Anhang

Lithiumorganische Verbindungen

Von der Struktur-Reaktivitätsbeziehung zu vielseitigen Synthesebausteinen und ihrer Anwendung

Dissertation

Vorgelegt von Diplom-Chemikerin

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Dortmund 2009

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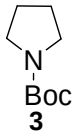
8. Anhang

8.1 Übersicht zentraler Verbindungen



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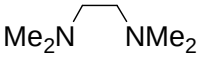

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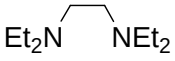

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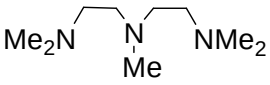

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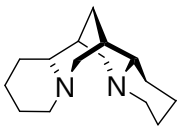

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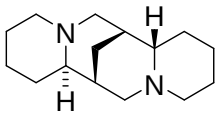
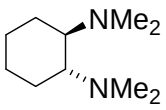


(+)-Spartein [(+)-**8**]



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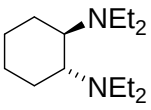

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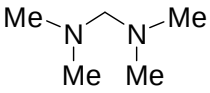

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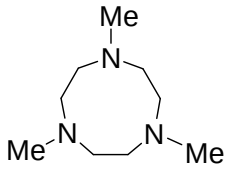
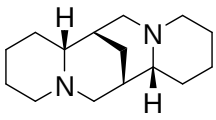
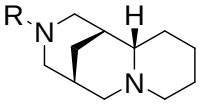


Me_3tacn (**27**)

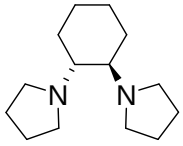


(–)-α-Isospartein (**30**)



R=Me (**40**)
R=Et (**41**)
R=*n*-Bu (**42**)

(+)-Spartein-Surrogate



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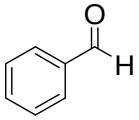

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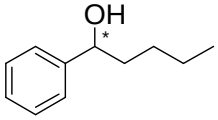

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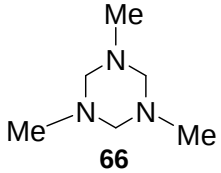

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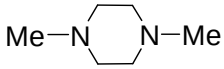

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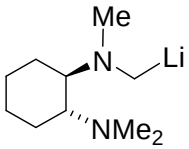
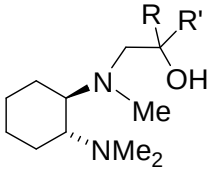
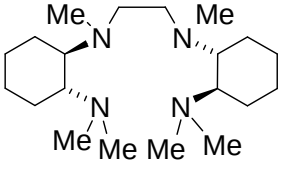


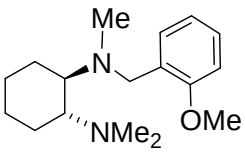
(*R*,*R*)-**68**



69a R = H R' = H
69b R = Me R' = Me
69c R = Ph R' = Ph
69d R = Ph R' = H
69e R = *i*-Pr R' = H
69f R = *i*-Bu R' = H
69g R = *t*-Bu R' = H



(*R*,*R*,*R*,*R*)-**70**



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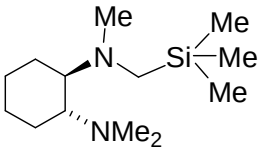
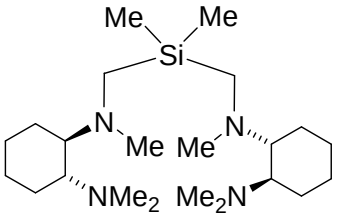
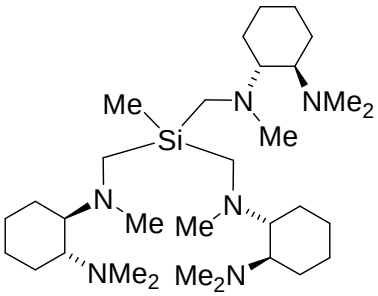


(*R*,*R*)-**73**



(*R*,*R*,*R*,*R*)-**74**



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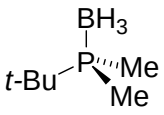

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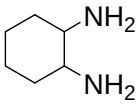

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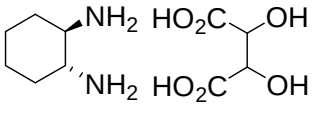

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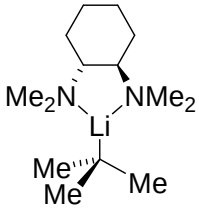

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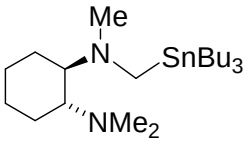

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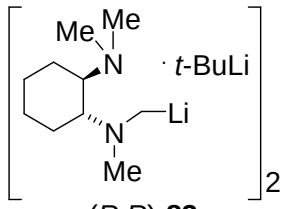

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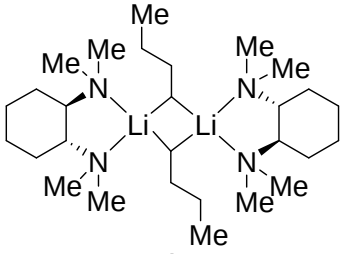

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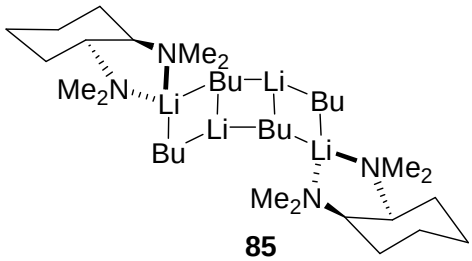

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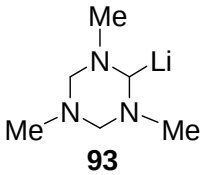

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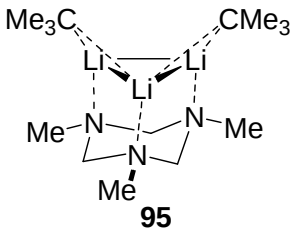

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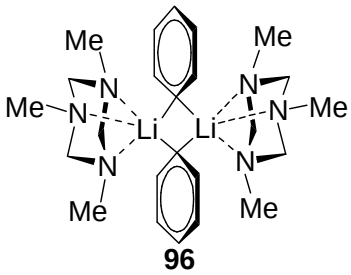

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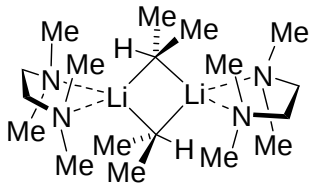

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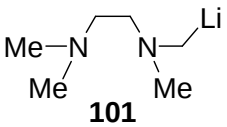
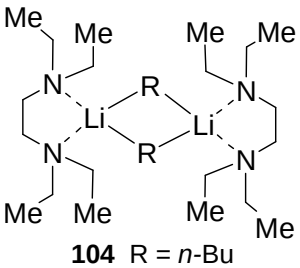
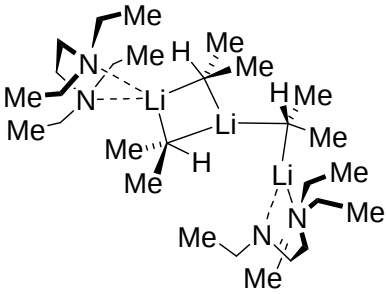


101

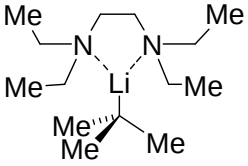
Fehler! Es ist nicht möglich, durch die Bearbeitung von Feldfunktionen Objekte zu erstellen.



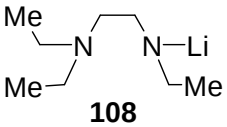
104 R = *n*-Bu
105 R = Ph



[(*i*-PrLi)$_3$·(TEEDA)$_2$] (**106**)



t-BuLi·TEEDA (**107**)



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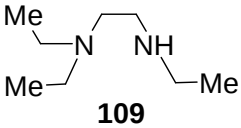

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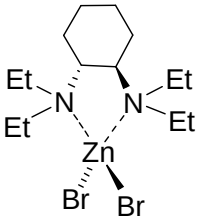
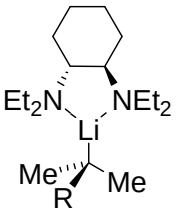
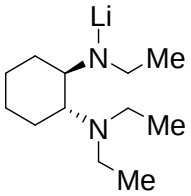


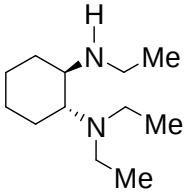
(*R*,*R*)-**110**



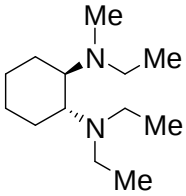
R = H: (*R*,*R*)-**111**
R = Me: (*R*,*R*)-**112**



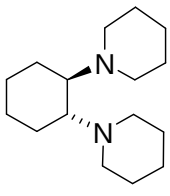
(*R*,*R*)-**113**



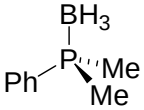
(*R*,*R*)-**114**



(*R*,*R*)-**115**



(*R*,*R*)-DPCH (**116**)



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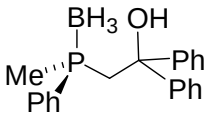

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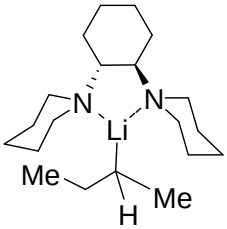
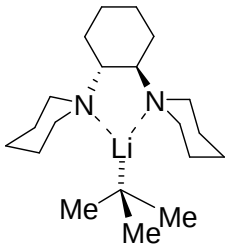
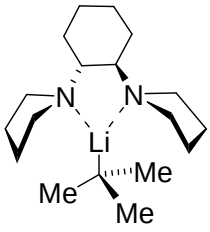


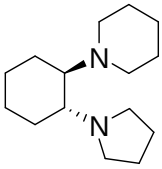
(*R*,*R*)-**123**



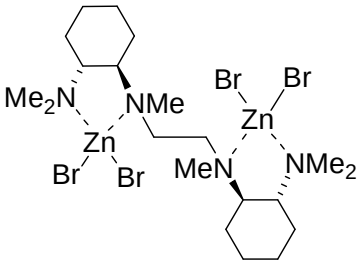
(*R*,*R*)-**124**



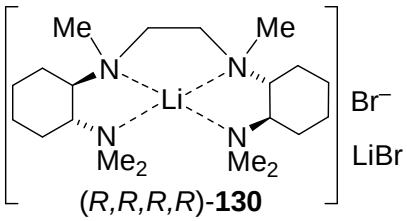
(*R*,*R*)-**125**



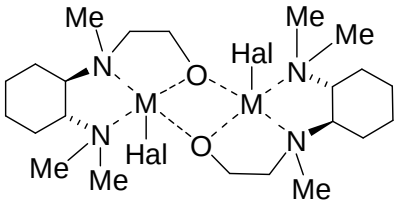
(*R*,*R*)-**127**



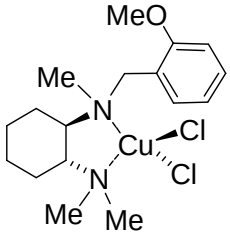
(*R*,*R*,*R*,*R*)-**129**



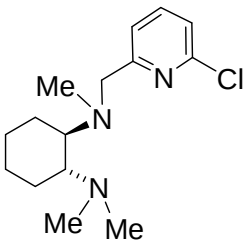
(*R*,*R*,*R*,*R*)-**130**



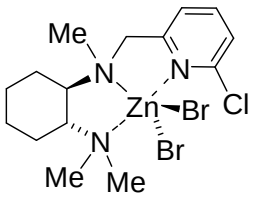
M = Zn, Hal = Br: **131**
M = Cu, Hal = I: **132**



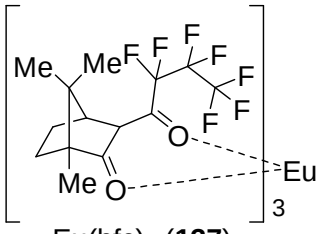
(*R*,*R*)-**134**



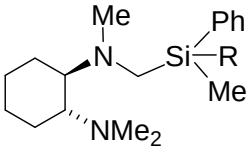
(*R*,*R*)-**135**



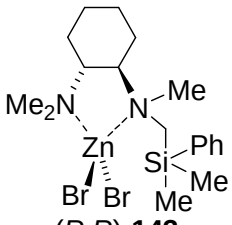
(*R*,*R*)-**136**



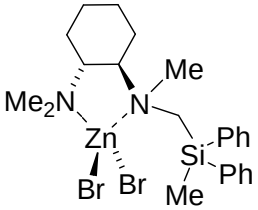
Eu(hfc)$_3$ (**137**)



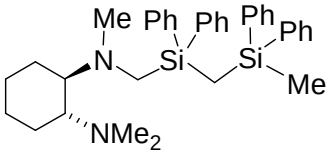
R = Me: (*R*,*R*)-**141**
R = Ph: (*R*,*R*)-**142**



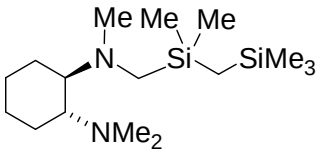
(*R*,*R*)-**143**



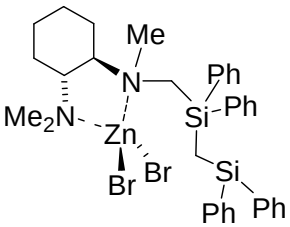
(*R*,*R*)-**145**



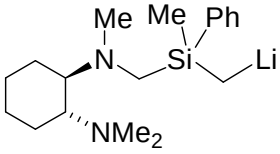
(*R*,*R*)-**146**



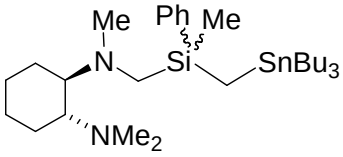
(*R*,*R*)-**147**



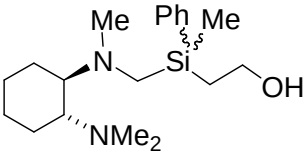
(*R*,*R*)-**148**



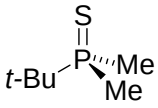
(*R*,*R*)-**149**



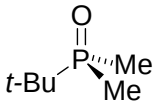
(*R*,*R*)-**150**



(*R*,*R*)-**151**



156



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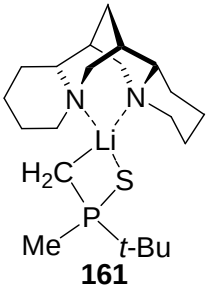

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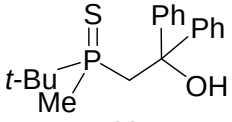

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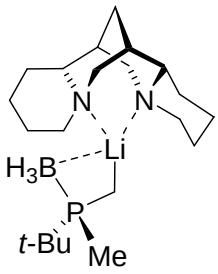

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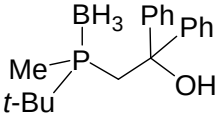

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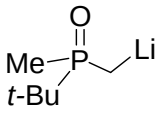
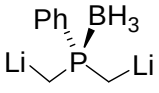


rac-**167**



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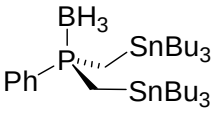

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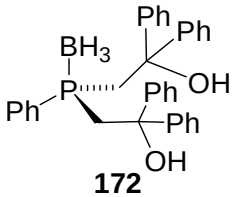

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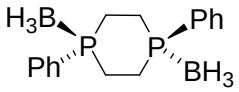

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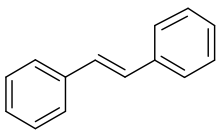
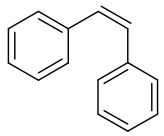
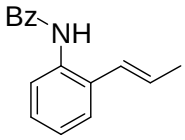


trans-Stilben (**177**)



cis-Stilben (**177**)



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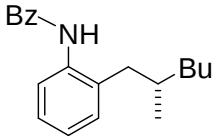
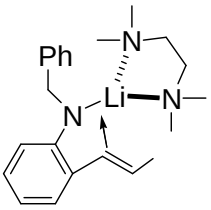


(*R*)-**182**



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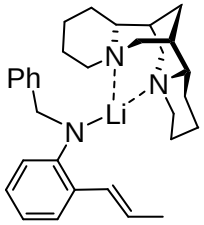
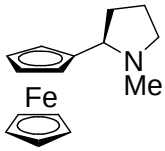
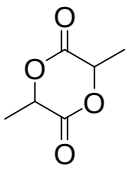


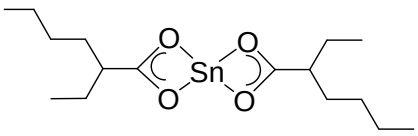
trans-**185**



(*R*)-**186**



D,*L*-Lactid (**189**)



$Sn(oct)_2$ (**191**)

8.2 Angaben zu den Kristallstrukturen

8.2.1 Kristallstrukturen aus Kapitel 4.1

Hydrobromid von (*R,R*)-TMCDA [(*R,R*)-9]

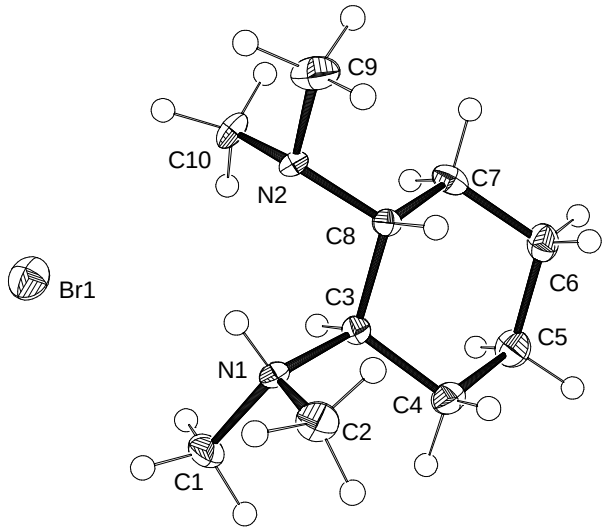


Abbildung 1 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Hydrobromids von (*R,R*)-TMCDA [(*R,R*)-**9**] im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 1 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für das Hydrobromid (*R,R*)-TMCDA [(*R,R*)-**9**]. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
Br(1)	7597(1)	3691(1)	6869(1)	25(1)
C(1)	8678(3)	5506(2)	9096(2)	26(1)
C(2)	5799(3)	5874(2)	8826(2)	25(1)
C(3)	7792(3)	7587(2)	8455(2)	15(1)
C(4)	7199(3)	8289(2)	9355(2)	21(1)
C(5)	7687(5)	9658(2)	9237(2)	26(1)
C(6)	7060(3)	10205(2)	8268(2)	23(1)
C(7)	7643(4)	9433(2)	7396(2)	19(1)
C(8)	7065(3)	8094(2)	7508(2)	14(1)
C(9)	6187(3)	7324(3)	5907(2)	28(1)
C(10)	8993(3)	7251(3)	6301(2)	28(1)
N(1)	7454(3)	6197(2)	8505(1)	15(1)
N(2)	7364(3)	7229(1)	6697(1)	17(1)

Tabelle 2 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für das Hydrobromid von (*R*,*R*)-TMCDA [(*R*,*R*)-**9**]. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	22(1)	29(1)	25(1)	–5(1)	–2(1)	1(1)
C(1)	34(2)	23(2)	20(2)	2(1)	–7(2)	7(1)
C(2)	26(2)	19(2)	29(2)	4(1)	8(2)	–9(1)
C(3)	14(2)	14(1)	15(1)	0(1)	0(1)	–1(1)
C(4)	24(2)	22(1)	17(1)	–1(1)	1(1)	0(1)
C(5)	32(2)	22(1)	24(2)	–6(1)	–3(2)	–1(2)
C(6)	25(2)	15(1)	28(2)	–2(1)	3(1)	–1(1)
C(7)	16(1)	20(1)	22(1)	7(1)	–2(2)	–2(2)
C(8)	11(2)	17(1)	13(2)	2(1)	0(1)	0(1)
C(9)	36(2)	31(2)	18(2)	2(2)	–3(2)	–7(1)
C(10)	36(2)	32(2)	18(2)	–5(2)	11(2)	10(1)
N(1)	20(1)	17(1)	10(1)	–1(1)	0(1)	1(2)
N(2)	23(1)	19(1)	9(1)	–1(1)	2(2)	5(1)

Tabelle 3 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für das Hydrobromid von (*R*,*R*)-TMCDA [(*R*,*R*)-**9**].

	x	y	z	U(eq)
H(1A)	8527	5690	9799	38
H(1B)	9760	5763	8893	38
H(1C)	8551	4612	8985	38
H(2A)	5579	5003	8668	37
H(2B)	5023	6407	8483	37
H(2C)	5703	6000	9540	37
H(4A)	7687	7939	9961	25
H(4B)	6015	8219	9410	25
H(5A)	7254	10143	9797	31
H(5B)	8875	9724	9253	31
H(6A)	7446	11070	8197	27
H(6B)	5869	10219	8277	27
H(7A)	7221	9787	6774	23
H(7B)	8833	9451	7367	23
H(9A)	5101	7321	6188	43
H(9B)	6309	6617	5457	43
H(9C)	6359	8099	5542	43
H(10A)	9178	6501	5907	43

H(10B)	9768	7279	6845	43
H(10C)	9130	7986	5883	43
H(3)	9020(20)	7608(16)	8419(14)	1(5)
H(8)	5820(20)	8123(16)	7592(15)	9(6)
H(1N)	7510(40)	5945(16)	7918(13)	13(6)

t-BuLi·(*R,R*)-TMCDA (80)

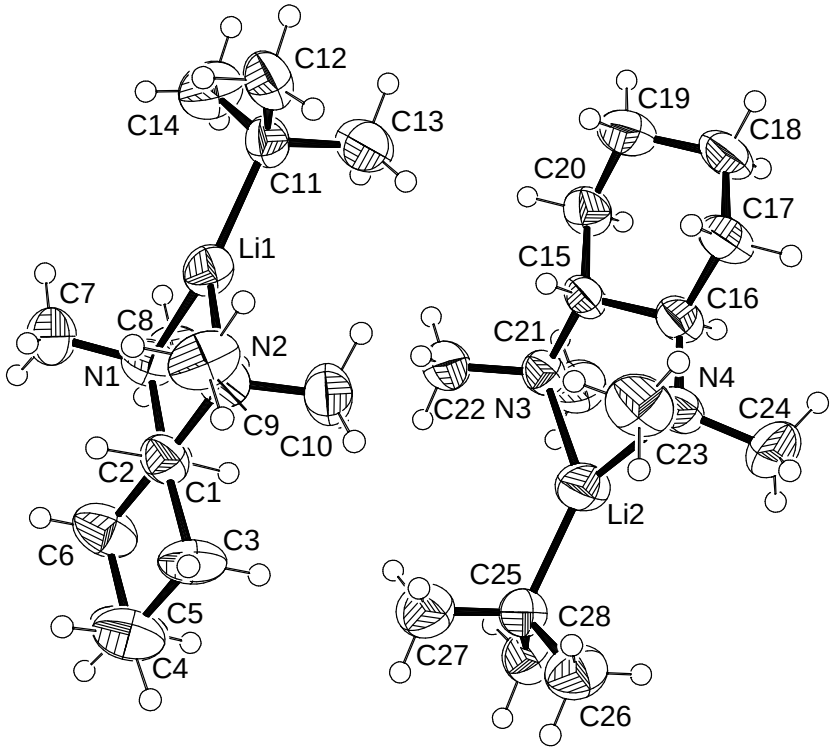


Abbildung 2 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von *t*-BuLi·(*R,R*)-TMCDA (**80**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 4 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung *t*-BuLi·(*R,R*)-TMCDA (**80**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	6373(7)	9784(4)	9028(8)	52(2)
C(2)	5789(7)	9541(4)	10166(7)	51(2)
C(3)	3997(7)	9774(5)	9864(9)	69(3)
C(4)	3787(9)	10561(5)	9629(11)	85(3)

C(5)	4365(9)	10809(5)	8512(11)	86(3)
C(6)	6112(8)	10578(5)	8781(10)	75(3)
C(7)	9279(7)	9915(4)	10271(11)	73(3)
C(8)	8440(8)	9523(5)	8012(8)	75(3)
C(9)	6000(8)	8559(5)	11761(9)	69(3)
C(10)	5026(8)	8277(4)	9418(10)	70(3)
C(11)	9479(7)	7585(4)	10167(8)	52(2)
C(12)	9684(7)	7133(5)	11432(8)	64(2)
C(13)	8753(8)	7114(5)	8920(9)	73(2)
C(14)	11161(7)	7783(5)	10175(9)	74(3)
C(15)	4789(6)	6645(3)	5726(8)	45(2)
C(16)	3344(7)	6135(4)	5356(9)	53(2)
C(17)	3743(8)	5409(4)	6084(10)	63(2)
C(18)	5178(8)	5054(4)	5799(10)	70(3)
C(19)	6648(8)	5570(4)	6279(10)	72(3)
C(20)	6236(7)	6269(4)	5517(9)	58(2)
C(21)	4208(8)	7354(5)	3638(9)	74(3)
C(22)	5492(7)	7921(4)	5802(10)	67(2)
C(23)	1987(9)	6591(5)	6929(9)	80(3)
C(24)	394(7)	6141(5)	4755(11)	82(3)
C(25)	866(7)	8534(4)	4964(8)	51(2)
C(26)	–716(7)	8359(5)	5173(9)	73(3)
C(27)	1774(8)	9049(5)	6023(9)	77(3)
C(28)	481(8)	8923(4)	3619(8)	60(2)
Li(1)	8201(11)	8514(8)	10164(14)	55(4)
Li(2)	2062(12)	7572(8)	5010(15)	65(4)
N(1)	8028(6)	9501(4)	9234(6)	55(2)
N(2)	6081(6)	8762(3)	10461(7)	51(2)
N(3)	4359(5)	7349(3)	5083(6)	47(2)
N(4)	1898(6)	6517(3)	5522(7)	55(2)

Tabelle 5 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung *t*-BuLi·(*R*,*R*)-TMCDA (**80**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	59(4)	52(5)	53(6)	7(4)	31(3)	9(3)
C(2)	56(4)	45(5)	58(6)	–7(4)	27(4)	1(3)
C(3)	54(4)	75(7)	85(8)	11(5)	34(4)	23(4)

C(4)	82(5)	83(8)	100(9)	5(6)	45(5)	26(5)
C(5)	93(6)	75(7)	99(9)	30(6)	45(5)	49(5)
C(6)	87(5)	53(6)	101(9)	16(5)	54(5)	7(4)
C(7)	62(4)	55(6)	98(8)	–2(5)	21(4)	–18(4)
C(8)	83(5)	97(7)	61(6)	–3(5)	45(5)	9(5)
C(9)	57(4)	94(7)	63(6)	23(5)	30(4)	3(4)
C(10)	67(4)	64(6)	82(8)	–19(5)	27(5)	–14(4)
C(11)	51(3)	48(5)	61(6)	–9(4)	23(4)	–9(3)
C(12)	74(4)	50(6)	73(7)	–12(5)	30(4)	–5(4)
C(13)	83(5)	61(6)	74(7)	1(5)	25(4)	12(4)
C(14)	56(4)	91(7)	86(8)	16(5)	39(4)	–5(4)
C(15)	48(3)	32(4)	62(6)	–5(4)	26(3)	–1(3)
C(16)	53(4)	40(5)	75(6)	1(4)	34(4)	0(3)
C(17)	72(4)	42(6)	83(8)	6(5)	37(4)	10(4)
C(18)	87(5)	40(5)	81(8)	–5(5)	27(5)	15(4)
C(19)	71(4)	60(6)	86(8)	5(5)	27(5)	20(4)
C(20)	56(4)	55(6)	71(6)	–12(4)	34(4)	1(3)
C(21)	69(4)	80(7)	75(7)	5(5)	27(4)	0(4)
C(22)	61(4)	50(5)	87(8)	4(5)	20(4)	–4(4)
C(23)	86(5)	84(7)	91(8)	–3(6)	59(5)	7(5)
C(24)	46(4)	80(7)	113(9)	6(6)	19(5)	–11(4)
C(25)	52(3)	49(5)	55(6)	7(4)	24(4)	–3(3)
C(26)	68(4)	80(7)	72(7)	15(5)	23(4)	6(4)
C(27)	74(5)	81(7)	67(7)	–2(5)	14(4)	10(4)
C(28)	65(4)	57(6)	66(6)	–2(4)	31(4)	–5(3)
Li(1)	42(5)	63(10)	66(10)	–3(7)	25(5)	–6(5)
Li(2)	53(6)	55(9)	95(13)	10(8)	35(7)	1(5)
N(1)	56(3)	58(5)	61(5)	5(4)	35(3)	7(3)
N(2)	59(3)	51(4)	49(4)	3(3)	24(3)	2(3)
N(3)	49(3)	42(4)	54(4)	0(3)	25(3)	–2(3)
N(4)	55(3)	43(4)	77(6)	–2(4)	36(3)	3(3)

Tabelle 6 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung *t*-BuLi·(*R*,*R*)-TMCDA (**80**).

	x	y	z	U(eq)
H(1)	5646	9544	8202	62
H(2)	6449	9807	10987	61
H(3A)	3299	9514	9064	82
H(3B)	3657	9641	10629	82
H(4A)	4395	10819	10462	102

H(4B)	2634	10684	9399	102
H(5A)	4286	11339	8437	103
H(5B)	3667	10601	7654	103
H(6A)	6427	10713	8004	90
H(6B)	6822	10842	9570	90
H(7A)	10329	9684	10452	110
H(7B)	9014	9929	11093	110
H(7C)	9320	10407	9951	110
H(8A)	8354	10018	7680	112
H(8B)	7696	9215	7331	112
H(8C)	9546	9351	8208	112
H(9A)	6756	8854	12460	103
H(9B)	6287	8051	11932	103
H(9C)	4904	8636	11765	103
H(10A)	3950	8263	9494	106
H(10B)	5485	7792	9542	106
H(10C)	4945	8457	8531	106
H(12A)	10414	6730	11471	96
H(12B)	8633	6947	11400	96
H(12C)	10136	7434	12228	96
H(13A)	9390	6674	9013	110
H(13B)	8764	7379	8127	110
H(13C)	7640	6990	8823	110
H(14A)	11645	8134	10885	111
H(14B)	11082	7991	9309	111
H(14C)	11833	7350	10336	111
H(15)	5102	6732	6710	55
H(16)	3055	6030	4381	63
H(17A)	2790	5090	5773	75
H(17B)	4020	5483	7058	75
H(18A)	4889	4960	4829	84
H(18B)	5449	4590	6279	84
H(19A)	6934	5663	7249	86
H(19B)	7587	5346	6128	86
H(20A)	5985	6173	4551	69
H(20B)	7182	6593	5815	69
H(21A)	3786	7819	3242	111
H(21B)	3470	6971	3166	111
H(21C)	5269	7273	3559	111
H(22A)	5586	7919	6747	100
H(22B)	5088	8389	5407	100
H(22C)	6552	7832	5728	100

H(23A)	1038	6852	6964	119
H(23B)	2964	6858	7432	119
H(23C)	2020	6114	7325	119
H(24A)	-201	6427	3969	123
H(24B)	-270	6075	5321	123
H(24C)	653	5671	4468	123
H(26A)	-1337	8801	5115	110
H(26B)	-492	8141	6057	110
H(26C)	-1336	8022	4482	110
H(27A)	2833	9141	5948	115
H(27B)	1914	8845	6904	115
H(27C)	1174	9501	5914	115
H(28A)	-130	8602	2893	91
H(28B)	1488	9063	3490	91
H(28C)	-161	9353	3615	91

[(*R,R*)-TMCDA-Li]$_3$ [(*R,R*)-68]

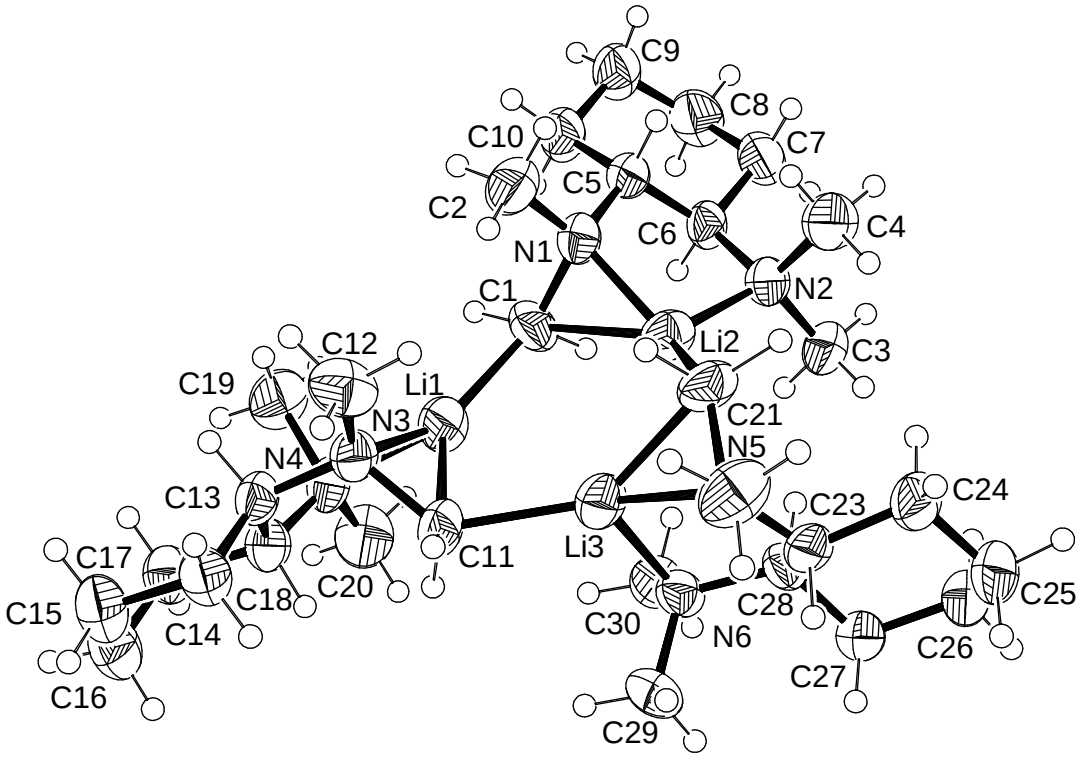


Abbildung 3 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von [(*R,R*)-TMCDA-Li]$_3$ [(*R,R*)-**68**] im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 7 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung [(*R*,*R*)-TMCDA-Li]$_3$ [(*R*,*R*)-**68**]. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	8177(9)	4018(4)	3084(2)	59(2)
C(2)	10208(8)	3623(5)	2553(2)	73(2)
C(3)	4987(8)	1585(4)	3132(2)	62(2)
C(4)	7084(9)	998(4)	2660(2)	72(2)
C(5)	7465(7)	3147(3)	2374(1)	47(1)
C(6)	6004(7)	2657(3)	2552(1)	44(1)
C(7)	4854(8)	2333(4)	2182(2)	65(2)
C(8)	4367(9)	3225(4)	1913(2)	72(2)
C(9)	5803(8)	3772(4)	1744(2)	67(2)
C(10)	6985(8)	4056(4)	2111(2)	64(2)
C(11)	11356(9)	4011(4)	4110(2)	59(2)
C(12)	13396(8)	4390(4)	3564(2)	67(2)
C(13)	12262(7)	5753(3)	3968(1)	48(1)
C(14)	13532(8)	5829(4)	4339(2)	58(2)
C(15)	13771(8)	6906(4)	4466(2)	69(2)
C(16)	12241(9)	7382(4)	4595(2)	70(2)
C(17)	10959(8)	7287(4)	4241(2)	58(2)
C(18)	10706(7)	6208(3)	4121(2)	49(1)
C(19)	9508(9)	6564(4)	3401(2)	75(2)
C(20)	7772(8)	6131(5)	4001(2)	76(2)
C(21)	10213(8)	1498(4)	3520(2)	60(2)
C(22)	12052(8)	728(5)	4058(2)	74(2)
C(23)	9182(7)	727(3)	4205(1)	49(1)
C(24)	8727(8)	–266(4)	4012(2)	61(2)
C(25)	7481(8)	–778(4)	4296(2)	64(2)
C(26)	6032(8)	–157(4)	4362(2)	63(2)
C(27)	6449(8)	862(4)	4524(1)	54(1)
C(28)	7686(6)	1357(3)	4234(1)	44(1)
C(29)	8596(9)	2521(4)	4796(1)	73(2)
C(30)	6718(8)	3039(4)	4247(2)	62(2)
Li(1)	9817(13)	4510(6)	3587(3)	58(3)
Li(2)	8506(12)	2406(6)	3197(2)	56(2)
Li(3)	10125(12)	2660(6)	3987(2)	55(2)
N(1)	8684(5)	3342(3)	2725(1)	46(1)
N(2)	6406(6)	1864(3)	2871(1)	51(1)
N(3)	11995(5)	4762(3)	3796(1)	47(1)
N(4)	9371(6)	5997(3)	3809(1)	51(1)

N(5)	10542(6)	1233(3)	3994(1)	52(1)
N(6)	8046(6)	2394(3)	4344(1)	48(1)

Tabelle 8 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung [(*R*,*R*)-TMCDA-Li]$_3$ [(*R*,*R*)-**68**]. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	85(6)	40(3)	54(3)	–11(2)	–4(3)	1(3)
C(2)	75(5)	79(4)	64(3)	9(3)	4(3)	–26(4)
C(3)	64(5)	57(4)	63(3)	6(3)	6(3)	–19(3)
C(4)	103(6)	45(3)	67(3)	7(3)	5(3)	15(4)
C(5)	61(4)	39(3)	43(2)	3(2)	–1(2)	–4(3)
C(6)	53(4)	30(2)	50(2)	3(2)	–4(2)	2(2)
C(7)	84(5)	50(3)	59(3)	–3(2)	–13(3)	–5(3)
C(8)	89(6)	65(4)	63(3)	5(3)	–28(3)	0(4)
C(9)	85(5)	54(3)	63(3)	11(3)	–18(3)	–9(4)
C(10)	85(5)	48(3)	57(3)	10(2)	–14(3)	–14(3)
C(11)	77(5)	38(3)	62(3)	13(2)	–5(3)	–10(3)
C(12)	77(5)	59(4)	64(3)	–8(3)	1(3)	24(3)
C(13)	55(4)	34(2)	56(2)	5(2)	2(2)	–5(3)
C(14)	62(4)	49(3)	63(3)	0(2)	–10(3)	–4(3)
C(15)	71(5)	52(3)	85(4)	–3(3)	–14(3)	–8(4)
C(16)	82(6)	46(3)	83(3)	–9(3)	–11(3)	0(4)
C(17)	58(4)	46(3)	72(3)	–5(3)	2(3)	4(3)
C(18)	54(4)	36(3)	58(3)	2(2)	–1(2)	1(3)
C(19)	97(6)	61(4)	69(3)	27(3)	–22(3)	2(4)
C(20)	65(5)	69(4)	93(4)	–5(3)	14(3)	8(4)
C(21)	81(5)	51(3)	47(3)	17(2)	5(3)	13(3)
C(22)	71(5)	74(4)	77(3)	26(3)	5(3)	17(4)
C(23)	70(4)	34(2)	42(2)	10(2)	–2(2)	7(3)
C(24)	80(5)	37(3)	67(3)	1(2)	19(3)	8(3)
C(25)	80(5)	36(3)	75(3)	4(3)	–1(3)	2(3)
C(26)	79(5)	49(3)	62(3)	3(3)	–4(3)	–14(3)
C(27)	64(4)	47(3)	50(2)	0(2)	2(2)	–2(3)
C(28)	54(4)	34(2)	43(2)	–5(2)	–2(2)	4(3)
C(29)	100(6)	73(4)	46(2)	–10(3)	–19(3)	–20(4)
C(30)	72(5)	51(3)	62(3)	–6(3)	15(3)	5(3)
Li(1)	77(8)	37(5)	60(4)	9(4)	–8(4)	4(5)

Li(2)	65(7)	50(5)	53(4)	10(4)	4(4)	11(5)
Li(3)	64(7)	43(5)	58(4)	9(4)	–1(4)	3(5)
N(1)	45(3)	38(2)	55(2)	3(2)	1(2)	0(2)
N(2)	68(4)	35(2)	51(2)	1(2)	3(2)	3(2)
N(3)	55(3)	35(2)	52(2)	3(2)	1(2)	2(2)
N(4)	54(3)	33(2)	66(2)	7(2)	0(2)	0(2)
N(5)	62(4)	43(2)	52(2)	13(2)	2(2)	11(2)
N(6)	62(3)	37(2)	44(2)	–2(2)	–5(2)	7(2)

Tabelle 9 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung [(*R*,*R*)-TMCDA-Li]$_3$ [(*R*,*R*)-**68**].

	x	y	z	U(eq)
H(1B)	7040(90)	3760(50)	3149(17)	90(20)
H(1A)	8050(80)	4750(50)	2985(16)	87(19)
H(2A)	10126	4274	2426	109
H(2B)	10538	3158	2329	109
H(2C)	11005	3630	2787	109
H(3A)	4152	1326	2941	92
H(3B)	4576	2157	3286	92
H(3C)	5295	1087	3344	92
H(4A)	7379	519	2881	108
H(4B)	8040	1182	2494	108
H(4C)	6286	715	2463	108
H(5)	7970	2681	2166	57
H(6)	5413	3165	2721	53
H(7A)	5397	1852	1994	77
H(7B)	3887	2023	2307	77
H(8A)	3697	3013	1665	87
H(8B)	3713	3666	2096	87
H(9A)	5435	4368	1594	81
H(9B)	6371	3362	1528	81
H(10A)	7955	4357	1983	76
H(10B)	6473	4538	2305	76
H(11A)	12450(100)	3720(60)	4227(19)	110(20)
H(11B)	10340(80)	4430(40)	4332(17)	90(20)
H(12A)	13725	4860	3342	100
H(12B)	13125	3770	3426	100
H(12C)	14278	4290	3770	100

H(13)	12664	6158	3722	58
H(14A)	13164	5455	4595	70
H(14B)	14563	5550	4240	70
H(15A)	14541	6946	4710	83
H(15B)	14238	7261	4216	83
H(16A)	12441	8079	4654	84
H(16B)	11842	7081	4867	84
H(17A)	11296	7655	3981	70
H(17B)	9936	7567	4347	70
H(18)	10418	5869	4397	59
H(19A)	8582	6427	3214	113
H(19B)	10496	6381	3249	113
H(19C)	9537	7260	3469	113
H(20A)	7687	5742	4267	113
H(20B)	6952	5921	3793	113
H(20C)	7612	6819	4071	113
H(21B)	11570(100)	1760(50)	3411(18)	110(20)
H(21A)	9990(70)	800(40)	3336(16)	72(17)
H(22A)	12214	610	4369	111
H(22B)	12932	1127	3946	111
H(22C)	12028	106	3904	111
H(23)	9525	599	4511	58
H(24A)	9698	-677	3989	74
H(24B)	8287	-173	3717	74
H(25A)	7159	-1397	4156	76
H(25B)	7963	-935	4581	76
H(26A)	5315	-475	4576	76
H(26B)	5441	-104	4085	76
H(27A)	6875	818	4823	65
H(27B)	5463	1262	4532	65
H(28)	7214	1365	3936	52
H(29A)	7742	2322	4996	109
H(29B)	8861	3206	4846	109
H(29C)	9550	2120	4846	109
H(30A)	6395	2955	3944	92
H(30B)	7050	3714	4295	92
H(30C)	5811	2885	4438	92

[*t*-BuLi·(*R,R*)-TMCDA-Li]$_2$ [(*R,R*)-83]

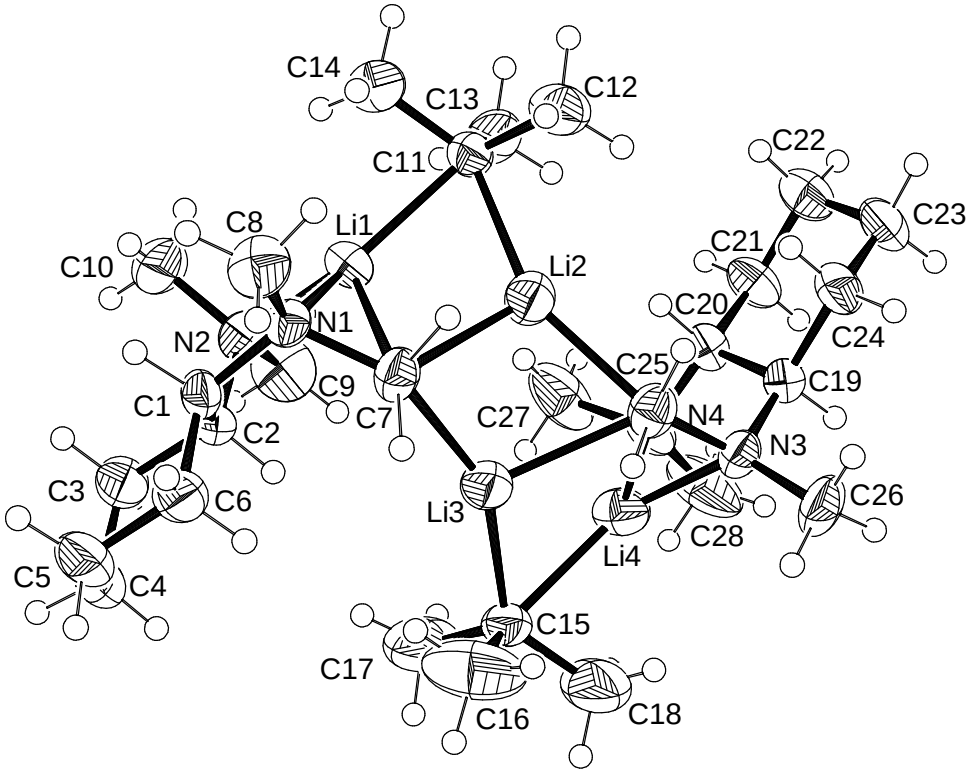


Abbildung 4 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von [*t*-BuLi·(*R,R*)-TMCDA-Li]$_2$ [(*R,R*)-**83**] im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 10 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für [*t*-BuLi·(*R,R*)-TMCDA-Li]$_2$ [(*R,R*)-**83**]. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	2213(4)	1168(2)	6272(3)	43(1)
C(2)	3736(4)	1582(2)	6005(3)	41(1)
C(3)	5036(5)	1060(2)	5655(3)	63(1)
C(4)	5387(6)	516(3)	6684(4)	76(1)
C(5)	3889(6)	115(2)	7003(4)	77(1)
C(6)	2556(5)	625(2)	7320(3)	58(1)
C(7)	1000(5)	2119(2)	7622(3)	47(1)
C(8)	–642(5)	1252(2)	6386(4)	59(1)
C(9)	4758(5)	2700(3)	5087(4)	74(1)
C(10)	3159(5)	1910(3)	3772(3)	70(1)
C(11)	94(4)	3583(2)	5469(3)	45(1)
C(12)	–1380(5)	3871(3)	6112(4)	68(1)
C(13)	916(5)	4215(2)	4866(3)	63(1)
C(14)	–526(5)	3114(2)	4370(3)	62(1)

C(15)	5003(5)	2820(2)	9706(3)	50(1)
C(16)	4347(8)	2136(4)	10310(6)	121(2)
C(17)	6344(7)	2583(4)	8946(5)	122(3)
C(18)	5584(9)	3272(3)	10784(5)	128(3)
C(19)	1647(4)	4974(2)	9522(3)	43(1)
C(20)	2487(4)	5016(2)	8265(3)	43(1)
C(21)	2367(5)	5765(2)	7693(4)	60(1)
C(22)	664(5)	6023(2)	7549(4)	64(1)
C(23)	-149(5)	5986(2)	8786(4)	65(1)
C(24)	-54(5)	5236(2)	9349(3)	55(1)
C(25)	1148(5)	3647(2)	9373(3)	49(1)
C(26)	1313(5)	4272(2)	11432(3)	59(1)
C(27)	4686(6)	4497(3)	7118(4)	90(2)
C(28)	5229(6)	5179(3)	9010(5)	94(2)
Li(1)	1396(7)	2582(3)	5703(5)	48(2)
Li(2)	725(8)	3342(3)	7442(5)	54(2)
Li(3)	2712(8)	2689(3)	8742(5)	54(2)
Li(4)	3759(8)	3830(3)	9422(5)	55(2)
N(1)	858(3)	1650(2)	6464(2)	39(1)
N(2)	3448(4)	2169(2)	5061(2)	47(1)
N(3)	1846(3)	4258(2)	10123(2)	42(1)
N(4)	4098(4)	4704(2)	8364(3)	52(1)

Tabelle 11 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für [*t*-BuLi·(*R*,*R*)-TMCDA-Li]$_2$ [(*R*,*R*)-**83**]. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	44(2)	33(2)	52(2)	–10(2)	–4(2)	4(2)
C(2)	40(2)	40(2)	44(2)	–5(2)	–7(2)	7(2)
C(3)	41(3)	76(3)	72(2)	–17(2)	–7(2)	14(2)
C(4)	71(3)	61(3)	93(3)	–18(2)	–25(2)	26(3)
C(5)	91(4)	45(3)	92(3)	–1(2)	–27(3)	18(3)
C(6)	75(3)	40(2)	58(2)	4(2)	–12(2)	1(2)
C(7)	57(3)	46(2)	38(2)	–5(2)	7(2)	–1(2)
C(8)	48(3)	58(3)	72(2)	–4(2)	0(2)	–15(2)
C(9)	56(3)	66(3)	101(3)	7(3)	12(2)	–20(2)
C(10)	77(3)	92(4)	41(2)	–7(2)	4(2)	12(3)
C(11)	47(2)	46(2)	41(2)	1(2)	1(2)	6(2)
C(12)	54(3)	89(4)	61(2)	1(2)	–1(2)	16(2)

C(13)	86(3)	54(3)	51(2)	8(2)	–4(2)	–6(2)
C(14)	60(3)	68(3)	57(2)	–1(2)	–6(2)	0(2)
C(15)	58(3)	45(2)	45(2)	4(2)	–8(2)	2(2)
C(16)	117(5)	113(5)	130(5)	67(4)	–27(4)	–7(4)
C(17)	91(4)	200(8)	74(3)	–5(4)	–8(3)	69(5)
C(18)	156(6)	88(5)	136(5)	–36(4)	–91(4)	38(4)
C(19)	44(2)	42(2)	42(2)	–5(2)	1(2)	5(2)
C(20)	45(2)	37(2)	46(2)	4(2)	10(2)	3(2)
C(21)	58(3)	44(3)	77(2)	14(2)	4(2)	9(2)
C(22)	66(3)	47(3)	77(2)	8(2)	0(2)	12(2)
C(23)	56(3)	58(3)	80(3)	–7(2)	–1(2)	22(2)
C(24)	45(3)	63(3)	58(2)	–2(2)	8(2)	14(2)
C(25)	58(3)	45(2)	45(2)	–2(2)	6(2)	–5(2)
C(26)	86(3)	61(3)	32(2)	–7(2)	12(2)	1(2)
C(27)	90(4)	93(4)	90(3)	34(3)	49(3)	40(3)
C(28)	52(3)	59(3)	171(5)	18(3)	–15(3)	–2(2)
Li(1)	47(4)	47(4)	51(3)	0(3)	–2(3)	10(3)
Li(2)	52(4)	57(4)	52(3)	–6(3)	0(3)	–3(3)
Li(3)	67(4)	47(4)	48(3)	2(3)	–5(3)	4(3)
Li(4)	57(4)	46(4)	61(3)	7(3)	–9(3)	–8(3)
N(1)	33(2)	40(2)	43(1)	–4(1)	0(1)	–7(1)
N(2)	48(2)	50(2)	44(2)	–1(1)	5(1)	–6(2)
N(3)	55(2)	39(2)	32(1)	–2(1)	4(1)	–3(2)
N(4)	39(2)	48(2)	70(2)	9(2)	15(2)	5(2)

Tabelle 12 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung [*t*-BuLi·(*R*,*R*)-TMCDA-Li]$_2$ [(*R*,*R*)-**83**].

	x	y	z	U(eq)
H(1)	1955	883	5497	52
H(2)	4079	1817	6811	50
H(3A)	4717	805	4872	75
H(3B)	6008	1334	5483	75
H(4A)	5812	763	7443	91
H(4B)	6192	172	6397	91
H(5A)	4107	–205	7731	92
H(5B)	3558	–188	6278	92
H(6A)	2838	885	8106	70
H(6B)	1591	343	7473	70
H(7A)	–310(40)	2280(20)	7790(30)	56(10)

H(7B)	1160(40)	1790(18)	8500(30)	43(8)
H(8A)	–688	972	5604	89
H(8B)	–1525	1591	6392	89
H(8C)	–710	928	7109	89
H(9A)	5721	2472	4790	111
H(9B)	4934	2872	5951	111
H(9C)	4480	3105	4539	111
H(10A)	4125	1693	3455	105
H(10B)	2844	2313	3230	105
H(10C)	2316	1551	3769	105
H(12A)	–2036	4134	5497	102
H(12B)	–1061	4194	6801	102
H(12C)	–1983	3469	6450	102
H(13A)	1825	4043	4401	95
H(13B)	1274	4551	5523	95
H(13C)	179	4459	4286	95
H(14A)	–1209	3402	3811	93
H(14B)	–1129	2711	4704	93
H(14C)	365	2930	3897	93
H(16A)	5198	1886	10771	181
H(16B)	3912	1821	9650	181
H(16C)	3515	2264	10892	181
H(17A)	6769	2994	8491	183
H(17B)	5985	2218	8342	183
H(17C)	7168	2381	9503	183
H(18A)	6265	2983	11343	192
H(18B)	4683	3450	11253	192
H(18C)	6184	3679	10462	192
H(19)	2187	5327	10096	51
H(20)	1878	4695	7677	51
H(21A)	2856	5762	6856	71
H(21B)	2966	6106	8236	71
H(22A)	650	6523	7237	76
H(22B)	93	5720	6923	76
H(23A)	–1270	6123	8661	77
H(23B)	347	6332	9380	77
H(24A)	–639	4898	8790	66
H(24B)	–568	5236	10175	66
H(25A)	1270(50)	3200(20)	9930(30)	76(12)
H(25B)	–100(50)	3720(20)	9330(30)	68(12)
H(26A)	162	4319	11436	89
H(26B)	1796	4680	11876	89

H(26C)	1625	3825	11856	89
H(27A)	4821	4928	6603	135
H(27B)	3926	4176	6700	135
H(27C)	5702	4252	7224	135
H(28A)	5408	5604	8490	141
H(28B)	6228	4925	9151	141
H(28C)	4808	5327	9821	141

[*trans*-TMCDA-Li]$_4$ (*trans*-68)

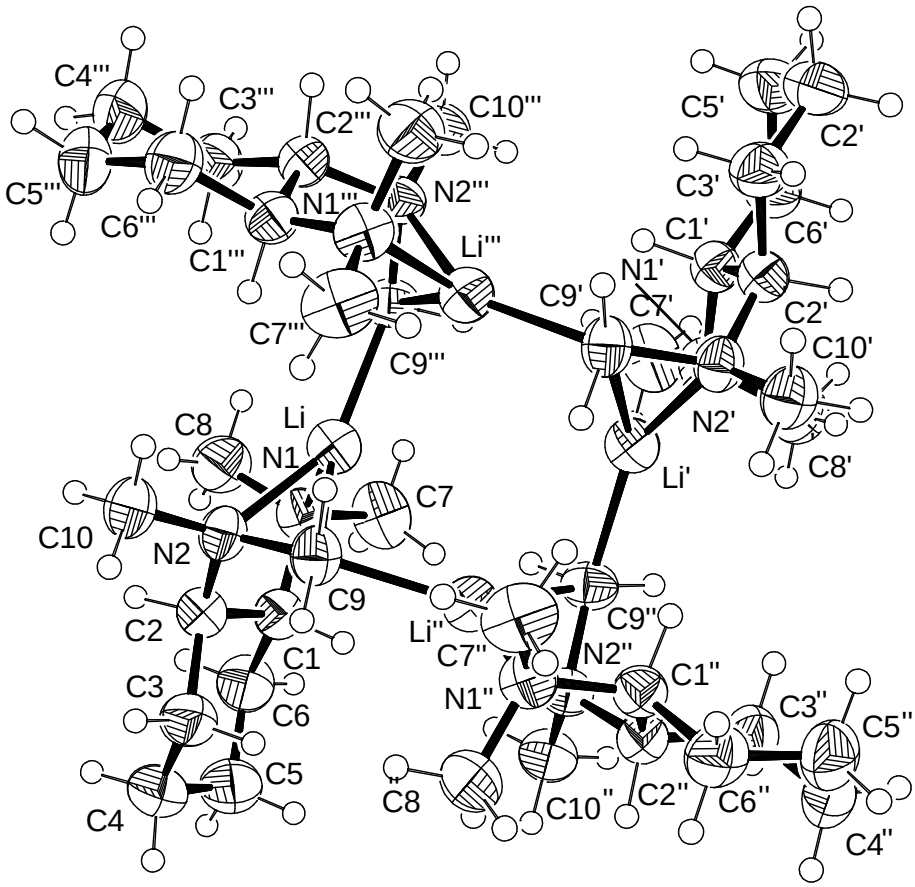


Abbildung 5 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von [*trans*-TMCDA-Li]$_4$ (*trans*-**68**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 13 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung [*trans*-TMCDA-Li]$_4$ (*trans*-**68**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	2870(3)	8772(3)	1035(4)	44(1)
C(2)	3432(3)	9035(2)	152(5)	45(2)
C(3)	3738(3)	7971(3)	-315(6)	62(2)
C(4)	4478(3)	7262(3)	269(7)	70(3)
C(5)	3958(4)	7032(3)	1157(6)	71(2)
C(6)	3628(3)	8082(3)	1618(6)	63(2)
C(7)	1750(4)	9529(4)	2217(6)	63(2)
C(8)	3263(3)	10574(4)	1682(6)	69(3)
C(9)	1774(3)	9336(3)	–-764(5)	51(2)
C(10)	3496(3)	10329(3)	–1070(5)	51(2)
Li(2)	1588(4)	10406(5)	342(8)	51(3)
N(1)	2430(2)	9775(3)	1456(4)	51(2)
N(2)	2807(2)	9813(2)	–397(4)	48(2)

Tabelle 14 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung [*trans*-TMCDA]-Li$_4$ (*trans*-**68**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	45(2)	45(2)	43(5)	2(2)	–6(2)	–1(2)
C(2)	41(2)	46(2)	48(6)	0(2)	–1(2)	1(1)
C(3)	56(2)	45(2)	85(7)	–5(2)	7(3)	4(2)
C(4)	62(2)	54(2)	93(9)	3(3)	5(3)	14(2)
C(5)	73(3)	57(2)	82(9)	14(3)	0(3)	10(2)
C(6)	62(2)	60(2)	68(8)	11(2)	–15(2)	6(2)
C(7)	68(3)	97(3)	23(8)	–2(3)	1(2)	1(2)
C(8)	65(2)	63(2)	79(9)	–24(3)	–11(3)	–3(2)
C(9)	45(2)	60(2)	48(6)	0(2)	–1(2)	–5(2)
C(10)	56(2)	57(2)	41(6)	3(2)	4(2)	–8(2)
Li(2)	48(3)	51(3)	54(10)	5(3)	6(3)	–1(2)
N(1)	50(2)	56(2)	48(6)	–8(2)	–5(2)	0(1)
N(2)	40(1)	46(1)	57(5)	3(2)	–3(2)	–7(1)

Tabelle 15 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung [*trans*TMCDA-Li]$_4$ (*trans*-**68**).

	x	y	z	U(eq)
H(9B)	2040(30)	8800(30)	−1340(70)	66(13)
H(1)	2220(30)	8310(30)	880(60)	47(10)
H(2)	4150(30)	9350(30)	370(60)	56(11)
H(3A)	4108	8135	−868	75
H(3B)	3081	7570	−457	75
H(4A)	4625	6581	−33	83
H(4B)	5165	7633	361	83
H(5A)	4466	6637	1530	85
H(5B)	3320	6579	1071	85
H(6A)	4275	8500	1759	76
H(6B)	3263	7910	2172	76
H(7A)	2197	9291	2703	94
H(7B)	1246	8963	2063	94
H(7C)	1355	10169	2389	94
H(8A)	2922	11228	1892	104
H(8B)	3689	10735	1163	104
H(8C)	3726	10285	2138	104
H(9A)	1580	9730	−1308	61
H(10A)	4115	10655	−787	77
H(10B)	3087	10879	−1375	77
H(10C)	3737	9791	−1489	77

[(*n*-BuLi)$_2$·(*R*,*R*)-TMCDA]$_2$ (85a)

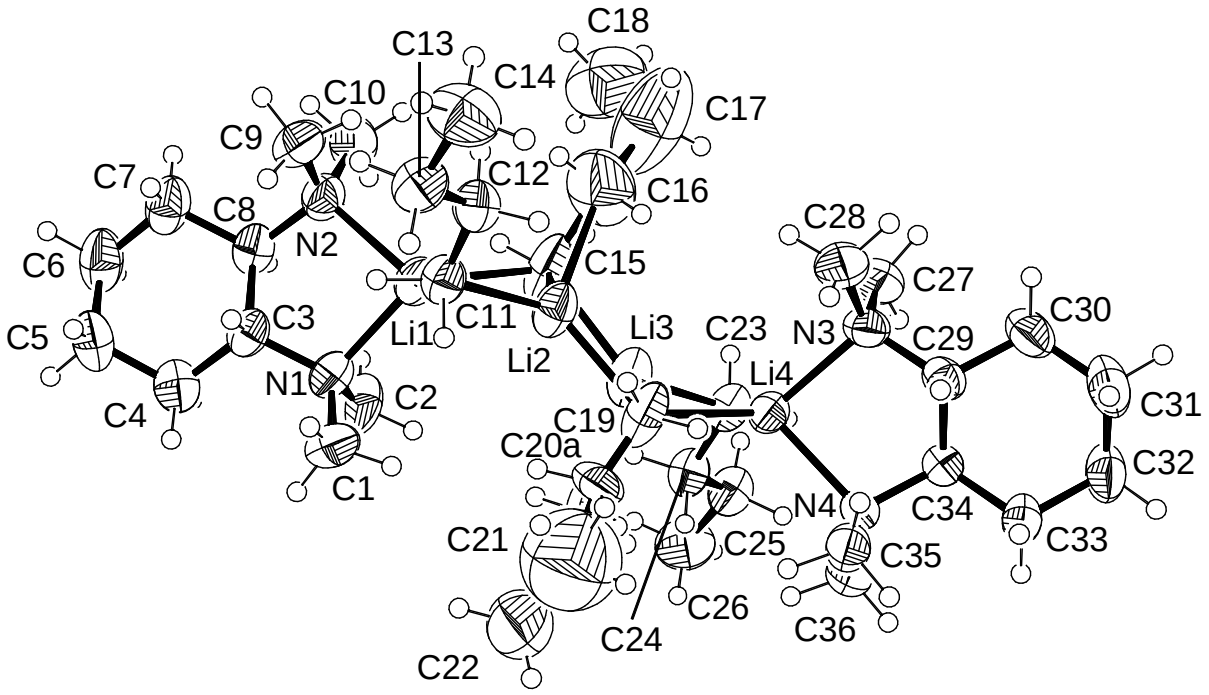


Abbildung 6 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von [(*n*-BuLi)$_2$·(*R*,*R*)-TMCDA]$_2$ (**85a**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 16 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung [(*n*-BuLi)$_2$·(*R*,*R*)-TMCDA]$_2$ (**85a**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	2264(4)	3478(2)	3986(4)	78(1)
C(2)	2453(5)	4152(1)	5761(5)	87(1)
C(3)	3486(3)	3255(1)	6286(3)	51(1)
C(4)	2068(4)	3065(1)	7023(4)	67(1)
C(5)	2441(5)	2618(1)	8062(4)	74(1)
C(6)	3664(5)	2793(2)	9159(4)	79(1)
C(7)	5086(5)	2964(1)	8458(3)	72(1)
C(8)	4763(4)	3412(1)	7381(3)	53(1)
C(9)	7142(4)	3169(2)	6303(4)	75(1)
C(10)	6986(5)	3985(2)	7594(4)	85(1)
C(11)	5975(4)	3485(1)	2754(3)	52(1)
C(12)	7517(4)	3359(1)	2202(3)	59(1)
C(13)	7837(4)	2774(1)	1857(4)	66(1)
C(14)	9305(5)	2683(2)	1147(5)	96(1)
C(15)	5966(6)	4820(1)	4312(4)	87(1)
C(16)	7771(7)	4842(3)	3798(7)	139(2)

C(17)	9073(14)	5218(3)	4238(9)	221(5)
C(18)	9342(8)	5241(3)	5678(9)	158(3)
C(19)	4560(6)	4697(2)	613(4)	79(1)
C(20A)	3228(12)	4478(8)	503(15)	133(7)
C(20B)	2418(13)	4691(2)	1053(8)	100(3)
C(21)	1867(15)	4361(6)	181(14)	259(5)
C(22)	427(7)	4264(2)	525(7)	128(2)
C(23)	4295(4)	6028(1)	2233(3)	55(1)
C(24)	2712(4)	6112(1)	2803(3)	57(1)
C(25)	2275(4)	6686(1)	3125(3)	64(1)
C(26)	804(5)	6737(2)	3851(5)	87(1)
C(27)	7574(4)	6252(1)	584(4)	70(1)
C(28)	8074(4)	5424(1)	-526(4)	74(1)
C(29)	6626(3)	6097(1)	-1902(3)	47(1)
C(30)	7792(4)	6503(1)	-2359(4)	67(1)
C(31)	7417(4)	6715(1)	-3831(4)	78(1)
C(32)	5821(4)	6965(1)	-3927(4)	70(1)
C(33)	4658(4)	6556(1)	-3520(3)	56(1)
C(34)	5019(3)	6337(1)	-2022(3)	42(1)
C(35)	3543(4)	5519(1)	-2606(3)	62(1)
C(36)	2446(3)	6215(2)	-1250(4)	66(1)
Li(1)	5328(6)	3916(2)	4646(5)	56(1)
Li(2)	5773(7)	4320(2)	2413(5)	63(1)
Li(3)	4591(7)	5193(2)	2561(6)	68(1)
Li(4)	4921(5)	5621(2)	315(5)	47(1)
N(1)	3190(3)	3676(1)	5214(3)	55(1)
N(2)	6119(3)	3605(1)	6679(3)	58(1)
N(3)	6980(3)	5862(1)	-477(3)	51(1)
N(4)	3878(2)	5949(1)	-1564(2)	45(1)

Tabelle 17 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung $[(n\text{-BuLi})_2 \cdot (R,R)\text{-TMCDA}]_2$ (**85a**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	62(2)	96(3)	74(2)	19(2)	–13(2)	6(2)
C(2)	102(3)	58(2)	105(3)	21(2)	30(2)	35(2)
C(3)	66(2)	36(1)	50(2)	–2(1)	3(1)	7(1)
C(4)	72(2)	60(2)	70(2)	4(2)	11(2)	–4(2)
C(5)	93(3)	57(2)	73(2)	6(2)	16(2)	–20(2)

C(6)	119(3)	66(2)	53(2)	8(2)	8(2)	–18(2)
C(7)	106(3)	60(2)	48(2)	4(2)	–7(2)	–13(2)
C(8)	75(2)	44(2)	39(1)	–4(1)	3(1)	–2(1)
C(9)	65(2)	81(2)	76(2)	20(2)	–4(2)	16(2)
C(10)	103(3)	87(3)	61(2)	11(2)	–25(2)	–38(2)
C(11)	63(2)	46(2)	48(2)	–1(1)	2(1)	0(1)
C(12)	64(2)	53(2)	59(2)	1(1)	6(2)	–1(1)
C(13)	72(2)	56(2)	69(2)	–6(2)	4(2)	10(2)
C(14)	75(3)	87(3)	126(4)	–22(3)	19(2)	13(2)
C(15)	162(5)	47(2)	48(2)	4(2)	–19(2)	–5(2)
C(16)	163(6)	135(5)	117(4)	–15(4)	–13(4)	–57(4)
C(17)	398(15)	129(6)	124(6)	–1(5)	–75(8)	–21(8)
C(18)	164(6)	112(5)	195(7)	–15(5)	–22(5)	25(4)
C(19)	136(4)	48(2)	50(2)	9(2)	–17(2)	–4(2)
C(20A)	54(6)	240(20)	103(9)	93(12)	–25(6)	–68(9)
C(20B)	201(10)	28(2)	77(5)	–3(3)	43(5)	12(4)
C(22)	113(4)	115(4)	155(5)	24(4)	11(4)	9(3)
C(23)	69(2)	50(2)	47(2)	2(1)	5(2)	8(2)
C(24)	70(2)	50(2)	50(2)	2(1)	10(1)	5(1)
C(25)	74(2)	63(2)	56(2)	1(2)	11(2)	12(2)
C(26)	77(2)	88(3)	96(3)	–14(2)	11(2)	25(2)
C(27)	58(2)	73(2)	76(2)	–4(2)	–7(2)	–13(2)
C(28)	52(2)	71(2)	99(3)	17(2)	6(2)	17(2)
C(29)	39(1)	44(2)	59(2)	–1(1)	11(1)	2(1)
C(30)	45(2)	61(2)	97(3)	9(2)	19(2)	–1(1)
C(31)	76(2)	62(2)	100(3)	21(2)	34(2)	–6(2)
C(32)	81(2)	55(2)	77(2)	22(2)	22(2)	–1(2)
C(33)	63(2)	51(2)	54(2)	12(1)	11(1)	0(1)
C(34)	43(1)	39(1)	45(1)	–3(1)	5(1)	0(1)
C(35)	72(2)	60(2)	53(2)	7(2)	–13(2)	–23(2)
C(36)	38(2)	82(2)	78(2)	20(2)	8(1)	2(2)
Li(1)	68(3)	51(3)	47(3)	–1(2)	–1(2)	4(2)
Li(2)	93(4)	43(3)	52(3)	3(2)	–4(3)	–2(3)
Li(3)	97(4)	55(3)	55(3)	5(3)	15(3)	11(3)
Li(4)	49(2)	47(2)	44(2)	5(2)	0(2)	2(2)
N(1)	62(2)	48(1)	54(1)	5(1)	1(1)	11(1)
N(2)	67(2)	57(2)	49(1)	6(1)	–5(1)	–6(1)
N(3)	40(1)	46(1)	66(2)	–1(1)	–1(1)	1(1)
N(4)	40(1)	46(1)	48(1)	4(1)	2(1)	–6(1)

Tabelle 18 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung [(*n*-BuLi)$_2$·(*R*,*R*)-TMCDA]$_2$ (**85a**).

	x	y	z	U(eq)
H(1A)	1220	3409	4253	117
H(1B)	2709	3146	3653	117
H(1C)	2241	3744	3228	117
H(2A)	1456	4054	6095	131
H(2B)	2312	4418	5006	131
H(2C)	3099	4301	6548	131
H(3)	3868	2939	5772	61
H(4A)	1635	3369	7530	80
H(4B)	1283	2941	6298	80
H(5A)	1509	2516	8533	89
H(5B)	2799	2303	7550	89
H(6A)	3916	2495	9819	95
H(6B)	3280	3094	9713	95
H(7A)	5513	2653	7973	87
H(7B)	5863	3086	9193	87
H(8)	4373	3722	7918	63
H(9A)	6536	2882	5842	112
H(9B)	7690	3032	7163	112
H(9C)	7879	3303	5654	112
H(10A)	7838	4128	7091	127
H(10B)	7386	3803	8457	127
H(10C)	6314	4277	7847	127
H(12A)	8319	3481	2915	70
H(12B)	7625	3571	1333	70
H(13A)	7871	2566	2747	79
H(13B)	6976	2636	1233	79
H(14A)	10169	2813	1761	143
H(14B)	9268	2875	244	143
H(14C)	9432	2300	974	143
H(15B)	6630(30)	5149(13)	4640(30)	53(8)
H(15A)	6080(30)	4679(12)	5260(30)	54(8)
H(16A)	8186	4481	4002	167
H(16B)	7656	4870	2754	167
H(17A)	10013	5098	3808	265
H(17B)	8823	5580	3872	265
H(18A)	9902	4922	6008	237
H(18B)	8365	5259	6124	237
H(18C)	9949	5559	5931	237

H(19B)	5190(60)	4390(20)	440(50)	132(19)
H(20A)	2439	4755	479	200
H(20B)	3111	4243	1317	200
H(20C)	3122	4268	–372	200
H(20D)	2299	4574	2038	121
H(20E)	1943	5047	907	121
H(21A)	2476	4028	227	310
H(21B)	1865	4506	–791	310
H(22A)	421	3952	1150	191
H(22B)	–222	4194	–338	191
H(22C)	35	4575	1013	191
H(24A)	1934	5966	2103	68
H(24B)	2662	5901	3682	68
H(25A)	3110	6849	3733	77
H(25B)	2180	6889	2227	77
H(26A)	880	6533	4736	130
H(26B)	–43	6598	3230	130
H(26C)	618	7113	4060	130
H(27A)	7607	6090	1528	104
H(27B)	6904	6565	563	104
H(27C)	8607	6361	369	104
H(28A)	9041	5559	–850	111
H(28B)	7663	5150	–1183	111
H(28C)	8253	5270	422	111
H(29)	6626	5796	–2595	57
H(30A)	7836	6805	–1683	80
H(30B)	8815	6335	–2320	80
H(31A)	7454	6420	–4525	94
H(31B)	8183	6985	–4063	94
H(32A)	5802	7275	–3283	84
H(32B)	5562	7091	–4905	84
H(33A)	4638	6257	–4205	67
H(33B)	3631	6721	–3573	67
H(34)	5019	6646	–1355	51
H(35A)	2998	5667	–3453	93
H(35B)	2906	5247	–2190	93
H(35C)	4503	5357	–2865	93
H(36A)	1927	6345	–2131	99
H(36B)	2674	6516	–611	99
H(36C)	1782	5962	–796	99
H(23A)	5130(40)	6137(13)	2920(40)	68(10)
H(11A)	5620(40)	3215(15)	3470(40)	78(10)

H(19A)	4690(40)	4834(16)	–260(50)	89(12)
H(11B)	5160(30)	3381(12)	1980(30)	55(8)
H(23B)	4430(30)	6291(14)	1500(30)	62(9)

[(*n*-BuLi)$_2$·(*R*,*R*)-TMCDA]$_2$ (85b)

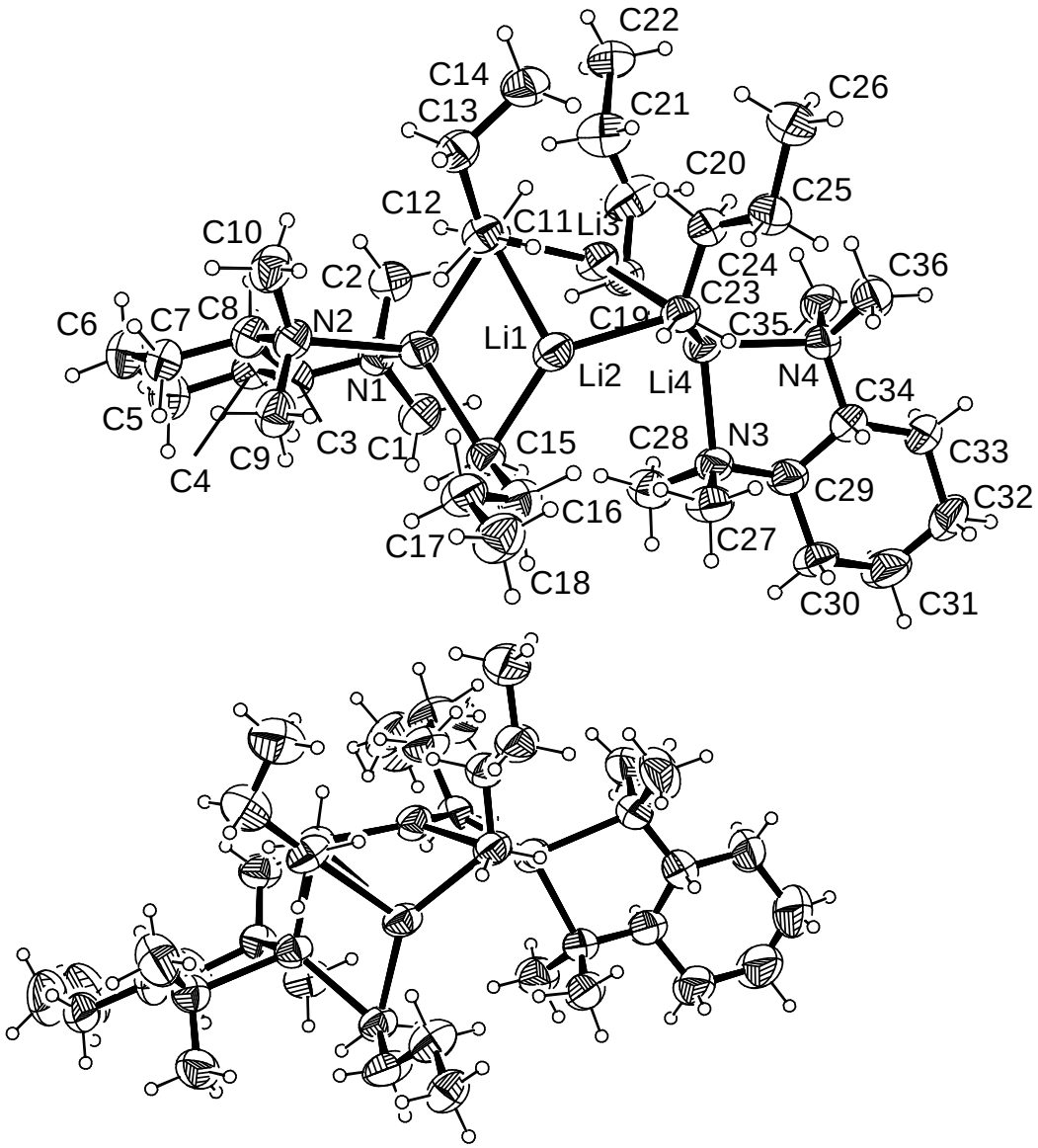


Abbildung 7 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von [(*n*-BuLi)$_2$·(*R*,*R*)-TMCDA]$_2$ und [(*n*-BuLi)$_2$·(*S*,*S*)-TMCDA]$_2$ (**85b**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 19 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für [(*n*-BuLi)$_2$·(*R*,*R*)-TMCDA]$_2$ und [(*n*-BuLi)$_2$·(*S*,*S*)-TMCDA]$_2$ (**85b**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	8761(3)	6529(3)	5367(2)	89(1)
C(2)	8706(3)	8204(3)	5197(2)	87(1)
C(3)	10406(2)	7906(3)	5500(1)	79(1)
C(4)	10449(2)	8514(2)	6094(1)	79(1)
C(5)	11567(3)	8919(3)	6413(2)	98(1)
C(6)	12273(3)	9595(3)	6116(2)	100(1)
C(7)	12243(2)	9036(2)	5528(1)	80(1)
C(8)	11134(2)	8577(2)	5199(1)	78(1)
C(9)	11740(2)	7336(3)	4536(2)	92(1)
C(10)	11349(3)	8838(3)	4280(2)	98(1)
C(11)	8487(3)	7480(2)	3704(2)	70(1)
C(12)	9116(3)	7402(2)	3224(2)	72(1)
C(13)	9379(3)	8354(2)	2953(1)	81(1)
C(14)	8439(3)	8457(3)	2596(2)	94(1)
C(15)	9259(3)	5233(2)	4081(2)	75(1)
C(16)	9448(3)	4428(3)	3616(2)	90(1)
C(17)	10451(3)	4825(3)	3415(2)	93(1)
C(18)	10649(3)	4026(3)	2930(2)	114(1)
C(19)	5883(3)	6261(3)	4332(2)	80(1)
C(20)	5288(4)	7118(3)	4361(2)	131(2)
C(21)	5665(4)	7967(4)	4142(2)	147(2)
C(22)	5042(3)	8808(3)	4223(2)	115(1)
C(23)	6702(3)	5099(3)	3033(1)	73(1)
C(24)	6267(3)	5739(3)	2670(2)	78(1)
C(25)	5997(3)	5267(3)	2050(2)	89(1)
C(26)	5620(4)	5975(3)	1717(2)	121(1)
C(27)	6505(3)	2951(3)	3645(2)	92(1)
C(28)	6332(3)	3742(3)	4569(2)	98(1)
C(29)	4758(3)	2678(2)	3935(2)	91(1)
C(30)	4706(2)	1538(2)	3959(2)	87(1)
C(31)	3603(3)	856(3)	3942(2)	124(2)
C(32)	2895(3)	867(3)	3456(2)	112(1)
C(33)	2923(2)	1985(2)	3405(2)	83(1)
C(34)	4037(3)	2720(2)	3464(2)	86(1)
C(35)	3467(3)	4317(3)	3764(2)	91(1)
C(36)	3772(3)	3817(3)	2838(2)	97(1)
C(37)	9028(4)	1627(3)	10426(2)	111(1)

C(38)	9304(3)	3408(3)	10338(2)	103(1)
C(39)	10801(4)	2771(4)	10626(2)	132(2)
C(40)	10919(3)	3374(3)	11215(2)	105(1)
C(41)	11976(5)	3604(6)	11550(2)	184(3)
C(42)	12830(5)	3884(5)	11289(2)	162(2)
C(43)	12751(3)	3311(3)	10703(2)	105(1)
C(44)	11679(3)	3013(4)	10353(2)	116(1)
C(45)	12168(4)	3113(4)	9447(2)	151(2)
C(46)	11886(3)	1476(3)	9730(2)	121(1)
C(47)	9401(3)	3073(3)	8922(2)	81(1)
C(48)	10006(4)	2940(3)	8429(2)	97(1)
C(49)	10838(4)	4010(4)	8343(2)	128(2)
C(50)	10259(5)	4489(4)	8032(2)	156(2)
C(51)	9269(4)	326(3)	9011(2)	86(1)
C(52)	9752(4)	-302(3)	8552(2)	129(2)
C(53)	9347(4)	-403(3)	7999(2)	115(1)
C(54)	9742(3)	-1118(3)	7581(2)	103(1)
C(55)	6462(4)	2227(3)	9359(2)	92(1)
C(56)	6480(6)	3379(4)	9462(3)	121(2)
C(57A)	6436(18)	3946(13)	10170(20)	185(14)
C(58A)	5226(12)	3508(12)	10079(12)	149(5)
C(57B)	5800(30)	3749(14)	9880(7)	125(5)
C(58B)	6070(30)	3767(19)	10398(12)	195(13)
C(59)	7278(4)	1338(3)	8036(2)	90(1)
C(60)	7149(4)	2328(3)	7852(2)	95(1)
C(61)	7071(4)	2301(3)	7229(2)	122(1)
C(62)	6951(4)	3297(4)	7087(2)	143(2)
C(63)	6009(4)	–591(3)	9298(2)	119(1)
C(64)	6170(3)	–1232(3)	8367(2)	110(1)
C(65)	4472(3)	–1063(3)	8592(2)	120(2)
C(66)	4039(3)	–2239(3)	8529(2)	134(2)
C(67)	2865(4)	–2646(4)	8417(4)	188(3)
C(68)	2398(4)	–2278(5)	7985(3)	188(3)
C(69)	2812(3)	–1081(4)	8036(2)	132(2)
C(70)	3995(3)	–665(3)	8160(2)	111(1)
C(71)	3926(4)	1121(4)	8555(2)	154(2)
C(72)	4361(4)	688(5)	7633(2)	166(2)
Li(1)	9906(5)	2019(4)	9454(2)	83(2)
Li(2)	8676(5)	1328(4)	8582(2)	87(2)
Li(3)	7680(5)	2431(4)	8874(2)	90(2)
Li(4)	6068(5)	923(4)	8616(2)	90(2)
Li(5)	9476(4)	6958(4)	4351(2)	72(1)

Li(6)	8265(4)	5741(4)	3553(2)	81(1)
Li(7)	6911(4)	6468(4)	3740(2)	82(2)
Li(8)	5691(4)	4761(4)	3718(2)	74(1)
N(1)	9762(2)	2523(2)	10285(1)	86(1)
N(2)	11562(2)	2452(2)	9776(1)	91(1)
N(3)	5628(2)	–636(2)	8722(2)	92(1)
N(4)	4450(2)	478(2)	8182(2)	107(1)
N(5)	9327(2)	7452(2)	5177(1)	73(1)
N(6)	11065(2)	8042(2)	4609(1)	73(1)
N(7)	5827(2)	3404(2)	3986(1)	75(1)
N(8)	4097(2)	3815(2)	3412(1)	73(1)

Tabelle 20 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für [(*n*-BuLi)$_2$·(*R*,*R*)-TMCDA]$_2$ und [(*n*-BuLi)$_2$·(*S*,*S*)-TMCDA]$_2$ (**85b**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	92(2)	85(2)	90(3)	25(2)	29(2)	18(2)
C(2)	92(2)	86(2)	87(3)	20(2)	21(2)	30(2)
C(3)	80(2)	82(2)	77(2)	17(2)	19(2)	24(2)
C(4)	88(2)	78(2)	73(2)	13(2)	21(2)	26(2)
C(5)	98(3)	106(3)	78(3)	8(2)	13(2)	20(2)
C(6)	94(2)	99(3)	85(3)	5(2)	4(2)	10(2)
C(7)	79(2)	74(2)	77(2)	10(2)	11(2)	12(2)
C(8)	78(2)	75(2)	76(2)	13(2)	18(2)	16(2)
C(9)	76(2)	90(2)	102(3)	3(2)	20(2)	19(2)
C(10)	98(2)	92(2)	93(3)	33(2)	15(2)	0(2)
C(11)	75(2)	63(2)	74(2)	19(2)	17(2)	19(2)
C(12)	77(2)	62(2)	77(2)	14(2)	15(2)	21(2)
C(13)	91(2)	74(2)	80(2)	24(2)	25(2)	17(2)
C(14)	111(3)	85(2)	96(3)	41(2)	21(2)	29(2)
C(15)	69(2)	66(2)	88(3)	19(2)	16(2)	18(2)
C(16)	95(3)	73(2)	103(3)	20(2)	16(2)	29(2)
C(17)	97(2)	73(2)	111(3)	20(2)	25(2)	25(2)
C(18)	118(3)	89(2)	133(4)	6(2)	37(3)	35(2)
C(19)	77(2)	64(2)	100(3)	20(2)	16(2)	21(2)
C(20)	179(4)	81(3)	136(4)	24(3)	47(3)	33(3)
C(21)	166(4)	120(4)	164(5)	52(3)	13(4)	50(3)
C(22)	122(3)	84(2)	146(4)	27(2)	7(3)	49(2)

C(23)	72(2)	65(2)	83(2)	22(2)	15(2)	20(2)
C(24)	77(2)	68(2)	88(3)	24(2)	8(2)	17(2)
C(25)	92(2)	88(2)	86(3)	30(2)	7(2)	24(2)
C(26)	141(4)	111(3)	110(3)	45(3)	-14(3)	32(3)
C(27)	91(2)	81(2)	121(3)	44(2)	35(2)	35(2)
C(28)	99(3)	103(3)	104(3)	43(2)	16(2)	38(2)
C(29)	74(2)	76(2)	132(3)	41(2)	16(2)	21(2)
C(30)	84(2)	66(2)	126(3)	39(2)	36(2)	26(2)
C(31)	107(3)	79(2)	195(5)	58(3)	37(3)	21(2)
C(32)	110(3)	69(2)	131(4)	20(2)	3(3)	-11(2)
C(33)	79(2)	66(2)	95(3)	19(2)	11(2)	8(2)
C(34)	82(2)	67(2)	102(3)	25(2)	-1(2)	10(2)
C(35)	78(2)	79(2)	115(3)	24(2)	16(2)	19(2)
C(36)	82(2)	104(3)	103(3)	39(2)	4(2)	16(2)
C(37)	152(4)	106(3)	91(3)	31(2)	42(3)	52(3)
C(38)	138(3)	96(3)	82(3)	14(2)	10(2)	51(2)
C(39)	110(3)	212(5)	68(3)	9(3)	0(3)	56(3)
C(40)	127(3)	113(3)	72(3)	3(2)	-3(2)	51(2)
C(41)	151(5)	289(8)	85(4)	-8(4)	-17(4)	70(5)
C(42)	146(5)	181(5)	113(5)	-14(4)	-29(4)	23(4)
C(43)	105(3)	99(3)	100(3)	21(2)	-10(2)	19(2)
C(44)	106(3)	128(3)	91(3)	-4(3)	0(3)	20(2)
C(45)	107(3)	197(5)	156(5)	100(4)	15(3)	17(3)
C(46)	127(3)	120(3)	115(4)	5(3)	-3(3)	58(3)
C(47)	106(3)	68(2)	72(3)	14(2)	10(2)	30(2)
C(48)	136(3)	69(2)	86(3)	22(2)	30(3)	23(2)
C(49)	144(4)	160(4)	97(3)	46(3)	29(3)	58(3)
C(50)	186(5)	169(5)	138(5)	40(4)	32(4)	91(4)
C(51)	108(3)	72(2)	77(3)	12(2)	13(2)	29(2)
C(52)	218(5)	73(2)	91(3)	13(2)	-11(3)	54(3)
C(53)	149(4)	92(3)	105(4)	22(2)	40(3)	31(2)
C(54)	119(3)	83(2)	99(3)	0(2)	35(2)	26(2)
C(55)	97(3)	80(2)	95(3)	16(2)	3(3)	28(2)
C(56)	160(5)	95(3)	119(4)	22(3)	29(4)	58(3)
C(57A)	119(12)	81(8)	330(40)	-11(15)	60(20)	26(8)
C(58A)	142(12)	165(12)	150(14)	29(11)	51(11)	57(10)
C(57B)	182(18)	85(8)	118(12)	11(7)	50(11)	57(11)
C(58B)	220(30)	203(18)	172(19)	72(14)	87(18)	36(18)
C(59)	117(3)	67(2)	81(3)	12(2)	2(2)	25(2)
C(60)	116(3)	81(3)	87(3)	19(2)	-6(3)	32(2)
C(61)	165(4)	96(3)	96(3)	29(2)	-21(3)	36(3)
C(62)	172(4)	123(3)	131(4)	55(3)	-14(3)	33(3)

C(63)	129(3)	109(3)	130(4)	48(3)	21(3)	40(3)
C(64)	101(3)	84(2)	145(4)	23(2)	23(3)	25(2)
C(65)	95(3)	81(3)	183(5)	35(3)	9(3)	27(2)
C(66)	91(3)	94(3)	217(5)	46(3)	30(3)	18(2)
C(67)	97(4)	110(4)	347(11)	49(5)	37(5)	20(3)
C(68)	99(4)	149(5)	274(9)	26(5)	-12(4)	-2(3)
C(69)	96(3)	120(3)	161(5)	1(3)	-13(3)	35(3)
C(70)	86(3)	109(3)	133(4)	28(3)	-3(2)	27(2)
C(71)	141(4)	127(4)	184(5)	-10(3)	-21(4)	76(3)
C(72)	142(4)	194(5)	143(5)	83(4)	-44(4)	8(4)
Li(1)	102(4)	75(3)	74(4)	15(3)	17(3)	30(3)
Li(2)	122(4)	67(3)	73(4)	11(3)	10(3)	32(3)
Li(3)	111(4)	73(3)	81(4)	5(3)	4(3)	28(3)
Li(4)	109(4)	66(3)	89(4)	12(3)	0(3)	24(3)
Li(5)	74(3)	69(3)	74(3)	17(2)	16(3)	23(2)
Li(6)	88(3)	63(3)	89(4)	14(3)	14(3)	21(2)
Li(7)	84(3)	65(3)	99(4)	22(3)	25(3)	20(2)
Li(8)	69(3)	67(3)	89(4)	27(3)	17(3)	16(2)
N(1)	100(2)	94(2)	66(2)	13(2)	11(2)	39(2)
N(2)	98(2)	95(2)	82(2)	23(2)	14(2)	30(2)
N(3)	85(2)	76(2)	116(3)	27(2)	6(2)	24(2)
N(4)	113(2)	90(2)	112(3)	15(2)	-16(2)	35(2)
N(5)	66(2)	72(2)	79(2)	16(1)	15(1)	17(1)
N(6)	74(2)	68(2)	74(2)	16(1)	20(1)	13(1)
N(7)	62(1)	68(2)	101(2)	34(1)	17(2)	18(1)
N(8)	69(2)	67(2)	85(2)	27(1)	7(1)	18(1)

Tabelle 21 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für [(*n*-BuLi)$_2$·(*R*,*R*)-TMCDA]$_2$ und [(*n*-BuLi)$_2$·(*S*,*S*)-TMCDA]$_2$ (**85b**).

	x	y	z	U(eq)
H(1A)	9164	6015	5344	133
H(1B)	8076	6199	5132	133
H(1C)	8666	6754	5751	133
H(2A)	8037	7867	4948	131
H(2B)	9090	8833	5081	131
H(2C)	8576	8413	5576	131
H(3)	10678	7291	5530	95
H(4A)	10169	9122	6083	95

H(4B)	10001	8041	6289	95
H(5A)	11572	9336	6787	118
H(5B)	11826	8309	6456	118
H(6A)	12999	9806	6316	119
H(6B)	12064	10248	6117	119
H(7A)	12566	8454	5529	96
H(7B)	12666	9542	5340	96
H(8)	10869	9202	5188	93
H(9A)	12476	7760	4633	139
H(9B)	11602	6941	4149	139
H(9C)	11589	6837	4776	139
H(10A)	12062	9298	4428	147
H(10B)	10861	9266	4299	147
H(10C)	11315	8481	3894	147
H(11A)	7830(20)	7740(20)	3584(11)	77(8)
H(11B)	8860(30)	8040(30)	4019(15)	102(12)
H(12A)	9810(20)	7240(20)	3354(11)	71(8)
H(12B)	8756(19)	6820(20)	2916(11)	57(7)
H(13A)	9675	9012	3247	98
H(13B)	9924	8284	2720	98
H(14A)	8171	7829	2289	142
H(14B)	8651	9092	2449	142
H(14C)	7891	8514	2821	142
H(15A)	8640(20)	4850(20)	4232(12)	87(9)
H(15B)	9890(30)	5420(20)	4397(14)	98(11)
H(16A)	9580(30)	3710(40)	3684(17)	146(15)
H(16B)	8950(30)	4230(30)	3208(18)	132(15)
H(17A)	11034	5004	3727	112
H(17B)	10455	5486	3294	112
H(18A)	10620	3359	3039	171
H(18B)	11340	4322	2835	171
H(18C)	10110	3893	2607	171
H(19A)	5390(30)	5670(30)	4480(13)	105(11)
H(19B)	6480(30)	6530(20)	4636(14)	92(11)
H(20A)	4558	6758	4174	158
H(20B)	5259	7391	4756	158
H(21A)	5651	7711	3741	176
H(21B)	6405	8319	4314	176
H(22A)	4321	8483	4030	172
H(22B)	5379	9410	4072	172
H(22C)	5038	9057	4619	172
H(23A)	6190(20)	4440(30)	2944(12)	85(10)

