0.61886596	-1.0979684713
H	-5.3492804699	-0.3000818032	0.5147230279
H	-4.2012614405	-2.2632780628	-0.5346750433
H	-3.7237885067	-1.2460021532	-1.8906239671
H	-0.7717301064	-3.5298389332	0.6073229529
H	-1.795615672	-2.6020439598	1.7042191422
H	-2.5320772651	-3.5426851472	0.3797450286
H	-0.3476116322	-2.7189834903	-1.633353325
H	-1.2745201583	-1.3569831172	-2.2592105263
H	-2.0938889089	-2.8968052376	-1.9082514128
H	-1.693263976	2.3029400209	1.7910999382
H	-0.1840983259	1.4117141386	2.0860164264

H	-1.713248309	0.5544362509	2.1448157582
H	-0.8981107579	3.1219782253	-0.2618874334
H	-0.4116043017	2.0228758545	-1.5445065557
H	3.2709635539	3.5808551755	-1.3051226848
H	1.674654258	4.2303571621	-1.7060936504
H	2.208984531	2.6853607176	-2.393621317
H	1.5456462956	2.8968283907	2.4460361905
H	2.7358917255	3.8494059004	1.5610660281
H	1.0329010803	4.3144788374	1.5126876056
H	1.6014524221	-0.0199066543	1.186385107
H	3.201794026	0.8726775604	0.8813605275
C	1.091745813	-1.0895339221	2.2508332015
C	1.9830187224	-2.3024342194	1.9783245049
C	1.6125531532	-0.3375395788	3.4722863528
Li	0.1674061221	-0.6330412963	0.3649701433
H	2.9931320255	-1.9708319048	1.7094164757
H	1.6281117565	-2.9131984254	1.1382384571
H	2.0900472424	-2.9710167408	2.8480475102
H	0.9317722486	0.4587571934	3.7939327071
H	2.5782058577	0.1379196744	3.2508019152
H	1.7780335382	-0.9899674914	4.3433633066
C	2.5620014814	-0.1608517472	-0.8607274811
C	1.6205600361	-0.3656237764	-1.8884077713
C	3.7598611264	-0.9009756497	-0.9565287895
C	1.8624830833	-1.2403948033	-2.9495445692
H	0.6911603022	0.197836226	-1.8793500925
C	4.0008415792	-1.7734860309	-2.0066831071
H	4.5073055488	-0.7766122746	-0.1805517887
C	3.0520719061	-1.9544973379	-3.0186178696
H	1.1148086416	-1.3550939626	-3.7271695121
H	4.936881629	-2.318995737	-2.0416063071
H	3.2435932616	-2.6325280488	-3.8407216592
H	0.0693811766	-1.438170213	2.4823554758

Tabelle 10.584 Standardorientierung von  $(S_N, R, R, R)$ -TS4 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	3.249569022	0.4113575672	-0.4567441926
C	2.6906396791	-0.9471426006	0.0076919311
C	3.7543745291	-1.708310235	0.8106270218
C	5.0270625057	-1.9187290905	-0.0113932506
C	5.5811332339	-0.5737414683	-0.4808152743
C	4.5239745831	0.1866186755	-1.2851674904
N	2.2117153517	1.2256906936	-1.1338807658
N	1.3944599304	-0.7901316683	0.698293099
C	2.5655648152	2.6472902558	-1.159389101
C	1.8938550498	0.7745501946	-2.4923239708
C	1.52002135	-0.3216421711	2.0830735685
C	0.5568277437	-2.0046938739	0.652776676
Si	-1.3214224218	-1.6438453017	0.8612427771
C	-2.2151632623	-3.1925803975	0.245767625

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C	-1.7886124828	-1.4176357155	2.6857625862
C	-1.6075167927	-0.1286705688	-0.1929239729
H	3.5283410107	0.9829057944	0.4363851667
H	2.47710419	-1.5365263995	-0.890828723
H	3.3419128194	-2.6667479869	1.1381144772
H	4.009049714	-1.1396248088	1.7114314369
H	5.7718472343	-2.4545577126	0.5817780814
H	4.8025745877	-2.5431558324	-0.8839794673
H	6.4775085158	-0.717896467	-1.0886373323
H	5.8770518342	0.0214440147	0.3908339637
H	4.9236378981	1.145029841	-1.6265986681
H	4.2787039756	-0.3991310992	-2.1779313383
H	1.7250519245	3.2172893431	-1.556350284
H	2.758731486	2.9948439583	-0.1442529406
H	3.446005061	2.8486734653	-1.7836091704
H	1.0136681529	1.3167501497	-2.8443490444
H	1.6597250883	-0.2908866883	-2.4952860403
H	2.7123842154	0.95936526	-3.1992375047
H	1.8960638751	-1.106983572	2.752409351
H	0.5413894281	-0.0011085629	2.4391299416
H	2.1874920894	0.5401371986	2.1361392495
H	0.9191773847	-2.7682535456	1.3598606536
H	0.6452679041	-2.436287406	-0.3504776729
H	-3.2926592761	-3.0068104424	0.2320141748
H	-2.0284246013	-4.0556710666	0.8914511479
H	-1.9118219701	-3.4489255883	-0.7726300223
H	-1.6672062108	-0.3851872501	3.0200423516
H	-2.8340804276	-1.6980556185	2.8397132371
H	-1.1780471778	-2.0631342564	3.3246696589
H	-1.0421520194	-0.2788781389	-1.1309703221
H	-1.1007965599	0.9715331569	0.446023692
C	-0.5629527665	2.3584411101	0.9442900504
C	-1.1655195714	3.2433234399	-0.1488791609
C	-1.3262147293	2.5297337491	2.2537554024
Li	0.4903108627	0.8513510259	-0.0782506251
H	-2.2098342153	2.9630980836	-0.3251558521
H	-0.651174321	3.1262913962	-1.1142685107
H	-1.1531981941	4.3168929379	0.0941019174
H	-0.854277657	1.9829487536	3.0781556376
H	-2.3492864838	2.1487174775	2.1556336813
H	-1.4106456081	3.5806351285	2.5718085509
C	-3.0187134346	0.1741666531	-0.5408262105
C	-3.4227465416	0.3859286053	-1.8712460365
C	-4.0117620807	0.2923035888	0.4494424154
C	-4.7378453818	0.7026569831	-2.1952322394
H	-2.6836512779	0.3014920916	-2.6619678998
C	-5.3290643009	0.6033251107	0.1271725716
H	-3.7379240634	0.1575616112	1.4900955353
C	-5.7063358439	0.8132806405	-1.1983559633
H	-5.0081310402	0.8612596715	-3.2331904196
H	-6.0639968066	0.689522279	0.9194967712

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H	-6.7308066238	1.0592909865	-1.4484848758
H	0.4824373686	2.6809527216	1.1212916407