H(23B)	7280(20)	4946(19)	2856(11)	64(8)
H(24A)	5640(20)	5900(20)	2788(12)	77(9)
H(24B)	6740(20)	6480(20)	2714(11)	75(8)
H(25A)	5445	4581	1982	106
H(25B)	6624	5123	1915	106
H(26A)	5000	6127	1849	182
H(26B)	5440	5612	1324	182
H(26C)	6176	6642	1765	182
H(27A)	7175	3491	3675	137
H(27B)	6162	2716	3257	137
H(27C)	6629	2345	3775	137
H(28A)	6446	3129	4696	147
H(28B)	5880	4043	4795	147
H(28C)	7005	4279	4605	147
H(29)	4482	2963	4271	110
H(30A)	4998	1220	3643	104
H(30B)	5146	1546	4304	104
H(31A)	3609	118	3933	148
H(31B)	3341	1119	4282	148
H(32A)	2171	473	3480	135
H(32B)	3091	496	3118	135
H(33A)	2566	2293	3694	100
H(33B)	2530	1947	3040	100
H(34)	4309	2413	3132	104
H(35A)	3608	5063	3747	137
H(35B)	3652	4275	4148	137
H(35C)	2723	3948	3634	137
H(36A)	4199	3495	2603	146
H(36B)	3866	4548	2802	146
H(36C)	3034	3409	2721	146
H(37A)	8935	1826	10812	167
H(37B)	9308	1017	10375	167
H(37C)	8352	1438	10184	167
H(38A)	9138	3578	10712	155
H(38B)	8663	3207	10066	155
H(38C)	9806	4030	10271	155
H(39)	10797	2053	10682	159
H(40A)	10767	4054	11213	126
H(40B)	10391	2962	11400	126
H(41A)	12049	4184	11877	220
H(41B)	12002	2967	11688	220
H(42A)	13438	3785	11509	195

H(42B)	12987	4650	11299	195
H(43A)	12955	2656	10704	127
H(43B)	13262	3762	10526	127
H(44)	11667	3728	10298	140
H(45A)	12002	3790	9495	227
H(45B)	11987	2745	9055	227
H(45C)	12917	3246	9571	227
H(46A)	12645	1664	9847	182
H(46B)	11703	1068	9345	182
H(46C)	11527	1047	9968	182
H(47A)	9920(30)	3480(30)	9256(17)	119(14)
H(47B)	9030(20)	3630(30)	8897(13)	100(11)
H(48A)	10430(30)	2400(30)	8456(15)	119(13)
H(48B)	9410(20)	2610(20)	8100(13)	76(10)
H(49A)	11177	4496	8705	153
H(49B)	11388	3823	8143	153
H(50A)	9956	4011	7668	233
H(50B)	10719	5155	7984	233
H(50C)	9696	4636	8226	233
H(51A)	8570(30)	-110(30)	9034(14)	105(12)
H(51B)	9720(20)	360(20)	9372(15)	93(11)
H(52A)	10514	53	8609	154
H(52B)	9660	-1024	8615	154
H(53A)	9520	311	7919	138
H(53B)	8575	-679	7949	138
H(54A)	10502	-830	7611	155
H(54B)	9404	-1160	7207	155
H(54C)	9577	-1829	7655	155
H(55A)	5790(30)	1810(30)	9413(13)	99(12)
H(55B)	6870(30)	2120(20)	9670(15)	89(11)
H(56A)	7230(40)	3860(40)	9490(20)	180(20)
H(56B)	6060(40)	3460(40)	9150(20)	160(20)
H(57A)	6789	3645	10441	222
H(57B)	6693	4731	10271	222
H(58A)	4929	3702	9753	223
H(58B)	4961	3811	10405	223
H(58C)	5022	2734	10021	223
H(57C)	5796	4474	9855	149
H(57D)	5076	3282	9758	149
H(58D)	5962	3039	10444	293
H(58E)	5646	4109	10623	293
H(58F)	6813	4165	10519	293

H(59A)	6670(20)	790(30)	7883(13)	85(10)
H(59B)	7800(20)	1100(20)	7819(13)	91(11)
H(60A)	7780(30)	2940(30)	8043(14)	92(10)
H(60B)	6560(20)	2460(20)	7974(12)	76(10)
H(61A)	7710	2170	7101	146
H(61B)	6465	1700	7025	146
H(62A)	6295	3408	7189	215
H(62B)	6936	3238	6689	215
H(62C)	7541	3899	7292	215
H(63A)	5806	–1307	9366	179
H(63B)	5703	–133	9543	179
H(63C)	6773	–304	9373	179
H(64A)	6921	–856	8440	166
H(64B)	5893	–1302	7978	166
H(64C)	6061	–1938	8442	166
H(65)	4230	–751	8934	144
H(66A)	4296	–2423	8872	161
H(66B)	4317	–2606	8221	161
H(67A)	2654	–3431	8316	225
H(67B)	2592	–2426	8760	225
H(68A)	1633	–2468	7981	226
H(68B)	2520	–2651	7625	226
H(69A)	2564	–916	7685	158
H(69B)	2518	–709	8334	158
H(70)	4211	–1017	7818	133
H(71A)	4301	1876	8615	230
H(71B)	3936	916	8912	230
H(71C)	3200	990	8383	230
H(72A)	3623	454	7462	250
H(72B)	4753	302	7405	250
H(72C)	4648	1450	7661	250

8.2.2 Kristallstrukturen aus Kapitel 4.2

[(*t*-BuLi)$_3$·C$_6$H$_{15}$N$_3$] (95)

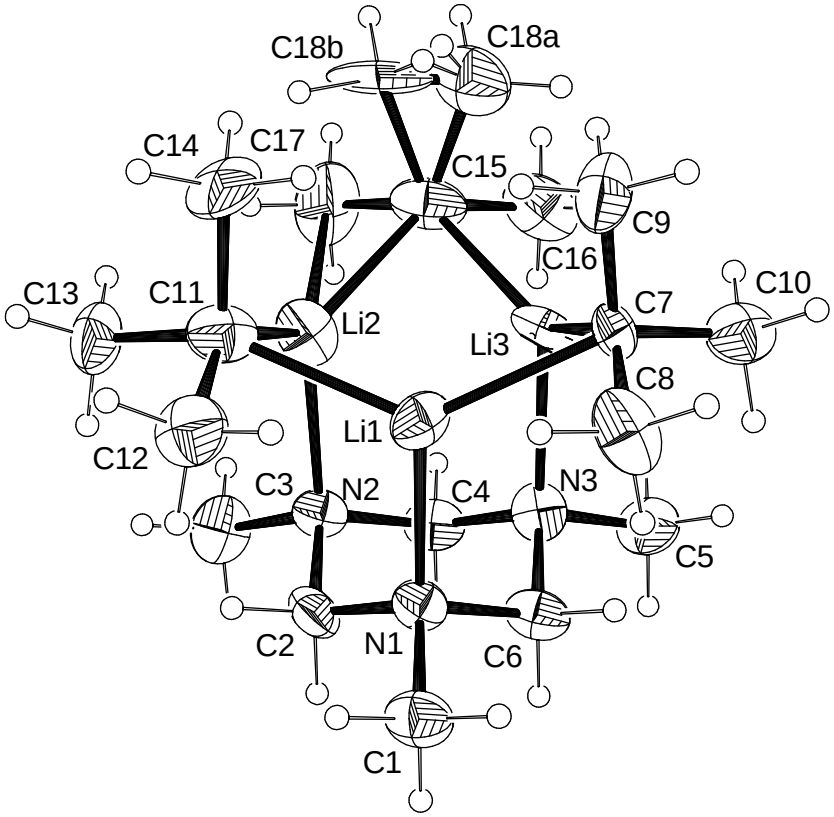


Abbildung 8 Thermische Auslenkungsellipsoide (30% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von [(*t*-BuLi)$_3$·C$_6$H$_{15}$N$_3$] (**95**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 22 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für [(*t*-BuLi)$_3$·C$_6$H$_{15}$N$_3$] (**95**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	–21(4)	4540(7)	3427(3)	68(1)
C(2)	2346(9)	5365(4)	5288(8)	58(2)
C(3)	4740(9)	6187(5)	7000(11)	77(2)
C(4)	4698(3)	4545(7)	7038(4)	60(1)
C(5)	4712(10)	2915(5)	7020(11)	74(2)
C(6)	2325(8)	3741(5)	5251(8)	58(2)
C(7)	240(7)	3184(3)	7631(8)	47(1)
C(8)	–1225(9)	3114(6)	6056(11)	86(3)
C(9)	–392(10)	3255(5)	8822(11)	85(3)
C(10)	1153(10)	2302(5)	7940(10)	76(2)
C(11)	296(9)	5885(5)	7644(9)	72(2)

C(12)	–1258(10)	6003(5)	6064(11)	84(3)
C(13)	1190(10)	6830(4)	7937(11)	77(2)
C(14)	–401(12)	5819(6)	8901(11)	98(3)
C(15)	4294(4)	4559(9)	10646(4)	78(1)
C(16)	5458(10)	3724(7)	11070(10)	99(3)
C(17)	5394(12)	5370(7)	11099(10)	128(4)
C(18A)	3570(20)	4211(15)	11740(20)	105(6)
C(18B)	3459(19)	4890(20)	11735(14)	104(8)
Li(1)	276(6)	4524(9)	6704(6)	57(1)
Li(2)	2800(14)	5417(9)	8597(15)	73(3)
Li(3)	2828(13)	3688(8)	8651(12)	59(3)
N(1)	1322(3)	4566(5)	5055(3)	51(1)
N(2)	3713(6)	5375(3)	6854(6)	51(1)
N(3)	3715(7)	3736(4)	6862(7)	62(1)

Tabelle 23 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für [(*t*-BuLi)$_3$·$C_6H_{15}N_3$] (**95**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	57(2)	86(2)	52(2)	8(5)	17(2)	10(5)
C(2)	71(4)	52(3)	61(4)	20(3)	40(3)	8(3)
C(3)	51(4)	78(5)	93(6)	–14(4)	22(4)	–18(4)
C(4)	42(2)	83(2)	56(2)	3(5)	22(2)	4(5)
C(5)	69(5)	86(5)	78(5)	1(4)	42(5)	22(4)
C(6)	38(3)	84(4)	48(4)	13(3)	16(3)	10(3)
C(7)	50(3)	36(2)	59(4)	5(3)	28(3)	–13(2)
C(8)	54(4)	79(5)	106(7)	22(5)	18(5)	–11(4)
C(9)	92(5)	55(4)	117(7)	–15(4)	54(5)	–8(4)
C(10)	69(5)	93(5)	76(5)	–7(4)	40(4)	–17(4)
C(11)	68(5)	88(4)	64(5)	–7(4)	33(4)	–25(4)
C(12)	73(5)	93(6)	82(6)	1(5)	32(5)	20(4)
C(13)	90(6)	45(3)	102(6)	–13(4)	48(5)	–14(3)
C(14)	134(8)	98(6)	121(8)	–22(5)	109(7)	–2(5)
C(15)	48(2)	127(3)	48(2)	16(6)	13(2)	13(6)
C(16)	71(5)	125(7)	70(6)	15(5)	3(4)	–27(5)
C(17)	131(8)	92(6)	74(6)	–23(5)	–32(5)	–13(6)
C(18A)	92(13)	124(14)	94(13)	33(10)	38(11)	35(11)
C(18B)	52(8)	240(20)	13(5)	15(9)	7(5)	21(12)
Li(1)	49(3)	62(3)	58(3)	–19(7)	22(3)	–20(6)
Li(2)	52(6)	75(7)	75(8)	7(6)	15(6)	–12(6)

Li(3)	55(6)	84(7)	44(6)	26(6)	27(5)	9(6)
N(1)	42(1)	58(2)	45(1)	3(3)	14(1)	–3(3)
N(2)	37(3)	64(3)	43(3)	–1(3)	11(2)	–9(2)
N(3)	48(3)	65(3)	72(4)	2(3)	27(3)	1(3)

Tabelle 24 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für [(*t*-BuLi)$_3$·$C_6H_{15}N_3$] (**95**).

	x	y	z	U(eq)
H(1A)	–731	5076	3248	102
H(1B)	–668	3980	3279	102
H(1C)	446	4547	2675	102
H(2A)	1678	5925	5134	69
H(2B)	2771	5368	4492	69
H(3A)	5676	6197	8052	116
H(3B)	4084	6744	6846	116
H(3C)	5141	6159	6199	116
H(4A)	5111	4541	6233	72
H(4B)	5656	4544	8093	72
H(5A)	5070	2913	6187	112
H(5B)	4054	2365	6925	112
H(5C)	5676	2918	8053	112
H(6A)	2750	3738	4455	69
H(6B)	1644	3186	5093	69
H(8A)	–861	3009	5240	130
H(8B)	–1857	3684	5830	130
H(8C)	–1917	2601	6065	130
H(9A)	–1049	2711	8761	128
H(9B)	–1078	3804	8614	128
H(9C)	533	3297	9878	128
H(10A)	430	1799	7915	115
H(10B)	2107	2326	8980	115
H(10C)	1524	2202	7128	115
H(12A)	–1912	5440	5817	126
H(12B)	–938	6130	5225	126
H(12C)	–1911	6515	6147	126
H(13A)	1556	6936	7123	116
H(13B)	2144	6829	8978	116
H(13C)	433	7319	7894	116

H(14A)	–1123	6343	8775	147
H(14B)	513	5824	9967	147
H(14C)	–1025	5248	8739	147
H(16A)	6188	3725	12206	149
H(16B)	6117	3760	10489	149
H(16C)	4809	3159	10784	149
H(17A)	6103	5360	12239	192
H(17B)	4731	5931	10818	192
H(17C)	6074	5355	10539	192
H(18A)	3327	3556	11557	157
H(18B)	2559	4547	11518	157
H(18C)	4370	4309	12843	157
H(18D)	2704	4411	11747	156
H(18E)	2849	5456	11311	156
H(18F)	4314	4992	12812	156

$(PhLi{\cdot}C_6H_{15}N_3)_2$ (96)

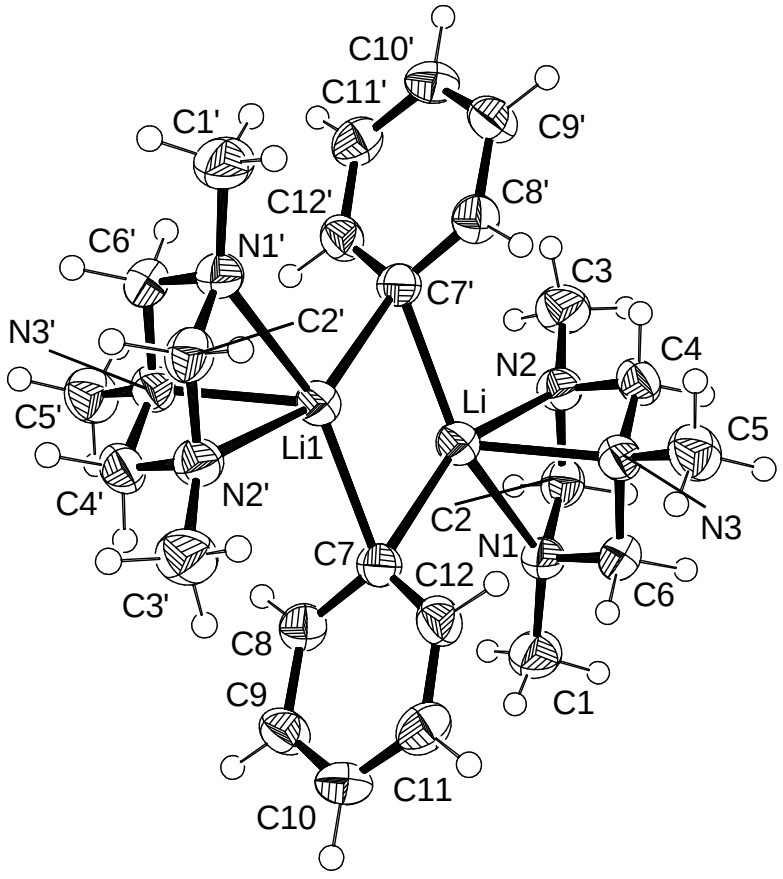


Abbildung 9 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von $(PhLi{\cdot}C_6H_{15}N_3)_2$ (**96**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 25 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für $(PhLi{\cdot}C_6H_{15}N_3)_2$ (**96**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	–1246(3)	4881(1)	2279(2)	56(1)
C(2)	–106(2)	5928(1)	3755(2)	41(1)
C(3)	1430(3)	6848(1)	5525(2)	54(1)
C(4)	2246(2)	6604(1)	3320(2)	41(1)
C(5)	3497(3)	6250(1)	1393(2)	52(1)
C(6)	1009(2)	5609(1)	1770(2)	39(1)
C(7)	4125(2)	4246(1)	3681(2)	37(1)
C(8)	3392(2)	3634(1)	4108(2)	38(1)
C(9)	2880(2)	3030(1)	3233(2)	44(1)
C(10)	3082(2)	3006(1)	1844(2)	45(1)
C(11)	3778(2)	3586(1)	1338(2)	45(1)
C(12)	4269(2)	4182(1)	2242(2)	41(1)
Li	3588(4)	5321(1)	4388(3)	39(1)
N(1)	320(2)	5342(1)	2927(2)	38(1)
N(2)	1581(2)	6307(1)	4464(2)	39(1)
N(3)	2664(2)	6013(1)	2492(2)	37(1)

Tabelle 26 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für $(PhLi{\cdot}C_6H_{15}N_3)_2$ (**96**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	54(1)	62(1)	49(1)	1(1)	11(1)	–20(1)
C(2)	34(1)	45(1)	42(1)	5(1)	10(1)	5(1)
C(3)	59(1)	47(1)	56(1)	–11(1)	18(1)	6(1)
C(4)	40(1)	31(1)	50(1)	4(1)	12(1)	2(1)
C(5)	57(1)	51(1)	53(1)	4(1)	25(1)	–6(1)
C(6)	40(1)	41(1)	33(1)	2(1)	7(1)	2(1)
C(7)	32(1)	31(1)	41(1)	–2(1)	4(1)	5(1)
C(8)	43(1)	40(1)	35(1)	–2(1)	17(1)	3(1)
C(9)	53(1)	34(1)	47(1)	–2(1)	21(1)	–9(1)
C(10)	51(1)	40(1)	45(1)	–13(1)	14(1)	–7(1)
C(11)	48(1)	58(1)	33(1)	–4(1)	17(1)	–2(1)
C(12)	38(1)	37(1)	46(1)	7(1)	11(1)	–4(1)
Li	40(2)	33(1)	40(2)	–1(1)	8(1)	1(1)
N(1)	37(1)	38(1)	36(1)	0(1)	9(1)	–4(1)
N(2)	37(1)	37(1)	41(1)	–3(1)	11(1)	3(1)

N(3)	37(1)	35(1)	39(1)	2(1)	13(1)	–1(1)

Tabelle 27 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für $(PhLi{\cdot}C_6H_{15}N_3)_2$ (**96**).

	x	y	z	U(eq)
H(1A)	–1721	4725	3072	85
H(1B)	–874	4466	1822	85
H(1C)	–2198	5141	1507	85
H(2A)	–1019	6245	3062	49
H(2B)	–609	5749	4526	49
H(3A)	2645	7035	6078	81
H(3B)	895	6638	6238	81
H(3C)	648	7234	4975	81
H(4A)	3354	6892	3794	49
H(4B)	1304	6913	2630	49
H(5A)	2621	6539	621	78
H(5B)	3847	5836	918	78
H(5C)	4584	6534	1902	78
H(6A)	83	5916	1062	47
H(6B)	1276	5208	1194	47
H(8)	3236	3633	5069	46
H(9)	2389	2634	3596	52
H(10)	2746	2592	1237	55
H(11)	3920	3579	372	54
H(12)	4739	4577	1858	49

[(*n*-BuLi)$_4$·C$_6$H$_{15}$N$_3$]$_\infty$ (98)

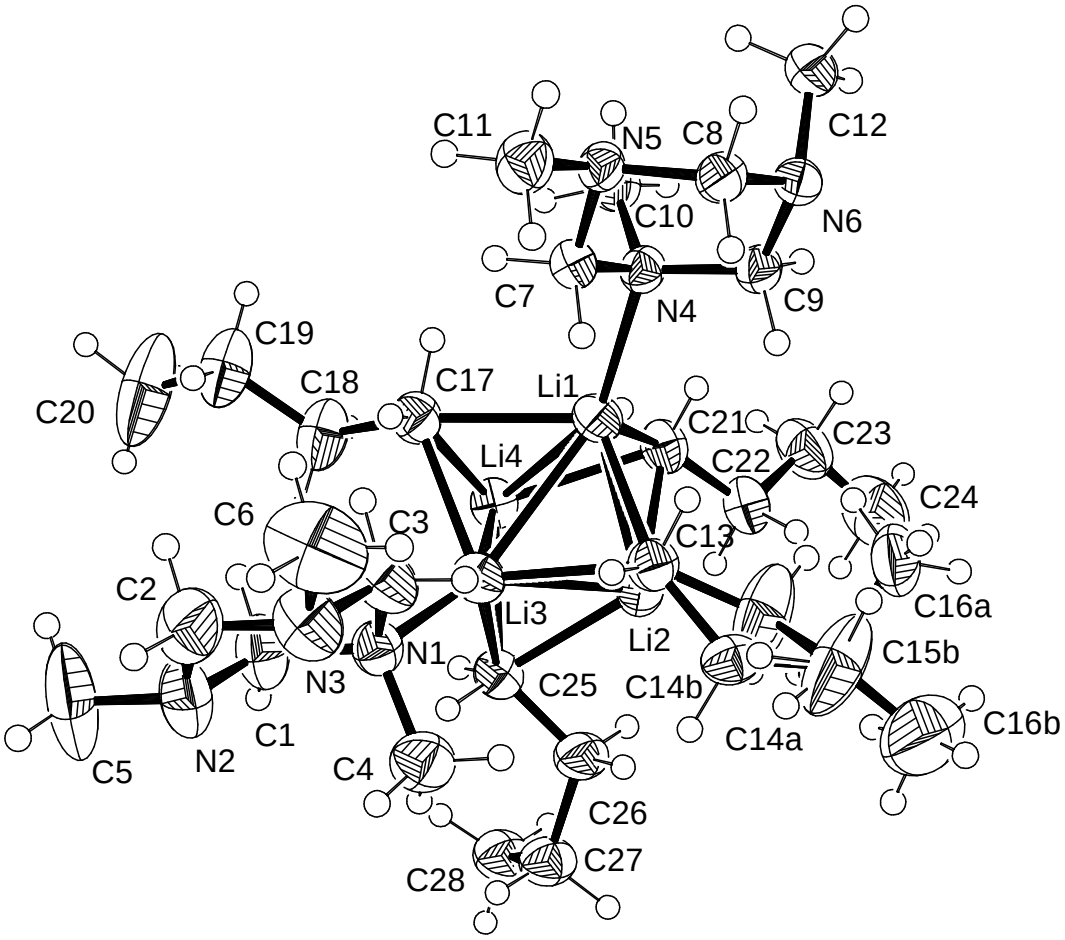


Abbildung 10 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von [(*n*-BuLi)$_4$·(C$_6$H$_{15}$N$_3$)$_2$]$_\infty$ (**98**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 28 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für [(*n*-BuLi)$_4$·(C$_6$H$_{15}$N$_3$)$_2$]$_\infty$ (**98**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(28A)	293(3)	6978(10)	–1860(6)	130(4)
C(27A)	497(3)	6012(7)	–1483(4)	98(3)
Li(4)	1577(1)	4685(4)	848(3)	39(1)
Li(2)	1034(1)	3993(4)	1164(3)	41(1)
Li(1)	1578(1)	5174(4)	2323(3)	41(1)
Li(3)	1134(1)	6040(4)	987(3)	43(1)
C(16)	1794(1)	9769(3)	1407(3)	95(1)
C(17)	1639(1)	3383(3)	1892(2)	43(1)
C(21)	946(1)	5441(2)	1946(2)	39(1)
C(20)	1998(2)	1930(3)	4169(2)	120(2)
C(19)	1923(1)	2047(3)	3245(2)	72(1)

C(18)	1716(1)	3137(3)	2820(2)	58(1)
C(15)	1936(1)	8561(3)	1514(2)	65(1)
C(14)	1623(1)	7669(2)	1324(2)	49(1)
C(6)	2282(1)	5991(2)	5764(2)	44(1)
C(13)	1745(1)	6412(2)	1470(2)	42(1)
C(10)	487(2)	306(4)	2143(3)	124(2)
C(12)	517(1)	94(3)	–610(3)	101(2)
C(8)	256(1)	3105(3)	432(2)	58(1)
C(11)	507(1)	200(3)	771(2)	73(1)
C(9)	688(1)	1913(3)	1578(2)	60(1)
C(7)	695(1)	1824(3)	217(2)	55(1)
N(5)	434(1)	923(2)	1359(2)	68(1)
C(4)	1738(1)	8897(2)	4153(2)	49(1)
N(6)	445(1)	827(2)	–2(2)	61(1)
C(2)	2318(1)	5834(2)	3928(2)	43(1)
C(1)	1797(1)	5375(2)	4342(2)	36(1)
N(4)	638(1)	2573(2)	824(1)	41(1)
C(3)	1768(1)	7080(2)	3560(2)	37(1)
C(5)	1736(1)	7179(2)	4907(2)	37(1)
N(3)	1878(1)	6016(2)	5133(1)	34(1)
N(1)	1906(1)	5907(2)	3704(1)	35(1)
N(2)	1886(1)	7739(2)	4355(1)	35(1)
C(25)	949(1)	4871(3)	–94(2)	42(1)
C(22)	692(1)	6493(3)	1585(2)	50(1)
C(23)	394(1)	6780(3)	1917(2)	50(1)
C(24)	568(1)	7143(3)	2847(2)	54(1)
C(26B)	602(2)	5546(7)	–680(5)	45(2)
C(26A)	802(4)	6020(9)	–548(5)	96(4)
C(28B)	980(2)	7004(6)	–1088(4)	68(2)
C(27B)	677(2)	6802(6)	–754(4)	50(2)

Tabelle 29 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für $[(n\text{-BuLi})_4 \cdot (C_6H_{15}N_3)_2]_\infty$ (**98**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(28A)	139(9)	189(11)	73(6)	34(6)	55(6)	81(8)
C(27A)	160(9)	73(5)	49(4)	3(4)	35(5)	47(6)
Li(4)	43(3)	45(3)	36(2)	–1(2)	23(2)	3(2)
Li(2)	41(3)	39(3)	44(3)	–5(2)	19(2)	–3(2)

Li(1)	42(3)	40(3)	40(2)	0(2)	18(2)	–3(2)
Li(3)	49(3)	40(3)	41(2)	3(2)	19(2)	3(2)
C(16)	123(4)	51(2)	143(4)	–7(2)	86(3)	–18(2)
C(17)	45(2)	45(2)	39(2)	2(1)	20(1)	2(1)
C(21)	38(2)	46(2)	33(2)	–5(1)	15(1)	–3(1)
C(20)	217(6)	55(2)	53(2)	12(2)	26(3)	12(3)
C(19)	100(3)	52(2)	54(2)	9(2)	22(2)	6(2)
C(18)	82(2)	42(2)	42(2)	1(1)	19(2)	–2(2)
C(15)	77(2)	49(2)	84(2)	–6(2)	51(2)	–15(2)
C(14)	57(2)	49(2)	43(2)	1(1)	24(2)	–6(1)
C(6)	41(2)	52(2)	37(2)	0(1)	16(1)	–2(1)
C(13)	50(2)	42(2)	37(2)	–3(1)	21(2)	–6(1)
C(10)	157(5)	113(4)	84(3)	40(3)	34(3)	–53(3)
C(12)	107(3)	78(3)	124(4)	–59(3)	57(3)	–35(2)
C(8)	47(2)	59(2)	63(2)	–3(2)	18(2)	–6(2)
C(11)	61(2)	47(2)	96(3)	4(2)	19(2)	–14(2)
C(9)	68(2)	60(2)	44(2)	4(2)	16(2)	–18(2)
C(7)	57(2)	56(2)	58(2)	–17(2)	30(2)	–20(2)
N(5)	77(2)	60(2)	63(2)	12(1)	25(2)	–21(2)
C(4)	54(2)	38(2)	54(2)	0(1)	23(2)	1(1)
N(6)	66(2)	49(2)	67(2)	–19(1)	28(2)	–20(1)
C(2)	42(2)	51(2)	39(2)	–3(1)	20(1)	–3(1)
C(1)	40(2)	37(2)	34(1)	–5(1)	17(1)	–7(1)
N(4)	40(1)	43(1)	37(1)	–1(1)	14(1)	–4(1)
C(3)	38(2)	39(2)	32(1)	0(1)	14(1)	–4(1)
C(5)	38(2)	40(2)	36(1)	–3(1)	18(1)	–2(1)
N(3)	34(1)	37(1)	31(1)	–1(1)	13(1)	–4(1)
N(1)	36(1)	36(1)	33(1)	–1(1)	16(1)	–3(1)
N(2)	39(1)	33(1)	35(1)	–2(1)	17(1)	–5(1)
C(25)	42(2)	48(2)	35(2)	1(1)	17(1)	3(1)
C(22)	45(2)	66(2)	40(2)	4(1)	21(1)	11(2)
C(23)	43(2)	65(2)	43(2)	–3(1)	19(1)	7(2)
C(24)	53(2)	65(2)	48(2)	–1(2)	26(2)	6(2)
C(26B)	40(4)	51(5)	41(4)	–5(3)	15(3)	4(3)
C(26A)	167(13)	69(8)	38(5)	11(5)	30(7)	36(8)
C(28B)	92(5)	65(4)	57(4)	17(3)	43(4)	12(4)
C(27B)	52(4)	45(4)	47(4)	7(3)	15(3)	11(3)

Tabelle 30 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für $[(n\text{-BuLi})_4 \cdot (C_6H_{15}N_3)_2]_\infty$ (**98**).

	x	y	z	U(eq)
H(28A)	127	7175	-1585	196
H(28B)	138	6834	-2471	196
H(28C)	468	7612	-1793	196
H(27A)	624	5759	-1843	117
H(27B)	311	5411	-1525	117
H(22A)	1621	9904	804	143
H(22B)	2009	10296	1581	143
H(22C)	1658	9895	1764	143
H(18A)	2159	2563	4498	180
H(18B)	2127	1203	4393	180
H(18C)	1757	1948	4219	180
H(17A)	1771	1383	2925	87
H(17B)	2168	2021	3203	87
H(16)	1453	2905	2722	70
H(15A)	2130	8455	2110	77
H(15B)	2060	8429	1127	77
H(14A)	1437	7759	718	58
H(14B)	1488	7847	1683	58
H(6A)	2432	6476	5560	66
H(6B)	2377	5204	5830	66
H(6C)	2305	6276	6318	66
H(10A)	313	-345	1995	187
H(10B)	435	822	2527	187
H(10C)	750	31	2430	187
H(12A)	781	-169	-346	151
H(12B)	472	531	-1129	151
H(12C)	346	-567	-760	151
H(8A)	62	2508	276	88
H(8B)	226	3529	-83	88
H(8C)	228	3630	843	88
H(11A)	337	-473	623	88
H(11B)	773	-76	1046	88
H(9A)	638	2408	1984	72
H(9B)	955	1647	1868	72
H(7A)	963	1565	467	66
H(7B)	647	2259	-312	66
H(4A)	1459	8873	3871	73
H(4B)	1832	9254	3769	73

H(4C)	1821	9344	4683	73
H(2A)	2361	6028	3424	65
H(2B)	2407	5055	4114	65
H(2C)	2457	6371	4393	65
H(1A)	1520	5221	4059	44
H(1B)	1927	4627	4504	44
H(3A)	1487	7073	3262	44
H(3B)	1863	7464	3179	44
H(5A)	1808	7633	5438	45
H(5B)	1455	7161	4607	45
H(35A)	860	7167	1691	60
H(35B)	557	6397	956	60
H(36A)	230	7403	1563	60
H(36B)	232	6101	1848	60
H(37A)	718	6512	3205	81
H(37B)	365	7345	3016	81
H(37C)	732	7807	2923	81
H(26A)	500	5200	–1259	54
H(26B)	405	5477	–465	54
H(26C)	1023	6453	–532	116
H(26D)	698	6456	–203	116
H(23A)	761(8)	4810(30)	1881(17)	59(9)
H(23B)	1061(7)	5530(20)	2560(17)	45(7)
H(28D)	1229	6771	–650	102
H(28E)	987	7818	–1218	102
H(28F)	918	6554	–1610	102
H(13A)	1869(7)	6240(20)	1083(16)	44(7)
H(13B)	1975(8)	6360(20)	2091(19)	57(8)
H(27C)	761	7165	–184	60
H(27D)	438	7175	–1147	60
H(21B)	1533(9)	2710(30)	1580(20)	70(10)
H(21A)	1887(10)	3260(30)	1850(20)	82(11)
H(31A)	1078(10)	4700(30)	–420(20)	83(11)
H(16B)	1920(12)	3710(40)	3160(30)	122(15)
H(31B)	804(12)	4140(40)	–270(30)	117(15)

(*i*-PrLi·TMEDA)$_2$ (100)

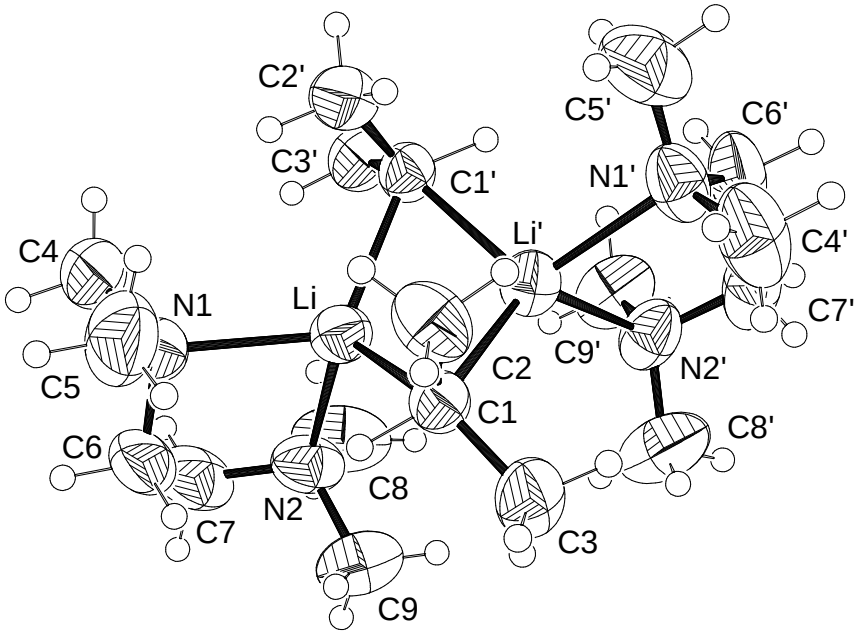


Abbildung 11 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von (*i*-PrLi·TMEDA)$_2$ (**100**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 31 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für (*i*-PrLi·TMEDA)$_2$ (**100**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	1730(2)	2112(1)	1074(5)	56(1)
C(2)	1562(3)	2172(1)	−664(7)	77(2)
C(3)	937(3)	2031(1)	1919(7)	77(2)
C(4)	4662(3)	1894(2)	445(10)	103(2)
C(5)	3500(4)	1605(2)	−744(9)	108(2)
C(6)	3777(3)	1471(2)	1949(9)	88(2)
C(7)	3946(3)	1644(2)	3514(8)	93(2)
C(8)	3706(4)	2216(2)	5129(8)	111(2)
C(9)	2648(4)	1756(2)	4622(7)	91(2)
Li	3020(4)	2247(2)	1687(9)	57(2)
N(1)	3825(2)	1772(1)	711(6)	72(1)
N(2)	3365(2)	1948(1)	3956(5)	73(1)

Tabelle 32 Anisotrope Auslenkungsparameter ($Å^2 \times 10^3$) für (*i*-PrLi·TMEDA)$_2$ (**100**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	48(2)	53(2)	65(3)	0(2)	–1(2)	–1(2)
C(2)	91(4)	63(3)	77(4)	–6(3)	–17(3)	2(2)
C(3)	52(3)	74(3)	104(4)	–9(3)	–7(3)	–4(2)
C(4)	62(3)	79(3)	168(6)	23(4)	45(4)	4(3)
C(5)	110(5)	100(5)	116(5)	–32(4)	29(4)	8(4)
C(6)	60(3)	61(3)	142(6)	25(3)	11(3)	10(2)
C(7)	70(3)	80(4)	131(6)	44(4)	–20(3)	3(3)
C(8)	125(5)	115(5)	95(5)	23(4)	–39(4)	–46(4)
C(9)	93(4)	107(4)	73(4)	19(3)	–2(3)	–26(3)
Li	55(4)	58(4)	58(4)	8(3)	–1(3)	–3(3)
N(1)	56(2)	56(2)	103(3)	6(2)	21(2)	5(2)
N(2)	64(2)	75(3)	80(3)	24(2)	–13(2)	–8(2)

Tabelle 33 Wasserstoffkoordinaten ($\times 10^4$) und isotrope Auslenkungsparameter ($Å^2 \times 10^3$) für (*i*-PrLi·TMEDA)$_2$ (**100**).

	x	y	z	U(eq)
H(1)	2070(20)	1840(11)	1180(50)	49(10)
H(2A)	1208	1957	–1037	115
H(2B)	2069	2164	–1245	115
H(2C)	1302	2433	–825	115
H(3A)	622	2279	1968	115
H(3B)	1048	1936	2979	115
H(3C)	633	1825	1350	115
H(4A)	4852	2053	1336	154
H(4B)	4694	2057	–506	154
H(4C)	4999	1655	328	154
H(5A)	3489	1815	–1546	163
H(5B)	2954	1506	–562	163
H(5C)	3842	1383	–1096	163
H(6A)	4168	1253	1731	105
H(6B)	3234	1350	1951	105
H(7A)	3941	1425	4299	112
H(7B)	4490	1764	3511	112
H(8A)	3920	2056	5995	167
H(8B)	3288	2397	5519	167

H(8C)	4140	2374	4661	167
H(9A)	2408	1576	3845	136
H(9B)	2257	1963	4916	136
H(9C)	2800	1600	5547	136

α-lithiiertesTMEDA (101)

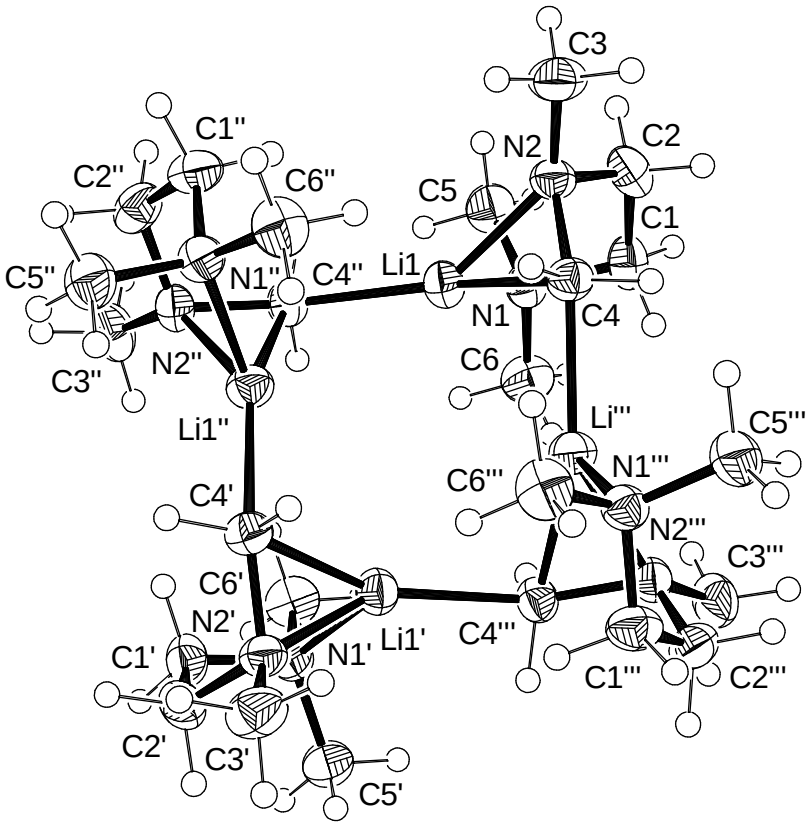


Abbildung 12 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von α-lithiiertemTMEDA (**101**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 34 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) von α-lithiiertemTMEDA (**101**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	3558(1)	3840(1)	10488(2)	40(1)
C(2)	3577(1)	4249(1)	9013(2)	41(1)
C(3)	4089(1)	4485(1)	6599(2)	47(1)
C(4)	4010(1)	3310(1)	7493(2)	33(1)

C(5)	4455(1)	4417(1)	11835(2)	43(1)
C(6)	4202(1)	3276(1)	12442(2)	47(1)
Li(1)	4786(1)	3512(1)	9209(2)	34(1)
N(1)	4224(1)	3775(1)	11203(1)	33(1)
N(2)	4098(1)	4033(1)	7934(1)	33(1)

Tabelle 35 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) von α-lithiiertemTMEDA (**101**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	29(1)	51(1)	40(1)	–9(1)	1(1)	3(1)
C(2)	37(1)	41(1)	45(1)	–8(1)	–10(1)	10(1)
C(3)	58(1)	35(1)	49(1)	10(1)	–12(1)	–6(1)
C(4)	37(1)	30(1)	32(1)	–1(1)	–2(1)	–2(1)
C(5)	47(1)	41(1)	43(1)	–9(1)	–3(1)	–2(1)
C(6)	55(1)	48(1)	38(1)	2(1)	–1(1)	–3(1)
Li(1)	30(1)	38(1)	36(1)	–2(1)	–2(1)	2(1)
N(1)	32(1)	35(1)	31(1)	–4(1)	–3(1)	0(1)
N(2)	36(1)	27(1)	35(1)	1(1)	–6(1)	–1(1

Tabelle 36 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) von α-lithiiertemTMEDA (**101**).

	x	y	z	U(eq)
H(1A)	3235(8)	4052(8)	11200(20)	49(4)
H(1B)	3402(7)	3377(8)	10255(18)	45(4)
H(2A)	3125(8)	4220(7)	8549(18)	51(4)
H(2B)	3650(7)	4726(8)	9234(18)	47(4)
H(3A)	3649(8)	4451(8)	6044(19)	51(4)
H(3B)	4475(8)	4366(8)	5878(19)	52(4)
H(3C)	4132(8)	4948(9)	6943(19)	58(5)
H(4B)	3518(8)	3250(7)	7135(18)	47(4)
H(4A)	4268(7)	3257(7)	6510(18)	41(4)
H(5A)	4515(8)	4763(8)	11007(19)	50(4)
H(5B)	4911(8)	4353(7)	12338(18)	49(4)
H(5C)	4150(8)	4604(8)	12620(20)	55(4)
H(6A)	4659(10)	3200(9)	12900(20)	65(5)

H(6B)	4050(8)	2838(9)	12020(20)	54(4)
H(6C)	3914(9)	3414(9)	13270(20)	61(5)

Hydrobromid des Abfangproduktes von lithiiertem TEMDA mit Benzophenon

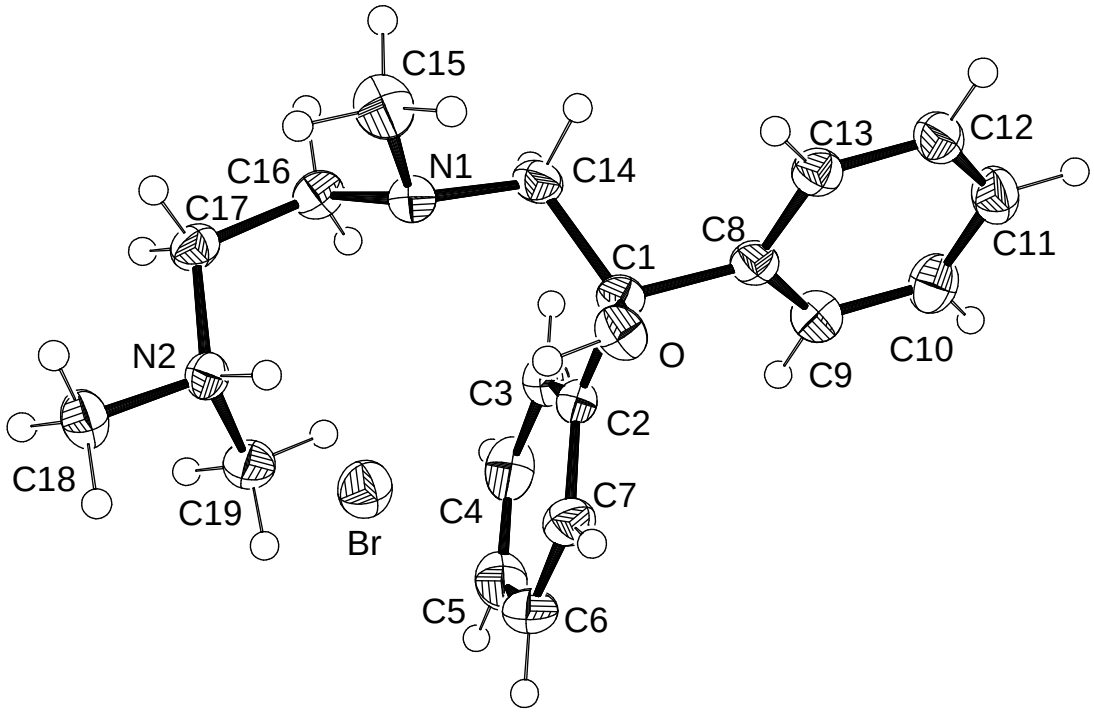


Abbildung 13 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Hydrobromids von Verbindung (**103**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 37 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für das Hydrobromids von Verbindung (**103**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
Br	5574(1)	6973(1)	5648(1)	32(1)
C(1)	5689(4)	9346(2)	6357(1)	25(1)
C(2)	6972(4)	8817(2)	6628(1)	25(1)
C(3)	8583(4)	9173(2)	6797(1)	32(1)
C(4)	9747(5)	8691(2)	7043(1)	41(1)
C(5)	9322(5)	7848(2)	7124(1)	45(1)
C(6)	7726(5)	7483(2)	6963(1)	43(1)
C(7)	6550(5)	7962(2)	6718(1)	33(1)

C(8)	4436(4)	9959(2)	6597(1)	26(1)
C(9)	4565(4)	10056(2)	7007(1)	34(1)
C(10)	3373(5)	10615(2)	7208(1)	38(1)
C(11)	2045(4)	11091(2)	7004(1)	37(1)
C(12)	1884(4)	10993(2)	6597(1)	34(1)
C(13)	3059(4)	10431(2)	6396(1)	29(1)
C(14)	6829(4)	9867(2)	6047(1)	28(1)
C(15)	6944(5)	9484(2)	5349(1)	40(1)
C(16)	9753(4)	9341(2)	5748(1)	29(1)
C(17)	10617(4)	8595(2)	5524(1)	29(1)
C(18)	10397(4)	7043(2)	5383(1)	34(1)
C(19)	10432(4)	7533(2)	6075(1)	34(1)
N(1)	7696(3)	9306(2)	5746(1)	26(1)
N(2)	9858(4)	7744(2)	5661(1)	26(1)
O	4416(3)	8802(1)	6145(1)	29(1)

Tabelle 38 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für das Hydrobromids von Verbindung (**103**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br	28(1)	33(1)	36(1)	–2(1)	1(1)	–3(1)
C(1)	25(1)	22(1)	28(1)	–1(1)	–3(1)	–3(1)
C(2)	24(1)	26(1)	25(1)	0(1)	3(1)	1(1)
C(3)	30(2)	33(2)	33(2)	–4(1)	0(1)	–1(1)
C(4)	30(2)	62(2)	30(2)	–6(2)	–6(1)	3(2)
C(5)	47(2)	58(2)	31(2)	8(2)	–3(2)	19(2)
C(6)	48(2)	37(2)	43(2)	16(1)	8(2)	8(2)
C(7)	32(2)	31(2)	37(2)	4(1)	2(1)	–4(1)
C(8)	25(1)	22(1)	32(1)	0(1)	–1(1)	–5(1)
C(9)	33(2)	35(2)	33(2)	–1(1)	–3(1)	0(1)
C(10)	39(2)	45(2)	31(2)	–7(1)	4(1)	–2(2)
C(11)	33(2)	31(2)	48(2)	–8(1)	8(1)	–1(1)
C(12)	26(2)	29(2)	46(2)	2(1)	2(1)	–1(1)
C(13)	28(1)	26(1)	32(1)	1(1)	–1(1)	–3(1)
C(14)	33(2)	20(1)	32(1)	1(1)	–1(1)	0(1)
C(15)	40(2)	47(2)	33(2)	–5(1)	–9(1)	5(2)
C(16)	28(2)	30(2)	29(1)	–1(1)	–2(1)	–7(1)
C(17)	25(1)	31(2)	30(1)	4(1)	2(1)	–3(1)
C(18)	33(2)	32(2)	38(2)	–8(1)	4(1)	3(1)
C(19)	34(2)	36(2)	33(2)	6(1)	0(1)	5(1)

N(1)	27(1)	26(1)	25(1)	–1(1)	–2(1)	–1(1)
N(2)	20(1)	27(1)	31(1)	1(1)	3(1)	0(1)
O	27(1)	25(1)	35(1)	–7(1)	–5(1)	–1(1)

Tabelle 39 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung (*n*-BuLi·TEEDA)$_2$ (**103**).

	x	y	z	U(eq)
H(3)	8891	9757	6742	38
H(4)	10839	8946	7155	49
H(5)	10123	7516	7290	54
H(6)	7427	6899	7021	51
H(7)	5450	7705	6611	40
H(9)	5477	9736	7151	40
H(10)	3472	10671	7489	46
H(11)	1250	11481	7143	45
H(12)	966	11313	6454	40
H(13)	2927	10365	6116	35
H(14A)	5987	10285	5913	34
H(14B)	7824	10198	6185	34
H(15A)	7316	10065	5267	60
H(15B)	5571	9444	5356	60
H(15C)	7442	9062	5160	60
H(16A)	10205	9332	6027	35
H(16B)	10169	9889	5626	35
H(17A)	10360	8664	5236	34
H(17B)	11996	8603	5562	34
H(18A)	11761	6958	5393	51
H(18B)	10023	7199	5112	51
H(18C)	9764	6508	5461	51
H(19A)	9797	7005	6161	51
H(19B)	10081	8009	6253	51
H(19C)	11795	7448	6085	51
H(2N)	8640(60)	7780(20)	5666(10)	44(10)
H(0)	5021	8417	6025	44

(*n*-BuLi·TEEDA)$_2$ (104)

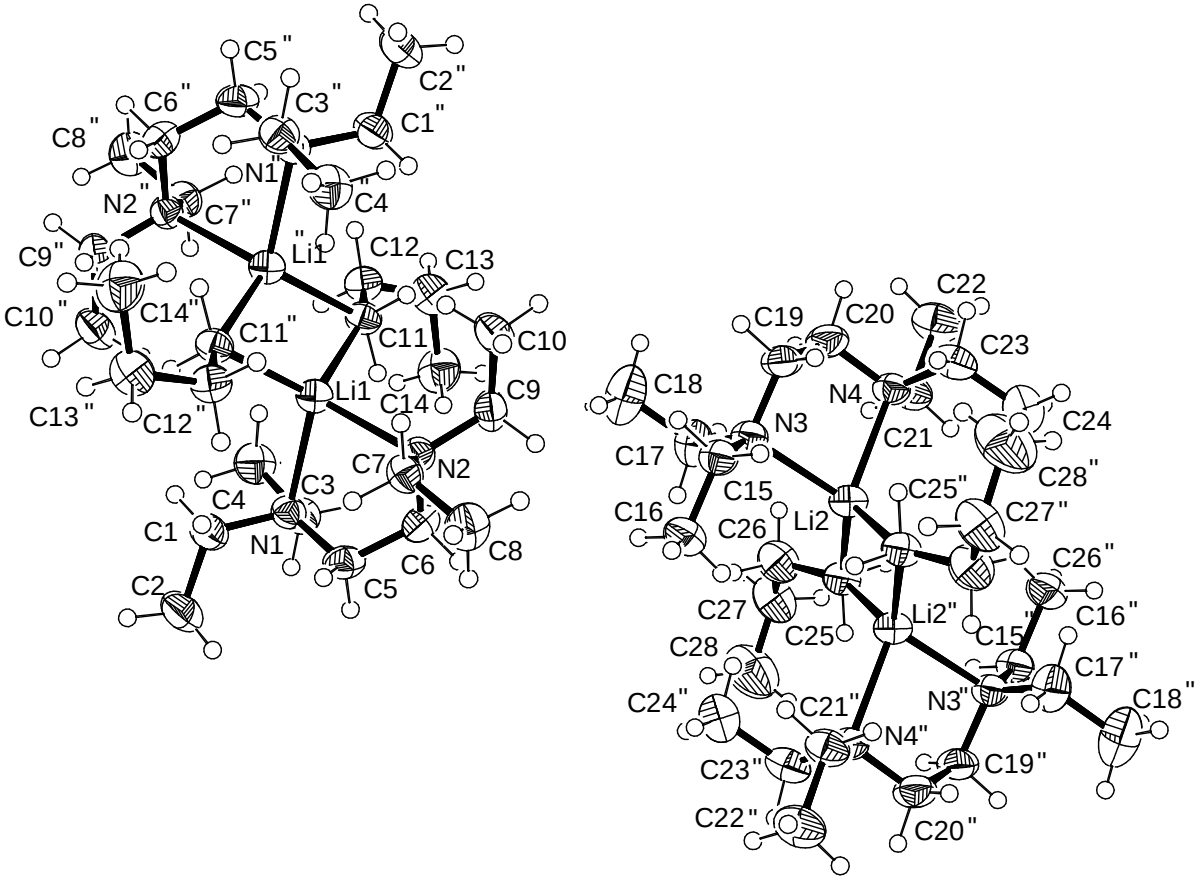


Abbildung 14 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von (*n*-BuLi·TEEDA)$_2$ (**104**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 40 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung (*n*-BuLi·TEEDA)$_2$ (**104**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	7052(2)	7486(2)	-657(2)	48(1)
C(2)	7973(2)	6490(2)	-742(2)	70(1)
C(3)	7166(2)	7681(2)	1160(2)	45(1)
C(4)	8035(2)	8723(2)	1340(2)	55(1)
C(5)	5398(2)	6577(2)	125(2)	46(1)
C(6)	4212(2)	6854(2)	636(2)	43(1)
C(7)	2654(2)	7258(2)	-836(1)	41(1)
C(8)	1718(2)	6256(2)	-883(2)	58(1)
C(9)	2427(2)	8111(2)	834(2)	45(1)
C(10)	1529(2)	9022(2)	449(2)	57(1)

C(11)	4988(2)	10218(2)	1391(1)	39(1)
C(12)	5732(2)	10978(2)	2271(1)	45(1)
C(13)	5512(2)	10761(2)	3322(2)	52(1)
C(14)	6167(2)	9704(2)	3668(2)	64(1)
C(15)	389(2)	6833(2)	2909(1)	44(1)
C(16)	1155(2)	5827(2)	2578(2)	57(1)
C(17)	2092(2)	7461(2)	4311(2)	57(1)
C(18)	2703(3)	8393(2)	3838(2)	85(1)
C(19)	–192(2)	8158(2)	4184(2)	53(1)
C(20)	–196(3)	8472(2)	5282(2)	56(1)
C(21)	–198(2)	7647(2)	6834(1)	50(1)
C(22)	–555(3)	8690(2)	7474(2)	64(1)
C(23)	–2208(2)	7602(2)	5584(2)	53(1)
C(24)	–2878(2)	6681(2)	6007(2)	68(1)
C(25)	1521(2)	5088(2)	5996(2)	45(1)
C(26)	2889(2)	5677(2)	6231(2)	62(1)
C(27)	3932(2)	5265(2)	7033(2)	68(1)
C(28)	4575(3)	4230(3)	6748(2)	104(1)
Li(1)	4904(3)	8988(2)	8(2)	39(1)
Li(2)	55(3)	6009(2)	4993(2)	43(1)
N(1)	6297(2)	7561(1)	188(1)	38(1)
N(2)	3355(1)	7701(1)	158(1)	36(1)
N(3)	671(2)	7201(1)	3979(1)	41(1)
N(4)	–733(2)	7570(1)	5765(1)	42(1)

Tabelle 41 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung (*n*-BuLi·TEEDA)$_2$ (**104**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	48(1)	50(1)	48(1)	6(1)	12(1)	13(1)
C(2)	72(2)	69(2)	80(2)	15(1)	36(1)	31(1)
C(3)	38(1)	48(1)	49(1)	9(1)	2(1)	5(1)
C(4)	40(1)	59(1)	65(2)	4(1)	1(1)	–1(1)
C(5)	41(1)	36(1)	59(1)	7(1)	0(1)	6(1)
C(6)	41(1)	40(1)	48(1)	12(1)	1(1)	–4(1)
C(7)	36(1)	47(1)	41(1)	4(1)	7(1)	4(1)
C(8)	50(1)	62(1)	58(2)	–1(1)	1(1)	–11(1)
C(9)	43(1)	50(1)	42(1)	–1(1)	15(1)	–7(1)
C(10)	45(1)	61(1)	65(2)	–4(1)	18(1)	8(1)

C(11)	39(1)	38(1)	38(1)	3(1)	3(1)	5(1)
C(12)	47(1)	42(1)	43(1)	3(1)	3(1)	1(1)
C(13)	54(1)	59(1)	38(1)	–4(1)	2(1)	–1(1)
C(14)	70(2)	76(2)	48(1)	17(1)	4(1)	4(1)
C(15)	54(1)	42(1)	38(1)	5(1)	8(1)	7(1)
C(16)	63(2)	52(1)	58(1)	–3(1)	18(1)	9(1)
C(17)	57(1)	71(2)	42(1)	5(1)	6(1)	–9(1)
C(18)	90(2)	103(2)	62(2)	6(2)	14(2)	–38(2)
C(19)	77(2)	36(1)	50(1)	10(1)	22(1)	13(1)
C(20)	84(2)	34(1)	52(1)	–3(1)	21(1)	2(1)
C(21)	58(1)	50(1)	40(1)	–1(1)	4(1)	10(1)
C(22)	83(2)	64(1)	42(1)	–9(1)	6(1)	13(1)
C(23)	61(1)	51(1)	46(1)	0(1)	4(1)	19(1)
C(24)	60(2)	81(2)	64(2)	6(1)	15(1)	2(1)
C(25)	44(1)	40(1)	48(1)	0(1)	4(1)	4(1)
C(26)	56(2)	70(2)	57(2)	4(1)	6(1)	8(1)
C(27)	52(1)	93(2)	54(2)	1(1)	0(1)	13(1)
C(28)	92(2)	134(3)	91(2)	32(2)	12(2)	51(2)
Li(1)	40(2)	37(2)	40(2)	4(1)	5(1)	3(1)
Li(2)	46(2)	36(2)	44(2)	3(1)	3(2)	4(2)
N(1)	34(1)	38(1)	42(1)	4(1)	5(1)	4(1)
N(2)	34(1)	38(1)	37(1)	5(1)	7(1)	2(1)
N(3)	50(1)	36(1)	38(1)	3(1)	9(1)	6(1)
N(4)	52(1)	36(1)	36(1)	2(1)	8(1)	7(1)

Tabelle 42 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung (*n*-BuLi·TEEDA)$_2$ (**104**).

	x	y	z	U(eq)
H(1A)	7593	8186	–607	58
H(1B)	6406	7459	–1284	58
H(2A)	8625	6504	–129	105
H(2B)	8440	6538	–1315	105
H(2C)	7447	5787	–838	105
H(3A)	7741	7014	1209	54
H(3B)	6605	7692	1694	54
H(4A)	8713	8654	900	83
H(4B)	8471	8816	2038	83
H(4C)	7488	9381	1199	83

H(5A)	5893	5959	440	56
H(5B)	5087	6310	–586	56
H(6A)	3680	6157	630	52
H(6B)	4528	7139	1342	52
H(7A)	3332	7045	–1266	49
H(7B)	2134	7877	–1129	49
H(8A)	2225	5613	–646	87
H(8B)	1286	6062	–1575	87
H(8C)	1039	6447	–459	87
H(9A)	2947	8402	1487	54
H(9B)	1870	7469	948	54
H(10A)	2062	9601	221	85
H(10B)	1071	9362	984	85
H(10C)	869	8698	–111	85
H(11A)	4029(19)	10315(14)	1426(13)	39(5)
H(11B)	5177(18)	9407(16)	1532(13)	45(5)
H(12A)	5485	11765	2173	53
H(12B)	6698	10918	2243	53
H(13A)	5869	11413	3797	62
H(13B)	4543	10701	3333	62
H(14A)	5806	9051	3209	96
H(14B)	5989	9610	4342	96
H(14C)	7131	9765	3677	96
H(15A)	589	7467	2537	53
H(15B)	–575	6653	2726	53
H(16A)	2099	6038	2636	86
H(16B)	806	5563	1880	86
H(16C)	1061	5224	3001	86
H(17A)	2593	6765	4186	69
H(17B)	2227	7666	5043	69
H(18A)	2581	8208	3111	127
H(18B)	3657	8468	4101	127
H(18C)	2266	9105	3996	127
H(19A)	–1114	7964	3854	63
H(19B)	112	8818	3889	63
H(20A)	727	8659	5615	67
H(20B)	–737	9154	5369	67
H(21A)	785	7613	6905	60
H(21B)	–512	6975	7107	60
H(22A)	–266	9367	7209	96
H(22B)	–106	8671	8163	96
H(22C)	–1521	8704	7462	96

H(23A)	–2517	7551	4855	64
H(23B)	–2490	8337	5880	64
H(24A)	–2528	5951	5780	102
H(24B)	–3841	6690	5777	102
H(24C)	–2701	6799	6738	102
H(25A)	1140(20)	5210(16)	6648(16)	54(6)
H(25B)	1770(20)	4280(20)	5989(17)	77(7)
H(26A)	3272	5631	5603	74
H(26B)	2746	6485	6425	74
H(27A)	4626	5862	7241	81
H(27B)	3503	5157	7622	81
H(28A)	3936	3600	6674	156
H(28B)	5330	4105	7265	156
H(28C)	4895	4284	6111	156

$(PhLi \cdot TEEDA)_2$ (105)

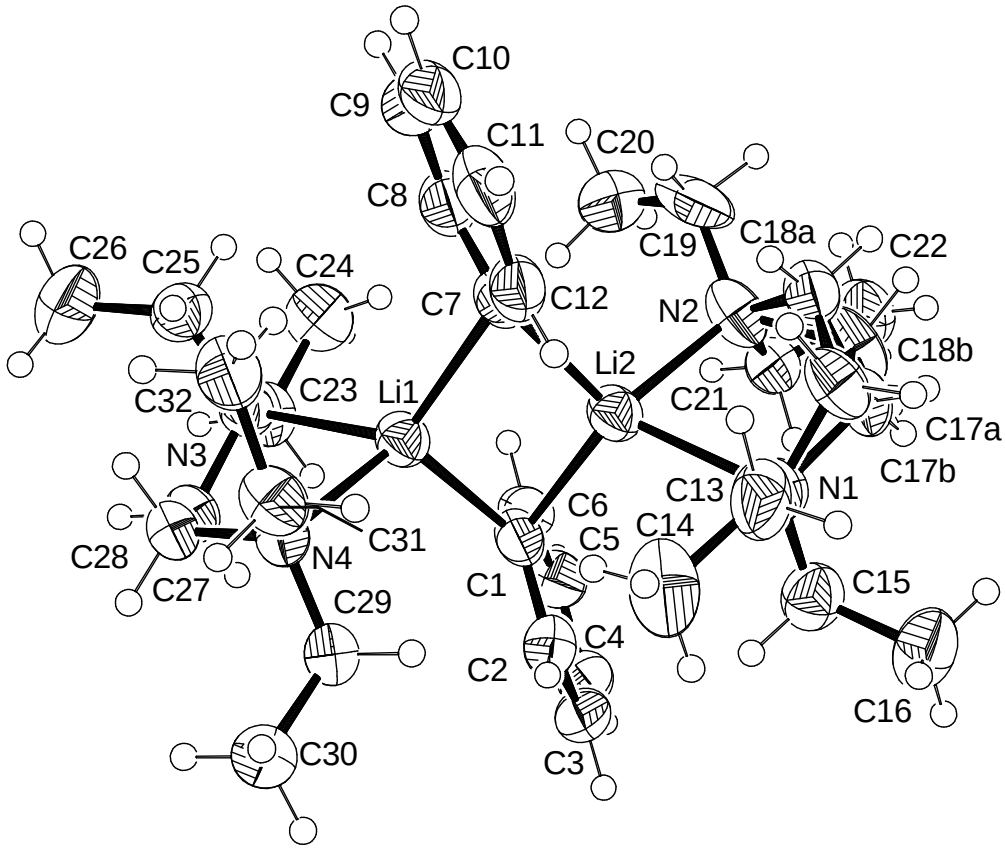


Abbildung 15 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von $(PhLi \cdot TEEDA)_2$ (**105**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 43 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für $(PhLi{\cdot}TEEDA)_2$ (**105**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	2412(2)	4483(3)	490(1)	49(1)
C(2)	3044(2)	3865(3)	201(1)	51(1)
C(3)	2963(2)	3256(3)	–396(1)	54(1)
C(4)	2216(2)	3213(3)	–747(1)	56(1)
C(5)	1568(2)	3777(3)	–499(1)	59(1)
C(6)	1676(2)	4399(3)	97(1)	54(1)
C(7)	2582(2)	7036(3)	1851(1)	49(1)
C(8)	1868(2)	7279(3)	2113(2)	59(1)
C(9)	1813(2)	7996(4)	2680(2)	74(1)
C(10)	2487(3)	8524(4)	3025(2)	76(1)
C(11)	3222(2)	8335(3)	2804(2)	67(1)
C(12)	3258(2)	7598(3)	2234(1)	55(1)
C(13)	4390(2)	7845(4)	876(2)	81(1)
C(14)	4695(2)	6387(4)	1118(2)	87(1)
C(15)	3964(2)	7010(4)	–188(2)	63(1)
C(16)	4655(2)	7684(4)	–492(2)	80(1)
C(17A)	3348(4)	9189(6)	106(3)	54(1)
C(18A)	2619(4)	9589(7)	421(3)	59(2)
C(17B)	3546(8)	9234(13)	485(7)	61(4)
C(18B)	2765(9)	9459(15)	40(8)	63(4)
C(19)	1330(3)	9098(4)	611(2)	83(1)
C(20)	619(3)	8126(5)	588(2)	98(1)
C(21)	1707(2)	8144(3)	–386(1)	57(1)
C(22)	1358(2)	9353(4)	–820(2)	80(1)
C(23)	792(2)	2898(3)	1366(2)	59(1)
C(24)	197(2)	4120(4)	1238(2)	71(1)
C(25)	1156(2)	3626(3)	2466(1)	58(1)
C(26)	659(2)	2509(4)	2778(2)	82(1)
C(27)	1981(2)	1926(3)	1944(1)	52(1)
C(28)	2740(2)	2141(3)	2400(1)	52(1)
C(29)	3765(2)	2644(3)	1715(1)	51(1)
C(30)	4380(2)	1490(3)	1950(2)	65(1)
C(31)	3794(2)	3942(3)	2701(1)	59(1)
C(32)	3348(2)	4677(3)	3190(1)	65(1)
Li(1)	2418(3)	4681(5)	1554(2)	47(1)
Li(2)	2651(3)	6759(5)	803(2)	49(1)
N(1)	3720(2)	7749(3)	363(1)	66(1)
N(2)	2001(2)	8525(3)	275(1)	61(1)

N(3)	1459(1)	3204(2)	1871(1)	46(1)
N(4)	3266(1)	3247(2)	2179(1)	46(1)

Tabelle 44 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für $(PhLi{\cdot}TEEDA)_2$ (**105**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	68(2)	36(2)	43(2)	4(1)	6(2)	–1(1)
C(2)	57(2)	51(2)	45(2)	3(2)	5(1)	–8(2)
C(3)	65(2)	53(2)	46(2)	–3(2)	16(2)	2(2)
C(4)	76(2)	55(2)	38(2)	–6(1)	6(2)	3(2)
C(5)	66(2)	60(2)	46(2)	–2(2)	–5(2)	7(2)
C(6)	66(2)	46(2)	51(2)	0(2)	8(2)	10(2)
C(7)	63(2)	37(2)	46(2)	4(1)	5(1)	1(1)
C(8)	70(2)	49(2)	56(2)	7(2)	7(2)	–1(2)
C(9)	98(3)	60(2)	69(2)	7(2)	33(2)	13(2)
C(10)	140(4)	43(2)	49(2)	–1(2)	24(2)	8(2)
C(11)	106(3)	44(2)	47(2)	3(2)	–8(2)	–13(2)
C(12)	72(2)	47(2)	47(2)	7(2)	9(2)	–1(2)
C(13)	122(3)	56(2)	71(2)	–11(2)	36(2)	–34(2)
C(14)	120(3)	79(3)	58(2)	0(2)	–6(2)	–33(2)
C(15)	55(2)	70(2)	63(2)	7(2)	7(2)	–1(2)
C(16)	77(2)	98(3)	68(2)	20(2)	16(2)	–6(2)
C(17A)	65(4)	43(3)	53(3)	4(3)	3(3)	–14(3)
C(18A)	82(4)	47(3)	48(3)	2(3)	8(3)	–6(3)
C(17B)	61(8)	41(7)	76(9)	2(8)	–12(8)	–7(5)
C(18B)	45(8)	43(7)	92(11)	19(8)	–31(9)	–2(6)
C(19)	132(4)	50(2)	63(2)	–8(2)	–3(2)	41(2)
C(20)	118(3)	84(3)	103(3)	15(2)	53(3)	28(3)
C(21)	60(2)	52(2)	59(2)	7(2)	11(2)	6(2)
C(22)	100(3)	74(2)	66(2)	15(2)	6(2)	12(2)
C(23)	58(2)	54(2)	62(2)	1(2)	1(2)	–12(2)
C(24)	59(2)	78(2)	72(2)	1(2)	–6(2)	2(2)
C(25)	55(2)	64(2)	58(2)	1(2)	13(2)	4(2)
C(26)	70(2)	109(3)	70(2)	14(2)	19(2)	–8(2)
C(27)	59(2)	38(2)	60(2)	0(1)	10(2)	–5(1)
C(28)	59(2)	42(2)	56(2)	10(1)	12(2)	4(1)
C(29)	56(2)	49(2)	50(2)	7(1)	9(1)	1(1)

C(30)	68(2)	61(2)	68(2)	7(2)	17(2)	12(2)
C(31)	65(2)	54(2)	57(2)	–1(2)	–6(2)	2(2)
C(32)	91(2)	52(2)	50(2)	–2(2)	1(2)	–5(2)
Li(1)	53(3)	41(3)	45(3)	–1(2)	4(2)	0(2)
Li(2)	61(3)	41(3)	45(3)	–1(2)	5(2)	1(2)
N(1)	69(2)	46(2)	87(2)	–6(2)	26(2)	–12(1)
N(2)	68(2)	43(2)	68(2)	3(1)	–13(1)	–5(1)
N(3)	51(1)	43(1)	45(1)	–2(1)	5(1)	0(1)
N(4)	49(1)	43(1)	45(1)	2(1)	5(1)	–3(1)

Tabelle 45 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für $(PhLi{\cdot}TEEDA)_2$ (**105**).

	x	y	z	U(eq)
H(2)	3569	3865	436	61
H(3)	3422	2869	-563	65
H(4)	2150	2793	-1159	67
H(5)	1045	3743	-735	70
H(6)	1213	4801	252	65
H(8)	1379	6926	1886	70
H(9)	1300	8118	2826	88
H(10)	2452	9016	3414	92
H(11)	3703	8703	3038	81
H(12)	3775	7468	2095	66
H(13A)	4211	8398	1232	97
H(13B)	4842	8379	721	97
H(14A)	4237	5802	1219	131
H(14B)	5082	6513	1502	131
H(14C)	4963	5902	790	131
H(15A)	3486	6946	-515	75
H(15B)	4121	6014	-61	75
H(16A)	5156	7616	-197	121
H(16B)	4532	8699	-587	121
H(16C)	4723	7173	-886	121
H(17A)	3759	9960	181	65
H(17B)	3190	9108	-359	65
H(18A)	2768	9645	887	71
H(18B)	2415	10544	268	71
H(17C)	3983	9877	376	74

H(17D)	3463	9388	935	74
H(18C)	2849	9156	-395	76
H(18D)	2626	10496	26	76
H(19A)	1541	9276	1062	99
H(19B)	1150	10033	419	99
H(20A)	325	8128	158	147
H(20B)	259	8461	891	147
H(20C)	803	7146	701	147
H(21A)	1284	7395	–379	68
H(21B)	2162	7705	–578	68
H(22A)	878	9752	–657	121
H(22B)	1206	8976	–1249	121
H(22C)	1765	10112	–831	121
H(23A)	497	2034	1486	71
H(23B)	1024	2671	969	71
H(24A)	–136	4189	1587	106
H(24B)	–151	3942	838	106
H(24C)	494	5024	1205	106
H(25A)	818	4500	2382	70
H(25B)	1626	3895	2776	70
H(26A)	198	2205	2474	123
H(26B)	460	2931	3153	123
H(26C)	1000	1673	2906	123
H(27A)	2135	1657	1523	63
H(27B)	1670	1115	2096	63
H(28A)	2589	2423	2821	62
H(28B)	3040	1220	2452	62
H(29A)	4060	3448	1540	62
H(29B)	3395	2233	1358	62
H(30A)	4791	1905	2269	98
H(30B)	4641	1125	1591	98
H(30C)	4104	698	2140	98
H(31A)	4137	4662	2517	71
H(31B)	4158	3203	2918	71
H(32A)	2913	5277	2974	97
H(32B)	3726	5284	3464	97
H(32C)	3115	3949	3449	97

[(*i*-PrLi)$_3$·(TEEDA)$_2$] (106)

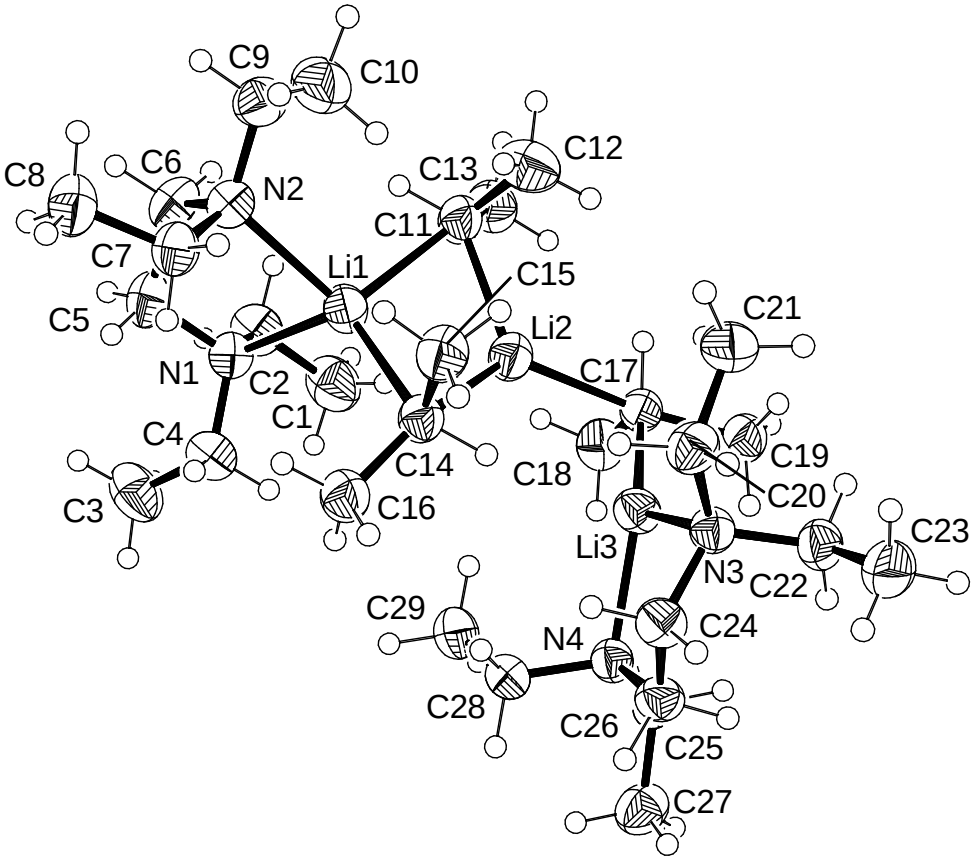


Abbildung 16 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von [(*i*-PrLi)$_3$·(TEEDA)$_2$] (**106**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 46 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für [(*i*-PrLi)$_3$·(TEEDA)$_2$] (**106**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	–1342(3)	8421(2)	9148(1)	71(1)
C(2)	–1082(3)	8691(2)	9815(1)	57(1)
C(3)	–2638(3)	7274(2)	10345(1)	69(1)
C(4)	–1199(3)	7234(2)	10187(1)	53(1)
C(5)	–302(3)	8352(2)	10875(1)	52(1)
C(6)	944(3)	8873(2)	11015(1)	54(1)
C(7)	2326(3)	7696(2)	11437(1)	48(1)
C(8)	2232(3)	7916(2)	12114(1)	59(1)
C(9)	3317(3)	9003(2)	11073(1)	57(1)
C(10)	4681(3)	8624(2)	11066(1)	68(1)
C(11)	2456(3)	8784(2)	9327(1)	50(1)

C(12)	3967(3)	8794(2)	9295(1)	69(1)
C(13)	1824(3)	9373(2)	8824(1)	60(1)
C(14)	2417(2)	6537(1)	9762(1)	44(1)
C(15)	3841(3)	6589(2)	10060(1)	57(1)
C(16)	1678(3)	5889(2)	10126(1)	53(1)
C(17)	2281(2)	7279(1)	7963(1)	41(1)
C(18)	824(3)	7473(2)	7763(1)	54(1)
C(19)	2926(3)	6950(1)	7398(1)	50(1)
C(20)	5354(3)	5556(2)	8837(1)	50(1)
C(21)	5935(3)	6402(2)	8685(1)	60(1)
C(22)	4910(2)	5099(2)	7759(1)	47(1)
C(23)	6087(3)	4491(2)	7770(1)	65(1)
C(24)	3681(2)	4484(1)	8580(1)	45(1)
C(25)	2438(2)	4236(1)	8172(1)	45(1)
C(26)	638(2)	4887(2)	7503(1)	47(1)
C(27)	–235(3)	4108(2)	7374(1)	60(1)
C(28)	575(2)	4874(1)	8634(1)	45(1)
C(29)	–399(3)	5598(2)	8654(1)	53(1)
Li(1)	1671(4)	7854(2)	10008(2)	47(1)
Li(2)	2318(4)	7482(2)	8988(2)	48(1)
Li(3)	2641(4)	6018(2)	8243(2)	44(1)
N(1)	–446(2)	8037(1)	10225(1)	44(1)
N(2)	2187(2)	8397(1)	10982(1)	45(1)
N(3)	4333(2)	5245(1)	8354(1)	40(1)
N(4)	1428(2)	4922(1)	8117(1)	39(1)

Tabelle 47 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für [(*i*-PrLi)$_3$·(TEEDA)$_2$] (**106**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	72(2)	85(2)	55(2)	14(2)	–1(1)	–13(2)
C(2)	55(2)	57(1)	58(2)	9(1)	0(1)	4(1)
C(3)	48(2)	91(2)	67(2)	15(2)	5(1)	–10(2)
C(4)	49(2)	54(1)	58(2)	4(1)	6(1)	–4(1)
C(5)	49(2)	64(2)	45(1)	–4(1)	11(1)	11(1)
C(6)	58(2)	54(1)	48(1)	–11(1)	2(1)	10(1)
C(7)	47(2)	52(1)	45(1)	0(1)	7(1)	6(1)
C(8)	55(2)	77(2)	45(1)	0(1)	8(1)	4(1)
C(9)	64(2)	55(1)	51(2)	–5(1)	1(1)	–8(1)
C(10)	56(2)	81(2)	66(2)	–1(2)	2(1)	–14(2)

C(11)	63(2)	46(1)	41(1)	1(1)	12(1)	–2(1)
C(12)	69(2)	64(2)	73(2)	11(1)	–2(2)	–13(2)
C(13)	71(2)	44(1)	67(2)	9(1)	19(1)	4(1)
C(14)	48(1)	45(1)	39(1)	1(1)	6(1)	–1(1)
C(15)	58(2)	61(2)	54(2)	–4(1)	9(1)	3(1)
C(16)	60(2)	52(1)	49(1)	3(1)	10(1)	–1(1)
C(17)	47(1)	38(1)	40(1)	1(1)	7(1)	1(1)
C(18)	54(2)	53(1)	54(2)	5(1)	6(1)	8(1)
C(19)	63(2)	44(1)	45(1)	4(1)	12(1)	2(1)
C(20)	49(2)	55(1)	45(1)	–4(1)	–1(1)	0(1)
C(21)	55(2)	64(2)	60(2)	–8(1)	2(1)	–13(1)
C(22)	40(1)	54(1)	47(1)	–5(1)	8(1)	0(1)
C(23)	55(2)	65(2)	79(2)	–17(2)	19(2)	2(1)
C(24)	44(1)	40(1)	51(1)	6(1)	4(1)	5(1)
C(25)	46(2)	37(1)	54(1)	0(1)	7(1)	0(1)
C(26)	47(2)	52(1)	42(1)	–4(1)	4(1)	5(1)
C(27)	49(2)	65(2)	65(2)	–16(1)	0(1)	–1(1)
C(28)	48(1)	43(1)	47(1)	1(1)	11(1)	–6(1)
C(29)	44(2)	59(1)	58(2)	–1(1)	14(1)	0(1)
Li(1)	47(2)	48(2)	46(2)	2(2)	10(2)	1(2)
Li(2)	53(3)	49(2)	41(2)	–2(2)	8(2)	0(2)
Li(3)	43(2)	39(2)	51(2)	4(2)	6(2)	2(2)
N(1)	44(1)	46(1)	42(1)	1(1)	5(1)	2(1)
N(2)	47(1)	45(1)	44(1)	–2(1)	3(1)	2(1)
N(3)	38(1)	43(1)	39(1)	0(1)	4(1)	0(1)
N(4)	39(1)	39(1)	40(1)	0(1)	7(1)	1(1)

Tabelle 48 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für g [(*i*-PrLi)$_3$·(TEEDA)$_2$] (**106**).

	x	y	z	U(eq)
H(1A)	–515	8187	9006	107
H(1B)	–1634	8912	8891	107
H(1C)	–2047	7986	9112	107
H(2A)	–497	9200	9836	68
H(2B)	–1947	8855	9970	68
H(3A)	–2660	7485	10771	103
H(3B)	–3035	6705	10311	103
H(3C)	–3152	7658	10054	103

H(4A)	–711	6820	10470	64
H(4B)	–1198	7011	9757	64
H(5A)	–275	7862	11164	63
H(5B)	–1097	8700	10947	63
H(6A)	925	9352	10716	64
H(6B)	940	9116	11438	64
H(7A)	3206	7419	11403	57
H(7B)	1621	7270	11312	57
H(8A)	2837	8391	12232	88
H(8B)	2493	7422	12374	88
H(8C)	1306	8078	12174	88
H(9A)	3269	9294	11478	69
H(9B)	3200	9440	10742	69
H(10A)	4886	8278	11441	101
H(10B)	5350	9078	11057	101
H(10C)	4706	8265	10695	101
H(12A)	4184	8509	8913	104
H(12B)	4409	8497	9658	104
H(12C)	4284	9383	9294	104
H(13A)	2293	9921	8849	90
H(13B)	873	9460	8884	90
H(13C)	1898	9119	8413	90
H(15A)	3848	6860	10470	86
H(15B)	4384	6925	9795	86
H(15C)	4217	6015	10110	86
H(16A)	2164	5347	10137	80
H(16B)	767	5807	9924	80
H(16C)	1629	6093	10553	80
H(18A)	763	7826	7387	81
H(18B)	430	7778	8098	81
H(18C)	334	6941	7675	81
H(19A)	2622	6367	7306	75
H(19B)	3907	6956	7485	75
H(19C)	2664	7314	7037	75
H(20A)	6091	5134	8895	60
H(20B)	4943	5603	9236	60
H(21A)	6495	6337	8338	90
H(21B)	6487	6619	9051	90
H(21C)	5204	6803	8566	90
H(22A)	5202	5655	7603	56
H(22B)	4186	4884	7454	56
H(23A)	6855	4726	8031	98

H(23B)	6335	4409	7345	98
H(23C)	5833	3943	7941	98
H(24A)	3436	4592	9008	54
H(24B)	4327	4006	8601	54
H(25A)	2690	4089	7751	55
H(25B)	2037	3724	8347	55
H(26A)	1269	4925	7177	57
H(26B)	51	5395	7462	57
H(27A)	326	3596	7422	90
H(27B)	–671	4135	6948	90
H(27C)	–922	4087	7670	90
H(28A)	1160	4860	9031	55
H(28B)	63	4334	8600	55
H(29A)	95	6137	8678	80
H(29B)	–900	5539	9022	80
H(29C)	–1029	5591	8277	80
H(11)	2300(30)	9063(17)	9731(13)	73(8)
H(14)	2490(20)	6293(13)	9319(10)	43(6)
H(17)	2740(20)	7833(14)	8058(10)	47(6)

t-BuLi·TEEDA (107)

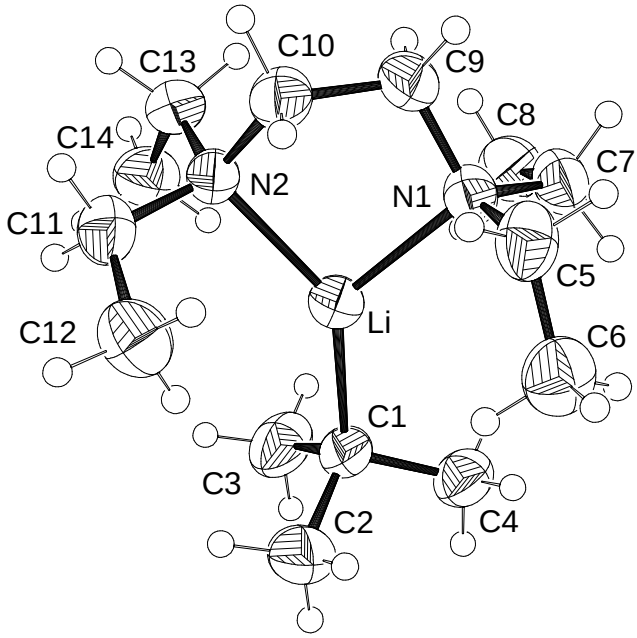


Abbildung 17 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von *t*-BuLi·TEEDA (**107**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 49 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter ($Å^2$ x 10^3) für *t*-BuLi·TEEDA (**107**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen Uij Tensors

	x	y	z	U(eq)
C(1)	255(3)	7128(1)	10378(1)	47(1)
C(2)	–1605(3)	6645(2)	10314(1)	72(1)
C(3)	1696(3)	6529(2)	10951(1)	73(1)
C(4)	155(3)	8063(1)	10819(1)	57(1)
C(5)	789(3)	9342(2)	8776(2)	57(1)
C(6)	–1252(4)	9119(2)	8638(2)	65(1)
C(7)	3891(3)	8723(2)	9027(2)	61(1)
C(8)	4410(4)	8707(2)	9960(2)	69(1)
C(9)	1665(3)	8241(1)	7797(1)	55(1)
C(10)	2124(3)	7214(1)	7700(1)	56(1)
C(11)	–820(3)	6450(2)	7575(1)	55(1)
C(12)	–2231(4)	6082(2)	8028(2)	61(1)
C(13)	1955(4)	5653(2)	8292(2)	59(1)
C(14)	3597(4)	5668(2)	9017(2)	67(1)
Li(1)	982(4)	7312(2)	9221(2)	46(1)
N(1)	1921(2)	8512(1)	8680(1)	46(1)
N(2)	1032(2)	6579(1)	8117(1)	43(1)

Tabelle 50 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung *t*-BuLi·TEEDA (**107**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	58(1)	45(1)	39(1)	–2(1)	12(1)	–4(1)
C(2)	89(2)	76(2)	57(2)	–14(1)	30(1)	–28(1)
C(3)	107(2)	63(2)	49(1)	4(1)	17(1)	8(1)
C(4)	63(2)	61(1)	48(1)	–7(1)	15(1)	–6(1)
C(5)	66(2)	42(1)	66(2)	4(1)	18(1)	2(1)
C(6)	64(2)	57(2)	72(2)	4(2)	11(1)	11(1)
C(7)	58(2)	55(2)	76(2)	–8(1)	24(1)	–14(1)
C(8)	51(2)	73(2)	78(2)	–2(2)	4(1)	–7(1)
C(9)	73(2)	47(1)	50(1)	5(1)	23(1)	–7(1)
C(10)	73(2)	53(1)	50(1)	–5(1)	30(1)	–8(1)
C(11)	64(2)	54(1)	43(1)	–1(1)	7(1)	–3(1)
C(12)	53(2)	71(2)	57(2)	3(2)	4(1)	–10(1)
C(13)	67(2)	47(1)	62(2)	–7(1)	12(1)	5(1)
C(14)	53(2)	64(2)	82(2)	7(2)	12(1)	6(1)

Li(1)	52(2)	44(2)	42(2)	1(2)	12(2)	–2(2)
N(1)	51(1)	39(1)	52(1)	–1(1)	16(1)	–2(1)
N(2)	50(1)	39(1)	41(1)	–1(1)	13(1)	–2(1)

Tabelle 51 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung *t*-BuLi·TEEDA (**107**).

	x	y	z	U(eq)
H(2A)	–1872	6597	10871	108
H(2B)	–1566	6009	10079	108
H(2C)	–2577	7018	9951	108
H(3A)	2918	6825	11012	110
H(3B)	1718	5894	10713	110
H(3C)	1383	6483	11499	110
H(4A)	–819	8458	10483	85
H(4B)	1349	8389	10895	85
H(4C)	–130	7945	11365	85
H(9A)	2471	8640	7530	66
H(9B)	363	8359	7507	66
H(10A)	1880	7055	7099	68
H(10B)	3460	7111	7937	68
H(18)	4580(40)	6116(17)	8940(15)	99(9)
H(9)	5690(30)	8801(15)	10151(13)	74(7)
H(10)	4150(30)	8089(17)	10195(14)	88(8)
H(8)	3730(30)	9234(17)	10230(15)	108(9)
H(5)	–1470(30)	8598(16)	8972(13)	73(7)
H(3)	–1780(30)	8946(17)	8061(17)	102(9)
H(15)	–2360(30)	6525(16)	8470(14)	80(8)
H(13)	–3450(30)	6045(13)	7671(12)	59(6)
H(14)	–1880(30)	5443(17)	8272(14)	86(8)
H(2)	1250(30)	9568(15)	9369(14)	82(8)
H(1)	960(20)	9854(14)	8385(12)	62(6)
H(16)	2330(30)	5453(14)	7764(14)	76(7)
H(17)	960(30)	5206(15)	8370(13)	78(7)
H(11)	–1230(30)	7104(14)	7332(12)	63(6)
H(12)	–710(30)	6015(13)	7117(12)	62(6)
H(4)	–1880(30)	9686(16)	8730(13)	74(7)
H(6)	4230(30)	9352(14)	8804(12)	60(6)
H(7)	4670(30)	8238(14)	8821(12)	65(6)

H(20)	3240(30)	5878(16)	9545(17)	105(10)
H(19)	4200(30)	5056(18)	9095(14)	96(9)

2-(Diethylamino)ethyl-(ethyl)lithiumamid (108)

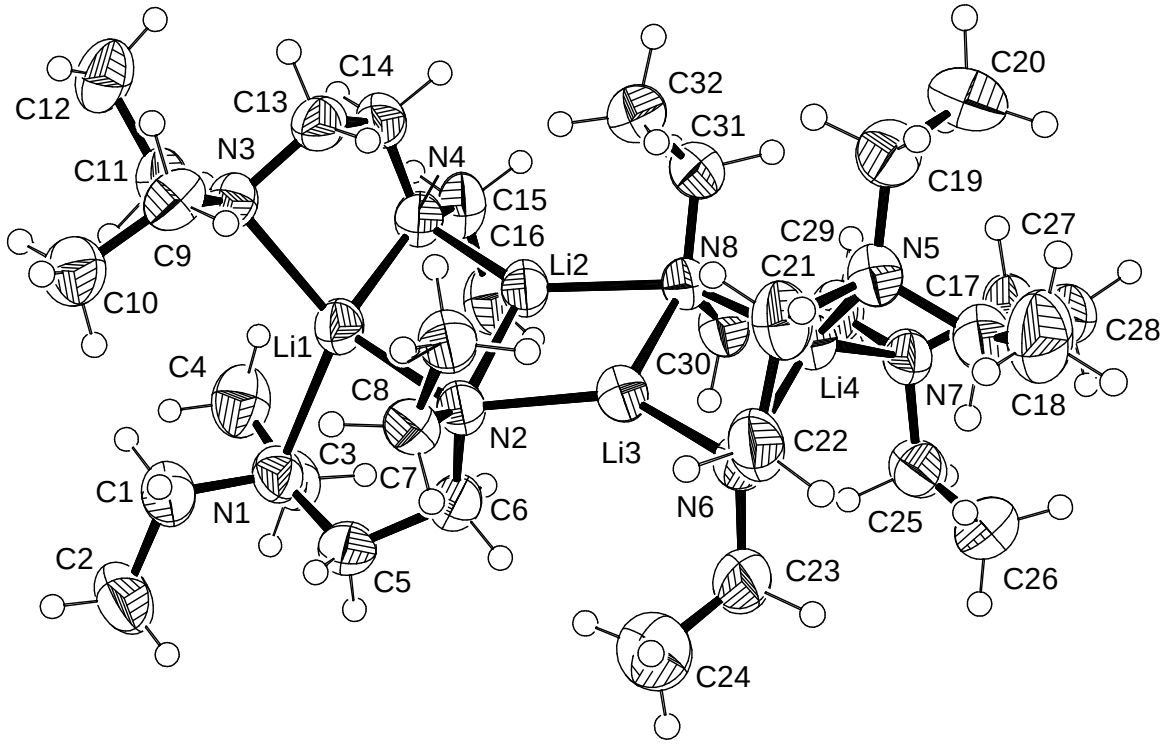


Abbildung 18 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von 2-(Diethylamino)ethyl-(ethyl)lithiumamid (**108**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 52 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für 2-(Diethylamino)ethyl-(ethyl)lithiumamid (**108**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	5414(3)	12611(2)	1757(2)	64(1)
C(2)	6664(4)	12524(3)	1246(2)	83(1)
C(3)	6339(3)	11807(2)	2734(2)	65(1)
C(4)	6967(3)	12771(2)	3507(2)	80(1)
C(5)	4327(3)	10785(2)	1483(2)	62(1)
C(6)	3135(3)	10065(2)	1747(2)	59(1)

C(7)	995(3)	10620(2)	1255(2)	56(1)
C(8)	-650(3)	10633(2)	1312(2)	58(1)
C(9)	1491(3)	13648(2)	2472(2)	56(1)
C(10)	2444(4)	14118(2)	1954(2)	71(1)
C(11)	3719(3)	14228(2)	3660(2)	58(1)
C(12)	3360(4)	15210(2)	4166(2)	75(1)
C(13)	1312(3)	12999(2)	3605(2)	54(1)
C(14)	2062(3)	12654(2)	4274(2)	56(1)
C(15)	3661(3)	11721(2)	4660(2)	63(1)
C(16)	4702(4)	11034(2)	4421(2)	75(1)
C(17)	–4684(3)	6373(2)	1361(2)	64(1)
C(18)	–6275(4)	5953(3)	753(2)	91(1)
C(19)	–5082(3)	7935(2)	2303(2)	63(1)
C(20)	–5211(4)	7569(3)	3036(2)	76(1)
C(21)	–3864(3)	8019(2)	1152(2)	66(1)
C(22)	–2756(4)	7676(2)	608(2)	71(1)
C(23)	–315(5)	7201(2)	598(2)	103(1)
C(24)	250(5)	7584(3)	–22(2)	119(2)
C(25)	97(3)	6255(2)	2427(2)	64(1)
C(26)	–968(4)	5397(2)	1662(2)	84(1)
C(27)	–1842(3)	6275(2)	3296(2)	64(1)
C(28)	–1196(4)	5692(2)	3811(2)	81(1)
C(29)	436(3)	7743(2)	3668(2)	60(1)
C(30)	1157(3)	8658(2)	3415(2)	57(1)
C(31)	–681(3)	9595(2)	3749(2)	59(1)
C(32)	–1535(3)	10300(2)	3535(2)	65(1)
Li(1)	3147(5)	11946(3)	2814(3)	52(1)
Li(2)	1554(5)	10527(3)	3124(3)	52(1)
Li(3)	104(5)	9092(3)	1900(3)	55(1)
Li(4)	–1612(5)	7755(3)	2241(3)	52(1)
N(1)	4997(2)	11817(2)	2141(1)	55(1)
N(2)	1786(2)	10412(1)	1955(1)	48(1)
N(3)	2377(2)	13361(2)	3110(1)	48(1)
N(4)	2854(2)	11893(2)	3944(1)	50(1)
N(5)	–4081(2)	7504(2)	1774(1)	53(1)
N(6)	–1289(3)	7758(2)	1107(1)	59(1)
N(7)	–711(2)	6893(2)	2967(1)	55(1)
N(8)	80(2)	9145(1)	3089(1)	47(1)

Tabelle 53 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für 2-(Diethylamino)ethyl-(ethyl)lithiumamid (**108**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2$ [$h^2a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	58(2)	64(2)	82(2)	39(2)	21(2)	18(1)
C(2)	71(2)	92(2)	104(3)	56(2)	38(2)	19(2)
C(3)	51(2)	71(2)	90(2)	42(2)	27(2)	23(2)
C(4)	57(2)	73(2)	102(2)	35(2)	4(2)	8(2)
C(5)	57(2)	58(2)	77(2)	22(1)	30(2)	22(1)
C(6)	60(2)	46(1)	71(2)	19(1)	20(1)	14(1)
C(7)	63(2)	57(2)	57(2)	24(1)	24(1)	19(1)
C(8)	59(2)	56(2)	60(2)	23(1)	15(1)	14(1)
C(9)	53(2)	48(1)	60(2)	12(1)	2(1)	17(1)
C(10)	83(2)	71(2)	69(2)	34(2)	15(2)	29(2)
C(11)	54(2)	54(2)	61(2)	25(1)	6(1)	6(1)
C(12)	86(2)	47(2)	70(2)	12(1)	–2(2)	3(2)
C(13)	49(2)	47(1)	62(2)	13(1)	14(1)	12(1)
C(14)	60(2)	48(1)	53(2)	14(1)	18(1)	3(1)
C(15)	71(2)	54(2)	60(2)	27(1)	6(2)	3(2)
C(16)	74(2)	75(2)	85(2)	45(2)	10(2)	20(2)
C(17)	66(2)	56(2)	65(2)	22(1)	18(2)	6(1)
C(18)	83(2)	73(2)	90(2)	24(2)	2(2)	–13(2)
C(19)	48(2)	64(2)	72(2)	22(2)	8(1)	15(1)
C(20)	68(2)	102(2)	69(2)	33(2)	26(2)	35(2)
C(21)	60(2)	65(2)	67(2)	31(2)	2(2)	3(2)
C(22)	84(2)	58(2)	51(2)	16(1)	15(2)	–11(2)
C(23)	157(4)	53(2)	73(2)	2(2)	55(2)	–9(2)
C(24)	139(4)	92(3)	100(3)	16(2)	46(3)	–1(3)
C(25)	70(2)	64(2)	80(2)	40(2)	33(2)	32(2)
C(26)	102(3)	58(2)	97(2)	22(2)	41(2)	27(2)
C(27)	72(2)	54(2)	82(2)	35(2)	35(2)	21(2)
C(28)	107(3)	64(2)	104(2)	50(2)	59(2)	40(2)
C(29)	61(2)	59(2)	69(2)	34(1)	12(2)	19(1)
C(30)	50(2)	56(2)	66(2)	28(1)	12(1)	10(1)
C(31)	67(2)	58(2)	57(2)	24(1)	22(1)	16(1)
C(32)	64(2)	55(2)	76(2)	19(1)	24(2)	18(1)
Li(1)	49(2)	44(2)	63(3)	19(2)	15(2)	9(2)
Li(2)	59(3)	44(2)	52(2)	20(2)	14(2)	6(2)
Li(3)	59(3)	49(2)	56(3)	19(2)	20(2)	9(2)
Li(4)	53(3)	46(2)	58(3)	20(2)	18(2)	11(2)
N(1)	47(1)	53(1)	73(2)	30(1)	21(1)	17(1)

N(2)	48(1)	45(1)	54(1)	22(1)	16(1)	12(1)
N(3)	43(1)	44(1)	54(1)	18(1)	7(1)	10(1)
N(4)	54(1)	45(1)	50(1)	19(1)	10(1)	9(1)
N(5)	50(1)	51(1)	58(1)	22(1)	13(1)	9(1)
N(6)	67(2)	48(1)	53(1)	10(1)	23(1)	3(1)
N(7)	56(1)	47(1)	70(1)	27(1)	24(1)	17(1)
N(8)	51(1)	43(1)	51(1)	21(1)	17(1)	13(1)

Tabelle 54 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für 2-(Diethylamino)ethyl-(ethyl)lithiumamid (**108**).

	x	y	z	U(eq)
H(1A)	5766	13295	2215	77
H(1B)	4462	12593	1382	77
H(2A)	7657	12639	1623	124
H(2B)	6766	13042	973	124
H(2C)	6372	11833	813	124
H(3A)	7181	11708	2431	78
H(3B)	6028	11210	2918	78
H(4A)	7412	13354	3338	119
H(4B)	7774	12677	3897	119
H(4C)	6123	12910	3787	119
H(5A)	5175	10469	1352	74
H(5B)	3822	10860	961	74
H(6A)	2759	9387	1281	70
H(6B)	3670	9958	2245	70
H(7A)	978	10086	716	67
H(7B)	1578	11296	1250	67
H(8D)	–1274	9936	1228	87
H(8E)	–1095	10867	874	87
H(8F)	–648	11104	1870	87
H(9A)	957	14145	2764	68
H(9B)	679	13023	2082	68
H(10A)	3145	14792	2319	106
H(10B)	1749	14204	1503	106
H(10C)	3055	13663	1703	106
H(11A)	4429	14407	3302	69
H(11B)	4286	13987	4063	69
H(12A)	2815	15469	3777	112

H(12B)	4333	15734	4497	112
H(12C)	2703	15058	4547	112
H(13A)	438	12416	3212	65
H(13B)	876	13563	3881	65
H(14A)	2815	13262	4720	67
H(14B)	1252	12363	4537	67
H(15A)	2885	11404	4928	76
H(15B)	4295	12394	5082	76
H(16A)	4112	10400	3951	112
H(16B)	5090	10860	4908	112
H(16C)	5582	11396	4248	112
H(17A)	–4732	6068	1809	77
H(17B)	–3923	6127	1045	77
H(18A)	–7055	6172	1057	137
H(18B)	–6551	5198	526	137
H(18C)	–6241	6219	288	137
H(19A)	–6135	7754	1946	75
H(19B)	–4675	8697	2524	75
H(20A)	–5777	6835	2824	114
H(20B)	–5772	7962	3404	114
H(20C)	–4169	7672	3358	114
H(21A)	–3466	8773	1457	79
H(21B)	–4886	7882	780	79
H(22A)	–3234	6951	227	85
H(22B)	–2581	8106	251	85
H(23A)	592	7205	997	123
H(23B)	–934	6472	305	123
H(24A)	–630	7584	–427	178
H(24B)	834	7142	–322	178
H(24C)	931	8289	258	178
H(25A)	685	5953	2769	77
H(25B)	856	6705	2236	77
H(26A)	–1576	4870	1841	126
H(26B)	–350	5089	1281	126
H(26C)	–1672	5674	1367	126
H(27A)	–2662	5770	2810	77
H(27B)	–2345	6743	3653	77
H(28A)	–800	5167	3449	121
H(28B)	–2023	5357	4034	121
H(28C)	–350	6176	4282	121
H(29A)	1275	7479	3876	72
H(29B)	–76	7986	4138	72

H(30A)	1915	9189	3915	68
H(30B)	1742	8420	2979	68
H(31A)	109	9985	4282	71
H(31B)	–1421	9035	3843	71
H(32A)	–791	10906	3516	97
H(32B)	–2122	10520	3966	97
H(32C)	–2253	9937	2982	97

$ZnBr_2$·(*R,R*)-TECDA (110)

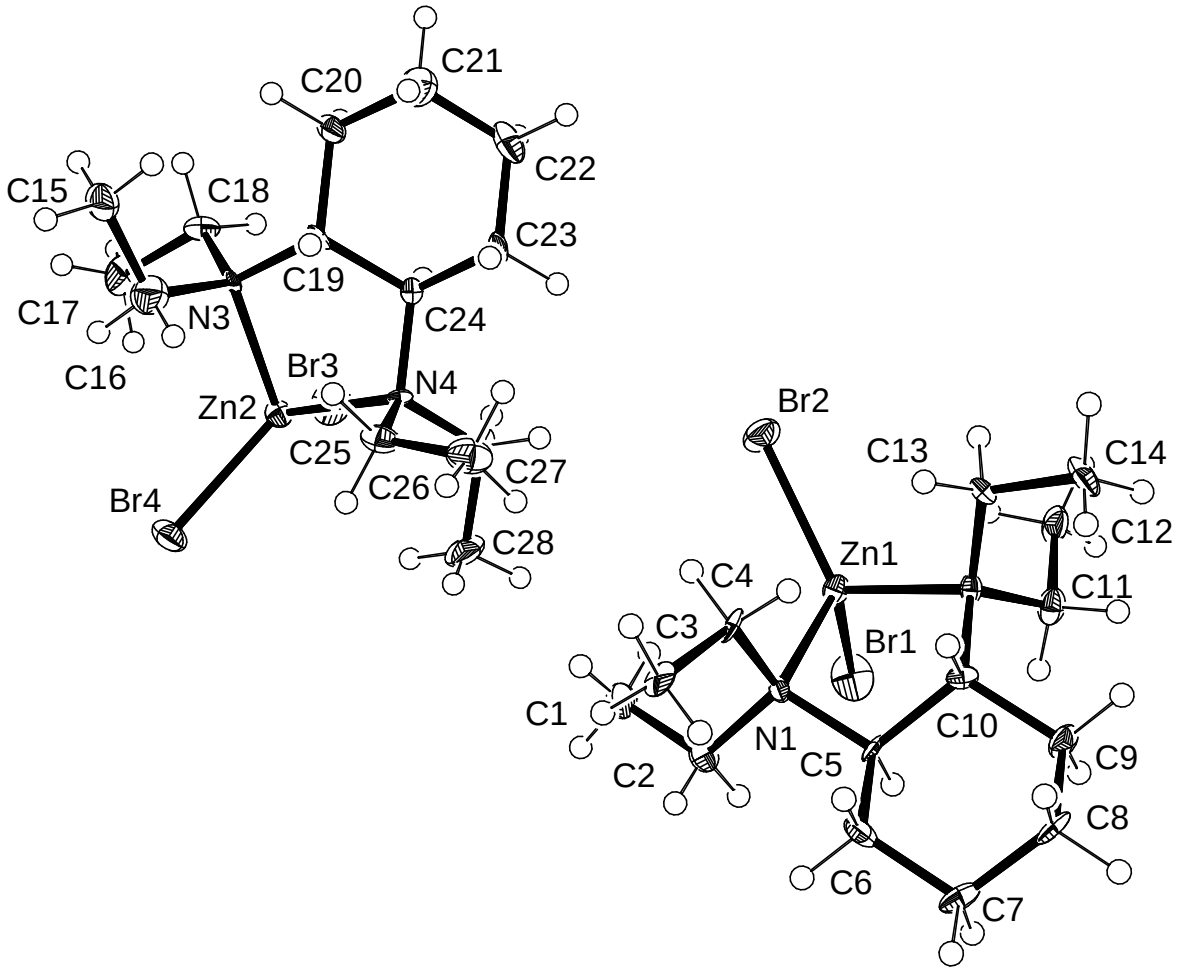


Abbildung 19 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von $ZnBr_2$·(*R,R*)-TECDA (**110**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 55 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für $ZnBr_2$·(*R*,*R*)-TECDA (**110**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
Br(1)	12030(1)	1105(1)	5336(1)	33(1)
Br(2)	8411(1)	2978(1)	4271(1)	25(1)
Br(3)	12167(1)	3588(1)	376(1)	30(1)
Br(4)	8846(1)	1622(1)	–734(1)	25(1)
C(1)	8791(7)	320(4)	3366(4)	27(2)
C(2)	8412(6)	–186(5)	4105(4)	22(2)
C(3)	4514(6)	72(4)	3660(3)	23(2)
C(4)	5790(5)	767(4)	4184(3)	15(1)
C(5)	7551(5)	–75(3)	5452(3)	12(1)
C(6)	6439(6)	–971(4)	5396(4)	19(2)
C(7)	6694(6)	–1464(3)	6226(3)	21(1)
C(8)	6226(6)	–804(4)	6872(3)	19(1)
C(9)	7286(6)	105(4)	6940(4)	19(2)
C(10)	7052(6)	602(3)	6087(3)	12(1)
C(11)	9489(5)	1642(5)	6849(3)	19(1)
C(12)	10457(6)	2577(4)	6858(4)	24(2)
C(13)	6679(6)	2321(4)	6086(4)	16(1)
C(14)	5799(6)	2394(4)	6828(4)	25(2)
C(15)	4451(6)	4264(4)	–1471(4)	26(2)
C(16)	5897(5)	3607(4)	–1040(3)	17(1)
C(17)	9081(6)	4326(4)	–1556(4)	26(2)
C(18)	8373(6)	4749(5)	–839(4)	19(2)
C(19)	6750(5)	4437(3)	308(3)	10(1)
C(20)	6477(6)	5504(4)	285(4)	20(2)
C(21)	5747(6)	5834(3)	1016(3)	29(2)
C(22)	6949(6)	5546(4)	1822(4)	27(2)
C(23)	7149(6)	4487(4)	1850(4)	19(2)
C(24)	7932(5)	4142(3)	1129(3)	14(1)
C(25)	6781(5)	2454(4)	1078(4)	20(2)
C(26)	6115(6)	2247(4)	1870(4)	30(2)
C(27)	9741(5)	2879(5)	1867(3)	22(2)
C(28)	10489(6)	1899(4)	1829(4)	32(2)
N(1)	7531(5)	412(3)	4645(3)	12(1)
N(2)	7969(4)	1556(4)	6118(3)	12(1)
N(3)	7394(5)	4043(3)	–435(3)	10(1)
N(4)	8323(4)	3108(3)	1140(3)	10(1)
Zn(1)	9058(1)	1595(1)	5048(1)	14(1)
Zn(2)	9255(1)	3007(1)	52(1)	15(1)

Tabelle 56 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für $ZnBr_2$·(*R,R*)-TECDA (**110**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	12(1)	50(1)	38(1)	–4(1)	5(1)	4(1)
Br(2)	31(1)	20(1)	25(1)	8(1)	5(1)	–3(1)
Br(3)	12(1)	42(1)	36(1)	1(1)	5(1)	–6(1)
Br(4)	23(1)	21(1)	28(1)	–10(1)	3(1)	5(1)
C(1)	39(3)	25(4)	19(4)	–1(3)	13(3)	4(3)
C(2)	31(3)	21(4)	17(4)	–1(3)	14(3)	9(3)
C(3)	23(3)	22(4)	15(3)	3(3)	–15(2)	1(2)
C(4)	12(2)	23(3)	7(3)	8(3)	–2(2)	2(2)
C(5)	13(2)	17(3)	7(3)	8(2)	4(2)	6(2)
C(6)	25(3)	12(4)	21(4)	–7(3)	9(3)	–2(2)
C(7)	22(3)	17(3)	26(3)	13(3)	8(2)	–1(2)
C(8)	20(3)	20(3)	17(3)	15(3)	5(3)	1(2)
C(9)	24(3)	21(4)	15(4)	7(3)	10(3)	2(3)
C(10)	10(2)	10(3)	18(3)	2(2)	4(2)	–2(2)
C(11)	19(2)	24(3)	14(4)	1(3)	5(2)	–7(3)
C(12)	34(3)	25(4)	11(4)	0(3)	–3(3)	–8(3)
C(13)	22(3)	13(3)	14(4)	–4(3)	6(3)	3(2)
C(14)	27(3)	28(4)	21(4)	–13(3)	9(3)	5(3)
C(15)	24(3)	26(4)	24(4)	–6(3)	–2(3)	–2(3)
C(16)	22(2)	18(3)	9(3)	–12(3)	–3(2)	–7(2)
C(17)	30(3)	36(4)	17(4)	6(3)	16(3)	–1(3)
C(18)	17(3)	12(4)	27(5)	2(3)	6(3)	1(3)
C(19)	11(2)	8(3)	13(3)	–7(2)	4(2)	–4(2)
C(20)	16(3)	19(4)	20(4)	–9(3)	–6(3)	5(3)
C(21)	29(3)	8(3)	49(4)	–11(3)	5(3)	12(2)
C(22)	27(3)	34(4)	23(4)	–13(3)	10(3)	0(3)
C(23)	25(3)	26(4)	8(4)	–4(3)	5(3)	5(3)
C(24)	16(2)	14(3)	10(3)	–1(2)	1(2)	1(2)
C(25)	15(3)	15(3)	31(4)	–3(3)	4(3)	1(2)
C(26)	28(3)	24(4)	41(5)	1(3)	16(3)	3(3)
C(27)	21(2)	29(4)	13(4)	6(3)	1(2)	3(3)
C(28)	35(3)	32(4)	29(5)	13(3)	8(3)	20(3)
N(1)	12(2)	14(3)	9(3)	–3(2)	1(2)	2(2)
N(2)	11(2)	17(3)	9(3)	–1(3)	1(2)	–3(2)
N(3)	13(2)	8(2)	8(3)	–4(2)	2(2)	–6(2)
N(4)	12(2)	5(3)	14(3)	3(2)	4(2)	–1(2)
Zn(1)	13(1)	17(1)	13(1)	1(1)	3(1)	–2(1)
Zn(2)	12(1)	16(1)	16(1)	–2(1)	3(1)	1(1)

Tabelle 57 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für $ZnBr_2$·(*R*,*R*)-TECDA (**110**).

	x	y	z	U(eq)
H(1A)	7684	499	2997	40
H(1B)	9455	–94	3068	40
H(1C)	9483	885	3549	40
H(2A)	7652	–734	3911	26
H(2B)	9528	–427	4441	26
H(3A)	5076	–216	3242	34
H(3B)	3453	406	3384	34
H(3C)	4199	–419	4020	34
H(4A)	6015	1278	3812	18
H(4B)	5182	1052	4594	18
H(5)	8794	–269	5676	14
H(6A)	5185	–807	5205	23
H(6B)	6771	–1402	4983	23
H(7A)	7932	–1667	6402	25
H(7B)	5940	–2030	6175	25
H(8A)	6454	–1123	7418	23
H(8B)	4959	–653	6721	23
H(9A)	8544	–38	7151	23
H(9B)	6898	531	7341	23
H(10)	5767	727	5900	15
H(11A)	10323	1121	6833	23
H(11B)	9048	1582	7368	23
H(12A)	10696	2698	6308	37
H(12B)	11567	2548	7267	37
H(12C)	9728	3084	7006	37
H(13A)	5752	2238	5580	19
H(13B)	7275	2924	6030	19
H(14A)	5049	1843	6842	37
H(14B)	5084	2966	6780	37
H(14C)	6701	2419	7341	37
H(15A)	3898	4566	–1057	39
H(15B)	3568	3904	–1859	39
H(15C)	4955	4747	–1776	39
H(16A)	5356	3122	–743	21
H(16B)	6385	3281	–1472	21
H(17A)	9631	3718	–1386	39
H(17B)	9953	4752	–1706	39
H(17C)	8113	4237	–2035	39

H(18A)	9364	5001	–419	22
H(18B)	7580	5278	–1049	22
H(19)	5574	4148	295	12
H(20A)	7612	5821	293	24
H(20B)	5657	5680	–237	24
H(21A)	5623	6527	998	35
H(21B)	4569	5557	985	35
H(22A)	6453	5760	2296	33
H(22B)	8113	5844	1866	33
H(23A)	7922	4300	2381	23
H(23B)	5987	4192	1820	23
H(24)	9075	4477	1169	17
H(25A)	7098	1847	854	24
H(25B)	5792	2719	665	24
H(26A)	7064	1969	2285	45
H(26B)	5129	1806	1744	45
H(26C)	5726	2833	2087	45
H(27A)	9272	2937	2379	26
H(27B)	10700	3344	1902	26
H(28A)	9548	1434	1794	48
H(28B)	11392	1783	2330	48
H(28C)	11011	1846	1339	48

i-PrLi·(*R*,*R*)-TECDA (111)

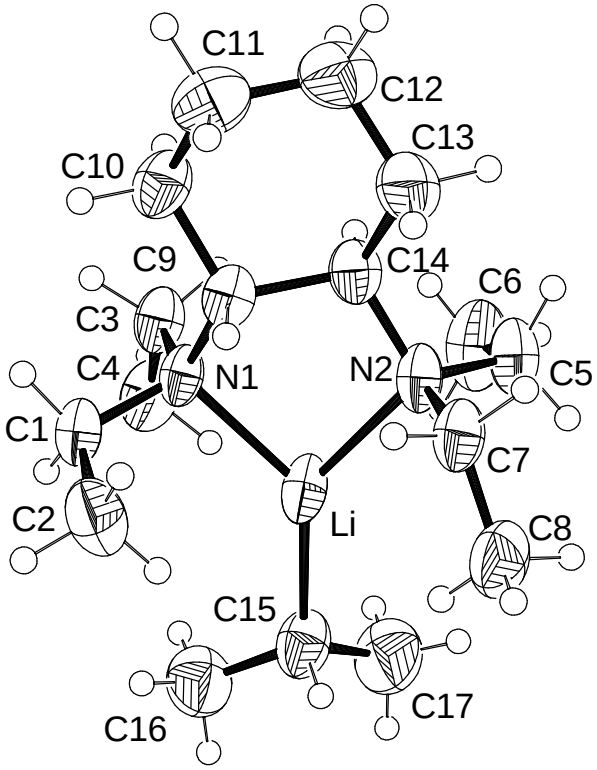


Abbildung 20 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von *i*-PrLi·(*R*,*R*)-TECDA (**111**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 58 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für *i*-PrLi·(*R*,*R*)-TECDA (**111**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
C(1)	889(4)	3092(2)	1217(2)	49(1)
C(2)	2343(5)	3315(2)	1783(2)	69(1)
C(3)	–1341(4)	3641(2)	321(2)	50(1)
C(4)	–426(5)	3590(2)	–494(2)	63(1)
C(5)	–948(5)	6575(2)	883(2)	63(1)
C(6)	–1465(6)	6347(2)	12(2)	85(1)
C(7)	795(4)	6067(2)	2030(2)	54(1)
C(8)	2514(5)	6465(2)	1766(2)	70(1)
C(9)	–1161(4)	4208(2)	1731(2)	44(1)
C(10)	–2686(4)	3614(2)	1977(2)	56(1)
C(11)	–3572(5)	3957(2)	2741(2)	68(1)
C(12)	–4209(4)	4910(2)	2591(2)	71(1)
C(13)	–2717(4)	5523(2)	2373(2)	61(1)

C(14)	–1757(4)	5194(2)	1603(2)	46(1)
C(15)	3572(5)	5053(2)	–68(2)	58(1)
C(16)	4210(5)	4204(2)	–492(2)	77(1)
C(17)	3528(5)	5811(2)	–694(2)	91(1)
Li	1301(7)	4948(3)	616(3)	50(1)
N(1)	–193(3)	3875(1)	1008(1)	41(1)
N(2)	–303(3)	5780(1)	1338(1)	48(1)

Tabelle 59 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung *i*-PrLi·(*R*,*R*)-TECDA (**111**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	67(2)	30(1)	50(2)	–3(1)	–3(2)	–2(1)
C(2)	79(2)	56(2)	73(2)	–13(2)	–14(2)	16(2)
C(3)	72(2)	40(1)	37(2)	–5(1)	–5(2)	–6(2)
C(4)	91(3)	59(2)	39(2)	–5(1)	–4(2)	–10(2)
C(5)	92(2)	36(1)	60(2)	2(1)	–5(2)	7(2)
C(6)	134(4)	61(2)	59(2)	19(2)	–20(2)	3(2)
C(7)	75(2)	38(1)	49(2)	–11(1)	–2(2)	–2(2)
C(8)	85(2)	51(2)	74(2)	–18(2)	0(2)	–11(2)
C(9)	59(2)	40(1)	33(1)	0(1)	–4(1)	–5(1)
C(10)	71(2)	50(2)	46(2)	7(1)	4(2)	–8(2)
C(11)	70(2)	81(2)	52(2)	7(2)	7(2)	–12(2)
C(12)	68(2)	88(2)	57(2)	–23(2)	13(2)	–7(2)
C(13)	71(2)	58(2)	55(2)	–19(2)	4(2)	1(2)
C(14)	61(2)	41(1)	37(2)	–5(1)	–4(1)	2(1)
C(15)	78(2)	48(2)	48(2)	–5(1)	11(2)	–7(2)
C(16)	85(3)	72(2)	73(2)	–2(2)	19(2)	3(2)
C(17)	106(3)	74(2)	92(3)	20(2)	27(3)	–6(2)
Li	78(3)	30(2)	42(2)	–1(2)	4(3)	–7(2)
N(1)	60(1)	28(1)	33(1)	–3(1)	–3(1)	–5(1)
N(2)	71(2)	32(1)	40(1)	–4(1)	–4(1)	1(1)

Tabelle 60 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für *i*-PrLi·(*R*,*R*)-TECDA (**111**).

	x	y	z	U(eq)
H(1A)	1363	2834	705	59
H(1B)	163	2626	1477	59
H(2A)	1886	3495	2319	104
H(2B)	3015	3812	1552	104
H(2C)	3080	2785	1849	104
H(3A)	–2263	4099	285	60
H(3B)	–1886	3052	436	60
H(4A)	330	3063	–501	94
H(4B)	257	4138	–575	94
H(4C)	–1272	3537	–936	94
H(5A)	–44	7044	872	75
H(5B)	–1951	6827	1177	75
H(6A)	–2402	5908	20	127
H(6B)	–480	6092	–280	127
H(6C)	–1847	6896	–269	127
H(7A)	1012	5540	2388	65
H(7B)	168	6521	2358	65
H(8A)	2325	7053	1509	105
H(8B)	3068	6059	1373	105
H(8C)	3253	6539	2248	105
H(9)	–346	4210	2205	53
H(10A)	–3521	3596	1521	67
H(10B)	–2278	2991	2075	67
H(11A)	–2760	3953	3207	81
H(11B)	–4550	3560	2879	81
H(12A)	–4786	5139	3090	85
H(12B)	–5054	4909	2138	85
H(13A)	–1909	5548	2840	74
H(13B)	–3153	6141	2275	74
H(14)	–2607	5188	1144	55
H(15)	4470(40)	5202(19)	364(18)	63(9)
H(15A)	5286	4335	–778	115
H(15B)	3349	4000	–889	115
H(15C)	4404	3731	–83	115
H(17A)	2660	5678	–1111	136
H(17B)	4655	5866	–955	136
H(17C)	3241	6378	–418	136

(1*R*,2*R*)-2-(Diethylamino)cyclohexyl(ethyl)lithiumamid [(*R,R*)-113]

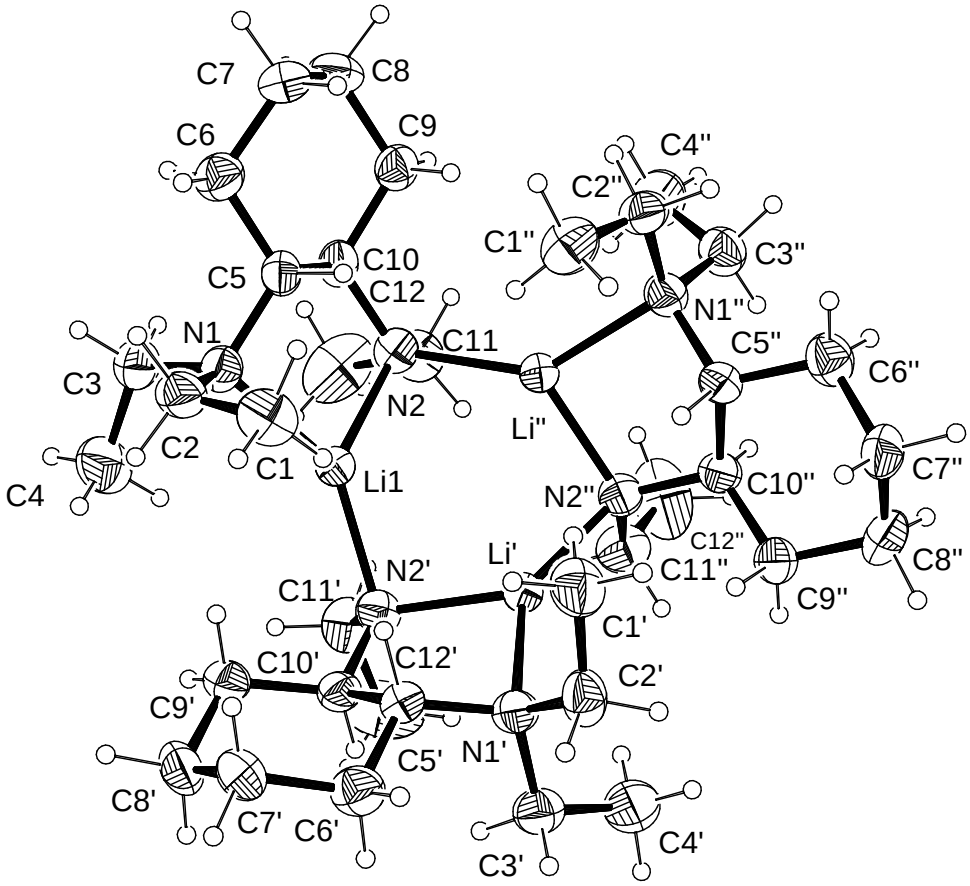


Abbildung 21 Thermische Auslenkungsellipsoide (30% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von (1*R*,2*R*)-2-(Diethylamino)cyclohexylethyllithiumamid (**113**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 61 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für (1*R*,2*R*)-2-(Diethylamino)cyclohexylethyllithiumamid (**113**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
Li(1)	6375(4)	4043(4)	8176(7)	62(2)
C(1)	6122(3)	4276(3)	11771(5)	87(2)
C(2)	6156(3)	4921(3)	10810(5)	73(1)
C(3)	6547(3)	5643(3)	8500(5)	77(1)
C(4)	5790(4)	5274(3)	7628(8)	111(2)
C(5)	7482(2)	5353(2)	9770(4)	58(1)
C(6)	7916(3)	6156(3)	10524(5)	74(1)
C(7)	8745(3)	6390(3)	10929(5)	79(1)
C(8)	9201(3)	6392(3)	9576(5)	76(1)
C(9)	8772(2)	5589(3)	8816(5)	69(1)
C(10)	7922(2)	5313(2)	8382(4)	57(1)

C(11)	7757(3)	4582(3)	6141(4)	83(1)
C(12)	7573(5)	5050(4)	5073(6)	126(3)
N(1)	6630(2)	5075(2)	9441(3)	59(1)
N(2)	7510(2)	4546(2)	7682(3)	58(1)

Tabelle 62 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für (1*R*,2*R*)-2-(Diethylamino)cyclohexylethyllithiumamid (**113**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Li(1)	61(4)	60(4)	60(3)	0(3)	–6(3)	27(3)
C(1)	72(3)	107(4)	62(2)	14(2)	9(2)	29(3)
C(2)	62(2)	74(3)	80(3)	–12(2)	12(2)	32(2)
C(3)	82(3)	76(3)	86(3)	7(2)	–1(2)	49(2)
C(4)	99(4)	93(4)	145(5)	16(4)	–33(4)	51(3)
C(5)	61(2)	54(2)	63(2)	4(2)	2(2)	32(2)
C(6)	80(3)	68(3)	75(3)	–10(2)	–7(2)	38(2)
C(7)	71(3)	68(3)	86(3)	–14(2)	–12(2)	26(2)
C(8)	59(3)	63(3)	94(3)	1(2)	–7(2)	22(2)
C(9)	58(2)	63(2)	80(2)	10(2)	8(2)	26(2)
C(10)	62(2)	52(2)	60(2)	15(2)	8(2)	31(2)
C(11)	97(3)	90(3)	59(2)	3(2)	17(2)	44(3)
C(12)	201(8)	96(4)	69(3)	6(3)	–4(4)	65(5)
N(1)	61(2)	58(2)	62(2)	1(1)	2(1)	32(2)
N(2)	59(2)	57(2)	59(2)	2(1)	6(1)	30(2)

Tabelle 63 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für (1*R*,2*R*)-2-(Diethylamino)cyclohexylethyllithiumamid (**113**).

	x	y	z	U(eq)
H(1A)	5953	3801	11170	131
H(1B)	5745	4160	12580	131
H(1C)	6645	4446	12187	131
H(2A)	5612	4778	10526	88
H(2B)	6379	5412	11400	88
H(3A)	6996	5889	7800	93
H(3B)	6569	6066	9136	93

H(4A)	5801	4915	6881	167
H(4B)	5732	5687	7132	167
H(4C)	5345	4978	8302	167
H(6A)	7922	6558	9850	88
H(6B)	7627	6144	11435	88
H(7A)	9007	6922	11380	95
H(7B)	8742	6016	11673	95
H(8A)	9736	6512	9874	91
H(8B)	9255	6806	8876	91
H(9A)	9069	5610	7910	83
H(9B)	8778	5193	9490	83
H(11A)	7512	4036	5761	100
H(11B)	8334	4800	6134	100
H(12A)	7002	4835	5036	189
H(12B)	7765	5021	4082	189
H(12C)	7832	5600	5398	189
H(5)	7510(20)	4980(20)	10420(40)	58(11)
H(10)	7936(17)	5680(20)	7840(30)	30(7)

8.2.3 Kristallstrukturen aus Kapitel 4.3

$ZnBr_2$·DPCH [(*R*,*R*)-122]

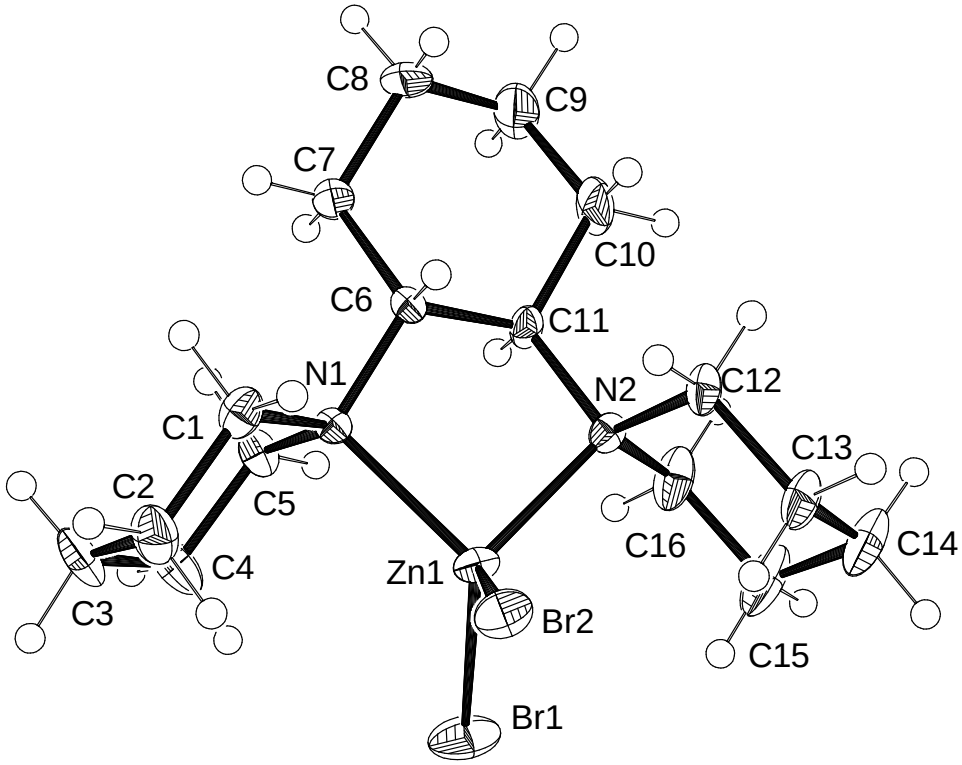


Abbildung 22 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von $ZnBr_2$·DPCH (**122**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 64 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für $ZnBr_2$·DPCH (**122**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
Br(1)	–2224(1)	2701(1)	7732(1)	40(1)
Br(2)	–2086(1)	–466(1)	7594(1)	25(1)
C(1)	1853(4)	721(3)	8052(3)	16(1)
C(2)	3201(5)	838(4)	8559(3)	30(1)
C(3)	4414(5)	541(5)	7986(4)	40(1)
C(4)	4441(5)	1234(6)	7140(4)	45(2)
C(5)	3139(5)	1055(5)	6619(3)	36(1)
C(6)	1895(4)	1352(4)	7168(3)	19(1)
C(7)	565(5)	311(3)	6034(3)	21(1)
C(8)	–689(6)	294(4)	5431(3)	28(1)
C(9)	–764(7)	1275(4)	4838(4)	40(1)
C(10)	–757(7)	2229(4)	5451(4)	44(2)
C(11)	474(6)	2243(4)	6064(4)	31(1)

C(12)	856(5)	1998(3)	9172(3)	20(1)
C(13)	–306(6)	2235(4)	9809(4)	34(1)
C(14)	–571(6)	1308(4)	10450(4)	36(1)
C(15)	–793(6)	314(4)	9891(3)	30(1)
C(16)	391(5)	109(4)	9272(3)	22(1)
N(1)	645(4)	997(3)	8629(2)	14(1)
N(2)	589(4)	1271(3)	6637(2)	16(1)
Zn(1)	–893(1)	1157(1)	7656(1)	19(1)

Tabelle 65 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für $ZnBr_2$·DPCH (**122**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	28(1)	26(1)	67(1)	–5(1)	–8(1)	11(1)
Br(2)	19(1)	23(1)	33(1)	1(1)	–3(1)	–5(1)
C(1)	11(2)	22(2)	14(2)	–1(2)	3(2)	1(2)
C(2)	15(3)	56(4)	19(3)	–4(2)	–2(2)	5(2)
C(3)	15(3)	71(4)	34(3)	–9(3)	–3(2)	13(3)
C(4)	18(3)	89(5)	26(3)	–4(3)	3(2)	–8(3)
C(5)	26(3)	67(4)	16(3)	5(3)	6(2)	–10(3)
C(6)	16(2)	26(2)	15(2)	–2(2)	–3(2)	–4(2)
C(7)	29(3)	18(2)	16(2)	–3(2)	–4(2)	–1(2)
C(8)	37(3)	28(3)	20(2)	–6(2)	–12(2)	–6(2)
C(9)	55(4)	40(3)	26(3)	1(2)	–25(3)	–2(3)
C(10)	67(4)	30(3)	34(3)	5(2)	–31(3)	3(3)
C(11)	48(4)	19(2)	24(3)	4(2)	–12(2)	–3(2)
C(12)	25(3)	16(2)	19(2)	–5(2)	5(2)	–5(2)
C(13)	41(3)	30(3)	31(3)	–12(2)	17(3)	–2(2)
C(14)	39(3)	47(3)	23(3)	–5(2)	18(2)	–4(3)
C(15)	30(3)	38(3)	23(3)	5(2)	8(2)	–6(2)
C(16)	24(3)	22(2)	20(2)	7(2)	–1(2)	–5(2)
N(1)	16(2)	11(2)	15(2)	0(1)	2(2)	1(2)
N(2)	18(2)	14(2)	15(2)	–3(2)	–5(2)	–2(2)
Zn(1)	13(1)	18(1)	25(1)	0(1)	–3(1)	1(1)

Tabelle 66 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung $ZnBr_2$·DPCH (**122**).

	x	y	z	U(eq)
H(1)	1762	–37	7881	19
H(2A)	3299	1577	8761	36
H(2B)	3183	388	9107	36
H(3A)	4358	–209	7809	48
H(3B)	5248	644	8340	48
H(4A)	4521	1983	7315	53
H(4B)	5221	1048	6756	53
H(5A)	3078	304	6444	44
H(5B)	3157	1478	6055	44
H(7A)	581	–330	6415	25
H(7B)	1378	306	5648	25
H(8A)	–668	–339	5040	34
H(8B)	–1501	253	5816	34
H(9A)	14	1299	4422	48
H(9B)	–1596	1264	4471	48
H(10A)	–767	2875	5075	52
H(10B)	–1579	2227	5828	52
H(11A)	1290	2311	5686	37
H(11B)	427	2867	6465	37
H(12A)	1692	1931	9530	24
H(12B)	971	2595	8748	24
H(13A)	–1125	2381	9449	41
H(13B)	–95	2872	10169	41
H(14A)	206	1210	10860	44
H(14B)	–1374	1454	10825	44
H(15A)	–919	–294	10301	36
H(15B)	–1618	393	9523	36
H(16A)	1204	–7	9645	26
H(16B)	222	–541	8920	26
H(6)	1840(50)	2080(40)	7300(30)	22(12)

t-BuLi·(*R*,*R*)-DPCH [(*R*,*R*)-124]

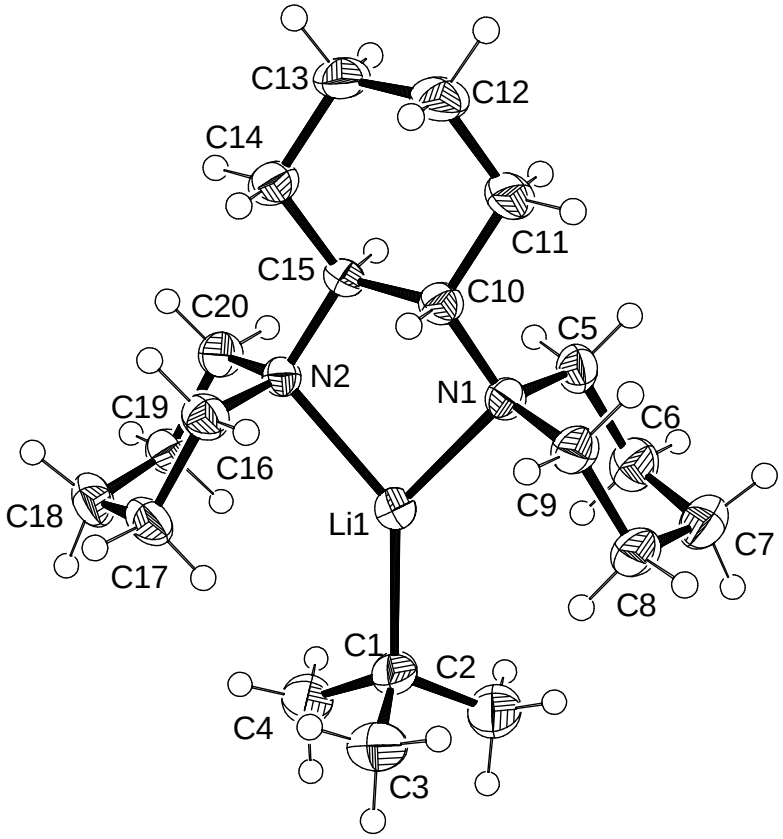


Abbildung 23 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von *t*-BuLi·DPCH (**124**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 67 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für *t*-BuLi·DPCH (**124**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
N(1)	8889(2)	3159(2)	11008(1)	26(1)
N(2)	8539(2)	3088(2)	8882(1)	27(1)
C(1)	9778(2)	3183(2)	11744(2)	34(1)
C(15)	7910(2)	1750(2)	7628(2)	40(1)
C(5)	7863(2)	2949(2)	11541(2)	34(1)
C(3)	8844(2)	1822(3)	12807(2)	42(1)
C(6)	8879(2)	4187(2)	10423(2)	28(1)
C(11)	8232(2)	4079(2)	9446(2)	30(1)
C(7)	8472(2)	5175(2)	11010(2)	39(1)
C(12)	9569(2)	3203(2)	8319(2)	36(1)
C(4)	7909(2)	1862(2)	12083(2)	39(1)
C(10)	8312(2)	5135(2)	8842(2)	41(1)
C(16)	7667(2)	2802(2)	8171(2)	36(1)
C(8)	8564(3)	6207(2)	10401(2)	44(1)

C(14)	8975(2)	1809(3)	7078(2)	48(1)
C(13)	9868(2)	2159(3)	7788(2)	44(1)
C(2)	9890(2)	2111(2)	12283(2)	36(1)
C(9)	7930(3)	6107(2)	9438(2)	47(1)
C(17)	8958(2)	102(2)	9947(2)	41(1)
C(19)	7790(3)	–310(2)	9948(3)	62(1)
C(18)	9500(3)	–422(3)	9050(2)	64(1)
C(20)	9495(3)	–389(2)	10866(2)	53(1)
Li(1)	8884(3)	1846(3)	9937(3)	32(1)

Tabelle 68 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für *t*-BuLi·DPCH (**124**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	28(1)	25(1)	24(1)	2(1)	–3(1)	0(1)
N(2)	28(1)	29(1)	26(1)	1(1)	–4(1)	–3(1)
C(1)	37(2)	34(2)	31(1)	2(1)	–8(1)	–1(1)
C(15)	43(2)	39(2)	36(2)	–5(1)	–12(1)	–7(1)
C(5)	35(2)	31(2)	37(2)	3(1)	5(1)	3(1)
C(3)	49(2)	43(2)	33(2)	12(1)	7(1)	11(2)
C(6)	32(2)	23(1)	28(1)	4(1)	0(1)	0(1)
C(11)	34(2)	26(1)	29(1)	2(1)	–4(1)	1(1)
C(7)	54(2)	29(2)	35(2)	–3(1)	–11(1)	2(1)
C(12)	37(2)	43(2)	28(1)	0(1)	3(1)	–9(1)
C(4)	40(2)	36(2)	40(2)	9(1)	13(1)	–1(1)
C(10)	56(2)	32(2)	34(2)	8(1)	–12(1)	–1(1)
C(16)	39(2)	37(2)	32(2)	–2(1)	–11(1)	–5(1)
C(8)	61(2)	25(2)	45(2)	–2(1)	–11(2)	2(1)
C(14)	58(2)	48(2)	39(2)	–11(2)	3(2)	–2(2)
C(13)	38(2)	52(2)	41(2)	–6(2)	9(1)	–5(1)
C(2)	40(2)	33(2)	35(2)	7(1)	–7(1)	5(1)
C(9)	67(2)	27(2)	48(2)	6(1)	–15(2)	5(1)
C(17)	62(2)	27(1)	34(1)	–2(1)	0(2)	3(1)
C(19)	88(3)	43(2)	56(2)	1(2)	–5(2)	–18(2)
C(18)	109(3)	33(2)	50(2)	–1(2)	6(2)	18(2)
C(20)	82(2)	32(2)	45(2)	5(1)	1(2)	12(2)
Li(1)	41(2)	29(2)	27(2)	1(2)	0(2)	–1(2)

Tabelle 69 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für *t*-BuLi·DPCH (**124**).

	x	y	z	U(eq)
H(1A)	9639	3760	12241	41
H(1B)	10465	3353	11397	41
H(15A)	7934	1152	8119	47
H(15B)	7323	1596	7144	47
H(5A)	7258	2945	11054	41
H(5B)	7728	3532	12033	41
H(3A)	8713	2334	13364	50
H(3B)	8902	1087	13094	50
H(7A)	7707	5060	11201	47
H(7B)	8900	5252	11634	47
H(12A)	10156	3406	8788	43
H(12B)	9495	3789	7818	43
H(4A)	7224	1746	12453	46
H(4B)	7986	1275	11585	46
H(10A)	7869	5068	8227	49
H(10B)	9073	5249	8636	49
H(16A)	7582	3389	7674	43
H(16B)	6976	2730	8540	43
H(8A)	9333	6351	10245	52
H(8B)	8283	6822	10797	52
H(14A)	8918	2330	6518	58
H(14B)	9152	1092	6793	58
H(13A)	9995	1586	8291	52
H(13B)	10547	2265	7406	52
H(2A)	10077	1540	11794	43
H(2B)	10481	2158	12781	43
H(9A)	7150	6030	9593	56
H(9B)	8025	6770	9032	56
H(19A)	7427	–80	9331	93
H(19B)	7405	–14	10529	93
H(19C)	7790	–1100	9986	93
H(18A)	9443	–1209	9106	96
H(18B)	10265	–214	9032	96
H(18C)	9143	–181	8433	96
H(20A)	9460	–1178	10823	80
H(20B)	9117	–146	11471	80
H(20C)	10253	–159	10895	80
H(1)	9644(18)	4327(16)	10232(15)	15(6)

H(2)	7470(20)	3958(19)	9648(17)	28(7)

s-BuLi·(*R*,*R*)-DPCH [(*R*,*R*)-123]

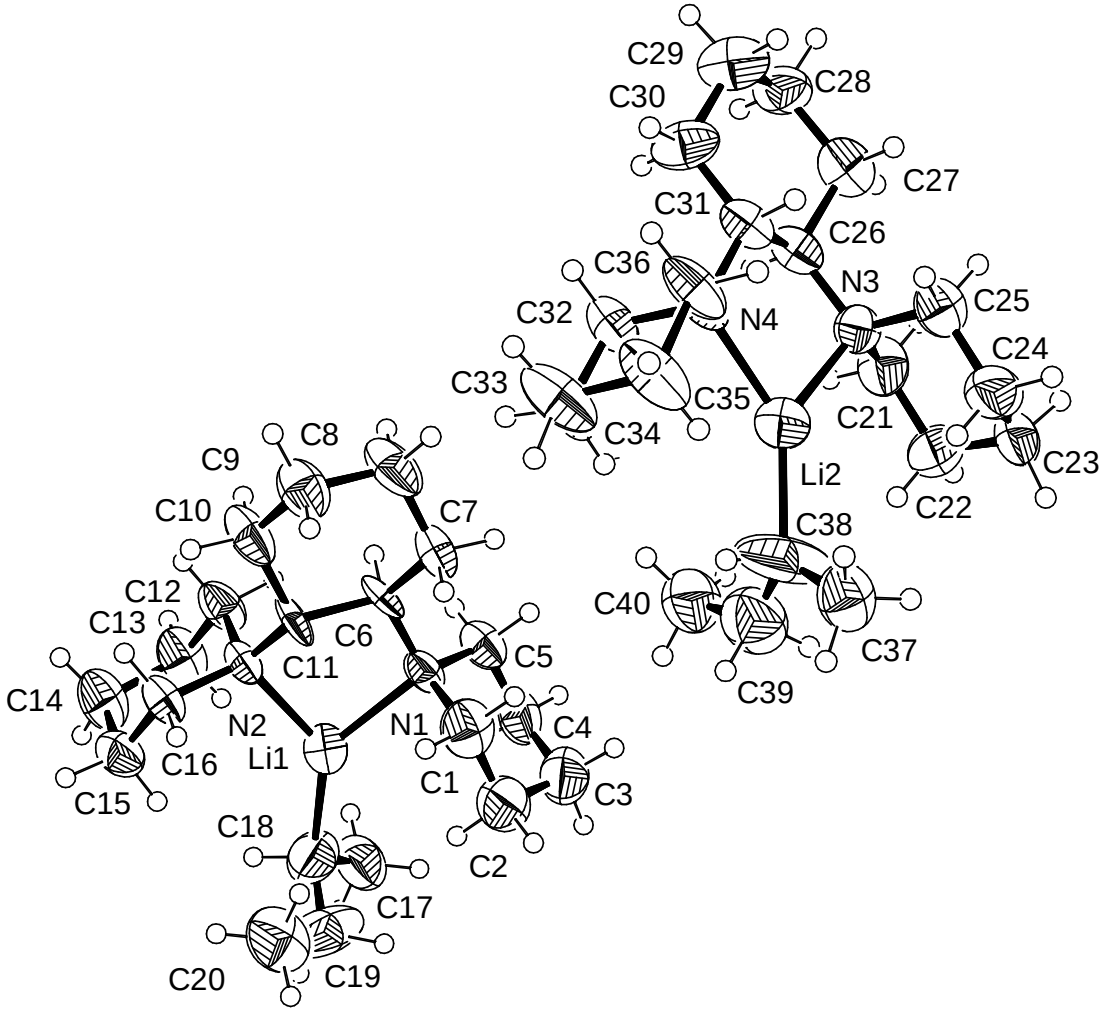


Abbildung 24 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von *s*-BuLi·DPCH (**123**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 70 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für *s*-BuLi·DPCH (**123**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(17)	–1307(5)	2339(4)	6547(4)	85(3)
C(18)	–259(8)	2136(5)	7076(4)	105(3)
C(19)	328(9)	1748(5)	6614(5)	178(6)
C(20)	1383(5)	1495(4)	7039(5)	99(3)

C(34)	5750(6)	6746(4)	9318(5)	101(3)
C(37)	6107(5)	7300(4)	6568(4)	82(2)
C(38)	5112(7)	7171(5)	6969(5)	134(4)
C(39)	4496(7)	6632(4)	6658(5)	105(3)
C(40)	3481(6)	6372(4)	6969(4)	93(3)
Li(1)	298(9)	2982(6)	7793(6)	61(3)
Li(2)	4628(9)	7984(7)	7704(7)	72(4)
C(1)	1731(5)	4110(4)	7253(4)	76(2)
C(2)	1416(6)	3843(4)	6485(4)	84(3)
C(3)	641(6)	4394(4)	6132(4)	85(3)
C(4)	–266(5)	4462(4)	6654(4)	69(2)
C(5)	91(5)	4706(4)	7421(3)	60(2)
C(6)	1075(4)	4391(3)	8520(3)	46(2)
C(7)	1867(5)	5046(3)	8582(4)	58(2)
C(8)	1996(5)	5310(4)	9386(4)	82(2)
C(9)	2376(4)	4612(4)	9846(4)	73(2)
C(10)	1587(5)	3952(4)	9795(4)	72(2)
C(11)	1426(4)	3688(4)	8974(4)	52(2)
C(12)	–345(4)	3215(4)	9291(4)	61(2)
C(13)	–1112(5)	2563(4)	9128(4)	73(2)
C(14)	–696(5)	1779(4)	9406(4)	76(2)
C(15)	368(5)	1620(4)	9080(4)	66(2)
C(16)	1080(5)	2312(4)	9238(3)	58(2)
N(1)	827(4)	4166(3)	7743(3)	46(1)
N(2)	653(4)	3041(3)	8922(3)	48(1)
C(21)	2976(5)	9048(4)	7162(4)	70(2)
C(22)	3367(6)	8846(4)	6383(4)	88(3)
C(23)	4174(6)	9388(4)	6123(4)	89(3)
C(24)	5011(5)	9453(4)	6706(4)	79(2)
C(25)	4578(5)	9652(4)	7454(4)	65(2)
C(26)	3442(5)	9172(4)	8474(4)	55(2)
C(27)	3061(5)	10012(4)	8626(4)	70(2)
C(28)	2646(4)	10102(4)	9424(4)	71(2)
C(29)	3474(5)	9881(4)	9977(3)	81(2)
C(30)	3817(5)	9071(4)	9816(3)	71(2)
C(31)	4251(5)	8962(4)	9041(4)	57(2)
C(32)	4160(5)	7538(4)	9220(3)	67(2)
C(33)	4658(6)	6752(4)	9058(4)	88(3)
C(35)	6326(5)	7434(4)	8992(4)	87(3)
C(36)	5790(5)	8185(3)	9187(4)	71(2)
N(3)	3834(4)	9055(3)	7691(3)	53(2)

N(4)	4737(4)	8189(3)	8883(3)	54(2)

Tabelle 71 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für *s*-BuLi·DPCH (**123**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(17)	104(7)	59(6)	92(6)	2(5)	–16(6)	–8(4)
C(18)	171(10)	80(7)	64(6)	–10(5)	17(7)	–51(6)
C(19)	273(15)	138(11)	123(10)	–78(8)	116(11)	–137(10)
C(20)	76(6)	84(7)	136(8)	0(6)	16(6)	–24(5)
C(34)	89(6)	48(7)	166(9)	–11(6)	–23(7)	14(5)
C(37)	65(5)	79(6)	101(6)	12(5)	8(5)	–4(4)
C(38)	100(8)	101(8)	201(11)	–97(7)	44(7)	–40(6)
C(39)	101(8)	89(8)	124(8)	2(6)	12(6)	14(6)
C(40)	93(7)	83(6)	103(7)	2(5)	10(5)	–17(5)
Li(1)	63(7)	56(9)	62(8)	8(7)	0(7)	–1(6)
Li(2)	84(9)	62(9)	70(9)	–5(7)	9(8)	4(7)
C(1)	60(5)	78(6)	88(6)	7(5)	7(5)	–5(4)
C(2)	85(6)	73(7)	93(7)	3(5)	24(5)	–1(5)
C(3)	93(6)	78(7)	84(6)	15(5)	18(5)	7(5)
C(4)	73(5)	58(6)	75(6)	18(4)	–17(5)	–1(4)
C(5)	62(5)	43(5)	76(6)	3(4)	–9(4)	6(4)
C(6)	48(4)	13(5)	78(5)	–2(4)	–8(4)	–5(3)
C(7)	59(4)	36(5)	78(6)	14(4)	–12(4)	–5(3)
C(8)	93(6)	41(6)	112(7)	–3(5)	–43(5)	–11(4)
C(9)	70(5)	56(6)	93(6)	7(4)	–23(5)	–9(4)
C(10)	72(5)	39(6)	105(7)	12(5)	–40(5)	–1(4)
C(11)	61(5)	15(5)	79(5)	11(4)	–23(4)	–13(3)
C(12)	46(4)	40(5)	96(6)	6(4)	17(4)	10(4)
C(13)	48(4)	63(6)	107(6)	14(5)	6(5)	–4(4)
C(14)	56(5)	60(6)	113(6)	16(5)	6(5)	–15(4)
C(15)	73(5)	48(6)	77(6)	0(4)	8(5)	15(4)
C(16)	67(5)	34(5)	74(5)	8(4)	–3(4)	9(4)
N(1)	43(3)	29(4)	65(4)	3(3)	5(3)	8(3)
N(2)	57(4)	27(4)	59(4)	6(3)	–3(3)	3(3)
C(21)	65(5)	73(6)	70(5)	11(5)	–12(5)	–8(4)
C(22)	130(8)	83(7)	50(5)	–7(5)	–9(5)	–15(6)
C(23)	127(7)	48(6)	93(7)	4(5)	44(6)	–18(5)
C(24)	83(6)	67(6)	87(6)	–12(5)	23(5)	–10(4)

C(25)	51(5)	61(6)	83(6)	6(4)	1(4)	–4(4)
C(26)	48(4)	42(5)	75(5)	–6(4)	–8(4)	0(3)
C(27)	50(4)	65(6)	95(7)	2(5)	–1(4)	4(4)
C(28)	78(5)	66(6)	68(5)	–12(4)	2(5)	21(4)
C(29)	65(5)	99(7)	78(5)	–23(5)	–15(5)	20(5)
C(30)	60(5)	94(7)	60(5)	–22(5)	–16(4)	13(4)
C(31)	50(4)	40(6)	80(5)	–6(4)	–1(4)	0(4)
C(32)	73(5)	42(6)	86(6)	5(5)	–14(5)	–5(5)
C(33)	121(7)	33(7)	109(7)	11(5)	–25(6)	–13(5)
C(35)	59(5)	48(6)	155(8)	–1(5)	–20(5)	1(4)
C(36)	48(4)	35(5)	130(7)	0(5)	–14(5)	9(4)
N(3)	46(3)	53(4)	59(4)	–1(3)	10(3)	–8(3)
N(4)	57(4)	29(4)	77(4)	–1(3)	–5(3)	0(3)

Tabelle 72 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für *s*-BuLi·DPCH (**123**).

	x	y	z	U(eq)
H(17A)	–1117	2707	6147	128
H(17B)	–1843	2575	6863	128
H(17C)	–1571	1853	6323	128
H(18)	–514	1720	7426	126
H(19A)	495	2079	6173	214
H(19B)	–38	1274	6434	214
H(20A)	1713	1962	7253	148
H(20B)	1853	1247	6679	148
H(20C)	1220	1124	7443	148
H(34A)	6086	6251	9159	121
H(34B)	5770	6772	9873	121
H(37A)	6350	6802	6358	123
H(37B)	6621	7505	6921	123
H(37C)	6003	7679	6160	123
H(38)	5406	6811	7357	160
H(39A)	4920	6151	6606	126
H(39B)	4354	6817	6141	126
H(40A)	3521	6352	7519	139
H(40B)	3314	5849	6775	139
H(40C)	2942	6743	6818	139
H(1A)	2232	3734	7468	91

H(1B)	2070	4630	7217	91
H(2A)	2034	3810	6160	100
H(2B)	1111	3311	6520	100
H(3A)	957	4916	6053	102
H(3B)	414	4187	5639	102
H(4A)	–759	4855	6456	82
H(4B)	–626	3951	6686	82
H(5A)	410	5232	7389	72
H(5B)	–514	4745	7759	72
H(6)	423	4587	8755	55
H(7A)	2539	4859	8386	69
H(7B)	1644	5496	8270	69
H(8A)	1329	5500	9587	98
H(8B)	2503	5744	9413	98
H(9A)	3050	4430	9650	88
H(9B)	2469	4769	10377	88
H(10A)	1826	3501	10098	86
H(10B)	921	4134	10005	86
H(12A)	–620	3720	9102	73
H(12B)	–242	3263	9840	73
H(13A)	–1776	2679	9381	87
H(13B)	–1242	2534	8581	87
H(14A)	–1174	1354	9257	92
H(14B)	–655	1786	9962	92
H(15A)	659	1138	9307	79
H(15B)	313	1537	8531	79
H(16A)	1169	2372	9787	70
H(16B)	1767	2209	9015	70
H(21A)	2641	9571	7153	84
H(21B)	2456	8657	7322	84
H(22A)	3647	8305	6387	105
H(22B)	2783	8859	6025	105
H(23A)	3870	9912	6030	107
H(23B)	4472	9195	5645	107
H(24A)	5509	9864	6553	95
H(24B)	5387	8949	6739	95
H(25A)	5143	9687	7826	78
H(25B)	4232	10170	7429	78
H(26)	2844	8809	8549	66
H(27A)	2510	10146	8262	84
H(27B)	3638	10385	8549	84
H(28A)	2429	10652	9509	85

H(28B)	2036	9759	9493	85
H(29A)	3200	9914	10495	97
H(29B)	4064	10247	9933	97
H(30A)	3223	8711	9881	86
H(30B)	4350	8920	10188	86
H(31)	4810	9362	8986	68
H(32A)	3447	7538	9021	80
H(32B)	4121	7616	9771	80
H(33A)	4269	6331	9317	105
H(33B)	4634	6647	8511	105
H(35A)	7039	7443	9193	105
H(35B)	6366	7380	8439	105
H(36A)	5763	8245	9740	85
H(36B)	6182	8633	8979	85

Protoniertes (*R*,*R*)-DPyCH [(*R*,*R*)-46] mit $ZnBr_4^{2-}$ als Gegenion

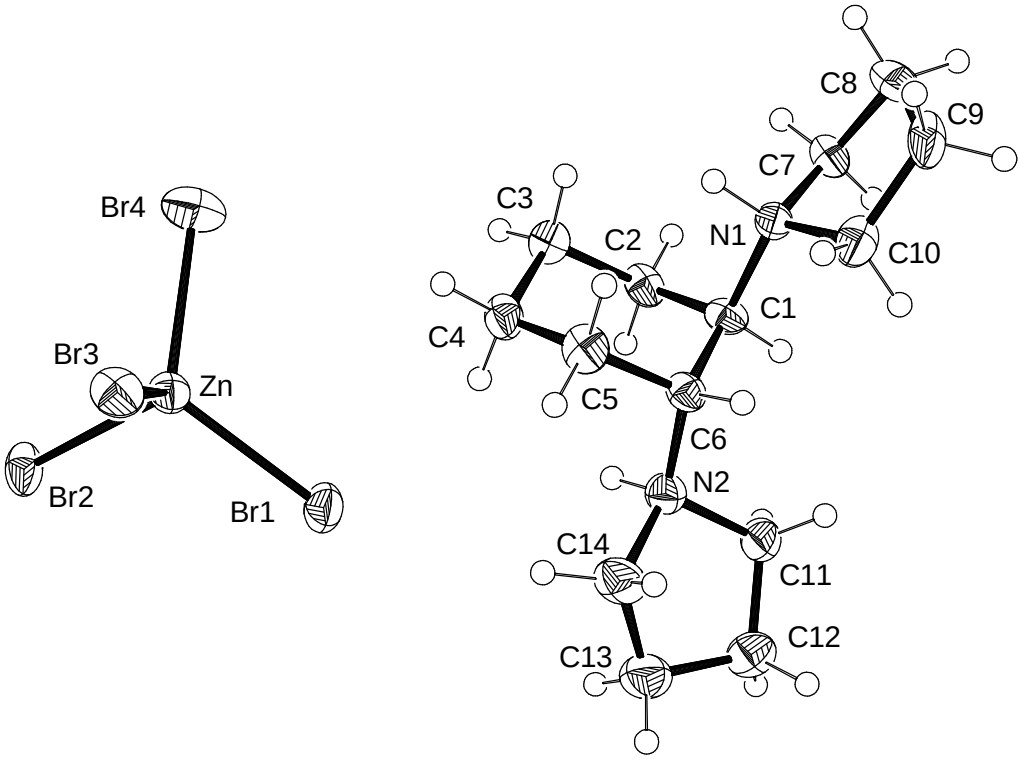


Abbildung 25 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von protonierten DPyCH (**46**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 73 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter ($Å^2$ x 10^3) für protoniertes DPyCH (**46**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
Br(1)	6416(1)	7094(1)	6451(1)	49(1)
Br(2)	8656(1)	5344(1)	7854(1)	38(1)
Br(3)	5523(1)	6207(1)	8983(1)	36(1)
Br(4)	8237(1)	8163(1)	8710(1)	37(1)
C(1)	3887(5)	8455(5)	7619(4)	36(1)
C(2)	4759(5)	9148(5)	8164(5)	50(2)
C(3)	4342(6)	9142(6)	9187(5)	55(2)
C(4)	3111(6)	8648(5)	9177(4)	41(1)
C(5)	1961(4)	7483(4)	8074(4)	27(1)
C(6)	1417(5)	6821(4)	8846(4)	33(1)
C(7)	2056(5)	5783(4)	8999(4)	32(1)
C(8)	2149(5)	5169(4)	8081(4)	37(1)
C(9)	2710(5)	5820(5)	7306(4)	36(1)
C(10)	2080(4)	6865(4)	7144(4)	30(1)
C(11)	204(5)	7734(4)	6496(5)	40(1)
C(12)	-498(6)	7544(5)	5604(4)	40(1)
C(13)	-357(6)	6392(5)	5380(4)	45(2)
C(14)	837(6)	6090(5)	5812(4)	43(2)
N(1)	3186(4)	7878(4)	8370(3)	31(1)
N(2)	856(4)	6718(4)	6724(3)	33(1)
Zn(1)	7175(1)	6743(1)	7998(1)	29(1)

Tabelle 74 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für protoniertes DPyCH. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	43(1)	68(1)	37(1)	7(1)	–4(1)	10(1)
Br(2)	24(1)	24(1)	68(1)	–2(1)	–2(1)	1(1)
Br(3)	24(1)	40(1)	43(1)	6(1)	2(1)	–2(1)
Br(4)	39(1)	26(1)	48(1)	–2(1)	–2(1)	–4(1)
C(1)	20(3)	36(3)	53(4)	12(3)	1(3)	–1(2)
C(2)	29(3)	34(3)	86(5)	17(3)	–4(3)	–3(3)
C(3)	50(4)	51(4)	63(5)	6(3)	–23(4)	–21(3)
C(4)	44(4)	38(3)	41(4)	–2(3)	–3(3)	–11(3)
C(5)	18(2)	29(3)	35(3)	–2(2)	0(2)	1(2)
C(6)	23(2)	33(3)	43(3)	–8(3)	2(2)	–5(2)

C(7)	28(3)	30(3)	37(3)	3(2)	8(2)	0(2)
C(8)	29(3)	28(3)	54(4)	3(3)	–3(3)	1(2)
C(9)	24(3)	38(3)	46(3)	–8(3)	3(2)	6(2)
C(10)	26(3)	31(3)	33(3)	–3(2)	0(2)	–3(2)
C(11)	40(3)	26(3)	54(4)	1(3)	–12(3)	2(2)
C(12)	43(4)	46(4)	33(3)	0(3)	3(3)	4(3)
C(13)	49(4)	56(4)	32(3)	2(3)	–1(3)	–9(3)
C(14)	53(4)	41(4)	35(3)	–9(3)	–4(3)	4(3)
N(1)	24(2)	31(2)	39(3)	3(2)	–5(2)	–1(2)
N(2)	34(3)	29(3)	37(3)	–2(2)	0(2)	–1(2)
Zn(1)	22(1)	28(1)	36(1)	1(1)	–1(1)	1(1)

Tabelle 75 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für protoniertes DPyCH (**46**).

	x	y	z	U(eq)
H(1A)	3346	8882	7222	44
H(1B)	4325	7959	7209	44
H(2A)	5584	8870	8116	60
H(2B)	4750	9867	7909	60
H(3A)	4898	8730	9585	66
H(3B)	4301	9862	9439	66
H(4A)	2481	9177	9061	49
H(4B)	2942	8288	9782	49
H(5)	1428	8097	7961	33
H(6A)	568	6681	8687	39
H(6B)	1431	7221	9445	39
H(7A)	2870	5915	9250	38
H(7B)	1612	5366	9472	38
H(8A)	2639	4536	8186	44
H(8B)	1339	4943	7881	44
H(9A)	2697	5416	6710	43
H(9B)	3558	5954	7469	43
H(10)	2572	7286	6693	36
H(11A)	–340	7927	7020	48
H(11B)	787	8307	6402	48
H(12A)	–181	7976	5081	49
H(12B)	–1353	7720	5700	49
H(13A)	–1017	5982	5663	55

H(13B)	–353	6275	4689	55
H(14A)	1511	6286	5394	52
H(14B)	874	5331	5941	52
H(100)	3600(60)	7260(50)	8610(40)	39(16)
H(101)	450(60)	6300(50)	7140(40)	37(17)

.

t-BuLi·(*R*,*R*)-DPyCH [(*R*,*R*)-125]

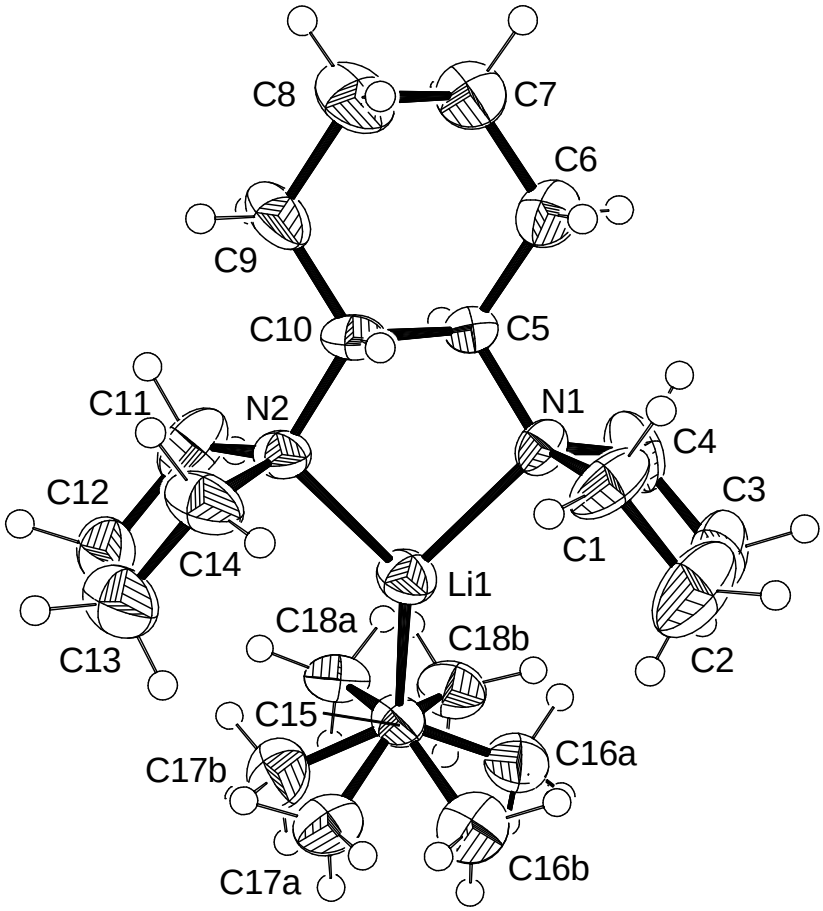


Abbildung 26 Thermische Auslenkungsellipsoide (25% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von *t*-BuLi·(*R*,*R*)-DPyCH (**125**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 76 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter ($Å^2$ x 10^3) von *t*-BuLi·(*R*,*R*)-DPyCH (**125**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
N(1)	5539(1)	4589(1)	1072(1)	34(1)
N(2)	5160(1)	4764(1)	–941(1)	36(1)
C(5)	6227(2)	5446(1)	533(1)	31(1)
C(9)	6308(2)	6592(1)	–958(1)	54(1)
C(6)	6528(2)	6477(2)	1117(2)	49(1)
C(12)	5338(3)	3642(2)	–2322(2)	68(1)
C(8)	6607(2)	7605(1)	–373(2)	63(1)
C(7)	7300(2)	7290(2)	535(2)	54(1)
C(1)	4350(2)	4918(2)	1511(2)	58(1)
C(3)	5309(3)	3546(2)	2492(2)	78(1)
C(4)	6260(2)	4105(2)	1864(1)	60(1)
C(14)	4028(2)	4948(2)	–1532(2)	58(1)
C(11)	6074(2)	4331(2)	–1638(2)	61(1)
C(13)	3974(2)	3955(2)	–2175(2)	70(1)
C(2)	4061(3)	3959(2)	2180(2)	86(1)
Li(1)	5125(3)	3450(2)	26(3)	43(1)
C(10)	5547(2)	5757(1)	–392(1)	37(1)
C(15)	5256(2)	1716(1)	–15(2)	37(1)
C(17A)	4242(5)	1222(4)	–604(4)	52(1)
C(16B)	4127(4)	1247(4)	557(4)	58(1)
C(17B)	5138(6)	1187(4)	–987(4)	66(2)
C(16A)	5249(5)	1208(3)	953(3)	56(1)
C(18A)	6406(4)	1301(4)	464(4)	57(1)
C(18B)	6532(4)	1354(3)	–491(4)	48(1)

Tabelle 77 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) von *t*-BuLi·(*R*,*R*)-DPyCH (**125**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	32(1)	34(1)	36(1)	–4(1)	7(1)	–5(1)
N(2)	38(1)	30(1)	40(1)	–6(1)	–8(1)	4(1)
C(5)	28(1)	27(1)	37(1)	–1(1)	1(1)	1(1)
C(9)	78(2)	35(1)	50(1)	13(1)	–20(1)	–12(1)
C(6)	56(2)	39(1)	51(1)	–10(1)	2(1)	–14(1)
C(12)	106(2)	55(2)	43(1)	–13(1)	–17(1)	15(2)
C(8)	83(2)	33(1)	71(2)	11(1)	–19(1)	–18(1)

C(7)	64(2)	37(1)	60(2)	–4(1)	–9(1)	–16(1)
C(1)	48(2)	49(1)	76(2)	–20(1)	32(1)	–12(1)
C(3)	121(3)	61(2)	51(2)	4(1)	34(2)	–23(2)
C(4)	71(2)	61(2)	49(2)	15(1)	–11(1)	–26(1)
C(14)	59(2)	43(1)	71(2)	–2(1)	–32(1)	2(1)
C(11)	60(2)	57(2)	65(2)	–21(1)	13(1)	–13(1)
C(13)	87(2)	55(2)	69(2)	–11(1)	–38(1)	1(2)
C(2)	90(2)	76(2)	92(2)	–15(2)	57(2)	–27(2)
Li(1)	46(2)	36(2)	47(2)	3(2)	–3(2)	0(1)
C(10)	35(1)	25(1)	51(1)	–2(1)	–5(1)	3(1)
C(15)	40(1)	32(1)	38(1)	–1(1)	–9(1)	–3(1)
C(17A)	61(4)	31(2)	64(4)	1(2)	7(3)	–6(3)
C(16B)	61(4)	43(3)	69(4)	–7(2)	3(3)	–17(2)
C(17B)	98(5)	45(3)	54(4)	–11(3)	–10(4)	–5(3)
C(16A)	71(4)	39(3)	57(3)	0(2)	–2(3)	1(3)
C(18A)	57(4)	43(3)	70(4)	0(3)	–5(3)	–1(3)
C(18B)	43(3)	40(3)	59(3)	–1(2)	–1(3)	6(2)

Tabelle 78 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) von *t*-BuLi·(*R*,*R*)-DPyCH (**125**).

	x	y	z	U(eq)
H(9A)	7097	6249	–1171	65
H(9B)	5835	6809	–1539	65
H(6A)	5739	6829	1321	59
H(6B)	6996	6268	1702	59
H(12A)	5465	2856	–2184	82
H(12B)	5597	3788	–2993	82
H(8A)	7127	8109	–760	75
H(8B)	5824	7988	–203	75
H(7A)	7462	7952	925	64
H(7B)	8113	6959	365	64
H(1A)	3691	5008	1019	70
H(1B)	4440	5608	1875	70
H(3A)	5358	2743	2411	93
H(3B)	5458	3724	3176	93
H(4A)	6708	4678	2229	72
H(4B)	6875	3571	1616	72
H(14A)	4104	5627	–1915	69

H(14B)	3274	4998	–1123	69
H(11A)	6715	3886	–1307	73
H(11B)	6495	4935	–1983	73
H(13A)	3570	4132	–2796	84
H(13B)	3507	3353	–1863	84
H(2A)	3565	4205	2740	103
H(2B)	3591	3383	1836	103
H(17A)	4319	1470	–1271	78
H(17B)	3430	1447	–348	78
H(17C)	4309	423	–581	78
H(16A)	3347	1484	254	86
H(16B)	4156	1514	1220	86
H(16C)	4167	446	556	86
H(17D)	5108	391	–911	99
H(17E)	5858	1386	–1384	99
H(17F)	4370	1439	–1299	99
H(16D)	4462	1379	1278	84
H(16E)	5948	1496	1331	84
H(16F)	5335	414	890	84
H(18A)	6438	503	409	85
H(18B)	6393	1508	1145	85
H(18C)	7142	1620	154	85
H(18D)	6569	555	–524	72
H(18E)	7229	1626	–103	72
H(18F)	6588	1658	–1142	72
H(5)	7030(13)	5105(11)	330(9)	23(5)
H(10)	4763(14)	6070(11)	–198(11)	24(5)

Protoniertes *Bis*-TMCDA (128)

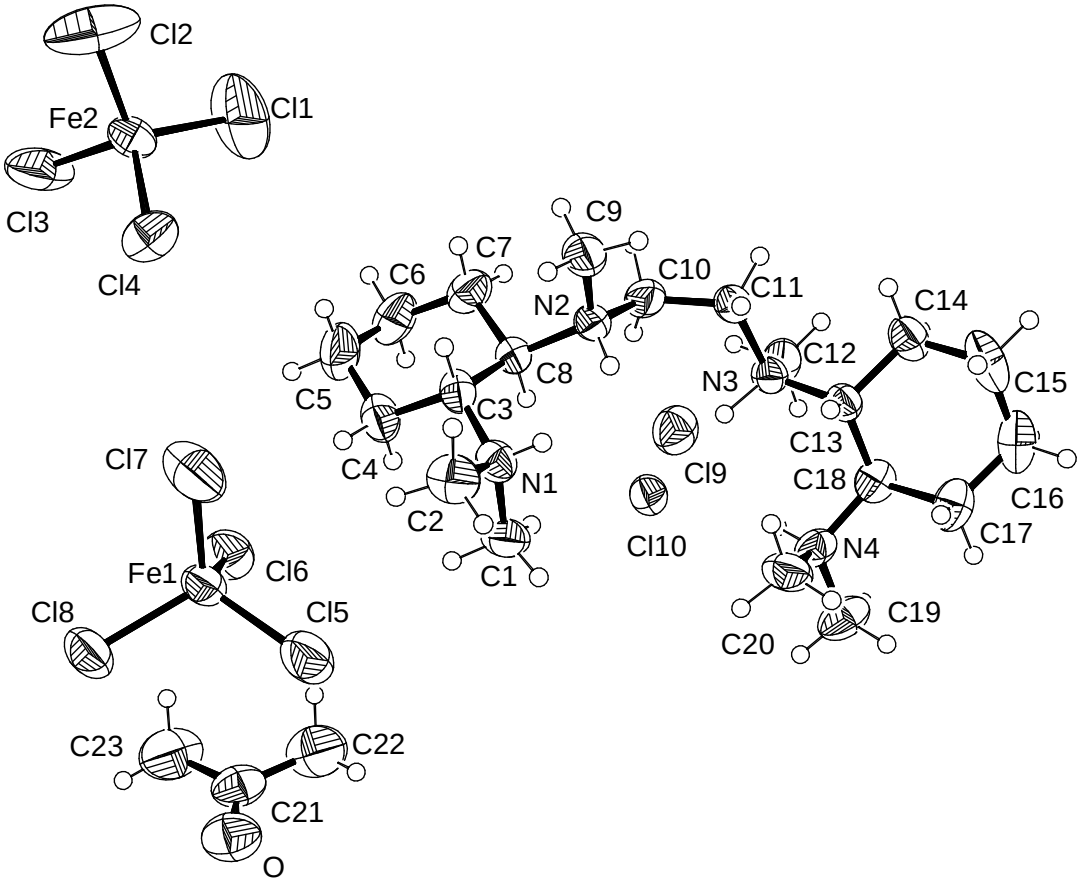


Abbildung 27 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von protoniertem *Bis*-TMCDA (**128**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 79 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für protoniertes *Bis*-TMCDA (**128**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen Uij Tensors.

	x	y	z	U(eq)
C(1)	3518(6)	3771(6)	2131(5)	61(2)
C(2)	4184(6)	5271(6)	3259(5)	65(2)
C(3)	2849(5)	3902(5)	3615(4)	48(1)
C(4)	3786(6)	3072(5)	4119(5)	60(2)
C(5)	3505(8)	2520(7)	4933(6)	83(2)
C(6)	2285(7)	1978(7)	4549(5)	75(2)
C(7)	1340(6)	2773(6)	4049(5)	61(2)
C(8)	1595(5)	3383(5)	3226(4)	43(1)
C(9)	441(6)	5041(6)	3407(5)	63(2)
C(10)	–602(5)	3595(6)	2283(4)	58(2)
C(11)	–1450(5)	4217(6)	1425(4)	53(2)
C(12)	–2262(5)	2771(6)	239(5)	57(2)

C(13)	–1838(5)	4578(4)	–337(4)	43(1)
C(14)	–3129(5)	4971(5)	–513(5)	56(2)
C(15)	–3498(6)	5854(5)	–1286(6)	74(2)
C(16)	–3347(6)	5469(6)	–2224(6)	71(2)
C(17)	–2082(6)	5101(5)	–2052(5)	60(2)
C(18)	–1703(6)	4198(5)	–1287(4)	49(1)
C(19)	–388(8)	3285(6)	–2087(5)	67(2)
C(20)	526(6)	4636(6)	–849(5)	63(2)
Cl(1)	2305(2)	1633(3)	7562(3)	151(2)
Cl(2)	3972(4)	3128(2)	9659(3)	146(2)
Cl(3)	5155(3)	706(2)	9195(2)	124(1)
Cl(4)	5018(2)	2880(2)	7649(1)	76(1)
Cl(5)	6978(2)	3493(2)	3291(2)	102(1)
Cl(6)	6426(2)	1226(2)	4535(2)	76(1)
Cl(7)	6821(2)	3781(3)	5665(2)	136(1)
Cl(8)	9342(2)	2434(2)	5366(2)	79(1)
Cl(9)	1193(2)	5816(1)	1467(1)	61(1)
Cl(10)	761(1)	2532(1)	708(1)	51(1)
Fe(3)	4082(1)	2070(1)	8509(1)	58(1)
Fe(4)	7413(1)	2744(1)	4718(1)	58(1)
N(1)	3205(4)	4478(4)	2839(4)	48(1)
N(2)	576(4)	4168(4)	2749(4)	44(1)
N(3)	–1490(4)	3747(4)	465(3)	44(1)
N(4)	–444(5)	3802(4)	–1184(4)	50(1)
O	8924(5)	1139(5)	2528(4)	85(2)
C(21)	8238(8)	552(6)	2728(6)	68(2)
C(22)	6918(9)	569(9)	2146(7)	101(3)
C(23)	8646(11)	–175(8)	3573(8)	111(4)

Tabelle 80 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für protoniertes *Bis*-TMCDA (**128**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	54(4)	74(4)	62(4)	–13(3)	28(3)	–2(3)
C(2)	62(4)	59(4)	73(5)	–14(3)	24(4)	–15(3)
C(3)	42(3)	48(3)	46(3)	–1(3)	6(2)	4(2)
C(4)	51(3)	61(4)	61(4)	2(3)	8(3)	11(3)
C(5)	83(5)	89(6)	64(5)	23(4)	6(4)	24(4)
C(6)	95(5)	75(5)	52(4)	21(4)	21(4)	–3(4)

C(7)	67(4)	71(4)	48(3)	4(3)	22(3)	–12(3)
C(8)	39(3)	49(3)	41(3)	3(2)	13(2)	2(2)
C(9)	55(4)	74(4)	54(4)	–17(3)	12(3)	11(3)
C(10)	43(3)	87(5)	45(3)	5(3)	18(3)	–7(3)
C(11)	37(3)	76(4)	45(3)	–8(3)	11(2)	2(3)
C(12)	46(3)	64(4)	56(4)	14(3)	12(3)	–10(3)
C(13)	35(3)	46(3)	45(3)	2(2)	12(2)	1(2)
C(14)	40(3)	59(4)	68(4)	7(3)	15(3)	3(3)
C(15)	42(3)	48(4)	117(7)	17(4)	6(4)	4(3)
C(16)	64(4)	57(4)	69(5)	16(4)	–8(4)	–5(3)
C(17)	75(4)	45(3)	50(4)	2(3)	8(3)	–3(3)
C(18)	58(3)	38(3)	50(3)	1(3)	17(3)	–4(2)
C(19)	110(6)	46(3)	55(4)	–1(3)	42(4)	3(4)
C(20)	47(3)	80(5)	70(5)	–8(4)	30(3)	–7(3)
Cl(1)	68(1)	161(3)	193(3)	25(3)	2(2)	–53(2)
Cl(2)	254(4)	93(2)	152(3)	–25(2)	150(3)	–13(2)
Cl(3)	150(2)	131(2)	131(2)	70(2)	102(2)	85(2)
Cl(4)	89(1)	77(1)	68(1)	–7(1)	33(1)	–30(1)
Cl(5)	67(1)	134(2)	114(2)	60(2)	43(1)	22(1)
Cl(6)	68(1)	73(1)	90(1)	8(1)	31(1)	–8(1)
Cl(7)	65(1)	201(3)	125(2)	–106(2)	10(1)	7(2)
Cl(8)	45(1)	96(1)	95(1)	15(1)	22(1)	2(1)
Cl(9)	69(1)	54(1)	58(1)	6(1)	20(1)	6(1)
Cl(10)	48(1)	53(1)	51(1)	2(1)	14(1)	7(1)
Fe(3)	51(1)	50(1)	78(1)	1(1)	30(1)	–3(1)
Fe(4)	44(1)	68(1)	64(1)	–3(1)	21(1)	–1(1)
N(1)	41(3)	49(3)	53(3)	–4(2)	13(2)	–3(2)
N(2)	35(2)	56(3)	41(3)	–2(2)	12(2)	–1(2)
N(3)	32(2)	56(3)	40(3)	–8(2)	8(2)	–3(2)
N(4)	66(3)	42(3)	47(3)	10(2)	28(2)	2(2)
O	91(4)	81(4)	94(4)	–3(3)	46(3)	–21(3)
C(21)	93(6)	55(4)	69(5)	–9(3)	44(4)	6(4)
C(22)	96(7)	121(8)	91(6)	–27(6)	38(5)	–39(6)
C(23)	148(10)	96(7)	112(8)	32(6)	73(7)	51(7)

Tabelle 81 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für protoniertes *Bis*-TMCDA (**128**).

	x	y	z	U(eq)
H(1A)	3605	4206	1601	92
H(1B)	2874	3244	1866	92
H(1C)	4279	3400	2464	92
H(2A)	3933	5780	3664	97
H(2B)	4347	5657	2732	97
H(2C)	4917	4900	3657	97
H(3)	2829	4444	4113	57
H(4A)	3831	2531	3637	72
H(4B)	4585	3421	4382	72
H(5A)	3503	3050	5436	100
H(5B)	4136	1982	5238	100
H(6A)	2309	1405	4088	90
H(6B)	2090	1647	5094	90
H(7A)	1264	3295	4535	73
H(7B)	557	2398	3778	73
H(8)	1612	2848	2722	52
H(9A)	171	4734	3916	94
H(9B)	–157	5561	3030	94
H(9C)	1219	5399	3706	94
H(10A)	–1001	3483	2773	69
H(10B)	–441	2884	2055	69
H(11A)	–2272	4212	1466	64
H(11B)	–1177	4969	1462	64
H(12A)	–1994	2274	790	85
H(12B)	–2194	2424	–342	85
H(12C)	–3104	2971	122	85
H(13)	–1287	5204	–105	51
H(14A)	–3190	5247	104	67
H(14B)	–3695	4361	–726	67
H(15A)	–4350	6056	–1409	89
H(15B)	–2990	6495	–1047	89
H(16A)	–3913	4872	–2495	85
H(16B)	–3547	6058	–2705	85
H(17A)	–1524	5714	–1828	72
H(17B)	–2014	4842	–2671	72
H(18)	–2274	3588	–1533	59
H(19A)	–479	3830	–2589	101
H(19B)	–1041	2760	–2319	101

H(19C)	391	2924	–1949	101
H(20A)	1319	4293	–677	95
H(20B)	455	5006	–279	95
H(20C)	436	5154	–1372	95
H(1N)	2630(60)	4940(50)	2570(40)	44(16)
H(2N)	870(40)	4470(30)	2320(30)	9(10)
H(3N)	–630(50)	3480(50)	630(40)	44(15)
H(4N)	–370(40)	3260(40)	–750(40)	22(11)
H(22A)	6451	676	2582	151
H(22B)	6687	–113	1802	151
H(22C)	6751	1154	1673	151
H(23A)	8464	–915	3354	166
H(23B)	8228	4	4031	166
H(23C)	9519	–94	3897	166

$ZnBr_2$-Addukt von *Bis*-TMCDA (129)