Tabelle 10.585 Standardorientierung von  $(R_M, S, R, R)$ -TS4 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	2.8445758644	-0.4472824535	-0.9088792668
C	2.8804861377	0.3991480773	0.3783690968
C	3.8520172717	1.5766131896	0.2112009442
C	5.2573833858	1.0983643021	-0.1573324909
C	5.2132986269	0.2720383977	-1.4419901924
C	4.2618754017	-0.9139192698	-1.2726618017
N	1.8502757071	-1.5425339378	-0.8087505251
N	1.5159269568	0.7862618889	0.8029364641
C	1.407442023	-2.0081057448	-2.1245943267
C	2.3018735556	-2.6893316668	-0.0118532752
C	1.456418395	1.0621730618	2.2390656412
C	0.9317813662	1.9125359086	0.0414304628
Si	-0.9932694493	1.9694959315	0.031591524
C	-1.6894383434	2.5816111007	1.6846640198
C	-1.4394113182	3.2641749882	-1.2732253838
C	-1.5165733847	0.2337341299	-0.4208655653
H	2.4870724389	0.1987511049	-1.71928018
H	3.2711123854	-0.2394175184	1.1802295106
H	3.8760735438	2.1643722836	1.1327683315
H	3.487183665	2.237390963	-0.5815687907
H	5.9239161646	1.9560682221	-0.2749276418
H	5.6649683689	0.4846577706	0.6544778434
H	6.2114733893	-0.0867226057	-1.7039743686
H	4.8716366553	0.9042424522	-2.2697366861
H	4.2324705927	-1.51471006	-2.1857953603
H	4.6490681442	-1.5567306768	-0.4747195486
H	0.5938533591	-2.723332415	-1.9925278133
H	1.0311405886	-1.1654762584	-2.7062187631
H	2.211210277	-2.5000717514	-2.6884459629
H	1.4509431815	-3.3486867211	0.1667036532
H	2.675605433	-2.3559094276	0.9570150023
H	3.0876197547	-3.2646978972	-0.5171949135
H	1.8415789737	0.2060161481	2.7954911293
H	0.4193151528	1.2141639234	2.5322388283
H	2.0281724528	1.9593577322	2.5155177532
H	1.2005043907	1.7938677453	-1.0139937211
H	1.3624278739	2.8730372818	0.3658168489
H	-2.6814392348	3.0131645297	1.5269215919
H	-1.0530558985	3.3653221073	2.1069389269
H	-1.7878870433	1.778900341	2.4187744474
H	-0.9806010954	3.0328618016	-2.2382299739
H	-2.5233607103	3.2712788778	-1.4173411205
H	-1.1304784984	4.2703089201	-0.9750655739
H	-0.892573677	-0.0743725096	-1.2790311168
H	-1.2730355644	-0.6453486103	0.5982268139

C	-0.9909142948	-1.800132489	1.6205538324
C	-1.7029572727	-2.9513692743	0.9092151548
C	-1.812398749	-1.3146317027	2.8118508519
Li	0.3482782309	-0.7886872544	0.3388087823
H	-2.6432336982	-2.6007862534	0.4683239809
H	-1.1069607398	-3.3618038853	0.0825185241
H	-1.9525660557	-3.7915710024	1.5756947954
H	-2.7556118383	-0.870254078	2.4732727425
H	-1.2825198762	-0.5481932085	3.3890342266
H	-2.0784151421	-2.1215257226	3.5123204542
C	-2.9421666294	0.0694889998	-0.8075313277
C	-3.3092849893	-0.4947830341	-2.0422773596
C	-3.9891921845	0.4481553025	0.0530207991
C	-4.642197117	-0.6753318866	-2.397261473
H	-2.5274030813	-0.7978223799	-2.7317930761
C	-5.3231332262	0.2751216837	-0.3030491708
H	-3.7495964212	0.8636305505	1.0251443632
C	-5.6641618122	-0.2890821153	-1.5313290871
H	-4.8833153537	-1.1175328277	-3.3573781783
H	-6.1012163789	0.5756959266	0.3894237037
H	-6.7024459414	-0.4279246835	-1.805787626
H	-0.0253146692	-2.1755954821	2.0139743272

Tabelle 10.586 Standardorientierung von  $(R_N, R, R, R)$ -TS4 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.225934533	0.7045457424	0.1126388684
C	-2.251882029	-0.8098551618	0.3925865126
C	-3.2535589663	-1.5181379651	-0.5309849737
C	-4.656894065	-0.9261425828	-0.3953347616
C	-4.6234881047	0.567598597	-0.713288383
C	-3.6456973877	1.2830446899	0.2199656665
N	-1.2294363015	1.3889021192	0.9693934377
N	-0.88421379	-1.3864817248	0.3729360759
C	-0.916208261	2.7375728224	0.4892360441
C	-1.5953395929	1.4595731991	2.387226167
C	-0.7841977745	-2.5097538274	1.3055676544
C	-0.410727852	-1.8019446704	-0.9644695285
Si	1.502842926	-1.9559344746	-1.136368511
C	2.1983082049	-3.5064536017	-0.3014248206
C	1.7836220456	-2.2439824693	-2.9937148978
C	2.2743228751	-0.4504279325	-0.349700292
H	-1.8708791084	0.8488780758	-0.9165018112
H	-2.6170978022	-0.9436455693	1.4168926132
H	-3.2625714772	-2.5881514757	-0.3046849439
H	-2.9335609941	-1.4135301922	-1.5719936418
H	-5.3471241939	-1.447493771	-1.0630448348
H	-5.0262681368	-1.0722194863	0.6264843139
H	-5.6195069532	1.0061733464	-0.6150070311
H	-4.311265641	0.7100090152	-1.754465798
H	-3.6274263365	2.3537254591	0.0026165909

H	-4.0039483126	1.1675325463	1.2489361967
H	-0.0611246356	3.1204922347	1.0480918623
H	-0.6377680891	2.7002838242	-0.5629083982
H	-1.7555997319	3.4333428826	0.6223259886
H	-0.7356279162	1.8304605911	2.9472409543
H	-1.8413431641	0.471085579	2.7748102804
H	-2.44147868	2.1352687946	2.5664726055
H	-1.0239718415	-2.176188938	2.3164028748
H	0.2363454071	-2.8851567282	1.3096341205
H	-1.4549483383	-3.3364508403	1.0283379433
H	-0.7080846048	-1.0343124953	-1.6852283167
H	-0.9014899627	-2.7348620045	-1.2871763777
H	3.1606251628	-3.7489531579	-0.7623333641
H	1.5388597699	-4.3673923636	-0.4443090838
H	2.3719820683	-3.3708989463	0.7668025724
H	1.2676402301	-1.5331010033	-3.6416202298
H	2.8516342408	-2.1794262729	-3.2184241483
H	1.44785899	-3.2498799504	-3.264687441
H	1.9835053791	-0.378457722	0.9547702696
H	3.3448042716	-0.6291997442	-0.1936523698
C	1.7109876959	-0.1930271178	2.5503438346
C	2.4281604826	1.0482257813	3.0814956079
C	2.4954375822	-1.4353942782	2.9660450214
Li	0.3912013318	0.1533473507	0.8879578782
H	3.4243626365	1.1373251881	2.6299933009
H	1.8938439114	1.9786787925	2.8564855472
H	2.5912396372	1.0147750405	4.1713155488
H	3.4272110947	-1.521320682	2.388942655
H	1.9302286722	-2.3579311406	2.8006503305
H	2.7861010629	-1.4233509195	4.0281866864
C	2.059804021	0.9045400135	-0.9337880459
C	1.2583475092	1.1664159766	-2.0627265389
C	2.6556863493	2.0244591009	-0.3171695223
C	1.0946384996	2.4550979345	-2.5666493807
H	0.7930018619	0.3447894132	-2.591550027
C	2.4940032047	3.3128997297	-0.8177291398
H	3.2735681829	1.862887691	0.5574600479
C	1.7131448986	3.5412479001	-1.9501370077
H	0.4909581591	2.6062221391	-3.4546666757
H	2.9852341802	4.1421649396	-0.3214615445
H	1.5936003793	4.5421271335	-2.3462459424
H	0.7193366535	-0.2516944337	3.035601712

Tabelle 10.587 Standardorientierung von pro-(S)-(S<sub>N</sub>,R,R)-E3 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.882345	-0.115761	0.346908
C	-1.973253	-1.061475	-0.459263
C	-2.815659	-1.814969	-1.501184
C	-3.931716	-2.621764	-0.835082
C	-4.826517	-1.701067	-0.007207