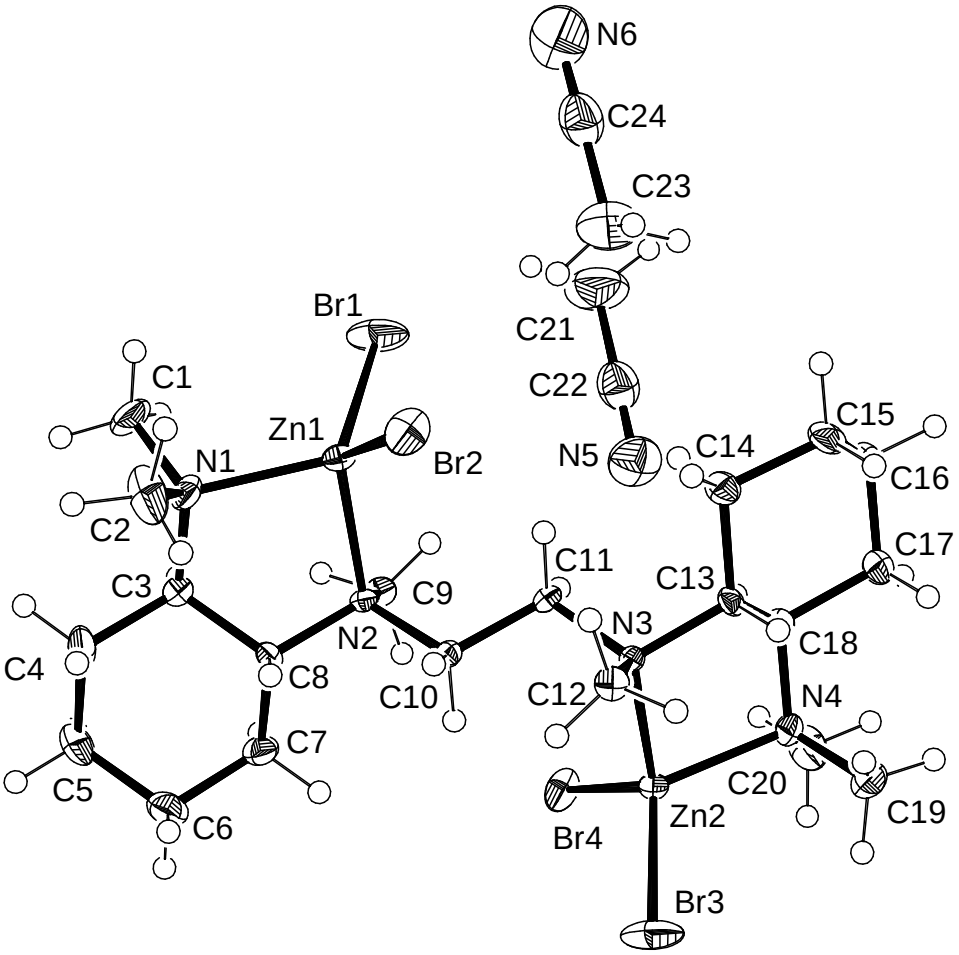


Abbildung 28 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des $ZnBr_2$-Adduktes (**129**) von *Bis*-TMCDA (x) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 82 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter ($Å^2$ x 10^3) für das $ZnBr_2$-Addukt von *Bis*-TMCDA (**129**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
Br(1)	6512(1)	3786(1)	10623(1)	47(1)
Br(2)	2028(1)	5865(1)	11333(1)	33(1)
Br(3)	2014(1)	13281(1)	6134(1)	43(1)
Br(4)	6624(1)	10804(1)	6114(1)	30(1)
C(1)	7529(6)	4308(4)	13307(4)	46(1)
C(2)	4843(6)	5792(6)	13536(4)	41(1)
C(3)	7165(4)	6911(4)	12087(3)	17(1)
C(4)	7479(5)	7449(4)	13039(3)	29(1)
C(5)	8461(5)	8701(4)	12434(4)	35(1)
C(6)	7486(5)	9915(4)	11271(4)	30(1)

C(7)	7223(5)	9367(4)	10322(3)	23(1)
C(8)	6223(4)	8127(4)	10911(3)	14(1)
C(9)	7430(4)	7355(4)	9236(3)	17(1)
C(10)	4439(5)	8710(4)	9098(3)	13(1)
C(11)	3801(5)	8246(4)	8186(3)	14(1)
C(12)	982(5)	9805(4)	8072(3)	19(1)
C(13)	1666(4)	8921(4)	6460(3)	16(1)
C(14)	1398(5)	7369(4)	7122(3)	22(1)
C(15)	497(5)	7010(4)	6235(4)	27(1)
C(16)	1620(5)	7242(4)	5060(3)	28(1)
C(17)	1870(5)	8786(4)	4376(3)	26(1)
C(18)	2701(4)	9243(4)	5230(3)	16(1)
C(19)	1266(5)	11808(4)	3958(4)	32(1)
C(20)	4286(6)	11016(5)	3599(3)	34(1)
C(21)	7068(14)	3437(8)	7497(8)	76(2)
C(22)	6552(7)	4998(7)	6987(5)	43(1)
C(23)	1702(15)	3479(9)	9563(9)	78(3)
C(24)	2044(7)	1930(7)	10230(5)	41(1)
N(1)	6248(4)	5659(3)	12639(3)	21(1)
N(2)	5852(4)	7615(3)	9966(2)	13(1)
N(3)	2431(4)	9408(3)	7310(2)	12(1)
N(4)	2900(4)	10789(3)	4578(2)	18(1)
N(5)	6174(6)	6198(5)	6576(4)	53(1)
N(6)	2315(6)	709(6)	10753(4)	62(1)
Zn(1)	5095(1)	5650(1)	11120(1)	17(1)
Zn(2)	3532(1)	11169(1)	6054(1)	17(1)

Tabelle 83 Anisotrope Auslenkungsparameter ($Å^2 \times 10^3$) für das $ZnBr_2$-Addukt von *Bis*-TMCDA (**129**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	65(1)	21(1)	56(1)	–22(1)	21(1)	–8(1)
Br(2)	18(1)	38(1)	33(1)	–6(1)	3(1)	–11(1)
Br(3)	61(1)	17(1)	50(1)	–16(1)	19(1)	–7(1)
Br(4)	20(1)	36(1)	25(1)	0(1)	–3(1)	–13(1)
C(1)	55(3)	26(3)	39(3)	7(2)	–31(2)	–7(2)
C(2)	42(3)	71(4)	20(2)	–20(2)	15(2)	–36(2)
C(3)	16(2)	16(2)	17(2)	–6(2)	0(1)	–3(2)
C(4)	33(2)	37(3)	19(2)	–14(2)	–7(2)	–5(2)
C(5)	37(2)	37(3)	40(2)	–22(2)	–14(2)	–10(2)

C(6)	28(2)	26(2)	43(2)	–19(2)	–6(2)	–8(2)
C(7)	27(3)	16(2)	23(2)	–4(2)	–1(2)	–7(2)
C(8)	13(2)	17(2)	15(2)	–10(2)	1(1)	–4(2)
C(9)	16(2)	16(2)	19(2)	–10(2)	2(1)	–2(2)
C(10)	13(2)	12(2)	13(2)	–4(1)	0(1)	–2(2)
C(11)	14(2)	12(2)	12(2)	–3(2)	2(1)	–1(2)
C(12)	16(2)	21(2)	19(2)	–11(2)	2(1)	0(2)
C(13)	12(2)	18(2)	20(2)	–10(2)	–4(1)	–2(2)
C(14)	20(2)	23(2)	26(2)	–12(2)	1(2)	–7(2)
C(15)	20(2)	21(2)	42(2)	–13(2)	–10(2)	–6(2)
C(16)	35(2)	21(2)	34(2)	–16(2)	–16(2)	–2(2)
C(17)	34(2)	25(2)	22(2)	–14(2)	–8(2)	–3(2)
C(18)	19(2)	14(2)	18(2)	–8(2)	–3(1)	–2(2)
C(19)	33(2)	23(2)	33(2)	–4(2)	–11(2)	–5(2)
C(20)	39(3)	49(3)	22(2)	–18(2)	11(2)	–23(2)
C(21)	114(7)	49(4)	69(5)	–32(4)	8(5)	–11(4)
C(22)	39(3)	51(4)	46(3)	–30(3)	–3(2)	–3(3)
C(23)	119(8)	45(5)	77(6)	–34(4)	–11(5)	–11(4)
C(24)	42(3)	47(4)	43(3)	–31(3)	–2(2)	–1(3)
N(1)	21(2)	20(2)	15(2)	1(1)	–1(1)	–5(1)
N(2)	15(2)	10(2)	13(1)	–5(1)	0(1)	–2(1)
N(3)	11(2)	11(2)	14(1)	–5(1)	–3(1)	0(1)
N(4)	20(2)	19(2)	14(2)	–5(1)	–2(1)	–4(1)
N(5)	44(3)	46(3)	62(3)	–24(2)	–1(2)	3(2)
N(6)	70(4)	60(3)	59(3)	–36(3)	0(2)	5(3)
Zn(1)	18(1)	14(1)	18(1)	–5(1)	2(1)	–5(1)
Zn(2)	18(1)	14(1)	17(1)	–5(1)	0(1)	–5(1)

Tabelle 84 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3 für das $ZnBr_2$-Addukt von *Bis*-TMCDA (**129**).

	x	y	z	U(eq)
H(1A)	8097	4357	13992	69
H(1B)	8414	4181	12702	69
H(1C)	6924	3492	13669	69
H(2A)	5358	5756	14281	62
H(2B)	4212	4997	13806	62
H(2C)	4028	6709	13111	62
H(3)	8341	6571	11804	20

H(4A)	8166	6651	13769	35
H(4B)	6342	7767	13366	35
H(5A)	8588	9058	13063	42
H(5B)	9646	8362	12185	42
H(6A)	6336	10308	11529	36
H(6B)	8160	10699	10870	36
H(7A)	8376	9036	10024	28
H(7B)	6566	10163	9575	28
H(8)	5067	8501	11195	17
H(9A)	7211	6795	8809	25
H(9B)	8427	6820	9819	25
H(9C)	7691	8278	8598	25
H(10A)	4873	9617	8599	16
H(10B)	3440	8905	9614	16
H(11A)	4798	8022	7682	17
H(11B)	3315	7363	8677	17
H(12A)	642	8930	8739	29
H(12B)	–23	10408	7515	29
H(12C)	1376	10339	8464	29
H(13)	474	9534	6204	19
H(14A)	676	7222	7892	27
H(14B)	2545	6711	7395	27
H(15A)	344	5996	6676	32
H(15B)	–671	7637	5986	32
H(16A)	1052	7007	4479	33
H(16B)	2774	6590	5313	33
H(17A)	720	9426	4068	31
H(17B)	2622	8906	3625	31
H(18)	3900	8638	5465	20
H(19A)	1013	11707	3205	48
H(19B)	1412	12796	3702	48
H(19C)	294	11595	4559	48
H(20A)	5390	10381	3993	52
H(20B)	4430	12021	3223	52
H(20C)	3955	10798	2932	52
H(21A)	6810(80)	3080(70)	8360(60)	90(20)
H(23A)	1850(80)	3770(70)	9880(60)	40(20)
H(21B)	7890(110)	3270(90)	7100(80)	130(40)
H(23B)	150(110)	3630(90)	9870(70)	150(30)
H(21C)	6120(80)	3010(70)	7080(60)	100(20)
H(23C)	1960(130)	3630(110)	8690(110)	220(50)

LiBr·Addukt von *Bis*-TMCDA (130)

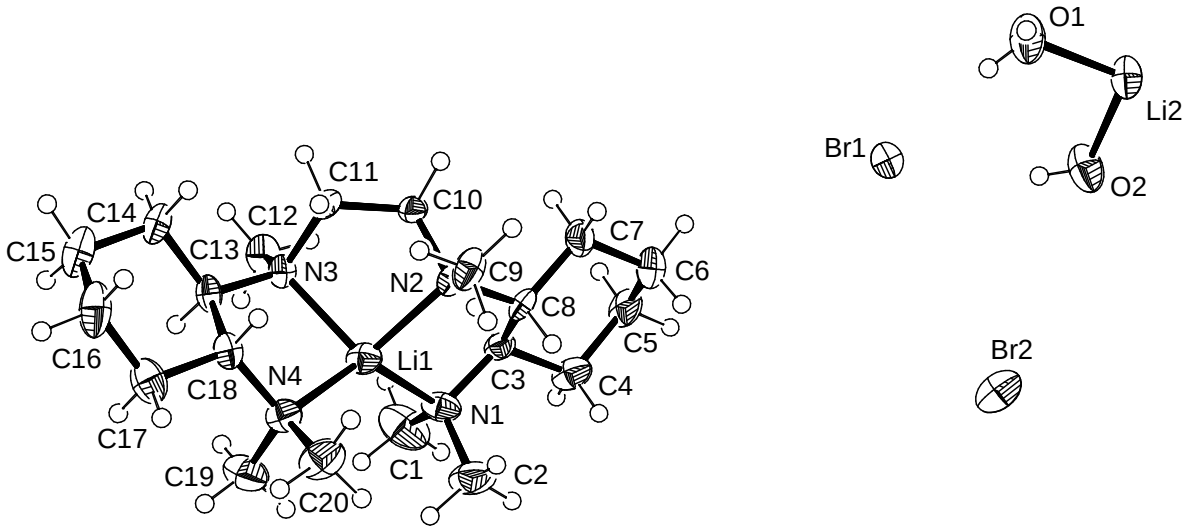


Abbildung 29 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des LiBr-Adduktes von *Bis*-TMCDA (**130**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 85 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für das LiBr-Addukt von *Bis*-TMCDA (**130**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
Br(1)	1466(1)	1805(1)	2433(1)	32(1)
Br(2)	5000	5000	2855(1)	51(1)
C(1)	8955(4)	2616(4)	5836(7)	66(2)
C(2)	9212(4)	1690(3)	4060(7)	60(2)
C(3)	7744(3)	1904(2)	5084(5)	29(1)
C(4)	7821(3)	1323(3)	6263(6)	40(1)
C(5)	6933(3)	1073(3)	6759(6)	46(1)
C(6)	6417(4)	830(3)	5406(6)	49(1)
C(7)	6330(3)	1402(3)	4223(6)	40(1)
C(8)	7214(3)	1667(2)	3694(5)	28(1)
C(9)	6998(4)	1907(3)	965(5)	38(1)
C(10)	6555(3)	2753(2)	2841(5)	27(1)
C(11)	6773(3)	3403(2)	1991(5)	28(1)
C(12)	7514(3)	4084(3)	3903(5)	38(1)
C(13)	8066(3)	4082(2)	1286(5)	29(1)
C(14)	7494(3)	4573(2)	376(5)	37(1)
C(15)	8010(4)	4991(3)	-768(5)	50(1)
C(16)	8515(4)	4532(3)	-1845(6)	53(2)

C(17)	9088(4)	4043(3)	-957(5)	43(1)
C(18)	8567(3)	3616(2)	181(5)	31(1)
C(19)	9823(3)	3384(3)	1847(6)	49(2)
C(20)	9359(4)	2542(3)	42(6)	50(2)
Li(1)	8274(4)	2775(4)	2720(8)	32(2)
Li(2)	0	0	2135(12)	38(3)
N(1)	8576(3)	2203(2)	4595(4)	35(1)
N(2)	7174(2)	2204(2)	2489(4)	26(1)
N(3)	7618(2)	3679(2)	2498(4)	25(1)
N(4)	9078(2)	3099(2)	1045(4)	33(1)
O(1)	-1(3)	766(2)	709(5)	48(1)
O(2)	921(3)	233(2)	3578(5)	49(1)

Tabelle 86 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für das LiBr-Addukt von *Bis*-TMCDA (**130**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	35(1)	33(1)	28(1)	–2(1)	2(1)	–4(1)
Br(2)	69(1)	56(1)	28(1)	0	0	22(1)
C(1)	53(4)	102(6)	43(3)	2(4)	–9(3)	–19(4)
C(2)	42(3)	75(5)	63(4)	26(3)	20(3)	22(3)
C(3)	27(3)	30(3)	30(2)	5(2)	6(2)	8(2)
C(4)	42(3)	49(3)	30(3)	8(2)	6(2)	16(3)
C(5)	53(3)	41(3)	44(3)	26(3)	13(3)	9(3)
C(6)	53(3)	33(3)	60(3)	16(3)	3(3)	–6(3)
C(7)	41(3)	32(3)	46(3)	13(2)	–7(2)	–8(2)
C(8)	37(3)	16(3)	30(2)	0(2)	–1(2)	8(2)
C(9)	57(3)	26(3)	32(2)	1(2)	–13(2)	2(3)
C(10)	22(2)	23(2)	36(2)	–1(2)	–6(2)	1(2)
C(11)	30(2)	22(2)	31(2)	–1(2)	–2(2)	7(2)
C(12)	50(3)	35(3)	28(2)	–6(2)	6(2)	–2(3)
C(13)	38(3)	21(3)	28(2)	–2(2)	1(2)	–9(2)
C(14)	52(3)	21(3)	37(3)	4(2)	–3(2)	2(2)
C(15)	78(4)	28(3)	43(3)	6(3)	–4(3)	0(3)
C(16)	84(4)	39(3)	36(3)	12(2)	–3(3)	–14(3)
C(17)	51(3)	50(4)	29(3)	4(2)	5(2)	–13(3)
C(18)	35(3)	29(3)	28(2)	2(2)	2(2)	–6(2)
C(19)	33(3)	71(4)	44(3)	4(3)	–2(2)	–4(3)
C(20)	57(4)	54(4)	39(3)	1(3)	12(3)	18(3)

Li(1)	31(4)	41(4)	24(4)	4(4)	–3(3)	4(3)
Li(2)	50(7)	29(6)	36(6)	0	0	–8(5)
N(1)	26(2)	52(3)	26(2)	1(2)	–4(2)	1(2)
N(2)	33(2)	21(2)	23(2)	0(2)	–3(2)	2(1)
N(3)	33(2)	22(2)	21(2)	–5(2)	2(2)	–2(1)
N(4)	34(2)	38(3)	28(2)	1(2)	2(2)	4(2)
O(1)	68(3)	38(2)	37(2)	1(2)	–6(2)	–13(2)
O(2)	62(3)	49(3)	37(2)	3(2)	–6(2)	–22(2)

Tabelle 87 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für das LiBr-Addukt von *Bis*-TMCDA (**130**).

	x	y	z	U(eq)
H(1A)	8527	2947	6201	100
H(1B)	9463	2859	5445	100
H(1C)	9127	2319	6687	100
H(2A)	9739	1921	3718	90
H(2B)	8966	1430	3202	90
H(2C)	9351	1378	4905	90
H(3)	7408	2277	5589	35
H(4A)	8149	941	5804	49
H(4B)	8144	1487	7174	49
H(5A)	7000	695	7505	55
H(5B)	6619	1447	7278	55
H(6A)	5837	684	5751	58
H(6B)	6708	433	4929	58
H(7A)	5997	1783	4680	48
H(7B)	6005	1232	3321	48
H(8)	7528	1270	3235	33
H(9A)	6451	1656	997	57
H(9B)	7467	1595	685	57
H(9C)	6959	2272	199	57
H(10A)	6559	2843	3961	33
H(10B)	5966	2604	2551	33
H(11A)	6793	3310	873	34
H(11B)	6316	3746	2180	34
H(12A)	7174	4493	3674	56
H(12B)	8084	4217	4291	56
H(12C)	7215	3811	4682	56

H(13)	8507	4369	1825	35
H(14A)	7047	4309	–181	44
H(14B)	7196	4884	1100	44
H(15A)	7613	5282	–1374	60
H(15B)	8414	5293	–207	60
H(16A)	8876	4816	–2533	64
H(16B)	8107	4270	–2492	64
H(17A)	9533	4305	–392	52
H(17B)	9387	3737	–1688	52
H(18)	8128	3360	–432	37
H(19A)	10095	3029	2475	74
H(19B)	9635	3759	2512	74
H(19C)	10241	3555	1094	74
H(20A)	9758	2719	–737	75
H(20B)	8854	2341	–467	75
H(20C)	9651	2193	657	75
H(201)	790(40)	240(30)	4540(70)	70(20)
H(200)	1130(40)	600(30)	3510(70)	70(20)
H(100)	380(40)	1030(30)	890(70)	70(20)
H(101)	0(40)	720(30)	-60(60)	50(20)

Protoniertes Ethanolderivat von TMCDA [(*R,R*)-69a]

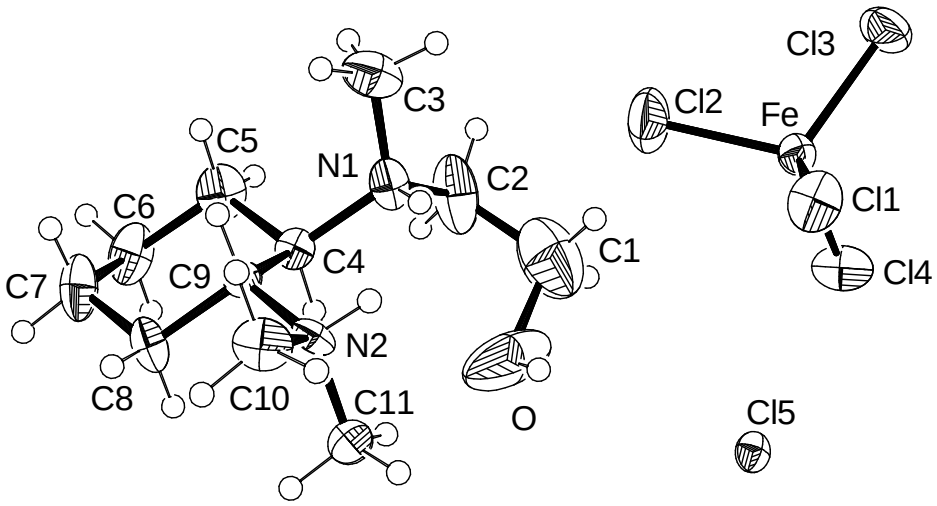


Abbildung 30 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des protonierten Ethanolderivats [(*R,R*)-**69a**] im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 88 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für das protonierte Ethanolderivat [(*R*,*R*)-**69a**]. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	5986(17)	10155(9)	656(5)	98(3)
C(2)	7808(11)	10557(6)	950(4)	64(2)
C(3)	10638(10)	9853(6)	519(3)	56(2)
C(4)	9392(6)	8958(4)	1493(2)	27(1)
C(5)	10807(10)	9638(5)	1836(3)	46(2)
C(6)	11138(10)	9138(6)	2463(3)	50(2)
C(7)	11614(10)	7889(6)	2419(3)	57(2)
C(8)	10246(9)	7216(5)	2076(2)	42(1)
C(9)	9958(6)	7693(4)	1435(2)	25(1)
C(10)	9519(9)	5816(4)	927(3)	43(1)
C(11)	6926(7)	6742(5)	1367(3)	39(1)
Cl(1)	5892(2)	6709(2)	3047(1)	54(1)
Cl(2)	8384(3)	8152(2)	4177(1)	79(1)
Cl(3)	6375(2)	9757(2)	2966(1)	66(1)
Cl(4)	3697(2)	8479(1)	4112(1)	53(1)
Cl(5)	8231(2)	7836(1)	9789(1)	37(1)
Fe	6104(1)	8285(1)	3583(1)	35(1)
N(1)	9044(7)	9544(4)	881(2)	35(1)
N(2)	8683(6)	6943(3)	1085(2)	27(1)
O	5511(10)	8887(9)	956(3)	129(4)

Tabelle 89 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für das protonierte Ethanolderivat [(*R*,*R*)-**69a**]. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2$ [$h^2a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	124(9)	95(7)	76(6)	9(5)	1(7)	40(7)
C(2)	93(6)	36(3)	64(4)	–15(3)	–29(4)	35(4)
C(3)	67(5)	49(4)	54(4)	9(3)	9(3)	–11(3)
C(4)	29(2)	27(2)	27(2)	–7(2)	1(2)	3(2)
C(5)	60(4)	33(3)	46(3)	–15(2)	–10(3)	–1(3)
C(6)	52(3)	59(4)	40(3)	–24(3)	–22(3)	–3(3)
C(7)	56(4)	71(4)	43(3)	–4(3)	–26(3)	12(4)
C(8)	53(3)	43(3)	31(3)	6(2)	–12(3)	8(3)
C(9)	23(2)	23(2)	28(2)	–1(2)	1(2)	–1(2)

C(10)	54(4)	26(3)	49(3)	–9(2)	7(3)	1(2)
C(11)	36(3)	41(3)	41(3)	3(3)	–6(2)	–8(2)
Cl(1)	53(1)	56(1)	51(1)	–20(1)	3(1)	12(1)
Cl(2)	74(1)	56(1)	107(2)	16(1)	–54(1)	–12(1)
Cl(3)	54(1)	62(1)	83(1)	39(1)	14(1)	14(1)
Cl(4)	62(1)	37(1)	60(1)	–11(1)	23(1)	0(1)
Cl(5)	39(1)	47(1)	24(1)	–3(1)	–3(1)	3(1)
Fe	34(1)	33(1)	38(1)	3(1)	–3(1)	2(1)
N(1)	48(3)	22(2)	35(2)	–5(2)	–13(2)	0(2)
N(2)	41(2)	19(2)	22(2)	5(1)	3(2)	–4(2)
O	93(5)	236(10)	57(4)	–42(5)	12(3)	–95(6)

Tabelle 90 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für das protonierte Ethanolderivat [(*R*,*R*)-**69a**].

	x	y	z	U(eq)
H(500)	8580(80)	9170(50)	690(30)	30(17)
H(400)	8490(70)	7190(40)	720(20)	19(12)
H(1A)	6097	10092	211	118
H(1B)	5055	10715	750	118
H(2A)	8272	11236	734	77
H(2B)	7652	10754	1383	77
H(3A)	10299	10016	100	84
H(3B)	11464	9213	526	84
H(3C)	11190	10532	696	84
H(4)	8292	8986	1736	33
H(5A)	11906	9626	1600	56
H(5B)	10431	10446	1876	56
H(6A)	12099	9563	2662	60
H(6B)	10076	9225	2715	60
H(7A)	11739	7568	2831	68
H(7B)	12752	7813	2210	68
H(8A)	9131	7240	2302	51
H(8B)	10618	6406	2047	51
H(9)	11104	7674	1219	30
H(10A)	9652	5354	1295	65
H(10B)	10670	5953	747	65
H(10C)	8781	5406	636	65
H(11A)	6212	6273	1094	59
H(11B)	6346	7478	1436	59

H(11C)	7073	6343	1754	59
H(0)	5242	8427	679	193

ZnBr-Addukt des Ethanolderivat von TMCDA (131)

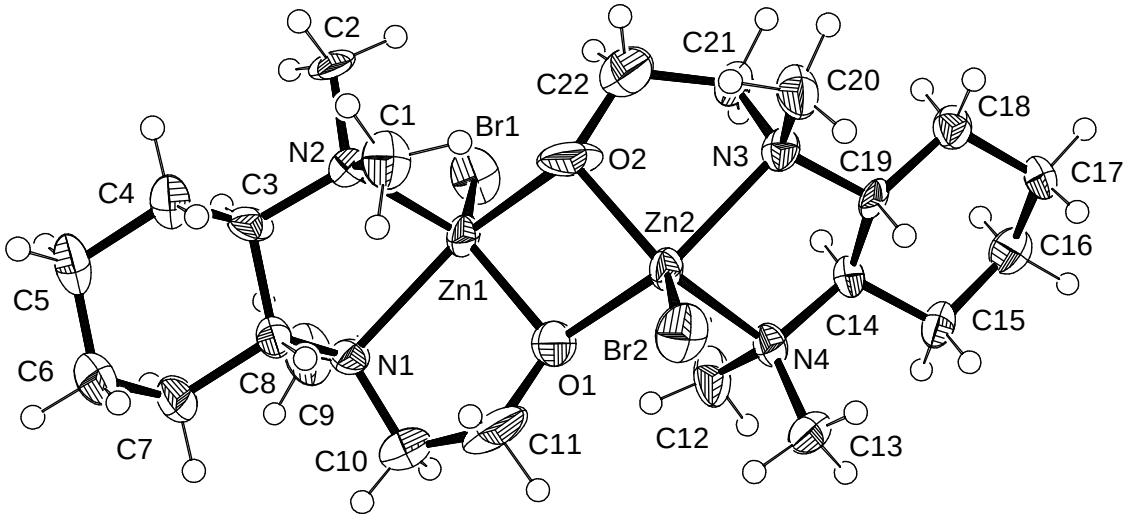


Abbildung 31 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des ZnBr-Adduktes des Ethanolderivats (**131**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).´

Tabelle 91 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für das ZnBr-Addukt des Ethanolderivats (**131**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
Br(1)	4360(2)	–821(1)	9059(1)	52(1)
Br(2)	7950(2)	5025(1)	8509(1)	47(1)
C(1)	9719(13)	809(11)	8677(4)	44(3)
C(2)	8880(13)	–1177(11)	9028(3)	38(3)
C(3)	8897(15)	–1200(9)	8307(3)	37(3)
C(4)	10578(14)	–1477(11)	8200(3)	40(3)
C(5)	10716(16)	–2355(12)	7833(3)	51(3)
C(6)	9873(18)	–1719(14)	7481(4)	56(4)
C(7)	8181(15)	–1448(13)	7580(3)	47(3)
C(8)	7954(13)	–602(11)	7957(3)	35(2)
C(9)	5230(15)	–1563(13)	8054(4)	54(3)
C(10)	5450(17)	703(14)	7821(4)	60(4)

C(11)	5900(30)	2099(16)	8004(5)	104(7)
C(12)	2607(13)	3260(13)	8668(4)	54(4)
C(13)	3653(15)	5445(11)	8528(3)	46(3)
C(14)	3081(13)	4763(10)	9224(3)	33(2)
C(15)	1816(13)	5798(10)	9227(3)	35(2)
C(16)	1313(13)	6142(11)	9654(3)	40(3)
C(17)	2764(14)	6664(11)	9883(3)	38(3)
C(18)	4086(12)	5677(10)	9880(3)	34(2)
C(19)	4612(12)	5269(8)	9462(3)	27(2)
C(20)	7471(13)	4846(13)	9577(4)	47(3)
C(21)	5601(15)	3014(11)	9678(3)	41(3)
C(22)	6666(18)	1935(15)	9518(4)	65(4)
N(1)	6225(11)	–347(8)	8063(2)	31(2)
N(2)	8627(10)	–340(8)	8665(2)	31(2)
N(3)	5896(9)	4250(8)	9451(2)	29(2)
N(4)	3651(10)	4348(8)	8815(2)	31(2)
O(1)	5478(10)	2139(7)	8432(2)	46(2)
O(2)	6962(15)	1882(8)	9083(3)	80(4)
Zn(1)	6253(1)	483(1)	8688(1)	29(1)
Zn(2)	6089(1)	3528(1)	8833(1)	29(1)

Tabelle 92 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für das ZnBr-Addukt des Ethanolderivats (**131**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	58(1)	43(1)	56(1)	0(1)	17(1)	–16(1)
Br(2)	50(1)	32(1)	58(1)	7(1)	10(1)	–9(1)
C(1)	38(6)	36(6)	58(7)	–7(6)	2(5)	–10(5)
C(2)	27(5)	61(7)	27(5)	13(5)	–3(5)	23(5)
C(3)	63(7)	22(5)	25(5)	–2(4)	–15(5)	–5(5)
C(4)	44(6)	33(6)	44(6)	–6(5)	10(5)	3(5)
C(5)	59(8)	46(7)	49(7)	–18(6)	16(6)	9(6)
C(6)	73(9)	61(9)	35(6)	–6(6)	14(6)	21(7)
C(7)	55(8)	49(7)	36(6)	–18(5)	–10(6)	12(6)
C(8)	49(6)	28(5)	27(5)	–1(4)	6(5)	8(5)
C(9)	40(7)	49(8)	73(9)	–26(7)	–4(6)	–16(6)
C(10)	69(9)	62(9)	50(7)	5(7)	–18(7)	26(8)

C(11)	167(19)	59(10)	84(12)	18(9)	–49(12)	48(12)
C(12)	38(7)	47(7)	78(9)	–37(7)	–19(6)	6(5)
C(13)	61(7)	38(6)	39(6)	9(5)	1(6)	20(6)
C(14)	44(6)	24(5)	31(5)	–8(4)	–1(5)	5(5)
C(15)	36(6)	23(5)	48(6)	–3(5)	–1(5)	6(5)
C(16)	34(6)	38(6)	49(6)	2(5)	0(5)	5(5)
C(17)	53(7)	34(6)	28(5)	–10(5)	2(5)	11(5)
C(18)	32(6)	30(5)	40(6)	–6(4)	–5(4)	0(5)
C(19)	37(6)	7(4)	38(5)	2(4)	–5(4)	0(4)
C(20)	34(6)	50(7)	58(7)	–24(6)	–13(5)	9(5)
C(21)	52(7)	29(5)	42(6)	1(5)	–2(5)	13(5)
C(22)	71(10)	56(8)	67(9)	–1(7)	–21(8)	16(8)
N(1)	37(5)	28(4)	29(4)	–4(3)	–11(4)	0(4)
N(2)	31(4)	29(4)	31(4)	1(3)	–3(4)	6(4)
N(3)	20(4)	31(4)	37(4)	–2(4)	1(3)	3(4)
N(4)	36(4)	24(4)	32(4)	–7(3)	1(4)	–4(4)
O(1)	67(5)	28(4)	43(5)	–4(3)	–11(4)	0(4)
O(2)	158(10)	27(4)	55(6)	10(4)	–63(7)	–4(6)
Zn(1)	35(1)	17(1)	36(1)	–2(1)	1(1)	1(1)
Zn(2)	36(1)	18(1)	32(1)	–2(1)	3(1)	0(1)

Tabelle 93 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für das ZnBr-Addukt des Ethanolderivats (**131**).

	x	y	z	U(eq)
H(1A)	10774	514	8767	66
H(1B)	9302	1482	8860	66
H(1C)	9810	1197	8412	66
H(2A)	8416	–2064	8987	58
H(2B)	8363	–748	9255	58
H(2C)	10026	–1264	9080	58
H(3)	8397	–2084	8366	44
H(4A)	11113	–1927	8424	49
H(4B)	11137	–621	8152	49
H(5A)	11856	–2491	7768	62
H(5B)	10237	–3240	7887	62
H(6A)	10413	–874	7410	68
H(6B)	9928	–2327	7251	68
H(7A)	7620	–2310	7615	56

H(7B)	7676	–978	7356	56
H(8)	8440	290	7901	42
H(9A)	4243	–1406	8202	81
H(9B)	5818	–2305	8175	81
H(9C)	4970	–1787	7780	81
H(10A)	4278	582	7824	72
H(10B)	5826	648	7545	72
H(11A)	7060	2258	7972	124
H(11B)	5322	2815	7862	124
H(12A)	1597	3639	8574	82
H(12B)	2395	2626	8882	82
H(12C)	3139	2796	8450	82
H(13A)	4140	5141	8281	69
H(13B)	4268	6197	8634	69
H(13C)	2553	5731	8478	69
H(14)	2656	3952	9360	39
H(15A)	876	5471	9078	43
H(15B)	2214	6614	9094	43
H(16A)	885	5335	9786	49
H(16B)	465	6829	9651	49
H(17A)	3135	7509	9763	46
H(17B)	2449	6853	10159	46
H(18A)	3742	4870	10026	41
H(18B)	5013	6061	10022	41
H(19)	5021	6087	9326	33
H(20A)	7560	5756	9473	71
H(20B)	8346	4300	9473	71
H(20C)	7528	4869	9865	71
H(21A)	4469	2745	9653	49
H(21B)	5834	3166	9961	49
H(22A)	7714	2017	9651	77
H(22B)	6207	1065	9599	77

CuI-Addukt des Ethanolderivat von TMCDA (132)

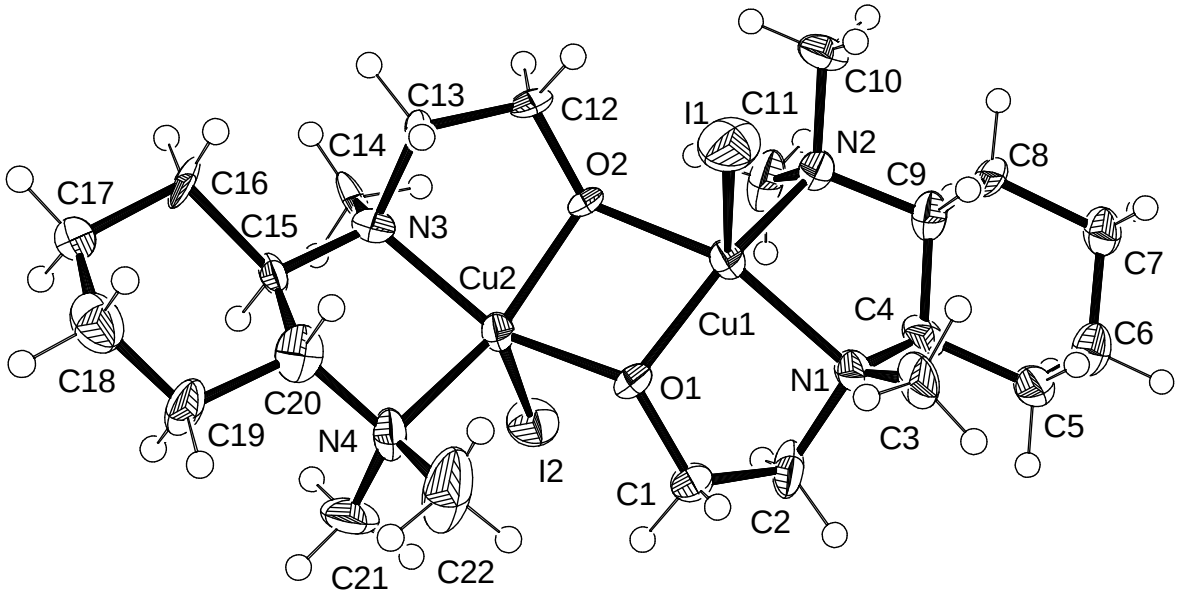


Abbildung 32 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des CuI-Adduktes des Ethanolderivat von TMCDA (**132**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 94 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für das CuI-Addukt des Ethanolderivats von TMCDA (**132**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	10444(16)	4695(16)	3246(9)	33(4)
C(2)	10965(13)	3820(20)	2566(9)	38(4)
C(3)	13377(15)	4740(20)	2840(8)	40(4)
C(4)	12401(12)	4211(18)	1464(8)	31(3)
C(5)	13417(15)	2870(20)	1458(9)	34(4)
C(6)	13591(15)	2390(20)	596(8)	35(3)
C(7)	14107(13)	3821(17)	164(7)	32(3)
C(8)	13068(13)	5261(19)	154(7)	26(3)
C(9)	12838(13)	5645(17)	1017(7)	31(3)
C(10)	12445(15)	8522(17)	845(9)	40(3)
C(11)	10584(15)	6730(20)	535(9)	46(4)
C(12)	9623(15)	10083(18)	1918(8)	29(3)
C(13)	8765(16)	10717(18)	2536(9)	34(4)
C(14)	6701(11)	9740(19)	1940(7)	30(4)
C(15)	6934(12)	9975(15)	3382(7)	25(3)
C(16)	6697(17)	11810(20)	3522(9)	40(4)
C(17)	5912(14)	12044(19)	4244(8)	36(3)
C(18)	6571(17)	11220(20)	4963(9)	45(4)

C(19)	6768(18)	9520(20)	4795(9)	40(4)
C(20)	7625(13)	9200(20)	4107(8)	34(3)
C(21)	6745(19)	6451(19)	3900(10)	54(5)
C(22)	8990(20)	6860(30)	4533(10)	84(9)
Cu(1)	11235(2)	6938(2)	2179(1)	27(1)
Cu(2)	8603(2)	7549(2)	2803(1)	25(1)
I(1)	12930(1)	9171(1)	3097(1)	49(1)
I(2)	7174(1)	5228(1)	1810(1)	42(1)
N(1)	12128(12)	4735(14)	2287(7)	31(3)
N(2)	11792(11)	6973(16)	1056(7)	30(3)
N(3)	7647(11)	9665(14)	2663(7)	28(3)
N(4)	7911(11)	7462(17)	3930(6)	31(3)
O(1)	10204(10)	6314(12)	3049(6)	27(2)
O(2)	9685(10)	8404(12)	1987(6)	27(2)

Tabelle 95 Anisotrope Auslenkungsparameter ($Å^2 \times 10^3$) für das CuI-Addukt des Ethanolderivats von TMCDA (**132**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2\, h\, k\, a^*\, b^*\, U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	38(8)	15(8)	49(9)	–2(6)	16(7)	–2(6)
C(2)	24(7)	29(9)	63(10)	–18(7)	9(6)	6(6)
C(3)	45(8)	57(11)	22(6)	2(6)	20(6)	15(7)
C(4)	20(6)	32(7)	41(7)	–2(6)	6(5)	–11(6)
C(5)	35(8)	27(9)	44(8)	0(6)	17(6)	0(6)
C(6)	36(7)	39(9)	31(7)	–9(6)	2(6)	11(7)
C(7)	34(7)	37(8)	28(6)	–7(6)	10(5)	7(6)
C(8)	33(7)	15(6)	31(6)	–6(6)	8(5)	6(6)
C(9)	25(7)	37(9)	30(7)	–2(6)	1(5)	10(6)
C(10)	40(8)	31(8)	51(8)	5(6)	18(7)	–11(6)
C(11)	41(8)	53(11)	44(8)	–3(7)	0(7)	26(8)
C(12)	38(7)	10(6)	42(7)	3(6)	10(6)	–2(6)
C(13)	41(8)	19(7)	47(8)	4(6)	32(7)	10(6)
C(14)	8(5)	54(10)	31(7)	–9(6)	8(5)	–8(5)
C(15)	22(6)	23(7)	33(6)	–11(5)	17(5)	–5(5)
C(16)	53(10)	18(8)	50(9)	–7(6)	18(7)	20(7)
C(17)	31(7)	30(8)	50(9)	6(7)	18(6)	4(6)
C(18)	45(9)	49(10)	42(9)	–13(7)	13(7)	–9(8)
C(19)	53(9)	42(11)	27(7)	8(6)	5(6)	32(7)
C(20)	27(7)	44(9)	30(7)	–4(7)	–9(5)	5(7)

C(21)	76(12)	28(8)	62(10)	6(7)	38(9)	–13(8)
C(22)	105(17)	110(20)	36(9)	18(11)	17(10)	77(16)
Cu(1)	22(1)	26(1)	34(1)	0(1)	10(1)	–1(1)
Cu(2)	20(1)	23(1)	34(1)	–1(1)	9(1)	1(1)
I(1)	39(1)	39(1)	66(1)	3(1)	–4(1)	–9(1)
I(2)	39(1)	40(1)	47(1)	–3(1)	0(1)	–10(1)
N(1)	34(6)	25(7)	35(6)	–3(5)	17(5)	1(5)
N(2)	26(6)	23(6)	42(6)	0(5)	8(5)	4(5)
N(3)	28(6)	24(7)	32(6)	5(5)	8(5)	–4(5)
N(4)	26(6)	39(8)	28(6)	–4(5)	7(4)	10(5)
O(1)	28(5)	15(5)	37(5)	5(4)	7(4)	5(4)
O(2)	31(5)	9(5)	43(5)	4(4)	13(4)	3(4)

Tabelle 96 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für das CuI-Addukt des Ethanolderivats von TMCDA (**132**).

	x	y	z	U(eq)
H(23E)	9594	4196	3382	40
H(23F)	11112	4624	3714	40
H(22A)	10239	3704	2131	46
H(22B)	11267	2737	2738	46
H(23A)	13177	5184	3349	60
H(23B)	14067	5393	2618	60
H(23C)	13711	3650	2916	60
H(130)	11531	3822	1190	37
H(10A)	13101	1945	1750	41
H(10B)	14296	3221	1723	41
H(12E)	14242	1501	588	42
H(12F)	12715	2035	330	42
H(33A)	14244	3516	–386	39
H(33B)	14989	4160	428	39
H(12C)	13439	6202	–102	31
H(12D)	12205	4963	–146	31
H(118)	13712	6034	1287	37
H(55A)	12722	8452	307	59
H(55B)	13238	8723	1218	59
H(55C)	11797	9393	873	59
H(12G)	10808	6757	–15	70
H(12H)	9936	7582	617	70
H(12I)	10186	5701	646	70

H(1A)	9223	10386	1384	35
H(1B)	10543	10540	1998	35
H(01D)	9335	10854	3041	40
H(01E)	8406	11774	2368	40
H(01A)	6480	10854	1815	46
H(01B)	5873	9159	2026	46
H(01C)	7123	9258	1499	46
H(121)	6022	9475	3288	30
H(11C)	7577	12367	3605	48
H(11D)	6185	12281	3051	48
H(11A)	5841	13195	4356	44
H(11B)	4986	11622	4127	44
H(11E)	7455	11724	5122	54
H(11F)	5998	11335	5406	54
H(12A)	5872	9018	4675	48
H(12B)	7205	9005	5277	48
H(122)	8513	9744	4231	41
H(12M)	6985	5385	3726	80
H(12N)	6032	6893	3527	80
H(12O)	6421	6385	4426	80
H(12J)	8657	6906	5058	126
H(12K)	9793	7531	4525	126
H(12L)	9213	5763	4408	126

Hydroiodid des Diphenylethanolderivats von TMCDA [(*R*,*R*)-69c]

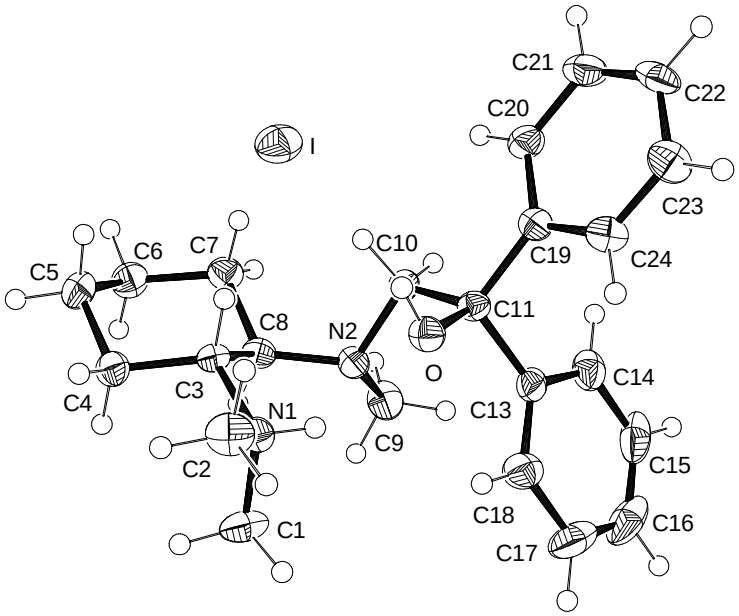


Abbildung 33 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Hydroiodids des Diphenylethanolderivats von TMCDA (**69c**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 97 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für das Hydroiodid des Diphenylethanolderivats von TMCDA (**69c**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
C(1)	1466(5)	6577(3)	5765(5)	40(1)
C(2)	4285(5)	6458(3)	6433(4)	37(1)
C(3)	3074(4)	8278(2)	5929(3)	23(1)
C(4)	2929(4)	8580(6)	7329(3)	29(1)
C(5)	3171(5)	9782(3)	7543(4)	33(1)
C(6)	2054(5)	10427(3)	6450(4)	33(1)
C(7)	2168(5)	10081(3)	5058(5)	29(1)
C(8)	1839(4)	8876(3)	4860(3)	25(1)
C(9)	112(3)	8582(6)	2655(3)	35(1)
C(10)	2904(4)	8741(2)	2842(3)	23(1)
C(11)	3594(4)	7769(3)	2275(3)	23(1)
C(13)	2303(4)	7088(3)	1376(4)	28(1)
C(14)	1521(4)	7488(4)	124(4)	36(1)
C(15)	293(5)	6922(4)	–685(5)	49(1)
C(16)	–146(7)	5963(6)	–235(6)	55(2)
C(17)	610(6)	5557(4)	987(6)	50(1)
C(18)	1858(4)	6117(3)	1811(4)	35(1)

C(19)	4759(5)	8086(4)	1470(4)	24(1)
C(20)	5171(5)	9133(4)	1274(5)	31(1)
C(21)	6229(6)	9356(4)	527(5)	37(1)
C(22)	6871(4)	8548(6)	–48(3)	36(1)
C(23)	6478(6)	7486(4)	160(5)	37(1)
C(24)	5432(4)	7275(3)	911(4)	30(1)
I	7501(1)	8515(1)	5594(1)	38(1)
N(1)	2927(4)	7074(3)	5633(3)	25(1)
N(2)	1706(3)	8431(5)	3511(2)	25(1)
O	4366(3)	7103(2)	3393(2)	28(1)

Tabelle 98 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für das Hydroiodid des Diphenylethanolderivats von TMCDA (**69c**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	36(3)	26(2)	59(3)	-3(2)	13(2)	-9(2)
C(2)	35(2)	28(2)	46(2)	9(2)	7(2)	8(2)
C(3)	23(2)	20(3)	27(2)	-1(1)	6(1)	-3(1)
C(4)	30(2)	28(2)	24(1)	3(2)	2(1)	-1(3)
C(5)	37(2)	31(2)	31(2)	-7(2)	7(2)	-2(2)
C(6)	38(3)	25(2)	37(2)	-2(2)	10(2)	1(2)
C(7)	33(2)	22(2)	34(2)	2(2)	11(2)	2(2)
C(8)	19(2)	27(2)	29(2)	1(1)	8(2)	0(1)
C(9)	20(2)	52(2)	31(2)	1(3)	3(1)	2(3)
C(10)	23(2)	22(3)	23(2)	0(1)	3(1)	1(1)
C(11)	24(2)	20(2)	24(2)	3(1)	4(1)	0(1)
C(13)	24(2)	33(2)	28(2)	-8(2)	11(2)	-3(2)
C(14)	26(2)	53(3)	30(2)	-7(2)	9(2)	-2(2)
C(15)	30(2)	79(4)	36(2)	-25(2)	9(2)	2(2)
C(16)	24(3)	69(4)	72(5)	-45(3)	12(3)	-11(2)
C(17)	35(3)	38(3)	83(4)	-26(3)	26(3)	-13(2)
C(18)	30(2)	33(2)	47(2)	-5(2)	17(2)	-1(2)
C(19)	17(2)	33(2)	21(2)	3(2)	-1(2)	-1(2)
C(20)	34(3)	23(2)	36(2)	-4(2)	12(2)	-3(2)
C(21)	35(3)	36(2)	38(3)	9(2)	8(2)	-10(2)
C(22)	23(2)	52(2)	36(2)	11(4)	10(1)	-9(3)
C(23)	28(2)	41(3)	45(3)	3(2)	14(2)	8(2)
C(24)	26(2)	27(2)	38(2)	5(2)	9(2)	2(2)
I	26(1)	39(1)	47(1)	-3(1)	10(1)	-4(1)

N(1)	29(2)	23(2)	25(2)	2(1)	8(1)	3(1)
N(2)	19(1)	32(2)	22(1)	2(2)	3(1)	0(2)
O	27(1)	28(1)	26(1)	4(1)	4(1)	1(1)

Tabelle 99 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für das Hydroiodid des Diphenylethanolderivats von TMCDA (**69c**).

	x	y	z	U(eq)
H(1)	2810(50)	7020(30)	4780(40)	27(12)
H(1A)	1402	5835	5430	60
H(1B)	580	6990	5237	60
H(1C)	1446	6575	6716	60
H(2A)	4316	6505	7393	56
H(2B)	5242	6761	6284	56
H(2C)	4190	5703	6149	56
H(3)	4118	8518	5850	28
H(4A)	1887	8378	7423	34
H(4B)	3714	8184	8021	34
H(5A)	4252	9966	7543	40
H(5B)	3018	9980	8435	40
H(6A)	2302	11203	6578	40
H(6B)	979	10318	6525	40
H(7A)	3221	10240	4957	35
H(7B)	1409	10491	4360	35
H(8)	821	8742	5075	30
H(9A)	-101	9353	2512	53
H(9B)	-632	8266	3101	53
H(9C)	13	8229	1783	53
H(10A)	3746	9124	3495	28
H(10B)	2452	9245	2097	28
H(14)	1831	8154	-181	43
H(15)	-241	7196	-1544	58
H(16)	-994	5576	-787	66
H(17)	291	4891	1281	60
H(18)	2394	5832	2662	42
H(20)	4725	9708	1656	37
H(21)	6509	10081	414	44
H(22)	7573	8704	-581	44
H(23)	6929	6910	-214	44

H(24)	5172	6549	1045	36
H(0)	5160(50)	7410(30)	3800(40)	34(12)

$ZnBr_2$·(*R,R*)-TMCDA [(*R,R*)-133]

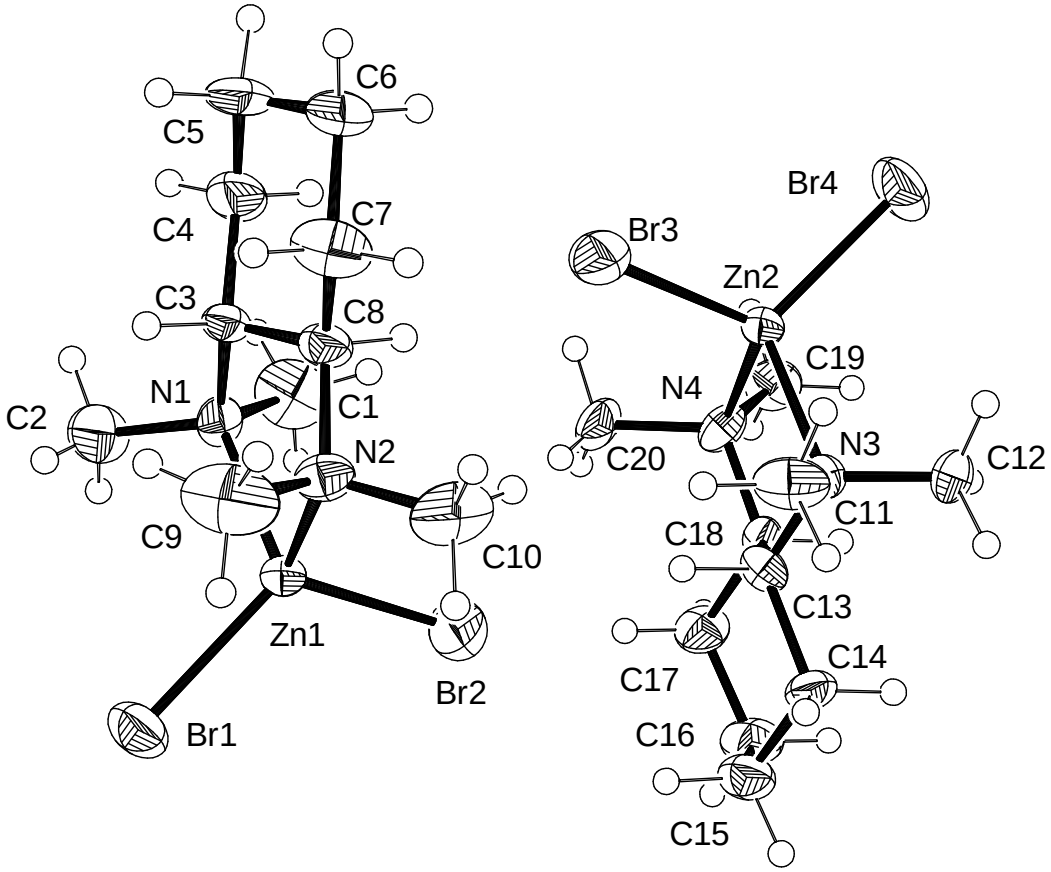


Abbildung 34 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von $ZnBr_2$·(*R,R*)-TMCDA (**133**). im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 100 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter ($Å^2$ x 10^3) für $ZnBr_2$·(*R,R*)-TMCDA (**133**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(12)	2223(14)	3891(8)	9566(10)	40(3)
N(4)	460(12)	6197(8)	9541(7)	35(2)
N(2)	4642(11)	7094(8)	5643(7)	34(2)
N(1)	2704(11)	8698(7)	6003(7)	31(2)
N(3)	2404(12)	4759(7)	9022(7)	28(2)

Zn(1)	5016(1)	8122(1)	6834(1)	27(1)
Zn(2)	26(1)	5270(1)	8255(1)	28(1)
Br(2)	4902(2)	7422(1)	8408(1)	72(1)
Br(3)	13(2)	5970(1)	6631(1)	58(1)
Br(1)	7289(1)	9121(1)	7015(1)	49(1)
Br(4)	–2176(2)	4224(1)	8113(1)	58(1)
C(4)	182(14)	8089(12)	4444(10)	55(4)
C(1)	1570(19)	8645(13)	6666(12)	62(4)
C(7)	2258(16)	6576(11)	4090(11)	53(4)
C(11)	3329(14)	4565(11)	8213(10)	47(3)
C(9)	5611(18)	7280(16)	4907(11)	72(5)
C(10)	5129(15)	6178(9)	6157(11)	56(4)
C(19)	–903(14)	6132(11)	10064(10)	47(3)
C(3)	2086(11)	8107(7)	4960(7)	32(2)
C(20)	450(15)	7176(8)	9081(9)	43(3)
C(8)	2759(11)	7139(8)	5107(8)	33(2)
C(13)	3280(11)	5513(7)	9731(7)	28(2)
C(5)	–366(16)	7540(11)	3427(11)	64(4)
C(18)	2073(11)	5962(7)	10321(7)	27(2)
C(14)	4958(12)	5238(11)	10534(8)	34(3)
C(6)	253(15)	6604(9)	3594(10)	57(3)
C(15)	5799(13)	6046(9)	11250(9)	42(3)
C(16)	4612(14)	6438(10)	11852(8)	49(3)
C(17)	2998(15)	6756(9)	11035(8)	41(3)
C(2)	2828(18)	9688(9)	5732(12)	57(4)

Tabelle 101 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für $ZnBr_2$·(*R*,*R*)-TMCDA (**133**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(12)	39(6)	21(6)	54(6)	7(5)	4(5)	9(4)
N(4)	33(5)	36(6)	35(5)	6(4)	8(4)	15(4)
N(2)	25(4)	44(6)	33(4)	–2(4)	7(3)	5(4)
N(1)	23(4)	28(5)	44(5)	8(4)	13(4)	10(4)
N(3)	30(5)	19(5)	32(4)	–4(4)	5(4)	0(4)
Zn(1)	22(1)	29(1)	29(1)	2(1)	5(1)	–1(1)
Zn(2)	21(1)	28(1)	32(1)	2(1)	5(1)	–2(1)
Br(2)	82(1)	71(1)	48(1)	13(1)	–2(1)	–27(1)
Br(3)	55(1)	71(1)	40(1)	8(1)	4(1)	–15(1)
Br(1)	32(1)	49(1)	66(1)	2(1)	17(1)	–9(1)

Br(4)	37(1)	47(1)	94(1)	3(1)	26(1)	–12(1)
C(4)	27(6)	50(9)	76(9)	15(8)	–5(6)	–3(6)
C(1)	59(9)	62(9)	73(9)	–13(8)	31(7)	9(7)
C(7)	40(7)	66(11)	54(7)	–20(7)	14(5)	–5(7)
C(11)	24(5)	74(10)	46(6)	–11(6)	17(5)	3(6)
C(9)	55(8)	120(16)	51(8)	–27(9)	29(7)	–13(9)
C(10)	48(7)	40(7)	72(8)	–18(6)	3(6)	27(6)
C(19)	28(6)	64(9)	52(7)	9(6)	20(5)	4(5)
C(3)	21(4)	43(6)	28(4)	4(5)	3(3)	–9(4)
C(20)	51(7)	26(6)	44(6)	7(5)	1(5)	12(5)
C(8)	24(5)	45(6)	29(5)	–1(4)	8(4)	–8(4)
C(13)	23(4)	36(6)	33(5)	–2(4)	20(4)	–5(4)
C(5)	33(6)	89(11)	52(8)	11(7)	–14(5)	–26(7)
C(18)	25(4)	31(5)	31(5)	7(4)	16(4)	3(4)
C(14)	21(5)	46(8)	33(5)	9(6)	3(4)	2(5)
C(6)	53(7)	62(9)	41(6)	–4(6)	–8(5)	–24(6)
C(15)	29(5)	57(7)	40(6)	1(5)	10(4)	–7(5)
C(16)	45(6)	65(8)	32(6)	–9(5)	2(5)	–8(6)
C(17)	48(7)	42(7)	28(5)	–9(5)	3(5)	0(6)
C(2)	52(7)	24(6)	83(10)	3(6)	0(7)	3(5)

Tabelle 102 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für $ZnBr_2$·(*R*,*R*)-TMCDA (**133**).

	x	y	z	U(eq)
H(10A)	1486	3468	9046	60
H(10B)	1739	4024	10147	60
H(10C)	3324	3603	9869	60
H(2A)	–338	7823	4967	66
H(2B)	–228	8733	4290	66
H(1A)	2116	8918	7375	94
H(1B)	1298	7995	6753	94
H(1C)	541	8988	6312	94
H(5A)	2642	5927	4248	64
H(5B)	2781	6834	3565	64
H(11A)	4425	4295	8583	70
H(11B)	3481	5146	7863	70
H(11C)	2680	4129	7668	70

H(6A)	6789	7372	5321	109
H(6B)	5182	7840	4489	109
H(6C)	5515	6753	4418	109
H(7A)	4390	6017	6585	85
H(7B)	6289	6204	6627	85
H(7C)	5032	5707	5599	85
H(8A)	–897	5511	10372	70
H(8B)	–1988	6245	9525	70
H(8C)	–713	6596	10638	70
H(3)	2554	8407	4421	38
H(9A)	574	7632	9657	65
H(9B)	–611	7281	8515	65
H(9C)	1380	7240	8778	65
H(4)	2238	6829	5613	40
H(23)	3520	6003	9256	33
H(21A)	–1604	7530	3156	77
H(21B)	48	7841	2875	77
H(22)	1852	5478	10810	33
H(24A)	4778	4726	10992	41
H(24B)	5710	5009	10133	41
H(20A)	–87	6269	2898	68
H(20B)	–255	6283	4090	68
H(34A)	6076	6540	10804	50
H(34B)	6853	5833	11778	50
H(32A)	4370	5954	12321	59
H(32B)	5154	6967	12311	59
H(33A)	3254	7244	10575	49
H(33B)	2260	7030	11420	49
H(31A)	3654	9757	5344	86
H(31B)	3175	10055	6396	86
H(31C)	1735	9906	5277	86

Kupfer(II)-chlorid-Addukt des TMCDA-Anisol-Liganden [(*R,R*)-134]

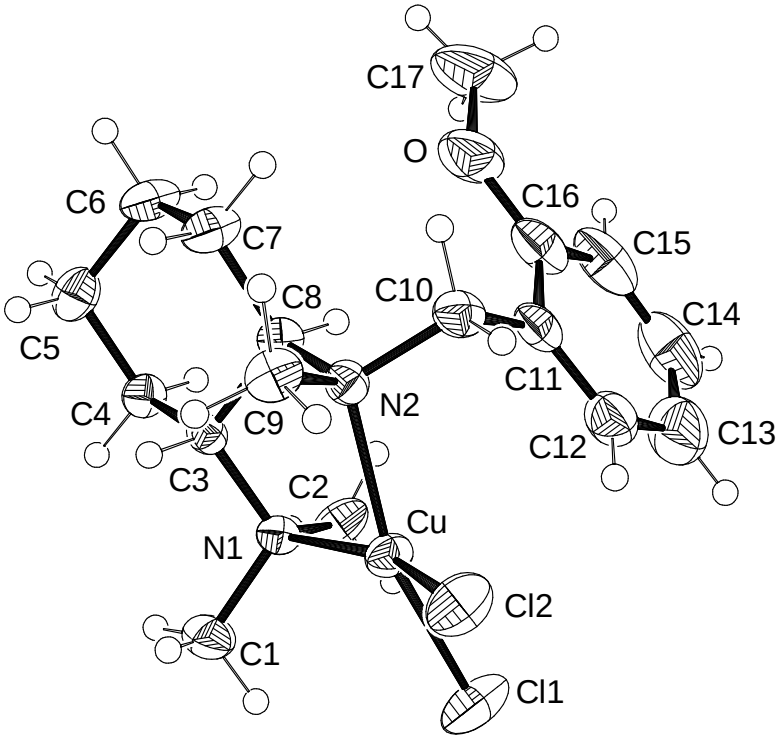


Abbildung 35 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Kupfer(II)-chlorid-Adduktes des TMCDA-Anisol-Liganden [(*R,R*)-**134**] im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 103 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für das Kupfer(II)-chlorid-Addukt des TMCDA-Anisol-Liganden [(*R,R*)-**134**]. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	4617(4)	6263(4)	1375(3)	44(1)
C(2)	6073(4)	5213(3)	491(2)	41(1)
C(3)	6756(3)	6712(3)	1517(2)	25(1)
C(4)	6990(4)	7432(3)	672(2)	29(1)
C(5)	7920(4)	8308(3)	892(3)	40(1)
C(6)	9088(4)	7773(3)	1197(3)	41(1)
C(7)	8871(4)	7091(3)	2069(3)	41(1)
C(8)	7915(3)	6213(3)	1885(2)	27(1)
C(9)	7524(4)	6200(3)	3558(2)	34(1)
C(10)	8548(4)	4651(3)	2868(2)	33(1)
C(11)	8633(4)	3829(3)	2097(3)	35(1)
C(12)	7863(4)	2947(4)	2050(3)	46(1)
C(13)	7910(6)	2179(5)	1346(4)	67(2)
C(14)	8778(6)	2319(5)	669(4)	71(2)
C(15)	9582(5)	3164(5)	701(3)	61(2)

C(16)	9526(4)	3920(4)	1409(3)	46(1)
C(17)	11271(5)	4894(6)	870(4)	83(2)
Cl(1)	4594(1)	3611(1)	1868(1)	57(1)
Cl(2)	5754(1)	4163(1)	3901(1)	47(1)
Cu	5974(1)	4775(1)	2454(1)	29(1)
N(1)	5854(3)	5813(2)	1365(2)	26(1)
N(2)	7617(3)	5523(2)	2710(2)	27(1)
O	10297(3)	4780(3)	1516(2)	59(1)

Tabelle 104 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für das Kupfer(II)-chlorid-Addukt des TMCDA-Anisol-Liganden [(*R,R*)-**134**]. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	27(2)	45(3)	60(3)	10(2)	–5(2)	2(2)
C(2)	50(3)	43(2)	30(2)	–4(2)	–1(2)	–19(2)
C(3)	24(2)	27(2)	25(1)	3(1)	2(1)	3(2)
C(4)	31(2)	31(2)	26(2)	6(1)	0(1)	–1(2)
C(5)	49(3)	33(2)	38(2)	6(2)	4(2)	–7(2)
C(6)	33(2)	50(3)	41(2)	8(2)	–6(2)	–16(2)
C(7)	36(3)	46(2)	39(2)	7(2)	–6(2)	–14(2)
C(8)	28(2)	32(2)	22(1)	1(1)	1(1)	–1(2)
C(9)	39(2)	41(2)	23(2)	–3(1)	–2(2)	–5(2)
C(10)	29(2)	40(2)	30(2)	9(2)	–4(1)	0(2)
C(11)	29(2)	41(2)	37(2)	7(2)	–1(2)	12(2)
C(12)	40(3)	44(3)	53(2)	–7(2)	1(2)	8(2)
C(13)	69(4)	53(3)	78(4)	–21(3)	–6(3)	8(3)
C(14)	80(5)	78(4)	54(3)	–25(3)	–10(3)	39(4)
C(15)	56(3)	84(4)	42(2)	3(2)	5(2)	37(3)
C(16)	38(3)	61(3)	40(2)	13(2)	3(2)	18(2)
C(17)	37(3)	132(6)	79(3)	35(4)	20(3)	9(3)
Cl(1)	63(1)	57(1)	51(1)	18(1)	–16(1)	–33(1)
Cl(2)	56(1)	51(1)	33(1)	9(1)	7(1)	–12(1)
Cu	29(1)	31(1)	28(1)	5(1)	0(1)	–4(1)
N(1)	23(2)	30(2)	25(1)	1(1)	1(1)	0(1)
N(2)	27(2)	28(2)	26(1)	2(1)	–1(1)	2(1)
O	35(2)	74(2)	68(2)	20(2)	15(2)	7(2)

Tabelle 105 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für das Kupfer(II)-chlorid-Addukt des TMCDA-Anisol-Liganden [(*R*,*R*)-**134**].

	x	y	z	U(eq)
H(1A)	4533	6805	882	66
H(1B)	4464	6614	1970	66
H(1C)	4035	5671	1280	66
H(2A)	5566	4556	474	62
H(2B)	6925	5001	455	62
H(2C)	5871	5685	-31	62
H(3)	6424	7197	2010	30
H(4A)	7286	6972	158	35
H(4B)	6226	7782	475	35
H(5A)	8069	8763	340	48
H(5B)	7611	8789	1387	48
H(6A)	9701	8343	1323	49
H(6B)	9398	7296	700	49
H(7A)	9636	6739	2261	49
H(7B)	8597	7573	2574	49
H(8)	8241	5715	1399	32
H(9A)	8326	6476	3725	51
H(9B)	7206	5753	4062	51
H(9C)	6980	6818	3446	51
H(10A)	8353	4260	3445	40
H(10B)	9346	5003	2949	40
H(12)	7274	2860	2520	55
H(13)	7365	1578	1329	80
H(14)	8815	1815	172	85
H(15)	10181	3234	237	73
H(17A)	11821	4269	930	124
H(17B)	11712	5572	997	124
H(17C)	10945	4917	244	124

Zink(II)bromid-Addukt des TMCDA-Pyridin-Liganden [(*R,R*)-136]

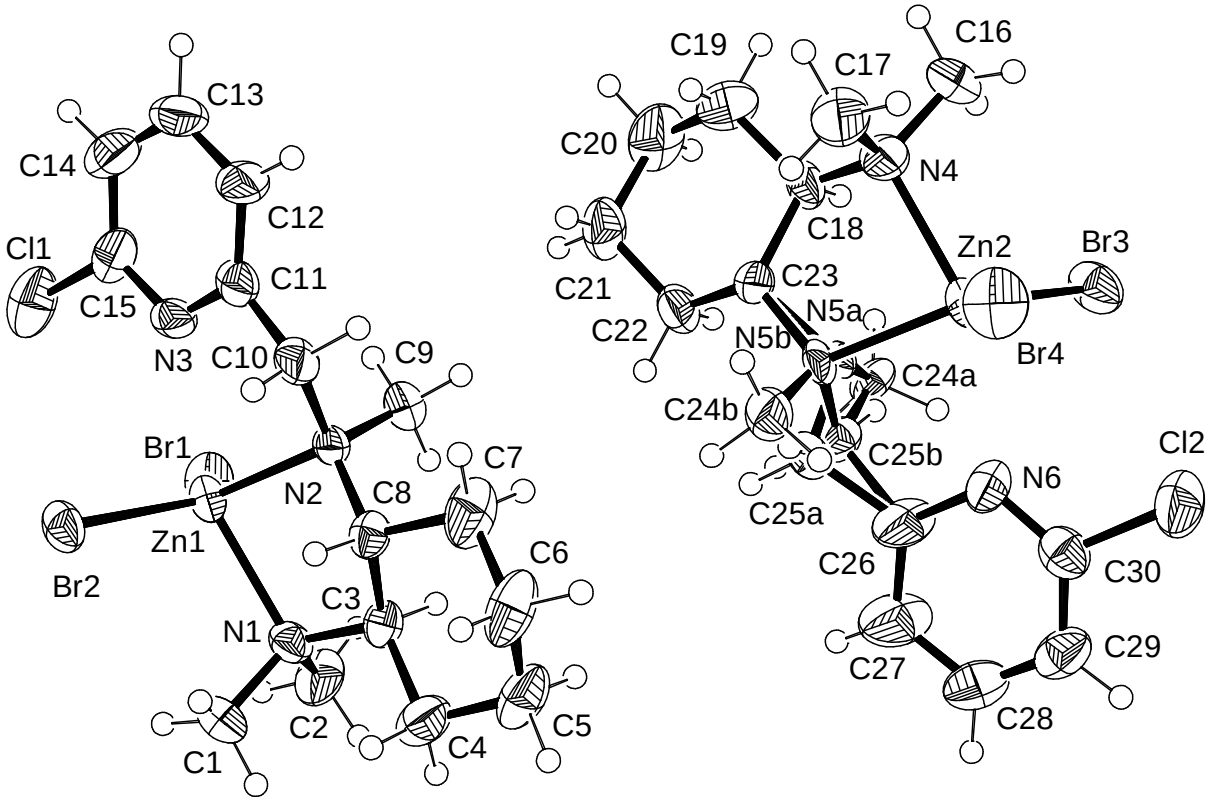


Abbildung 36 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zink(II)bromid-Adduktes des TMCDA-Pyridin-Liganden [(*R,R*)-**136**] im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 106 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für das Zink(II)bromid-Addukt des TMCDA-Pyridin-Liganden [(*R,R*)-**136**]. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
Br(1)	1702(1)	7606(1)	–1342(1)	50(1)
Br(2)	4518(1)	5190(1)	–1146(1)	42(1)
Br(3)	5471(1)	11315(1)	6207(1)	53(1)
Br(4)	7921(1)	8799(1)	6306(1)	64(1)
C(1)	6684(12)	7079(8)	–1421(7)	68(3)
C(2)	5269(12)	8447(6)	–1272(6)	59(3)
C(3)	6387(8)	7742(5)	101(5)	34(2)
C(4)	8137(9)	7920(7)	125(6)	54(2)
C(5)	8747(10)	8127(7)	1071(7)	60(3)
C(6)	8396(11)	7367(7)	1714(7)	68(3)
C(7)	6685(11)	7212(8)	1693(6)	62(3)
C(8)	5990(8)	6996(5)	746(5)	35(2)

C(9)	3424(9)	7622(7)	1058(6)	47(2)
C(10)	3916(10)	5991(6)	1194(5)	44(2)
C(11)	2320(9)	5678(5)	1010(5)	41(2)
C(12)	1532(11)	5266(6)	1650(7)	55(2)
C(13)	125(13)	4888(7)	1432(8)	68(3)
C(14)	–472(11)	4944(7)	555(8)	68(3)
C(15)	399(9)	5398(6)	–64(7)	49(2)
C(16)	3086(12)	9477(8)	6487(6)	64(3)
C(17)	4257(13)	8104(7)	5948(7)	67(3)
C(18)	3042(9)	9225(5)	4870(5)	39(2)
C(19)	1633(10)	8622(9)	4716(7)	70(3)
C(20)	801(10)	8794(9)	3826(7)	77(3)
C(21)	1846(9)	8603(7)	3089(6)	59(2)
C(22)	3201(10)	9242(7)	3199(5)	47(2)
C(23)	4080(9)	9092(6)	4104(5)	42(2)
C(26)	7633(11)	10540(8)	3928(6)	68(3)
C(27)	8392(12)	10989(9)	3283(7)	82(4)
C(28)	9664(11)	11509(8)	3549(8)	63(3)
C(29)	10124(10)	11568(7)	4423(7)	53(2)
C(30)	9282(10)	11090(6)	5015(6)	46(2)
C(24A)	4615(16)	10858(9)	4003(10)	37(3)
C(25A)	6526(16)	9727(12)	3683(9)	35(3)
C(24B)	6813(18)	8736(14)	3969(13)	50(5)
C(25B)	5929(19)	10261(13)	3758(11)	40(4)
Cl(1)	–263(3)	5435(2)	–1176(2)	69(1)
Cl(2)	9825(3)	11155(2)	6155(2)	72(1)
N(1)	5667(7)	7564(5)	–825(4)	37(1)
N(2)	4285(7)	6843(4)	706(4)	31(1)
N(3)	1743(7)	5759(4)	154(4)	39(2)
N(4)	3909(8)	9097(5)	5746(5)	46(2)
N(6)	8056(7)	10592(5)	4805(5)	44(2)
N(5A)	5203(14)	9925(8)	4227(8)	25(2)
N(5B)	5695(16)	9419(10)	4267(8)	33(3)
Zn(1)	3634(1)	6661(1)	–661(1)	33(1)
Zn(2)	6101(1)	9834(1)	5613(1)	39(1)

Tabelle 107 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für für das Zink(II)bromid-Addukt des TMCDA-Pyridin-Liganden [(*R*,*R*)-**136**]. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	53(1)	41(1)	54(1)	2(1)	–8(1)	13(1)
Br(2)	58(1)	29(1)	40(1)	–5(1)	9(1)	7(1)
Br(3)	76(1)	37(1)	49(1)	–2(1)	19(1)	8(1)
Br(4)	68(1)	48(1)	75(1)	1(1)	–2(1)	19(1)
C(1)	73(7)	84(8)	51(6)	–25(6)	31(5)	–19(6)
C(2)	93(7)	40(5)	45(5)	13(4)	–2(5)	–23(5)
C(3)	38(4)	26(3)	38(4)	–2(3)	–2(3)	1(3)
C(4)	38(5)	48(5)	76(7)	–5(5)	7(4)	–7(4)
C(5)	36(5)	52(5)	89(7)	–12(5)	–15(5)	–4(4)
C(6)	61(6)	61(6)	76(7)	–5(5)	–36(5)	–9(5)
C(7)	73(7)	57(6)	51(6)	7(5)	–30(5)	–9(5)
C(8)	38(4)	33(4)	33(4)	–1(3)	–4(3)	–2(3)
C(9)	55(5)	46(5)	42(5)	–12(4)	10(4)	–3(4)
C(10)	68(5)	41(5)	25(4)	4(3)	5(3)	–9(4)
C(11)	56(5)	26(4)	41(5)	–3(3)	13(4)	3(4)
C(12)	81(7)	32(4)	55(6)	4(4)	30(5)	–10(5)
C(13)	86(7)	43(5)	83(8)	–7(5)	57(6)	–8(5)
C(14)	55(6)	38(5)	113(10)	–14(6)	37(6)	–10(5)
C(15)	30(4)	39(5)	78(7)	–17(5)	2(4)	2(4)
C(16)	80(7)	75(7)	39(5)	–5(5)	24(5)	–17(6)
C(17)	103(8)	46(5)	53(6)	13(4)	4(5)	–18(5)
C(18)	49(5)	34(4)	36(4)	–12(3)	7(3)	4(3)
C(19)	32(5)	97(9)	83(8)	–11(7)	17(4)	–14(5)
C(20)	30(5)	97(9)	102(9)	–32(7)	–3(5)	2(5)
C(21)	48(5)	72(6)	54(6)	–21(5)	–13(4)	1(5)
C(22)	63(5)	49(5)	30(4)	–4(4)	4(4)	–4(4)
C(23)	38(4)	57(5)	30(4)	–4(4)	–1(3)	–16(4)
C(26)	69(6)	93(8)	40(5)	36(5)	–12(4)	–35(6)
C(27)	69(7)	119(11)	57(7)	42(7)	–7(5)	–24(7)
C(28)	58(6)	57(6)	75(8)	16(6)	12(5)	–12(5)
C(29)	41(5)	38(5)	82(7)	–8(5)	11(4)	–3(4)
C(30)	55(5)	40(5)	44(5)	–2(4)	7(4)	7(4)
C(24A)	34(8)	31(7)	43(8)	12(6)	–10(6)	–8(6)
C(25A)	29(8)	51(9)	25(7)	1(7)	–7(6)	10(8)
C(24B)	43(9)	51(11)	57(11)	–19(9)	10(8)	1(8)
C(25B)	38(9)	42(10)	38(10)	6(8)	–5(7)	–7(8)
Cl(1)	59(1)	54(2)	90(2)	–13(1)	–23(1)	1(1)

Cl(2)	59(1)	91(2)	63(2)	–21(1)	–11(1)	–13(1)
N(1)	48(4)	36(3)	29(3)	2(3)	10(3)	0(3)
N(2)	37(3)	24(3)	33(3)	–5(3)	10(2)	0(3)
N(3)	41(4)	31(3)	47(4)	–2(3)	19(3)	4(3)
N(4)	64(4)	31(3)	46(4)	2(3)	13(3)	–7(3)
N(6)	46(4)	39(4)	45(4)	3(3)	–9(3)	–9(3)
N(5A)	39(7)	14(5)	24(6)	–7(5)	10(5)	0(5)
N(5B)	53(9)	33(7)	13(6)	0(5)	–3(5)	–5(7)
Zn(1)	42(1)	29(1)	26(1)	–3(1)	–1(1)	5(1)
Zn(2)	49(1)	39(1)	29(1)	–5(1)	1(1)	3(1)

Tabelle 108 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für das Zink(II)bromid-Addukt des TMCDA-Pyridin-Liganden [(*R*,*R*)-**136**].

	x	y	z	U(eq)
H(1A)	6128	6952	–1997	102
H(1B)	7023	6498	–1142	102
H(1C)	7572	7465	–1518	102
H(2A)	6185	8830	–1288	89
H(2B)	4503	8767	–940	89
H(2C)	4855	8328	–1885	89
H(3)	5915	8321	315	41
H(4A)	8659	7372	–101	65
H(4B)	8346	8447	–269	65
H(5A)	9866	8214	1080	72
H(5B)	8293	8709	1272	72
H(6A)	8785	7536	2328	81
H(6B)	8911	6793	1544	81
H(7A)	6191	7769	1921	74
H(7B)	6471	6695	2097	74
H(8)	6469	6414	546	42
H(9A)	2328	7516	938	71
H(9B)	3716	8192	765	71
H(9C)	3656	7674	1705	71
H(10A)	4615	5496	1026	53
H(10B)	4099	6101	1845	53
H(12)	1954	5240	2250	66
H(13)	–429	4593	1875	82
H(14)	–1437	4684	379	81

H(16A)	2775	10111	6345	96
H(16B)	3754	9471	7037	96
H(16C)	2179	9103	6573	96
H(17A)	3302	7767	6008	101
H(17B)	4894	8059	6508	101
H(17C)	4802	7836	5459	101
H(18)	2686	9879	4845	47
H(19A)	1943	7967	4752	84
H(19B)	934	8739	5196	84
H(20A)	451	9441	3791	92
H(20B)	–107	8390	3756	92
H(21A)	1297	8704	2499	71
H(21B)	2194	7956	3121	71
H(22A)	2846	9887	3154	57
H(22B)	3888	9131	2711	57
H(27)	8053	10944	2669	99
H(28)	10211	11823	3115	76
H(29)	10989	11923	4622	64
H(24A)	5293	11320	4293	55
H(24B)	3589	10926	4216	55
H(24C)	4573	10946	3353	55
H(25A)	6216	9724	3035	42
H(25B)	6999	9128	3849	42
H(24D)	6743	8703	3314	75
H(24E)	6589	8131	4217	75
H(24F)	7846	8925	4180	75
H(25C)	5258	10757	3958	48
H(25D)	5687	10151	3111	48

8.2.4 Kristallstrukturen aus Kapitel 4.4

Dimethyl[N^1,N^2,N^3-Trimethylcyclohexan-(1*R*,2*R*)-diamino-N^1-methyl]phenylsilan-hydrochlorid [(*R*,*R*)-141·HBr]

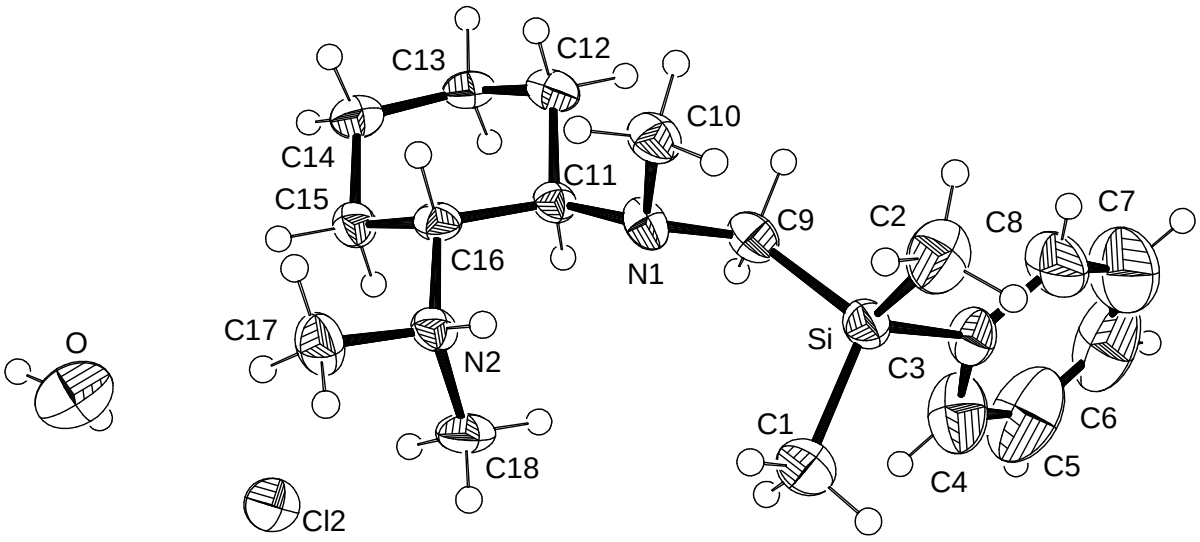


Abbildung 37 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von Dimethyl[N^1,N^2,N^3-Trimethylcyclohexan-(1*R*,2*R*)-diamino-N^1-methyl]phenylsilan-hydrochlorid [(*R*,*R*)-**141**·HBr] im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 109 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für Dimethyl[N^1,N^2,N^3-Trimethylcyclohexan-(1*R*,2*R*)-diamino-N^1-methyl]phenylsilan-hydrochlorid [(*R*,*R*)-**141**·HBr]. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
C(1)	1378(10)	3080(9)	7932(3)	68(2)
C(2)	–1600(7)	5632(9)	8288(3)	60(2)
C(3)	1735(7)	4920(8)	9344(2)	42(1)
C(4)	3279(9)	3929(11)	9565(3)	72(2)
C(5)	3944(12)	3892(14)	10259(5)	105(3)
C(6)	3104(16)	4849(16)	10732(4)	108(4)
C(7)	1600(15)	5779(14)	10514(4)	103(3)
C(8)	959(11)	5840(9)	9834(3)	68(2)
C(9)	2427(7)	6877(7)	8087(3)	39(1)
C(10)	650(7)	8142(7)	7096(3)	38(1)
C(11)	4005(6)	7945(6)	7127(2)	27(1)
C(12)	4379(7)	9841(7)	7316(3)	37(1)
C(13)	6300(6)	10377(7)	7149(3)	35(1)
C(14)	6498(7)	10052(7)	6388(3)	37(1)

C(15)	6020(6)	8188(6)	6172(3)	32(1)
C(16)	4096(6)	7765(6)	6343(2)	28(1)
C(17)	3294(8)	5860(8)	5318(3)	45(1)
C(18)	4526(7)	4503(6)	6411(3)	40(1)
Cl(2)	9478(2)	4299(2)	5997(1)	46(1)
N(1)	2309(5)	7175(6)	7338(2)	31(1)
N(2)	3448(6)	5976(5)	6086(2)	29(1)
O	8069(6)	6157(6)	4554(3)	68(1)
Si	923(2)	5125(2)	8393(1)	36(1)

Tabelle 110 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für Dimethyl[*N*^{1},*N*^{2},*N*^{3}-Trimethylcyclohexan-(1*R*,2*R*)-diamino-*N*^{1}-methyl]phenylsilan-hydrochlorid [(*R*,*R*)-**141**·HBr]. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2$ [h^{2}a*^{2}U^{11} + ... + 2 h k a* b* U^{12}].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	109(6)	46(4)	52(4)	–12(3)	27(4)	–2(4)
C(2)	34(3)	76(5)	71(4)	16(4)	6(3)	2(3)
C(3)	49(3)	52(3)	23(3)	3(3)	–1(2)	–2(3)
C(4)	58(4)	109(6)	48(4)	16(4)	–1(3)	10(4)
C(5)	85(6)	142(10)	80(6)	48(6)	–24(5)	–14(6)
C(6)	141(9)	139(10)	40(4)	1(6)	–5(5)	–66(8)
C(7)	141(8)	122(8)	47(5)	–6(5)	12(5)	7(7)
C(8)	97(5)	74(5)	33(4)	–9(3)	6(3)	15(4)
C(9)	33(3)	43(3)	40(3)	–5(2)	4(2)	6(2)
C(10)	31(3)	41(3)	42(3)	–1(3)	4(2)	9(2)
C(11)	23(2)	28(3)	30(3)	0(2)	3(2)	4(2)
C(12)	40(3)	32(3)	38(3)	–7(2)	–1(2)	8(2)
C(13)	34(3)	25(3)	46(3)	3(2)	1(2)	6(2)
C(14)	35(3)	29(3)	47(3)	2(3)	2(2)	–1(2)
C(15)	32(3)	32(3)	34(3)	–1(2)	9(2)	0(2)
C(16)	30(3)	25(3)	29(3)	1(2)	–3(2)	7(2)
C(17)	50(3)	53(3)	32(3)	–9(3)	8(2)	–8(3)
C(18)	35(3)	25(3)	60(3)	–1(3)	8(2)	7(2)
Cl(2)	36(1)	47(1)	56(1)	–3(1)	7(1)	–5(1)
N(1)	22(2)	45(2)	26(2)	–4(2)	–1(2)	7(2)
N(2)	23(2)	28(2)	37(2)	–3(2)	9(2)	1(2)
O	56(3)	60(3)	81(3)	6(3)	–14(2)	–18(2)
Si	40(1)	38(1)	31(1)	–1(1)	6(1)	6(1)

Tabelle 111 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für Dimethyl[N^1,N^2,N^3-Trimethylcyclohexan-(1*R*,2*R*)-diamino-N^1-methyl]phenylsilan-hydrochlorid [(*R*,*R*)-**141**·HBr].

	x	y	z	U(eq)
H(1A)	874	3178	7444	101
H(1B)	788	2102	8147	101
H(1C)	2714	2879	7963	101
H(2A)	–1792	6826	8445	91
H(2B)	–2245	4815	8566	91
H(2C)	–2088	5520	7798	91
H(4)	3878	3276	9239	87
H(5)	4993	3198	10411	126
H(6)	3585	4851	11208	129
H(7)	975	6403	10841	124
H(8)	–79	6557	9692	82
H(9A)	2123	7984	8311	46
H(9B)	3727	6593	8255	46
H(10A)	677	9279	7327	57
H(10B)	–438	7488	7204	57
H(10C)	591	8311	6592	57
H(11)	5061	7256	7362	32
H(12A)	4291	10010	7818	45
H(12B)	3435	10587	7054	45
H(13A)	6500	11630	7255	42
H(13B)	7249	9702	7441	42
H(14A)	7786	10302	6300	45
H(14B)	5676	10860	6099	45
H(15A)	6081	8049	5667	39
H(15B)	6921	7376	6420	39
H(16)	3234	8646	6104	34
H(17A)	4531	5750	5168	67
H(17B)	2697	6915	5115	67
H(17C)	2553	4838	5163	67
H(18A)	4561	4582	6917	60
H(18B)	5789	4549	6282	60
H(18C)	3945	3402	6250	60
H(100)	2350(60)	5800(50)	6180(20)	10(11)
H(200)	8920(60)	6740(60)	4350(20)	34(15)
H(300)	9100(300)	5900(400)	4860(130)	530(190)

$ZnCl_2$-Addukt von Dimethyl[*N*^{1},*N*^{2},*N*^{3}-Trimethylcyclohexan-(1*R*,2*R*)-diamino-N^1-methyl]phenylsilan [(*R*,*R*)-144]

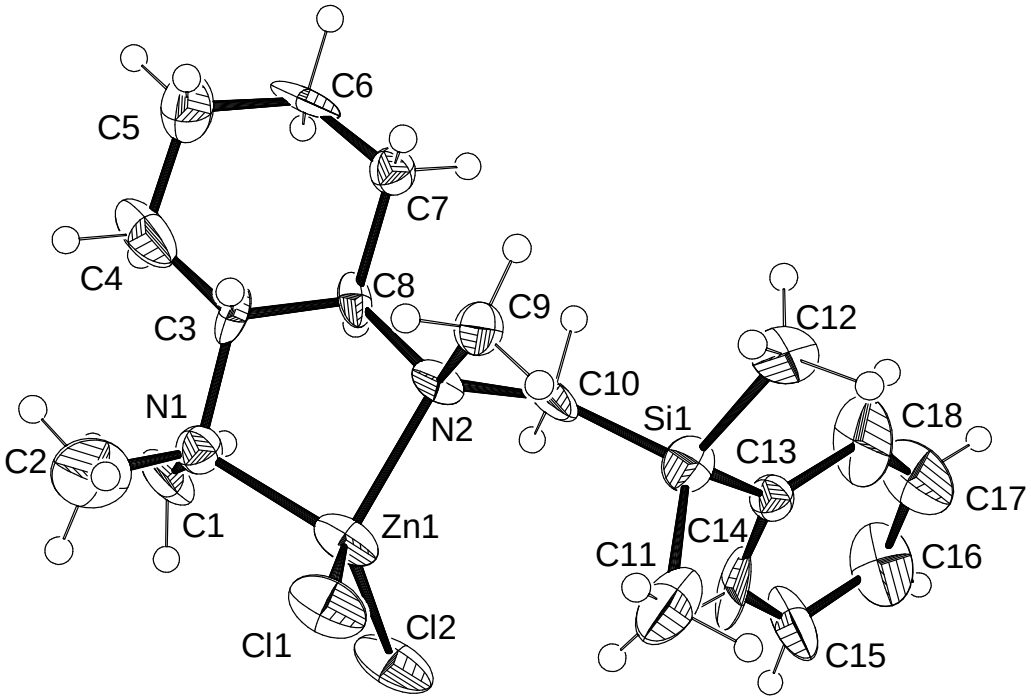


Abbildung 38 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des $ZnCl_2$-Addukts von Dimethyl[N^1,N^2,N^3-Trimethylcyclohexan-(1*R*,2*R*)-diamino-N^1-methyl]phenylsilan (**144**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 112 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für das $ZnCl_2$-Addukt von Dimethylphenylsilan [(*R*,*R*)-**144**]. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
C(1)	4655(11)	9903(16)	11170(10)	58(5)
C(2)	3206(12)	11809(18)	11478(13)	66(5)
C(3)	2577(12)	8955(18)	11379(12)	33(4)
C(4)	2913(12)	8472(17)	12634(14)	58(5)
C(5)	2078(12)	7172(18)	13000(11)	53(4)
C(6)	2078(10)	5754(15)	12213(12)	46(4)
C(7)	1655(11)	6231(16)	11006(9)	39(4)
C(8)	2409(9)	7616(15)	10570(10)	26(3)
C(9)	700(10)	8430(14)	9242(10)	32(3)
C(10)	2211(10)	6996(16)	8438(10)	46(4)
C(11)	1571(13)	9148(19)	6301(11)	69(5)
C(12)	23(9)	6278(17)	6799(10)	46(4)
C(13)	2452(14)	5690(20)	6093(10)	65(6)
C(14)	3563(15)	6250(20)	5863(12)	68(5)