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C	-3.99287	-0.937415	1.023536
N	-2.103621	0.741462	1.265501
N	-0.788741	-0.362767	-1.015356
C	-2.890902	1.877217	1.74956
C	-1.542598	0.022661	2.412576
C	-1.109233	0.433125	-2.208169
C	0.292536	-1.316374	-1.305372
Si	2.026898	-0.709327	-1.834622
C	2.928633	-2.338617	-2.17033
C	2.078001	0.302111	-3.42683
C	2.858343	0.263588	-0.43181
H	-3.363172	0.574691	-0.356805
H	-1.573004	-1.805497	0.237683
H	-2.173421	-2.472605	-2.09207
H	-3.268378	-1.097153	-2.19353
H	-4.516985	-3.146484	-1.594031
H	-3.493366	-3.385781	-0.182636
H	-5.608014	-2.27463	0.496902
H	-5.32933	-0.989173	-0.672031
H	-4.634941	-0.281714	1.616501
H	-3.541903	-1.660003	1.712379
H	-2.237298	2.543721	2.312671
H	-3.293331	2.43428	0.903494
H	-3.715268	1.566543	2.405064
H	-0.88915	0.70482	2.959522
H	-0.94139	-0.824699	2.082922
H	-2.317439	-0.331697	3.104646
H	-1.284085	-0.194813	-3.091875
H	-0.285669	1.114404	-2.415181
H	-1.997608	1.041626	-2.028164
H	-0.022335	-2.045452	-2.072032
H	0.48786	-1.892315	-0.392896
H	3.995435	-2.166652	-2.337428
H	2.524573	-2.807458	-3.072243
H	2.823342	-3.046512	-1.345234
H	1.802865	1.34564	-3.269199
H	3.097659	0.28374	-3.822746
H	1.418907	-0.122607	-4.188946
H	2.338753	1.221732	-0.339062
H	3.886431	0.477115	-0.745462
C	0.406699	3.208902	-0.158116
C	1.248238	3.695965	1.021613
C	-0.845355	4.092174	-0.20297
C	1.187572	3.531414	-1.430724
Li	-0.437066	1.310757	0.147507
H	2.211036	3.174	1.095137
H	0.734213	3.562378	1.983912
H	1.485481	4.778745	0.939456
H	-1.527178	3.818223	-1.021387
H	-1.419355	4.055482	0.729544
H	-0.583411	5.160814	-0.361133

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H	0.617833	3.296974	-2.340284
H	2.14566	3.001584	-1.496523
H	1.429894	4.614216	-1.490746
C	2.842345	-0.459285	0.8869
C	2.021546	-0.01598	1.929581
C	3.636177	-1.591957	1.110165
C	1.978498	-0.692863	3.147466
H	1.445363	0.894676	1.790526
C	3.596049	-2.269944	2.325195
H	4.301014	-1.936155	0.325598
C	2.760537	-1.827	3.349746
H	1.346184	-0.322746	3.946484
H	4.223805	-3.140266	2.475344
H	2.732522	-2.349668	4.297881

Tabelle 10.588 Standardorientierung von  $\text{pro-}(R)\text{-}(S_N, R, R)\text{-E3}$  [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.1586940699	-0.0980620153	-1.1998127585
C	-2.1767149126	-0.5991792911	0.2534069619
C	-3.1335718335	-1.793462557	0.4022024793
C	-4.5395678892	-1.4697092988	-0.1054712568
C	-4.4852171979	-1.0276897387	-1.5658705782
C	-3.5811279242	0.1974286713	-1.6978185981
N	-1.2132948311	1.0348975816	-1.3557008098
N	-0.797817567	-0.8633520442	0.7446341262
C	-0.5716636265	1.0069523786	-2.6699273209
C	-1.8231057615	2.354384339	-1.1441439334
C	-0.7993947412	-1.1541443609	2.1789790005
C	-0.0744814035	-1.8932971813	-0.0093111433
Si	1.6653634019	-2.4212390572	0.57076784
C	1.6717971167	-3.4555936138	2.1524734847
C	2.2583739527	-3.5495330922	-0.8261708936
C	2.8218541131	-0.9318625516	0.8147512813
H	-1.7695175156	-0.9106003633	-1.8224679163
H	-2.5517625639	0.2205794069	0.8823481688
H	-3.1768123565	-2.1006419877	1.449458425
H	-2.7487268746	-2.644417173	-0.1698233627
H	-5.1852020358	-2.3435297525	0.0115966492
H	-4.9742557393	-0.6658651884	0.4996938627
H	-5.4860440329	-0.7935436483	-1.9366597833
H	-4.0966420241	-1.8472414855	-2.1818920566
H	-3.5385521011	0.5357654745	-2.7372513845
H	-4.017709775	1.0111840821	-1.1107349281
H	0.0981062907	1.8608568879	-2.7593298675
H	0.0281872388	0.101569474	-2.7767109947
H	-1.3058326778	1.0520972743	-3.4877617161
H	-1.0267600058	3.097766602	-1.09565002
H	-2.3498813024	2.3812580314	-0.1911660805
H	-2.5135851068	2.6297244476	-1.9524976803
H	-1.4480189084	-0.4437747699	2.6911813296

H	0.206085425	-1.0185795208	2.5761892669
H	-1.130782919	-2.1770472209	2.4037392741
H	0.0798670014	-1.5419387948	-1.0340858595
H	-0.6495848782	-2.8316531693	-0.083002209
H	2.6127698007	-4.0095177627	2.2148694276
H	0.8582989783	-4.1860468922	2.1451958212
H	1.5785511248	-2.8532040502	3.0573741295
H	2.1491775974	-3.0875356297	-1.8095285933
H	3.3084781316	-3.8224154496	-0.691109405
H	1.6750564648	-4.4748877866	-0.8229525726
H	2.5102882574	-0.3918947833	1.714715036
H	3.8164512479	-1.3413828896	1.0269870595
C	-0.0970931538	2.4640622253	2.0302703365
C	-1.4883970883	2.6777386488	2.629240452
C	0.3945797804	3.8407523987	1.5787351896
C	0.8079796674	2.040215166	3.1895262273
Li	-0.0952483312	1.0479093322	0.4434869973
H	-1.9196810874	1.7560377375	3.0424660149
H	-2.2066009171	3.0745640126	1.8999294241
H	-1.4671756096	3.4095729814	3.4660583457
H	1.426497039	3.819760862	1.2024892015
H	-0.2328919039	4.2734247127	0.7886824255
H	0.389850669	4.5728489181	2.4153187799
H	1.8584275072	1.9148578177	2.890496482
H	0.486492374	1.0978861057	3.6505538908
H	0.8129478339	2.7979589572	4.0029141946
C	2.8902456774	0.0196574116	-0.3518800075
C	2.425601569	1.3341194618	-0.2262037467
C	3.4416569383	-0.3704011309	-1.5794651886
C	2.4973849922	2.2279587518	-1.294628395
H	2.0317595425	1.6780917199	0.7260405586
C	3.5189093941	0.5217573847	-2.6460022341
H	3.8379809449	-1.3733395107	-1.6915317006
C	3.0446892749	1.8261079525	-2.5099503816
H	2.1370529261	3.241657047	-1.1602600082
H	3.9616066832	0.2007464222	-3.5815250931
H	3.1126980698	2.5213798836	-3.3378570962

Tabelle 10.589 Standardorientierung von pro-(S)-(R<sub>N</sub>,R,R)-E3 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-1.978719749	-0.8123151793	-0.7686858435
C	-2.3078790767	-0.5614547328	0.715660604
C	-3.0099027395	-1.7862662447	1.3219716779
C	-4.2685386015	-2.1643977415	0.5396817069
C	-3.914578427	-2.4427634946	-0.9201416472
C	-3.2469813655	-1.2133821623	-1.5372767941
N	-1.2520141584	0.3361333231	-1.3549086809
N	-1.1055894694	-0.1165193936	1.4629421065
C	-0.4042265618	-0.0589855157	-2.4788907663
C	-2.1214764117	1.4433142661	-1.7734587668

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C	-1.4749787885	0.605439393	2.6840731514
C	-0.1640590804	-1.2048259445	1.782264071
Si	1.6645473732	-0.7147060006	2.0650209626
C	1.9860939537	0.3098939522	3.6119126956
C	2.5751810675	-2.3603467487	2.2151599711
C	2.2632131522	0.2184613933	0.5154603953
H	-1.284280728	-1.659111436	-0.8145641632
H	-3.0081205708	0.2822542528	0.7585926666
H	-3.255654732	-1.5889896181	2.3685020757
H	-2.3246677868	-2.6401597566	1.3081270123
H	-4.7407109201	-3.0378729364	0.9956836526
H	-4.995362598	-1.3452635548	0.5868901589
H	-4.808346021	-2.7062629234	-1.4906754909
H	-3.234777416	-3.3012850341	-0.9726455158
H	-2.9988810637	-1.395082111	-2.5869038025
H	-3.962985612	-0.3854165743	-1.5139276657
H	0.193037542	0.7996021728	-2.7905095219
H	0.2734717404	-0.8562563271	-2.1704187346
H	-0.9876121538	-0.4060704346	-3.3432202409
H	-1.4958137944	2.3040618403	-2.0097800071
H	-2.7862263997	1.7364469866	-0.9599968722
H	-2.7226219874	1.1876436846	-2.6556404787
H	-2.1191845867	1.4485562489	2.4314589499
H	-0.5768501075	1.0050145824	3.1508008303
H	-1.9852799331	-0.0417973191	3.4111851443
H	-0.1140970574	-1.8888058949	0.9283585373
H	-0.5261516958	-1.804974557	2.6328954555
H	3.0615676591	0.3293191604	3.8084729482
H	1.4931704108	-0.1298024284	4.4834253539
H	1.6493285602	1.3426143086	3.5040674437
H	2.4458950571	-2.9778948556	1.3219646837
H	3.6457722218	-2.1919076148	2.3519923594
H	2.2083624778	-2.9279220365	3.0749083202
H	1.8995949937	-0.3045233139	-0.3761420692
H	1.8415252815	1.2312061196	0.5100776167
C	0.0526198323	3.3365993539	0.5235799211
C	-1.2378354639	4.157568299	0.5348345074
C	0.9259689413	3.8840128126	-0.6065507708
C	0.772774635	3.651133114	1.8338036247
Li	-0.3339590016	1.3122718102	0.2159874881
H	-1.9145408206	3.8608529438	1.3478261787
H	-1.8006691416	4.0762219404	-0.4034870364
H	-1.032346949	5.2407124524	0.678620935
H	1.9096305934	3.3970536861	-0.6507724031
H	0.4609490353	3.7601008368	-1.5943874383
H	1.1202081714	4.972507097	-0.4884800475
H	1.7507100828	3.1571353026	1.9070987635
H	0.1882968776	3.3520714035	2.7141973853
H	0.9686794271	4.7399983942	1.9437363781
C	3.7674334622	0.2957058878	0.4922223733
C	4.5302727315	-0.6971000284	-0.1323239779

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C	4.4389201197	1.3418493319	1.1343671134
C	5.9216858478	-0.6502090439	-0.1142121162
H	4.0262421978	-1.5138423223	-0.639090575
C	5.8306659259	1.39111283	1.1547027651
H	3.8640595889	2.1290121506	1.6098357359
C	6.5791254551	0.3943594161	0.5325089329
H	6.4916013465	-1.4278072632	-0.6087228406
H	6.3291033046	2.2147834447	1.6514074431
H	7.6612343334	0.4347165205	0.5449936104

Tabelle 10.590 Standardorientierung von pro-(R)-(R<sub>N</sub>R,R)-E3 [globales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	3.35883	0.180558	-0.512423
C	2.644905	-1.07567	0.017044
C	3.598643	-1.883704	0.908463
C	4.850174	-2.298949	0.132587
C	5.562821	-1.064996	-0.419291
C	4.614991	-0.239732	-1.293036
N	2.429401	1.053208	-1.258597
N	1.337151	-0.751943	0.636622
C	3.013529	2.36169	-1.557573
C	1.889868	0.464269	-2.48512
C	1.466273	-0.256829	2.014836
C	0.421876	-1.905311	0.604683
Si	-1.453061	-1.559723	0.777167
C	-2.263699	-3.207459	0.340707
C	-2.007469	-1.056129	2.504974
C	-1.917055	-0.243046	-0.514232
H	3.685222	0.777343	0.349024
H	2.414647	-1.703026	-0.850091
H	3.079028	-2.763912	1.297227
H	3.903319	-1.278957	1.768971
H	5.519327	-2.870616	0.780007
H	4.566471	-2.957291	-0.696826
H	6.443316	-1.35562	-0.997207
H	5.917067	-0.448871	0.415225
H	5.130895	0.645845	-1.671266
H	4.320403	-0.840327	-2.160992
H	2.221008	3.037767	-1.880852
H	3.462474	2.775486	-0.65475
H	3.774001	2.310463	-2.347894
H	1.14483	1.148806	-2.896081
H	1.394647	-0.483597	-2.270701
H	2.658308	0.29984	-3.251557
H	1.769731	-1.050177	2.710606
H	0.509506	0.148643	2.339787
H	2.194709	0.555239	2.061184
H	0.72793	-2.677264	1.33086
H	0.500539	-2.36931	-0.385484
H	-3.351677	-3.117744	0.382838

H	-1.9604	-3.988005	1.044108
H	-1.995466	-3.53611	-0.667134
H	-1.728002	-0.032207	2.75672
H	-3.096838	-1.128582	2.56597
H	-1.584308	-1.728377	3.256851
H	-1.399257	-0.480381	-1.451084
H	-1.557847	0.734607	-0.171451
C	-0.104447	2.848955	0.798887
C	-0.887727	3.621604	-0.263735
C	1.044862	3.752185	1.254088
C	-1.025718	2.688847	2.004764
Li	0.798389	1.165127	-0.031083
H	-1.777774	3.078166	-0.60731
H	-0.280831	3.841107	-1.152857
H	-1.24706	4.601394	0.119877
H	1.660027	3.286879	2.037388
H	1.714391	4.026909	0.43023
H	0.670241	4.708859	1.679274
H	-0.523577	2.210452	2.856858
H	-1.919735	2.095313	1.776725
H	-1.391464	3.671671	2.373245
C	-3.405787	-0.212731	-0.737544
C	-4.000807	-0.999798	-1.729936
C	-4.236532	0.568969	0.073063
C	-5.381833	-1.010072	-1.906718
H	-3.372215	-1.609308	-2.37126
C	-5.618426	0.560638	-0.100983
H	-3.79336	1.198286	0.836715
C	-6.198612	-0.230466	-1.090061
H	-5.818983	-1.624336	-2.684976
H	-6.240572	1.180102	0.533795
H	-7.272816	-0.234191	-1.227641

Tabelle 10.591 Standardorientierung von  $(S_N, S, R, R)$ -T55 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.8603582728	-0.4616528074	0.4341938083
C	-2.061719303	-1.2582555892	-0.6136133679
C	-3.006853591	-1.7674280524	-1.7133590415
C	-4.117014869	-2.646048616	-1.1366783904
C	-4.9081930832	-1.8668347575	-0.0884288388
C	-3.9733456255	-1.3552131432	1.0091655142
N	-1.9799539468	0.1516733655	1.4594237163
N	-0.894336703	-0.5015052013	-1.1190839435
C	-2.7072884335	1.1600470879	2.2392705187
C	-1.4041368746	-0.8221376809	2.3959900913
C	-1.2575814615	0.5096775536	-2.1216762829
C	0.1350445242	-1.3922404179	-1.6861627199
Si	1.8269781746	-0.5560084627	-2.0659317029
C	3.0295767714	-2.0189257507	-2.0866839989
C	1.8085906626	0.207665707	-3.7995457893