C(15)	4276(11)	5340(20)	5118(12)	65(4)
C(16)	3822(13)	3890(20)	4707(14)	71(5)
C(17)	2770(16)	3331(18)	4978(16)	72(5)
C(18)	2119(18)	4190(20)	5678(14)	101(8)
Cl(1)	1653(3)	12412(4)	8790(3)	48(1)
Cl(2)	4470(3)	10122(5)	8194(3)	59(1)
N(1)	3332(7)	10346(16)	10886(9)	43(3)
N(2)	2050(7)	8180(12)	9376(9)	25(3)
Si(1)	1591(3)	7068(5)	6952(3)	38(1)
Zn(1)	2898(1)	10368(2)	9181(1)	39(1)

Tabelle 113 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für das $ZnCl_2$-Addukt von Dimethylphenylsilan [(*R*,*R*)-**144**]. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2$ [$h^2a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	60(10)	45(12)	70(10)	–16(8)	12(8)	–32(8)
C(2)	58(12)	71(13)	65(12)	24(11)	–17(9)	3(10)
C(3)	43(9)	42(10)	12(8)	–6(8)	–5(7)	7(8)
C(4)	42(10)	37(10)	100(15)	–29(10)	21(9)	–10(8)
C(5)	66(11)	51(11)	40(10)	–5(10)	–8(8)	4(10)
C(6)	33(8)	25(11)	83(11)	8(9)	21(7)	–16(6)
C(7)	59(9)	59(9)	5(8)	29(7)	28(6)	30(7)
C(8)	10(7)	36(9)	32(9)	–16(8)	–3(6)	0(6)
C(9)	33(8)	32(8)	31(9)	–3(7)	4(6)	2(7)
C(10)	41(9)	42(10)	59(10)	–20(9)	25(7)	–29(8)
C(11)	62(11)	109(14)	35(9)	2(10)	1(8)	3(10)
C(12)	3(7)	80(12)	54(10)	17(8)	–4(6)	–1(7)
C(13)	77(11)	105(17)	19(9)	–47(10)	38(8)	–79(12)
C(14)	104(15)	71(12)	27(11)	–38(9)	–3(9)	11(11)
C(15)	49(9)	63(10)	86(12)	–43(14)	9(8)	–21(12)
C(16)	42(11)	84(14)	90(14)	–41(12)	16(10)	17(11)
C(17)	78(14)	29(9)	112(16)	–30(11)	26(11)	8(9)
C(18)	150(20)	84(15)	74(14)	–70(13)	36(13)	–15(14)
Cl(1)	39(2)	26(2)	81(3)	5(2)	11(2)	9(2)
Cl(2)	29(2)	41(3)	111(3)	–1(3)	28(2)	–7(2)
N(1)	33(6)	0(5)	101(9)	–21(8)	41(6)	–5(7)
N(2)	3(5)	30(7)	42(8)	7(6)	–6(5)	–1(5)
Si(1)	34(2)	44(3)	36(3)	–1(2)	2(2)	4(2)

Zn(1)	25(1)	24(1)	68(1)	0(1)	12(1)	0(1)

Tabelle 114 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für das $ZnCl_2$-Addukt von Dimethylphenylsilan [(*R*,*R*)-**144**].

	x	y	z	U(eq)
H(1A)	5143	10581	10708	87
H(1B)	4778	8753	10992	87
H(1C)	4878	10097	11990	87
H(2A)	2451	12317	11211	99
H(2B)	3855	12545	11333	99
H(2C)	3223	11589	12306	99
H(3)	1772	9442	11390	40
H(4A)	3733	8055	12717	70
H(4B)	2873	9438	13136	70
H(5A)	2326	6820	13797	64
H(5B)	1269	7623	12988	64
H(6A)	1559	4893	12482	55
H(6B)	2888	5307	12226	55
H(7A)	821	6587	10982	47
H(7B)	1693	5276	10494	47
H(8)	3213	7134	10532	31
H(9A)	455	8780	8454	48
H(9B)	482	9265	9785	48
H(9C)	306	7404	9402	48
H(10A)	1960	5933	8734	55
H(10B)	3075	6917	8399	55
H(11A)	981	9820	6644	103
H(11B)	1369	9067	5469	103
H(11C)	2352	9648	6449	103
H(12A)	-24	5275	7247	69
H(12B)	-213	6051	5986	69
H(12C)	-506	7098	7083	69
H(14)	3856	7239	6199	81
H(15)	5020	5731	4924	79
H(16)	4265	3262	4214	85
H(17)	2483	2320	4672	86
H(18)	1402	3728	5891	121

$ZnBr_2$-Addukt von Dimethyl[*N*',*N*',*N*'-Trimethylcyclohexan-(1*R*,2*R*)-diamino-N^1-methyl]phenylsilan [(*R*,*R*)-143]

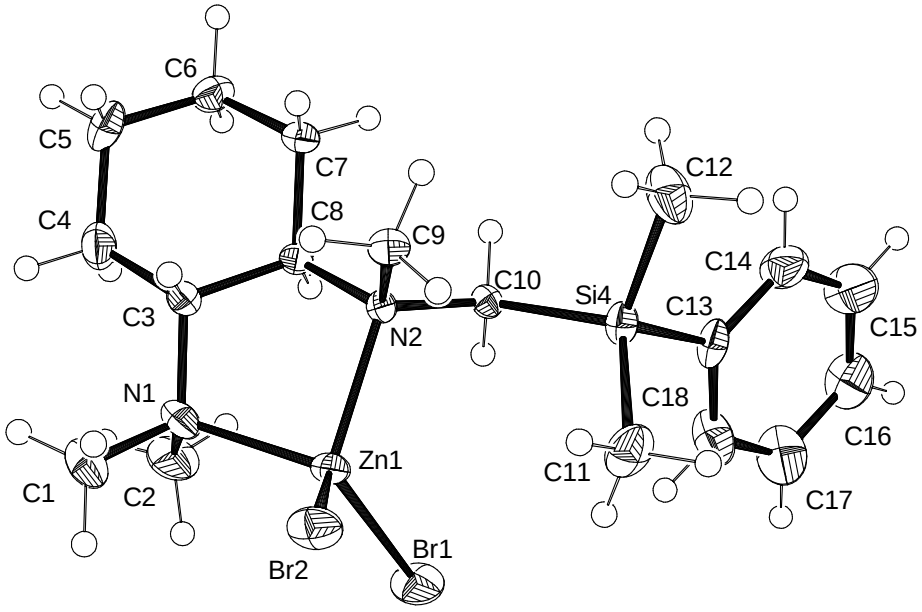


Abbildung 39 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des $ZnBr_2$-Addukts von Dimethylphenylsilan [(*R*,*R*)-**144**] im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 115 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter ($Å^2$ x 10^3) für das $ZnBr_2$-Addukt von Dimethylphenylsilan [(*R*,*R*)-144]. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
Zn(1)	2882(1)	11830(1)	9213(1)	21(1)
Br(1)	4539(1)	11620(1)	8211(1)	39(1)
Br(2)	1583(1)	13951(1)	8689(1)	32(1)
Si(4)	1605(1)	8589(1)	6902(1)	24(1)
N(1)	3310(2)	11745(4)	11008(3)	29(1)
C(8)	2423(3)	9080(4)	10546(3)	16(1)
C(3)	2516(3)	10469(4)	11409(3)	21(1)
C(7)	1676(3)	7713(4)	10957(3)	22(1)
C(5)	2006(3)	8649(5)	12992(3)	33(1)
C(4)	2850(4)	9920(5)	12658(3)	34(1)
C(6)	2038(3)	7221(4)	12201(3)	26(1)
N(2)	1996(2)	9669(3)	9340(2)	15(1)
C(13)	2549(3)	7242(4)	6091(3)	28(1)
C(10)	2311(3)	8483(4)	8454(3)	17(1)

C(9)	719(3)	9961(4)	9196(3)	20(1)
C(14)	2154(4)	5758(5)	5687(4)	41(1)
C(2)	4568(3)	11361(6)	11297(4)	45(1)
C(1)	3076(4)	13298(5)	11539(4)	47(1)
C(12)	66(3)	7769(5)	6745(4)	41(1)
C(18)	3611(3)	7782(5)	5813(4)	41(1)
C(11)	1601(4)	10627(5)	6241(4)	39(1)
C(17)	4267(3)	6886(6)	5117(4)	49(1)
C(16)	3858(4)	5418(5)	4705(4)	45(1)
C(15)	2816(4)	4862(5)	4993(4)	50(1)

Tabelle 116 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für das $ZnBr_2$-Addukt von Dimethylphenylsilan [(*R*,*R*)-144]. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2$ [$h^2a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	20(1)	17(1)	28(1)	–1(1)	8(1)	–2(1)
Br(1)	24(1)	42(1)	54(1)	–3(1)	20(1)	–4(1)
Br(2)	35(1)	18(1)	46(1)	3(1)	13(1)	5(1)
Si(4)	27(1)	26(1)	17(1)	–2(1)	0(1)	3(1)
N(1)	29(2)	22(2)	37(2)	–6(2)	1(1)	–9(2)
C(8)	12(2)	19(2)	19(2)	–2(2)	1(1)	–1(1)
C(3)	20(2)	22(2)	22(2)	–3(2)	2(2)	–4(1)
C(7)	21(2)	21(2)	25(2)	0(2)	5(2)	–1(1)
C(5)	43(2)	42(2)	16(2)	4(2)	7(2)	5(2)
C(4)	45(2)	31(2)	25(2)	–6(2)	1(2)	–1(2)
C(6)	27(2)	28(2)	24(2)	6(2)	3(2)	–1(2)
N(2)	16(1)	14(1)	15(2)	–2(1)	0(1)	0(1)
C(13)	38(2)	29(2)	16(2)	–1(2)	1(2)	11(2)
C(10)	16(2)	17(2)	20(2)	–2(1)	2(1)	0(1)
C(9)	14(2)	20(2)	27(2)	1(2)	4(2)	1(1)
C(14)	53(3)	31(2)	44(3)	–3(2)	23(2)	–2(2)
C(2)	32(2)	59(3)	42(3)	2(2)	–10(2)	–22(2)
C(1)	68(3)	31(2)	42(3)	–12(2)	10(2)	–13(2)
C(12)	28(2)	48(3)	44(3)	–10(2)	–6(2)	2(2)
C(18)	27(2)	50(3)	43(3)	–17(2)	–2(2)	1(2)
C(11)	55(3)	34(2)	28(2)	9(2)	4(2)	10(2)
C(17)	26(2)	67(3)	54(3)	–15(3)	6(2)	6(2)
C(16)	51(3)	42(3)	44(3)	–9(2)	14(2)	16(2)

C(15)	69(3)	30(2)	56(3)	–11(2)	27(3)	1(2)

Tabelle 117 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für das $ZnBr_2$-Addukt von Dimethylphenylsilan [(*R*,*R*)-**144**].

	x	y	z	U(eq)
H(8)	3231	8652	10520	20
H(3)	1718	10950	11378	26
H(7A)	846	8050	10878	27
H(7B)	1737	6777	10447	27
H(5A)	2228	8318	13806	40
H(5B)	1203	9089	12929	40
H(4A)	3655	9483	12739	41
H(4B)	2836	10843	13187	41
H(6A)	1501	6386	12430	32
H(6B)	2840	6772	12272	32
H(10A)	2148	7408	8750	21
H(10B)	3168	8552	8434	21
H(9A)	503	10562	8480	31
H(9B)	504	10575	9858	31
H(9C)	303	8939	9155	31
H(14)	1431	5355	5884	49
H(2A)	5041	12115	10903	68
H(2B)	4717	10274	11042	68
H(2C)	4776	11442	12137	68
H(1A)	3216	13208	12385	70
H(1B)	2260	13605	11313	70
H(1C)	3597	14110	11272	70
H(12A)	–460	8548	7043	61
H(12B)	50	6774	7187	61
H(12C)	–189	7559	5926	61
H(18)	3899	8784	6102	49
H(11A)	1333	10557	5412	59
H(11B)	2395	11068	6349	59
H(11C)	1074	11323	6618	59
H(17)	4996	7279	4925	59
H(16)	4300	4803	4223	54
H(15)	2538	3849	4717	60

Methyl[N^1,N^2,N^3-Trimethylcyclohexan-(1*R*,2*R*)-diamino-N^1-methyl]diphenylsilan-dihydrochlorid [(*R*,*R*)-142·2HCl]

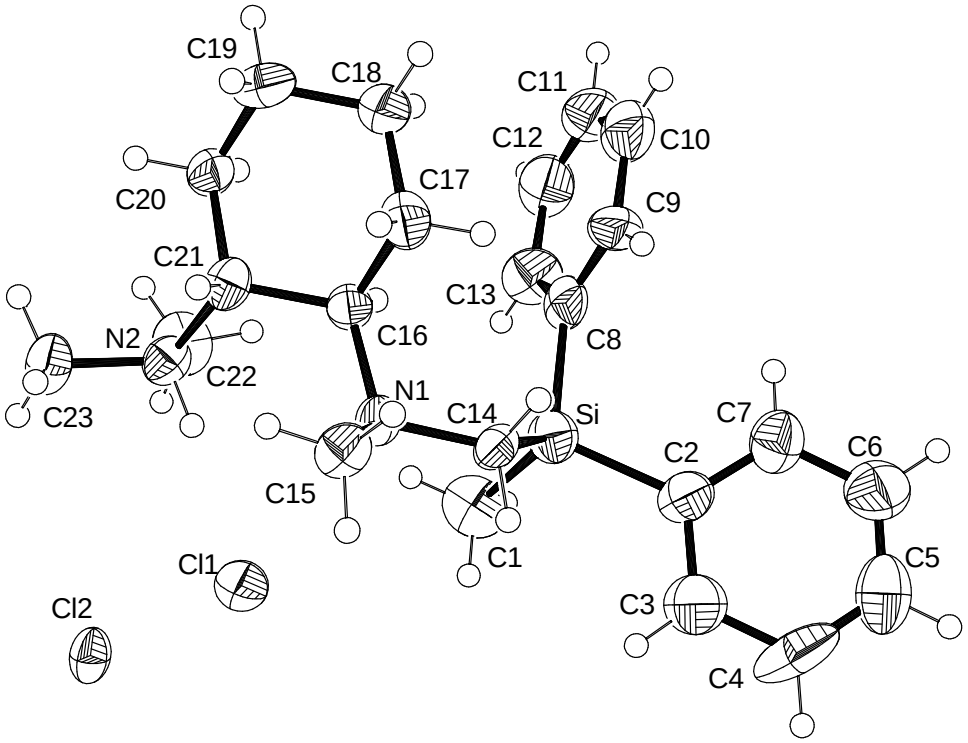


Abbildung 40 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von Methyl[N^1,N^2,N^3-Trimethylcyclohexan-(1*R*,2*R*)-diamino-N^1-methyl]diphenylsilan-dihydrochlorid [(*R*,*R*)-**142**·2HCl] im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 118 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung Methyl[N^1,N^2,N^3-Trimethylcyclohexan-(1*R*,2*R*)-diamino-N^1-methyl]diphenylsilan-dihydrochlorid [(*R*,*R*)-**142**·2HCl]. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
C(1)	4931(7)	4902(8)	2845(5)	60(2)
C(2)	5779(6)	7952(7)	3385(5)	47(2)
C(3)	4627(7)	8519(10)	2754(5)	71(2)
C(4)	4177(9)	9846(9)	2911(6)	77(3)
C(5)	4862(9)	10641(8)	3703(7)	70(2)
C(6)	6006(8)	10154(9)	4328(6)	69(2)
C(7)	6454(7)	8799(7)	4177(5)	57(2)
C(8)	7718(6)	5518(6)	4207(4)	43(2)
C(9)	7502(7)	4391(7)	4833(5)	57(2)
C(10)	8449(8)	3999(7)	5677(5)	65(2)
C(11)	9654(9)	4694(8)	5894(5)	69(2)
C(12)	9938(8)	5813(8)	5305(5)	65(2)

C(13)	8941(6)	6223(8)	4455(4)	53(2)
C(14)	7102(6)	6457(6)	1827(4)	35(1)
C(15)	7864(7)	5807(7)	158(5)	38(2)
C(16)	8611(5)	4335(6)	1823(4)	32(1)
C(17)	9927(6)	5143(7)	2114(5)	42(2)
C(18)	11026(6)	4299(7)	2809(5)	49(2)
C(19)	11307(6)	2974(7)	2251(5)	56(2)
C(20)	9997(6)	2169(6)	1952(5)	42(2)
C(21)	8883(5)	2992(6)	1240(4)	34(1)
C(22)	7177(10)	1276(9)	1772(6)	53(2)
C(23)	7820(8)	1126(9)	1(6)	46(2)
Cl(1)	4985(2)	3628(2)	173(1)	56(1)
Cl(2)	245(2)	8549(2)	1377(1)	50(1)
N(1)	7505(5)	5254(5)	1188(3)	33(1)
N(2)	7646(5)	2087(5)	898(4)	36(1)
Si(1)	6384(2)	6161(2)	3087(1)	42(1)

Tabelle 119 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für Methyl[N^1,N^2,N^3-Trimethylcyclohexan-(1*R*,2*R*)-diamino-N^1-methyl]diphenylsilan-dihydrochlorid [(*R*,*R*)-**142**·2HCl]. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2$ [$h^2a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	53(4)	77(5)	52(4)	2(4)	12(3)	–18(4)
C(2)	51(4)	52(4)	38(3)	1(3)	8(3)	12(3)
C(3)	73(4)	91(6)	50(4)	–10(5)	9(3)	35(5)
C(4)	82(6)	92(7)	61(5)	12(5)	23(4)	48(5)
C(5)	84(6)	56(5)	79(6)	–4(4)	38(5)	10(4)
C(6)	63(5)	76(6)	71(5)	–13(4)	22(4)	2(4)
C(7)	64(4)	52(5)	56(4)	–6(4)	12(3)	4(4)
C(8)	51(4)	49(4)	28(3)	–5(3)	6(3)	11(3)
C(9)	70(5)	57(4)	45(4)	8(3)	11(3)	9(4)
C(10)	91(5)	59(5)	42(4)	9(3)	4(4)	12(4)
C(11)	90(6)	69(5)	41(4)	–5(4)	–12(4)	32(5)
C(12)	72(5)	71(6)	47(4)	–11(4)	–1(4)	19(4)
C(13)	53(4)	62(4)	40(3)	–5(4)	–6(3)	10(4)
C(14)	32(3)	36(4)	36(3)	0(3)	0(2)	5(3)
C(15)	43(4)	38(4)	33(3)	8(3)	7(3)	11(3)
C(16)	35(3)	32(3)	28(3)	2(3)	3(2)	2(3)
C(17)	41(4)	39(4)	45(4)	–4(3)	6(3)	0(3)
C(18)	42(4)	45(4)	55(4)	–6(3)	–6(3)	1(3)

C(19)	39(4)	57(4)	68(4)	0(4)	–2(3)	16(3)
C(20)	44(4)	32(3)	45(4)	1(3)	–5(3)	10(3)
C(21)	36(3)	33(3)	35(3)	3(3)	10(3)	1(2)
C(22)	56(5)	47(5)	57(4)	8(4)	15(4)	–18(4)
C(23)	59(5)	33(4)	45(4)	–8(4)	10(3)	–2(4)
Cl(1)	42(1)	52(1)	66(1)	–16(1)	–11(1)	5(1)
Cl(2)	72(1)	33(1)	47(1)	–1(1)	17(1)	–2(1)
N(1)	39(3)	30(3)	30(3)	–2(2)	3(2)	2(2)
N(2)	40(3)	27(3)	41(3)	3(2)	6(2)	4(2)
Si(1)	44(1)	48(1)	35(1)	–1(1)	6(1)	3(1)

Tabelle 120 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung Methyl[N^1,N^2,N^3-Trimethylcyclohexan-(1*R*,2*R*)-diamino-N^1-methyl]diphenylsilan-dihydrochlorid [(*R*,*R*)-**142**·2HCl].

	x	y	z	U(eq)
H(22C)	7140(70)	1940(90)	2410(60)	80(20)
H(1A)	5265	4013	2640	90
H(1B)	4229	5244	2277	90
H(1C)	4545	4793	3490	90
H(3)	4135	7980	2202	86
H(4)	3394	10198	2466	93
H(5)	4541	11536	3819	84
H(6)	6501	10719	4862	82
H(7)	7237	8459	4630	68
H(9)	6677	3888	4667	69
H(10)	8272	3252	6108	78
H(11)	10320	4399	6468	83
H(12)	10779	6288	5471	77
H(13)	9106	6994	4044	64
H(17A)	9748	5989	2494	50
H(17B)	10258	5417	1462	50
H(18A)	11872	4845	2972	59
H(18B)	10723	4075	3483	59
H(19A)	11688	3194	1609	67
H(19B)	11983	2414	2723	67
H(20A)	9660	1898	2602	50
H(20B)	10186	1319	1581	50
H(1N)	6700(60)	4680(60)	970(40)	47(18)

H(2N)	7010(50)	2670(50)	720(40)	19(14)
H(14A)	7840(40)	7150(50)	1920(30)	9(11)
H(16)	8240(40)	4110(40)	2430(30)	10(11)
H(14B)	6450(50)	6930(60)	1490(40)	28(15)
H(21)	9210(60)	3180(60)	640(50)	50(17)
H(15A)	7090(50)	6180(60)	–180(40)	23(13)
H(15C)	8620(60)	6520(60)	330(40)	37(16)
H(23A)	7010(60)	600(50)	–170(40)	28(15)
H(23C)	7940(60)	1650(60)	–530(50)	41(18)
H(23B)	8370(70)	470(70)	170(50)	50(20)
H(15B)	8230(60)	5090(70)	–210(50)	49(17)
H(22B)	7690(70)	590(80)	1950(50)	60(20)
H(22A)	6390(70)	950(70)	1580(50)	50(20)

$ZnBr_2$-Addukt von Methyl[*N*^{1},*N*^{2},*N*^{3}-Trimethylcyclohexan-(1*R*,2*R*)-diamino-*N*^{1}-methyl]diphenylsilan [(*R*,*R*)-145]

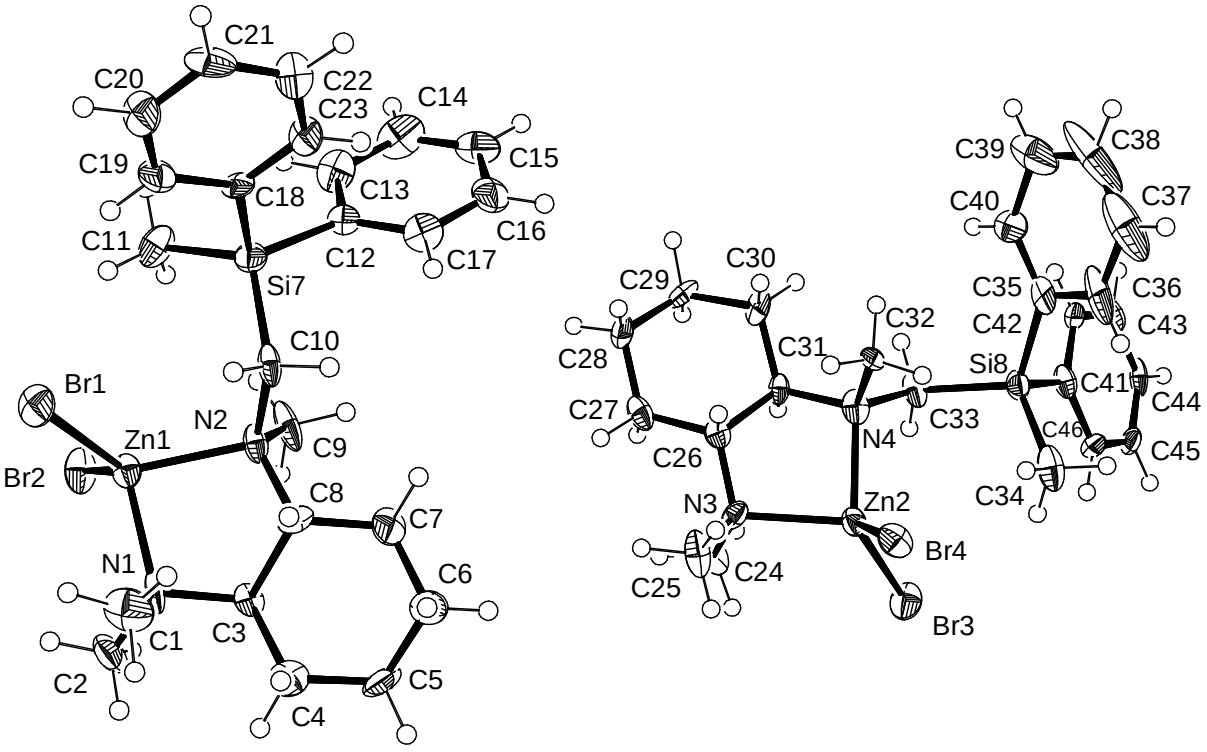


Abbildung 41 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des $ZnBr_2$-Addukts des Methyldiphenylsilan (**145**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 121 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für das $ZnBr_2$-Addukt von Methyldiphenylsilan (**145**)**.** U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
Br(1)	7677(1)	–2552(1)	8130(1)	38(1)
Br(2)	4449(1)	–2630(1)	8183(1)	38(1)
Br(3)	–1731(1)	8948(1)	5379(1)	39(1)
Br(4)	1576(1)	8755(1)	5464(1)	32(1)
C(1)	6266(6)	–2204(7)	6312(4)	49(3)
C(2)	4439(6)	–2870(6)	6345(4)	41(2)
C(3)	4741(5)	–685(6)	6350(4)	21(2)
C(4)	4509(6)	–467(7)	5561(4)	36(2)
C(5)	3975(7)	770(7)	5345(4)	44(2)
C(6)	4718(7)	1763(7)	5734(4)	49(2)
C(7)	4962(6)	1571(7)	6549(4)	36(2)
C(8)	5485(6)	339(6)	6789(4)	26(2)
C(9)	4799(5)	572(6)	7859(5)	41(3)
C(10)	6853(5)	701(6)	7994(4)	28(2)
C(11)	6938(5)	–387(6)	9494(4)	36(2)
C(12)	6624(5)	2347(7)	9230(4)	25(2)
C(13)	6296(6)	2451(8)	9844(5)	41(2)
C(14)	5972(6)	3540(10)	10072(5)	49(3)
C(15)	5992(6)	4587(8)	9692(5)	42(3)
C(16)	6308(6)	4519(7)	9081(5)	40(2)
C(17)	6607(5)	3397(7)	8847(4)	34(2)
C(18)	8841(5)	1125(7)	9262(4)	23(2)
C(19)	9554(6)	126(7)	9394(4)	36(2)
C(20)	10738(6)	258(8)	9656(4)	40(2)
C(21)	11200(6)	1386(8)	9778(4)	39(2)
C(22)	10517(6)	2387(8)	9613(4)	36(2)
C(23)	9334(5)	2257(7)	9371(4)	31(2)
C(24)	–951(5)	6222(6)	6350(4)	43(2)
C(25)	854(6)	5885(6)	6102(4)	43(3)
C(26)	845(6)	6849(6)	7228(4)	22(2)
C(27)	752(6)	5807(6)	7724(4)	30(2)
C(28)	1371(6)	5951(6)	8494(4)	31(2)
C(29)	1001(6)	7116(6)	8768(4)	30(2)
C(30)	1175(5)	8168(6)	8325(4)	29(2)
C(31)	549(5)	8055(6)	7536(4)	20(2)
C(32)	1893(5)	9465(6)	7244(4)	21(2)
C(33)	–22(5)	10170(5)	7176(4)	26(2)

C(34)	182(6)	11656(6)	5893(4)	42(2)
C(35)	1556(6)	12417(7)	7377(5)	30(2)
C(36)	2236(6)	13077(6)	7051(6)	55(3)
C(37)	3195(9)	13696(10)	7435(7)	83(4)
C(38)	3464(8)	13634(10)	8181(9)	106(6)
C(39)	2857(8)	12956(8)	8551(6)	72(3)
C(40)	1879(6)	12337(7)	8125(4)	38(2)
C(41)	–1004(6)	12673(6)	6932(5)	27(2)
C(42)	–948(5)	13262(6)	7575(4)	25(2)
C(43)	–1801(6)	14031(6)	7636(4)	31(2)
C(44)	–2738(6)	14198(6)	7043(4)	27(2)
C(45)	–2838(5)	13638(7)	6418(4)	27(2)
C(46)	–1973(6)	12853(6)	6348(4)	26(2)
N(1)	5272(4)	–1910(5)	6602(3)	24(2)
N(2)	5732(4)	113(5)	7572(3)	25(2)
N(3)	242(5)	6693(5)	6471(3)	23(2)
N(4)	669(4)	9086(5)	7067(3)	25(2)
Si(7)	7256(2)	911(2)	8985(1)	26(1)
Si(8)	211(2)	11706(2)	6828(1)	25(1)
Zn(1)	5825(1)	–1792(1)	7699(1)	25(1)
Zn(2)	139(1)	8433(1)	6027(1)	23(1)

Tabelle 122 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für das $ZnBr_2$-Addukt von Methyldiphenylsilan (**145**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	22(1)	38(1)	52(1)	0(1)	6(1)	11(1)
Br(2)	29(1)	30(1)	60(1)	10(1)	21(1)	1(1)
Br(3)	23(1)	40(1)	48(1)	11(1)	2(1)	–2(1)
Br(4)	29(1)	32(1)	38(1)	–5(1)	16(1)	–7(1)
C(1)	41(5)	60(6)	52(6)	–14(5)	21(5)	7(4)
C(2)	58(6)	20(5)	46(6)	–8(4)	17(5)	–10(4)
C(3)	11(4)	21(4)	34(6)	0(4)	10(4)	–10(3)
C(4)	23(4)	42(5)	39(6)	2(5)	2(4)	–18(4)
C(5)	52(6)	46(6)	21(5)	16(5)	–11(4)	–21(5)
C(6)	64(6)	37(5)	36(6)	1(5)	–4(5)	–15(5)
C(7)	27(5)	28(5)	48(7)	3(5)	1(5)	–13(4)
C(8)	19(4)	37(5)	19(5)	3(4)	2(4)	–3(4)

C(9)	19(4)	14(4)	92(8)	–7(5)	20(5)	2(4)
C(10)	14(4)	14(4)	56(6)	6(4)	11(4)	2(3)
C(11)	34(5)	45(5)	35(6)	17(5)	17(4)	4(4)
C(12)	23(4)	29(4)	24(5)	–2(5)	9(4)	0(4)
C(13)	29(5)	47(5)	50(7)	8(6)	17(5)	4(5)
C(14)	43(5)	74(7)	40(6)	3(6)	26(5)	17(6)
C(15)	29(5)	54(6)	41(7)	–21(6)	5(5)	17(5)
C(16)	29(5)	34(5)	50(7)	–5(5)	0(5)	–6(4)
C(17)	26(4)	44(5)	37(5)	–1(5)	18(4)	3(5)
C(18)	11(4)	30(5)	22(5)	–3(4)	–2(4)	6(4)
C(19)	28(5)	31(5)	43(6)	–6(5)	–2(4)	–7(4)
C(20)	26(5)	36(5)	58(7)	–2(5)	10(5)	12(4)
C(21)	12(4)	59(6)	41(6)	–21(5)	1(4)	–3(5)
C(22)	32(5)	35(5)	48(6)	4(5)	24(4)	0(5)
C(23)	21(4)	30(5)	43(6)	0(5)	9(4)	11(4)
C(24)	34(5)	28(5)	61(7)	5(5)	4(5)	–30(4)
C(25)	51(6)	21(4)	66(7)	8(5)	31(5)	6(4)
C(26)	19(4)	21(4)	28(6)	0(4)	10(4)	–3(4)
C(27)	29(5)	18(4)	46(6)	–5(5)	13(4)	3(4)
C(28)	38(5)	22(4)	31(6)	11(4)	8(5)	0(4)
C(29)	30(4)	41(5)	16(5)	12(4)	1(4)	5(4)
C(30)	33(4)	25(5)	33(5)	8(4)	17(4)	22(4)
C(31)	16(4)	16(4)	30(5)	6(4)	9(4)	5(3)
C(32)	21(4)	17(4)	23(5)	–2(4)	0(4)	–6(4)
C(33)	9(4)	18(4)	50(6)	2(4)	8(4)	–1(3)
C(34)	41(5)	22(4)	68(7)	7(5)	25(5)	6(4)
C(35)	30(4)	12(4)	50(6)	0(5)	13(4)	17(4)
C(36)	31(5)	14(4)	125(9)	6(6)	33(6)	11(4)
C(37)	46(7)	30(6)	187(13)	–22(10)	55(9)	0(6)
C(38)	26(6)	34(7)	262(18)	–62(12)	47(10)	–5(5)
C(39)	44(6)	39(6)	105(10)	–31(7)	–21(6)	21(5)
C(40)	29(5)	29(5)	46(6)	–4(6)	–7(4)	18(5)
C(41)	28(4)	19(5)	40(6)	3(4)	16(4)	–7(4)
C(42)	31(4)	19(4)	22(5)	7(4)	5(4)	–4(4)
C(43)	25(4)	22(5)	49(6)	–3(5)	16(4)	–10(4)
C(44)	16(4)	15(4)	55(6)	13(5)	17(4)	5(4)
C(45)	26(4)	21(4)	27(5)	11(4)	–4(4)	0(4)
C(46)	32(5)	27(5)	16(5)	5(4)	3(4)	–3(4)
N(1)	12(3)	9(3)	55(5)	3(3)	13(3)	2(3)
N(2)	19(3)	16(3)	43(5)	3(4)	14(3)	3(3)
N(3)	25(4)	26(4)	20(4)	5(3)	6(3)	10(3)
N(4)	12(3)	25(4)	42(4)	4(3)	14(3)	–3(3)

Si(7)	21(1)	28(1)	27(2)	0(1)	4(1)	–1(1)
Si(8)	27(1)	17(1)	31(2)	2(1)	6(1)	2(1)
Zn(1)	18(1)	23(1)	34(1)	1(1)	8(1)	1(1)
Zn(2)	21(1)	19(1)	29(1)	1(1)	6(1)	–2(1)

Tabelle 123 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für das $ZnBr_2$-Addukt von Dimethylphenylsilan (**145**).

	x	y	z	U(eq)
H(1A)	6671	–2913	6562	74
H(1B)	6781	–1509	6388	74
H(1C)	5986	–2379	5799	74
H(2A)	4294	–2966	5828	61
H(2B)	3733	–2656	6451	61
H(2C)	4729	–3633	6585	61
H(3)	3998	–658	6458	26
H(4A)	5225	–520	5431	43
H(4B)	3994	–1105	5294	43
H(5A)	3238	808	5451	52
H(5B)	3836	883	4824	52
H(6A)	5437	1765	5605	59
H(6B)	4342	2555	5596	59
H(7A)	4247	1646	6680	44
H(7B)	5482	2213	6805	44
H(8)	6224	314	6676	31
H(9A)	4755	1457	7816	62
H(9B)	4958	343	8363	62
H(9C)	4079	215	7585	62
H(10A)	6874	1514	7783	33
H(10B)	7465	222	7889	33
H(11A)	6120	–444	9416	55
H(11B)	7314	–270	10005	55
H(11C)	7213	–1136	9332	55
H(13)	6292	1746	10122	49
H(14)	5733	3568	10493	59
H(15)	5790	5342	9853	51
H(16)	6326	5232	8812	48
H(17)	6803	3363	8411	41
H(19)	9238	–663	9306	43

H(20)	11211	–438	9747	48
H(21)	11993	1480	9977	47
H(22)	10844	3173	9662	43
H(23)	8869	2959	9282	37
H(24A)	–923	5388	6527	65
H(24B)	–1348	6237	5837	65
H(24C)	–1353	6735	6606	65
H(25A)	946	5083	6327	64
H(25B)	1600	6229	6136	64
H(25C)	422	5809	5597	64
H(26)	1664	6907	7255	26
H(27A)	–59	5684	7684	36
H(27B)	1027	5060	7549	36
H(28A)	2195	5974	8556	37
H(28B)	1209	5255	8768	37
H(29A)	1444	7242	9273	36
H(29B)	193	7059	8748	36
H(30A)	923	8918	8512	35
H(30B)	1993	8251	8378	35
H(31)	–273	8007	7505	24
H(32A)	2131	9814	7725	32
H(32B)	1981	10070	6896	32
H(32C)	2361	8756	7224	32
H(33A)	94	10254	7697	31
H(33B)	–828	9962	6961	31
H(34A)	243	12481	5722	63
H(34B)	–530	11292	5611	63
H(34C)	818	11169	5842	63
H(36)	2032	13105	6544	66
H(37)	3648	14140	7203	100
H(38)	4099	14082	8453	127
H(39)	3083	12909	9058	86
H(40)	1440	11862	8352	46
H(42)	–313	13131	7978	30
H(43)	–1749	14437	8073	37
H(44)	–3324	14727	7083	32
H(45)	–3489	13770	6025	33
H(46)	–2044	12447	5908	31

$ZnCl_2$-Addukt des Diphenylmethylsilans 142

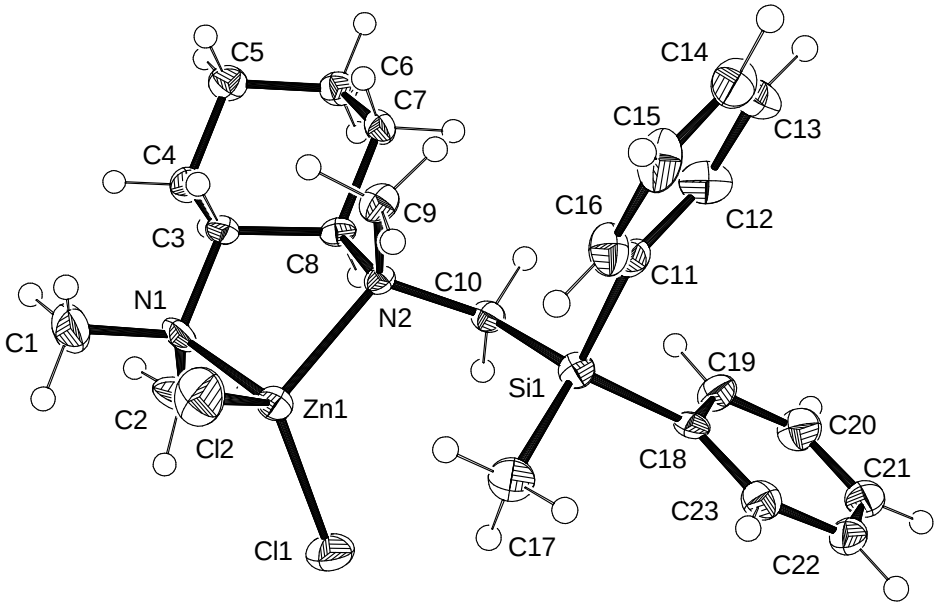


Abbildung 42 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des $ZnCl_2$-Adduktes des Diphenylmethylsilans **142** im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 124 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) des $ZnCl_2$-Adduktes des Diphenylmethylsilans **142**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
Zn(1)	8138(1)	8987(1)	9214(1)	24(1)
Cl(1)	9858(1)	8751(2)	8500(1)	39(1)
Cl(2)	7042(1)	11058(1)	8837(1)	44(1)
Si(1)	7294(1)	6226(1)	6876(1)	21(1)
N(2)	7196(2)	6882(3)	9170(2)	15(1)
C(10)	7591(2)	5767(3)	8311(2)	18(1)
N(1)	8291(2)	8687(4)	10845(2)	26(1)
C(8)	7394(2)	6149(3)	10245(2)	16(1)
C(3)	7425(3)	7421(4)	11116(3)	19(1)
C(1)	7997(3)	10189(4)	11399(3)	44(1)
C(6)	6770(2)	4161(5)	11611(2)	24(1)
C(11)	5757(3)	5898(4)	6514(2)	22(1)
C(12)	5296(3)	4373(4)	6505(2)	33(1)
C(5)	6733(3)	5443(3)	12452(2)	24(1)
C(7)	6536(2)	4858(3)	10527(2)	21(1)
C(9)	5969(2)	7275(3)	8992(2)	23(1)
C(4)	7635(2)	6675(4)	12205(2)	22(1)

C(13)	4182(3)	4121(6)	6178(2)	37(1)
C(18)	8122(3)	4744(4)	6113(3)	18(1)
C(19)	8474(3)	3275(4)	6523(3)	26(1)
C(16)	5051(3)	7135(4)	6186(2)	27(1)
C(15)	3930(3)	6855(5)	5870(3)	35(1)
C(14)	3499(3)	5355(5)	5870(3)	35(1)
C(17)	7731(2)	8244(3)	6479(2)	29(1)
C(20)	9034(3)	2165(4)	5910(3)	33(1)
C(2)	9486(3)	8235(4)	11127(3)	46(1)
C(22)	8921(2)	3871(6)	4425(2)	26(1)
C(23)	8364(3)	5000(4)	5039(3)	26(1)
C(21)	9245(3)	2472(4)	4861(3)	29(1)

Tabelle 125 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) des $ZnCl_2$-Adduktes des Diphenylmethylsilans **142**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	28(1)	19(1)	26(1)	1(1)	5(1)	–4(1)
Cl(1)	26(1)	51(1)	39(1)	–3(1)	8(1)	–9(1)
Cl(2)	62(1)	22(1)	48(1)	4(1)	7(1)	10(1)
Si(1)	20(1)	21(1)	22(1)	–1(1)	0(1)	2(1)
N(2)	12(2)	14(2)	19(2)	–2(1)	1(1)	3(1)
C(10)	12(2)	13(2)	27(2)	–5(2)	5(2)	2(2)
N(1)	31(2)	18(2)	29(2)	2(2)	–2(1)	–14(2)
C(8)	10(2)	19(2)	20(2)	5(2)	2(2)	4(2)
C(3)	16(2)	16(2)	23(2)	2(2)	4(2)	–4(2)
C(1)	65(3)	26(3)	40(3)	–5(2)	11(2)	–15(2)
C(6)	22(2)	25(2)	26(2)	4(2)	2(1)	0(2)
C(11)	25(2)	28(2)	14(2)	0(2)	3(2)	–1(2)
C(12)	22(2)	36(3)	40(2)	11(2)	–4(2)	3(2)
C(5)	27(2)	23(2)	22(2)	4(2)	–2(2)	–2(2)
C(7)	24(2)	17(2)	22(2)	–1(2)	2(2)	–4(2)
C(9)	16(2)	25(2)	27(2)	1(2)	1(2)	7(2)
C(4)	25(2)	23(2)	17(2)	1(2)	2(2)	0(2)
C(13)	28(2)	38(3)	46(2)	–4(3)	–1(2)	–18(3)
C(18)	11(2)	25(2)	20(2)	1(2)	0(2)	–8(2)
C(19)	30(3)	30(2)	18(2)	0(2)	4(2)	0(2)
C(16)	30(2)	23(2)	29(2)	–7(2)	–4(2)	5(2)
C(15)	32(3)	39(3)	33(2)	–9(2)	–13(2)	25(2)

C(14)	16(2)	56(3)	34(3)	–15(2)	–8(2)	8(2)
C(17)	28(2)	26(2)	32(2)	2(2)	0(2)	1(2)
C(20)	35(2)	28(2)	36(3)	1(2)	8(2)	3(2)
C(2)	34(2)	65(3)	38(3)	14(2)	–14(2)	–27(2)
C(22)	18(2)	36(2)	24(2)	–7(3)	4(2)	–6(3)
C(23)	18(2)	26(2)	33(3)	–1(2)	–7(2)	–3(2)
C(21)	16(2)	33(2)	37(3)	–8(2)	6(2)	1(2)

Tabelle 126 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) des $ZnCl_2$-Adduktes des Diphenylmethylsilans **142**.

	x	y	z	U(eq)
H(10A)	7252	4719	8461	21
H(10B)	8428	5650	8391	21
H(8)	8166	5644	10231	20
H(3)	6657	7935	11133	22
H(1A)	7241	10548	11166	66
H(1B)	8566	10999	11228	66
H(1C)	7991	10010	12167	66
H(6A)	7531	3651	11617	29
H(6B)	6192	3342	11771	29
H(12)	5752	3503	6725	39
H(5A)	6880	4977	13160	29
H(5B)	5968	5941	12459	29
H(7A)	5755	5308	10513	25
H(7B)	6570	4008	9988	25
H(9A)	5894	7947	8362	34
H(9B)	5673	7838	9612	34
H(9C)	5534	6298	8886	34
H(4A)	8399	6174	12218	26
H(4B)	7624	7509	12756	26
H(13)	3885	3076	6168	45
H(19)	8322	3036	7245	31
H(16)	5340	8184	6180	33
H(15)	3460	7713	5652	42
H(14)	2732	5168	5657	43
H(17A)	7587	8389	5718	43
H(17B)	8546	8388	6627	43
H(17C)	7290	9024	6881	43

H(20)	9273	1192	6215	40
H(2A)	10018	8992	10809	69
H(2B)	9647	7172	10856	69
H(2C)	9579	8245	11900	69
H(22)	9074	4080	3699	31
H(23)	8141	5971	4721	31
H(21)	9619	1703	4438	34

$ZnBr_2$-Addukt der (Silymethyl)silylverbindung 148

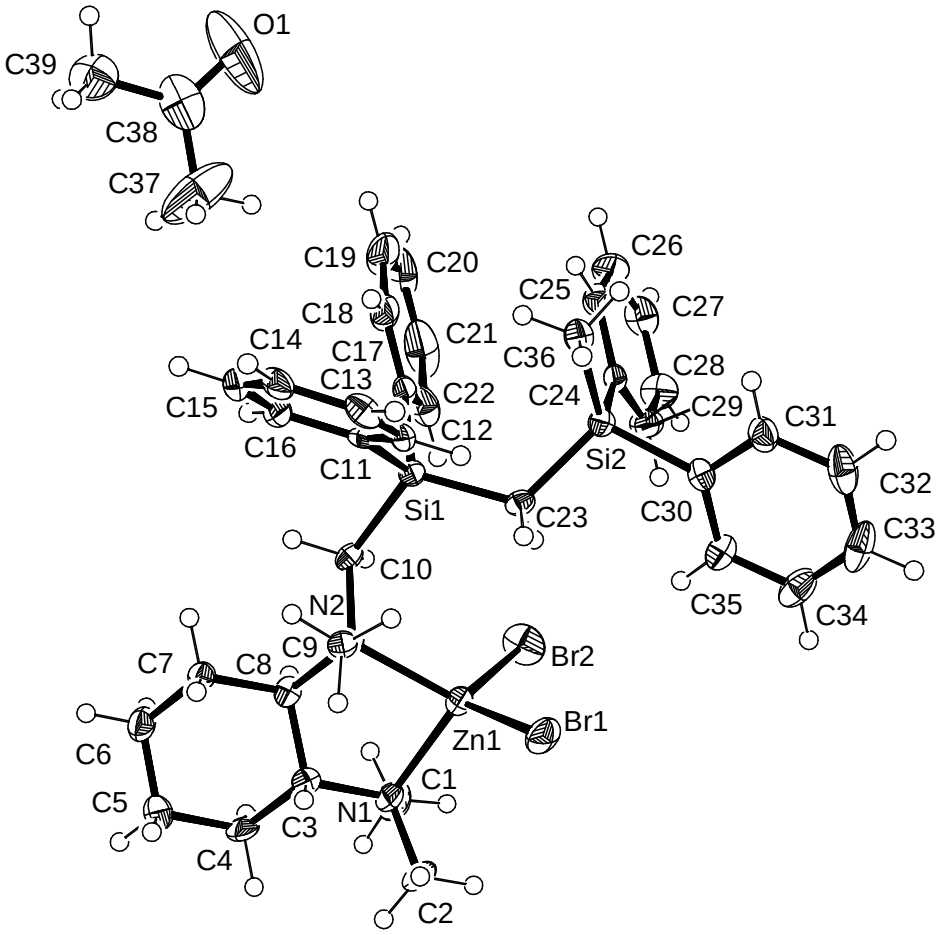


Abbildung 43 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des $ZnBr_2$-Adduktes **148** der (Silymethyl)silylverbindung im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 127 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) $ZnBr_2$-Adduktes der Silylmethyl)silylverbindung (**148**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
Br(1)	9651(1)	7105(1)	–55(1)	36(1)
Br(2)	10155(1)	4716(1)	–272(1)	45(1)
C(1)	12324(3)	5226(2)	778(1)	48(1)
C(2)	12282(3)	6686(2)	719(2)	52(1)
C(3)	11388(2)	6019(2)	1677(1)	25(1)
C(4)	12359(2)	5815(2)	2138(1)	37(1)
C(5)	12059(2)	5896(2)	2882(1)	37(1)
C(6)	11110(2)	5358(2)	3040(1)	32(1)
C(7)	10135(2)	5587(2)	2607(1)	24(1)
C(8)	10402(2)	5504(2)	1853(1)	20(1)
C(9)	8884(2)	6455(2)	1594(1)	21(1)
C(10)	8661(2)	4992(2)	1400(1)	20(1)
C(11)	6353(2)	5706(2)	1539(1)	21(1)
C(12)	5832(2)	6406(2)	1319(1)	22(1)
C(13)	5168(2)	6865(2)	1735(1)	30(1)
C(14)	5001(2)	6625(2)	2401(1)	31(1)
C(15)	5512(2)	5931(2)	2635(1)	33(1)
C(16)	6178(2)	5486(2)	2220(1)	26(1)
C(17)	6765(3)	4012(2)	956(1)	26(1)
C(18)	5744(3)	3805(2)	1183(1)	42(1)
C(19)	5360(4)	3015(2)	1138(2)	69(1)
C(20)	6006(4)	2421(2)	857(2)	73(2)
C(21)	7040(4)	2610(2)	621(2)	66(1)
C(22)	7405(3)	3400(2)	671(1)	40(1)
C(23)	7342(2)	5525(2)	115(1)	21(1)
C(24)	6285(2)	4229(2)	–800(1)	22(1)
C(25)	5467(3)	3676(2)	–656(1)	29(1)
C(26)	5491(3)	2882(2)	–897(1)	39(1)
C(27)	6350(3)	2624(2)	–1297(1)	38(1)
C(28)	7164(3)	3161(2)	–1448(2)	35(1)
C(29)	7138(3)	3955(2)	–1201(1)	31(1)
C(30)	6476(2)	5984(2)	–1268(1)	22(1)
C(31)	5616(3)	6313(2)	–1641(1)	30(1)
C(32)	5789(3)	6731(2)	–2245(2)	41(1)
C(33)	6833(4)	6837(2)	–2480(2)	43(1)
C(34)	7705(3)	6544(2)	–2111(2)	38(1)
C(35)	7531(3)	6121(2)	–1516(1)	29(1)

C(36)	4847(2)	5521(1)	–158(1)	28(1)
N(1)	11664(2)	5953(2)	937(1)	29(1)
N(2)	9444(2)	5688(1)	1394(1)	16(1)
Si(1)	7270(1)	5091(1)	982(1)	20(1)
Si(2)	6230(1)	5319(1)	–508(1)	21(1)
Zn(1)	10169(1)	5866(1)	444(1)	23(1)
C(38)	2987(4)	3577(2)	3051(2)	54(1)
C(39)	2743(3)	3514(2)	3780(2)	57(1)
O(1)	2357(3)	3355(2)	2636(2)	119(1)
C(37)	4049(4)	3957(3)	2887(2)	101(2)

Tabelle 128 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) des $ZnBr_2$-Adduktes der (Silylmethyl)-silylverbindung (**148**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	41(1)	28(1)	38(1)	15(1)	1(1)	–2(1)
Br(2)	46(1)	41(1)	47(1)	–22(1)	4(1)	7(1)
C(1)	31(2)	75(3)	38(2)	0(2)	10(2)	13(2)
C(2)	40(2)	77(3)	40(2)	26(2)	–1(2)	–28(2)
C(3)	24(2)	27(2)	24(2)	1(1)	2(1)	–4(2)
C(4)	16(2)	58(2)	35(2)	16(2)	0(2)	–12(2)
C(5)	35(2)	47(2)	29(2)	12(2)	–13(2)	–5(2)
C(6)	31(2)	42(2)	24(2)	9(2)	–1(2)	2(2)
C(7)	22(2)	28(2)	23(1)	4(1)	–1(1)	–1(2)
C(8)	21(2)	16(2)	22(2)	3(1)	2(1)	9(2)
C(9)	23(2)	16(2)	24(2)	0(1)	0(1)	–1(2)
C(10)	22(2)	16(2)	22(2)	4(1)	5(1)	1(2)
C(11)	17(2)	23(2)	23(2)	1(1)	–5(1)	–10(2)
C(12)	21(2)	29(2)	15(2)	–3(1)	0(1)	–5(2)
C(13)	30(2)	27(2)	34(2)	–8(1)	–8(2)	0(2)
C(14)	22(2)	47(2)	24(2)	–17(1)	1(1)	–3(2)
C(15)	29(2)	53(2)	18(2)	–1(2)	–2(1)	–9(2)
C(16)	22(2)	34(2)	23(2)	5(1)	–2(1)	0(2)
C(17)	39(2)	20(2)	20(2)	6(1)	–9(1)	–13(2)
C(18)	62(3)	38(2)	25(2)	7(2)	–5(2)	–26(2)
C(19)	109(4)	66(3)	33(2)	9(2)	–7(2)	–62(3)
C(20)	147(5)	37(3)	37(2)	10(2)	–33(3)	–54(3)
C(21)	127(4)	25(2)	46(2)	2(2)	–32(3)	–4(3)

C(22)	61(3)	24(2)	36(2)	–1(2)	–17(2)	–4(2)
C(23)	23(2)	15(1)	24(2)	0(1)	2(1)	–3(1)
C(24)	22(2)	29(2)	16(2)	3(1)	–3(1)	1(2)
C(25)	33(2)	31(2)	24(2)	–1(1)	2(1)	–2(2)
C(26)	46(2)	29(2)	41(2)	–3(2)	–1(2)	–14(2)
C(27)	53(3)	25(2)	34(2)	–10(2)	–6(2)	3(2)
C(28)	35(2)	32(2)	40(2)	–9(2)	6(2)	8(2)
C(29)	25(2)	34(2)	34(2)	–1(2)	2(2)	–3(2)
C(30)	29(2)	20(2)	17(2)	–10(1)	0(1)	2(2)
C(31)	38(2)	29(2)	23(2)	–3(2)	–5(2)	–3(2)
C(32)	67(3)	27(2)	30(2)	1(2)	–17(2)	9(2)
C(33)	88(3)	18(2)	21(2)	0(2)	9(2)	0(2)
C(34)	52(3)	32(2)	31(2)	–4(2)	19(2)	–5(2)
C(35)	33(2)	28(2)	26(2)	4(2)	7(2)	4(2)
C(36)	31(2)	30(2)	23(1)	–2(1)	–1(1)	0(2)
N(1)	23(2)	41(2)	22(1)	4(1)	6(1)	–5(1)
N(2)	17(1)	15(1)	17(1)	2(1)	2(1)	–1(1)
Si(1)	22(1)	19(1)	20(1)	2(1)	–1(1)	–3(1)
Si(2)	21(1)	23(1)	19(1)	–1(1)	1(1)	–1(1)
Zn(1)	25(1)	23(1)	21(1)	1(1)	2(1)	–1(1)
C(38)	63(3)	40(2)	58(3)	–15(2)	–12(2)	31(2)
C(39)	46(3)	59(3)	64(3)	–2(2)	6(2)	13(2)
O(1)	143(3)	124(3)	89(2)	–66(2)	–66(2)	51(3)
C(37)	91(4)	74(3)	138(4)	58(3)	62(3)	33(3)

Tabelle 129 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) des $ZnBr_2$-Adduktes der (Silylmethyl)silylverbindung (**148**).

	x	y	z	U(eq)
H(1A)	12411	5181	286	72
H(1B)	11957	4740	951	72
H(1C)	13040	5277	991	72
H(2A)	11845	7174	804	78
H(2B)	12445	6646	235	78
H(2C)	12963	6720	975	78
H(3)	11187	6598	1766	30
H(4A)	12603	5253	2047	44
H(4B)	12969	6187	2034	44
H(5A)	12688	5739	3167	45
H(5B)	11872	6468	2985	45

H(6A)	10918	5411	3524	38
H(6B)	11309	4784	2953	38
H(7A)	9921	6156	2706	29
H(7B)	9513	5230	2721	29
H(8)	10609	4923	1773	24
H(9A)	8351	6603	1246	31
H(9B)	9422	6892	1639	31
H(9C)	8512	6375	2027	31
H(10A)	8535	4844	1879	24
H(10B)	9032	4523	1186	24
H(12)	5936	6577	864	26
H(13)	4827	7342	1566	37
H(14)	4542	6933	2691	37
H(15)	5401	5760	3089	40
H(16)	6530	5017	2395	32
H(18)	5292	4213	1374	50
H(19)	4654	2884	1301	83
H(20)	5743	1879	825	88
H(21)	7489	2200	428	79
H(22)	8109	3532	507	48
H(23A)	8030	5333	-90	25
H(23B)	7403	6122	163	25
H(25)	4871	3844	-384	35
H(26)	4919	2516	-787	46
H(27)	6373	2083	-1465	45
H(28)	7755	2992	-1724	42
H(29)	7715	4316	-1309	37
H(31)	4894	6251	-1478	36
H(32)	5189	6941	-2493	50
H(33)	6955	7112	-2895	51
H(34)	8426	6634	-2267	46
H(35)	8137	5918	-1270	35
H(36A)	4296	5323	-477	42
H(36B)	4753	6107	-90	42
H(36C)	4765	5239	275	42
H(39A)	2013	3287	3841	85
H(39B)	2778	4055	3986	85
H(39C)	3278	3157	3997	85
H(37A)	4241	3836	2417	152
H(37B)	4611	3738	3188	152
H(37C)	3998	4547	2949	152

Diastereomerenreines α-lithiiertes (*R,R,S*$_{Si}$)-Silan 149

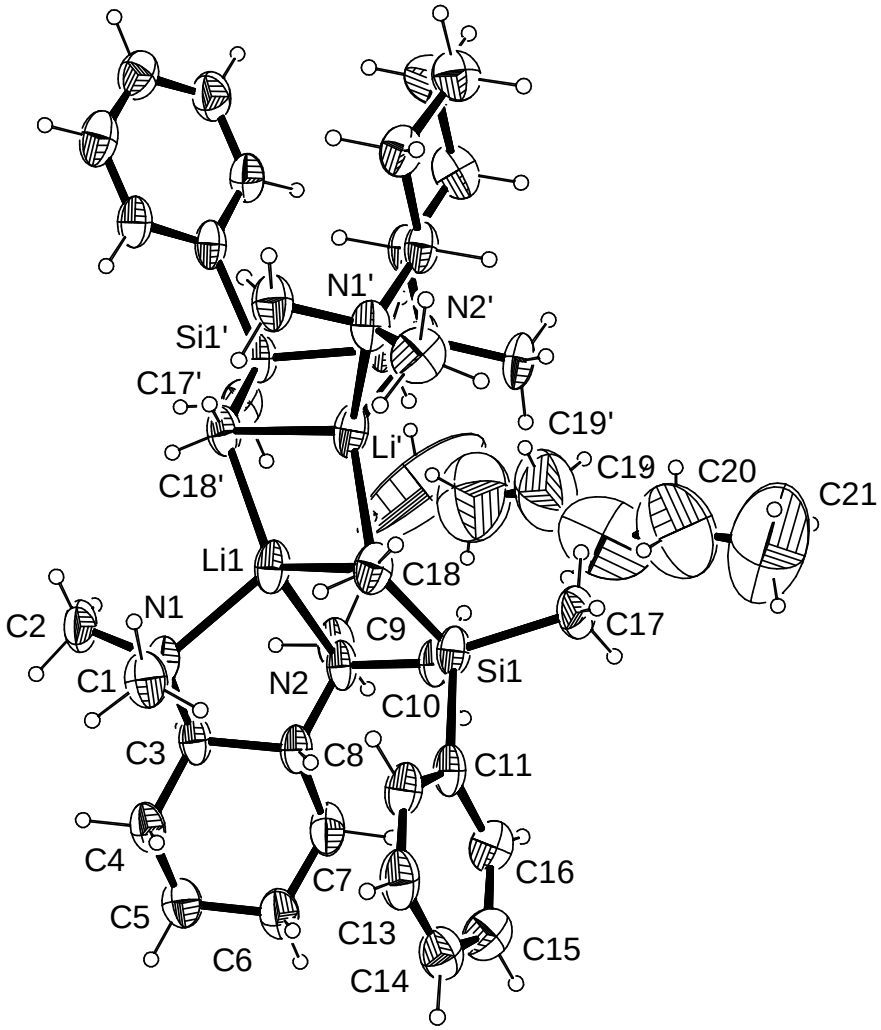


Abbildung 44 Thermische Auslenkungsellipsoide (25% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des diasteromerenreinen α-lithiierten Silans **149** im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 130 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) des diasteromerenreinen α-lithiierten Silans **149**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
C(1)	3799(2)	753(3)	6077(4)	97(1)
C(2)	4227(2)	1396(3)	8478(4)	100(1)
C(3)	3415(2)	2570(3)	7078(3)	72(1)
C(4)	2820(2)	1916(3)	7219(4)	83(1)
C(5)	2289(2)	2760(4)	7328(4)	98(1)
C(6)	2191(2)	3534(5)	6008(4)	116(1)

C(7)	2766(2)	4231(4)	5865(4)	98(1)
C(8)	3323(2)	3424(3)	5781(3)	69(1)
C(9)	4075(2)	4935(3)	6780(4)	87(1)
C(10)	3883(2)	4591(3)	4174(3)	70(1)
C(11)	3111(2)	2968(3)	1936(3)	70(1)
C(12)	2985(2)	1794(4)	1581(3)	79(1)
C(13)	2404(3)	1399(4)	1090(4)	94(1)
C(14)	1915(2)	2155(5)	949(4)	92(1)
C(15)	2018(2)	3319(5)	1270(4)	98(1)
C(16)	2599(2)	3727(4)	1753(3)	86(1)
C(17)	4144(2)	4470(3)	1136(3)	94(1)
C(18)	4475(2)	2407(4)	3246(5)	80(1)
N(1)	3955(2)	1784(3)	7001(3)	74(1)
N(2)	3900(1)	4062(2)	5632(2)	68(1)
Si(1)	3917(1)	3515(1)	2626(1)	72(1)
Li(1)	4566(3)	2674(5)	5752(6)	81(2)
C(19)	4802(8)	8109(11)	4280(13)	334(12)
C(20)	4798(7)	8051(11)	2710(12)	344(8)
C(21)	4661(8)	8395(16)	1083(14)	620(20)

Tabelle 131 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) des diasteromerenreinen α-lithiierten Silans **149**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	139(4)	66(3)	88(3)	–5(2)	26(3)	–4(2)
C(2)	126(4)	104(3)	69(3)	37(2)	10(2)	–3(3)
C(3)	115(3)	64(2)	36(2)	0(2)	12(2)	–9(3)
C(4)	114(3)	79(3)	56(2)	8(2)	15(2)	–16(3)
C(5)	113(4)	106(3)	78(3)	14(3)	23(2)	–2(3)
C(6)	117(4)	130(3)	107(3)	46(4)	34(3)	15(4)
C(7)	135(4)	87(3)	78(3)	27(2)	33(2)	20(3)
C(8)	108(3)	63(2)	37(2)	2(2)	12(2)	–2(3)
C(9)	147(4)	70(3)	44(2)	–12(2)	9(2)	–18(2)
C(10)	104(3)	67(2)	38(2)	3(2)	11(2)	–4(2)
C(11)	114(4)	68(3)	28(2)	0(2)	10(2)	–1(3)
C(12)	120(4)	73(3)	41(2)	–2(2)	4(2)	4(3)
C(13)	147(5)	82(3)	50(2)	1(2)	8(3)	–16(4)
C(14)	116(4)	99(4)	62(3)	–4(3)	11(2)	–17(3)

C(15)	113(4)	108(4)	72(3)	–16(3)	6(2)	14(3)
C(16)	113(3)	78(3)	63(2)	–13(2)	5(2)	8(3)
C(17)	122(3)	119(3)	42(2)	8(2)	14(2)	–9(3)
C(18)	116(4)	84(3)	39(2)	–5(2)	11(2)	12(3)
N(1)	107(3)	59(2)	55(2)	7(2)	8(2)	3(2)
N(2)	116(2)	59(2)	27(1)	–2(1)	10(1)	–8(2)
Si(1)	109(1)	75(1)	32(1)	1(1)	8(1)	3(1)
Li(1)	127(6)	64(4)	47(3)	–2(3)	1(3)	–6(4)
C(19)	360(20)	246(11)	420(40)	–136(19)	130(20)	–34(11)
C(20)	447(19)	225(15)	370(20)	–19(13)	100(20)	–76(11)
C(21)	620(30)	520(20)	600(40)	280(20)	–320(30)	–370(30)

Tabelle 132 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) des diasteromerenreinen α-lithiierten Silans **149**.

	x	y	z	U(eq)
H(1A)	3539	221	6552	145
H(1B)	4178	343	5931	145
H(1C)	3576	1002	5127	145
H(2A)	4395	2079	9054	150
H(2B)	4558	830	8405	150
H(2C)	3908	1021	8958	150
H(3)	3519	3058	7982	86
H(4A)	2888	1411	8102	100
H(4B)	2710	1398	6357	100
H(5A)	1909	2307	7394	117
H(5B)	2384	3248	8222	117
H(6A)	1847	4084	6081	140
H(6B)	2076	3044	5122	140
H(7A)	2862	4763	6718	118
H(7B)	2690	4723	4972	118
H(8)	3218	2935	4878	83
H(9A)	4479	5267	6677	131
H(9B)	4098	4558	7741	131
H(9C)	3767	5565	6693	131
H(10A)	4233	5145	4211	84
H(10B)	3499	5058	3947	84
H(12)	3316	1247	1684	95
H(13)	2338	592	845	113

H(14)	1508	1876	631	111
H(15)	1681	3854	1157	118
H(16)	2658	4541	1969	103
H(17A)	4558	4788	1449	141
H(17B)	3850	5121	936	141
H(17C)	4142	4001	245	141
H(101)	4600(16)	2100(30)	2470(40)	111(16)
H(100)	4326(17)	1780(30)	3630(40)	108(18)
H(19A)	4513	7461	4415	401
H(19B)	4559	8835	4355	401
H(20A)	4646	7231	2583	412
H(20B)	5250	7965	2753	412
H(21A)	4216	8360	752	927
H(21B)	4871	7846	505	927
H(21C)	4809	9197	957	927

1:1-Aggregat des α-lithiierten Silans 149 aus beiden Diastereomernen (*R,R,R*$_{Si}$) und (*R,R,S*$_{Si}$)

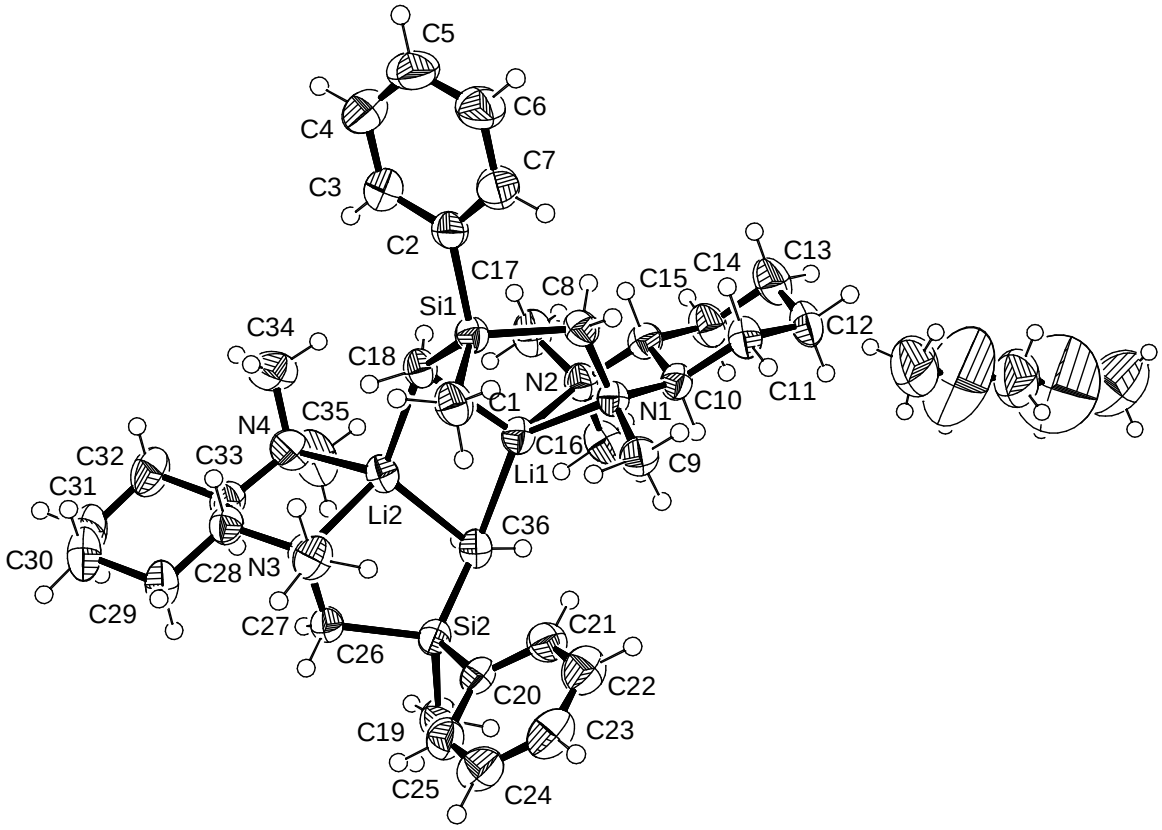


Abbildung 45 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des 1:1-Aggregats des α-lithiierten Silans **149**. im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 133 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) des 1:1-Aggregats des α-lithiierten Silans **149**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
C(1)	–2440(3)	1067(2)	7769(2)	47(1)
C(2)	–796(4)	1189(1)	6614(1)	42(1)
C(3)	43(4)	722(2)	6342(2)	59(1)
C(4)	–51(5)	605(2)	5740(2)	70(1)
C(5)	–985(5)	954(2)	5398(2)	70(1)
C(6)	–1818(5)	1414(2)	5649(2)	66(1)
C(7)	–1731(4)	1528(2)	6249(2)	55(1)
C(8)	–447(3)	2218(1)	7469(1)	39(1)
C(9)	–1539(3)	2567(2)	8382(1)	45(1)
C(10)	734(3)	3067(1)	8063(1)	38(1)
C(11)	53(4)	3588(1)	7688(1)	46(1)
C(12)	979(4)	4184(1)	7709(2)	55(1)
C(13)	2536(4)	4052(2)	7494(2)	63(1)
C(14)	3248(4)	3552(2)	7880(2)	54(1)
C(15)	2337(3)	2941(1)	7879(1)	40(1)
C(16)	3556(4)	2647(2)	8810(2)	54(1)
C(17)	4175(4)	2106(2)	7921(2)	60(1)
C(18)	930(4)	982(2)	7818(2)	40(1)
C(19)	1447(4)	1009(2)	10729(1)	51(1)
C(20)	–1362(3)	1209(1)	10020(1)	41(1)
C(21)	–1872(4)	1747(2)	9735(1)	48(1)
C(22)	–3335(4)	1937(2)	9780(2)	60(1)
C(23)	–4329(4)	1594(2)	10106(2)	59(1)
C(24)	–3847(4)	1062(2)	10398(2)	57(1)
C(25)	–2381(4)	871(2)	10352(2)	49(1)
C(26)	743(4)	99(1)	9782(1)	41(1)
C(27)	–1065(3)	–45(2)	9014(2)	49(1)
C(28)	1216(3)	–656(1)	8971(2)	43(1)
C(29)	747(4)	–1220(1)	9342(2)	57(1)
C(30)	1468(5)	–1820(2)	9136(2)	69(1)
C(31)	3152(5)	–1755(2)	9148(2)	71(1)
C(32)	3616(4)	–1210(2)	8758(2)	64(1)
C(33)	2904(4)	–595(2)	8967(2)	47(1)
C(34)	3545(5)	–134(2)	8007(2)	76(1)
C(35)	4767(4)	215(2)	8879(2)	79(1)
C(36)	1605(4)	1399(2)	9376(2)	44(1)
C(37)	7298(8)	7676(4)	9068(4)	158(3)

C(38)	6966(10)	7073(6)	8997(6)	263(7)
C(39)	6206(9)	6607(3)	8836(3)	120(2)
C(40)	5847(10)	6027(5)	8743(6)	248(6)
C(41)	5137(10)	5551(3)	8548(3)	161(3)
Li(1)	1250(6)	1776(2)	8449(2)	40(1)
Li(2)	1580(6)	655(2)	8701(2)	42(1)
N(1)	–141(2)	2476(1)	8068(1)	34(1)
N(2)	2986(3)	2431(1)	8237(1)	42(1)
N(3)	521(3)	–57(1)	9152(1)	38(1)
N(4)	3381(3)	–33(1)	8644(1)	52(1)
Si(1)	–635(1)	1331(1)	7439(1)	37(1)
Si(2)	657(1)	972(1)	9952(1)	40(1)

Tabelle 134 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) des 1:1-Aggregats des α-lithiierten Silans **149**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	43(2)	42(2)	57(2)	4(2)	–1(2)	–4(2)
C(2)	50(2)	36(2)	40(2)	–1(1)	0(2)	–13(2)
C(3)	77(3)	46(2)	53(2)	–4(2)	2(2)	3(2)
C(4)	93(3)	61(2)	57(2)	–13(2)	9(2)	–3(2)
C(5)	94(3)	74(3)	41(2)	–7(2)	3(2)	–28(3)
C(6)	82(3)	68(3)	46(2)	1(2)	–12(2)	–7(2)
C(7)	63(2)	51(2)	50(2)	–1(2)	–9(2)	–1(2)
C(8)	39(2)	38(2)	39(2)	3(1)	–3(2)	–1(1)
C(9)	38(2)	45(2)	50(2)	1(2)	4(2)	1(2)
C(10)	41(2)	33(2)	41(2)	–4(1)	–5(2)	1(2)
C(11)	49(2)	36(2)	55(2)	2(2)	–6(2)	2(2)
C(12)	67(2)	33(2)	66(2)	7(2)	–8(2)	–1(2)
C(13)	66(2)	44(2)	80(3)	17(2)	4(2)	–12(2)
C(14)	45(2)	47(2)	71(2)	10(2)	4(2)	–8(2)
C(15)	39(2)	37(2)	43(2)	–4(2)	–1(1)	–8(2)
C(16)	46(2)	53(2)	63(2)	9(2)	–15(2)	–5(2)
C(17)	38(2)	55(2)	88(3)	2(2)	13(2)	4(2)
C(18)	35(2)	36(2)	49(2)	3(2)	–1(2)	3(2)
C(19)	56(2)	49(2)	49(2)	–7(2)	–6(2)	5(2)
C(20)	45(2)	40(2)	40(2)	–10(2)	–1(2)	2(2)
C(21)	47(2)	51(2)	45(2)	3(2)	–3(2)	5(2)

C(22)	55(2)	63(2)	62(2)	–4(2)	–12(2)	16(2)
C(23)	43(2)	70(2)	65(2)	–17(2)	–8(2)	8(2)
C(24)	46(2)	62(2)	63(2)	–11(2)	10(2)	–11(2)
C(25)	49(2)	42(2)	55(2)	–6(2)	2(2)	–2(2)
C(26)	48(2)	35(2)	40(2)	1(1)	–1(2)	4(2)
C(27)	40(2)	50(2)	57(2)	–7(2)	–2(2)	4(2)
C(28)	45(2)	38(2)	46(2)	–2(2)	–4(2)	5(2)
C(29)	64(2)	34(2)	73(2)	–2(2)	0(2)	0(2)
C(30)	81(3)	37(2)	90(3)	–5(2)	–8(2)	5(2)
C(31)	80(3)	45(2)	88(3)	–5(2)	–9(2)	22(2)
C(32)	59(2)	55(2)	79(3)	–11(2)	–7(2)	25(2)
C(33)	48(2)	45(2)	48(2)	–1(2)	–3(2)	15(2)
C(34)	73(3)	90(3)	66(3)	16(2)	29(2)	42(2)
C(35)	42(2)	72(3)	124(4)	19(3)	0(2)	–3(2)
C(36)	44(2)	35(2)	52(2)	–1(2)	0(2)	1(2)
C(37)	114(5)	172(7)	188(7)	–48(6)	27(5)	–17(5)
C(38)	131(8)	252(14)	406(19)	–38(14)	0(9)	–103(9)
C(39)	138(6)	101(4)	122(5)	1(4)	–19(4)	45(4)
C(40)	136(7)	174(9)	433(18)	–88(11)	101(9)	–56(7)
C(41)	251(10)	114(5)	118(5)	13(4)	–28(6)	76(6)
Li(1)	41(3)	36(3)	44(3)	–2(2)	–3(2)	0(2)
Li(2)	43(3)	35(3)	48(3)	5(2)	–1(2)	2(3)
N(1)	32(1)	32(1)	38(1)	–1(1)	–3(1)	1(1)
N(2)	37(1)	38(2)	50(2)	1(1)	1(1)	1(1)
N(3)	36(1)	35(1)	42(1)	–4(1)	–1(1)	3(1)
N(4)	38(2)	56(2)	63(2)	9(2)	8(1)	10(2)
Si(1)	38(1)	34(1)	39(1)	0(1)	–3(1)	–1(1)
Si(2)	42(1)	35(1)	41(1)	–4(1)	0(1)	3(1)

Tabelle 135 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) des 1:1-Aggregats des α-lithiierten Silans **149**.

	x	y	z	U(eq)
H(1A)	–2597	624	7678	71
H(1B)	–3255	1314	7602	71
H(1C)	–2411	1125	8198	71
H(3)	698	477	6575	70
H(4)	531	283	5566	84
H(5)	–1053	877	4986	84

H(6)	–2464	1657	5410	79
H(7)	–2330	1848	6415	65
H(8A)	367	2346	7201	46
H(8B)	–1376	2407	7318	46
H(9A)	–1341	2753	8770	67
H(9B)	–2035	2163	8434	67
H(9C)	–2181	2847	8153	67
H(10)	764	3222	8479	46
H(11A)	–28	3445	7274	56
H(11B)	–961	3679	7834	56
H(12A)	514	4507	7457	66
H(12B)	1015	4344	8119	66
H(13A)	3135	4440	7510	76
H(13B)	2504	3908	7078	76
H(14A)	3331	3710	8289	65
H(14B)	4263	3465	7733	65
H(15)	2307	2790	7461	48
H(16A)	4443	2904	8747	81
H(16B)	3813	2286	9056	81
H(16C)	2793	2896	9010	81
H(17A)	3793	1948	7544	90
H(17B)	4534	1756	8160	90
H(17C)	4994	2397	7846	90
H(18A)	710(40)	554(17)	7889(14)	55(9)
H(18B)	1760(30)	1069(14)	7629(13)	37(9)
H(19A)	2452	833	10731	77
H(19B)	813	767	10997	77
H(19C)	1483	1445	10861	77
H(21)	–1198	1987	9505	58
H(22)	–3653	2307	9585	72
H(23)	–5338	1719	10130	71
H(24)	–4525	828	10630	68
H(25)	–2067	503	10552	58
H(26A)	1723	–63	9908	49
H(26B)	–25	–117	10018	49
H(27A)	–1212	–153	8598	73
H(27B)	–1459	374	9090	73
H(27C)	–1586	–349	9263	73
H(28)	899	–740	8555	52
H(29A)	1018	–1144	9760	69
H(29B)	–346	–1266	9322	69
H(30A)	1136	–1918	8730	83

H(30B)	1162	–2168	9397	83
H(31A)	3493	–1683	9558	85
H(31B)	3617	–2145	9002	85
H(32A)	3314	–1294	8345	77
H(32B)	4711	–1167	8767	77
H(33)	3215	–535	9387	56
H(34A)	4402	–406	7934	115
H(34B)	3699	269	7809	115
H(34C)	2645	–332	7851	115
H(35A)	5563	–91	8820	119
H(35B)	4653	298	9303	119
H(35C)	5018	604	8674	119
H(36A)	2590(40)	1314(17)	9413(14)	60(11)
H(36B)	1480(40)	1785(19)	9391(16)	68(12)
H(37A)	6799	7922	8762	237
H(37B)	8375	7733	9035	237
H(37C)	6964	7815	9458	237
H(38A)	7912	6946	8810	316
H(38B)	7095	6946	9415	316
H(39A)	6015	6755	8428	144
H(39B)	5289	6723	9051	144
H(40A)	6839	5891	8605	297
H(40B)	5837	5901	9163	297
H(41A)	4525	5675	8210	241
H(41B)	4498	5385	8861	241
H(41C)	5845	5228	8425	241

8.2.5 Kristallstrukturen aus Kapitel 4.5

Monolithiiertes Dimethyl(*tert*-Butyl)phosphinsullfid mit (–)-Spartein 161

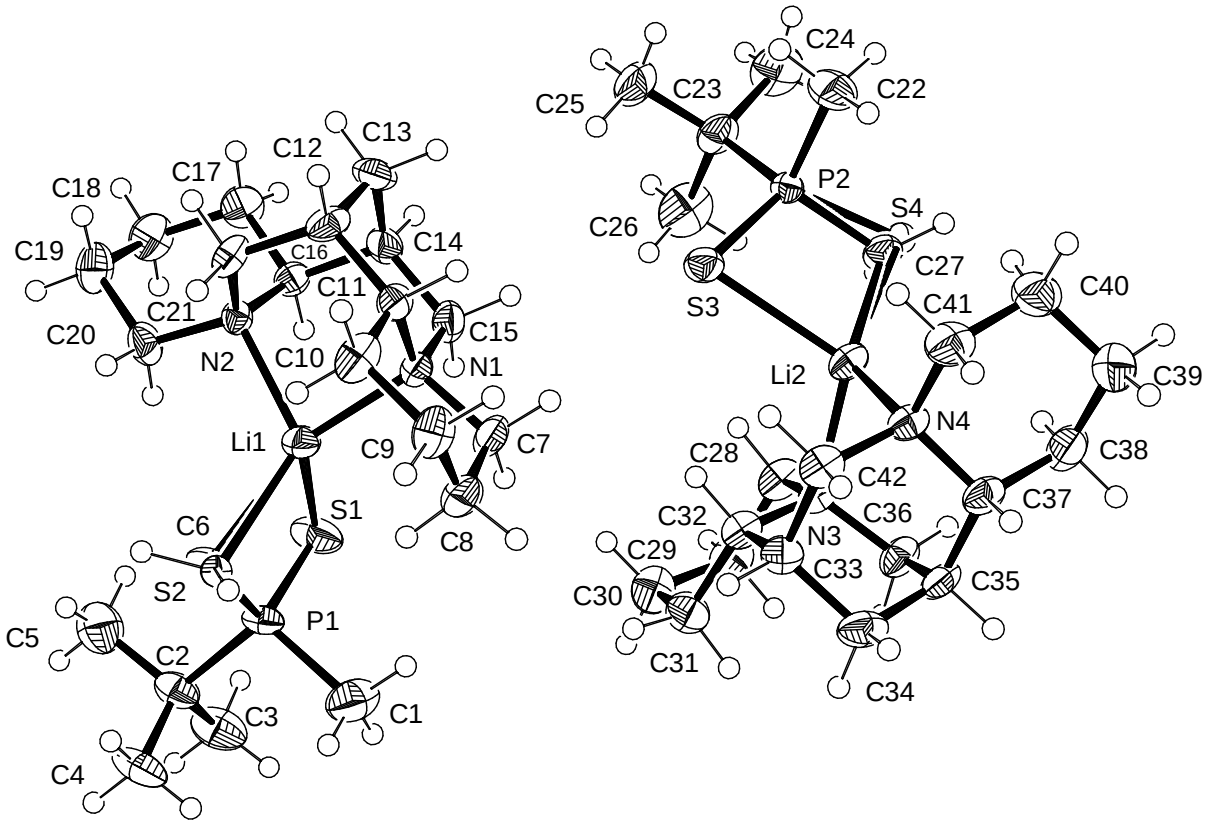


Abbildung 46 Thermische Auslenkungsellipsoide (25% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des (–)-Spartein-Addukts des lithiierten Dimethyl(*tert*-butyl)phosphinsulfids **161** im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 136 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) des (–)-Spartein-Addukts des lithiierten Dimethyl(*tert*-butyl)phosphinsulfids **161**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
C(1)	4644(3)	4636(3)	8364(1)	53(1)
C(2)	4524(2)	3048(2)	7695(1)	37(1)
C(3)	5113(3)	3902(3)	7420(1)	52(1)
C(4)	5420(3)	2310(3)	7906(1)	52(1)
C(5)	3716(3)	2287(3)	7456(1)	59(1)
C(6)	2845(5)	2787(6)	8388(2)	28(1)
C(7)	1390(2)	5859(2)	8925(1)	36(1)
C(8)	2099(2)	5096(2)	9192(1)	39(1)

C(9)	1332(3)	4395(2)	9462(1)	39(1)
C(10)	431(2)	3770(2)	9220(1)	38(1)
C(11)	–255(2)	4586(2)	8963(1)	30(1)
C(12)	–1247(2)	4025(2)	8734(1)	35(1)
C(13)	–1911(2)	4938(3)	8510(1)	44(1)
C(14)	–1077(2)	5428(2)	8206(1)	34(1)
C(15)	–74(2)	5988(2)	8429(1)	34(1)
C(16)	–698(2)	4506(2)	7911(1)	28(1)
C(17)	–1685(2)	4182(3)	7626(1)	41(1)
C(18)	–1340(3)	3227(3)	7345(1)	46(1)
C(19)	–902(3)	2217(3)	7580(1)	44(1)
C(20)	100(2)	2591(2)	7841(1)	35(1)
C(21)	–900(2)	3083(2)	8446(1)	31(1)
C(22)	–2739(2)	9648(3)	9591(1)	48(1)
C(23)	–2411(2)	9397(2)	8743(1)	37(1)
C(24)	–3273(3)	10376(3)	8688(1)	62(1)
C(25)	–3038(3)	8244(3)	8737(1)	49(1)
C(26)	–1507(3)	9424(3)	8410(1)	59(1)
C(27)	–797(4)	10896(4)	9250(1)	33(1)
C(28)	2043(2)	10006(2)	8842(1)	35(1)
C(29)	3050(2)	9695(3)	8576(1)	40(1)
C(30)	3403(3)	8452(3)	8642(1)	44(1)
C(31)	3646(2)	8251(3)	9082(1)	39(1)
C(32)	2625(2)	8623(2)	9343(1)	29(1)
C(33)	2903(2)	8449(2)	9784(1)	31(1)
C(34)	3819(2)	9287(3)	9922(1)	40(1)
C(35)	3294(2)	10477(2)	9873(1)	34(1)
C(36)	3033(2)	10689(2)	9434(1)	35(1)
C(37)	2261(2)	10592(2)	10156(1)	32(1)
C(38)	1722(3)	11782(2)	10159(1)	43(1)
C(39)	778(3)	11872(3)	10468(1)	51(1)
C(40)	–108(3)	10930(3)	10406(1)	47(1)
C(41)	464(2)	9765(3)	10382(1)	41(1)
C(42)	1858(2)	8563(2)	10058(1)	32(1)
Li(2)	593(4)	9884(4)	9522(1)	32(1)
Li(1)	1398(3)	4086(4)	8326(1)	31(1)
N(2)	–190(2)	3514(2)	8120(1)	23(1)
N(4)	1364(2)	9728(2)	10073(1)	29(1)
N(1)	540(2)	5191(2)	8694(1)	25(1)
N(3)	2243(2)	9820(2)	9271(1)	26(1)
P(2)	–1620(1)	9598(1)	9219(1)	23(1)
P(1)	3627(1)	3812(1)	8070(1)	28(1)

S(1)	2604(1)	4884(1)	7801(1)	48(1)
S(3)	–639(1)	8234(1)	9322(1)	32(1)
S(2)	2948(8)	2778(7)	8462(2)	21(1)
S(4)	–982(6)	11148(6)	9260(2)	21(1)

Tabelle 137 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) des (–)-Spartein-Addukts des lithiierten Dimethyl(*tert*-butyl)phosphinsulfids **161**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	39(2)	72(2)	48(2)	–6(2)	2(1)	–10(2)
C(2)	31(1)	43(2)	37(1)	6(1)	10(1)	8(1)
C(3)	44(2)	68(2)	45(2)	15(2)	20(1)	10(2)
C(4)	36(2)	56(2)	63(2)	13(2)	13(1)	22(2)
C(5)	61(2)	60(2)	55(2)	–14(2)	5(2)	5(2)
C(6)	19(2)	39(2)	27(3)	16(2)	8(2)	8(1)
C(7)	36(1)	30(1)	41(1)	–6(1)	–6(1)	–10(1)
C(8)	35(1)	44(2)	37(1)	–9(1)	–9(1)	–5(1)
C(9)	53(2)	43(2)	22(1)	–4(1)	–7(1)	–4(1)
C(10)	49(2)	44(2)	21(1)	2(1)	1(1)	–15(1)
C(11)	29(1)	36(1)	24(1)	–11(1)	8(1)	–6(1)
C(12)	27(1)	53(2)	24(1)	–8(1)	7(1)	–14(1)
C(13)	22(1)	62(2)	49(2)	–24(1)	0(1)	7(1)
C(14)	30(1)	31(1)	42(1)	–4(1)	–10(1)	10(1)
C(15)	39(1)	23(1)	38(1)	–3(1)	–7(1)	2(1)
C(16)	27(1)	31(1)	25(1)	0(1)	–3(1)	–2(1)
C(17)	41(2)	49(2)	35(1)	–3(1)	–16(1)	5(1)
C(18)	52(2)	57(2)	30(1)	–10(1)	–13(1)	–3(2)
C(19)	59(2)	42(2)	32(1)	–14(1)	–6(1)	–3(1)
C(20)	43(2)	34(1)	28(1)	–11(1)	–1(1)	7(1)
C(21)	38(1)	29(1)	26(1)	1(1)	–3(1)	–14(1)
C(22)	38(2)	62(2)	44(2)	–7(2)	17(1)	0(2)
C(23)	35(1)	41(2)	35(1)	1(1)	–14(1)	–2(1)
C(24)	56(2)	54(2)	76(2)	8(2)	–36(2)	12(2)
C(25)	41(2)	48(2)	57(2)	–11(2)	–18(1)	–7(1)
C(26)	71(2)	80(2)	25(1)	5(1)	–3(1)	–13(2)
C(27)	28(2)	33(2)	38(2)	1(2)	–10(1)	1(2)
C(28)	40(1)	40(2)	25(1)	9(1)	–5(1)	–9(1)
C(29)	46(2)	47(2)	27(1)	5(1)	6(1)	–12(1)

C(30)	51(2)	48(2)	33(1)	0(1)	10(1)	–7(1)
C(31)	37(1)	42(2)	36(1)	0(1)	4(1)	2(1)
C(32)	30(1)	33(1)	25(1)	5(1)	–1(1)	–5(1)
C(33)	30(1)	34(1)	28(1)	5(1)	–3(1)	2(1)
C(34)	27(1)	60(2)	32(1)	1(1)	–7(1)	0(1)
C(35)	27(1)	42(2)	33(1)	–6(1)	–5(1)	–13(1)
C(36)	35(1)	37(2)	33(1)	–1(1)	2(1)	–14(1)
C(37)	29(1)	43(2)	24(1)	–2(1)	–7(1)	–5(1)
C(38)	43(2)	37(2)	48(2)	–5(1)	–8(1)	–8(1)
C(39)	47(2)	53(2)	51(2)	–16(2)	–2(1)	2(2)
C(40)	39(2)	61(2)	41(2)	–7(1)	5(1)	1(2)
C(41)	38(1)	55(2)	31(1)	1(1)	6(1)	–6(1)
C(42)	35(1)	36(1)	25(1)	7(1)	–2(1)	–4(1)
Li(2)	29(2)	36(2)	29(2)	–1(2)	–7(2)	–6(2)
Li(1)	23(2)	36(2)	34(2)	–4(2)	4(2)	–2(2)
N(2)	26(1)	23(1)	20(1)	–2(1)	0(1)	–1(1)
N(4)	26(1)	35(1)	25(1)	3(1)	–2(1)	–6(1)
N(1)	26(1)	23(1)	26(1)	–1(1)	–3(1)	–3(1)
N(3)	26(1)	30(1)	22(1)	7(1)	–4(1)	–6(1)
P(2)	21(1)	24(1)	24(1)	0(1)	0(1)	1(1)
P(1)	19(1)	35(1)	30(1)	9(1)	4(1)	3(1)
S(1)	32(1)	48(1)	62(1)	20(1)	7(1)	11(1)
S(3)	26(1)	31(1)	40(1)	2(1)	–4(1)	2(1)

Tabelle 138 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) des (–)-Spartein-Addukts des lithiierten Dimethyl(*tert*-butyl)phosphinsulfids **161**.

	x	y	z	U(eq)
H(1A)	5140	4114	8515	79
H(1B)	4217	5130	8547	79
H(1C)	5123	5108	8190	79
H(3A)	5620	4403	7575	78
H(3B)	4524	4364	7286	78
H(3C)	5572	3488	7224	78
H(4A)	5026	1766	8080	77
H(4B)	5932	2801	8063	77
H(4C)	5878	1891	7710	77
H(5A)	4144	1946	7236	88
H(5B)	3075	2746	7353	88