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C	2.2265816232	0.7549211445	-0.8116106938
H	-3.3384614731	0.383025598	-0.0770227746
H	-1.6453712449	-2.1384361992	-0.1111387629
H	-2.4314070931	-2.3195247359	-2.4605015715
H	-3.4664481106	-0.9143719313	-2.2238421211
H	-4.7747432978	-2.9918151456	-1.9377027307
H	-3.6788840568	-3.5377804394	-0.6734935488
H	-5.6886229919	-2.492530281	0.3511919109
H	-5.4097565914	-1.0183666811	-0.5682395897
H	-4.545382911	-0.8069172074	1.7609312306
H	-3.5215016251	-2.2179179432	1.5109662622
H	-2.007691572	1.6932324809	2.8823441543
H	-3.1759531534	1.8827881412	1.5719613313
H	-3.4793729718	0.7116125818	2.8768265555
H	-0.6433432134	-0.3220268449	2.9978148928
H	-0.9238357354	-1.6382733338	1.8565107005
H	-2.1591541845	-1.2424167164	3.0722093114
H	-1.4754976784	0.0578693215	-3.098167794
H	-0.4275126352	1.2072947707	-2.2366847413
H	-2.1263815707	1.0802831953	-1.7934869204
H	-0.2334272647	-1.8886159401	-2.5995017441
H	0.3361151435	-2.1891193719	-0.9623721418
H	4.0183585485	-1.6941371223	-2.4202356196
H	2.6904255076	-2.8143219067	-2.7576524858
H	3.1401938732	-2.4387954134	-1.0832268302
H	1.2892754864	1.1681101172	-3.8260960824
H	2.8369473266	0.3803150396	-4.1292639645
H	1.3355291686	-0.4592646412	-4.5258639903
H	1.2214317541	1.6300214133	-0.5066269397
H	2.9478410292	1.4457952131	-1.2607785303
C	0.4390558841	2.8530108319	0.1294358671
C	0.5949456737	2.8827569107	1.6536744399
C	-0.9671679139	3.3204890811	-0.2481071908
C	1.4320187385	3.8451490582	-0.4617909683
Li	-0.2383738302	0.8196449019	0.3544179658
H	1.6182671342	2.642536938	1.9534271389
H	-0.0583069931	2.1704511389	2.1783986799
H	0.3484757303	3.879574742	2.0664808896
H	-1.0747919535	3.4346522177	-1.3317238775
H	-1.7620227828	2.6386202148	0.0840818207
H	-1.1988913646	4.3033711488	0.2042689692
H	1.3968130958	3.8444505456	-1.5580579338
H	2.4589005119	3.604169802	-0.1671761408
H	1.2280630838	4.8759030784	-0.1246120711
C	2.6815899937	0.3164628519	0.5213620555
C	1.9630167596	-0.6398968018	1.2660450302
C	3.7845683449	0.9121664134	1.167408204
C	2.3151108619	-0.9764346585	2.5728922815
H	1.125448266	-1.1515633145	0.7988021197
C	4.1355970124	0.5813104997	2.4688443358
H	4.362363654	1.6545626442	0.6271949631

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C	3.4010319387	-0.3645927842	3.1903111972
H	1.7389658467	-1.7249838775	3.1068207588
H	4.989444605	1.0651010215	2.9294598616
H	3.6770112779	-0.6210825515	4.2053287386

Tabelle 10.592 Standardorientierung von  $(S_N, R, R, R)$ -TS5 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.5616446636	-0.4332284434	0.4919046834
C	-1.864810342	-1.2213652713	-0.6308329455
C	-2.9051076718	-1.8890685731	-1.5408426995
C	-3.8133135728	-2.8263335092	-0.7442849911
C	-4.5091957612	-2.0531174081	0.3744101468
C	-3.4800530092	-1.3782997924	1.2846989472
N	-1.5842910908	0.3155001741	1.3210276694
N	-0.8681822682	-0.3902442967	-1.3400923961
C	-2.2594161657	1.22436143	2.2524058138
C	-0.6574271433	-0.5370810174	2.0741831534
C	-1.4644915723	0.4686888416	-2.370914681
C	0.2197025942	-1.1925774551	-1.9349112636
Si	1.8288023278	-0.1945333378	-2.2532350789
C	3.1804895942	-1.4824576195	-2.5527062185
C	1.6961724571	0.8604704906	-3.8259275766
C	2.0339509364	0.8034930423	-0.6929092261
H	-3.1912230911	0.3368560852	0.0275220264
H	-1.2973774105	-2.0279171578	-0.1556659857
H	-2.3896802064	-2.4339068976	-2.3367336778
H	-3.5251758007	-1.123794511	-2.019303514
H	-4.548974738	-3.2885524693	-1.4066993488
H	-3.2171397709	-3.6376263867	-0.3107273922
H	-5.145502954	-2.716879217	0.9645019671
H	-5.162897539	-1.2907104844	-0.0651159356
H	-3.9916475115	-0.8281931492	2.0773976305
H	-2.8749331335	-2.1547920054	1.7656097741
H	-1.5277312777	1.9062583624	2.6858023248
H	-3.0023361736	1.8163120007	1.7169430032
H	-2.7550836558	0.6887372796	3.0713802109
H	0.0679205551	0.1042516062	2.5796808002
H	-0.1099691235	-1.1987512663	1.4022832309
H	-1.1638244484	-1.1419229226	2.8365563905
H	-1.7702029851	-0.1037192063	-3.2566890244
H	-0.7332710799	1.2164387458	-2.6779835893
H	-2.3326120695	0.9953915935	-1.9725617225
H	-0.1277465706	-1.7311168409	-2.8313710336
H	0.5151177982	-1.9536534283	-1.2039712474
H	4.1507526355	-0.9833026887	-2.6220982402
H	3.0162079378	-2.0351664569	-3.482372295
H	3.2366302988	-2.1978691762	-1.7282250177
H	1.294109249	1.8542657513	-3.616612127
H	2.6840983206	0.9887075591	-4.2764394742
H	1.0569977733	0.3772536298	-4.5711494613

H	1.7264012853	0.1644257119	0.1526905153
H	1.1564142787	1.870585476	-0.7616890063
C	0.3082934952	3.1523402227	-0.4930951077
C	0.7263319657	3.3866740781	0.9583199753
C	-1.1851568243	3.4577891526	-0.6453951759
C	1.0797992297	4.1098597176	-1.3910482489
Li	-0.2428751591	1.1334092742	-0.0760201156
H	1.8089736792	3.2807130259	1.0748795266
H	0.2623141588	2.6707976923	1.6568614154
H	0.4453413183	4.3920850186	1.3171095445
H	-1.5080479244	3.3908334354	-1.6892439916
H	-1.8373950327	2.7920461458	-0.0593530003
H	-1.4201397286	4.4832732044	-0.3032363514
H	0.8124285051	3.9764134019	-2.4458251343
H	2.1594884476	3.9622391105	-1.3008332244
H	0.869585089	5.1643477071	-1.1368263475
C	3.3871405908	1.3384761245	-0.4106358986
C	3.9665720994	1.2401797625	0.8681135698
C	4.1480509277	1.9913309398	-1.3994033744
C	5.2256416068	1.7620951904	1.1448300568
H	3.4088492371	0.7442611125	1.6570196368
C	5.4092879583	2.5109535545	-1.1261538685
H	3.7313636337	2.1093314866	-2.3942914782
C	5.9623608432	2.4024772899	0.1489441297
H	5.6347890561	1.6660288231	2.1443265464
H	5.9614339878	3.0087076929	-1.9153179407
H	6.9432184179	2.8087879848	0.3620256486

Tabelle 10.593 Standardorientierung von  $(R_N, S, R, R)$ -TSS [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-1.9766914875	-0.7964030358	-0.7777207617
C	-2.4022205066	-0.5212364959	0.6763188617
C	-3.1544829466	-1.7273586963	1.2597533596
C	-4.3506127779	-2.1322765367	0.3984155991
C	-3.8830326942	-2.4547751948	-1.0191945365
C	-3.1836275897	-1.2359001402	-1.6211476164
N	-1.2332642387	0.3581358846	-1.3488892808
N	-1.2435954605	-0.0826833094	1.4929177422
C	-0.3365266473	-0.0633671891	-2.4308520803
C	-2.1109789627	1.4230741089	-1.851539945
C	-1.6782186069	0.6638616939	2.6767765029
C	-0.3475141531	-1.1874280513	1.9083129525
Si	1.4670137978	-0.6761159451	2.2784846826
C	1.6043811122	0.2794677819	3.9103573321
C	2.4074860136	-2.3020414983	2.4967717507
C	1.9645189659	0.3105126429	0.7776975797
H	-1.2630017956	-1.6275404143	-0.7611101687
H	-3.0942938401	0.3302271273	0.6595030503
H	-3.4757138112	-1.4971550002	2.2788867091
H	-2.4722234685	-2.5804118826	1.324130564

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H	-4.8544173754	-2.9929504972	0.844659574
H	-5.0809754052	-1.3154581235	0.3628934712
H	-4.7268981672	-2.7457147838	-1.6492120846
H	-3.1932576217	-3.3062023316	-0.9913458899
H	-2.8621749401	-1.4435936235	-2.6454799468
H	-3.9107668835	-0.4189304325	-1.6706809014
H	0.2605761144	0.7909882966	-2.7534269909
H	0.3413481456	-0.8375435425	-2.0701409166
H	-0.8862049223	-0.4483486211	-3.3000768358
H	-1.5068896039	2.3011026429	-2.0812772737
H	-2.8423123762	1.7051773201	-1.0937496276
H	-2.6425228015	1.1243090185	-2.7631993643
H	-2.3548744766	1.4660857093	2.3806034158
H	-0.8097855812	1.1125333805	3.1567004475
H	-2.1830537793	0.0201970177	3.4103990621
H	-0.2535391749	-1.8937034424	1.0769207658
H	-0.7866994138	-1.7507097408	2.7461933096
H	2.6109248645	0.1711732439	4.3230231642
H	0.903245616	-0.1123499405	4.653472918
H	1.412125376	1.3462964656	3.7767622708
H	2.2667525292	-2.962244413	1.6369261675
H	3.4775977633	-2.0929366199	2.5786773303
H	2.0960701424	-2.8358247592	3.3993444006
H	1.5361621206	-0.1940628216	-0.1045448395
H	1.3825603063	1.5450996405	0.8710199475
C	0.8149995926	3.001728608	0.692330867
C	-0.5839408102	3.5775157011	0.9290004064
C	1.2484278539	3.2971582163	-0.7421611466
C	1.7788803584	3.6965780213	1.6450545978
Li	-0.1494194798	1.1382174248	0.2637417102
H	-0.8919849373	3.472168657	1.9742072487
H	-1.3684328388	3.1124186646	0.3106378653
H	-0.6212233596	4.6580529324	0.6921486392
H	2.2557747985	2.913510031	-0.9354954455
H	0.5813029482	2.8408169216	-1.4887905653
H	1.2579054184	4.3807327845	-0.9581725603
H	2.8070351464	3.3550372889	1.4947893662
H	1.5172479377	3.5112534134	2.6933793464
H	1.7725685388	4.7923018243	1.500169018
C	3.4135367387	0.5163469442	0.5400373134
C	3.982479036	0.3263355147	-0.7327799612
C	4.2822733235	0.9378835213	1.5642232106
C	5.3354103015	0.5438671129	-0.970605696
H	3.3419339015	0.0039151168	-1.5484291479
C	5.6368270718	1.1517563825	1.3298393937
H	3.8808350594	1.1223004443	2.5548774591
C	6.1786451554	0.95690084	0.0601986167
H	5.7337317468	0.3877216101	-1.9668576134
H	6.2719137181	1.4794259403	2.1450932371
H	7.2325539121	1.1256525216	-0.1223879805

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Tabelle 10.594 Standardorientierung von  $(R_M, R, R, R)$ -T55 [lokales Minimum; M05-2X/6-31+G(d)].

	x	y	z
C	-2.4381929636	-0.7650038319	-0.8252055637
C	-2.5348068865	-0.444583193	0.6767839468
C	-3.2796955068	-1.5630324962	1.4215652439
C	-4.66467334	-1.8239210115	0.8308603374
C	-4.5297280009	-2.1998925308	-0.6430902788
C	-3.8310011472	-1.0709144681	-1.4007407283
N	-1.7091186004	0.3040716998	-1.5575774634
N	-1.2000466442	-0.1284361662	1.2422773729
C	-1.1696400786	-0.1915319288	-2.8291190717
C	-2.5490107367	1.4757000222	-1.8451221349
C	-1.3085012138	0.694282268	2.4506032648
C	-0.3762404913	-1.3181987832	1.5375022549
Si	1.4676065428	-0.9772608585	1.9816538863
C	1.6175858082	-0.5424081429	3.8203045514
C	2.2833507305	-2.6666044273	1.7243192251
C	2.1833601072	0.4004393372	0.9568749251
H	-1.8259437016	-1.6681559754	-0.9314013207
H	-3.1268369899	0.4729793576	0.7772800526
H	-3.3519071144	-1.3065783229	2.482189079
H	-2.7014393489	-2.4893209111	1.3532374943
H	-5.1630436706	-2.6197669852	1.3894949297
H	-5.2885563082	-0.9271121526	0.9223154628
H	-5.5095820796	-2.3915541778	-1.0869279547
H	-3.9494439086	-3.1256277868	-0.731399979
H	-3.7463102298	-1.3168733322	-2.4626266877
H	-4.4584931462	-0.1769749894	-1.3258802733
H	-0.5105401015	0.5637018402	-3.2595291161
H	-0.584380061	-1.0937595624	-2.6578038373
H	-1.9625940674	-0.4154760123	-3.5549616698
H	-1.917426495	2.2889249338	-2.202250989
H	-3.0585499608	1.8152571896	-0.9439874536
H	-3.2994238009	1.2615947723	-2.6158359138
H	-2.0053855555	1.5145227423	2.2794590813
H	-0.3337239842	1.126189277	2.6774603206
H	-1.6438903719	0.1119301759	3.320192421
H	-0.375262752	-1.9761029029	0.6621397525
H	-0.8149261289	-1.9027736241	2.3624706011
H	2.6335992686	-0.763878946	4.1588427571
H	0.9279047047	-1.1306406231	4.4322389416
H	1.4304441079	0.5160042726	4.0137678901
H	2.292190966	-2.9464748243	0.6680157699
H	3.3213342009	-2.6371217248	2.0652581899
H	1.7652516146	-3.4506600937	2.2852959044
H	1.366151195	1.4450583194	0.690544116
H	2.9411298297	0.9111063008	1.5600925262
C	0.7997864073	2.835397327	0.1379802623
C	-0.5234077831	3.4757818359	0.5579686677
C	0.983875255	2.9879365667	-1.3750672096
C	1.9250982762	3.5974539885	0.8250138571

Li	-0.1628084644	0.9405279384	-0.1891488022
H	-0.6240489337	3.5059214069	1.6475276286
H	-1.4108574434	2.9568690266	0.1680109411
H	-0.5996088286	4.5197979417	0.1983450873
H	1.9485058615	2.5897821098	-1.7025158867
H	0.2142254008	2.4686805406	-1.9640597004
H	0.9372664973	4.0502020505	-1.6835348486
H	2.9065491267	3.2225660576	0.5154064543
H	1.8674263034	3.5039124918	1.9163820485
H	1.8954945074	4.6742339933	0.5836357298
C	2.717423521	0.0590441758	-0.3769854813
C	1.9668248432	-0.6988972784	-1.2952515224
C	3.9485360909	0.5658762661	-0.8382268754
C	2.412821584	-0.9363366621	-2.5944974137
H	1.0216475901	-1.1332327627	-0.9738239486
C	4.3942547058	0.3347540721	-2.1326028267
H	4.5535647483	1.1568543161	-0.1590087009
C	3.6285576296	-0.4168199266	-3.0278829076
H	1.8096498904	-1.5329499617	-3.2704100201
H	5.3465987275	0.7443680575	-2.4494247976
H	3.9773036375	-0.5965230845	-4.0370089578

### 10.2.6. Details zu Kapitel 6.2

Tabelle 10.595. Absolute Energien der optimierten Strukturen.