H(5C)	3410	1679	7626	88
H(6A)	3160	2707	8659	34
H(6B)	2688	2034	8265	34
H(7A)	977	6433	9087	43
H(7B)	1912	6272	8743	43
H(8A)	2627	5571	9353	46
H(8B)	2576	4575	9028	46
H(9A)	1807	3836	9610	47
H(9B)	946	4904	9655	47
H(10A)	818	3196	9050	46
H(10B)	–103	3359	9399	46
H(11)	–605	5172	9142	36
H(12)	–1788	3681	8931	42
H(13A)	–2178	5544	8692	53
H(13B)	–2593	4600	8377	53
H(14)	–1493	6040	8056	41
H(15A)	483	6303	8235	40
H(15B)	–378	6634	8587	40
H(16)	–68	4848	7746	33
H(17A)	–2366	3936	7782	50
H(17B)	–1910	4864	7471	50
H(18A)	–2016	2994	7185	55
H(18B)	–728	3500	7164	55
H(19A)	–641	1607	7397	53
H(19B)	–1534	1905	7745	53
H(20A)	377	1921	7993	42
H(20B)	744	2851	7671	42
H(21A)	–463	2486	8590	37
H(21B)	–1607	2723	8337	37
H(22A)	–3216	10331	9551	72
H(22B)	–2383	9677	9853	72
H(22C)	–3224	8963	9570	72
H(24A)	–3590	10349	8419	93
H(24B)	–2879	11109	8729	93
H(24C)	–3903	10298	8879	93
H(25A)	–3612	8223	8950	73
H(25B)	–2475	7627	8776	73
H(25C)	–3427	8145	8483	73
H(26A)	–1893	9317	8155	88
H(26B)	–943	8809	8451	88
H(26C)	–1107	10164	8412	88
H(27A)	–1138	11479	9427	40

H(27B)	–591	11229	8991	40
H(28A)	1851	10823	8799	42
H(28B)	1361	9550	8760	42
H(29A)	3714	10204	8633	48
H(29B)	2826	9806	8296	48
H(30A)	4106	8278	8486	53
H(30B)	2776	7938	8553	53
H(31A)	4345	8685	9160	46
H(31B)	3803	7428	9126	46
H(32)	1957	8112	9277	35
H(33)	3223	7659	9816	37
H(34A)	4528	9211	9760	48
H(34B)	4019	9145	10202	48
H(35)	3891	11047	9956	40
H(36A)	2680	11456	9403	42
H(36B)	3766	10680	9283	42
H(37)	2556	10441	10429	39
H(38A)	2329	12358	10214	51
H(38B)	1393	11949	9895	51
H(39A)	396	12627	10448	61
H(39B)	1121	11803	10735	61
H(40A)	–667	10937	10628	56
H(40B)	–541	11077	10159	56
H(41A)	818	9580	10641	50
H(41B)	–131	9179	10325	50
H(42A)	1250	8024	9970	39
H(42B)	2092	8337	10329	39

Abfangprodukt von lithiiertem Dimethyl(*tert*-Butyl)phosphinsulfid mit Benzophenon 162

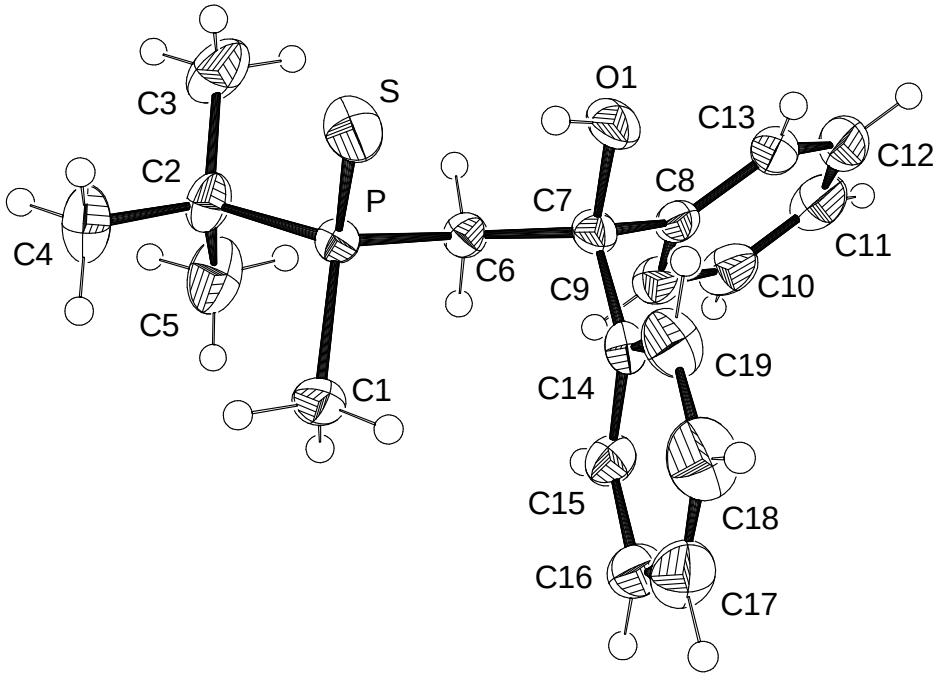


Abbildung 47 Thermische Auslenkungsellipsoide (25% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Abfangproduktes von monolithiiertem Phosphinsulfids **162** im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 139 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) des Abfangproduktes von monolithiiertem Phosphinsulfids **162**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
O(1)	896(2)	1769(1)	2822(1)	40(1)
C(1)	3642(3)	2172(1)	695(1)	35(1)
C(2)	2707(3)	3971(1)	1153(1)	35(1)
C(3)	1418(4)	4523(2)	1677(1)	54(1)
C(4)	1997(4)	4159(1)	380(1)	50(1)
C(5)	4963(3)	4190(2)	1242(2)	55(1)
C(6)	3519(3)	2611(1)	2220(1)	27(1)
C(7)	2994(3)	1763(1)	2642(1)	28(1)
C(8)	4141(3)	1755(1)	3367(1)	30(1)
C(9)	6145(3)	2035(1)	3430(1)	37(1)
C(10)	7142(4)	2007(1)	4090(1)	46(1)
C(11)	6125(4)	1702(2)	4691(1)	51(1)
C(12)	4155(4)	1420(2)	4632(1)	49(1)

C(13)	3147(4)	1442(1)	3974(1)	38(1)
C(14)	3556(3)	939(1)	2206(1)	29(1)
C(15)	5521(3)	808(1)	1954(1)	33(1)
C(16)	6005(4)	73(1)	1540(1)	42(1)
C(17)	4543(4)	–544(1)	1392(1)	51(1)
C(18)	2622(5)	–429(2)	1647(1)	58(1)
C(19)	2102(4)	310(1)	2050(1)	44(1)
P	2250(1)	2799(1)	1356(1)	24(1)
S	–667(1)	2481(1)	1348(1)	42(1)

Tabelle 140 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) des Abfangproduktes von monolithiiertem Phosphinsulfids **162**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2$ [$h^2a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	24(1)	59(1)	36(1)	12(1)	6(1)	3(1)
C(1)	41(1)	36(1)	28(1)	–4(1)	2(1)	7(1)
C(2)	44(1)	23(1)	37(1)	2(1)	–10(1)	–2(1)
C(3)	72(2)	35(1)	55(1)	–12(1)	–16(1)	17(1)
C(4)	75(2)	36(1)	40(1)	8(1)	–15(1)	–7(1)
C(5)	50(1)	38(1)	78(2)	18(1)	–14(1)	–18(1)
C(6)	26(1)	28(1)	26(1)	0(1)	–2(1)	0(1)
C(7)	22(1)	35(1)	27(1)	4(1)	2(1)	1(1)
C(8)	35(1)	28(1)	26(1)	–1(1)	0(1)	8(1)
C(9)	36(1)	41(1)	33(1)	–1(1)	–4(1)	7(1)
C(10)	48(1)	47(1)	44(1)	–11(1)	–14(1)	13(1)
C(11)	73(2)	49(1)	32(1)	–8(1)	–16(1)	21(1)
C(12)	76(2)	47(1)	26(1)	1(1)	3(1)	15(1)
C(13)	47(1)	36(1)	31(1)	1(1)	5(1)	8(1)
C(14)	31(1)	29(1)	25(1)	6(1)	–2(1)	–3(1)
C(15)	32(1)	28(1)	40(1)	0(1)	–2(1)	0(1)
C(16)	48(1)	40(1)	38(1)	–2(1)	–1(1)	9(1)
C(17)	76(2)	35(1)	43(1)	–10(1)	–5(1)	–1(1)
C(18)	73(2)	44(1)	56(1)	–9(1)	–5(1)	–24(1)
C(19)	43(1)	46(1)	44(1)	1(1)	1(1)	–17(1)
P	23(1)	26(1)	24(1)	–1(1)	–1(1)	–1(1)
S	25(1)	61(1)	41(1)	11(1)	–6(1)	–8(1)

Tabelle 141 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) des des Abfangproduktes von monolithiiertem Phosphinsulfids **162**.

	x	y	z	U(eq)
H(1O)	390(40)	1913(19)	2470(16)	61(9)
H(1A)	5099	2299	739	53
H(1B)	3174	2332	212	53
H(1C)	3407	1544	775	53
H(3A)	1830	4394	2172	81
H(3B)	–25	4378	1614	81
H(3C)	1630	5148	1577	81
H(4A)	2204	4782	270	75
H(4B)	548	4015	334	75
H(4C)	2787	3801	43	75
H(5A)	5193	4807	1116	83
H(5B)	5772	3813	924	83
H(5C)	5371	4090	1742	83
H(6A)	5007	2613	2133	32
H(6B)	3213	3118	2535	32
H(9)	6844	2247	3018	44
H(10)	8516	2196	4128	56
H(11)	6792	1689	5144	61
H(12)	3466	1207	5046	59
H(13)	1780	1242	3941	46
H(15)	6551	1224	2065	40
H(16)	7349	0	1361	51
H(17)	4870	–1047	1113	62
H(18)	1614	–860	1548	69
H(19)	747	381	2219	53

Monolithiiertes Dimethyl(*tert*-Butyl)phosphinoboran mit (–)-Spartein 164

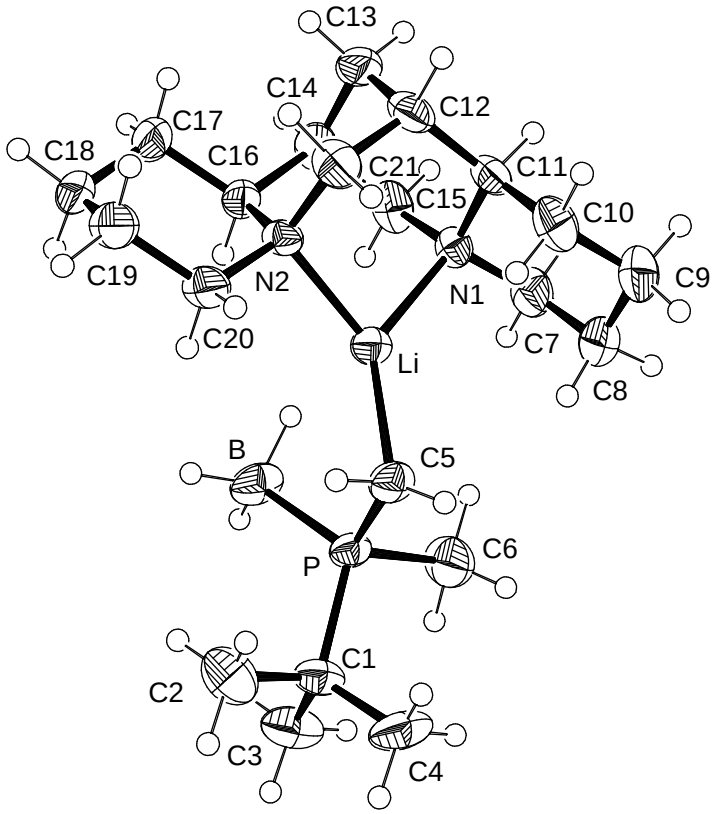


Abbildung 48 Thermische Auslenkungsellipsoide (25% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des (–)-Spartein-Adduktes des monolithiierten Phosphinoborans **164** im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 142 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) des (–)-Spartein-Adduktes des monolithiierten Phosphinoborans **164**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
B	3734(4)	9771(2)	9431(2)	48(1)
C(1)	4716(3)	11838(2)	8903(2)	41(1)
C(2)	4051(4)	12281(2)	9612(2)	68(1)
C(3)	6253(3)	11584(2)	9070(2)	58(1)
C(4)	4628(3)	12569(2)	8279(2)	57(1)
C(5)	1892(3)	10969(2)	8427(2)	39(1)
C(6)	4513(4)	10271(3)	7847(2)	61(1)
C(7)	1457(3)	8327(2)	7258(2)	47(1)
C(8)	1289(4)	9195(2)	6763(2)	58(1)
C(9)	–264(4)	9359(3)	6556(2)	59(1)
C(10)	–1162(3)	9372(2)	7256(2)	50(1)

C(11)	–947(3)	8459(2)	7713(1)	36(1)
C(12)	–1940(3)	8356(2)	8382(2)	47(1)
C(13)	–1677(3)	7402(2)	8768(2)	55(1)
C(14)	–172(3)	7442(2)	9067(2)	45(1)
C(15)	837(3)	7535(2)	8406(2)	44(1)
C(16)	–18(3)	8239(2)	9657(1)	36(1)
C(17)	–790(4)	7987(2)	10385(2)	57(1)
C(18)	–666(4)	8789(2)	10957(2)	61(1)
C(19)	–1192(4)	9715(2)	10631(2)	58(1)
C(20)	–395(3)	9946(2)	9913(2)	42(1)
C(21)	–1838(3)	9157(2)	8962(2)	45(1)
Li	1103(4)	9557(3)	8596(2)	35(1)
N(1)	561(2)	8386(1)	7936(1)	32(1)
N(2)	–448(2)	9182(1)	9337(1)	30(1)
P	3636(1)	10754(1)	8684(1)	32(1)

Tabelle 143 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) des (–)-Spartein-Adduktes des monolithiierten Phosphinoborans **164**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B	42(2)	39(2)	63(2)	27(2)	–9(2)	–1(2)
C(1)	39(2)	28(1)	55(2)	2(1)	–5(1)	–7(1)
C(2)	88(3)	51(2)	65(2)	–25(2)	1(2)	–4(2)
C(3)	43(2)	42(1)	88(2)	4(2)	–16(2)	–6(1)
C(4)	47(2)	40(2)	84(2)	25(2)	–2(2)	–11(1)
C(5)	39(2)	34(1)	44(2)	13(1)	–7(1)	–2(1)
C(6)	58(2)	73(2)	52(2)	–19(2)	14(2)	–9(2)
C(7)	41(2)	62(2)	37(1)	–12(1)	7(1)	5(1)
C(8)	61(2)	79(2)	34(1)	0(2)	5(1)	–16(2)
C(9)	71(2)	70(2)	37(2)	11(1)	–15(2)	–6(2)
C(10)	51(2)	54(2)	45(2)	–2(1)	–17(1)	8(1)
C(11)	33(1)	40(1)	35(1)	–11(1)	–5(1)	–4(1)
C(12)	29(1)	66(2)	45(2)	–19(1)	0(1)	–10(1)
C(13)	70(2)	52(2)	44(2)	–13(1)	11(2)	–33(2)
C(14)	75(2)	21(1)	39(1)	–1(1)	0(1)	–6(1)
C(15)	61(2)	30(1)	41(2)	–10(1)	–4(1)	13(1)
C(16)	47(2)	29(1)	31(1)	0(1)	2(1)	–8(1)
C(17)	86(2)	53(2)	34(2)	–1(1)	8(2)	–33(2)

C(18)	78(2)	73(2)	33(2)	–11(1)	18(2)	–39(2)
C(19)	60(2)	64(2)	49(2)	–29(2)	23(2)	–21(2)
C(20)	44(2)	37(1)	45(2)	–16(1)	13(1)	–6(1)
C(21)	30(1)	58(2)	47(2)	–15(1)	4(1)	6(1)
Li	35(2)	34(2)	36(2)	–1(2)	2(2)	–5(2)
N(1)	33(1)	32(1)	30(1)	–5(1)	1(1)	4(1)
N(2)	30(1)	26(1)	35(1)	–9(1)	4(1)	–3(1)
P	32(1)	26(1)	38(1)	6(1)	0(1)	–3(1)

Tabelle 144 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) des (–)-Spartein-Adduktes des monolithiierten Phosphinoborans **164**.

	x	y	z	U(eq)
H(100)	3100(30)	9180(20)	9176(16)	50(8)
H(101)	3210(30)	10020(20)	9968(17)	58(9)
H(102)	4820(30)	9540(20)	9549(17)	62(9)
H(2A)	4590	12854	9758	102
H(2B)	4076	11810	10020	102
H(2C)	3063	12461	9509	102
H(3A)	6700	11322	8618	86
H(3B)	6287	11103	9471	86
H(3C)	6765	12163	9229	86
H(4A)	5100	13164	8435	86
H(4B)	3628	12704	8165	86
H(4C)	5097	12314	7831	86
H(5A)	1790(30)	11300(20)	8033(17)	46(8)
H(5B)	1440(30)	11300(20)	8871(17)	54(8)
H(6A)	4020(40)	9600(30)	7690(20)	84(12)
H(6B)	5620(50)	10410(30)	7920(20)	119(16)
H(6C)	4330(40)	10740(30)	7410(20)	96(13)
H(7A)	1199	7743	6972	56
H(7B)	2466	8267	7410	56
H(8A)	1854	9104	6300	70
H(8B)	1660	9770	7025	70
H(9A)	–363	9979	6288	71
H(9B)	–593	8839	6219	71
H(10A)	–2177	9432	7116	60
H(10B)	–904	9938	7564	60
H(11)	–1145	7905	7371	43
H(12)	–2937	8349	8187	56

H(13A)	–2362	7308	9182	66
H(13B)	–1782	6865	8408	66
H(14)	30	6814	9318	54
H(15A)	1824	7569	8597	52
H(15B)	758	6951	8092	52
H(16)	1017	8287	9780	43
H(17A)	–1806	7866	10276	69
H(17B)	–380	7390	10595	69
H(18A)	–1232	8625	11407	73
H(18B)	339	8862	11112	73
H(19A)	–1053	10242	10997	69
H(19B)	–2222	9663	10524	69
H(20A)	–795	10543	9697	50
H(20B)	612	10073	10039	50
H(21A)	–2007	9783	8713	54
H(21B)	–2591	9065	9342	54

Monolithiiertes Dimethyl(*tert*-Butyl)phosphinoboran mit (*R,R*)-TMCDA 165

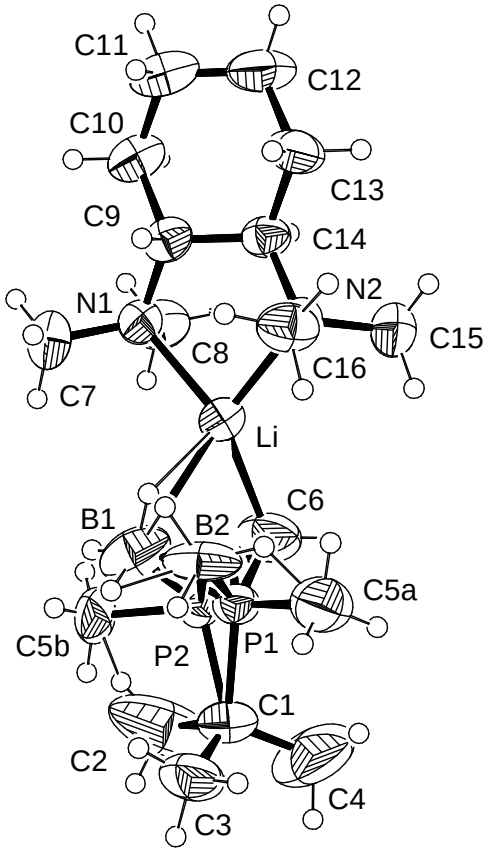


Abbildung 49 Thermische Auslenkungsellipsoide (25% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des (*R,R*)-TMCDA-Adduktes von lithiiertem Phosphinoboran **165** im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 145 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) des (*R,R*)-TMCDA-Adduktes von lithiiertem Phosphinoboran **165**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
B(1)	2300(5)	6901(6)	8263(4)	90(2)
B(2)	2388(19)	7870(30)	8225(15)	75(9)
C(1)	1004(3)	7569(3)	6485(2)	69(1)
C(2)	592(6)	6448(6)	6337(4)	175(4)
C(3)	2153(3)	7679(4)	5996(2)	89(1)
C(4)	186(5)	8378(6)	6127(4)	177(3)
C(6)	–58(3)	7561(4)	8394(2)	90(1)
C(7)	1801(4)	5324(3)	10444(3)	85(1)
C(8)	–154(3)	5857(3)	10648(3)	74(1)
C(9)	1383(2)	6767(2)	11523(2)	51(1)

C(10)	1099(3)	6137(3)	12396(2)	71(1)
C(11)	1518(4)	6736(3)	13247(2)	82(1)
C(12)	1008(4)	7833(4)	13298(2)	90(1)
C(13)	1301(4)	8473(3)	12436(2)	75(1)
C(14)	873(2)	7885(2)	11572(2)	51(1)
C(15)	254(3)	9374(3)	10630(3)	80(1)
C(16)	2251(3)	8893(3)	10619(2)	68(1)
C(5A)	1663(5)	9147(3)	7816(3)	101(2)
C(5B)	1370(30)	5839(17)	7535(19)	102(10)
Li	983(4)	7383(4)	9655(3)	57(1)
N(1)	1055(2)	6222(2)	10659(2)	53(1)
N(2)	1061(2)	8489(2)	10713(2)	50(1)
P(1)	1184(1)	7745(1)	7738(1)	49(1)
P(2)	1082(5)	7198(5)	7681(4)	44(1)

Tabelle 146 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) des (*R,R*)-TMCDA-Adduktes von lithiiertem Phosphinoboran **165**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2$ [$h^2a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	71(4)	120(5)	78(4)	31(4)	–16(3)	–13(3)
B(2)	35(12)	150(30)	35(11)	–2(15)	–7(9)	–27(16)
C(1)	78(2)	87(2)	42(1)	2(2)	–5(1)	–9(2)
C(2)	214(7)	204(7)	108(4)	–80(4)	57(4)	–132(6)
C(3)	111(3)	98(3)	58(2)	3(2)	31(2)	–1(3)
C(4)	137(5)	282(9)	113(4)	89(5)	12(4)	99(5)
C(6)	69(2)	140(4)	63(2)	3(2)	13(2)	16(3)
C(7)	107(3)	62(2)	87(3)	6(2)	0(2)	29(2)
C(8)	69(2)	85(2)	67(2)	3(2)	–10(2)	–21(2)
C(9)	38(2)	63(2)	51(2)	6(1)	–5(1)	–4(1)
C(10)	77(2)	77(2)	58(2)	17(2)	–8(2)	–6(2)
C(11)	86(3)	107(3)	52(2)	21(2)	–14(2)	–20(2)
C(12)	119(3)	110(3)	42(2)	7(2)	–2(2)	–12(3)
C(13)	101(3)	77(2)	45(2)	–8(2)	4(2)	–2(2)
C(14)	46(2)	64(2)	41(1)	3(1)	4(1)	–1(1)
C(15)	98(3)	70(2)	72(2)	6(2)	8(2)	31(2)
C(16)	76(2)	72(2)	55(2)	0(2)	4(2)	–22(2)
C(5A)	168(5)	62(2)	73(3)	2(2)	19(3)	–13(3)
C(5B)	160(30)	53(12)	91(18)	33(12)	51(19)	44(16)

Li	64(3)	58(3)	48(2)	4(2)	–4(2)	8(3)
N(1)	56(2)	52(1)	51(1)	4(1)	2(1)	4(1)
N(2)	53(1)	49(1)	48(1)	2(1)	1(1)	6(1)
P(1)	48(1)	59(1)	41(1)	4(1)	4(1)	2(1)
P(2)	51(3)	37(3)	45(3)	7(3)	2(2)	–5(3)

Tabelle 147 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) des (*R*,*R*)-TMCDA-Adduktes von lithiiertem Phosphinoboran **165**.

	x	y	z	U(eq)
H(0A)	2435	7139	8892	134
H(0B)	3012	6965	7911	134
H(0C)	2048	6151	8265	134
H(2A)	2621	7471	8768	112
H(2B)	2191	8611	8399	112
H(2C)	3021	7887	7785	112
H(2A)	–247	6433	6362	263
H(2B)	904	5981	6814	263
H(2C)	850	6194	5738	263
H(3A)	2073	7436	5363	134
H(3B)	2728	7239	6308	134
H(3C)	2394	8432	6003	134
H(4A)	338	9074	6414	266
H(4B)	–599	8153	6266	266
H(4C)	280	8442	5464	266
H(6A)	–493	6906	8231	109
H(6B)	–568	8197	8402	109
H(7A)	1658	4738	10875	128
H(7B)	2603	5552	10491	128
H(7C)	1645	5077	9821	128
H(8A)	–345	5581	10040	110
H(8B)	–659	6461	10796	110
H(8C)	–259	5286	11101	110
H(9)	2235	6856	11509	61
H(10A)	260	6030	12436	85
H(10B)	1467	5422	12368	85
H(11A)	1303	6325	13800	98
H(11B)	2364	6793	13231	98
H(12A)	1309	8212	13841	109

H(12B)	166	7777	13361	109
H(13A)	2141	8574	12398	89
H(13B)	939	9191	12471	89
H(14)	26	7794	11641	61
H(15A)	406	9903	11110	120
H(15B)	–530	9101	10694	120
H(15C)	343	9713	10031	120
H(16A)	2367	9166	9998	101
H(16B)	2792	8308	10738	101
H(16C)	2380	9473	11059	101
H(5A)	1061	9621	7584	151
H(5B)	2361	9242	7452	151
H(5C)	1825	9325	8455	151
H(5B1)	915	5421	7971	153
H(5B2)	2187	5706	7642	153
H(5B3)	1170	5625	6911	153

Abfangprodukt von lithiiertem Dimethyl(*tert*-Butyl)phosphinoboran mit Benzophenon 166

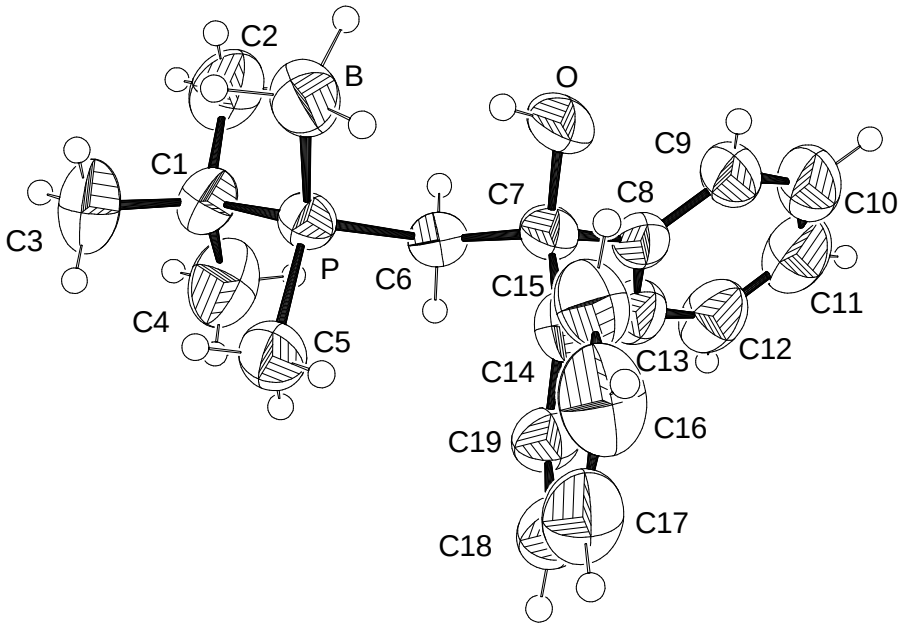


Abbildung 50 Thermische Auslenkungsellipsoide (25% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Abfangproduktes von lithiiertem Phosphinoboran **166** im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 148 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) des Abfangproduktes von lithiiertem Phosphinoboran **166**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
B	5498(4)	7526(2)	1409(2)	80(1)
C(1)	2251(4)	6072(1)	1187(1)	63(1)
C(2)	3483(5)	5515(2)	1699(2)	98(1)
C(3)	2935(5)	5896(2)	430(2)	93(1)
C(4)	82(4)	5854(2)	1270(2)	100(1)
C(5)	1488(5)	7867(2)	733(2)	72(1)
C(6)	1426(3)	7426(1)	2237(1)	53(1)
C(7)	1904(3)	8265(1)	2657(1)	54(1)
C(8)	793(4)	8272(1)	3362(1)	58(1)
C(9)	1728(4)	8557(1)	3969(1)	75(1)
C(10)	734(7)	8576(2)	4614(2)	98(1)
C(11)	–1200(7)	8301(2)	4656(2)	100(1)
C(12)	–2151(5)	8026(2)	4060(2)	88(1)
C(13)	–1170(4)	8009(1)	3416(1)	71(1)
C(14)	1376(3)	9085(1)	2227(1)	55(1)
C(15)	2750(4)	9736(1)	2110(1)	81(1)
C(16)	2259(7)	10466(2)	1704(2)	104(1)
C(17)	429(6)	10558(2)	1426(2)	97(1)
C(18)	–937(4)	9927(1)	1540(2)	81(1)
C(19)	–489(4)	9203(1)	1948(1)	65(1)
O	3939(2)	8264(1)	2840(1)	76(1)
P	2734(1)	7233(1)	1400(1)	50(1)

Tabelle 149 Anisotrope Auslenkungsparameter (Å^2 x 10^3) des Abfangproduktes von lithiiertem Phosphinoboran **166**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2$ [$h^2a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B	57(2)	113(2)	70(2)	–15(2)	10(2)	–12(1)
C(1)	68(2)	53(1)	67(2)	0(1)	14(1)	2(1)
C(2)	131(3)	68(1)	94(2)	17(1)	16(2)	25(2)
C(3)	131(3)	70(1)	79(2)	–14(1)	28(2)	–6(2)
C(4)	100(2)	73(1)	128(3)	–28(2)	18(2)	–27(1)
C(5)	88(2)	69(1)	60(2)	4(1)	–4(1)	9(1)
C(6)	49(1)	53(1)	57(1)	3(1)	–1(1)	2(1)

C(7)	45(1)	64(1)	55(1)	–5(1)	–6(1)	–1(1)
C(8)	66(1)	55(1)	53(1)	2(1)	–3(1)	11(1)
C(9)	95(2)	77(1)	53(2)	–3(1)	–12(1)	16(1)
C(10)	149(3)	92(2)	52(2)	0(1)	–11(2)	30(2)
C(11)	143(3)	91(2)	65(2)	15(1)	26(2)	34(2)
C(12)	101(2)	85(1)	78(2)	11(1)	29(2)	17(1)
C(13)	75(2)	74(1)	64(2)	0(1)	9(1)	7(1)
C(14)	63(1)	53(1)	50(1)	–9(1)	2(1)	–10(1)
C(15)	86(2)	75(1)	82(2)	–9(1)	0(2)	–29(1)
C(16)	144(3)	70(1)	99(2)	7(1)	15(2)	–41(2)
C(17)	147(3)	61(1)	82(2)	12(1)	8(2)	2(2)
C(18)	100(2)	67(1)	76(2)	5(1)	1(2)	16(1)
C(19)	66(2)	55(1)	75(2)	3(1)	–2(1)	2(1)
O	49(1)	109(1)	70(1)	–20(1)	–15(1)	2(1)
P	49(1)	53(1)	49(1)	2(1)	–1(1)	–2(1)

Tabelle 150 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) des Abfangproduktes von lithiiertem Phosphinoboran **166**.

	x	y	z	U(eq)
H(0A)	6030(50)	7273(19)	930(20)	128(11)
H(0B)	6200(40)	7245(17)	1905(19)	103(9)
H(0C)	5660(40)	8286(17)	1429(18)	111(9)
H(2A)	3071	5632	2186	147
H(2B)	4880	5660	1644	147
H(2C)	3283	4897	1591	147
H(3A)	2758	5278	320	140
H(3B)	4330	6049	384	140
H(3C)	2155	6248	101	140
H(4A)	–699	6229	958	151
H(4B)	–317	5948	1762	151
H(4C)	–137	5243	1142	151
H(5A)	210(50)	7752(18)	764(17)	102(10)
H(5B)	2090(40)	7693(15)	301(17)	92(8)
H(5C)	1790(40)	8508(16)	777(15)	86(7)
H(6A)	–4	7428	2134	63
H(6B)	1685	6924	2551	63
H(9)	3062	8742	3947	90
H(10)	1389	8779	5026	117

H(11)	–1866	8303	5098	120
H(12)	–3488	7845	4086	105
H(13)	–1846	7815	3006	85
H(15)	4033	9686	2306	97
H(16)	3222	10903	1623	125
H(17)	106	11058	1154	116
H(18)	–2212	9982	1338	97
H(19)	–1481	8782	2039	78
H(0)	4617	8174	2476	114

Monolithiiertes Dimethyl(*tert*-Butyl)phosphinoxid 167

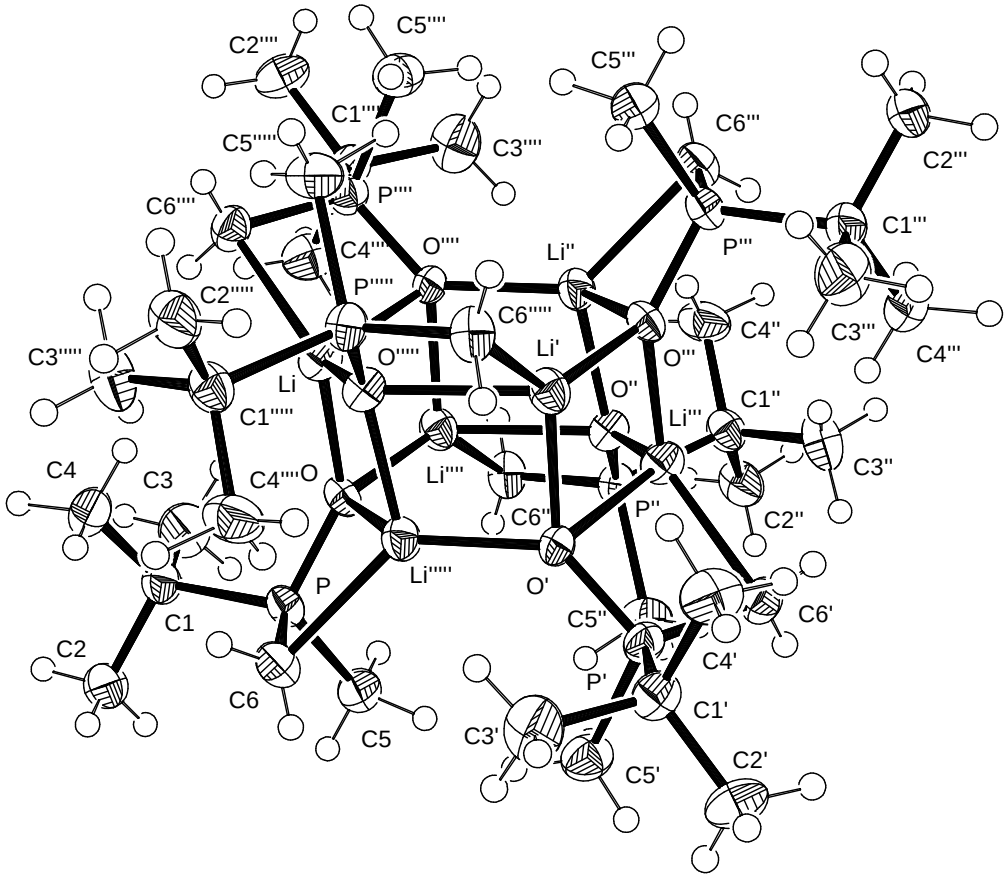


Abbildung 51 Thermische Auslenkungsellipsoide (25% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des α-lithiierten Phosphinoxids **167** im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 151 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) des des α-lithiierten Phosphinoxids **167**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
Li	5107(4)	7056(4)	1976(2)	29(1)
C(1)	7286(2)	7355(3)	933(1)	31(1)
C(2)	8155(3)	7929(4)	511(1)	40(1)
C(3)	6845(4)	5978(3)	953(2)	50(1)
C(4)	7966(3)	7983(4)	1391(1)	43(1)
C(5)	5242(3)	6875(3)	314(1)	38(1)
C(6)	6285(3)	9079(3)	865(1)	32(1)
O	5085(2)	6896(2)	1289(1)	25(1)
P	5975(1)	7605(1)	872(1)	27(1)

Tabelle 152 Anisotrope Auslenkungsparameter (Å^2 x 10^3) des α-lithiierten Phosphinoxids **167**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Li	32(2)	24(2)	32(2)	0(2)	–2(2)	16(2)
C(1)	28(1)	35(2)	35(2)	4(1)	2(1)	18(1)
C(2)	34(2)	59(2)	37(2)	7(2)	9(1)	30(2)
C(3)	51(2)	46(2)	65(3)	10(2)	4(2)	34(2)
C(4)	34(2)	59(2)	37(2)	–1(2)	–7(1)	23(2)
C(5)	34(2)	47(2)	30(2)	–1(1)	–2(1)	17(2)
C(6)	29(2)	28(2)	39(2)	5(1)	8(1)	15(1)
O	20(1)	22(1)	28(1)	0(1)	4(1)	7(1)
P	23(1)	27(1)	30(1)	2(1)	5(1)	12(1)

Tabelle 153 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) des α-lithiierten Phosphinoxids **167**.

	x	y	z	U(eq)
H(2A)	8840(30)	7830(30)	570(10)	35(8)
H(2B)	8460(30)	8790(40)	485(12)	61(11)
H(2C)	7780(30)	7570(30)	245(11)	34(8)
H(3A)	6370(30)	5510(30)	673(12)	50(10)
H(3B)	6260(40)	5540(30)	1192(13)	60(11)
H(3C)	7510(30)	5860(30)	1005(11)	56(10)
H(4A)	7450(30)	7720(30)	1648(13)	60(11)

H(4B)	8220(30)	8800(30)	1361(12)	50(10)
H(4C)	8750(30)	7890(30)	1416(11)	60(10)
H(5A)	4600(40)	7080(40)	221(15)	96(14)
H(5B)	5730(30)	7150(40)	63(14)	66(12)
H(5C)	4870(30)	6030(30)	346(12)	54(10)
H(6B)	6280(30)	9320(30)	610(13)	48(11)
H(6A)	6900(30)	9610(30)	1058(11)	43(9)

Diliithiierten Phosphinoboran (170)

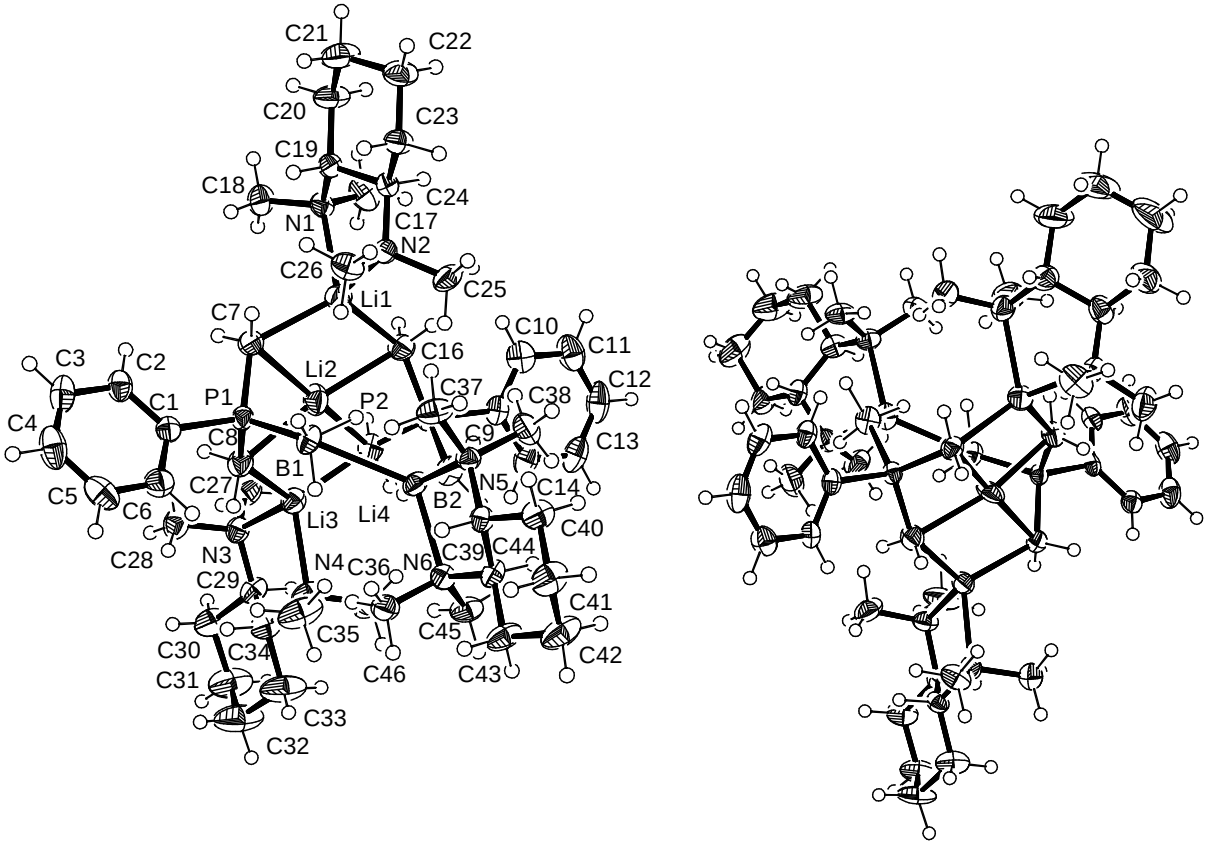


Abbildung 52 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des diliithiierten Phosphinoboran **170** im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 154 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) von diliithiiertem Phosphinoboran **170**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
B(1)	8020(4)	8785(4)	7711(3)	35(1)
B(2)	7192(4)	6673(4)	7061(4)	38(1)
B(3)	2367(4)	337(4)	3372(3)	32(1)
B(4)	3063(4)	2510(4)	4029(3)	36(1)
C(1)	7724(3)	9482(3)	9433(3)	29(1)
C(2)	7078(4)	10281(3)	9985(3)	36(1)
C(3)	7574(4)	10699(4)	10328(3)	46(1)
C(4)	8723(5)	10323(4)	10119(3)	52(1)
C(5)	9392(4)	9521(4)	9568(3)	49(1)
C(6)	8890(4)	9112(3)	9227(3)	40(1)
C(7)	5661(3)	9687(3)	9085(3)	33(1)
C(8)	6986(4)	7745(3)	9609(3)	37(1)
C(9)	5063(3)	6336(3)	7348(3)	32(1)
C(10)	4100(4)	6885(4)	7126(3)	44(1)
C(11)	3685(4)	6433(4)	6742(3)	54(1)
C(12)	4238(4)	5403(4)	6571(3)	55(1)
C(13)	5192(4)	4848(4)	6787(3)	49(1)
C(14)	5598(4)	5302(3)	7167(3)	41(1)
C(15)	5560(4)	6389(3)	8974(3)	35(1)
C(16)	4813(4)	8252(3)	7976(3)	36(1)
C(17)	2326(4)	10484(4)	8494(3)	48(1)
C(18)	2691(4)	11072(4)	9545(3)	43(1)
C(19)	3179(3)	11842(3)	7992(2)	29(1)
C(20)	2049(4)	12710(3)	8030(3)	49(1)
C(21)	2207(4)	13667(3)	7400(3)	59(1)
C(22)	2853(4)	13375(3)	6444(3)	47(1)
C(23)	4003(3)	12560(3)	6381(3)	36(1)
C(24)	3903(3)	11585(3)	7016(2)	28(1)
C(25)	5485(4)	10185(3)	6191(3)	41(1)
C(26)	5846(3)	11163(3)	6969(3)	40(1)
C(27)	5167(4)	5530(4)	11389(3)	48(1)
C(28)	6458(4)	6073(3)	11596(3)	44(1)
C(29)	7152(3)	4415(3)	10963(2)	35(1)
C(30)	7234(4)	3812(3)	11860(3)	48(1)
C(31)	8070(4)	2708(4)	11749(3)	71(2)
C(32)	9229(5)	2716(5)	11130(4)	85(2)
C(33)	9162(4)	3268(4)	10227(4)	71(2)
C(34)	8327(3)	4379(3)	10305(3)	39(1)
C(35)	9209(4)	5343(4)	8968(4)	63(1)
C(36)	8221(5)	4375(4)	8828(3)	64(2)
C(37)	8853(4)	9520(3)	5335(3)	42(1)

C(38)	8467(4)	8362(4)	4765(3)	43(1)
C(39)	10365(3)	7879(3)	4850(2)	28(1)
C(40)	10836(4)	8123(3)	3826(3)	39(1)
C(41)	12110(4)	7580(3)	3430(3)	49(1)
C(42)	12411(4)	6418(3)	3663(3)	57(1)
C(43)	11976(4)	6186(3)	4679(3)	44(1)
C(44)	10689(3)	6723(3)	5083(2)	31(1)
C(45)	10127(4)	5414(3)	6233(3)	39(1)
C(46)	10844(3)	6504(3)	6574(3)	37(1)
C(47)	2660(3)	–408(3)	1672(2)	27(1)
C(48)	1501(3)	–18(3)	1858(3)	34(1)
C(49)	994(4)	–426(4)	1525(3)	46(1)
C(50)	1638(4)	–1238(4)	1000(3)	49(1)
C(51)	2794(4)	–1634(3)	787(3)	47(1)
C(52)	3314(4)	–1227(3)	1124(3)	32(1)
C(53)	4733(3)	–602(3)	2009(3)	32(1)
C(54)	3382(4)	1348(3)	1505(3)	33(1)
C(55)	5233(3)	2759(3)	3793(2)	28(1)
C(56)	4704(3)	3798(3)	3957(2)	32(1)
C(57)	5143(4)	4248(3)	4330(3)	42(1)
C(58)	6097(4)	3668(4)	4545(3)	49(1)
C(59)	6631(4)	2651(4)	4377(3)	42(1)
C(60)	6200(3)	2195(3)	4005(2)	31(1)
C(61)	4784(4)	2693(3)	2165(3)	31(1)
C(62)	5412(4)	849(3)	3217(3)	38(1)
C(63)	4840(4)	3950(4)	–79(3)	53(1)
C(64)	4542(4)	2716(4)	–608(3)	57(1)
C(65)	2927(3)	4245(3)	–21(2)	41(1)
C(66)	3039(4)	4954(4)	–913(3)	65(1)
C(67)	1880(5)	5716(6)	–942(4)	110(3)
C(68)	1278(7)	6354(6)	–165(4)	131(4)
C(69)	1119(5)	5655(5)	726(4)	93(2)
C(70)	2266(4)	4908(3)	787(3)	47(1)
C(71)	1266(4)	3834(4)	1965(4)	60(1)
C(72)	2045(5)	4805(4)	2357(3)	60(1)
C(73)	8131(3)	–1088(3)	2413(3)	40(1)
C(74)	7587(4)	–2050(3)	1767(3)	44(1)
C(75)	7470(3)	–2462(3)	3362(2)	30(1)
C(76)	8556(3)	–3403(3)	3133(3)	47(1)
C(77)	8638(3)	–4192(3)	3940(3)	55(1)
C(78)	7606(4)	–4517(3)	4343(3)	50(1)
C(79)	6551(4)	–3591(3)	4590(3)	43(1)

C(80)	6423(3)	–2788(3)	3792(2)	30(1)
C(81)	4406(4)	–2173(4)	4110(4)	57(1)
C(82)	5139(4)	–1402(3)	4777(3)	55(1)
C(83)	–511(4)	2631(4)	4331(3)	47(1)
C(84)	155(3)	3428(3)	5036(3)	39(1)
C(85)	–528(3)	2005(3)	5876(3)	36(1)
C(86)	–1645(4)	2780(4)	6420(3)	60(1)
C(87)	–2200(4)	2261(4)	7332(3)	73(2)
C(88)	–1397(4)	1781(4)	7862(3)	66(1)
C(89)	–305(4)	983(4)	7331(3)	49(1)
C(90)	277(3)	1469(3)	6408(2)	33(1)
C(91)	2241(4)	469(5)	6234(3)	65(2)
C(92)	1263(4)	–200(3)	5742(3)	48(1)
Li(1)	4761(6)	9755(5)	8199(4)	35(2)
Li(2)	5720(7)	8021(6)	8941(5)	44(2)
Li(3)	6707(6)	6279(5)	9675(4)	33(2)
Li(4)	8558(5)	7604(5)	6578(4)	30(1)
Li(5)	3661(6)	2819(5)	1437(5)	37(2)
Li(6)	4613(6)	1061(5)	2199(5)	41(2)
Li(7)	5580(6)	–676(5)	2921(4)	33(2)
Li(8)	1791(6)	1484(5)	4508(4)	35(2)
N(1)	3069(3)	10901(2)	8593(2)	29(1)
N(2)	5003(2)	10771(2)	6977(2)	29(1)
N(3)	6339(3)	5485(2)	11034(2)	32(1)
N(4)	8267(3)	4970(3)	9431(2)	44(1)
N(5)	9120(2)	8427(2)	5271(2)	28(1)
N(6)	10200(3)	6451(2)	6068(2)	29(1)
N(7)	4008(3)	3487(2)	48(2)	32(1)
N(8)	2193(3)	4244(3)	1642(2)	40(1)
N(9)	7369(3)	–1647(2)	2604(2)	31(1)
N(10)	5363(3)	–1887(2)	3986(2)	35(1)
N(11)	55(3)	2457(2)	4981(2)	33(1)
N(12)	1360(3)	746(2)	5852(2)	32(1)
P(1)	7073(1)	8918(1)	8970(1)	28(1)
P(2)	5633(1)	6939(1)	7859(1)	30(1)
P(3)	3320(1)	162(1)	2124(1)	25(1)
P(4)	4642(1)	2177(1)	3285(1)	26(1)

Tabelle 155 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) von diliithiiertem Phosphinoboran **170**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	37(3)	38(3)	27(2)	–10(2)	–3(2)	–13(2)
B(2)	31(3)	44(3)	39(3)	–10(2)	–3(2)	–19(2)
B(3)	39(3)	33(3)	30(2)	–7(2)	–11(2)	–15(2)
B(4)	39(3)	40(3)	34(3)	–2(2)	–7(2)	–24(2)
C(1)	40(2)	23(2)	28(2)	4(2)	–15(2)	–14(2)
C(2)	47(3)	39(2)	27(2)	0(2)	–13(2)	–21(2)
C(3)	71(4)	48(3)	30(2)	–2(2)	–16(2)	–33(3)
C(4)	81(4)	62(3)	41(3)	8(2)	–28(3)	–51(3)
C(5)	47(3)	57(3)	53(3)	13(2)	–28(2)	–28(2)
C(6)	42(3)	37(2)	42(3)	–2(2)	–16(2)	–13(2)
C(7)	35(2)	30(2)	28(2)	–2(2)	–10(2)	–9(2)
C(8)	45(3)	30(2)	38(3)	–4(2)	–16(2)	–15(2)
C(9)	35(2)	39(2)	24(2)	–2(2)	–3(2)	–23(2)
C(10)	44(3)	51(3)	41(3)	–1(2)	–10(2)	–26(2)
C(11)	49(3)	80(4)	47(3)	–3(3)	–19(2)	–36(3)
C(12)	68(4)	82(4)	38(3)	–15(3)	–9(3)	–53(3)
C(13)	59(3)	51(3)	41(3)	–15(2)	–3(2)	–32(3)
C(14)	44(3)	43(3)	39(2)	–11(2)	–7(2)	–23(2)
C(15)	41(3)	34(2)	31(2)	–1(2)	–10(2)	–18(2)
C(16)	41(3)	29(2)	43(3)	–2(2)	–17(2)	–14(2)
C(17)	49(3)	59(3)	40(2)	9(2)	–18(2)	–29(2)
C(18)	48(3)	49(3)	24(2)	–2(2)	–7(2)	–16(2)
C(19)	34(2)	28(2)	22(2)	1(1)	–8(2)	–10(2)
C(20)	39(2)	40(2)	29(2)	6(2)	1(2)	5(2)
C(21)	56(3)	37(2)	43(2)	3(2)	–5(2)	7(2)
C(22)	45(2)	37(2)	37(2)	8(2)	–11(2)	–4(2)
C(23)	29(2)	37(2)	25(2)	1(2)	–4(2)	–3(2)
C(24)	31(2)	30(2)	26(2)	–2(1)	–12(2)	–10(2)
C(25)	46(2)	30(2)	28(2)	–6(2)	–2(2)	–5(2)
C(26)	36(2)	39(2)	44(2)	5(2)	–16(2)	–14(2)
C(27)	39(2)	47(3)	49(3)	–11(2)	–3(2)	–15(2)
C(28)	61(3)	37(2)	37(2)	–3(2)	–16(2)	–21(2)
C(29)	41(2)	26(2)	33(2)	–1(2)	–6(2)	–15(2)
C(30)	49(3)	38(2)	34(2)	6(2)	0(2)	–13(2)
C(31)	66(3)	50(3)	53(3)	21(2)	–3(3)	–8(2)
C(32)	58(3)	62(4)	74(4)	21(3)	–4(3)	6(3)
C(33)	46(3)	58(3)	53(3)	16(2)	6(2)	2(2)
C(34)	37(2)	32(2)	34(2)	4(2)	–4(2)	–10(2)

C(35)	45(3)	45(3)	60(3)	1(2)	14(2)	–14(2)
C(36)	69(4)	50(3)	45(3)	–16(2)	–9(3)	3(3)
C(37)	35(2)	27(2)	50(3)	1(2)	–8(2)	–6(2)
C(38)	41(2)	58(3)	35(2)	–1(2)	–18(2)	–18(2)
C(39)	30(2)	29(2)	26(2)	–2(1)	–8(2)	–12(2)
C(40)	43(2)	32(2)	31(2)	7(2)	–6(2)	–15(2)
C(41)	50(3)	43(2)	33(2)	3(2)	3(2)	–18(2)
C(42)	57(3)	37(2)	44(3)	–4(2)	7(2)	–8(2)
C(43)	39(2)	30(2)	36(2)	–2(2)	5(2)	–5(2)
C(44)	37(2)	27(2)	24(2)	–6(1)	–5(2)	–12(2)
C(45)	41(2)	22(2)	41(2)	6(2)	–10(2)	–9(2)
C(46)	32(2)	40(2)	30(2)	–2(2)	–9(2)	–7(2)
C(47)	38(2)	27(2)	19(2)	7(2)	–12(2)	–18(2)
C(48)	42(2)	37(2)	28(2)	4(2)	–18(2)	–17(2)
C(49)	42(3)	64(3)	42(3)	2(2)	–16(2)	–28(2)
C(50)	67(3)	60(3)	47(3)	5(2)	–32(3)	–41(3)
C(51)	75(4)	40(3)	41(3)	–5(2)	–24(3)	–28(3)
C(52)	43(2)	27(2)	27(2)	2(2)	–13(2)	–14(2)
C(53)	36(2)	30(2)	30(2)	–6(2)	–12(2)	–9(2)
C(54)	47(3)	28(2)	31(2)	5(2)	–16(2)	–20(2)
C(55)	34(2)	34(2)	19(2)	–1(2)	–5(2)	–20(2)
C(56)	41(2)	31(2)	25(2)	–3(2)	–6(2)	–19(2)
C(57)	52(3)	40(3)	36(2)	–12(2)	–3(2)	–24(2)
C(58)	62(3)	65(3)	37(3)	–10(2)	–9(2)	–46(3)
C(59)	38(2)	55(3)	41(3)	–3(2)	–15(2)	–23(2)
C(60)	35(2)	39(2)	25(2)	–6(2)	–9(2)	–17(2)
C(61)	35(2)	27(2)	32(2)	–5(2)	–10(2)	–11(2)
C(62)	48(3)	32(2)	41(3)	–4(2)	–22(2)	–15(2)
C(63)	53(3)	60(3)	58(3)	8(2)	–23(2)	–32(2)
C(64)	79(3)	50(3)	33(2)	–7(2)	–11(2)	–22(3)
C(65)	41(2)	51(2)	30(2)	3(2)	–12(2)	–20(2)
C(66)	56(3)	78(4)	41(3)	9(2)	–18(2)	–9(3)
C(67)	69(4)	150(6)	46(3)	36(4)	–19(3)	0(4)
C(68)	96(5)	118(6)	59(4)	35(4)	–14(4)	42(4)
C(69)	77(4)	71(4)	58(4)	11(3)	–16(3)	26(3)
C(70)	51(3)	37(2)	38(2)	3(2)	–11(2)	–7(2)
C(71)	42(3)	63(3)	54(3)	–5(2)	–4(2)	–9(2)
C(72)	71(4)	49(3)	46(3)	–15(2)	–23(3)	1(3)
C(73)	37(2)	41(2)	45(2)	12(2)	–18(2)	–20(2)
C(74)	47(3)	46(3)	35(2)	–5(2)	–14(2)	–12(2)
C(75)	34(2)	25(2)	34(2)	2(2)	–18(2)	–11(2)
C(76)	34(2)	35(2)	63(3)	4(2)	–13(2)	–12(2)

C(77)	34(2)	29(2)	83(3)	17(2)	–23(2)	–1(2)
C(78)	43(3)	29(2)	73(3)	16(2)	–23(2)	–13(2)
C(79)	42(2)	30(2)	51(3)	14(2)	–15(2)	–17(2)
C(80)	35(2)	27(2)	33(2)	–2(2)	–15(2)	–12(2)
C(81)	29(2)	55(3)	72(3)	23(2)	–19(2)	–14(2)
C(82)	65(3)	30(2)	38(2)	–4(2)	–8(2)	4(2)
C(83)	38(2)	54(3)	48(3)	–3(2)	–21(2)	–8(2)
C(84)	34(2)	26(2)	44(2)	9(2)	–7(2)	–10(2)
C(85)	33(2)	29(2)	42(2)	–1(2)	–6(2)	–15(2)
C(86)	37(3)	49(3)	56(3)	2(2)	5(2)	–5(2)
C(87)	45(3)	62(3)	59(3)	5(3)	19(2)	–10(3)
C(88)	71(3)	59(3)	36(2)	–5(2)	15(2)	–24(3)
C(89)	55(3)	49(3)	29(2)	–3(2)	–1(2)	–20(2)
C(90)	41(2)	34(2)	28(2)	–5(2)	–8(2)	–20(2)
C(91)	50(3)	104(4)	39(3)	–9(3)	–19(2)	–23(3)
C(92)	63(3)	28(2)	37(2)	–2(2)	–8(2)	–11(2)
Li(1)	40(4)	28(4)	35(4)	0(3)	–13(3)	–10(3)
Li(2)	57(5)	43(4)	42(4)	–6(3)	–22(4)	–22(4)
Li(3)	36(4)	33(4)	29(4)	–2(3)	–8(3)	–13(3)
Li(4)	35(4)	21(3)	28(3)	–4(3)	–8(3)	–6(3)
Li(5)	51(4)	25(3)	36(4)	4(3)	–17(3)	–15(3)
Li(6)	53(4)	26(4)	50(4)	12(3)	–35(4)	–11(3)
Li(7)	39(4)	29(3)	35(4)	–1(3)	–20(3)	–10(3)
Li(8)	33(4)	44(4)	34(4)	–3(3)	–9(3)	–24(3)
N(1)	30(2)	34(2)	20(2)	3(1)	–7(1)	–12(1)
N(2)	27(2)	31(2)	24(2)	–4(1)	–7(1)	–8(1)
N(3)	35(2)	33(2)	27(2)	–3(1)	–7(2)	–14(2)
N(4)	43(2)	35(2)	33(2)	1(2)	1(2)	–8(2)
N(5)	28(2)	25(2)	30(2)	–2(1)	–12(1)	–8(1)
N(6)	35(2)	26(2)	25(2)	3(1)	–10(1)	–13(1)
N(7)	40(2)	28(2)	28(2)	–4(1)	–6(2)	–16(2)
N(8)	44(2)	38(2)	30(2)	–4(2)	–8(2)	–11(2)
N(9)	37(2)	29(2)	29(2)	–1(1)	–14(2)	–12(1)
N(10)	29(2)	30(2)	36(2)	4(1)	–12(1)	–6(1)
N(11)	31(2)	26(2)	37(2)	0(1)	–9(1)	–11(1)
N(12)	29(2)	38(2)	31(2)	–1(1)	–11(1)	–15(2)
P(1)	36(1)	23(1)	28(1)	–2(1)	–13(1)	–11(1)
P(2)	33(1)	31(1)	31(1)	–4(1)	–8(1)	–17(1)
P(3)	33(1)	24(1)	23(1)	–2(1)	–12(1)	–12(1)
P(4)	31(1)	24(1)	27(1)	–2(1)	–11(1)	–13(1)

Tabelle 156 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) von diliithiiertem Phosphinoboran **170**.

	x	y	z	U(eq)
H(1A)	8740(30)	8100(30)	7650(30)	35(10)
H(1B)	8280(30)	9480(30)	7420(30)	41(11)
H(1C)	7480(30)	8700(30)	7330(30)	40(11)
H(2A)	7180(30)	7260(30)	6470(20)	25(9)
H(2B)	7550(50)	5930(50)	6800(40)	92(18)
H(2C)	7650(40)	6660(30)	7530(30)	56(13)
H(3A)	2020(40)	–220(30)	3620(30)	48(12)
H(3B)	1570(40)	1170(40)	3420(30)	78(16)
H(3C)	2950(30)	380(30)	3710(20)	22(9)
H(4A)	2620(30)	2360(30)	3680(20)	30(10)
H(4B)	2660(40)	3370(30)	4180(30)	51(12)
H(4C)	3010(40)	1990(30)	4660(30)	51(12)
H(2)	6281	10548	10133	43
H(3)	7115	11246	10707	55
H(4)	9062	10610	10352	63
H(5)	10189	9254	9426	58
H(6)	9351	8567	8846	48
H(10)	3713	7590	7240	53
H(11)	3022	6827	6595	65
H(12)	3957	5088	6307	66
H(13)	5575	4143	6673	58
H(14)	6262	4903	7312	49
H(17A)	2342	9845	8886	71
H(17B)	2581	10341	7866	71
H(17C)	1552	10985	8662	71
H(18A)	1944	11615	9711	64
H(18B)	3230	11280	9639	64
H(18C)	2646	10433	9920	64
H(19)	3596	12115	8201	35
H(20A)	1626	12906	8656	59
H(20B)	1592	12455	7860	59
H(21A)	1460	14203	7439	71
H(21B)	2627	13950	7585	71
H(22A)	2948	13991	6036	56
H(22B)	2423	13106	6255	56
H(23A)	4444	12847	6537	43
H(23B)	4417	12370	5753	43

H(24)	3497	11294	6812	34
H(25A)	4927	9934	6179	62
H(25B)	6162	9597	6228	62
H(25C)	5690	10630	5640	62
H(26A)	6094	11546	6387	61
H(26B)	6498	10583	7063	61
H(26C)	5506	11620	7452	61
H(27A)	5050	5188	10998	72
H(27B)	4659	6251	11408	72
H(27C)	5004	5181	11998	72
H(28A)	5967	6794	11552	66
H(28B)	7246	6031	11386	66
H(28C)	6241	5784	12224	66
H(29)	6882	4044	10700	42
H(30A)	7470	4173	12155	58
H(30B)	6476	3798	12260	58
H(31A)	8105	2356	12344	85
H(31B)	7813	2326	11493	85
H(32A)	9769	2000	11049	102
H(32B)	9502	3070	11398	102
H(33A)	8928	2886	9950	85
H(33B)	9922	3272	9824	85
H(34)	8601	4740	10574	46
H(35A)	9911	4760	8756	94
H(35B)	9272	5692	9385	94
H(35C)	9076	5827	8453	94
H(36A)	8045	4832	8313	97
H(36B)	7633	4071	9158	97
H(36C)	8954	3825	8611	97
H(37A)	9172	9580	5753	63
H(37B)	8031	9869	5556	63
H(37C)	9180	9841	4739	63
H(38A)	7659	8609	5122	64
H(38B)	8705	7645	4647	64
H(38C)	8604	8790	4192	64
H(39)	10748	8120	5121	34
H(40A)	10459	7912	3535	47
H(40B)	10657	8876	3691	47
H(41A)	12499	7836	3676	59
H(41B)	12369	7732	2768	59
H(42A)	12067	6154	3382	69
H(42B)	13241	6070	3425	69

H(43A)	12354	6419	4954	52
H(43B)	12169	5433	4825	52
H(44)	10344	6479	4779	37
H(45A)	9652	5399	5926	59
H(45B)	9795	5252	6882	59
H(45C)	10887	4904	6002	59
H(46A)	11578	5940	6431	55
H(46B)	10423	6441	7220	55
H(46C)	10963	7165	6408	55
H(48)	1045	543	2222	41
H(49)	198	–144	1660	56
H(50)	1285	–1528	783	59
H(51)	3240	–2184	410	56
H(52)	4111	–1506	981	39
H(56)	4039	4201	3814	38
H(57)	4782	4956	4435	51
H(58)	6388	3972	4810	58
H(59)	7299	2254	4516	51
H(60)	6574	1488	3895	38
H(63A)	5058	4269	–697	80
H(63B)	5510	3415	30	80
H(63C)	4506	4476	346	80
H(64A)	4011	2383	–535	85
H(64B)	5224	2196	–508	85
H(64C)	4745	3053	–1220	85
H(65)	2461	3849	6	49
H(66A)	3521	5341	–975	78
H(66B)	3411	4525	–1428	78
H(67A)	1983	6169	–1510	132
H(67B)	1418	5330	–931	132
H(68A)	530	6833	–193	158
H(68B)	1718	6768	–191	158
H(69A)	711	6085	1241	111
H(69B)	656	5259	760	111
H(70)	2711	5334	743	57
H(71A)	539	4394	2168	90
H(71B)	1351	3308	2468	90
H(71C)	1294	3526	1474	90
H(72A)	2695	5022	2184	90
H(72B)	1991	4355	2918	90
H(72C)	1352	5413	2444	90
H(73A)	7977	–799	2961	61

H(73B)	8009	–530	1940	61
H(73C)	8916	–1561	2211	61
H(74A)	7441	–1475	1311	66
H(74B)	7089	–2434	1888	66
H(74C)	8377	–2508	1544	66
H(75)	7487	–2142	3838	36
H(76A)	8588	–3733	2647	56
H(76B)	9214	–3175	2903	56
H(77A)	9330	–4804	3749	66
H(77B)	8694	–3891	4402	66
H(78A)	7588	–4875	3900	60
H(78B)	7651	–5000	4885	60
H(79A)	6554	–3267	5064	52
H(79B)	5889	–3816	4846	52
H(80)	6427	–3145	3330	36
H(81A)	4594	–2562	3611	85
H(81B)	3742	–1549	4123	85
H(81C)	4239	–2600	4680	85
H(82A)	4912	–1844	5324	82
H(82B)	4530	–731	4803	82
H(82C)	5825	–1309	4731	82
H(83A)	–1288	3114	4556	71
H(83B)	–521	1976	4253	71
H(83C)	–99	2920	3751	71
H(84A)	602	3659	4442	59
H(84B)	529	3316	5469	59
H(84C)	–601	3954	5234	59
H(85)	–721	1459	5757	43
H(86A)	–2166	3063	6073	71
H(86B)	–1497	3359	6523	71
H(87A)	–2900	2779	7683	88
H(87B)	–2407	1722	7230	88
H(88A)	–1765	1447	8444	79
H(88B)	–1219	2325	7990	79
H(89A)	–479	415	7241	59
H(89B)	214	690	7680	59
H(90)	464	2018	6532	40
H(91A)	2313	1096	6309	97
H(91B)	2961	45	5828	97
H(91C)	2042	79	6821	97
H(92A)	1018	–566	6334	72
H(92B)	1999	–642	5370	72

H(92C)	707	–23	5448	72
H(54B)	3870(40)	1170(40)	970(30)	55(15)
H(53A)	5220(40)	–630(40)	1310(40)	64(15)
H(62A)	6180(50)	750(40)	2890(40)	66(16)
H(8B)	6560(40)	7890(30)	10230(30)	47(12)
H(54A)	2540(40)	1770(30)	1650(30)	33(11)
H(8A)	7780(40)	7300(30)	9580(30)	34(11)
H(15A)	4720(40)	6520(30)	9310(30)	43(12)
H(7A)	5660(30)	10380(30)	8730(30)	37(11)
H(53B)	4810(30)	–1260(30)	2240(20)	26(10)
H(7B)	5250(30)	9740(30)	9700(30)	20(9)
H(15B)	5990(40)	5590(40)	8880(30)	53(13)
H(62B)	5260(30)	600(30)	3800(30)	40(11)
H(61A)	5550(40)	2560(30)	1850(30)	32(11)
H(16A)	4050(40)	8310(30)	8290(30)	40(12)
H(161)	4310(30)	3370(30)	2200(20)	20(9)
H(16B)	4710(30)	8570(30)	7440(30)	38(11)

Kupplungsprodukt 173 des dilithiiertem Phosphinoborans

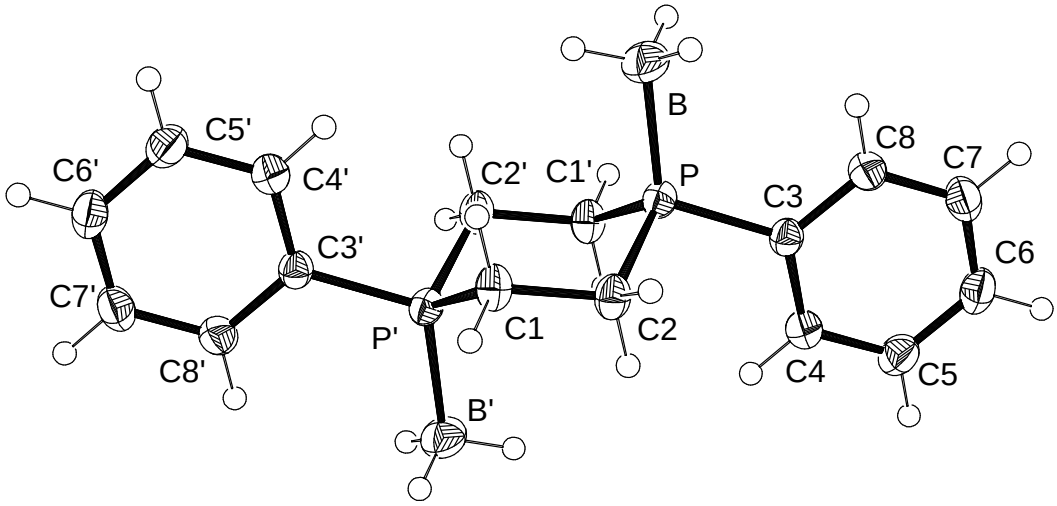


Abbildung 53 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) des Kupplungsproduktes von dilithiiertem Phosphinoboran **173** im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 157 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) des Kupplungsproduktes von dilithiiertem Phosphinoboran **173**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
B	11609(3)	3635(3)	7566(2)	39(1)
C(1)	12087(2)	5173(2)	11601(2)	28(1)
C(2)	10711(2)	3245(2)	10625(2)	28(1)
C(3)	7602(2)	934(2)	7637(2)	24(1)
C(4)	5912(2)	448(2)	8150(2)	29(1)
C(5)	4431(2)	–1238(2)	7450(2)	34(1)
C(6)	4623(3)	–2451(2)	6243(2)	34(1)
C(7)	6289(3)	–1989(2)	5728(2)	34(1)
C(8)	7776(2)	-301(2)	6417(2)	29(1)
P	9516(1)	3145(1)	8504(1)	24(1)

Tabelle 158 Anisotrope Auslenkungsparameter (Å^2 x 10^3) des Kupplungsproduktes von dilithiiertem Phosphinoboran **173**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2$ [$h^2a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B	34(1)	40(1)	47(1)	11(1)	23(1)	6(1)
C(1)	26(1)	23(1)	30(1)	5(1)	4(1)	7(1)
C(2)	29(1)	21(1)	29(1)	6(1)	5(1)	7(1)
C(3)	26(1)	21(1)	25(1)	6(1)	8(1)	6(1)
C(4)	31(1)	27(1)	30(1)	4(1)	12(1)	6(1)
C(5)	31(1)	31(1)	37(1)	9(1)	12(1)	2(1)
C(6)	38(1)	23(1)	31(1)	5(1)	5(1)	1(1)
C(7)	45(1)	26(1)	28(1)	2(1)	11(1)	9(1)
C(8)	34(1)	27(1)	28(1)	6(1)	13(1)	8(1)
P	23(1)	21(1)	28(1)	6(1)	9(1)	5(1)

Tabelle 159 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) des Kupplungsproduktes von dilithiiertem Phosphinoboran **173**.

	x	y	z	U(eq)
H(0A)	12390	2672	7615	58
H(0B)	12625	4824	8151	58
H(0C)	10884	3660	6452	58
H(1A)	13232	5554	11196	33

H(1B)	12790	5137	12727	33
H(2A)	9551	2874	11018	34
H(2B)	11622	2363	10785	34
H(4)	5777	1276	8981	35
H(5)	3283	–1561	7800	41
H(6)	3607	–3606	5767	41
H(7)	6418	–2827	4900	41
H(8)	8916	15	6057	35

Dilithiiertes Phosphorsulfid 174

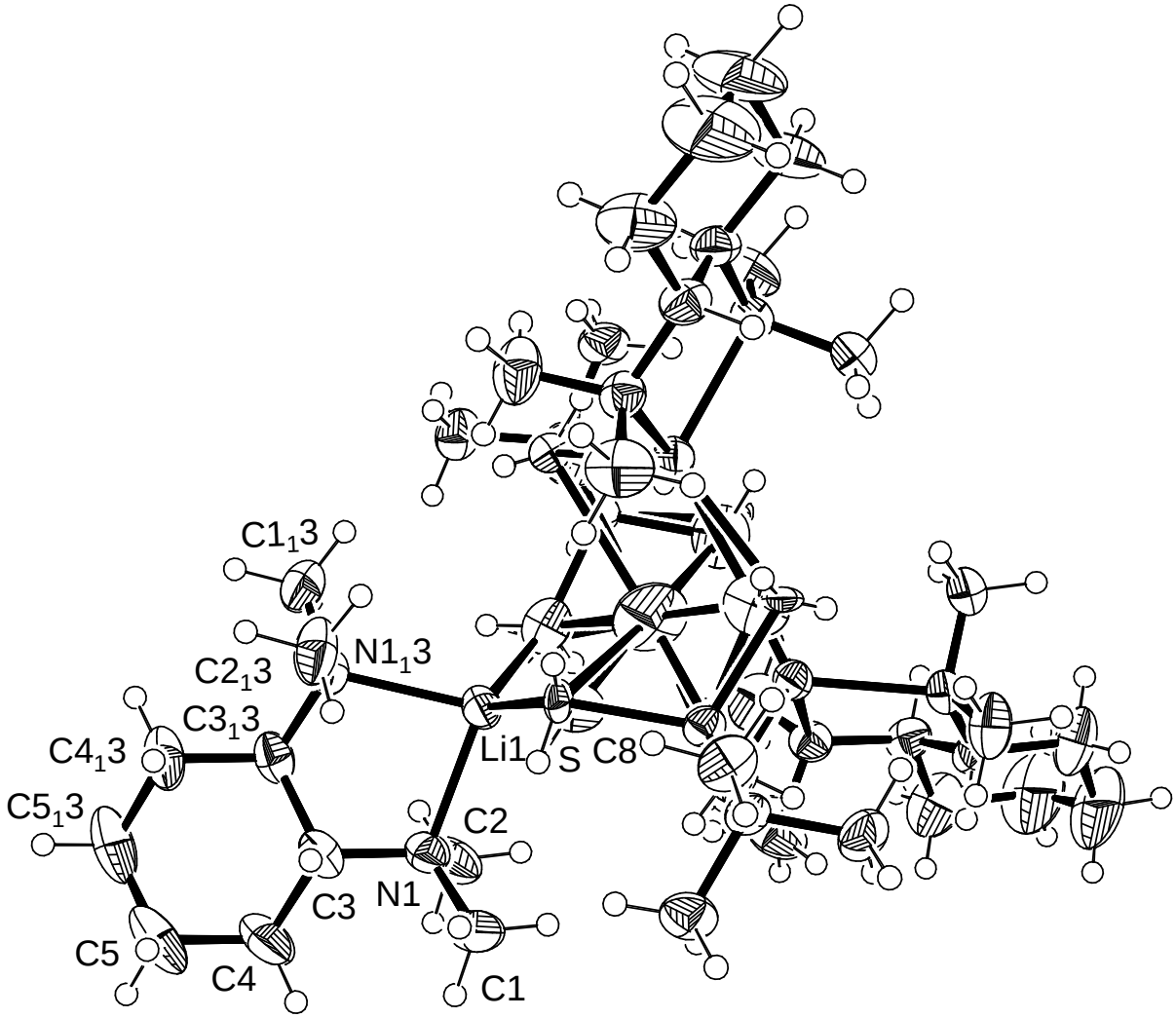


Abbildung 54 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des dilithiierten Phosphinsulfids **174** im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 160 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) des dilithiierten Phosphinsulfids **174**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
Li(1)	2676(3)	5176(3)	1250	35(2)
P(1)	4577(1)	5423(1)	423(1)	31(1)
S	4001(3)	4742(4)	1133(4)	26(1)
C(6)	5201(2)	4799(2)	–201(2)	32(1)
N(1)	2018(1)	4518(2)	432(1)	38(1)
C(3)	1623(2)	3884(2)	839(2)	41(1)
C(7)	5757(2)	4334(2)	304(2)	48(1)
C(2)	1497(2)	5136(2)	184(2)	59(1)
C(1)	2446(2)	4222(2)	–238(2)	59(1)
C(4)	928(3)	3534(3)	413(3)	72(1)
C(5)	590(3)	2850(3)	849(3)	108(2)
Li(2)	3750	6250	1250	92(6)
C(8)	3951(9)	4901(9)	1018(10)	67(6)

Tabelle 161 Anisotrope Auslenkungsparameter (Å^2 x 10^3) des dilithiierten Phosphinsulfids **174**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Li(1)	33(2)	33(2)	38(4)	4(2)	–4(2)	–4(3)
P(1)	31(1)	31(1)	31(1)	–5(1)	5(1)	5(1)
S	17(2)	30(2)	31(2)	2(2)	10(2)	–3(1)
C(6)	32(1)	32(1)	32(1)	–7(1)	7(1)	7(1)
N(1)	37(1)	39(1)	38(1)	–2(1)	–6(1)	–3(1)
C(3)	35(2)	32(2)	57(2)	–6(2)	0(1)	–4(1)
C(7)	43(2)	52(2)	50(2)	–4(2)	7(2)	18(2)
C(2)	65(2)	48(2)	64(2)	–1(2)	–33(2)	–4(2)
C(1)	61(2)	73(3)	43(2)	–18(2)	–1(2)	–14(2)
C(4)	67(3)	70(3)	79(3)	–21(3)	–3(2)	–33(2)
C(5)	104(4)	91(4)	128(5)	–16(4)	–6(4)	–68(3)
Li(2)	92(6)	92(6)	92(6)	–28(6)	28(6)	28(6)
C(8)	78(8)	69(11)	55(8)	–14(7)	–1(5)	–11(6)

Tabelle 162 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) des dilithiierten Phosphinsulfids **174**.

	x	y	z	U(eq)
H(8A)	3750(20)	4490(20)	790(20)	13(10)
H(8B)	4230(30)	4660(30)	1420(30)	40(20)
H(3)	2011	3459	898	49
H(7A)	5463	4045	692	72
H(7B)	6116	4688	563	72
H(7C)	6049	3973	−20	72
H(2A)	1141	4936	−210	89
H(2B)	1799	5562	−34	89
H(2C)	1200	5323	629	89
H(1A)	2081	4020	−621	89
H(1B)	2795	3807	−72	89
H(1C)	2749	4642	−469	89
H(4A)	525	3935	348	86
H(4B)	1092	3364	−108	86
H(5A)	137	2647	566	129
H(5B)	981	2433	883	129

8.2.6 Kristallstrukturen aus Kapitel 4.6

$(MeLi \cdot Et_2O)_4$

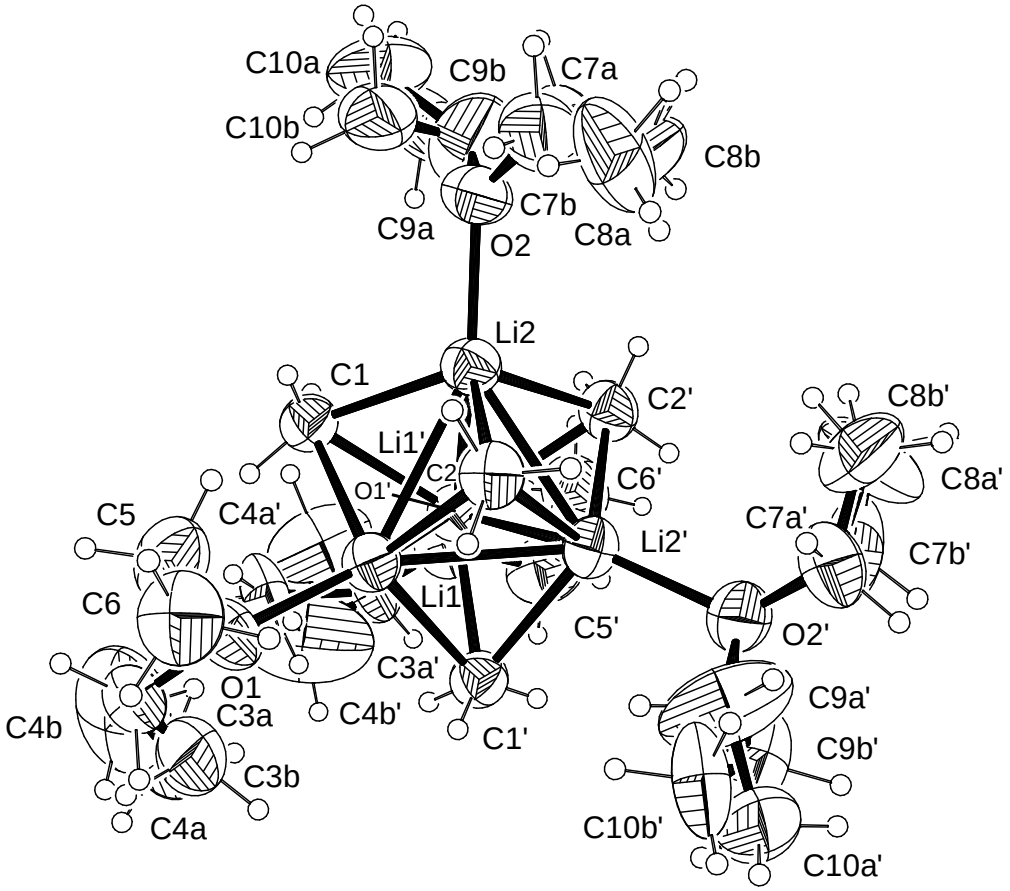


Abbildung 55 Thermische Auslenkungsellipsoide (30% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von $(MeLi \cdot Et_2O)_4$ (**175**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 163 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) von $(MeLi \cdot Et_2O)_4$ (**175**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	926(2)	8644(2)	7297(2)	84(1)
C(2)	583(2)	6352(2)	8758(2)	90(1)
C(3A)	1068(5)	10654(4)	9613(4)	93(1)
C(4B)	806(17)	11330(30)	9034(14)	308(13)
C(3B)	487(11)	10696(16)	9431(10)	195(7)
C(4A)	365(7)	11323(7)	8938(9)	140(4)
C(5)	1805(2)	8956(3)	10019(2)	142(1)
C(6)	1857(2)	8580(3)	10914(2)	147(1)
C(7A)	1361(9)	4345(10)	6913(6)	128(3)
C(7B)	1628(8)	4353(15)	7481(17)	209(9)
C(8A)	1329(13)	3724(13)	7718(15)	213(8)

C(8B)	1126(9)	3618(18)	7444(19)	210(10)
C(9A)	1348(10)	5769(15)	6115(9)	227(9)
C(9B)	2011(5)	6184(8)	6622(7)	161(3)
C(10A)	2020(9)	6211(12)	5972(10)	185(5)
C(10B)	1485(8)	6281(8)	5767(10)	167(6)
Li(1)	394(2)	8339(3)	8364(2)	80(1)
Li(2)	634(2)	6659(3)	7353(2)	84(1)
O(1)	996(1)	9413(1)	9443(1)	106(1)
O(2)	1376(1)	5587(2)	7027(1)	114(1)

Tabelle 164 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) von $(MeLi{\cdot}Et_2O)_4$ (**175**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	79(2)	89(1)	82(1)	1(1)	31(1)	0(1)
C(2)	88(2)	96(2)	78(1)	7(1)	22(1)	2(1)
C(3A)	107(4)	83(3)	77(3)	2(2)	22(3)	3(3)
C(4B)	410(30)	370(30)	150(13)	–83(16)	115(17)	–160(20)
C(3B)	177(11)	251(16)	178(11)	–128(12)	94(10)	–89(12)
C(4A)	144(7)	90(4)	131(6)	25(4)	–5(5)	29(4)
C(5)	110(2)	190(3)	108(2)	–11(2)	23(2)	–24(2)
C(6)	137(3)	155(3)	123(2)	22(2)	22(2)	7(2)
C(7A)	150(10)	86(4)	132(6)	–5(4)	36(5)	10(5)
C(7B)	115(8)	122(9)	360(30)	–35(15)	53(12)	32(7)
C(8A)	350(20)	97(6)	213(12)	6(7)	131(14)	–58(9)
C(8B)	125(8)	201(17)	350(30)	1(14)	142(12)	5(8)
C(9A)	205(11)	360(20)	157(9)	–132(12)	115(9)	–106(13)
C(9B)	103(5)	158(6)	195(9)	–46(7)	28(6)	26(4)
C(10A)	220(13)	214(10)	185(11)	47(8)	150(11)	57(8)
C(10B)	157(10)	110(5)	167(10)	–13(5)	–11(8)	55(6)
Li(1)	76(2)	92(2)	69(2)	–3(1)	22(1)	–1(1)
Li(2)	79(2)	88(2)	81(2)	–3(2)	27(2)	7(2)
O(1)	119(1)	100(1)	80(1)	–13(1)	18(1)	2(1)
O(2)	127(1)	98(1)	133(2)	–11(1)	68(1)	10(1)

Tabelle 165 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) von $(MeLi{\cdot}Et_2O)_4$ (**175**).

	x	y	z	U(eq)
H(1A)	965(17)	9460(30)	7510(20)	136(9)
H(1B)	840(20)	8800(30)	6700(30)	161(12)
H(1C)	1340(20)	8360(30)	7490(20)	142(13)
H(2A)	555(16)	6690(30)	9300(20)	136(10)
H(2B)	1111(19)	6160(20)	8906(18)	116(8)
H(2C)	346(18)	5610(30)	8760(20)	145(10)
H(3A)	835	10826	10075	111
H(3B)	1643	10834	9915	111
H(4D)	1231	11685	8882	463
H(4E)	533	11968	9230	463
H(4F)	426	10915	8487	463
H(3C)	−29	10440	9443	233
H(3D)	780	11112	10027	233
H(4A)	−111	11085	8404	210
H(4B)	815	11400	8748	210
H(4C)	271	12103	9178	210
H(5A)	1934	8262	9701	170
H(5B)	2199	9604	10090	170
H(6A)	1797	9287	11260	221
H(6B)	2375	8201	11250	221
H(6C)	1434	7994	10845	221
H(7A)	1842	4086	6817	154
H(7B)	891	4118	6355	154
H(7C)	1974	3975	7202	251
H(7D)	1960	4494	8143	251
H(8A)	1730	4068	8284	319
H(8B)	1436	2859	7683	319
H(8C)	800	3827	7730	319
H(8D)	1042	3634	8025	315
H(8E)	1302	2808	7351	315
H(8F)	628	3817	6927	315
H(9A)	1202	4984	5787	272
H(9B)	905	6336	5798	272
H(9C)	2222	6978	6905	193
H(9D)	2453	5628	6677	193
H(10A)	2100	7070	6144	277
H(10B)	1934	6121	5317	277
H(10C)	2492	5749	6355	277
H(10D)	1184	5523	5584	251
H(10E)	1759	6443	5350	251

H(10F)	1120	6949	5729	251

(MeLi·*trans*-TMCDA)$_2$ (176)

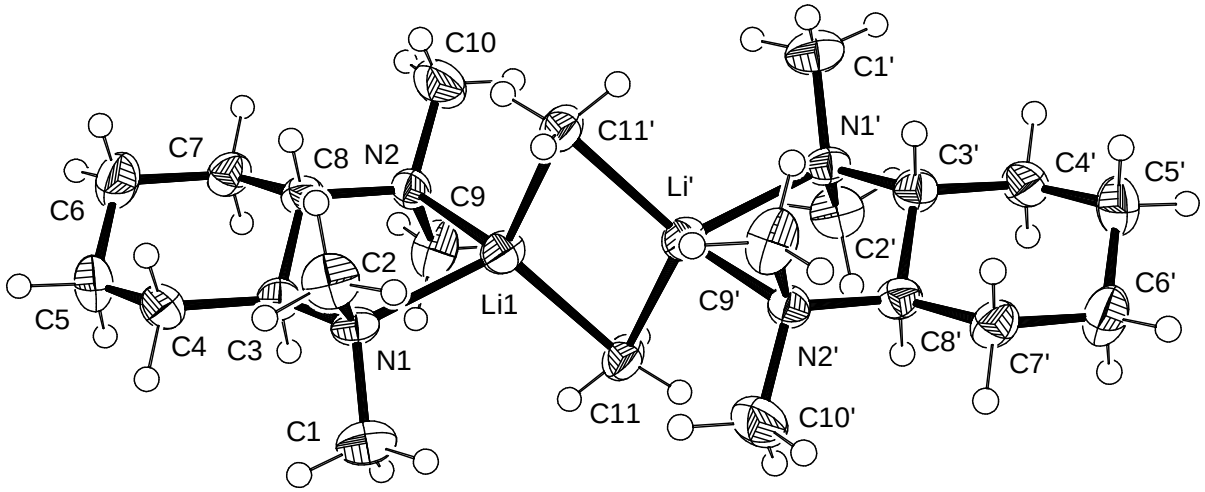


Abbildung 56 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von (MeLi·*trans*-TMCDA)$_2$ (**176**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 166 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) von (MeLi·*trans*-TMCDA)$_2$ (**176**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
C(3)	7146(3)	5825(3)	1341(2)	31(1)
C(8)	7312(3)	7513(3)	964(2)	30(1)
C(7)	6045(3)	8616(3)	910(2)	35(1)
C(6)	5722(3)	8778(4)	1747(2)	48(1)
C(5)	5527(3)	7093(4)	2090(2)	44(1)
C(4)	6795(3)	6006(3)	2175(2)	36(1)
C(2)	9529(3)	4940(4)	2118(2)	43(1)
C(1)	7899(3)	2960(4)	1314(2)	48(1)
C(9)	6502(3)	6806(4)	–554(2)	45(1)
C(10)	8234(4)	8896(4)	–64(2)	53(1)
C(11)	8701(3)	3649(4)	–749(2)	37(1)
Li(1)	9145(4)	5406(5)	331(3)	32(1)

N(1)	8335(2)	4717(2)	1370(1)	30(1)
N(2)	7661(2)	7345(3)	160(1)	28(1)

Tabelle 167 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) von (MeLi·*trans*-TMCDA)$_2$ (**176**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(3)	28(1)	30(1)	32(1)	3(1)	5(1)	3(1)
C(8)	30(1)	26(1)	31(1)	1(1)	5(1)	0(1)
C(7)	36(2)	29(2)	38(2)	1(1)	7(1)	7(1)
C(6)	50(2)	48(2)	49(2)	–5(1)	18(1)	13(2)
C(5)	44(2)	56(2)	36(2)	–1(1)	18(1)	5(1)
C(4)	39(2)	36(2)	33(1)	5(1)	11(1)	–2(1)
C(2)	36(2)	48(2)	39(2)	6(1)	–1(1)	5(1)
C(1)	53(2)	30(2)	58(2)	2(1)	12(2)	–1(1)
C(9)	39(2)	57(2)	31(2)	–2(1)	–2(1)	14(1)
C(10)	59(2)	42(2)	66(2)	15(2)	31(2)	0(2)
C(11)	26(1)	41(2)	43(2)	–18(1)	8(1)	–4(1)
Li(1)	23(2)	34(2)	37(2)	–5(2)	4(2)	2(2)
N(1)	29(1)	22(1)	36(1)	4(1)	4(1)	3(1)
N(2)	30(1)	27(1)	28(1)	4(1)	8(1)	2(1)

Tabelle 168 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) von (MeLi·*trans*-TMCDA)$_2$ (**176**).

	x	y	z	U(eq)
H(1)	6314	5295	936	37
H(2)	8127	8067	1373	36
H(3A)	6217	9740	712	42
H(3B)	5225	8141	484	42
H(4A)	6494	9368	2159	58
H(4B)	4863	9446	1668	58
H(5A)	4698	6549	1704	53
H(5B)	5364	7221	2652	53
H(6A)	6622	4888	2379	43
H(6B)	7603	6499	2605	43
H(7A)	9299	4519	2621	65

H(7B)	9761	6128	2193	65
H(7C)	10329	4324	2042	65
H(8A)	8666	2252	1260	72
H(8B)	7089	2805	817	72
H(8C)	7651	2651	1829	72
H(9A)	6117	5763	–407	67
H(9B)	6834	6626	–1053	67
H(9C)	5777	7666	–682	67
H(10A)	7496	9739	–223	80
H(10B)	8607	8695	–545	80
H(10C)	8981	9293	424	80
H(11)	8080(40)	3280(50)	–500(30)	89(14)
H(12)	8220(40)	4240(50)	–1250(30)	76(12)
H(13)	9060(40)	2830(60)	–960(20)	86(13)

(*E*)-Benzyl-(2-propenylaryl)amin (180)