Struktur	Min./TS	SCF [Hartree]	ZPE [Hartree]
<b>112</b>	Min.	-1675.79768	-1675.45832
<b>114</b>	Min.	-1291.78704	-1291.42141
<b>113</b>	Min.	-1215.32006	-1214.98171
<b>115</b>	Min.	-1291.76520	-1291.40287
<b>TS39</b>	TS	-1291.75863	-1291.39579

Tabelle 10.596 Standardorientierung von **112** [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
C	1.0494889778	-0.0001519147	-3.032191861
C	3.5244315754	1.3353145835	-2.5441157486
C	-2.4657937775	-0.2732357439	-2.1738446125
C	1.0398729823	2.7037675589	-1.9029673105
C	-2.7924302994	2.0231240065	-1.4833550854
C	2.7420299583	-0.9319412158	-0.9172503405
C	-3.515611614	0.201341862	-0.038858246
C	2.8646924049	1.8099977298	0.2111433608
C	-3.040465932	-1.0017752864	0.7533823455
C	-3.9387348626	-1.9714100014	1.2169700968
C	-1.6852227365	-1.0835851934	1.0998049073

C	-3.4857183313	-3.0019350279	2.0458087882
C	-1.2392936976	-2.0979935966	1.9569707325
C	-2.1423265883	-3.058333552	2.4293780588
C	0.2209701497	-2.1108158892	2.3699585687
C	2.2046229503	-0.7509892313	2.7061505169
C	0.1416671026	-0.1140861162	3.7661972875
H	-1.7026793564	0.0483757829	-2.8833189851
H	-3.4395572066	-0.2927724461	-2.688342269
H	-2.0409084207	2.3278951803	-2.2157796728
H	-3.7858066344	2.0785869984	-1.9560191487
H	-2.2311759247	-1.2858760364	-1.83536756
H	-2.7538070431	2.7099600246	-0.635212957
H	-4.4719181755	-0.0062645076	-0.5453943811
H	-3.6833481214	1.0351294403	0.6533772056
H	-4.991211739	-1.9161798968	0.9449761703
H	0.8336068274	-2.5809091173	1.5892606556
H	2.6645854142	-1.204204339	1.8260844513
H	-4.1840161603	-3.752079303	2.4079011773
H	-1.801965316	-3.8447235331	3.1004729855
H	2.5736371145	0.271729246	2.813516108
H	0.3593385154	-2.7077376506	3.2870138605
H	2.51031535	-1.3269406966	3.595252701
H	-0.9452185728	-0.0846239983	3.6770045328
H	0.503334999	0.9119449675	3.8611209547
H	0.4142246226	-0.6816597653	4.6714115135
N	-2.5023107709	0.6508660524	-1.0223701838
N	0.7376036077	-0.7346040623	2.5652741101
O	0.6081655427	-0.4995357592	-3.9806673909
O	4.4465595484	1.5889892233	-3.1998374839
O	0.5563372145	3.7061951441	-2.2157619097
O	3.2057824729	-1.9672521173	-0.6759845102
O	3.4217016206	2.3240038223	1.0843666562
Cl	-1.050655625	2.3631721596	1.6510251669
Sn	-0.2997787401	0.404073183	0.3396718965
W	1.9209466949	0.8971490324	-1.3931051519

Tabelle 10.597 Standardorientierung von **114** [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
C	-1.0330835142	-3.2165924774	-3.3714297163
C	1.2221094201	1.7452809579	-3.0057718883
C	3.2872640067	-2.7922636063	-2.0222613539
C	3.5227863752	-1.4212093258	-1.9116472835
C	-2.7511433412	-3.2050345007	-1.5971471991
C	2.0314823293	-3.3093277714	-1.6975270898
C	2.5130015112	-0.5740639942	-1.4381897735
C	1.0087968365	-2.4643979406	-1.2381763687
C	2.7693935874	0.916128428	-1.285955206
C	1.7009163222	3.1085812245	-1.0486646899
C	-0.3520083769	-3.0580946524	-0.9482059398
C	1.25493416	-1.0862403892	-1.0735973511

C	-1.1552155568	3.3636484684	1.4438996262
C	-3.0450254884	1.137784102	1.2866409001
C	0.7711907935	1.624045727	2.8232193263
C	-1.1558261304	-0.58880549	2.6913003689
C	-1.9393935054	1.9396909362	3.861844734
H	-1.791037257	-2.8752822302	-4.0788828507
H	-0.0591635552	-2.8159177759	-3.6502718675
H	-1.0003969729	-4.3088745963	-3.3584492275
H	2.0282842536	2.2526486281	-3.5514269283
H	1.1138858579	0.7269957962	-3.3813766052
H	0.2846885138	2.2812725076	-3.1694381843
H	-3.4804850904	-2.9029696999	-2.3510994764
H	4.0732200284	-3.4540708112	-2.3738843648
H	4.4925971992	-1.0150993137	-2.1904532396
H	-1.4520686844	-1.6563246283	-2.057138062
H	1.8496049407	-4.3768296037	-1.8032581106
H	-2.270832476	0.4786836365	-1.9018529787
H	3.5731547298	1.253255468	-1.9543019651
H	-2.7341930396	-4.294100469	-1.5126843201
H	2.5485500036	3.5942455195	-1.54868498
H	0.7946410204	3.6843674097	-1.2494714833
H	-0.3108774047	-4.1499450519	-0.8943276187
H	-3.0134004035	-2.7615595628	-0.6349373228
H	3.0878866407	1.1451930264	-0.2609974425
H	1.8809034236	3.0958877496	0.0286422968
H	-0.7655569045	-2.6931812804	-0.0025617127
N	-1.3967503128	-2.7169497937	-2.0095130222
N	1.531614326	1.7190893539	-1.5504828164
O	-1.4262889758	-0.0010534759	-1.9125306917
O	-1.1637659863	4.4661949017	1.1019651305
O	-4.0991965901	0.9866112682	0.8344605585
O	1.8388134619	1.7627242858	3.2411117594
O	-1.1733431217	-1.6972028702	3.0242447707
O	-2.3900631797	2.2501934226	4.8760784861
Sn	-0.1152662557	0.4670909087	-0.3478476499
W	-1.1461076185	1.3815175851	2.0651588232

Tabelle 10.598 Standardorientierung von **113** [globales Minimum; B3LYP/6-31+G(d)].

	x	y	z
C	1.4647831123	-2.8702896241	1.6917251816
C	-0.6479739889	-3.477407388	0.6714626078
C	-0.6224572225	-2.4492202207	2.8725271994
C	-0.2591102856	-1.1855210353	5.0352365865
C	-0.2675100854	-1.1904070596	3.6372449965
C	0.	0.	5.7291631185
C	1.268998469	-1.6409337726	-2.0003297348
C	0.	0.	2.9358736565
C	0.2591102856	1.1855210353	5.0352365865
C	0.2675100854	1.1904070596	3.6372449965
C	-1.6463768179	-1.2709587802	-2.0069502672