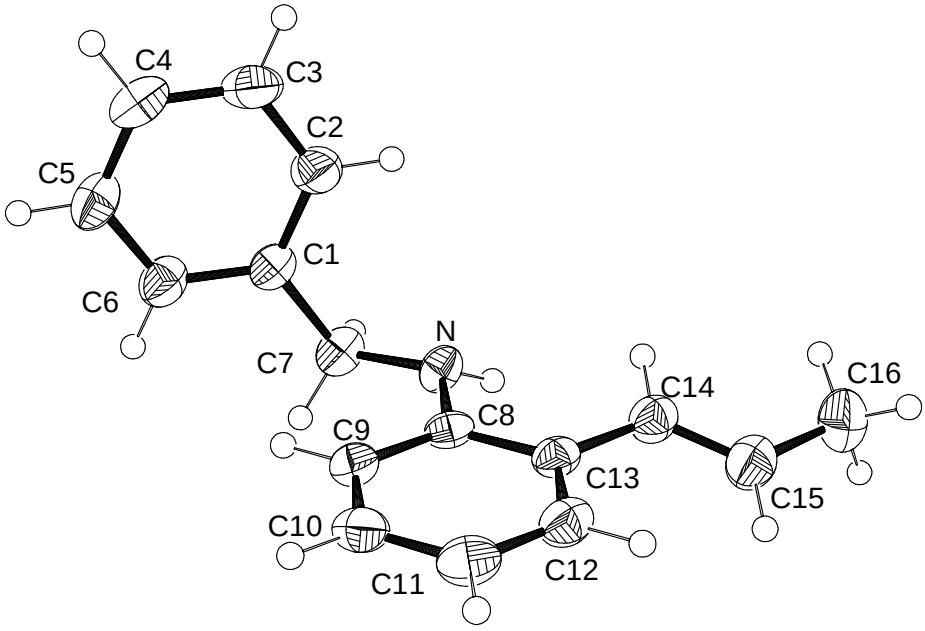


Abbildung 57 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des freien Amins **180** im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 169 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) des freien Amins **180**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
C(1)	8232(3)	8553(1)	174(1)	31(1)
C(2)	7112(4)	9167(1)	–296(1)	42(1)
C(3)	5092(4)	9085(1)	–1011(1)	49(1)
C(4)	4145(4)	8380(1)	–1261(1)	45(1)
C(5)	5231(4)	7765(1)	–797(1)	44(1)
C(6)	7271(3)	7853(1)	-86(1)	41(1)
C(7)	10481(3)	8638(1)	942(1)	37(1)
C(8)	8312(3)	9150(1)	2336(1)	29(1)
C(9)	6681(3)	8523(1)	2370(1)	34(1)
C(10)	4933(4)	8446(1)	3083(1)	39(1)
C(11)	4760(4)	8989(1)	3771(1)	42(1)
C(12)	6351(4)	9615(1)	3740(1)	39(1)
C(13)	8135(3)	9716(1)	3035(1)	31(1)
C(14)	9760(4)	10393(1)	3004(1)	37(1)
C(15)	10538(4)	10835(1)	3709(1)	48(1)
C(16)	12168(4)	11526(1)	3636(2)	59(1)
N	10055(3)	9239(1)	1612(1)	33(1)

Tabelle 170 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) des freien Amins **180**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	27(1)	41(1)	27(1)	–5(1)	7(1)	2(1)
C(2)	42(1)	45(1)	38(1)	6(1)	1(1)	–9(1)
C(3)	47(1)	58(1)	40(1)	14(1)	–7(1)	–2(1)
C(4)	37(1)	68(2)	31(1)	–5(1)	–2(1)	–1(1)
C(5)	41(1)	50(1)	42(1)	–16(1)	–1(1)	2(1)
C(6)	40(1)	42(1)	39(1)	–10(1)	–3(1)	10(1)
C(7)	30(1)	46(1)	35(1)	–6(1)	4(1)	3(1)
C(8)	24(1)	38(1)	25(1)	4(1)	–3(1)	5(1)
C(9)	34(1)	37(1)	30(1)	1(1)	–2(1)	1(1)
C(10)	38(1)	44(1)	35(1)	10(1)	–1(1)	–4(1)
C(11)	38(1)	55(1)	34(1)	6(1)	9(1)	2(1)
C(12)	40(1)	45(1)	31(1)	–2(1)	2(1)	6(1)
C(13)	30(1)	36(1)	27(1)	1(1)	–2(1)	6(1)
C(14)	39(1)	41(1)	33(1)	–3(1)	4(1)	3(1)
C(15)	56(1)	47(1)	40(1)	–5(1)	4(1)	–4(1)
C(16)	68(2)	46(1)	62(1)	–11(1)	–2(1)	–8(1)
N	29(1)	39(1)	30(1)	–6(1)	2(1)	–5(1)

Tabelle 171 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) des freien Amins **180**.

	x	y	z	U(eq)
H(2)	7739	9654	−126	50
H(3)	4352	9514	−1331	58
H(4)	2751	8323	−1752	54
H(5)	4586	7278	−961	53
H(6)	8024	7423	228	49
H(7A)	10701	8162	1304	44
H(7B)	12149	8734	629	44
H(9)	6771	8143	1896	41
H(10)	3843	8013	3097	47
H(11)	3560	8935	4262	51
H(12)	6224	9991	4217	47
H(14)	10316	10526	2389	45
H(15)	10019	10705	4330	57
H(16A)	12496	11616	2961	88
H(16B)	13867	11463	4014	88
H(16C)	11213	11954	3885	88
H(1)	11440(40)	9494(10)	1798(12)	40(6)

Dimeres Lithiumamid 183

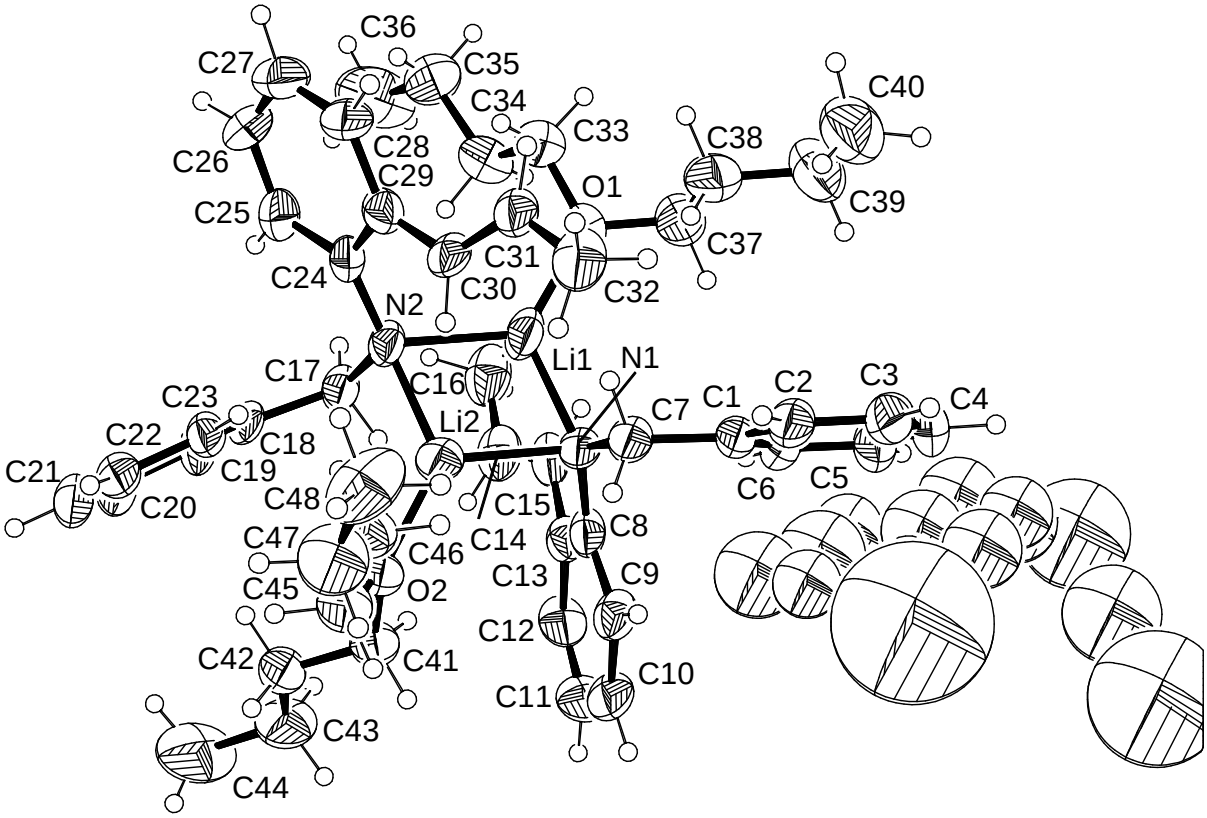


Abbildung 58 Thermische Auslenkungsellipsoide (25% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des dimeren Lithiumamids **183** im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 172 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) des dimeren Lithiumamids **183**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
C(1)	4074(3)	4577(2)	2601(2)	75(1)
C(2)	2941(3)	4038(2)	2462(2)	90(1)
C(3)	2587(4)	3159(3)	1981(3)	104(1)
C(4)	3397(5)	2806(3)	1625(3)	110(1)
C(5)	4542(4)	3326(2)	1760(2)	98(1)
C(6)	4868(3)	4209(2)	2243(2)	89(1)
C(7)	4384(3)	5542(2)	3113(2)	82(1)
C(8)	6551(3)	5849(2)	3713(2)	77(1)
C(9)	6465(3)	5301(2)	4366(2)	89(1)
C(10)	7504(4)	5172(2)	4947(2)	102(1)
C(11)	8626(4)	5551(3)	4909(3)	108(1)
C(12)	8726(3)	6027(2)	4242(3)	98(1)

C(13)	7711(3)	6184(2)	3639(2)	81(1)
C(14)	7861(3)	6649(2)	2899(2)	86(1)
C(15)	8781(4)	7287(3)	2911(3)	100(1)
C(16)	8937(4)	7735(3)	2144(3)	125(1)
C(17)	6945(3)	8704(2)	3598(2)	77(1)
C(18)	7265(3)	9474(2)	4400(2)	72(1)
C(19)	8421(3)	10034(2)	4677(2)	88(1)
C(20)	8779(3)	10692(2)	5435(3)	102(1)
C(21)	7987(4)	10819(2)	5927(2)	95(1)
C(22)	6837(3)	10279(2)	5659(2)	86(1)
C(23)	6471(3)	9612(2)	4891(2)	77(1)
C(24)	4945(3)	8779(2)	2807(2)	78(1)
C(25)	5391(3)	9650(2)	2651(2)	94(1)
C(26)	4638(4)	10131(3)	2179(2)	108(1)
C(27)	3417(4)	9777(3)	1856(2)	110(1)
C(28)	2941(3)	8945(2)	2017(2)	97(1)
C(29)	3672(3)	8430(2)	2494(2)	81(1)
C(30)	3095(3)	7578(2)	2700(2)	80(1)
C(31)	2085(3)	6997(2)	2219(2)	89(1)
C(32)	1434(3)	6191(2)	2500(3)	108(1)
C(33)	4671(4)	7479(3)	633(2)	110(1)
C(34)	5830(4)	8113(3)	753(2)	115(1)
C(35)	5717(5)	8915(3)	274(3)	142(2)
C(36)	6843(6)	9593(4)	471(4)	220(3)
C(37)	4415(4)	5871(2)	642(2)	105(1)
C(38)	3086(4)	5562(3)	464(3)	115(1)
C(39)	2566(4)	4602(3)	−68(3)	128(1)
C(40)	1250(4)	4282(3)	−203(3)	155(2)
C(41)	7514(3)	7489(2)	5722(2)	92(1)
C(42)	8249(3)	8339(2)	6344(2)	97(1)
C(43)	9599(4)	8329(3)	6602(3)	127(1)
C(44)	10367(4)	9169(3)	7267(3)	173(2)
C(45)	5566(3)	7581(3)	5875(2)	103(1)
C(46)	4267(3)	7430(2)	5364(2)	97(1)
C(47)	3430(4)	7477(3)	5939(3)	135(1)
C(48)	2109(4)	7270(3)	5422(3)	141(2)
Li(1)	5443(5)	7026(3)	2411(3)	91(2)
Li(2)	5714(5)	7324(3)	4021(3)	85(2)
N(1)	5568(2)	6102(2)	3186(2)	75(1)
N(2)	5666(2)	8247(1)	3226(2)	75(1)
O(1)	4874(2)	6777(2)	1140(1)	100(1)

O(2)	6272(2)	7509(1)	5287(1)	87(1)

Tabelle 173 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) des dimeren Lithiumamids **183**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	74(2)	65(2)	72(2)	1(2)	0(2)	18(2)
C(2)	86(2)	76(2)	92(2)	7(2)	0(2)	20(2)
C(3)	99(3)	81(3)	105(3)	8(2)	–2(2)	6(2)
C(4)	135(4)	69(2)	98(3)	–7(2)	0(3)	18(3)
C(5)	114(3)	78(2)	89(2)	–6(2)	15(2)	26(2)
C(6)	95(2)	71(2)	87(2)	–3(2)	9(2)	21(2)
C(7)	78(2)	73(2)	82(2)	3(2)	1(2)	23(2)
C(8)	78(2)	60(2)	81(2)	–5(2)	6(2)	25(2)
C(9)	90(2)	73(2)	92(2)	–1(2)	6(2)	33(2)
C(10)	114(3)	86(2)	98(3)	2(2)	8(3)	47(2)
C(11)	92(3)	115(3)	103(3)	–2(2)	–1(2)	49(3)
C(12)	81(2)	99(3)	103(3)	–9(2)	8(2)	37(2)
C(13)	74(2)	72(2)	89(2)	–5(2)	11(2)	26(2)
C(14)	68(2)	74(2)	105(3)	–13(2)	17(2)	24(2)
C(15)	91(3)	84(2)	122(3)	–7(2)	31(2)	28(2)
C(16)	111(3)	96(3)	174(4)	10(3)	49(3)	34(2)
C(17)	80(2)	60(2)	83(2)	–6(2)	13(2)	20(2)
C(18)	71(2)	57(2)	83(2)	–2(2)	12(2)	24(2)
C(19)	80(2)	68(2)	107(3)	–12(2)	18(2)	20(2)
C(20)	78(2)	75(2)	130(3)	–23(2)	12(2)	19(2)
C(21)	94(3)	69(2)	101(3)	–22(2)	2(2)	30(2)
C(22)	79(2)	74(2)	91(2)	–9(2)	4(2)	30(2)
C(23)	70(2)	64(2)	87(2)	–6(2)	9(2)	24(2)
C(24)	90(2)	68(2)	67(2)	–7(2)	8(2)	28(2)
C(25)	116(3)	72(2)	83(2)	3(2)	13(2)	26(2)
C(26)	133(4)	86(2)	98(3)	21(2)	14(3)	37(3)
C(27)	132(4)	95(3)	95(3)	22(2)	6(3)	45(3)
C(28)	110(3)	87(2)	85(2)	5(2)	2(2)	43(2)
C(29)	96(3)	73(2)	67(2)	–7(2)	10(2)	34(2)
C(30)	77(2)	73(2)	84(2)	0(2)	11(2)	32(2)
C(31)	83(2)	83(2)	93(2)	–3(2)	12(2)	32(2)
C(32)	76(2)	93(3)	144(3)	3(2)	15(2)	27(2)
C(33)	142(4)	99(3)	84(2)	13(2)	18(2)	39(3)

C(34)	138(4)	108(3)	90(3)	13(2)	16(2)	33(3)
C(35)	194(5)	121(3)	102(3)	28(3)	24(3)	38(3)
C(36)	235(7)	175(5)	171(5)	66(4)	–14(4)	–60(5)
C(37)	121(3)	92(3)	91(2)	–9(2)	11(2)	40(2)
C(38)	117(3)	114(3)	109(3)	15(2)	10(2)	48(3)
C(39)	140(4)	109(3)	109(3)	–16(3)	3(3)	34(3)
C(40)	116(4)	142(4)	166(4)	–12(3)	3(3)	9(3)
C(41)	82(2)	94(2)	85(2)	2(2)	1(2)	30(2)
C(42)	99(3)	93(2)	83(2)	6(2)	3(2)	22(2)
C(43)	103(3)	131(3)	122(3)	27(3)	–9(2)	25(3)
C(44)	133(4)	160(4)	158(4)	30(4)	–30(3)	–26(3)
C(45)	102(3)	111(3)	88(2)	9(2)	21(2)	23(2)
C(46)	94(3)	92(2)	99(2)	8(2)	14(2)	28(2)
C(47)	106(3)	142(4)	150(4)	8(3)	32(3)	33(3)
C(48)	105(3)	128(3)	200(4)	42(3)	39(3)	50(3)
Li(1)	111(4)	72(3)	81(3)	–2(3)	12(3)	32(3)
Li(2)	90(4)	69(3)	82(3)	–7(3)	6(3)	25(3)
N(1)	67(2)	65(2)	81(2)	–1(1)	4(1)	23(1)
N(2)	78(2)	60(1)	77(2)	–7(1)	9(1)	24(1)
O(1)	139(2)	80(2)	70(1)	0(1)	12(1)	32(1)
O(2)	96(2)	86(1)	73(1)	–1(1)	13(1)	31(1)

Tabelle 174 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) des dimeren Lithiumamids **183**.

	x	y	z	U(eq)
H(2)	2377	4279	2705	108
H(3)	1794	2801	1897	125
H(4)	3162	2204	1287	132
H(5)	5110	3083	1525	117
H(6)	5661	4569	2328	107
H(7A)	3760	5853	2823	99
H(7B)	4323	5514	3728	99
H(9)	5689	5019	4407	106
H(10)	7426	4805	5387	122
H(11)	9329	5487	5337	129
H(12)	9510	6260	4184	118
H(14)	7220	6466	2353	103

H(15)	9412	7486	3460	121
H(16A)	8248	7458	1612	188
H(16B)	9692	7655	2018	188
H(16C)	8974	8388	2296	188
H(17A)	7231	8953	3115	93
H(17B)	7404	8240	3777	93
H(19)	8973	9962	4337	106
H(20)	9581	11064	5623	122
H(21)	8238	11279	6450	114
H(22)	6288	10359	5999	103
H(23)	5665	9247	4700	93
H(25)	6237	9918	2877	113
H(26)	4974	10716	2078	129
H(27)	2905	10107	1522	131
H(28)	2088	8704	1801	117
H(30)	3498	7423	3249	96
H(31)	1734	7100	1633	107
H(32A)	600	6242	2457	162
H(32B)	1856	6171	3122	162
H(32C)	1418	5632	2107	162
H(33A)	4110	7808	839	132
H(33B)	4296	7208	-11	132
H(34A)	6371	7777	528	138
H(34B)	6217	8348	1402	138
H(35A)	5418	8685	-382	170
H(35B)	5104	9208	447	170
H(36A)	7461	9306	316	330
H(36B)	7115	9859	1112	330
H(36C)	6716	10074	119	330
H(37A)	4819	5452	981	126
H(37B)	4613	5842	64	126
H(38A)	2686	5986	129	138
H(38B)	2892	5594	1044	138
H(39A)	2719	4578	-662	154
H(39B)	2994	4181	249	154
H(40A)	1090	4297	381	233
H(40B)	970	3656	-543	233
H(40C)	815	4680	-538	233
H(41A)	7916	7357	5253	110
H(41B)	7504	6981	6061	110
H(42A)	7978	8401	6892	116
H(42B)	8128	8870	6053	116

H(43A)	9710	7781	6865	152
H(43B)	9874	8291	6055	152
H(44A)	10129	9191	7823	259
H(44B)	10247	9715	7014	259
H(44C)	11225	9149	7396	259
H(45A)	5844	8194	6259	123
H(45B)	5663	7123	6270	123
H(46A)	4010	6823	4970	117
H(46B)	4184	7893	4975	117
H(47A)	3656	8097	6307	161
H(47B)	3550	7041	6355	161
H(48A)	1875	6658	5054	211
H(48B)	1970	7720	5033	211
H(48C)	1620	7296	5843	211

Monomeres Lithiumamid 184

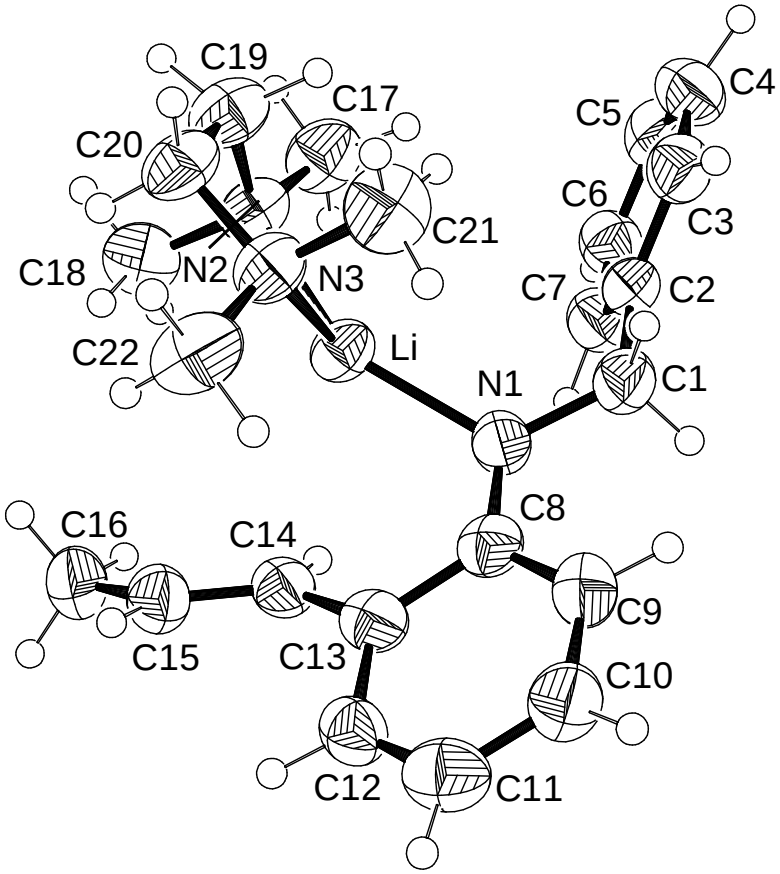


Abbildung 59 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des monomeren Lithiumamids **184** im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 175 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter ($Å^2$ x 10^3) des monomeren Lithiumamids **184**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
C(1)	3195(3)	4685(2)	2070(6)	52(1)
C(2)	2292(2)	4900(2)	2348(5)	47(1)
C(3)	2049(3)	5529(2)	3350(6)	56(1)
C(4)	1227(3)	5753(3)	3526(7)	64(1)
C(5)	637(3)	5350(3)	2640(7)	66(1)
C(6)	838(3)	4719(2)	1637(6)	59(1)
C(7)	1663(3)	4498(2)	1485(6)	56(1)
C(8)	4095(2)	3597(2)	1822(5)	45(1)
C(9)	4778(3)	4074(2)	1373(6)	57(1)
C(10)	5555(3)	3778(3)	1009(6)	60(1)

C(11)	5694(3)	2983(3)	1032(7)	64(1)
C(12)	5040(2)	2488(2)	1427(6)	53(1)
C(13)	4254(2)	2768(2)	1822(5)	48(1)
C(14)	3563(3)	2223(2)	2142(5)	48(1)
C(15)	3607(3)	1535(2)	2939(6)	55(1)
C(16)	2937(4)	940(3)	3059(8)	68(1)
C(17)	1094(3)	3464(4)	5299(8)	71(1)
C(18)	1705(3)	2210(3)	5808(8)	65(1)
C(19)	2157(3)	3341(3)	7423(6)	62(1)
C(20)	3028(3)	3109(3)	7805(6)	60(1)
C(21)	3803(4)	4170(3)	6522(9)	73(1)
C(22)	4368(3)	2876(4)	6562(8)	74(1)
Li	2916(4)	3252(4)	4216(8)	46(1)
N(1)	3331(2)	3849(2)	2273(4)	47(1)
N(2)	1869(2)	3055(2)	5754(4)	52(1)
N(3)	3604(2)	3338(2)	6419(4)	53(1)

Tabelle 176 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) des monomeren Lithiumamids **184**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	63(3)	50(2)	43(2)	3(2)	0(2)	–2(2)
C(2)	57(2)	45(2)	37(2)	2(2)	3(2)	2(2)
C(3)	62(3)	53(2)	53(3)	–1(2)	–3(2)	–11(2)
C(4)	70(3)	54(2)	69(3)	–5(2)	–1(2)	10(2)
C(5)	61(3)	71(3)	65(3)	17(2)	0(2)	19(2)
C(6)	63(3)	54(2)	59(3)	0(2)	–7(2)	2(2)
C(7)	67(3)	49(2)	52(2)	–1(2)	–3(2)	1(2)
C(8)	49(2)	54(2)	32(2)	0(2)	–6(2)	2(2)
C(9)	62(2)	48(2)	61(3)	7(2)	4(2)	–2(2)
C(10)	47(2)	66(3)	66(3)	11(2)	2(2)	3(2)
C(11)	54(3)	78(3)	60(3)	–8(2)	–4(2)	9(2)
C(12)	60(2)	50(2)	48(2)	0(2)	–6(2)	10(2)
C(13)	53(2)	55(2)	36(2)	–4(2)	–9(2)	9(2)
C(14)	58(2)	47(2)	38(2)	–5(2)	–6(2)	6(2)
C(15)	64(3)	51(2)	51(2)	3(2)	–3(2)	2(2)
C(16)	93(4)	47(2)	64(3)	7(2)	6(3)	2(2)
C(17)	54(3)	87(4)	70(3)	7(3)	4(3)	1(2)
C(18)	48(3)	74(3)	73(3)	–3(3)	–3(3)	0(2)
C(19)	59(3)	79(3)	49(3)	–7(2)	2(2)	–17(2)

C(20)	70(3)	76(3)	35(2)	–2(2)	–3(2)	–9(2)
C(21)	65(3)	76(3)	77(3)	–5(3)	–10(3)	–18(2)
C(22)	53(3)	111(4)	57(3)	8(3)	–3(3)	13(3)
Li	38(3)	57(4)	44(4)	4(3)	2(3)	0(3)
N(1)	52(2)	41(2)	47(2)	2(1)	–2(2)	0(1)
N(2)	46(2)	65(2)	45(2)	–2(2)	0(2)	–13(2)
N(3)	50(2)	63(2)	45(2)	1(2)	–3(2)	–7(1)

Tabelle 177 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) des monomeren Lithiumamids **184**.

	x	y	z	U(eq)
H(1A)	3480(30)	5020(30)	2960(70)	64(13)
H(1B)	3320(20)	4850(20)	930(60)	40(9)
H(3)	2460(20)	5800(20)	3590(50)	24(8)
H(4)	1080(50)	6260(50)	4010(140)	160(30)
H(5)	130(30)	5560(30)	2700(70)	76(15)
H(6)	420(40)	4460(30)	990(100)	103(19)
H(7)	1810(30)	4050(30)	710(70)	74(14)
H(9)	4710(20)	4620(20)	1290(60)	49(10)
H(10)	6010(30)	4120(30)	810(70)	70(13)
H(11)	6190(30)	2740(20)	820(60)	50(11)
H(12)	5090(20)	1940(20)	1480(60)	46(9)
H(14)	3050(20)	2360(20)	1700(60)	43(10)
H(15)	4110(30)	1370(20)	3490(60)	49(11)
H(16A)	3100(30)	450(30)	2600(70)	84(16)
H(16B)	2740(30)	840(30)	4210(80)	76(16)
H(16C)	2450(30)	1140(20)	2560(60)	51(12)
H(17A)	690(30)	3360(30)	6240(80)	80(15)
H(17B)	1310(30)	4070(30)	5260(70)	75(15)
H(17C)	900(30)	3220(30)	4220(90)	80(16)
H(18A)	1250(30)	2040(20)	6780(60)	53(11)
H(18B)	1500(30)	2050(30)	4800(70)	60(14)
H(18C)	2190(30)	1960(20)	5930(70)	63(13)
H(19A)	2140(30)	3950(30)	7280(70)	82(15)
H(19B)	1730(40)	3080(30)	8270(90)	103(19)
H(20A)	3010(30)	2540(30)	7820(70)	76(14)
H(20B)	3240(30)	3340(30)	8790(70)	55(12)
H(21A)	4130(40)	4360(30)	7540(80)	84(16)

H(21B)	4250(30)	4210(30)	5760(70)	66(14)
H(21C)	3270(40)	4450(30)	6200(90)	94(17)
H(22A)	4660(30)	2940(30)	7810(80)	75(14)
H(22B)	4170(30)	2320(30)	6370(70)	70(14)
H(22C)	4750(30)	2980(30)	5600(80)	77(15)

Ferrocenderivat (*R*)-186

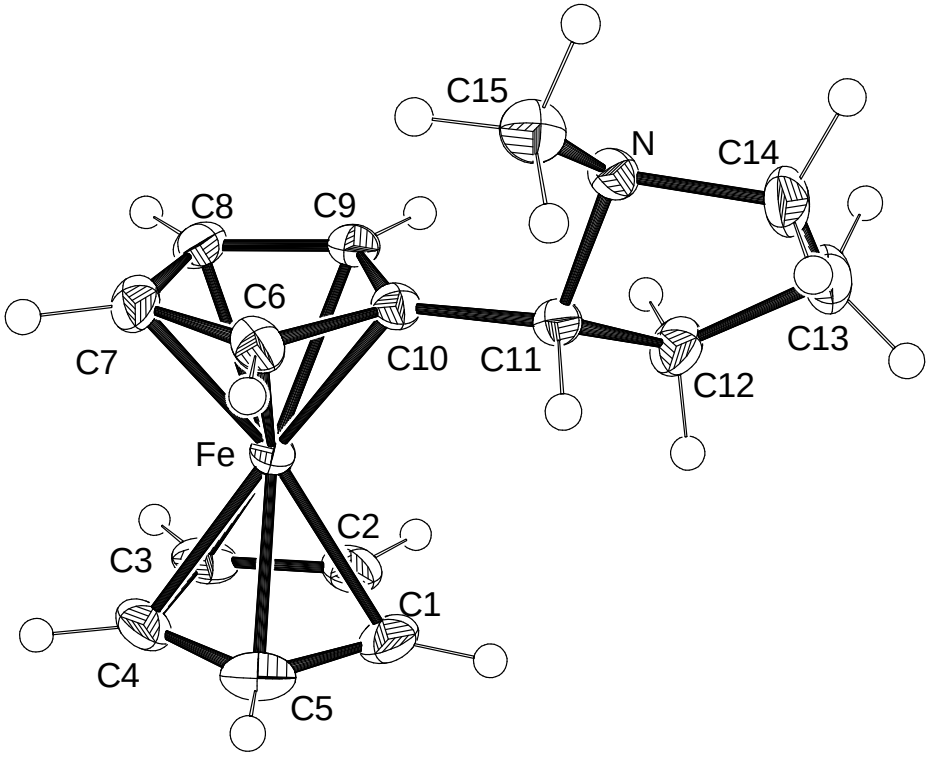


Abbildung 60 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Ferrocenderivats **186** im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 178 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) des Ferrocenderivats **186**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors

	x	y	z	U(eq)
C(1)	7130(5)	4697(3)	3298(3)	34(1)
C(2)	7807(4)	5222(3)	2464(3)	31(1)
C(3)	7052(4)	6275(3)	2435(2)	30(1)
C(4)	5923(4)	6387(3)	3242(3)	31(1)
C(5)	5969(4)	5411(3)	3781(3)	35(1)

C(6)	9176(4)	6401(3)	5103(2)	24(1)
C(7)	9083(5)	7378(3)	4561(2)	27(1)
C(8)	10264(4)	7285(2)	3761(3)	25(1)
C(9)	11102(4)	6257(2)	3813(2)	21(1)
C(10)	10419(4)	5703(2)	4651(2)	19(1)
C(11)	10980(4)	4615(2)	5044(2)	19(1)
C(12)	11623(5)	3781(2)	4288(2)	28(1)
C(13)	12918(5)	3053(3)	4858(3)	32(1)
C(14)	13050(5)	3593(3)	5871(3)	30(1)
C(15)	12154(4)	5291(3)	6604(2)	26(1)
Fe	8423(1)	6083(1)	3704(1)	18(1)
N	12527(3)	4723(2)	5694(2)	20(1)

Tabelle 179 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) des Ferrocenderivats **186**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	32(2)	25(2)	46(2)	–2(2)	–14(2)	–9(1)
C(2)	23(2)	38(2)	33(2)	–12(2)	–6(1)	–2(1)
C(3)	23(2)	42(2)	24(2)	6(2)	–11(1)	–7(1)
C(4)	19(1)	35(2)	37(2)	–7(2)	–8(1)	4(1)
C(5)	26(2)	44(2)	34(2)	–1(2)	–2(2)	–12(2)
C(6)	22(1)	29(2)	20(1)	–6(1)	–3(1)	5(1)
C(7)	30(2)	21(2)	29(2)	–9(1)	–10(1)	4(1)
C(8)	27(2)	19(1)	29(2)	2(1)	–7(2)	–5(1)
C(9)	18(1)	24(2)	21(1)	–2(1)	–2(1)	–3(1)
C(10)	19(1)	21(1)	17(1)	–1(1)	–3(1)	0(1)
C(11)	18(1)	19(2)	21(1)	1(1)	–1(1)	–1(1)
C(12)	35(2)	21(2)	27(2)	–4(1)	–5(1)	0(2)
C(13)	34(2)	24(2)	38(2)	–1(2)	–3(1)	10(1)
C(14)	35(2)	21(2)	34(2)	4(1)	–9(1)	9(1)
C(15)	28(2)	30(2)	18(1)	3(1)	–2(1)	–1(1)
Fe	17(1)	19(1)	19(1)	–1(1)	–3(1)	0(1)
N	19(1)	22(1)	20(1)	2(1)	–3(1)	1(1)

Tabelle 180 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) des Ferrocenderivats **186**.

	x	y	z	U(eq)
H(1)	7432	3944	3516	41
H(2)	8659	4912	1982	37
H(3)	7281	6840	1924	36
H(4)	5209	7045	3405	37
H(5)	5295	5253	4394	42
H(6)	8479	6230	5705	28
H(7)	8318	8017	4713	32
H(8)	10470	7849	3246	30
H(9)	11995	5967	3343	25
H(11)	9985	4293	5425	23
H(12A)	12222	4146	3735	33
H(12B)	10628	3349	4030	33
H(13A)	12461	2303	4913	39
H(13B)	14081	3033	4531	39
H(14A)	12246	3240	6344	36
H(14B)	14267	3554	6127	36
H(15A)	11777	6034	6458	38
H(15B)	13217	5310	7010	38
H(15C)	11215	4911	6957	38

$ZnCl_2$·(*R*,*R*)-TMCDA (194)

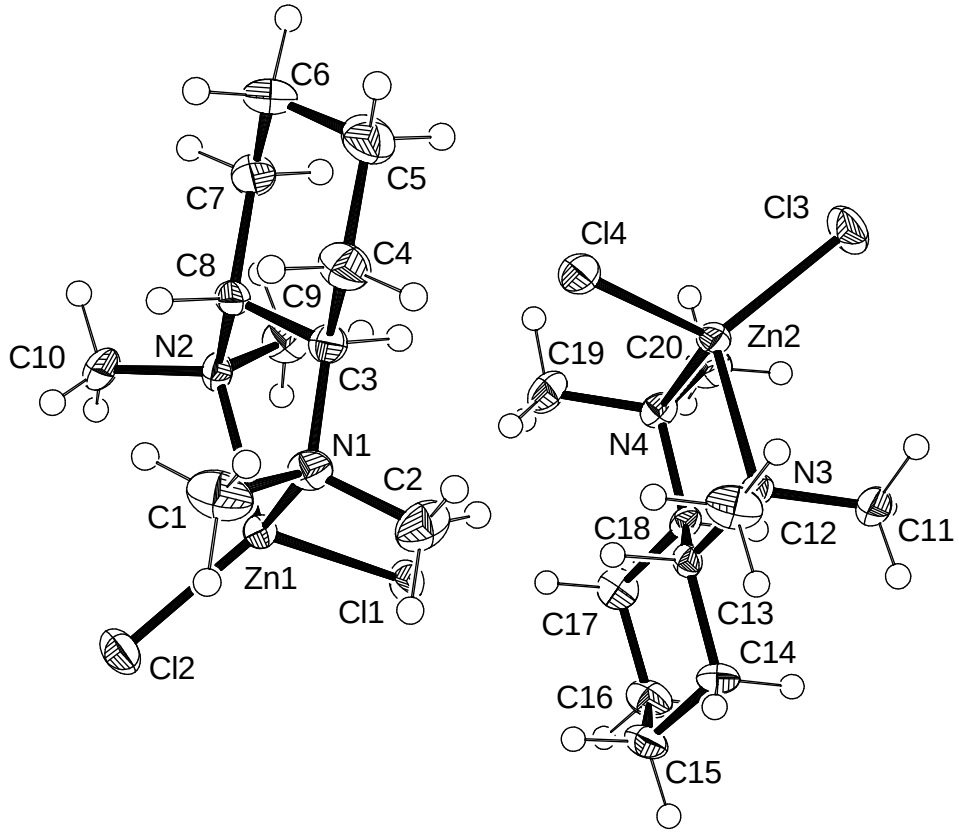


Abbildung 61 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur von $ZnCl_2$·(*R*,*R*)-TMCDA (**194**) im Kristall (Ortep-Darstellung der asymmetrischen Einheit).

Tabelle 181 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für $ZnCl_2$·(*R*,*R*)-TMCDA (**194**). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	5829(5)	5931(3)	5019(3)	40(1)
C(2)	5344(4)	4769(2)	6271(3)	37(1)
C(3)	2885(4)	5682(2)	5151(2)	21(1)
C(4)	2408(5)	5112(3)	4097(3)	34(1)
C(5)	482(5)	5075(2)	3564(3)	39(1)
C(6)	-232(4)	6065(3)	3341(3)	38(1)
C(7)	228(5)	6650(3)	4368(3)	33(1)
C(8)	2157(4)	6681(2)	4937(2)	21(1)
C(9)	1445(5)	7185(3)	6616(3)	32(1)
C(10)	2843(5)	8277(2)	5707(3)	32(1)
C(11)	2243(5)	2434(3)	9596(3)	34(1)
C(12)	3384(5)	3071(3)	8219(3)	32(1)
C(13)	3291(4)	4108(2)	9732(2)	17(1)

C(14)	4989(4)	3819(3)	10570(2)	23(1)
C(15)	5828(4)	4658(2)	11275(3)	28(1)
C(16)	4624(4)	5079(3)	11850(2)	31(1)
C(17)	2962(5)	5389(3)	11017(3)	26(1)
C(18)	2090(4)	4560(2)	10289(2)	18(1)
C(19)	416(4)	5789(2)	9002(3)	31(1)
C(20)	-986(5)	4763(3)	9977(3)	34(1)
Cl(1)	4791(1)	6058(1)	8419(1)	30(1)
Cl(2)	7203(1)	7712(1)	7109(1)	32(1)
Cl(3)	–2116(1)	2854(1)	8059(1)	39(1)
Cl(4)	110(1)	4530(1)	6648(1)	30(1)
N(1)	4774(4)	5702(2)	5738(2)	24(1)
N(2)	2667(4)	7261(2)	5971(2)	19(1)
N(3)	2432(4)	3307(2)	8994(2)	18(1)
N(4)	407(4)	4821(2)	9461(2)	21(1)
Zn(1)	5022(1)	6737(1)	6911(1)	19(1)
Zn(2)	24(1)	3848(1)	8190(1)	20(1)

Tabelle 182 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für $ZnCl_2$·(*R*,*R*)-TMCDA (**194**). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2 [h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	26(2)	60(3)	38(2)	–10(2)	16(2)	0(2)
C(2)	38(2)	29(2)	41(2)	1(2)	8(2)	14(2)
C(3)	21(2)	26(2)	18(2)	2(1)	7(1)	–1(1)
C(4)	33(2)	36(2)	32(2)	–5(2)	7(2)	–6(2)
C(5)	42(2)	41(2)	30(2)	–7(2)	5(2)	–13(2)
C(6)	27(2)	46(2)	32(2)	1(2)	-6(2)	–6(2)
C(7)	22(2)	31(2)	42(2)	7(2)	5(2)	2(2)
C(8)	18(2)	26(2)	18(1)	3(1)	5(1)	–4(1)
C(9)	27(2)	35(2)	36(2)	–1(2)	15(2)	7(2)
C(10)	33(2)	20(2)	36(2)	11(2)	2(2)	5(2)
C(11)	35(2)	21(2)	35(2)	5(2)	–5(2)	–2(2)
C(12)	23(2)	43(2)	34(2)	–10(2)	13(2)	4(2)
C(13)	16(2)	18(2)	19(2)	2(1)	9(1)	–1(1)
C(14)	14(2)	30(2)	23(2)	–2(2)	4(1)	2(2)
C(15)	18(2)	37(2)	30(2)	–2(1)	5(1)	–6(1)
C(16)	29(2)	45(2)	19(2)	–4(1)	6(1)	–9(2)
C(17)	31(2)	29(2)	23(2)	–6(1)	12(2)	1(2)
C(18)	18(2)	20(2)	17(2)	5(1)	7(1)	3(1)

C(19)	35(2)	23(2)	33(2)	5(1)	8(2)	11(2)
C(20)	23(2)	50(3)	34(2)	4(2)	17(2)	6(2)
Cl(1)	35(1)	32(1)	20(1)	6(1)	4(1)	−12(1)
Cl(2)	25(1)	30(1)	44(1)	2(1)	13(1)	−7(1)
Cl(3)	22(1)	32(1)	65(1)	3(1)	17(1)	−7(1)
Cl(4)	32(1)	37(1)	19(1)	5(1)	5(1)	−7(1)
N(1)	19(2)	30(2)	24(2)	1(1)	10(1)	3(1)
N(2)	20(2)	16(2)	24(2)	4(1)	10(1)	3(1)
N(3)	16(2)	19(2)	19(2)	3(1)	6(1)	3(1)
N(4)	18(2)	24(2)	22(1)	2(1)	10(1)	7(1)
Zn(1)	17(1)	20(1)	19(1)	2(1)	5(1)	−1(1)
Zn(2)	15(1)	23(1)	21(1)	3(1)	6(1)	0(1)

Tabelle 183 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für $ZnCl_2$·(*R*,*R*)-TMCDA (**194**).

	x	y	z	U(eq)
H(1A)	7036	5984	5461	60
H(1B)	5445	6536	4645	60
H(1C)	5706	5424	4475	60
H(2A)	5109	4269	5713	55
H(2B)	4718	4632	6797	55
H(2C)	6578	4792	6656	55
H(3)	2320	5368	5651	26
H(4A)	2953	5402	3582	41
H(4B)	2857	4456	4256	41
H(5A)	-62	4740	4053	46
H(5B)	218	4715	2867	46
H(6A)	227	6374	2794	46
H(6B)	-1498	6032	3029	46
H(7A)	-349	6381	4879	39
H(7B)	-201	7306	4186	39
H(8)	2693	6989	4417	25
H(9A)	1947	7480	7335	47
H(9B)	1207	6512	6711	47
H(9C)	373	7511	6227	47
H(10A)	1774	8496	5175	47
H(10B)	3791	8347	5395	47
H(10C)	3078	8658	6377	47
H(11A)	1460	1992	9093	51

H(11B)	1776	2602	10192	51
H(11C)	3368	2132	9902	51
H(12A)	4515	2816	8623	49
H(12B)	3527	3647	7824	49
H(12C)	2743	2595	7695	49
H(13)	3565	4608	9255	20
H(14A)	5776	3568	10182	27
H(14B)	4776	3307	11043	27
H(15A)	6901	4447	11827	34
H(15B)	6128	5150	10812	34
H(16A)	5179	5633	12296	38
H(16B)	4378	4599	12348	38
H(17A)	3204	5902	10556	32
H(17B)	2178	5647	11404	32
H(18)	1837	4065	10780	21
H(19A)	-657	5894	8411	46
H(19B)	1390	5850	8711	46
H(19C)	521	6263	9579	46
H(20A)	-1071	4110	10222	50
H(20B)	-2077	4947	9442	50
H(20C)	-731	5195	10607	50

8.3 Angaben zu den quantenchemischen Rechnungen

8.3.1 Angaben zu den quantenchemischen Rechnungen der Deprotonierung von (*R,R*)-TMCDA (Kapitel 4.1.1)

Tabelle 184 Energien der berechneten Verbindungen.

Verbindung	Methode	Min./TS	SCF [Hartree]	ZPE [Hartree]
(*R,R*)-TMCDA	B3LYP/6-31+G(d)	Globales Min.	–503,804794	–503.487766
t-BuLi·(*R,R*)-TMCDA	B3LYP/6-31+G(d)	Globales Min.	–669.194369	–668.755132
t-BuLi·(*R,R*)-TMCDA-	B3LYP/6-31+G(d)	TS	–669.151472	–668.717810
s-BuLi·(*R,R*)-TMCDA	B3LYP/6-31+G(d)	Globales Min.	–669.193247	–668.753489
s-BuLi·(*R,R*)-TMCDA-	B3LYP/6-31+G(d)	TS	–669.152496	–668.717567

Tabelle 185 Standardorientierung von (*R,R*)-TMCDA [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.6860384761	–0.3604876021	–0.1190602029
C	–0.6894826372	0.3604293279	–0.0974826762
C	–1.4916230753	–0.0519554335	–1.3599957021
C	–0.744411433	0.3078207339	–2.6534510635
C	0.659743304	–0.3098454387	–2.6755104242
C	1.4476565409	0.0509525724	–1.4067220238
C	2.5956065727	–1.0862291461	1.230854179
C	1.748442406	1.1524847484	1.5390449416
C	–1.6984683889	–1.1512617509	1.5948028486
C	–2.5553648509	1.0870734963	1.3117450584
N	1.4387127776	–0.2103449486	1.1336256593
N	–1.4019922091	0.2112611255	1.1785899893
H	0.4888934343	–1.4402283749	–0.2055483961
H	–0.4951947762	1.4400975258	–0.1910239371
H	–2.4715402049	0.4411154722	–1.350912121
H	–1.6847346972	–1.1343023275	–1.3381369247
H	–0.6597587757	1.4028922499	–2.7283654574
H	–1.3219024289	–0.0196138093	–3.5283869486
H	0.5727841823	–1.4049765709	–2.7468185678
H	1.2091437324	0.0168856865	–3.5686107337
H	2.4273990611	–0.4420625706	–1.4284100477
H	1.6412827794	1.1333284279	–1.3918196431
H	2.954318587	–1.0970314495	2.2674203717

H	3.4490038729	–0.7913676937	0.5881599743
H	2.3104862461	–2.1107734451	0.962413129
H	2.1902838674	1.1294491689	2.5422875834
H	2.4668839887	1.6684239629	0.8715043504
H	0.8308564375	1.742986914	1.5982606141
H	–2.1090511229	–1.1273380945	2.6112180517
H	–0.779240387	–1.7413470091	1.6261806776
H	–2.4370550137	–1.6681552883	0.9503883669
H	–2.8806826664	1.0991273415	2.3592585692
H	–2.2792007815	2.1113186533	1.0330110504
H	–3.4288408007	0.7912689467	0.6970708887

Tabelle 186 Standardorientierung von *t*-BuLi·(*R,R*)-TMCDA (**80**) [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.2227832614	4.0466149537	0.5665751453
C	2.1803671385	0.5108187831	–1.5029995014
C	–2.240434446	0.0958478876	–0.8485355885
C	1.1816003616	2.8517832059	0.4566156355
C	–0.9868954883	3.6949984562	1.4424093914
C	0.4765844488	1.5885086229	–0.0858106774
C	–1.7012652717	2.4449011388	0.9080198421
N	1.3672622871	0.4106092066	–0.2813203578
C	–0.7490380849	1.2331418326	0.7990698221
Li	0.1306348583	–1.2683238047	–0.3486876312
N	–1.3960006798	–0.0315939567	0.3518004329
C	2.2292044875	0.0898019607	0.8695256014
C	–2.1511554025	–0.6932812472	1.4266489338
C	0.3179840699	–3.2738370318	–0.8351935885
C	–1.05780528	–3.9283393425	–1.0232793336
C	1.1110263529	–3.4763391658	–2.1339835418
C	1.046525114	–4.0372831261	0.2806934334
H	–0.1243103981	4.3366874742	–0.436502428
H	0.7552708066	4.9145951566	0.9756193654
H	1.5327680507	0.6882391704	–2.3676075587
H	2.9316186623	1.3174184591	–1.4539508698
H	2.7030335095	–0.4368963508	–1.6630383913
H	–1.697494166	0.6081107666	–1.6486116265
H	–3.1769767074	0.6442461467	–0.6578365379

H	–2.4980320632	–0.9068580798	–1.2043865503
H	2.0312659841	3.1055580541	–0.1893498427
H	1.5954299187	2.6416425459	1.4524389231
H	–1.6900675899	4.5364896854	1.4838169829
H	–0.6511332326	3.5168167558	2.4750249064
H	0.0990969997	1.8302402775	–1.0890253724
H	–2.1165851631	2.6749310798	–0.0827647694
H	–2.5509917153	2.1889301818	1.5530229777
H	–0.3742924912	1.0201924333	1.8098132886
H	3.0391997215	0.8224051229	1.0156880178
H	2.6825428456	–0.8932484836	0.7067805064
H	1.6395085152	0.0383947787	1.7896238176
H	–2.4880284895	–1.6727305102	1.0744693497
H	–3.0360166899	–0.1174831086	1.7475362184
H	–1.5027979208	–0.8503792703	2.2946734426
H	–0.9839533135	–5.0152293405	–1.2731919462
H	–1.6352377057	–3.4676546741	–1.8419724542
H	–1.6801303574	–3.8690103989	–0.1147737676
H	1.2213165195	–4.5555288448	–2.4029245317
H	2.1355631186	–3.0740055431	–2.0683226461
H	0.6306926977	–2.9926195623	–3.0000244366
H	1.1534469688	–5.1265693971	0.0535581493
H	0.5183684941	–3.97726509	1.2463520106
H	2.0693017978	–3.6615763387	0.4500346966

Tabelle 187 Standardorientierung von *t*-BuLi·(*R,R*)-TMCDA (**80**) [TS, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–3.6497168166	–1.0725406985	1.330687345
C	–3.9814600175	0.1295965036	0.4364333147
C	–2.452810697	–1.8643639259	0.7777249258
C	–2.7497286849	1.021325447	0.214635608
C	–1.2181477889	–0.9525629449	0.6119613414
C	–1.5510930736	0.2232091907	–0.3459187141
N	–0.3431296512	1.0139904903	–0.6494015791
N	0.050266097	–1.6526528231	0.225831807
C	–0.4896844546	1.8824903646	–1.8118112565
C	0.3368968171	1.7332485636	0.4842470212
C	–0.0594113069	–2.4556874124	–1.0041558174
C	0.5789535373	–2.4803040733	1.3215075058

Li	1.2735880752	–0.0245142103	–0.2522359945
C	3.1212799743	1.1213362989	–0.2737534815
C	3.746634783	2.5090507992	–0.1486561503
C	3.723750913	0.1893975299	0.7843766443
C	3.3913393497	0.5671952336	–1.6812626018
H	–3.412901329	–0.7187939413	2.3452819397
H	–4.5211665112	–1.7332927785	1.4256883841
H	–4.3504110931	–0.2339914426	–0.5349719917
H	–4.7974662606	0.7174459104	0.8769957112
H	–2.2214824307	–2.7028336928	1.4464808099
H	–2.7301007829	–2.2994982039	–0.1926096953
H	–2.9979276832	1.8363045017	–0.4763382535
H	–2.4532855572	1.4943033843	1.1604601461
H	–1.0010851626	–0.5187534069	1.5967433541
H	–1.870333135	–0.2113998163	–1.3068150745
H	–1.1735512368	2.7321888475	–1.6314305681
H	–0.861567969	1.3108544625	–2.6716338052
H	0.488841738	2.2994513492	–2.0706264202
H	–0.0087446282	1.3306413027	1.445409936
H	0.0887007419	2.8045247017	0.4736357325
H	1.7672052107	1.5123351254	0.1558468649
H	–0.4463922369	–1.8434400755	–1.8227700322
H	–0.710881025	–3.3359392134	–0.8838718618
H	0.93651044	–2.8141546353	–1.2881208495
H	–0.0632855057	–3.3434499454	1.5610471968
H	0.6945575409	–1.8703748343	2.2230421935
H	1.5655246732	–2.8646306329	1.0406832674
H	3.3277633195	3.2070525059	–0.8883048305
H	4.8434542974	2.4936000141	–0.3003624535
H	3.5619916382	2.9442751632	0.844436085
H	4.8251414817	0.1002255778	0.6997927103
H	3.3395300615	–0.8460124029	0.7197810653
H	3.5086046214	0.5462245188	1.8027964364
H	4.4766401196	0.50184832	–1.9104500347
H	2.943466851	1.1980094718	–2.4623145945
H	3.0011152596	–0.4568864314	–1.8318990874

Tabelle 188 Standardorientierung von *s*-BuLi·(*R*,*R*)-TMCDA [Globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–2.1103416253	–0.1155222656	1.2038030546
C	2.2236914481	–1.131010131	0.6706205912
C	0.1329533098	–1.5116642318	–0.5706505048
C	–0.6338472563	–3.5890712662	–1.8491115129
C	2.0226445511	3.022321627	2.4208978342
C	–0.4609688052	3.08485073	2.7369453993
Li	0.3111228244	1.1361759817	0.6229066036
N	1.2268985637	–0.5532793468	–0.2440495299
N	–1.5000515418	0.3257556677	–0.0623950317
C	–2.2991974454	–1.7820726016	–1.266382563
C	0.5114060659	–2.5952188518	–1.6055983352
C	3.2351245783	3.0183230191	1.4793980875
C	0.6691947529	2.8617965276	1.7120767473
C	–1.1584127247	–0.7719171017	–1.0081441805
C	–1.9048599127	–2.8543932059	–2.2927043497
C	–2.3300061076	1.3701865667	–0.6803364634
C	1.9012749702	0.0295230315	–1.4172884512
H	–1.5180241514	–0.9152020165	1.6588540996
H	–2.1248403816	0.728945496	1.8993466547
H	–3.1437960391	–0.4774665302	1.0783880944
H	1.7278861664	–1.5048279633	1.5723107902
H	2.9285422312	–0.3503812901	0.9712559997
H	2.7964866977	–1.957036399	0.215582536
H	–0.0868366067	–2.025929243	0.3750017417
H	–0.8393902198	–4.1516457906	–0.9260167025
H	–0.331882637	–4.3266602634	–2.6035080953
H	2.1579167821	2.219890247	3.1683382659
H	2.0692212872	3.9658248699	3.0124916983
H	–0.5015690516	2.2797999978	3.4914750616
H	–0.3640107014	4.0298696859	3.3175524235
H	–1.4564294515	3.1217686198	2.2635701364
H	–2.5665331171	–2.2809299481	–0.3248382168
H	–3.1953574693	–1.2464157844	–1.603338106
H	1.4102200059	–3.1279044044	–1.2710988995
H	0.7669434824	–2.1161882454	–2.5606683643
H	3.3136956883	2.0665931321	0.9329891159
H	4.1809314634	3.1726090938	2.0180723436
H	3.1468935069	3.8157280226	0.728098296
H	0.6006099015	3.7071358786	0.9935387631

H	–0.9436167144	–0.2706965802	–1.9622274593
H	–2.7323809063	–3.5623901232	–2.4278656477
H	–1.7319863488	–2.384224172	–3.2724978116
H	–2.4272665395	2.2067336814	0.0178335163
H	–3.3419551731	1.0157481846	–0.9409037065
H	–1.8451146834	1.7422296023	–1.588699014
H	2.5372378618	0.8554648671	–1.0838286095
H	2.5337269963	–0.6967392794	–1.9528724279
H	1.1674456991	0.4336433839	–2.1210964753

Tabelle 189 Standardorientierung der Deprotonierung von (*R*,*R*)-TMCDA (**9**) über *s*-BuLi·(*R*,*R*)-TMCDA [TS, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–3.8736604211	0.3918804398	–0.8634352717
C	–3.787327451	–1.1180912631	–0.6040573751
C	–2.9375054307	1.1726848546	0.0741054233
C	–2.3366224917	–1.6191202631	–0.6843807434
C	–1.4813676192	0.6787367472	–0.0631865847
C	–1.4014677718	–0.8368118012	0.2654923876
N	–0.0001501819	–1.299177957	0.3064603212
N	–0.4607741709	1.4758162153	0.6916717431
C	0.167440611	–2.5907456733	0.9641583756
C	0.8064254247	–1.2232804024	–0.9623901793
C	–0.7343471927	1.5894980211	2.1344395588
C	–0.2606761703	2.8127780242	0.1107171554
Li	1.2014528618	0.2346876949	0.528209112
C	3.3226404643	–0.2355798924	0.1888622713
C	3.9991773392	–1.5116851056	0.6971111638
C	4.0497634475	0.3535592989	–1.0255994351
C	3.4968533649	1.7195274979	–1.4545987735
H	–3.5962123672	0.5989968858	–1.9077002509
H	–4.9053892138	0.7453805723	–0.7383562791
H	–4.1958127881	–1.3369883599	0.3945225294
H	–4.4144037462	–1.6636835446	–1.3214390675
H	–2.9985017581	2.2450761049	–0.1494677608
H	–3.2802915229	1.0446332813	1.1104978672
H	–2.2959070672	–2.6865389084	–0.4352223988
H	–1.9626935416	–1.5246412539	–1.7126172935
H	–1.1963711562	0.7996094126	–1.1164440475
H	–1.7884155246	–0.9751810611	1.287878182

H	–0.2465982808	–3.4301773132	0.3758058345
H	–0.3164288228	–2.5829888244	1.9491955847
H	1.2354866186	–2.783910135	1.1027421719
H	0.3028652112	–0.5722367576	–1.6890774524
H	0.8973977504	–2.2157975671	–1.4260276382
H	2.1209505006	–0.7213086893	–0.457546655
H	–0.8727484557	0.5979995118	2.5730465626
H	–1.6245008736	2.2002613654	2.3543267368
H	0.1240904191	2.0625527324	2.6249415582
H	–1.1377181699	3.4705018574	0.225280876
H	–0.028700917	2.7221706742	–0.9549240107
H	0.5886179943	3.297734147	0.6042020258
H	3.3712441988	0.5241727626	1.0001816913
H	5.0896928555	–1.4036282196	0.8362425827
H	3.8540363378	–2.3404554982	–0.0144186059
H	3.5838812175	–1.8424039764	1.6598980732
H	5.1363503261	0.4495836683	–0.8447345676
H	3.9515064709	–0.3462127034	–1.8733777893
H	3.5904545398	2.4548812497	–0.6423791537
H	2.4333079694	1.6482795014	–1.7232035184
H	4.0269670629	2.1236852976	–2.3268054101

8.3.2 Angaben zu den quantenchemischen Berechnungen der Deprotonierung von Benzol durch Mischungen von *n*-BuLi und (*R,R*)-TMCDA (Kapitel 4.1.3 und 4.1.4)

Tabelle 190 Ergebnisse der Deprotonierung von Benzol mit *n*-BuLi und (*R,R*)-TMCDA (**9**).

Verbindung	Methode/Basis	Min./TS	SCF [Hartree]	ZPE [Hartree]
$[(n\text{-BuLi})_2 \cdot (R,R)\text{-TMCDA}]_2$ (**85a**)	B3LYP/6-31+G(d) B3LYP/6-31G	Global Min.	–1669.212758	–1668,078597
$[(n\text{-BuLi})_2 \cdot (R,R)\text{-TMCDA}]_2$ (**85b**)	B3LYP/6-1+G(d) B3LYP/6-31G	Global Min.	–1669.211363	–1668.076077
(*R,R*)-TMCDA (**9**)	B3LYP/6-31+G(d) B3LYP/6-31G	Global Min.	–503.804794	–503.485898
$(n\text{-BuLi})_6$	B3LYP/6-31+G(d) B3LYP/6-31G	Global Min.	–992.374458	–991.633932
$[n\text{-BuLi} \cdot (R,R)\text{-TMCDA}]_2$ (**84**)	B3LYP/6-31+G(d) B3LYP/6-31G	Global Min.	–1338.422342	–1337.534100
$n\text{-BuLi} \cdot (R,R)\text{-TMCDA}$ (**87**)	B3LYP/6-31+G(d) B3LYP/6-31G	Global Min.	–669.198069	–668.756822
$n\text{-BuLi} \cdot (R,R)\text{-TMCDA} \cdot C_6H_6$ (**88**)	B3LYP/6-31+G(d) B3LYP/6-31G	Global Min.	–901.458747	–900.913492
$n\text{-BuLi} \cdot (R,R)\text{-TMCDA} \cdot C_6H_6$ TS	B3LYP/6-31+G(d) B3LYP/6-31G	TS	–901.429079	–900.886985
$[n\text{-BuLi} \cdot (R,R)\text{-TMCDA}]_2 \cdot C_6H_6$ (**89**)	B3LYP/6-31+G(d) B3LYP/6-31G	Global Min.	–1570.678990	–1569.688346
$[n\text{-BuLi} \cdot (R,R)\text{-TMCDA}]_2 \cdot C_6H_6$ TS	B3LYP/6-1+G(d) B3LYP/6-31G	TS	–1570.633154	–1569.646184
C_6H_6	B3LYP/6-1+G(d) B3LYP/6-31G	Global Min.	–232.258933	–232.157096
Halbe Leiterstruktur (**90**)	B3LYP/6-1+G(d) B3LYP/6-31G	Global Min.	–834.594981	–834.028872
Halbe Leiterstruktur $\cdot C_6H_6$ (**91**)	B3LYP/6-31+G(d) B3LYP/6-31G	Global Min.	–1066.857484	–1066.188976
Halbe Leiterstruktur $\cdot C_6H_6$ TS	B3LYP/6-31+G(d) B3LYP/6-31G	TS	–1066.816464	–1066.151788

Tabelle 191 Standardorientierung von [(*n*-BuLi)$_2$·(*R*,*R*)-TMCDA]$_2$ (**85a**) [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.702566	2.780080	–5.100141
C	0.570551	2.014473	–3.776915
C	1.596743	0.883100	–3.606504
C	–2.814022	–0.857319	–2.331489
C	1.425427	0.063781	–2.301734
C	–4.990502	–2.843359	–1.941372
C	–6.412384	–3.336320	–1.642811
C	–7.329698	–2.151640	–1.321254
N	–2.996524	–1.539239	–1.037718
C	–2.014643	–2.626984	–0.913358
C	–4.386827	–2.013490	–0.782685
Li	0.485508	1.278901	–0.802451
C	–5.325255	–0.839900	–0.402642
C	–6.764213	–1.345839	–0.143868
Li	2.533319	0.050887	–0.350318
C	–5.268275	1.357915	0.678091
Li	–2.523961	–0.089417	0.481390
N	–4.757814	–0.020511	0.709651
Li	–0.440643	0.822420	1.286183
C	–4.980363	–0.589249	2.050044
C	–1.309182	–0.903772	2.174176
C	–0.840213	–0.617031	3.625185
C	–1.797081	0.276239	4.429932
C	–1.303818	0.599250	5.846326
H	0.559649	2.111538	–5.959350
H	1.699195	3.231330	–5.196895
H	–0.036967	3.587375	–5.178340
H	–0.445618	1.597388	–3.701975
H	0.669667	2.727262	–2.942829
H	1.543803	0.255542	–4.517831
H	2.598875	1.342433	–3.634274
H	–2.875991	–1.545546	–3.189765
H	–1.827961	–0.386649	–2.343986
H	–3.560410	–0.069428	–2.461112
H	2.186369	–0.744396	–2.340073
H	0.482727	–0.515514	–2.413894
H	–5.025069	–2.227860	–2.850333
H	–4.334982	–3.693728	–2.164781

H	–6.397944	–4.030405	–0.788948
H	–6.796849	–3.903248	–2.500538
H	–8.342999	–2.498588	–1.080817
H	–7.420724	–1.507344	–2.208677
H	–1.011444	–2.211320	–1.037576
H	–2.149034	–3.417017	–1.671883
H	–2.079263	–3.073997	0.083168
H	–4.309188	–2.672473	0.093346
H	–5.368063	–0.162981	–1.265928
H	–6.771456	–1.989896	0.745452
H	–7.417742	–0.493829	0.081361
H	–6.357354	1.415236	0.848755
H	–5.038329	1.820340	–0.285832
H	–4.773845	1.943368	1.458327
H	–4.660480	–1.633887	2.083330
H	–6.034065	–0.532146	2.368658
H	–4.373984	–0.036274	2.771552
H	–0.598215	–1.641659	1.747185
H	–2.244296	–1.494634	2.258991
H	0.148025	–0.120667	3.616760
H	–0.680597	–1.540336	4.215983
H	–1.969841	1.213101	3.878355
H	–2.776669	–0.221569	4.495557
H	–0.341216	1.127083	5.818463
H	–2.015345	1.235029	6.389164
H	–1.159810	–0.316721	6.434627
C	4.970882	0.185926	–1.968605
N	4.766287	0.155020	–0.509889
C	5.316207	1.382887	0.083339
C	6.734849	–1.455334	–0.309303
C	5.312829	–1.063954	0.156872
C	1.960837	–2.837874	–0.072636
C	4.344887	–2.268049	0.034638
C	7.284025	–2.680844	0.433482
C	6.334813	–3.872725	0.268511
N	2.964067	–1.906610	0.464919
C	4.926797	–3.506765	0.756944
C	2.792701	–1.789271	1.924233
H	6.025433	0.342147	–2.248653
H	4.380923	1.003392	–2.390016
H	4.619232	–0.741695	–2.427209
H	4.843486	2.251703	–0.383154

H	6.407363	1.474850	–0.056593
H	5.094856	1.413124	1.154185
H	6.717640	–1.685001	–1.383009
H	7.411405	–0.601066	–0.182292
H	5.379408	–0.804224	1.221522
H	2.070213	–3.863148	0.320260
H	2.025989	–2.865894	–1.164527
H	0.965675	–2.480029	0.203416
H	4.256878	–2.514786	–1.032629
H	7.400925	–2.450427	1.503142
H	8.284815	–2.926364	0.055207
H	6.705890	–4.744056	0.823483
H	6.298639	–4.167726	–0.791086
H	4.977786	–3.307366	1.835856
H	4.249311	–4.359385	0.628275
H	2.848158	–2.761414	2.440031
H	1.812867	–1.352204	2.129854
H	3.549984	–1.125266	2.349016
C	–1.594609	1.945412	–0.238517
C	–1.915742	5.197659	–0.542687
C	–2.670342	4.278128	0.425232
C	–1.884714	3.012625	0.847098
H	–1.117671	2.472609	–1.091412
H	–2.571629	1.675302	–0.692554
H	–1.663091	4.680078	–1.475416
H	–2.515591	6.078905	–0.803960
H	–0.978414	5.555042	–0.095629
H	–3.619435	3.969299	–0.037933
H	–2.937430	4.855562	1.324977
H	–0.939537	3.355282	1.302932
H	–2.442389	2.547261	1.678668
C	3.003978	5.371162	0.701275
C	1.959434	3.025094	0.456873
C	1.619280	1.644299	1.072956
C	2.671539	4.035068	1.379500
H	3.664664	5.224101	–0.164074
H	2.094987	5.867773	0.337218
H	3.507188	6.062300	1.389670
H	2.584104	2.890238	–0.444282
H	1.041873	3.516149	0.088641
H	2.574597	1.210913	1.435853
H	1.116041	1.857989	2.042567

H	3.593838	3.576319	1.765915
H	2.034902	4.215528	2.258077

Tabelle 192 Standardorientierung von [(*n*-BuLi)$_2$·(*R,R*)-TMCDA]$_2$ (**85b**) [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.0539335618	0.0048001673	0.0473803946
C	–0.0269492353	–0.0247203681	1.5850702434
C	1.3966505346	–0.008041836	2.1780444627
C	–1.3177875188	–3.297474961	4.4735252107
C	1.4401255656	–0.1165394982	3.7292861221
C	–1.9100670503	–5.8344120459	5.970932038
C	–2.8083541252	–6.9300056927	6.5725626522
C	–4.290872423	–6.59437222	6.3388823922
N	–1.362031609	–3.341794046	5.9589866467
C	0.0118283095	–3.3580104143	6.5175054572
C	–2.2288726158	–4.4237764369	6.5334765075
Li	–0.3613252275	0.721105352	4.5178806429
C	–3.7318192894	–4.0857496826	6.364253389
C	–4.6272645315	–5.2155273795	6.9362770045
Li	1.803145587	1.4549012655	5.3242566018
C	–5.2417908536	–2.1228150929	6.2643640435
Li	–2.2467398898	–1.5142318177	6.563748761
N	–4.053018963	–2.7239499481	6.9180285566
Li	–1.3625478944	0.7276181643	6.5991815103
C	–4.2061761093	–2.6795153526	8.3958566953
C	–1.2549826587	–0.5131991253	8.3130212427
C	–1.4563649926	0.6467468099	9.333128628
C	–2.9347672637	0.9703745017	9.6263912623
C	–3.1282432881	2.1485158856	10.595384646
H	0.4676960491	–0.8659965418	–0.3702594766
H	0.4458047072	0.9043296448	–0.3353773351
H	–1.0796190545	0.0008058627	–0.3417007621
H	–0.5556980362	–0.9231548145	1.9405906991
H	–0.5931275342	0.8383132517	1.9703005421
H	1.9675561592	–0.8129415762	1.6733458031
H	1.8767457976	0.9315857301	1.8558520285
H	–0.752330247	–4.1367217814	4.0393062747

H	–0.8401155627	–2.3639920004	4.1695430772
H	–2.3287441502	–3.304044318	4.0603758036
H	2.5126013122	–0.1458467485	4.0226367935
H	1.0858712807	–1.1374741386	4.0005073056
H	–2.0516131143	–5.8298646701	4.8815965751
H	–0.8537516787	–6.0689203399	6.1508385133
H	–2.6195411723	–7.017337284	7.6531569851
H	–2.5578289715	–7.9022492146	6.1297718792
H	–4.9365790264	–7.3609263533	6.785612501
H	–4.5001433416	–6.5955775875	5.258618833
H	0.5569481078	–2.4974875635	6.1240105363
H	0.572236409	–4.2696504637	6.2506658161
H	–0.0328031677	–3.2702773635	7.6062769296
H	–2.0051949894	–4.4315622481	7.6098483739
H	–3.9367323592	–4.0141665495	5.287768764
H	–4.4940616631	–5.2699986978	8.0250586469
H	–5.6819659788	–4.9707093587	6.7581637633
H	–6.1698531019	–2.6824161812	6.4709212395
H	–5.0870165474	–2.0785584001	5.1838807921
H	–5.3712206356	–1.1010302053	6.6292100499
H	–3.3502477645	–3.1528409797	8.8817214118
H	–5.1285987584	–3.1716901422	8.7425276746
H	–4.2298733294	–1.6348614683	8.712003624
H	–0.1651091961	–0.7249400031	8.253333538
H	–1.6748213522	–1.4305095763	8.7771626817
H	–0.9813325147	1.5723084949	8.9550333947
H	–0.9639631504	0.4559667045	10.3073303932
H	–3.4521547949	1.1814436184	8.6778422333
H	–3.4164175438	0.0732189287	10.0457467917
H	–2.686215857	3.0669867689	10.1874447776
H	–4.1900151595	2.3462153086	10.7886446899
H	–2.643768291	1.9480912146	11.55980201
C	3.9722508889	2.3601028251	3.6230435383
N	3.440705357	2.8685065415	4.9149980946
C	2.9509293794	4.2600198167	4.7538299715
C	5.8285586471	3.2206402674	5.7567057973
C	4.389258115	2.7387884583	6.0748711334
C	2.9150670992	–0.6522127185	7.0304790945
C	4.3998273189	1.2972770999	6.6426655896
C	6.7686680477	3.1084016742	6.9709278963
C	6.8007455574	1.6612714568	7.4909259738
N	3.0103003036	0.8261171353	6.9577383415

C	5.3791529231	1.1844511851	7.8407173054
C	2.3972090224	1.4451508198	8.1627053477
H	4.7646607338	3.0020209921	3.2070099433
H	3.1526484535	2.3114238017	2.9036328217
H	4.3639757544	1.3479667478	3.7436195152
H	2.2042974789	4.285966931	3.9566849354
H	3.7562696906	4.967574252	4.4930510831
H	2.4717189314	4.5925666164	5.6778680236
H	6.2438325186	2.6134016007	4.9412283753
H	5.796180119	4.2563864209	5.3959901472
H	3.9842025603	3.3995249373	6.8530228871
H	3.4845285251	–1.077944357	7.8735570657
H	3.2762028051	–1.0902615919	6.0962202585
H	1.8657812388	–0.9261435687	7.1585122935
H	4.7577740513	0.6260312386	5.8490356803
H	6.4246925052	3.7781037734	7.7734121018
H	7.7765581622	3.4419145981	6.6933130365
H	7.448155668	1.5818923887	8.373336785
H	7.2351223424	1.0061369847	6.7207966049
H	5.003050836	1.7946998152	8.6731966643
H	5.4038366884	0.1469429771	8.19541469
H	2.8609897548	1.1005875423	9.1001556414
H	1.3376052601	1.1844643348	8.1861901524
H	2.4724509878	2.5335743263	8.1127256938
C	–2.5304474004	0.1131197666	4.8234136692
C	–4.579456868	1.912611294	3.0069460139
C	–4.8828536855	1.2572638858	4.3635566466
C	–3.639471721	1.1031172344	5.281493199
H	–2.243128396	0.3884269028	3.785017191
H	–3.0078608086	–0.878515812	4.667875599
H	–3.8412471069	1.3312919509	2.4425647242
H	–5.4834618511	1.9950023112	2.390711427
H	–4.1747771305	2.9242149832	3.1437470363
H	–5.3241397786	0.263066095	4.1947871877
H	–5.6483062087	1.8552008928	4.8844796211
H	–3.2093271457	2.1105124912	5.420038531
H	–4.0032406773	0.8052385631	6.2812106539
C	–1.2873277869	5.541898149	3.4402054661
C	–0.6193045015	3.305519434	4.5485935711
C	–0.2347904824	2.510780796	5.8297615968
C	–0.9253938287	4.8094661117	4.7437142932
H	–0.4671473929	5.4812532332	2.7120765621

H	–2.1746973763	5.0954758567	2.9729521404
H	–1.5005846599	6.6037419806	3.6152690604
H	0.1856814527	3.2141472684	3.7965289407
H	–1.5079874357	2.852906774	4.0745053299
H	0.6581596985	2.9991427366	6.2752744307
H	–1.0171447626	2.7369064647	6.5910784879
H	–0.0552908438	5.2923537912	5.2136820282
H	–1.7510583074	4.9049207024	5.4645005767

Tabelle 193 Standardorientierung von (*R,R*)-TMCDA (**9**) [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.6860384761	–0.3604876021	–0.1190602029
C	–0.6894826372	0.3604293279	–0.0974826762
C	–1.4916230753	–0.0519554335	–1.3599957021
C	–0.744411433	0.3078207339	–2.6534510635
C	0.659743304	–0.3098454387	–2.6755104242
C	1.4476565409	0.0509525724	–1.4067220238
C	2.5956065727	–1.0862291461	1.230854179
C	1.748442406	1.1524847484	1.5390449416
C	–1.6984683889	–1.1512617509	1.5948028486
C	–2.5553648509	1.0870734963	1.3117450584
N	1.4387127776	–0.2103449486	1.1336256593
N	–1.4019922091	0.2112611255	1.1785899893
H	0.4888934343	–1.4402283749	–0.2055483961
H	–0.4951947762	1.4400975258	–0.1910239371
H	–2.4715402049	0.4411154722	–1.350912121
H	–1.6847346972	–1.1343023275	–1.3381369247
H	–0.6597587757	1.4028922499	–2.7283654574
H	–1.3219024289	–0.0196138093	–3.5283869486
H	0.5727841823	–1.4049765709	–2.7468185678
H	1.2091437324	0.0168856865	–3.5686107337
H	2.4273990611	–0.4420625706	–1.4284100477
H	1.6412827794	1.1333284279	–1.3918196431
H	2.954318587	–1.0970314495	2.2674203717
H	3.4490038729	–0.7913676937	0.5881599743
H	2.3104862461	–2.1107734451	0.962413129
H	2.1902838674	1.1294491689	2.5422875834
H	2.4668839887	1.6684239629	0.8715043504
H	0.8308564375	1.742986914	1.5982606141

H	–2.1090511229	–1.1273380945	2.6112180517
H	–0.779240387	–1.7413470091	1.6261806776
H	–2.4370550137	–1.6681552883	0.9503883669
H	–2.8806826664	1.0991273415	2.3592585692
H	–2.2792007815	2.1113186533	1.0330110504
H	–3.4288408007	0.7912689467	0.6970708887

Tabelle 194 Standardorientierung von (*n*-BuLi)$_6$ (**86**) [global minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
H	–5.6247489288	0.797558634	1.3151581267
H	–5.6593959785	0.8738139902	3.7950499308
H	–2.3844305881	0.8241161552	–6.7599215823
H	–2.8174319001	1.5195207531	–4.3832251212
C	–4.7836201352	0.3516046556	1.8671468073
H	–5.0096317681	–0.7200938961	1.9648434129
H	–4.4937754702	2.0633425506	3.1915239903
C	–4.7091687715	0.9883749186	3.2594248957
H	–2.5887103994	–0.6093830675	–5.7399153217
H	–3.7337291605	0.1521867994	0.0066297175
C	–1.9491897576	0.2641477724	–5.9231667712
C	–1.8269192019	1.1368623102	–4.6677457827
H	–3.3192358247	1.5956330595	0.9314989837
H	–1.2098785101	2.0200604111	–4.8872227733
C	–3.4959887271	0.5037226121	1.0253407999
H	–3.9264702032	0.5289971213	3.8737218991
H	–2.097341416	1.6060377933	–1.9312387669
H	–0.9678830074	–0.1068779459	–6.2475836015
H	–1.8412377213	–0.490357884	–3.2614918489
C	–1.2221778892	0.4032827906	–3.4554369186
C	–1.0743032764	1.2352785794	–2.1558850019
H	–0.5492995111	2.1704936379	–2.4471329523
Li	–1.535658242	1.0807700046	–0.0479394689
H	–2.5152562554	–1.2796698451	1.6524426846
C	–2.2197726274	–0.2148125811	1.5334003969
H	–1.1158102722	2.9990627855	0.8728187879
H	–2.063845115	0.1047195378	2.5841739289
H	–0.2374706242	0.0155529056	–3.7900626795
H	–0.2221245698	5.3647696396	0.764521082
H	–2.8456321864	–5.624469333	–0.5108365677
H	0.7777539652	3.6462751554	–0.7216056869

H	1.6855333857	6.0494372639	–0.7583575426
H	–0.9280549075	–4.9478736595	–2.0264010587
H	–1.7167947265	–6.9670279549	–0.7558143874
H	–1.9270102096	–3.2026906189	–0.5393813938
C	–0.1120748573	2.5296750186	0.9584206948
C	–1.816808836	–5.9618177066	–0.328335897
C	0.8936718826	3.5567070789	0.3787927391
C	0.7972562974	4.990183537	0.9357153166
Li	0.0944279115	–0.537949307	–1.7952776715
H	–0.0570464206	–2.5475750859	–2.0564307279
C	1.816808836	5.9618177066	0.328335897
H	1.7167947265	6.9670279549	0.7558143874
C	–0.7972562974	–4.990183537	–0.9357153166
Li	–0.702129457	–1.556370656	0.783091272
Li	0.702129457	1.556370656	–0.783091272
H	0.0570464206	2.5475750859	2.0564307279
C	–0.8936718826	–3.5567070789	–0.3787927391
Li	–0.0944279115	0.537949307	1.7952776715
H	–1.6855333857	–6.0494372639	0.7583575426
H	0.9280549075	4.9478736595	2.0264010587
H	1.9270102096	3.2026906189	0.5393813938
C	0.1120748573	–2.5296750186	–0.9584206948
H	2.8456321864	5.624469333	0.5108365677
H	0.2221245698	–5.3647696396	–0.764521082
H	–0.7777539652	–3.6462751554	0.7216056869
H	0.2374706242	–0.0155529056	3.7900626795
H	2.063845115	–0.1047195378	–2.5841739289
H	1.1158102722	–2.9990627855	–0.8728187879
H	2.5152562554	1.2796698451	–1.6524426846
C	2.2197726274	0.2148125811	–1.5334003969
Li	1.535658242	–1.0807700046	0.0479394689
H	0.5492995111	–2.1704936379	2.4471329523
C	1.0743032764	–1.2352785794	2.1558850019
C	1.2221778892	–0.4032827906	3.4554369186
H	0.9678830074	0.1068779459	6.2475836015
H	1.8412377213	0.490357884	3.2614918489
H	3.9264702032	–0.5289971213	–3.8737218991
H	1.2098785101	–2.0200604111	4.8872227733
H	2.097341416	–1.6060377933	1.9312387669
C	1.9491897576	–0.2641477724	5.9231667712
C	1.8269192019	–1.1368623102	4.6677457827
H	2.5887103994	0.6093830675	5.7399153217

C	3.4959887271	–0.5037226121	–1.0253407999
H	3.3192358247	–1.5956330595	–0.9314989837
H	3.7337291605	–0.1521867994	–0.0066297175
C	4.7091687715	–0.9883749186	–3.2594248957
H	2.3844305881	–0.8241161552	6.7599215823
H	4.4937754702	–2.0633425506	–3.1915239903
H	5.0096317681	0.7200938961	–1.9648434129
H	2.8174319001	–1.5195207531	4.3832251212
C	4.7836201352	–0.3516046556	–1.8671468073
H	5.6593959785	–0.8738139902	–3.7950499308
H	5.6247489288	–0.797558634	–1.3151581267

Tabelle 195 Standardorientierung von [*n*-BuLi·(*R,R)*-TMCDA]$_2$ (**84**) [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	7.7581138847	2.5733928513	–3.5559400703
C	5.4166002798	3.0136982827	–3.2821204576
C	7.3926825392	5.4718015351	–3.031786962
N	6.7281986672	3.0482779382	–2.619740214
C	7.677823646	6.8314459305	–2.3804386282
C	7.0181039141	4.3748570338	–2.0056482245
C	8.7921046244	6.6979844454	–1.3366864439
C	8.101069262	4.2643057877	–0.898799886
C	8.408788665	5.6502409245	–0.2836774231
N	7.754668773	3.220254207	0.1073870514
C	8.9479288495	2.657953846	0.7517271857
C	6.8043223502	3.6617833713	1.1397554692
H	7.7692075653	3.1385162783	–4.503093752
H	7.5651453132	1.5223503891	–3.7860915553
H	8.7509837677	2.6330933976	–3.1037642009
H	5.368466595	3.6602611038	–4.1760100401
H	5.2069203527	1.9866480995	–3.5980215768
H	4.6335507073	3.3131535035	–2.5806061029
H	6.5893885183	5.5684522619	–3.7725170493
H	8.2907989566	5.1619525719	–3.5832101984
H	7.9531707313	7.5627376144	–3.1516520898
H	6.7670204932	7.2145027194	–1.8957987821
H	6.0804341812	4.6781676245	–1.5200334985

H	9.7282834164	6.4049536995	–1.8356443759
H	8.985558928	7.6623579942	–0.8489407266
H	9.0228162646	3.9098732236	–1.37873503
H	7.5246533772	6.0155056499	0.2554080323
H	9.2089667856	5.548932676	0.4604749515
H	9.6278269512	2.2553905034	–0.0031845484
H	8.645508968	1.831461938	1.4028970499
H	9.4919889488	3.3952824666	1.3693466045
H	5.9345773366	4.1408195848	0.6846197404
H	6.4432110273	2.7838776191	1.6820426398
H	7.2555051758	4.359989004	1.8649971817
C	11.3882673904	–1.1687230646	–2.2433321071
C	9.8615918404	–1.3198210944	–2.3077186571
C	9.0872756083	–0.2800363729	–1.4687340813
C	7.5488877456	–0.3707527841	–1.4935553082
H	11.9023523084	–1.9276866	–2.8478336871
H	11.7045562866	–0.1829091168	–2.6116732583
H	11.7526349964	–1.2642576188	–1.2111086224
H	9.526806345	–1.2495653467	–3.3538839512
H	9.5775262833	–2.3281703037	–1.968771894
H	9.4153552487	0.7184796674	–1.8088404713
H	9.4543804648	–0.3563789197	–0.4295598794
H	7.2346667556	–0.311918208	–2.559071317
H	7.3105637387	–1.4252812639	–1.2371821214
C	4.7351838556	–2.5047415645	–2.1817678017
N	4.4965708522	–2.2551866409	–0.7531121102
C	3.0883170702	–1.8813114327	–0.5536305105
C	4.0406165236	–4.6242839922	0.061890135
C	4.9626193543	–3.3814448604	0.1044219951
C	4.5428354276	–5.7752336348	0.9435314778
C	7.5282974758	–2.0432811611	1.5451002022
C	5.1983490117	–2.9213781749	1.5682956163
N	6.0935176892	–1.731058533	1.6334279543
C	4.7071120549	–5.3029269222	2.3922514208
C	5.6611893871	–4.1031194907	2.4532516671
C	5.8443315821	–0.9184827921	2.830440323
H	4.4929363413	–1.597431264	–2.7445280076
H	4.1189874545	–3.3281623009	–2.5838423902
H	5.7909961695	–2.7309056598	–2.3522970778
H	2.90278693	–0.9303237361	–1.059699311
H	2.3853544149	–2.6300864544	–0.9558250398
H	2.8718420958	–1.7358198099	0.5074004744

H	3.9316629023	–4.9627355067	–0.9758378877
H	3.0360343833	–4.3432903792	0.4061924379
H	5.9371039803	–3.6743158554	–0.3098869889
H	5.5094301065	–6.1429111506	0.5671303158
H	3.8433012391	–6.6195182221	0.8868855145
H	7.729178663	–2.6997503921	0.6955296119
H	8.0790401765	–1.1146000059	1.3735617873
H	7.9192356649	–2.517922695	2.4610269757
H	4.2321828629	–2.5793924465	1.9621789373
H	3.7239589147	–5.0229644192	2.800035619
H	5.0891235798	–6.1147642637	3.0249623333
H	6.6537075394	–4.4390306701	2.1249255291
H	5.7742623159	–3.7597678833	3.4894165051
H	6.4528092927	–0.0098951391	2.7776145568
H	4.7951725126	–0.6148921735	2.8664937571
H	6.0992645859	–1.4438624569	3.7685771267
C	4.5417508874	1.3937796543	–0.1914637774
C	2.4221205143	2.391221019	1.0020207885
C	3.6651372913	1.4777578764	1.0734426097
C	1.5906051013	2.4236316609	2.292466302
H	3.8804112527	1.0755463042	–1.0274654387
H	4.7716391298	2.4464606346	–0.4626324678
H	1.7900552108	2.0626344262	0.1629692948
H	2.7489724373	3.4119438571	0.7497591826
H	3.3103943623	0.471157284	1.3584922753
H	4.2720265911	1.8144528007	1.9329724503
H	0.7201034675	3.087062073	2.2040447626
H	1.2181790575	1.4220928907	2.548907384
H	2.1914448701	2.7763568695	3.1421451772
Li	6.6590540459	1.5896153355	–0.9491825031
Li	5.7152295421	–0.4915556522	–0.1827429023

Tabelle 196 Standardorientierung von *n*-BuLi·(*R,R)*-TMCDA [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.5523601189	–1.516491613	1.2921787607
C	0.3446085183	2.850773572	0.8226513381
C	1.6491015504	0.75994146	0.90226054
C	3.9113650527	0.2892011633	1.9966756796
N	0.7983799477	1.6652743997	0.0814896586
N	0.2208938627	–1.1432858587	0.0957015857

C	2.4310116124	–1.6298225124	1.2828520052
C	3.1090287693	1.2308468722	1.0858773353
C	1.6144216574	–0.6951035385	0.3624486497
C	3.878162722	–1.1477421216	1.4605531701
C	0.1490505537	–2.2188619348	–0.903686992
C	1.3850585269	2.0698318568	–1.2064364849
C	–3.6802896744	–0.2933944653	–1.3770499614
Li	–0.8470741855	0.5344176514	–0.542794852
C	–2.6979088762	0.8934584108	–1.3285473729
C	–5.0828916527	–0.009245363	–1.9575144135
C	–6.016076219	–1.2287107454	–1.9781393238
H	–0.4864934167	–0.7329302829	2.0531351825
H	–1.6047225309	–1.6223922667	1.009922436
H	–0.2171752314	–2.4657149429	1.7411096425
H	–0.1497547072	2.5429212789	1.7495814363
H	–0.3873890299	3.3910986293	0.2148924405
H	1.1665276933	3.5430961385	1.0743740105
H	1.1804052159	0.7526789544	1.8961258545
H	3.4904015287	0.3096958114	3.0132054205
H	4.9460528442	0.6453327873	2.0806250407
H	1.9535750594	–1.6790826506	2.2711454909
H	2.4181969551	–2.6491309162	0.8771185787
H	3.1190612829	2.2499480727	1.4922130283
H	3.6049000501	1.2781991228	0.1064977106
H	2.1068121987	–0.6928189054	–0.620057528
H	4.4158381496	–1.8237605083	2.1375209798
H	4.403571028	–1.1896189721	0.4945648372
H	–0.9000033569	–2.4017768521	–1.1549262001
H	0.5914689991	–3.1660171254	–0.549344386
H	0.6675512469	–1.9118509675	–1.8178918516
H	0.608414962	2.5519948277	–1.8091188286
H	2.2231264456	2.7770416847	–1.0945632676
H	1.7425903103	1.1953670833	–1.7584417289
H	–3.2443806684	–1.1228272306	–1.9655509718
H	–3.8251410142	–0.7083374443	–0.3613490152
H	–2.603467785	1.2967114696	–2.3583348076
H	–3.1866412974	1.7143815744	–0.7631494558
H	–4.9661424391	0.3840791011	–2.9787439632
H	–5.5460104867	0.8004387722	–1.3733024303
H	–7.0026297262	–0.9859809316	–2.3958791689
H	–6.174168555	–1.6237998234	–0.9647140831

H	–5.5917623718	–2.0422044767	–2.5833561384

Tabelle 197 Standardorientierung von *n*-BuLi·(*R,R)*-TMCDA·Benzol (**88**) [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.0199997989	0.193157575	0.0630090551
C	–0.6675943216	0.625080672	–1.2796688142
C	–1.3509957838	2.0028906628	–1.1299078434
C	–2.382846887	2.0184400305	0.0077373238
C	–1.7373852366	1.596515346	1.3338319917
C	–1.0671429254	0.2212558934	1.1989235849
C	1.7778437364	–1.2522536285	0.9246260477
C	–0.1398336472	–2.2949652523	–0.097005202
C	1.295090601	1.6158893508	–2.4635880747
C	–0.354711779	0.3797709114	–3.7117844962
N	0.713836009	–1.0948518945	–0.0770412815
N	0.3023479968	0.5306783587	–2.4057646165
H	0.7507811955	0.9360598319	0.3107135607
H	–1.4515611904	–0.1070069237	–1.5166167469
H	–1.8284228038	2.2822678862	–2.0773980726
H	–0.5901278625	2.7680319952	–0.9233432184
H	–3.208290176	1.3313468446	–0.2315293376
H	–2.8249771902	3.0191446492	0.0954441899
H	–0.9889994827	2.3465168415	1.6313480509
H	–2.4868366156	1.5686637296	2.13513005
H	–0.591379443	–0.0634895791	2.1457159135
H	–1.8443166488	–0.5287297458	0.9987778927
H	2.3612274499	–2.1470423944	0.6873021736
H	1.3890137482	–1.3546646383	1.9526902051
H	2.452661181	–0.3908394991	0.89014097
H	0.4667643171	–3.1509892273	–0.4085275329
H	–0.5793592574	–2.5252037109	0.8872018579
H	–0.9518450023	–2.1831676655	–0.8208516218
H	2.0756248545	1.3389846559	–3.1796683869
H	1.7703379914	1.755569203	–1.4880089119
H	0.8619747788	2.5790484767	–2.7798727772
H	0.4067628774	0.1761144065	–4.4709564462
H	–1.0425539969	–0.4713388347	–3.6850214545

H	–0.9168884413	1.2791517162	–4.0175328143
Li	1.5082237938	–1.1313569559	–2.0174226986
H	–0.3423321762	–3.9355531691	–4.2389824241
C	2.9403247162	–2.1692189116	–3.0468551842
C	3.0590181068	–3.6881434428	–2.8132920515
C	4.1934196271	–4.4190408838	–3.5645274035
C	4.2591806993	–5.9291958041	–3.2926526586
H	3.9259309786	–1.7155374614	–2.8094925388
H	2.8268589526	–2.0030478365	–4.1384011294
H	2.1102350866	–4.1882382369	–3.0854463863
H	3.192077928	–3.8974190475	–1.734985661
H	5.1520275232	–3.9527777546	–3.2909306202
H	4.0693451038	–4.242838754	–4.6438089697
H	3.3251230012	–6.4265642894	–3.5897320671
H	4.4121777106	–6.1324797939	–2.2233990493
H	5.0791579376	–6.4117262428	–3.8416647892
C	–3.6977820752	–4.7805850265	–2.4696271435
C	–2.5052439917	–5.3651019844	–2.029452553
C	–1.2984554075	–5.0595037765	–2.6671944567
C	–1.2825109576	–4.1704114949	–3.7472087795
C	–2.4759275561	–3.5897724152	–4.1897142948
C	–3.683238343	–3.8931134176	–3.5506371126
H	–4.6363517379	–5.0212621889	–1.9759447739
H	–2.5174991146	–6.0608946841	–1.1937585991
H	–0.3702392551	–5.5130010837	–2.3289587419
H	–2.4663348156	–2.9080207596	–5.0371048773
H	–4.6109519815	–3.4446816271	–3.8984522539

Tabelle 198 Standardorientierung von *n*-BuLi·(*R,R)*-TMCDA·Benzol (**88**) [Übergangszustand, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.0971116835	0.106228424	0.0583035819
C	–0.697181323	0.6213374545	–1.2768894551
C	–0.5029590404	2.1484784871	–1.4137873537
C	–1.0689746463	2.922010813	–0.2149465482
C	–0.4313116952	2.4286609151	1.0890071101
C	–0.6456505773	0.9179033374	1.2542635551
C	0.7174620457	–1.9579857241	1.1229570647