C	0.6224572225	2.4492202207	2.8725271994
C	1.6463768179	1.2709587802	-2.0069502672
C	0.	0.	-4.0063617462
C	0.6479739889	3.477407388	0.6714626078
C	-1.268998469	1.6409337726	-2.0003297348
C	-1.4647831123	2.8702896241	1.6917251816
H	1.5599736676	-3.880944893	2.1145273788
H	-0.6327367361	-4.4798911313	1.1229108558
H	1.9552674878	-2.8578838163	0.7152288482
H	1.9711788352	-2.1682157104	2.3596399475
H	-0.1434484666	-3.5294328149	-0.2951076651
H	-0.3682747472	-3.3460524984	3.4568882275
H	-0.4606653046	-2.101903568	5.5849210403
H	-1.688166351	-3.1802730035	0.5148945143
H	-1.7067283157	-2.4799677418	2.7051471991
H	0.	0.	6.8154231487
H	0.4606653046	2.101903568	5.5849210403
H	1.7067283157	2.4799677418	2.7051471991
H	1.688166351	3.1802730035	0.5148945143
H	0.3682747472	3.3460524984	3.4568882275
H	-1.9711788352	2.1682157104	2.3596399475
H	0.1434484666	3.5294328149	-0.2951076651
H	0.6327367361	4.4798911313	1.1229108558
H	-1.9552674878	2.8578838163	0.7152288482
H	-1.5599736676	3.880944893	2.1145273788
N	0.035680081	-2.4960623031	1.5443557122
N	-0.035680081	2.4960623031	1.5443557122
O	1.9701269195	-2.555282753	-2.0515277196
O	-2.5573878376	-1.9735148867	-2.0655293321
O	2.5573878376	1.9735148867	-2.0655293321
O	0.	0.	-5.1555175233
O	-1.9701269195	2.555282753	-2.0515277196
Sn	0.	0.	0.7970675129
W	0.	0.	-1.9526855983

Tabelle 10.599 Standardorientierung von **115** [lokales Minimum; B3LYP/6-31+G(d)].

	x	y	z
C	0.7076601912	3.4666259843	-0.7033052327
C	1.4980429544	2.8430467569	1.5010842565
C	2.9064094867	2.4514405	-0.4442203081
C	5.0225909109	1.1842527288	0.1430536366
C	3.6314368204	1.19047276	-0.0134199985
C	5.6822469711	-0.0001565173	0.4812892748
C	-2.1065347351	1.252503962	-1.5361516217
C	2.9037973042	0.0047159595	0.1829788315
C	4.9602920453	-1.1821851381	0.6706323314
C	3.5681669264	-1.1834465606	0.5295331276
C	-2.0808080211	1.6089289921	1.3823187884
C	2.7619689621	-2.4393603781	0.7967935435
C	-2.0479783589	-1.6302924133	-1.1984600211

C	-4.0646408087	-0.0626129049	0.1301851995
C	1.9571397755	-2.9350561849	-1.4432088005
C	-1.9818452573	-1.2879866945	1.7378080751
C	0.6120571599	-3.5182349081	0.4741629605
N	1.5112890985	2.4852691643	0.0598337632
N	1.5653138224	-2.5290101937	-0.0756635939
O	-2.1514926721	1.9440406533	-2.4627437761
O	-2.1437180331	2.5146443447	2.0947678736
O	-2.0753131518	-2.5231856141	-1.932495207
O	-5.2153861648	-0.090341437	0.1463645898
O	-1.9805527544	-1.9890410372	2.6528651546
Sn	0.7667985708	0.0348334157	-0.0616871553
W	-2.0221236204	-0.0150426058	0.091494887
H	1.140243759	4.4741411739	-0.622379423
H	-0.3101132615	3.4963575591	-0.309028434
H	0.6733583023	3.1812482233	-1.7575739062
H	1.9025058259	3.8539444345	1.6518577661
H	0.4742107307	2.8203114857	1.8796440383
H	2.1102916933	2.1376915465	2.0692972086
H	2.8592464284	2.4965388594	-1.5390833311
H	3.4516251288	3.3479786537	-0.1140652696
H	5.5923194253	2.0996021324	-0.000702699
H	6.7621933027	-0.0022753768	0.5985053855
H	5.4820287997	-2.0991690165	0.9347581325
H	3.3890067714	-3.3368376416	0.6827117003
H	2.409906034	-2.4341056442	1.836450833
H	2.7147065422	-2.2498542504	-1.8333253028
H	1.0815902336	-2.9245933635	-2.0982733498
H	2.3809383308	-3.9506220347	-1.4460592142
H	0.2743918923	-3.204249938	1.4644547574
H	-0.2531022826	-3.6061382178	-0.1854615636
H	1.0813703843	-4.5093982574	0.5623331773
O	1.151081433	0.2779313961	-2.4861542657
H	1.9606207819	0.0030556395	-2.9510517421
H	0.4198863224	0.2538610029	-3.1284460764

Tabelle 10.600 Standardorientierung von **TS39** [Übergangszustand; B3LYP/6-31+G(d)].

	x	y	z
C	2.1626564055	2.5775708814	-1.9769253811
C	0.4566798341	3.5365327472	-0.5392663524
C	2.5342135296	2.6794956799	0.4322685982
C	4.663800827	1.4890223543	1.1304420521
C	3.3395029875	1.4177999788	0.6814632943
C	5.3500571989	0.3156630072	1.4488309196
C	-2.4596961753	1.2716755543	-1.286154536
C	2.7144520189	0.1683409826	0.5395371347
C	4.7213961206	-0.9279912082	1.3240802288
C	3.4000463769	-1.0135482453	0.8713969405
C	-2.0482309697	1.3959435418	1.6134062365
C	2.6915162631	-2.3529834603	0.7893801653

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C	-2.025568524	-1.6054714713	-1.2475842982
C	-4.0251386365	-0.4120938835	0.4956132702
C	3.043959025	-2.8443026527	-1.5513842048
C	-1.6167947583	-1.5138936355	1.6692697185
C	1.0933700518	-3.7140915726	-0.4292554923
N	1.5079437603	2.4891686176	-0.6421555845
N	2.0260365863	-2.5725945982	-0.515893476
O	-2.7022917757	2.0417578155	-2.1127266251
O	-2.0730692037	2.2419047142	2.3968934122
O	-2.0118793827	-2.4215248192	-2.0669534237
O	-5.150291167	-0.5807498741	0.6666101676
O	-1.3993879291	-2.2964789753	2.4884410899
Sn	0.6911263235	0.232044359	-0.1757374623
W	-2.0219653882	-0.116578429	0.1863034439
H	2.5933911395	3.5780437729	-2.1135293339
H	1.4270312848	2.400327747	-2.7638429726
H	2.9552662151	1.8317704283	-2.053544413
H	0.9031152747	4.5352168646	-0.6285655348
H	-0.2737614237	3.4051864419	-1.3401950042
H	-0.052763248	3.4625056219	0.4243065126
H	3.1834527984	3.5259284025	0.171748388
H	1.9970114399	2.9599030785	1.3468693312
H	5.1563713352	2.4528513466	1.2361323118
H	6.378946488	0.3679939429	1.793089243
H	5.2650141519	-1.8340741518	1.5809997201
H	3.3993899746	-3.1700576178	1.0049934085
H	1.9156186391	-2.4021881168	1.5641086071
H	3.7257212871	-1.9938050678	-1.6478748936
H	2.5605904948	-3.0371672812	-2.5178303414
H	3.6422456973	-3.7380418328	-1.3094979731
H	0.3363908554	-3.5215009657	0.3352017189
H	0.5883055491	-3.8534479221	-1.3895271355
H	1.6158158995	-4.6498582912	-0.1732266452
O	1.1986877506	-0.3115902264	-2.4587756699
H	1.5578524125	-1.2169496583	-2.3811318599
H	0.4469075854	-0.3621849238	-3.0770323002

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