C	–1.622754601	–1.802055276	0.5667829555
C	1.1433713027	0.2336838722	–2.9172942482
C	–1.1442837563	–0.146931579	–3.5671071833
N	–0.2627835745	–1.3711020942	0.1943337086
N	–0.1946235939	–0.1669185395	–2.442884297
H	0.9886686503	0.269833389	0.0162519352
H	–1.7781429486	0.4297688062	–1.2463582442
H	–0.9686400337	2.49593706	–2.3443967082
H	0.5681942155	2.3759967368	–1.4947377494
H	–2.1599855716	2.7880861826	–0.163524022
H	–0.8918747482	3.9966292967	–0.3500109811
H	0.6456510181	2.6546369984	1.0782073469
H	–0.8533552228	2.9597839069	1.9516934107
H	–0.1760287109	0.5676112071	2.1816011743
H	–1.7229306736	0.7313458943	1.3583121683
H	0.6249417272	–3.0479358169	1.0987380319
H	0.5733862802	–1.6246893152	2.1644485758
H	1.7323526543	–1.7018581722	0.8049764482
H	–1.7015989628	–2.8835526538	0.4264571283
H	–1.872863295	–1.567582412	1.6138774509
H	–2.3667515119	–1.3324204567	–0.0823852977
H	1.507471729	–0.5188414187	–3.6226586792
H	1.8505576492	0.2740497696	–2.0844855918
H	1.1409332363	1.2111840615	–3.4253710253
H	–0.7674056719	–0.7906319631	–4.3671777064
H	–2.1123758648	–0.5426683784	–3.2458873368
H	–1.2911247468	0.8637241498	–3.9841632376
Li	0.1072637354	–2.1265289307	–1.7164303172
H	0.5426478312	–3.5858450085	–2.320550909
C	1.9869748466	–3.2206724906	–2.1002403066
C	2.6354652296	–3.5582836352	–3.4481731215
C	4.1673242346	–3.7161712695	–3.4485273429
C	4.7531448547	–4.0715045405	–4.8220453204
H	2.2845662637	–3.9717310116	–1.3477481333
H	2.4018826817	–2.2595107212	–1.7305883206
H	2.3727404864	–2.785607951	–4.1934310295
H	2.1930386373	–4.490828828	–3.8367337502
H	4.4419649443	–4.4928707215	–2.7193564796
H	4.6240945789	–2.7835992731	–3.0831277576
H	4.5188312463	–3.2974004329	–5.5656556198
H	4.3408804014	–5.0187537376	–5.1944278031
H	5.8453484702	–4.1758546412	–4.784644278

C	–3.030509212	–5.6549610737	–3.0837654588
C	–2.3772360278	–5.7658556212	–1.8512658396
C	–1.2655065839	–4.9584637729	–1.5802448157
C	–0.7734760647	–4.0141576946	–2.5012964181
C	–1.4409008063	–3.9482223895	–3.73935456
C	–2.5544287585	–4.7457064377	–4.0345580054
H	–3.8923114846	–6.2806447963	–3.3064062937
H	–2.7309381348	–6.4843471447	–1.112661916
H	–0.7541887785	–5.086780559	–0.6221673785
H	–1.0808853875	–3.2636760422	–4.5107920216
H	–3.0469612581	–4.6665172373	–5.0030947846

Tabelle 199 Standardorientierung von [*n*-BuLi·(*R*,*R*)-TMCDA]$_2$·Benzol (**89**) [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.4765624052	–0.9125830991	–1.0906096851
Li	–0.47690154	–0.9143783179	1.2244628609
C	3.35696764	–0.9078752647	–3.2970929914
C	–1.2293170761	0.935755758	2.1654873726
C	3.2681278264	–0.8043898272	–4.6914725527
C	4.3893920042	–0.4257698968	–5.440151117
C	5.6015239585	–0.1490459079	–4.7949718099
C	5.6918874231	–0.2515453381	–3.4011750659
C	4.5700002655	–0.6307371574	–2.653123813
Li	–1.0556717603	1.0184389666	–0.150801338
N	1.400592967	–1.9832040408	1.8857897144
N	–1.4516291524	–2.7118649868	1.9355864138
C	–0.8424165747	–5.0658111397	2.6947605331
C	2.0098251862	–4.3321578917	2.6750463497
N	0.1485810331	2.720103328	–0.8135890096
C	1.5190651563	–5.5871089919	3.4186776552
N	–2.7649235274	2.3403699719	–0.7128058653
H	–1.7394431723	–5.4588267991	2.2004072214
C	–0.7859490105	3.7897369129	–1.2980911458
H	2.9075135014	–3.9272982682	3.1597826959
H	2.3050115661	–4.6293094758	1.6598508631
H	–1.1310993057	–4.8226768098	3.7266563496
C	–2.1640806682	3.7127607306	–0.5896345227

C	0.928422042	–3.2224123039	2.5913838921
C	–0.3874141203	–3.7675766036	1.9749130292
C	2.1917687004	–1.0956706585	2.7694988857
C	2.1417972313	–2.2302257982	0.6243038034
C	–2.5223233693	–3.0050187332	0.9544434771
C	–2.0370630204	–2.3579734749	3.2505542413
C	0.2551668865	–6.1436098604	2.7421415203
C	1.0783729663	2.2604225255	–1.8713249688
H	0.5021093115	–6.4718940283	1.7212200613
C	0.8925272829	3.0485441695	0.4281862533
H	–0.1132407043	–7.028355216	3.2769870551
C	–3.8536892062	2.1030198927	0.2663249486
H	1.2938909187	–5.3384613681	4.4668910961
C	–3.2253537979	1.9810396323	–2.0753995775
C	–1.4173706522	–1.0902748607	–2.3072426362
H	–0.3411024548	–1.9273404872	–0.6560134542
H	0.5302669128	–0.652030012	–1.4842643053
H	2.4840502655	–1.1998560938	–2.7203662554
H	–2.2610679002	0.5780399506	2.3835203897
H	–1.3833172395	1.9612530041	1.7659843918
C	–0.4966630459	1.1116217251	3.5158444026
H	2.3277097019	–1.0201719156	–5.1894578899
H	4.3197759903	–0.3471054751	–6.5209539429
H	6.4711971856	0.1441871532	–5.3753523391
H	6.631780673	–0.0376403265	–2.9010360426
H	4.6411293436	–0.7123019032	–1.5723476356
H	–0.9505403749	3.5725218475	–2.3617440972
H	2.3137958311	–6.3437610996	3.4380202732
C	–0.1840531837	5.2166093969	–1.2111554948
H	–1.9976372601	3.8553564515	0.4871767637
C	–3.1059369743	4.8422591719	–1.0871865927
H	0.7043846915	–2.9030163738	3.6178682868
H	–0.1865202057	–4.0128943164	0.922737234
H	1.6226202465	–0.8660156178	3.671422407
H	2.3846530393	–0.1545765924	2.2468507644
H	3.1633178763	–1.5353861809	3.0573848116
H	2.2410785893	–1.2827135002	0.0892510725
H	1.5855470749	–2.9096216	–0.023141194
H	3.1498763523	–2.6417769966	0.7974504229
H	–2.0795745947	–3.2217194515	–0.0198303385
H	–3.1543996585	–2.1187873665	0.8474923656
H	–3.1623658923	–3.8515993744	1.2573724049

H	–2.6323341211	–1.4499644424	3.1319240599
H	–1.2494537258	–2.1403685499	3.9746860936
H	–2.6848780569	–3.1509051841	3.6596331765
H	0.5104902886	1.8981453644	–2.7320507094
H	1.6698928149	1.4258337092	–1.4898140221
H	1.7712772393	3.0522335311	–2.2064443528
H	1.3301209528	2.1285095227	0.8241901573
H	0.2115992653	3.4353452449	1.1881748518
H	1.6989981765	3.7816501411	0.2617490115
H	–3.4984197712	2.3261559284	1.2737308703
H	–4.1303830255	1.0449988384	0.2329692266
H	–4.75755683	2.6997187895	0.0549025817
H	–3.4781604586	0.9189787516	–2.087731393
H	–2.4301957221	2.139005212	–2.8063325912
H	–4.1143394607	2.5517859063	–2.391453228
C	–1.1449560808	6.2985896076	–1.7346699538
H	0.761944069	5.243255296	–1.7670507974
H	0.0567266881	5.447433337	–0.1650104162
H	–4.0486372	4.8032117632	–0.528018216
H	–3.3569405367	4.6661768385	–2.1425510064
C	–2.4759779685	6.241937001	–0.9667642388
H	–1.3345965206	6.1448093258	–2.8078346764
H	–0.6822207071	7.2888131246	–1.6353908357
H	–3.1745099001	6.9990268308	–1.3455620506
H	–2.2960488662	6.4801262615	0.0924481832
H	–2.4492611502	–1.2936858722	–1.9653611182
C	–1.0357638454	–2.2066905023	–3.3124949249
H	–1.4768928368	–0.1464148405	–2.8756865761
C	–2.0028871655	–2.3385218983	–4.5022681024
H	–0.9829932969	–3.1644239249	–2.7708717126
H	–0.0167857873	–2.0123626604	–3.6823923831
H	–3.0219118892	–2.559348304	–4.1571292976
H	–1.7029313816	–3.1399410187	–5.1895124538
H	–2.0463795272	–1.404410851	–5.0785223043
C	–1.169724205	2.0499678467	4.5501986477
H	0.5262670485	1.4904196439	3.341341514
H	–0.3648873893	0.1307466917	4.0080380006
H	–1.2888110825	3.045854714	4.0950062898
C	–0.3973686202	2.1758315674	5.8751717821
H	–2.1885013575	1.6823300551	4.7475525022
H	–0.901522483	2.8460809388	6.5829883983
H	0.613757313	2.569568465	5.705080464

H	–0.2913918957	1.1967974354	6.3619863775

Tabelle 200 Standardorientierung von [*n*-BuLi·*(R,R)*-TMCDA]$_2$·Benzol (**89**) [Übergangszustand, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	0.4817459296	–1.6994493263	–1.2737113358
C	0.278137538	–3.1054228005	–1.8536229218
C	1.5542103172	–3.9269910092	–2.1193898792
C	1.2823892835	–5.3241895917	–2.6948346953
H	0.9827070995	–1.7805318816	–0.2915641177
H	1.2076687616	–1.1866420369	–1.932066826
H	–0.2909975419	–3.0346001132	–2.7955966482
H	–0.3666871582	–3.6934819361	–1.1809497701
H	2.1226302072	–4.0197211353	–1.1814441458
H	2.2029129756	–3.3675968212	–2.8114032221
H	2.2120958894	–5.8799393066	–2.873793015
H	0.7427687632	–5.260630148	–3.6491968209
H	0.6651642864	–5.920484996	–2.009490036
Li	0.4900198131	0.624524175	–1.310440971
C	–2.3590418376	–1.14445263	–1.3018750423
C	–3.0907263282	–2.352665253	–1.2814169766
C	–4.3214045676	–2.5073608464	–1.9319329098
C	–4.8732473487	–1.4388510813	–2.6480130548
C	–4.177291182	–0.2273019187	–2.703824249
C	–2.947396296	–0.0987820874	–2.0443771203
H	–2.6874792871	–3.2144752397	–0.7483636568
H	–4.8493365613	–3.4595081812	–1.8868454675
H	–5.82754236	–1.5513697076	–3.1583598619
H	–4.5960333971	0.6145397524	–3.2551895037
H	–2.4388464641	0.8651822245	–2.0961308124
C	–0.6133984815	1.9292739438	0.07094747
C	–0.1146756949	2.5608409158	1.3885042507
C	–0.2398994615	4.0935400948	1.5164231849
C	0.2632755996	4.6562851893	2.8532911097
H	–0.1330697794	2.5098645757	–0.7465880322
H	–1.6754231795	2.2315000282	–0.0547288596
H	0.9423731583	2.2957083303	1.5629031784
H	–0.6462833995	2.1166093436	2.2464438632

H	–1.2934138769	4.3755956881	1.369814647
H	0.3125171078	4.5635183899	0.6883917099
H	1.3232436774	4.4147492627	3.0120860024
H	–0.2977809054	4.2341391107	3.6984265826
H	0.1616031075	5.7482604891	2.9021375683
Li	–1.6444102	0.0458893058	0.602536233
N	0.5968822342	1.3116189068	–3.4868851492
N	2.6794440153	1.1358695747	–1.4415346601
C	1.9983555457	1.7352903372	–3.7886948802
C	3.0335910588	1.0149349302	–2.8868761951
C	–0.3470840918	2.4093992695	–3.7474120637
C	0.1599909821	0.1093235602	–4.2230245239
C	3.4315799048	0.1860317004	–0.6072419733
C	2.8448116488	2.4907266578	–0.8909341057
C	2.3826838478	1.6101136258	–5.2822377444
C	4.4694263379	1.4888177336	–3.2226263284
C	3.803972898	2.1085274858	–5.5715518766
C	4.8159214024	1.3458101924	–4.710643942
H	2.0390755624	2.8034663776	–3.5403989065
H	2.9740892087	–0.0603711849	–3.1061690872
H	–0.1043735628	3.2712502094	–3.1185937729
H	–1.3598568656	2.0844770955	–3.4969203526
H	–0.3469416892	2.729110577	–4.804613249
H	–0.7819597506	–0.2455440126	–3.7975881395
H	0.8935740751	–0.6926981832	–4.1154101941
H	0.0041822677	0.3039061205	–5.2967182938
H	3.3212039567	–0.8273774979	–1.0014180107
H	3.019559026	0.2015298256	0.4073291178
H	4.5051860602	0.4308462269	–0.5377967456
H	2.4338406581	2.5092753759	0.1205489917
H	2.2928459504	3.2235977436	–1.4836659152
H	3.9000925941	2.8054105946	–0.8351776841
H	1.6552410323	2.160354265	–5.8922660163
H	2.3190337742	0.5589599538	–5.5917378706
H	5.1921908504	0.9306723076	–2.6156122545
H	4.5781783082	2.5462194855	–2.9453808149
H	4.030971684	1.9858324684	–6.6386008024
H	3.8769555227	3.1855501506	–5.3568676792
H	5.8347967847	1.7127517899	–4.8908748145
H	4.8108061996	0.2829003396	–4.9953120284
N	–3.5632421685	0.4115392658	1.8286793416
N	–1.1555727912	–1.1618792236	2.3859697778

C	–3.5424076835	–0.5849202129	2.9394303619
C	–2.1081064948	–0.8112833672	3.4817199189
C	–4.733541597	0.216823384	0.9569448097
C	–3.5364085112	1.8116021749	2.2827159489
C	0.2382738646	–0.8847966	2.7654709891
C	–1.2647353042	–2.5560744936	1.9210929435
C	–4.5228641548	–0.254492279	4.0918411108
C	–2.1134505243	–1.8280556001	4.6493729597
C	–3.0879672495	–1.449623801	5.772409892
C	–4.5062468676	–1.3002148232	5.213317654
H	–3.8751477139	–1.5276582349	2.4859491245
H	–1.7496764562	0.1484697346	3.8784065213
H	–4.7252437971	–0.7904514419	0.5342794894
H	–4.6830339852	0.9236314378	0.1251477609
H	–5.6874535146	0.381527327	1.4880531877
H	–3.3340632184	2.4580259864	1.4243642773
H	–2.738507798	1.968979512	3.0120978582
H	–4.4906491153	2.1313187615	2.7333577375
H	0.3427279902	0.1612160873	3.0655040219
H	0.8829508025	–1.0566670455	1.8988575685
H	0.5943146172	–1.5292788629	3.5879549237
H	–0.6889802011	–2.664513869	0.9998690006
H	–2.3042573997	–2.8045606118	1.695852271
H	–0.8785081844	–3.2813230185	2.6561680185
H	–5.5370953406	–0.1472210358	3.6882420717
H	–4.2564087079	0.7166875603	4.5294672502
H	–1.0972843378	–1.9320781444	5.049282194
H	–2.4022946292	–2.8165428155	4.2681980237
H	–3.0580450428	–2.2119944362	6.5618318939
H	–2.7763829925	–0.5025637363	6.2385388658
H	–4.8538416946	–2.2712251276	4.8294665717
H	–5.2078648994	–1.0071837478	6.0052798741
H	–0.9800055371	–1.2256944772	–1.150236097

Tabelle 201 Standardorientierung von Benzol [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–1.2111807352	0.	–0.6992755235
C	–1.2111807352	0.	0.6992755235
C	0.	0.	–1.398551047

C	0.	0.	1.398551047
C	1.2111807352	0.	–0.6992755235
C	1.2111807352	0.	0.6992755235
H	–2.1527954605	0.	–1.2429170386
H	–2.1527954605	0.	1.2429170386
H	0.	0.	–2.4858340773
H	0.	0.	2.4858340773
H	2.1527954605	0.	–1.2429170386
H	2.1527954605	0.	1.2429170386

Tabelle 202 Standardorientierung der halben Leiterstruktur **90** [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.0974807878	–0.0943889619	1.3961750283
C	1.3238839847	–0.5503722617	1.752416301
C	–1.7556192773	0.5345914904	–0.5568497437
H	0.4418063962	0.7778043323	–0.4773815644
H	–0.0993209175	–0.8844912213	–0.6085599139
H	–0.3188051763	0.8598128162	1.8964758353
H	–0.8292797437	–0.8173619915	1.7854756815
H	2.0730688144	0.171293658	1.399124921
H	1.5576351959	–1.5189008065	1.2900124102
H	1.4561733951	–0.6598310635	2.8365047755
H	–2.0336840352	1.4077495527	0.0694395371
H	–2.4674718617	–0.2528489394	–0.2475652548
C	–1.4801929604	1.4841637012	–4.1415814031
C	–0.3079995705	1.0171214096	–5.0353172835
C	–0.357540793	1.4396622308	–6.517789522
C	0.8389475103	0.9549650011	–7.3483800572
H	–1.5392926762	2.5909434342	–4.2275740763
H	–2.4165069084	1.1562383493	–4.6403965262
H	–0.2217449379	–0.0840754206	–5.0040741544
H	0.651376907	1.3818321731	–4.6224738545
H	–0.422932123	2.5368799812	–6.5690221942
H	–1.2919722532	1.0610341555	–6.9603596597
H	0.765227371	1.2731612042	–8.3965773021
H	0.9108350441	–0.1413153033	–7.3388495636

H	1.7835421036	1.3480917613	–6.9485876812
C	–5.1608262294	1.1500408665	–1.1343824812
C	–5.0686847551	2.159457985	–3.318474154
N	–4.8855402199	0.9128161647	–2.5615608753
C	–7.1428967398	–0.2505444758	–2.8063249875
C	–5.6372709051	–0.2289127545	–3.1576187858
C	–7.886903868	–1.4205486391	–3.4650941092
C	–4.9720473696	–1.5883976405	–2.8104486666
N	–3.514609712	–1.580933807	–3.1248357369
C	–7.2388896807	–2.7549419519	–3.0770760403
C	–2.7716815338	–2.5798523864	–2.3428996077
C	–5.7515341248	–2.7587086939	–3.4537283708
C	–3.1954624314	–1.7341841622	–4.5537444463
H	–4.4181340908	1.8519302247	–0.7453389426
H	–6.1649797671	1.5687598345	–0.9569354052
H	–5.0610509392	0.2231031491	–0.5638483732
H	–4.4109297266	2.9288865085	–2.9024468961
H	–6.1052166955	2.5376955801	–3.2810410066
H	–4.7835236911	2.0072528087	–4.3634708058
H	–7.2623620161	–0.3350361102	–1.717936577
H	–7.5998870336	0.7031641886	–3.0988319129
H	–5.5559651179	–0.0915172073	–4.2442616502
H	–8.9436783158	–1.4024004177	–3.1688107359
H	–7.8666301567	–1.3083640581	–4.559618542
H	–5.0285687256	–1.7118257238	–1.7202794279
H	–7.3506746673	–2.9149712181	–1.9940534604
H	–7.7499411959	–3.5913305096	–3.5711186832
H	–2.9482204208	–2.4241712695	–1.2749048906
H	–1.7003342907	–2.4543074285	–2.5284396109
H	–3.0424927289	–3.617832662	–2.6027685469
H	–5.2903509032	–3.7108361823	–3.1634975266
H	–5.671817229	–2.6923530109	–4.5472239608
H	–3.7734055776	–1.0286098907	–5.1560218716
H	–2.1369622395	–1.5043569746	–4.7041045102
H	–3.3845273742	–2.7538051011	–4.9276837398
Li	–0.8374352702	1.3635572517	–2.1801013185
Li	–2.8258503944	0.3638240117	–2.5763106442

Tabelle 203 Standard Orientierung der halben Leiterstruktur und Benzol **91** [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	2.987561875	–0.1400697767	–4.0421330978
C	3.0131007271	0.2113050878	–2.5478410164
C	1.8211136051	–0.3523992383	–1.7467746704
C	3.7797847995	–3.8090317592	0.4208802968
C	2.717786115	–4.1532143103	–0.4197171889
C	–3.3871171419	–2.8006834928	1.1874047298
C	3.5479476797	–3.5619416563	1.7782278923
C	–0.4106209729	2.7890576123	–0.947026854
C	–4.4717647682	–1.8078021435	1.6212773128
C	1.7893244014	–0.0366610845	–0.2341528405
C	–2.117963038	–2.1385407982	0.59666222
C	1.4205930042	–4.2543215448	0.0974189611
C	2.2531987036	–3.6593156484	2.2963490752
C	1.1868933952	–4.0090872179	1.4569763866
C	–2.488548145	1.7772427308	–0.2838872712
Li	0.6232880578	–1.5474113688	0.6363340622
N	–1.1879657163	2.2709638833	0.1909707947
Li	–0.0537152383	0.600515106	0.945708164
C	–1.7551800242	4.6513833281	0.9039958993
C	–1.257989535	–1.2609484423	1.534899078
C	–1.329095057	3.2264945538	1.3275216718
C	–1.9235024955	5.5992980059	2.098945887
C	–0.0435534264	3.2726461285	2.1957042904
N	0.3879615487	1.9056270986	2.6025487987
C	–0.6276336083	5.6653984932	2.9152417334
C	1.8292736134	1.8359246499	2.8823744202
C	–0.2120070242	4.2608755377	3.3737825033
C	–0.3636935866	1.33708759	3.7335684281
H	3.8511258433	0.2772334935	–4.5767077925
H	2.0798206458	0.2470547848	–4.5251719341
H	2.998374999	–1.2282746101	–4.1934195855
H	3.0334261157	1.3054093086	–2.4266034502
H	3.9458914084	–0.1584031316	–2.0959799612
H	0.8941194752	0.0058795294	–2.2301206747
H	1.8090553333	–1.44638434	–1.9049213023
H	4.7857802731	–3.7257920926	0.0179999283
H	2.8972583008	–4.3403658716	–1.4750583121
H	–3.8178403309	–3.495664358	0.4478749624

H	–3.0920667124	–3.4124417856	2.0538990098
H	4.3747542367	–3.2893347679	2.429158623
H	–0.1894635207	1.962331667	–1.6276221276
H	–0.9476660179	3.5675210678	–1.5135360526
H	0.543983003	3.1989903542	–0.6075359381
H	–4.8077915608	–1.1968250758	0.7714617107
H	–5.3515526319	–2.3253801922	2.02486704
H	–4.0999232998	–1.1272966882	2.3963720245
H	1.8763573568	1.0654372805	–0.1309835512
H	2.748574996	–0.3937206749	0.1979834612
H	–2.4252910907	–1.5477128982	–0.2838884866
H	–1.5097487644	–2.9624743552	0.1753610578
H	0.5949071135	–4.532832517	–0.5529955098
H	2.0710852629	–3.4688555557	3.3509554605
H	–2.3224427761	1.0030903003	–1.0393683892
H	–3.1104523841	2.5681992697	–0.738318818
H	–3.04119046	1.3243180376	0.5438248314
H	0.1822246031	–4.0982646126	1.8616080425
H	–0.9950197611	5.0750550613	0.2338755975
H	–2.6868911594	4.599509751	0.3269373209
H	–1.0946326221	–1.832063423	2.4745381472
H	–1.8873957636	–0.4132667879	1.8683935125
H	–2.1322329768	2.8131033925	1.9527012876
H	–2.2089666977	6.5979969906	1.7437991642
H	–2.7447575265	5.2490552193	2.7424216008
H	0.767862114	3.6532633113	1.5606387012
H	0.1695246539	6.1101794884	2.3005265386
H	–0.75176346	6.319900539	3.7876989102
H	2.3963345789	2.1912843389	2.0174702009
H	2.1087441293	0.7922014326	3.0558050162
H	2.1229475201	2.422638614	3.7706173838
H	0.7227000229	4.3087173288	3.9464645624
H	–0.9807626301	3.8822602722	4.0608065787
H	–1.4397986177	1.4296278535	3.56691368
H	–0.1369209811	0.2696539321	3.8053139886
H	–0.1131249876	1.8137427951	4.6958588758

Tabelle 204 Standard Orientierung der halben Leiterstruktur und Benzol **91** [Übergangszustand, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	0.3485045437	0.3350289027	0.5419642762
C	–0.2399093738	0.2246635058	1.9549224592
C	–1.422333536	–0.7575006974	2.0638029469
C	1.1564590627	–6.2454004737	2.6354594587
C	0.3131020867	–5.8937296459	1.5757714183
C	0.7857894064	–5.9273855883	3.9465371461
C	–5.28759281	0.8723416268	2.1234303159
C	–2.0490645343	–0.9136098356	3.4704968592
C	–0.8879553911	–5.2219218005	1.8367061864
C	–0.4210408939	–5.2568604913	4.1838049235
C	–1.2866626692	–4.8729631792	3.1415651753
C	–6.0342253555	–1.3649142216	1.6400165611
Li	–2.3195974652	–2.9934922933	3.4233899261
N	–5.7309526648	–0.4037322943	2.7152715223
Li	–4.1007171014	–0.9987768542	3.8469301601
C	–8.0684890367	0.5188620277	3.1777451387
C	–6.850685845	–0.2785067044	3.6973155357
C	–9.2069650413	0.5853791471	4.2057785142
C	–6.3565781662	0.303156327	5.0486188408
N	–5.1461700116	–0.4190217578	5.54704292
C	–8.709370644	1.1845190651	5.5264561689
C	–4.3110247679	0.4302178719	6.4128478046
C	–7.5167142816	0.3822029862	6.0655091651
C	–5.4348647	–1.6939902737	6.232169765
H	1.1858242031	1.0436196796	0.5051390575
H	–0.4074175922	0.6770255205	–0.1783394982
H	0.7202714101	–0.636989713	0.1923996935
H	–0.5719950061	1.2170332409	2.2971593724
H	0.5445819424	–0.0918512478	2.6575873288
H	–2.195245736	–0.4427545178	1.3403089777
H	–1.0719637033	–1.7358826455	1.6886875518
H	2.090468382	–6.7690053266	2.4418280661
H	0.5927578492	–6.1456706964	0.5535113514
H	1.4350887163	–6.2045602191	4.7762132497
H	–4.3559787835	0.700788906	1.5751957479
H	–6.0230475942	1.2958329661	1.421878336
H	–5.0866473332	1.6128592457	2.9029114173
H	–2.3293530225	0.1079597836	3.8122218776

H	–1.2274123842	–1.1655512333	4.1735384403
H	–1.5324027609	–4.9699093258	0.9907007114
H	–0.6939188799	–5.0354312029	5.2191339405
H	–5.1341290909	–1.5218297264	1.0373269738
H	–6.8363890188	–1.0162610423	0.9693958564
H	–6.3263580446	–2.3267025651	2.0711223754
H	–2.652728181	–4.5903267073	3.4364940531
H	–7.7579037779	1.544517295	2.9360425927
H	–8.4302252699	0.0716048231	2.2441123104
H	–7.1809244451	–1.3097038488	3.8825918165
H	–	1.1780825624	3.8009901766
H	–9.6031361235	–0.4245714975	4.3883325627
H	–6.0190206832	1.3310557537	4.8598370762
H	–8.4133858349	2.2321721077	5.3661505453
H	–9.5143137134	1.197838536	6.2720114053
H	–4.0373108493	1.3485451819	5.8839302274
H	–3.3889168416	–0.1051690624	6.6587731904
H	–4.8125790667	0.702237231	7.3565425732
H	–7.1539708173	0.8236957813	7.0020893492
H	–7.8619399853	–0.6315106231	6.3082093804
H	–6.0693362713	–2.3322859045	5.6118385702
H	–4.4935946111	–2.227198268	6.3963345244
H	–5.9206641862	–1.5512984982	7.2099174495
C	–6.1816924818	–5.8428636033	3.6084103024
C	–4.7083537877	–5.6045773783	3.2315354936
C	–4.0639965211	–4.3249046946	3.7788814209
C	–6.7640398918	–7.1436264597	3.0384434686
H	–6.7847387516	–4.989131292	3.2597872797
H	–6.2722468916	–5.8498364189	4.7052698702
H	–4.6249093254	–5.6119872317	2.1321257005
H	–4.1196286404	–6.4727743982	3.5694012682
H	–4.1671566999	–4.2953744537	4.8784333433
H	–4.6284337481	–3.450994127	3.3882414038
H	–6.7148728808	–7.1518470003	1.9413952508
H	–7.814555872	–7.2806431952	3.3261815492
H	–6.2039442555	–8.0169088393	3.3975188298

8.3.3 Angaben zu den quantenchemischen Rechnungen der Deprotonierung von *N,N'*-Dimethylpiperazin (**67**) (Kapitel 4.2.1)

Tabelle 205 Energien der berechneten Verbindungen; [B3LYP/6–31+G(d)].

Compound	Min./TS	SCF (Hartree)	ZPE (Hartree)
t-BuLi·Piperazin Monomer	Global Min.	–511.934167	–511.609466
t-BuLi·Piperazin Monomer TS	TS	–511.878310	–511.559451
Piperazin	Global Min.	–346.564557	–346.361071
$(t\text{-BuLi})_6$	Global Min.	–661.533790	–661.048268
t-BuLi·Piperazin Dimer	Global Min.	–1023.901010	–1023.249911
t-BuLi·Piperazin Dimer–TS	TS	–1023.845528	–1023.199592

Tabelle 206 Standardorientierung von *t*-BuLi·Piperazin Monomer [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
Li	0.466869	–0.004974	–0.027707
C	2.527618	–0.004125	–0.009744
C	3.100162	–1.029139	–0.999344
C	3.054869	–0.358711	1.388824
C	3.088135	1.375118	–0.384794
H	2.803995	–0.819514	–2.039968
H	2.776768	–2.058028	–0.772758
H	4.217467	–1.046593	–0.992164
H	2.731129	–1.358950	1.719974
H	2.724533	0.358891	2.157420
H	4.171653	–0.365640	1.431629
H	2.755262	2.165824	0.306945
H	2.791481	1.687721	–1.399164
H	4.205238	1.398024	–0.367780
N	–1.247616	–1.269683	–0.015065
C	–1.866362	–0.777931	1.228311
C	–1.965482	0.772054	1.183803
N	–1.238251	1.271993	0.006291
C	–2.008320	–0.764192	–1.168938
C	–1.900760	0.785241	–1.216006
C	–1.106637	2.730319	0.009612

C	–1.128997	–2.729111	–0.022356
H	–1.240732	–1.103739	2.066406
H	–2.866888	–1.224102	1.371560
H	–1.514792	1.210736	2.079394
H	–3.021075	1.097650	1.155947
H	–3.064542	1.097650	–1.108345
H	–1.588877	–1.205460	–2.078398
H	–1.301269	1.107818	–2.074360
H	–2.902588	1.237912	–1.326402
H	–0.532919	3.045122	–0.867107
H	–0.561372	3.045273	0.904055
H	–2.087568	3.237690	–0.007266
H	–0.614123	–3.048882	–0.933003
H	–2.113343	–3.227911	0.024603
H	–0.532332	–3.048995	0.837121

Tabelle 207 Standardorientierung von *t*-BuLi·Piperazin Monomer TS [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.887520	0.885908	–1.370500
C	2.094993	–1.484089	–0.923028
C	–2.411140	0.235399	1.025652
C	–1.649336	1.573896	0.777572
C	2.388928	–0.336146	0.055982
C	–1.937333	–0.258593	–1.272785
C	–2.674250	–2.044573	0.221214
C	0.764818	2.088982	–0.003959
C	2.372148	–0.849815	1.504670
C	3.763254	0.252239	–0.254944
N	–0.468885	1.262019	–0.024841
N	–1.899258	–0.808355	0.100709
H	0.004158	0.563373	–1.921652
H	–1.306033	1.749312	–1.922450
H	2.074499	–1.127627	–1.962352
H	1.129072	–2.004689	–0.748505
H	2.852357	–2.004689	–0.871234
H	–3.498161	0.367273	0.882117
H	–2.258392	–0.124005	2.050829
H	–1.326459	2.012212	1.725319
H	–2.303838	2.316264	0.281368

H	1.679695	0.868593	–0.100542
H	–2.953872	0.103543	–1.507948
H	–1.710172	–1.063501	–1.980255
H	–2.253898	–2.809923	–0.439544
H	–3.737592	–1.901842	–0.041075
H	–2.622186	–2.410848	1.252237
H	0.893907	2.460836	1.023732
H	0.667887	2.967408	–0.670999
H	1.422129	–1.341292	1.813808
H	2.545569	–0.031615	2.216767
H	3.142811	–1.621195	1.694171
H	4.576927	–0.488550	–0.150247
H	3.989830	1.094083	0.413535
H	3.798448	0.642623	0.413535
Li	0.274318	–0.494981	0.384654

Tabelle 208 Standardorientierung von Piperazin **67** [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
N	1.402886	–0.000001	0.311756
C	0.739078	–1.200817	–0.192350
C	0.739085	1.200821	–0.192342
C	2.828751	–0.000008	0.021980
C	–2.828751	–0.000009	–0.022221
H	0.826641	–1.276471	–1.295619
C	–0.739089	–1.200794	0.192463
H	1.229216	–2.080050	0.243324
H	1.229232	2.080052	0.243328
C	–0.739090	1.200807	0.192455
H	0.826644	1.276475	–1.295610
H	–1.229241	2.080056	–0.243174
H	–0.826647	1.276432	1.295730
N	–1.402852	0.000004	–0.311683
H	–0.826653	–1.276411	1.295738
H	–0.826653	–2.080044	–0.243161
H	3.295566	0.887318	0.464287
H	3.048210	0.000035	–1.065204
H	3.295548	–0.887381	0.464214
H	–3.048488	–0.00007	1.064915
H	–3.295474	–0.887325	–0.464649
H	–3.295474	0.887376	–0.464527

Tabelle 209 Standardorientierung von (*t*-BuLi)$_6$ [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–1.591202	–2.148706	1.807477
C	–1.756247	–2.614332	–0.619100
C	0.336159	–3.132739	0.600089
C	–0.800869	–2.092946	0.477742
H	–1.948856	–3.176337	2.020980
H	–2.494716	–1.516087	1.806571
H	–0.983707	–1.857245	2.678348
H	–2.121046	–3.639743	–0.405571
H	–2.658143	–1.992481	–0.727700
H	–1.283872	–2.685333	–1.614716
H	–0.049230	–4.140626	0.856429
H	1.064130	–2.896197	1.395604
H	0.900974	–3.257801	–0.336575
C	–2.960711	1.202300	0.330522
C	–1.737579	1.346245	–0.603125
C	–2.237761	1.040363	–2.033772
C	–1.346609	2.842255	–0.587286
H	–3.392056	0.190271	0.309829
H	–2.739700	1.444166	1.385108
H	–3.783176	1.889587	0.045584
H	–2.594473	0.002970	–2.163807
H	–3.102426	1.674804	–2.315647
H	–1.468981	1.221437	–2.800148
H	–1.076244	3.199511	0.417682
H	–2.177828	3.492677	–0.927726
H	–0.504781	3.086080	–1.260208
C	–0.002504	1.311082	2.911613
C	1.957849	–0.157573	2.544119
C	1.026443	0.861548	1.848959
C	1.893978	2.100250	1.528296
H	–0.662757	0.496631	3.259727
H	0.486905	1.689517	3.831905
H	–0.649764	2.127256	2.557205
H	1.417807	–1.039669	2.919925
H	2.469122	0.282738	3.424225
H	2.773440	–0.522894	1.895197
H	2.342141	2.539894	2.442589
H	1.327801	2.927924	1.065031
H	2.737574	1.866701	0.861826

Li	–0.958591	0.072738	1.097403
Li	1.119328	–0.871630	0.392037
Li	–0.653070	–0.557718	–1.194967
Li	0.509904	1.347646	–0.311788
C	1.003455	–0.947805	–2.932541
C	2.825084	–0.768065	–1.261218
C	1.502812	–0.116501	–1.726331
C	1.873451	1.277626	–2.282269
H	0.733316	–1.980377	–2.659455
H	0.132317	–0.500894	–3.438812
H	1.789106	–1.045157	–3.708953
H	2.701168	–1.802697	–0.896249
H	3.325074	–0.195177	–0.464831
H	3.562766	–0.844428	–2.085720
H	1.013623	1.796874	–2.7329277
H	2.304695	1.953079	–1.522669
H	2.642582	1.219893	–3.079162

Tabelle 210 Standardorientierung von *t*-BuLi·Piperazin Dimer [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	1.969885828	1.3201749061	–3.2578476031
C	–0.44555629	1.3607925702	–2.8228015921
C	0.927905699	1.5214100744	–2.1390519338
C	1.0381348286	2.9797424737	–1.6709928239
H	1.8096032946	2.0168603038	–4.1114303735
H	1.9426495572	0.3064525853	–3.691310916
H	3.0029882667	1.5058465857	–2.9227201728
H	–0.594320719	2.0844424691	–3.6549675777
H	–0.5890662899	0.3618480579	–3.2649079127
H	–1.2957259844	1.5366409708	–2.1419730333
H	0.8990759032	3.7059699829	–2.504696416
H	2.018732321	3.2038507373	–1.2259786421
H	0.2850550514	3.2405497968	–0.9110795237
C	5.1113400187	–0.348777682	–1.7273337313
N	4.3348832549	0.1550035942	–0.5803430818
C	4.6893713032	1.5721512784	–0.3341589442
C	4.6719962316	–0.6364185569	0.6252408279
C	4.0011832847	2.110038725	0.9170178293

C	3.9846092725	–0.0844203734	1.8701269373
N	4.3608468346	1.3106792704	2.0861573807
C	3.7981501559	1.8508461314	3.3159353394
H	4.8598807864	0.2226767961	–2.6259232915
H	4.8740286011	–1.4008412449	–1.9070655383
H	6.1974650165	–0.262164227	–1.5505667327
H	4.3904316084	2.1623280808	–1.2066082824
H	5.7830198336	1.6698074036	–0.2134146823
H	4.3628199567	–1.6737341659	0.4569918319
H	5.764860356	–0.6268082536	0.786061225
H	2.904845705	2.126388807	0.756251027
H	4.3236779725	3.144915063	1.0831816256
H	2.8866313596	–0.2007083015	1.7687385415
H	4.2973613574	–0.6741783902	2.7400313541
H	2.6898869638	1.8606433621	3.3162655831
H	4.1483893498	2.8789058553	3.4605647621
H	4.1355313559	1.2524682059	4.1694838678
C	1.9265067703	–2.4712959465	–1.7508217895
C	–0.48321157	–2.269239975	–1.3407673131
C	0.8957837817	–1.8763472755	–0.7703245168
C	1.0649571185	–2.6121808555	0.5663745897
H	1.8775997745	–2.0204946921	–2.7561440613
H	1.7791155496	–3.5640615945	–1.9017354675
H	2.9631021314	–2.3684400634	–1.3929606785
H	–0.6746790293	–1.8388684556	–2.3371975657
H	–0.5833248739	–3.3707987134	–1.4638236505
H	–1.3233266144	–1.9737448714	–0.6910678635
H	0.9669448788	–3.7169891467	0.4598646313
H	2.0499850321	–2.431417143	1.0222326448
H	0.3158539179	–2.3106270866	1.3147654627
Li	2.1653742393	–0.0659974278	–1.1646612606
Li	–0.1308843409	0.0863798663	–0.7986652644
C	–3.5673761824	1.6323364462	–0.1126757874
C	–5.6151090376	0.3449766549	–0.0716951521
C	–2.2945534746	1.9637620351	0.6598926933
N	–1.4580630943	0.7638850907	0.8858811502
N	–4.3512145149	0.6245857166	0.5969524706
C	–3.5512834463	–0.5832336944	0.7854884346
C	–0.3118830216	1.119343232	1.7390738712
C	–2.2741608715	–0.2704543167	1.5612057402
H	–3.3105131629	1.2971285482	–1.1373510172
H	–4.1686291783	2.5443253624	–0.2094419143

H	–5.4806026925	–0.0694891216	–1.0906577244
H	–6.2013680043	1.2671037382	–0.1509495135
H	–6.1905717922	–0.3769551608	0.518114276
H	–1.7028575846	2.6994261005	0.1052180835
H	–2.5735821816	2.413209665	1.6299273123
H	–3.2976963572	–1.0532577719	–0.185418141
H	–4.1398443992	–1.3114299258	1.3562104532
H	0.2956884614	1.8798399042	1.238935323
H	0.3060425686	0.2325679542	1.9117696122
H	–0.6375027176	1.5169460935	2.716967343
H	–1.6687403788	–1.1765479639	1.6664749494
H	–2.5487877492	0.0736519023	2.5745143121

Tabelle 211 Standardorientierung von *t*-BuLi·Piperazin Dimer-TS [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.7582786917	–1.9986486242	–2.947556489
C	–0.5188862311	0.3939082828	–3.4762326072
C	–0.1236492206	–0.6823805703	–2.4449087732
C	1.4044834518	–0.8489017943	–2.5107448748
Li	–0.8030057331	–1.555762522	–0.6636256529
Li	–0.7625044015	1.1172260772	–1.2988839816
C	1.6315614541	2.4242311779	1.3198675575
C	4.0141323402	2.8185661089	1.1861619737
C	0.260976912	2.8937989498	0.8349391932
N	0.1519815028	2.813293106	–0.6275194912
N	2.6989018039	3.2069871618	0.70395262
C	2.6052383392	3.1470940111	–0.7536935524
C	–1.2217686157	3.1875537056	–1.0712918951
C	1.2300948793	3.6158157717	–1.2286942404
H	–0.4024993414	–2.2711499388	–3.9621897105
H	–1.8565905515	–1.9490581286	–3.0089268725
H	–0.5036715659	–2.8795082748	–2.3263061229
H	–0.1865871024	0.1240417295	–4.4992076832
H	–1.6063807608	0.5532471739	–3.5368215936
H	–0.0532668551	1.3750019032	–3.2817517391
H	1.7558594327	–1.0994940721	–3.5351803379
H	1.7724560856	–1.6543661926	–1.8555653948
H	1.932511723	0.0657018021	–2.208778316

H	1.7499927478	1.3414846557	1.0962900971
H	1.6937392995	2.5445636201	2.408899896
H	4.2706781974	1.7675357782	0.9382594781
H	4.0585449496	2.9336484114	2.2752814447
H	4.7776039543	3.467753666	0.7429007211
H	–0.5273181036	2.2799504879	1.2834772657
H	0.0954158378	3.9353146388	1.1707417365
H	2.789929872	2.1171842959	–1.1239468562
H	3.3802660744	3.7955347346	–1.1806895373
H	–1.5436221552	4.1349502122	–0.6040979381
H	–1.1918700924	3.3551784975	–2.1592427213
H	1.1669861634	3.52267496	–2.3185322619
H	1.0934561829	4.6826598972	–0.9745575401
C	–1.8438020202	–4.0508485183	0.2105807032
N	–0.6987667046	–3.2253964731	0.6438231414
C	0.5656707913	–3.981513662	0.4686195061
C	–0.8509435859	–2.883775915	2.0796889242
C	1.7614305081	–3.1930784122	0.9978857796
C	0.3512172584	–2.0958197282	2.5905094876
N	1.579008941	–2.8626609214	2.4080494862
C	2.7422272106	–2.1872158964	2.9707584364
H	–1.7327118887	–4.3181098314	–0.8449415694
H	–2.7737693613	–3.4864334418	0.3339736259
H	–1.917521066	–4.9799586693	0.7991452344
H	0.7003259284	–4.1938175009	–0.5980516702
H	0.5005207587	–4.9450088641	1.001694019
H	–1.7677140006	–2.2984810383	2.2036838581
H	–0.9547996342	–3.8085180766	2.6719743303
H	1.9112153141	–2.2810415115	0.3846105895
H	2.6637158309	–3.8061379638	0.8905858142
H	0.404079436	–1.1136150154	2.0736752094
H	0.2143422809	–1.8914099205	3.658528913
H	2.9521570373	–1.2153373671	2.4843189075
H	3.6255844936	–2.8251471616	2.8600882081
H	2.5814486304	–2.00971401	4.0395021608
C	–2.9552898479	–0.3741609086	0.0114958409
C	–4.2471235924	1.4083142495	–1.1565463468
C	–3.1204356797	1.1369865649	–0.1587917373
C	–3.4695646833	1.7501952299	1.1978055159
H	–2.7741556398	–0.8767044768	–0.9546906703
H	–3.8610967792	–0.8657743086	0.4338110732
H	–2.1401130699	–0.6135355347	0.7189621299

H	–4.043932926	0.9550227469	–2.1389056477
H	–5.2256147285	1.0154581273	–0.8152562286
H	–4.3742490346	2.4876537639	–1.3229403614
H	–4.4321120992	1.3743650514	1.5993907317
H	–2.7030204779	1.5352876486	1.9589616513
H	–3.5552841408	2.8439018792	1.1299047885
H	–2.1280231132	2.0835347038	–0.6378069162

8.3.4 Angaben zu den quantenchemischen Rechnungen der Deprotonierung von 1,3,5-Trimethylhexahydro-1,3,5-triazin (**66**) (Kapitel 4.2.2)

Tabelle 212 Ergebnisse der Deprotonierung von 1,3,5–Trimethylhexahydro–1,3,5–triazin (**66**); [B3LYP6-31+G(d)]

Compound	Min./TS	SCF (Hartree)	ZPE (Hartree)
[(*t*-BuLi)$_3$·$C_6H_{15}N_3$] (**95**)	Global Min.	–898.059999	–897.47465
[(*t*-BuLi)$_3$·$C_6H_{15}N_3$] Methyl	TS	–898.005893	–897.425909
[(*t*-BuLi)$_3$·$C_6H_{15}N_3$] Methylen	TS	–898.013479	–897.433899
[*t*-BuLi·$C_6H_{15}N_3$] (**97**)	Global Min.	–567.282774	–566.942434
[*t*-BuLi·$C_6H_{15}N_3$] Methyl	TS	–567.240413	–566.904485
[*t*-BuLi·$C_6H_{15}N_3$] Methylen	TS	–567.243553	–566.907181
[(*t*-BuLi)$_2$·($C_6H_{15}N_3$)$_2$]	Global Min.	–1134.578321	–1133.894904
[(*t*-BuLi)$_2$·($C_6H_{15}N_3$)$_2$] Methyl	TS.	–1134.534953	–1133,856515
[(*t*-BuLi)$_2$·($C_6H_{15}N_3$)$_2$] Methylen	TS	–1134.540029	–1133.863098
$C_6H_{15}N_3$ (**66**)	Global Min.	–401.897768	–401.678123
(*t*-BuLi)$_4$	Global Min.	–661.533790	–661.048268
(MeLi·$C_6H_{15}N_3$)$_2$	Global Min.	–898.729543	–898.217870
(MeLi·$C_6H_{15}N_3$)$_2$ Methyl	TS.	–898.672146	(898.166056
(MeLi·C6H15N3)2 Methylen	TS	(898.686165	(898.180281

Tabelle SEQ Tabelle * ARABIC 213 Standardorientierung von [(t-BuLi)3·C6H15N3] (95) [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	1.814852811	0.047432799	3.1538661585
C	0.9162078457	2.2647743241	2.5426096371
C	0.6229459687	0.7534332502	2.4762104212
C	–0.6034231243	0.4947876362	3.3740824129
C	3.259764026	1.088395287	–0.8123346687
C	1.5871834878	2.8613128434	–1.2617743378
Li	1.4975717511	0.2806343109	0.5308075809
C	1.8450830607	1.3459073826	–1.3696306041
Li	–0.9894698922	0.2189184204	1.0593729698
C	1.9057518466	1.0163556697	–2.8745357813
Li	–0.2064685336	0.5875777243	–1.3349083378
C	–2.1258988039	1.2667391842	–0.481836396
C	–3.4099507372	0.6280074364	0.0847664103
C	–2.3329259384	1.3776534529	–2.0058368493
C	–2.0698296133	2.7039719182	0.0703116379
H	2.006002431	0.4422323635	4.1755419876
H	2.767183101	0.1832391712	2.610491772
H	1.6660388436	–1.0369114859	3.2732038425
H	1.0688188054	2.6100508132	3.5888758306
H	1.8305727133	2.5410486619	1.9964029816
H	0.1053549338	2.8719534505	2.1215571386
H	–0.4601775856	0.8827605094	4.4050677488
H	–0.8347890562	–0.5771896837	3.4882140277
H	–1.5246869215	0.9939666603	3.0187362781
H	3.3649317033	1.326775544	0.2634632196
H	4.0289220588	1.7174811258	–1.3087255139
H	3.5903172563	0.0459007504	–0.9496130385
H	1.5502167926	3.2118867101	–0.2229098675
H	2.376677294	3.452934538	–1.7755264583
H	0.6351076992	3.1585493217	–1.7258892574
H	2.6291031523	1.6648515242	–3.4153249591
H	2.2206191218	–0.0190423641	–3.0774298368
H	0.9420939599	1.1666378767	–3.3938981051
H	–3.3884493043	0.5041997254	1.1827033864
H	–4.3096016312	1.2492676728	–0.1173024459
H	–3.6255840177	–0.3623844811	–0.3446565085
H	–1.4911479406	1.8649287498	–2.5336602227
H	–3.2166571756	1.9979982633	–2.2665187363

H	–2.5001698176	0.4008223084	–2.4890182654
H	–2.9771147081	3.2876205539	–0.2007951814
H	–1.2051882368	3.2662574445	–0.3028578978
H	–2.0093866	2.7306384926	1.1685239571
C	2.6805441946	–2.5482067894	0.5351549039
N	1.3810050751	–1.9590874272	0.17078648
C	0.3208003029	–2.558744901	0.990124975
C	1.1005162606	–2.2125101811	–1.2467876525
N	–0.9862445525	–1.99685675	0.6323837285
C	–2.0386957888	–2.6228849155	1.4507602729
N	–0.2018798203	–1.6476645221	–1.6220193478
C	–1.2503212026	–2.2488300602	–0.7893725233
C	–0.47206305	–1.9264378496	–3.042680452
H	3.4681826021	–2.0998955216	–0.0763089409
H	2.894126125	–2.3352257535	1.5855858073
H	2.6988093611	–3.6415333682	0.3842760907
H	0.5213671324	–2.3404283312	2.0404076162
H	0.3127139332	–3.6646184329	0.8529631314
H	1.8772403122	–1.7386759139	–1.8495635611
H	1.1134195662	–3.3082633681	–1.4495244031
H	–1.8407988882	–2.4299649524	2.5086011752
H	–2.0909532784	–3.7146429504	1.2970539785
H	–3.0068732226	–2.1854211282	1.1943210153
H	–1.3067644589	–3.3456732961	–0.9774564101
H	–2.2094538503	–1.8007473684	–1.0539514133
H	0.2983391055	–1.4549185285	–3.6578761141
H	–0.4858271791	–3.0087477483	–3.2588248202
H	–1.442065705	–1.5043207986	–3.3187666664

Tabelle 214 Standardorientierung von [(*t*-BuLi)$_3$·$C_6H_{15}N_3$] (**95**) Methyl [Übergangszustand, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	1.0214077765	–3.7216744284	1.409504472
C	0.2931272492	3.9345690181	1.199805104
C	2.523944472	–1.8776423076	1.0856450683
C	0.4467777916	–1.500627461	2.2188008648
C	–0.3082366683	2.7641261474	0.4167896705
C	0.5945409545	2.4623930647	–0.7906311789

C	4.0901318285	–0.0605004947	0.8393215592
C	1.9253981604	0.3209118458	1.8677739071
C	–0.3066029478	0.8684051623	2.6416412209
C	–1.7032781506	3.166909952	–0.0801926037
H	3.0116569065	–2.4267784873	0.275958408
H	1.4946914072	–4.2704472916	0.5892019236
H	–0.0303513361	–4.0153389556	1.4585928339
H	0.9137809686	–1.7098645987	3.2071099469
H	–0.6031269684	–1.7955957537	2.2609368372
H	4.5715701697	–0.290781683	1.8037160591
H	3.0374310556	–2.1326895357	2.0387701567
H	4.6161259565	–0.601615159	0.0472623811
H	4.1889455324	1.0135140606	0.6529490577
H	2.3917200695	0.1486246018	2.8644163259
H	1.9861016713	1.3890670114	1.64865946
H	0.2038837197	1.2167977936	3.5525945696
H	–2.3910160131	3.3400145855	0.7604809291
H	–1.2223903877	0.3500410703	2.9545513005
H	–0.3933876979	1.868400778	1.5967901283
H	0.1941022338	1.6586251407	–1.4311598895
H	–0.3239481742	4.190094207	2.0727568611
H	0.7223577783	3.3349030887	–1.4648577564
H	1.6240703323	2.2023882413	–0.4749191435
H	1.5113711427	–4.0110339618	2.3550997793
H	1.3005735207	3.7031193131	1.5806683778
H	0.3847692109	4.8490702731	0.5839197911
H	–2.1669932878	2.4076984011	–0.7292065526
H	–1.6846190495	4.1021029177	–0.6740128705
N	0.5370411749	–0.0913867447	1.8698870164
N	2.6637189162	–0.4300312481	0.8276019527
N	1.1124812488	–2.2767928498	1.1513797437
C	1.1989533636	–1.26401599	–2.4289515169
C	0.7017900614	–2.6913966179	–2.7165957048
C	2.7376917267	–1.294781669	–2.5734564399
C	0.6710530085	–0.3430990472	–3.5461300783
H	1.0680510785	–3.430293893	–1.984084775
H	3.2150986336	–2.034592717	–1.9138388043
H	–0.396949661	–2.7641602514	–2.7364988167
H	1.0341294515	–3.0579090436	–3.710262418
H	3.0551900133	–1.5451786502	–3.6062678787
H	3.2302017642	–0.3193823236	–2.3708447574
H	0.9712653507	–0.6978462547	–4.5552521289

H	–0.423071278	–0.2670812426	–3.5453593089
H	1.0559581205	0.6866872671	–3.4633671458
C	–3.2320689795	–0.4493810098	0.764256681
C	–2.2495965337	–1.0410053585	–0.2703529555
C	–2.3644912082	–2.5732792889	–0.1215345172
C	–2.7948993603	–0.6793304211	–1.6648848282
H	–2.1284766329	–2.9185917132	0.8965738671
H	–2.9923473321	–0.7405168816	1.7983069829
H	–1.7210919574	–3.1471573649	–0.8144516565
H	–3.3929619522	–2.9338770261	–0.3368103127
H	–4.2726243243	–0.7917589585	0.5820406099
H	–3.2893231301	0.6527374662	0.7435718351
H	–3.8424821988	–1.0258394366	–1.8032139391
H	–2.2109188216	–1.1313741966	–2.4784371727
H	–2.7978923824	0.4046273504	–1.8490199051
Li	1.7150197426	0.0506638542	–0.9384690462
Li	–0.1628869915	–1.6170811983	–0.6590819287
Li	–1.0490901382	0.5742389031	0.606810348

Tabelle 215 Standardorientierung von [(*t*-BuLi)$_3$·$C_6H_{15}N_3$] (**95**) Methylen [Übergangszustand, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	3.4415439161	0.8201019213	–1.3296302937
C	2.1836650026	2.9417315653	–1.0524798718
C	–3.23931119	1.2957053564	–0.3738261645
C	2.0520760458	1.472562035	–1.4939850797
C	–2.344585468	1.2384998765	–2.6725259951
C	–1.7187062749	3.0944901049	–1.1446693365
C	1.7549653489	1.4789300776	–3.007062463
C	–1.9738926834	1.5785973613	–1.2155029507
H	–2.663433144	0.192611262	–2.7947846757
H	–0.8874820892	3.4082751913	–1.7903631805
H	–1.4709659605	3.4341369532	–0.1285436307
H	2.4802589571	3.0426007395	0.001640131
H	4.2382494482	1.4007356862	–1.8392376349
H	3.4879325152	–0.197135278	–1.746058664
H	2.9551123767	3.4832217072	–1.6420224154
H	3.7808292083	0.7549842607	–0.2773911336

H	1.2467564125	3.500217163	–1.1680383539
H	2.5306965057	2.0230947736	–3.5845021233
H	1.7105943934	0.4673626801	–3.4441590615
H	0.8104765129	1.9921595264	–3.2622190966
H	–3.119182572	1.5321432952	0.701706738
H	–1.520196228	1.4097350225	–3.3868040306
H	–2.6053329138	3.680629586	–1.4695612056
H	–4.1021961395	1.9141300713	–0.6944739237
H	–3.5784659783	0.2491767565	–0.444112938
H	–3.1830714361	1.8636208254	–3.0467194558
Li	–1.2803220201	0.452092444	0.4345880175
Li	1.7269950479	0.2400386045	0.2187468355
Li	–0.0052686371	0.6763116971	–1.7342916903
C	–0.4110736395	1.3542866788	2.5139605514
C	0.7025752559	0.299619178	2.5755690352
C	0.6028711256	–0.4444449226	3.911750469
C	–0.3556763102	–2.0104464394	–3.3087029936
C	1.1136915501	–2.2082619991	–1.4122502548
C	0.2569690967	–2.013379579	0.903809051
C	–1.2379141549	–2.0574632383	–1.0654207773
C	2.5771474367	–2.4204861668	0.47321386
C	–2.1212562431	–2.0943515829	1.1632025591
C	2.0685356196	1.0019043735	2.5212513472
H	–0.3728696242	2.0731745358	3.3565276789
H	0.5019919629	–0.9126677803	1.7897938833
H	2.9048999046	0.2851477276	2.517787522
H	–0.3658535946	1.9829525964	1.6072155446
H	–1.4163391268	0.9003116496	2.583940024
H	0.6999858013	0.2354378323	4.7782555393
H	1.3881586817	–1.208282822	4.0053573712
H	–0.3588285162	–0.9681434937	4.0148931241
H	0.2046475391	–3.1064715034	1.1113137704
H	2.7718851322	–2.0729481444	1.4921033396
H	1.0324916446	–3.3176864444	–1.4482088081
H	–1.9749111957	–1.735179761	2.1857957723
H	–1.3008477585	–3.1680710723	–1.0858854176
H	–2.1724039514	–1.6473806789	–1.4630680327
H	2.4542750042	–3.5169570341	0.5090405197
H	1.940142519	–1.9000845578	–2.0621572255
H	3.4405954224	–2.1856989747	–0.1586044493
H	–2.1300936583	–3.1973570483	1.1911317357
H	2.1897789798	1.6748015792	1.6554577627

H	0.4755368218	–1.6640268599	–3.930427756
H	–0.4374732674	–3.1058453602	–3.4141768206
H	–1.2779710584	–1.5541654182	–3.6782393976
H	2.2377636223	1.6570884786	3.3987357769
H	–3.0932170573	–1.749151627	0.7939288793
N	1.3713208701	–1.7568196604	–0.0438086334
N	–0.1278629318	–1.6012313817	–1.9139668721
N	–1.0364108586	–1.5824823446	0.3091659687

Tabelle 216 Standardorientierung von [*t*-BuLi·$C_6H_{15}N_3$] (**97**) [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
N	–1.1899298795	0.6675016853	–1.1820168465
C	–0.017123165	1.3853148514	–1.6826518108
N	1.1730383563	0.6967586617	–1.1820168465
C	–1.191156271	–0.7074865216	–1.6826518108
N	0.0168915232	–1.364260347	–1.1820168465
C	1.2082794361	–0.6778283298	–1.6826518108
C	–2.4429329301	1.3699785406	–1.4526515194
C	2.4079026839	1.4306527068	–1.4526515194
C	0.0350302462	–2.8006312475	–1.4526515194
C	0.	0.	2.6910773887
Li	0.	0.	0.6309354417
C	–1.3801941832	–0.3815764151	3.2439098478
C	1.0205519605	–1.0044950173	3.2439098478
C	0.3596422227	1.3860714323	3.2439098478
H	–0.0178038704	1.4451900072	–2.7961524458
H	–0.0295265197	2.4031616517	–1.2815266151
H	–2.0664357799	–1.227151542	–1.2815266151
H	–1.2426693243	–0.7380136077	–2.7961524458
H	1.2604731948	–0.7071763995	–2.7961524458
H	2.0959622997	–1.1760101097	–1.2815266151
H	–2.4041614336	2.3651607486	–0.9999628373
H	–2.647285828	1.4806418572	–2.532387204
H	–3.2706242218	0.821411675	–0.9935651562
H	2.6059163762	1.5522958495	–2.532387204
H	2.3466754884	2.4217378248	–0.9935651562
H	3.2503700091	0.899484502	–0.9999628373
H	–0.8462085755	–3.2646452506	–0.9999628373

H	0.0413694518	–3.0329377067	–2.532387204
H	0.9239487334	–3.2431494998	–0.9935651562
H	–2.1687258149	0.3191971246	2.9244937901
H	–1.6959851846	–1.3889252766	2.9265067199
H	–1.4045011225	–0.3873997827	4.3619823487
H	0.8079300887	–2.0377702118	2.9244937901
H	2.0508371658	–0.774303616	2.9265067199
H	1.0377486145	–1.0226337604	4.3619823487
H	1.3607957262	1.7185730872	2.9244937901
H	–0.3548519811	2.1632288926	2.9265067199
H	0.366752508	1.4100335431	4.3619823487

Tabelle 217 Standardorientierung von [*t*-BuLi·$C_6H_{15}N_3$] (**97**) Methyl [Übergangszustand, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
N	–1.6863406051	–0.2198896316	–0.4394214833
C	–1.8145101036	1.2403386924	–0.3661714837
N	–0.4563776271	1.7864432533	–0.4810262303
C	–1.1584367	–0.5774363139	–1.8004680618
N	0.1319341459	0.0124696814	–2.048474728
C	0.0706318306	1.4356118845	–1.8442603499
C	–2.9427943502	–0.9056818496	–0.1395012207
C	–0.4127042547	3.2259192827	–0.2280556995
C	1.2609051946	–0.6671848921	–1.305020936
C	1.5819473041	–1.1791216145	1.6074591312
Li	0.1817393433	0.0217609655	0.524577764
C	0.7907562986	–2.4304638056	1.9950604006
C	3.0761538385	–1.4983566994	1.5630413877
C	1.3469669412	–0.0692338719	2.6482198354
H	–2.4840029014	1.6358442921	–1.1649338383
H	–2.2412750549	1.5214336291	0.6042488195
H	–1.0828543327	–1.6667342875	–1.853976296
H	–1.8786210757	–0.2298676208	–2.5639772416
H	–0.5875410929	1.8919839831	–2.606783064
H	1.0712005661	1.8663558974	–1.9380127042
H	–3.2887708836	–0.626969855	0.8615878874
H	–3.7398305181	–0.6641550708	–0.8647687972
H	–2.7764156986	–1.9869769607	–0.1549864126

H	–1.0053815218	3.8021633161	–0.9604741691
H	–0.7979304522	3.4391992304	0.7747880648
H	0.6249580886	3.5701151835	–0.2760530779
H	1.323949244	–1.6823009645	–1.7244272274
H	2.1811962939	–0.1539552875	–1.6207680408
H	1.3993756094	–0.9037891248	0.1269346136
H	–0.2919603078	–2.2372335967	2.0753670115
H	0.9177515848	–3.2303444246	1.250844286
H	1.1056745393	–2.8494082788	2.9731605499
H	3.2978896515	–2.2925134195	0.835486995
H	3.6714437781	–0.619748531	1.2728176069
H	3.4633031956	–1.8413441619	2.5435414403
H	1.8660324581	0.8667253379	2.3853546139
H	0.2765664285	0.1761890839	2.792690415
H	1.7120169823	–0.3494592648	3.6592443458

Tabelle 218 Standardorientierung von [*t*-BuLi·$C_6H_{15}N_3$] Methylen [Übergangszustand, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	0.0184012215	0.3121475495	0.1345897532
N	–0.1938152959	–1.0977475247	0.4407532419
C	0.1448913174	–1.3585029804	1.8349758865
N	1.545936864	–1.0032545233	2.0690714838
N	1.4202732504	0.6566762578	0.3795190915
C	1.8593098549	0.4173897608	1.7766757231
C	1.9460955175	–1.3514662941	3.4317945743
C	1.6894640847	2.0379768876	–0.0179141951
Li	2.7329830598	–0.9082732283	0.4091569726
C	4.673007733	–0.0855509404	1.0732125366
C	–1.549341761	–1.5277367078	0.1191292254
C	4.9373591308	–1.1609559658	–0.004590655
C	5.3841309172	–0.5018939905	2.3627367125
C	5.2520373229	1.2450384047	0.5872251921
H	–0.65214076	0.9616316027	0.7463147941
H	–0.2146235709	0.4768770881	–0.9247129316
H	0.0053919796	–2.4285966528	2.0324579241
H	–0.519921121	–0.7851068446	2.5241100853
H	3.2919012573	0.3026417629	1.5573930993

H	1.3458117937	1.1011733087	2.4865732299
H	1.8256792363	–2.4289559701	3.5933222086
H	1.3423032264	–0.8158780911	4.1864535256
H	2.9933634789	–1.0849187619	3.5806724605
H	1.0720597684	2.7565080786	0.5508158146
H	1.4772488003	2.1682700584	–1.0854173437
H	2.7394594063	2.2694373023	0.1662533073
H	–1.7425882888	–1.3587745242	–0.945652836
H	–2.3248487675	–0.9939013783	0.7013698489
H	–1.6485673738	–2.6002650081	0.3178539648
H	4.4838359987	–0.9119196619	–0.9821926697
H	4.5799039632	–2.1648822576	0.2916353872
H	6.0174916247	–1.2942368417	–0.2171941979
H	5.0832675263	–1.5043646608	2.7005469793
H	5.1697498673	0.1981365575	3.1841778444
H	6.4853702925	–0.5251464601	2.2435866127
H	5.0286849986	2.0615119231	1.2902538682
H	4.8531949363	1.5403815433	–0.3942408667
H	6.3543725098	1.2075141824	0.4827883474

Tabelle 219 Standardorientierung von [(*t*-BuLi)$_2$·($C_6H_{15}N_3$)$_2$] [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.0061427525	0.006649802	0.0018797279
C	0.0258618088	–0.0114635923	2.4581207259
C	0.9423501365	0.0010064131	1.2161021763
C	1.6872746638	1.3430028026	1.2038710224
H	–0.736751034	0.8472256774	0.044794899
H	–0.6069863997	–0.9129872825	–0.0781335002
H	0.5251052434	0.1345233794	–0.9553001571
H	–0.650345	0.8730267	2.4854847839
H	–0.634617927	–0.8926136488	2.4811200834
H	0.5704681103	0.0084012467	3.417861999
H	0.9932181784	2.2162445973	1.2046266758
H	2.3301452183	1.4552503038	0.3182790057
H	2.3423289172	1.4746894803	2.0780437425
C	1.7145870453	–1.8386638279	–2.9047722166
N	2.7688759899	–1.6612957096	–1.8914320742
C	3.4172811777	–0.3510093803	–2.0776488278
C	3.7823100317	–2.7189352805	–2.0514282365

N	4.4960309289	–0.1795800772	–1.1184158858
N	4.862205295	–2.5381837463	–1.0958553125
C	5.487949076	–1.2350386935	–1.2716698946
C	5.0967320133	1.1453943177	–1.2226479855
C	5.8352543417	–3.621100304	–1.1782535194
H	0.9596954722	–1.0568976201	–2.7892492214
H	1.2293611223	–2.8075955095	–2.7601420516
H	2.1162331369	–1.7938743449	–3.9315871197
H	2.6723540317	0.4342410367	–1.9206614844
H	3.7939420872	–0.2672762155	–3.1263622777
H	3.3082529572	–3.6887121099	–1.8740465599
H	4.1672628431	–2.7079735771	–3.1003879652
H	6.2593676721	–1.1079250608	–0.5045697047
H	5.9877290746	–1.1662802248	–2.2728620164
H	4.3332781436	1.9078199271	–1.0403505316
H	5.5554442986	1.3371723719	–2.2122154658
H	5.8735990205	1.2536700022	–0.4584519341
H	6.3344905896	–3.6812754226	–2.1649756676
H	5.336780005	–4.5753891118	–0.9826211993
H	6.6046806012	–3.4778039546	–0.412338457
N	2.33312971	–0.2477025334	5.4751764643
C	3.40787289	–0.0669845194	4.5152863045
N	3.5504315877	–1.2757797166	3.6882559947
C	2.5968535187	–1.3897928243	6.339351508
N	2.7838375414	–2.5911207463	5.5375134177
C	4.622197403	–1.0977468619	2.6965116376
C	3.8560495622	–2.4097516927	4.5747454752
C	2.0734486616	0.9671705282	6.2364976797
C	2.9897760938	–3.7736279022	6.363341073
H	3.1670453372	0.7786336906	3.8664296585
H	4.3776108312	0.1536837043	5.0260454133
H	3.4953142581	–1.1996672343	6.9831676176
H	1.7357952679	–1.5379762259	6.9994438948
H	4.3687674866	–0.2633951819	2.0371096753
H	4.6966671051	–1.9990530939	2.0815882261
H	5.5995209914	–0.9011578698	3.1724002003
H	3.9479594806	–3.3149767224	3.9694128629
H	4.8350896961	–2.2322990912	5.0847219237
H	1.8163983229	1.7796207786	5.5492052355
H	2.9366780736	1.2888996375	6.8516902361
H	1.2191962573	0.8034573932	6.9016592026
H	2.1317527813	–3.9045569051	7.0308926219

H	3.9069440826	–3.7181251463	6.982099234
H	3.0577869078	–4.6582003686	5.722012723
C	0.6864135939	–3.9742770461	0.1799520545
C	0.7151401321	–3.835524211	2.6322827419
C	1.5781428085	–3.5898628661	1.3768682477
C	2.7387148596	–4.593584347	1.4088398569
H	–0.2012568486	–3.329559498	0.0827353482
H	0.3004070786	–5.016041224	0.2652495189
H	1.2210870132	–3.9412023008	–0.7838188166
H	–0.2076347211	–3.2337433856	2.6316041358
H	0.3821563702	–4.8958087278	2.7085364826
H	1.2373279939	–3.622745087	3.5800713208
H	2.3856165646	–5.6512448	1.4436936971
H	3.3905510341	–4.5064461189	0.5276980925
H	3.3893787331	–4.4632244052	2.2868364581
Li	1.9251578131	–1.7295515045	0.1790881782
Li	1.7774038402	–1.6552738878	2.4766206172

Tabelle 220 Standardorientierung von [(*t*-BuLi)$_2$·($C_6H_{15}N_3$)$_2$] Methyl [Übergangszustand, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	0.0232558967	0.0038762216	–0.0021895052
C	–0.0081080739	2.4770931463	0.0222417397
C	–0.9105042863	1.2253284161	–0.0028005773
C	–1.6892062881	1.1736702205	1.3298645699
H	0.7255952083	0.0300001964	0.8581527673
H	0.652719743	–0.0672616233	–0.9014838337
H	–0.5241655913	–0.9461127698	0.0920246004
H	0.6549700091	2.4947973186	0.9145804417
H	0.640131849	2.5342048474	–0.8621113419
H	–0.5663675772	3.4318825099	0.064823249
H	–1.0081793024	1.1765712539	2.2089735763
H	–2.3128506818	0.2724754308	1.4037632868
H	–2.3609960962	2.0368686586	1.4921463292
C	–1.5477883942	–1.9694716056	–2.6290621154
N	–2.8700851626	–1.5005050818	–2.1168312656
C	–3.4423130413	–2.3550310166	–1.0761254069
C	–3.8105055395	–1.4142253052	–3.2298523844

N	–4.7335441291	–1.8349720882	–0.622484362
N	–5.1136959765	–0.9035878922	–2.7963523246
C	–5.6603166651	–1.7527137162	–1.7419830899
C	–5.2810324497	–2.6429928476	0.4591432089
C	–6.0359312627	–0.8146772171	–3.9230964765
H	–0.9382906424	–2.2772234157	–1.7682322378
H	–1.0817185269	–0.7863347231	–3.3521737885
H	–1.6631357942	–2.8503143254	–3.285402821
H	–2.7568589351	–2.3814627235	–0.2238670941
H	–3.5479290757	–3.3979633714	–1.46231089
H	–3.4014729915	–0.7474401491	–3.9920185905
H	–3.9298625516	–2.4250129868	–3.6935519923
H	–6.6047108859	–1.3181452591	–1.3911469584
H	–5.8887515464	–2.7739857039	–2.1436896962
H	–4.5773210028	–2.6535349045	1.2983067525
H	–5.4804917619	–3.6922274736	0.1632817764
H	–6.222165283	–2.2030790327	0.8092467329
H	–6.2405544326	–1.7949325028	–4.3958301362
H	–5.617714747	–0.1504175995	–4.686926952
H	–6.9903894493	–0.3932182395	–3.5865855997
N	–3.3575850437	4.4851192187	0.4748291724
C	–4.6165990001	3.7423842537	0.4339524157
N	–4.5466573632	2.8095040208	–0.6926206317
C	–3.1767877715	5.241100239	–0.7623385181
N	–3.1487158761	4.2972010678	–1.8819998757
C	–5.6671203144	1.8635969046	–0.7168197165
C	–4.4145234833	3.559843891	–1.9446024071
C	–3.2336207716	5.3212331452	1.6667413522
C	–2.8321019528	4.9642161286	–3.1474752046
H	–4.7193692296	3.1695717004	1.3602877245
H	–5.4938491577	4.4236454825	0.3424024141
H	–3.9824983192	6.0003480749	–0.8975439881
H	–2.2165423734	5.7639393632	–0.7196877705
H	–5.6921212142	1.3197410917	0.2315166598
H	–5.5006363767	1.1319805949	–1.5132545003
H	–6.6362303847	2.3720876757	–0.8641629604
H	–4.3724757018	2.8534027372	–2.7780411083
H	–5.2794254226	4.2440473266	–2.1021963604
H	–3.3102877664	4.6931128762	2.5593926981
H	–4.0076863935	6.1074235527	1.7216489334
H	–2.2497564138	5.8001041155	1.6730251511
H	–1.8543334657	5.4480740151	–3.0657007631

H	–3.5823490022	5.727207856	–3.4192229177
H	–2.7752186693	4.2212723021	–3.9462825883
C	0.7724127877	0.6887885236	–3.8463203822
C	–1.4933304116	1.7066600543	–4.1753724738
C	–0.700635034	0.3960050847	–4.1402779909
C	–0.8094614181	–0.2852127819	–5.5062683158
H	0.9105169583	1.2530014928	–2.9123312727
H	1.2533512062	1.2870069501	–4.6478805203
H	1.3531786884	–0.2411954681	–3.7520536227
H	–1.418809358	2.2682905098	–3.2302547432
H	–1.1318162792	2.3984637349	–4.9705558345
H	–2.5635390815	1.5380702189	–4.3800997489
H	–0.3916172453	0.3385709998	–6.3212630732
H	–0.268177364	–1.242424083	–5.5210711279
H	–1.8539810605	–0.5045723854	–5.776840166
Li	–1.5379235567	0.1006459314	–1.854716685
Li	–2.4080919257	2.5220189381	–0.5909808444

Tabelle 221 Standardorientierung von [(*t*-BuLi)$_2$·($C_6H_{15}N_3$)$_2$] Methylen [Übergangszustand, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	2.7867402058	–1.0018785126	2.3940933249
C	2.761561194	1.4449939168	2.482172379
C	1.8353204355	0.2094292536	2.447787003
C	1.088872554	0.1316339802	3.7957779804
Li	0.5428128074	1.6669389907	1.5858421234
H	3.4928774275	–0.9925792517	3.2511135027
H	3.4012049831	–1.0212017714	1.4824872552
H	2.260806787	–1.9660948387	2.4605762041
H	3.4582985225	1.4055225403	3.3468402583
H	3.3789236581	1.5230673435	1.5766191399
H	2.2334647772	2.4074985434	2.5964499201
H	1.7895635613	0.1112624496	4.6601918442
H	0.470200835	–0.7741138749	3.8686178864
H	0.4204404755	0.9902554762	3.968659674
C	2.6686965831	–3.0858885715	–1.1542273361
N	1.4928709671	–2.7546174203	–0.3505926581
C	1.1708950491	–3.8325809555	0.5857430969

C	0.3370242941	–2.3966837837	–1.193804113
N	0.1035096456	–3.3565214419	1.4725802437
N	–0.7196544003	–1.9507840031	–0.2559815788
C	–1.0845481367	–3.0083730091	0.6913268651
C	–0.1944405842	–4.3079222305	2.5372989925
C	–1.8997755852	–1.4957371004	–0.9874155043
H	3.5313750401	–3.2551986976	–0.4989568798
H	2.8874503156	–2.2565471469	–1.826927685
H	2.5098048353	–3.9948057382	–1.7627895559
H	2.0493484478	–4.0665128366	1.2010950877
H	0.863512288	–4.7553727461	0.0423261221
H	–0.0178292845	–3.2923115566	–1.7615636347
H	–1.8545271132	–2.6398226839	1.3832477881
H	–1.4897791647	–3.8971839436	0.1540665019
H	0.7101781795	–4.491485255	3.1266766056
H	–0.5634517844	–5.2779470319	2.1559238157
H	–0.9563939209	–3.8865884047	3.2018780078
H	–2.3573460758	–2.3091366288	–1.5795526152
H	–1.611829201	–0.7001089948	–1.6757275516
H	–2.6534761356	–1.1176856736	–0.2860138051
H	0.6848564267	–1.3523532653	–2.0033149345
N	0.4679963398	3.739894625	0.7031984933
C	0.3310195427	4.3951305647	2.0053149054
N	–0.3543428421	3.4657328249	2.9041602955
C	–0.8628049502	3.4624692791	0.1580489876
N	–1.5151896092	2.5145249701	1.0705790433
C	–0.3930634114	3.9462251197	4.2840246415
C	–1.6812686269	3.1376270337	2.3868938076
C	1.3086924106	4.5029042295	–0.2245544532
C	–2.7865846168	2.0219196041	0.5354769471
H	1.3274842564	4.6022985918	2.4066348445
H	–0.2180559613	5.3605628655	1.9161242131
H	–1.4607547679	4.3954689588	0.0502872872
H	–0.7553232627	2.9978859066	–0.8234851569
H	0.6288162201	4.1091749096	4.6394144904
H	–0.8552748173	3.185560691	4.9204198326
H	–0.9590386436	4.8882422249	4.3932583753
H	–2.1548419266	2.4186144024	3.0628493256
H	–2.3324346285	4.0401223139	2.3244285351
H	2.3066067542	4.6198430979	0.2086059236
H	0.8973117753	5.5039251728	–0.4404454408
H	1.4019883537	3.9496202886	–1.1627558495

H	–2.6091930955	1.5391412987	–0.4283218945
H	–3.5269405889	2.8287473089	0.3973984732
H	–3.2038863113	1.2785110846	1.2213803906
C	2.5136094546	–0.0465306037	–3.2806232394
C	0.627578805	1.1701795209	–2.224850992
C	1.0356549697	–0.1180573818	–2.9182822929
C	0.2072908549	–0.3046284377	–4.1832985656
H	3.155064185	0.0937484717	–2.395325265
H	2.749562932	0.7990839539	–3.9714485968
H	2.8580498631	–0.9597711058	–3.7909397883
H	1.1833099899	1.3244607319	–1.2829773535
H	0.8031095978	2.0876503468	–2.8465214232
H	–0.4477138113	1.1736643173	–1.9795533331
H	0.3291105769	0.5295593198	–4.9145560662
H	0.4816136647	–1.2282922569	–4.7158564682
H	–0.8725401499	–0.3707560113	–3.9691284752
Li	0.9396225658	–1.1440233572	0.9074020715

Tabelle 222 Standardorientierung von $C_6H_{15}N_3$ (**66**) [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–2.4579307353	1.0988108452	0.6921112619
N	–1.0560727986	0.7120411791	0.639582888
C	–0.8923506097	–0.7284380116	0.7717177243
C	–0.4138312102	1.1915880103	–0.5755684612
N	0.518466171	–1.0876643974	0.7602621481
N	0.9968596835	0.8315601011	–0.5872865056
C	1.6695125861	1.340599552	–1.77299763
C	1.1589707581	–0.609228258	–0.4562976186
C	0.7084377569	–2.5192119156	0.9388275187
H	–2.5376562132	2.1904075365	0.6473974054
H	–2.8934457363	0.7659590954	1.6404775426
H	–3.0618892575	0.6730410764	–0.1348074806
H	–1.3279300255	–1.0453602955	1.7256665113
H	–1.441758427	–1.2636840344	–0.0490103863
H	–0.4981426584	2.28333403	–0.6099572339
H	–0.9325934666	0.7809188542	–1.4834936873
H	1.5724833128	2.431156999	–1.8078706562
H	1.2654025992	0.9263097359	–2.718933542
H	2.7362885548	1.0972636128	–1.7207313442

H	0.7398059084	–1.1358667785	–1.3555705127
H	2.2288669221	–0.8390902009	–0.4040880752
H	0.258419544	–3.1265206046	0.1273686853
H	0.2605579869	–2.8311548012	1.8885746726
H	1.779968289	–2.7429937396	0.9803116171

Tabelle 223 Standardorientierung von (*t*-BuLi)$_4$ [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–1.591202	–2.148706	1.807477
C	–1.756247	–2.614332	–0.619100
C	0.336159	–3.132739	0.600089
C	–0.800869	–2.092946	0.477742
H	–1.948856	–3.176337	2.020980
H	–2.494716	–1.516087	1.806571
H	–0.983707	–1.857245	2.678348
H	–2.121046	–3.639743	–0.405571
H	–2.658143	–1.992481	–0.727700
H	–1.283872	–2.685333	–1.614716
H	–0.049230	–4.140626	0.856429
H	1.064130	–2.896197	1.395604
H	0.900974	–3.257801	–0.336575
C	–2.960711	1.202300	0.330522
C	–1.737579	1.346245	–0.603125
C	–2.237761	1.040363	–2.033772
C	–1.346609	2.842255	–0.587286
H	–3.392056	0.190271	0.309829
H	–2.739700	1.444166	1.385108
H	–3.783176	1.889587	0.045584
H	–2.594473	0.002970	–2.163807
H	–3.102426	1.674804	–2.315647
H	–1.468981	1.221437	–2.800148
H	–1.076244	3.199511	0.417682
H	–2.177828	3.492677	–0.927726
H	–0.504781	3.086080	–1.260208
C	–0.002504	1.311082	2.911613
C	1.957849	–0.157573	2.544119
C	1.026443	0.861548	1.848959
C	1.893978	2.100250	1.528296

H	–0.662757	0.496631	3.259727
H	0.486905	1.689517	3.831905
H	–0.649764	2.127256	2.557205
H	1.417807	–1.039669	2.919925
H	2.469122	0.282738	3.424225
H	2.773440	–0.522894	1.895197
H	2.342141	2.539894	2.442589
H	1.327801	2.927924	1.065031
H	2.737574	1.866701	0.861826
Li	–0.958591	0.072738	1.097403
Li	1.119328	–0.871630	0.392037
Li	–0.653070	–0.557718	–1.194967
Li	0.509904	1.347646	–0.311788
C	1.003455	–0.947805	–2.932541
C	2.825084	–0.768065	–1.261218
C	1.502812	–0.116501	–1.726331
C	1.873451	1.277626	–2.282269
H	0.733316	–1.980377	–2.659455
H	0.132317	–0.500894	–3.438812
H	1.789106	–1.045157	–3.708953
H	2.701168	–1.802697	–0.896249
H	3.325074	–0.195177	–0.464831
H	3.562766	–0.844428	–2.085720
H	1.013623	1.796874	–2.7329277
H	2.304695	1.953079	–1.522669
H	2.642582	1.219893	–3.079162

Tabelle 224 Standardorientierung von MeLi-Dimer [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	0.2580604727	0.8648091371	4.2255374056
N	0.6647735874	1.4826550035	2.961388518
C	2.1239233779	1.6005283245	2.8636816319
C	0.048316597	2.801982796	2.7830222824
N	2.4720084853	2.1333300595	1.5556824279
N	0.4130600332	3.3258529384	1.4760139201
C	3.9116303385	2.151422596	1.336027427
C	1.8598934671	3.4391784175	1.3513370569
C	–0.2725288518	4.5749107032	1.1746821492

H	0.7025986238	–0.1321876607	4.2982017706
H	0.5669910146	1.4566980764	5.1056175708
H	–0.83048166	0.7559831548	4.2392297365
H	2.5626373201	0.6039408209	2.9671021276
H	2.5164695536	2.2473545692	3.6866603237
H	0.3655310713	3.4920228804	3.6034169932
H	–1.038735079	2.6885533856	2.8270970305
H	4.3039227464	1.1336905459	1.4267797272
H	4.4536629792	2.8029443361	2.049353526
H	4.1197186461	2.5055984856	0.3209186344
H	2.2666533611	4.1898763106	2.0775564901
H	2.0994209146	3.7852640351	0.3403541687
H	–0.0188019994	5.3926352619	1.8775893857
H	–1.3541610563	4.4107010821	1.2075843017
H	–0.0096121281	4.8983768725	0.1620514748
C	–0.2856491832	–5.3454215174	–1.2078537684
C	–2.393769173	–4.1708007025	–1.3856785372
C	–4.4723708382	–2.9317711479	–1.3404153186
N	–0.9562479423	–4.0525734162	–1.180869547
N	–3.0202874845	–2.8629519716	–1.2478843451
C	–0.3756784097	–3.1176649501	–2.133279857
C	–2.4569929484	–1.9193924851	–2.2021352963
N	–1.0133553782	–1.8075997922	–1.9740508833
C	–0.4052464536	–0.8014096734	–2.8471360498
H	–0.7154989143	–5.9942778318	–0.4374932729
H	–0.3720892872	–5.8606533955	–2.1846808687
H	0.7763032186	–5.2075135078	–0.980921491
H	–2.803871603	–4.839568451	–0.6216133484
H	–2.6182804136	–4.617066973	–2.3893602202
H	–4.8545245333	–3.6066147429	–0.5672396273
H	–4.8296858531	–3.2928134176	–2.3248441966
H	–4.8940087407	–1.9376278543	–1.1612360211
H	–0.4919497145	–3.482139467	–3.1839765328
H	0.6919497108	–3.0126431567	–1.9190578294
H	–2.6616828956	–2.2341889941	–3.255324052
H	–2.9112900656	–0.9378313965	–2.0386226806
H	–0.5141682123	–1.0497287752	–3.9182504917
H	0.6589458983	–0.7173764669	–2.6090216965
H	–0.8756570067	0.167600267	–2.6576044
C	1.220189653	–1.4146349492	0.7842395283
H	2.0124008126	–1.1268678251	0.0640063358
H	1.084105634	–2.5052435458	0.6354074684

H	1.7096050025	–1.3585478836	1.7777947446
C	–1.9738726724	0.4126306221	0.6312387817
H	–2.2182540571	0.9582659918	1.5651192419
H	–2.8324981342	–0.2801436538	0.5161284321
H	–2.1044993794	1.1644081523	–0.1732489305
Li	–0.81961935	–1.3286954894	0.0710363013
Li	0.1209318992	0.4098142683	1.205552348

Tabelle 225 Standardorientierung von MeLi-Dimer Methyl-TS [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	-0.5233094601	0.1385279358	0.2944898748
N	-0.1638385258	1.5364663043	0.0526966615
C	1.2632366466	1.787605262	0.2748454351
C	-0.9586277792	2.4616787963	0.8649879242
N	1.5696423225	3.1568412148	-0.1122009616
N	-0.6579812589	3.8137814425	0.3888172799
C	2.9933800975	3.4549346297	-0.0424685788
C	0.7565425947	4.1140343337	0.6229288013
C	-1.5448539627	4.8161262608	0.9784294681
H	0.0590404099	-0.5047846817	-0.3723461453
H	-0.336621816	-0.1738852431	1.3370820477
H	-1.5838240864	-0.0027015183	0.0676732518
H	1.8427860513	1.1075635574	-0.3574667573
H	1.533889992	1.5883181176	1.3403323393
H	-0.7327329977	2.3504757199	1.9505593597
H	-2.0188043456	2.2585108734	0.6899018812
H	3.541597243	2.7559767264	-0.6819576299
H	3.4027205642	3.3876214837	0.9838658392
H	3.1712183202	4.4666176273	-0.4208528451
H	0.9852624632	4.0970553129	1.7166488337
H	0.9715733363	5.1188381555	0.2454163384
H	-1.4493891147	4.876401293	2.0772663855
H	-2.5798367956	4.5682420756	0.7257418069
H	-1.3125878283	5.7985884942	0.555243935
C	-1.3944001224	3.164199022	-8.2276538194
C	-3.0473774928	2.5316525255	-6.5458386687
C	-4.3331053599	1.8120590911	-4.4962189891
N	-1.9061790823	3.4027494882	-6.8834444986

N	-3.3855050008	2.7500922889	-5.1436114221
C	-2.2604695637	4.8038079724	-6.6753153144
C	-3.8112367721	4.1295277564	-4.9664201759
N	-2.6562966154	4.9962883964	-5.2769815066
C	-2.9163462525	6.4008847461	-4.9760984574
H	-1.1013506708	2.113612126	-8.3217975446
H	-2.134095466	3.3900030013	-9.0189743667
H	-0.5056809972	3.7817188854	-8.399078831
H	-2.7432588291	1.4897793081	-6.6776468591
H	-3.9188799109	2.7295873811	-7.2133311177
H	-3.9769812432	0.7893007858	-4.6906537449
H	-5.3463222664	1.917986279	-4.9360368995
H	-3.9413951313	2.1162464554	-3.1088824132
H	-3.0818083596	5.1211942038	-7.3626061695
H	-1.3828012567	5.4257786043	-6.8831930997
H	-4.6844969442	4.3807800184	-5.6133608539
H	-4.0995262152	4.274018247	-3.9227076993
H	-3.7427829948	6.8205458973	-5.5782588958
H	-2.01360396	6.9913608653	-5.1660175286
H	-3.1766249923	6.501975502	-3.917802243
H	0.906849086	4.0644712156	-3.1842854199
H	0.5275811487	3.1045268651	-4.5898278766
H	0.9989854826	2.3143707494	-3.1243072767
C	0.3704332089	3.1480599454	-3.4935560504
H	-2.4451074794	1.6216878924	-1.8510839981
H	-3.9147213033	2.2803066239	-1.0800717857
H	-2.7794558691	3.4072534724	-1.8661485577
C	-3.2276079001	2.3969915028	-1.9327009139
Li	-1.5255325161	3.2781867007	-4.3792301011
Li	-0.6566804296	2.8507620115	-1.6880914467

Tabelle 226 Standardorientierung von MeLi-Dimer Methylen-TS [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	-0.6790686836	-0.2484693483	-0.2634671048
N	-0.7358819111	-0.6705702451	1.1359139477
C	0.2933176785	-0.024148839	1.9544665255
C	-0.6543862614	-2.1249399838	1.2896226414
N	0.0100870908	-0.3599032129	3.3524307781
N	-0.8879985591	-2.4484790577	2.6919938223

C	0.8518071688	0.3892606946	4.2851377641
C	0.1053779216	-1.8086276183	3.5461557957
C	-1.008056243	-3.8818491962	2.9332464932
H	-0.8097017389	0.8362271446	-0.3148490267
H	0.2751180654	-0.5161499403	-0.7506698036
H	-1.4974974143	-0.7195516391	-0.816554041
H	0.2068871356	1.0591864323	1.831650812
H	1.3165105273	-0.3491029813	1.655681374
H	0.3313992767	-2.5099089174	0.934734875
H	-1.4413110787	-2.587660503	0.6861658601
H	0.6871408206	1.459895338	4.1338259742
H	1.9269979152	0.1723121903	4.1570796311
H	0.5652148178	0.1393347336	5.3113231722
H	1.1369440408	-2.1743293228	3.3269476711
H	-0.1266845595	-2.0405934571	4.5901224326
H	-0.0822457164	-4.4397022076	2.6992272805
H	-1.8217592851	-4.2843490736	2.3222412872
H	-1.2613083488	-4.0515939373	3.9842060032
C	-4.1102480858	3.676004203	5.4889810773
C	-4.8910747354	3.5274375201	3.2053219129
C	-5.6351245805	3.0598655165	0.9525158346
N	-4.9572589086	2.9384584842	4.5591583683
N	-5.7010115226	2.6380588028	2.3466903961
C	-6.325711442	2.8249478351	5.0632928632
C	-7.0865275597	2.5177603864	2.8001197895
N	-7.1091121955	1.9886242676	4.1598662647
C	-8.4665612662	1.7892746064	4.6432517218
C	-4.0411825428	-0.8072395378	3.5087231099
Li	-4.3922012083	1.2941308178	3.3410169752
Li	-2.1717209116	-0.2811279048	2.818138104
H	-3.0943212123	3.720299194	5.0880577171
H	-4.4642042063	4.7131864469	5.6436898389
H	-4.0882311988	3.1708535251	6.4625430734
H	-5.3082672782	4.5643361772	3.2050262563
H	-4.5874407368	3.1172798867	0.6461187286
H	-6.0943605198	4.0544545666	0.7948640743
H	-6.1548741833	2.3354161931	0.3133547337
H	-6.7820910829	3.8400397275	5.1701713348
H	-6.3176630713	2.3454489708	6.0511696671
H	-7.5971427003	3.5109393957	2.7456791947
H	-7.6284721961	1.8162165008	2.1520289908
H	-9.0485529889	2.7303354056	4.7112434447

H	-8.4373954333	1.3325778461	5.638908545
H	-8.9980549139	1.1063481559	3.9710373965
H	-4.1547368164	-1.5719820171	2.7145203487
H	-5.0813645037	-0.6159200092	3.8320014343
H	-3.6015485227	-1.3540918433	4.3666720113
H	-3.5360435682	3.1315057706	2.8037936098
C	-2.3228121113	2.4655078474	2.4866639884
H	-1.8078056765	1.9888613501	3.3398533434
H	-1.6896999603	3.3037240774	2.156210446
H	-2.3798388191	1.7530117824	1.6443252397

8.3.5 Angaben zu den quantenchemischen Rechnungen der Strukturen und Deprotonierung von TMEDA und TEEDA (Kapitel 4.2.3)

Tabelle 227 Berechnete Energien der optimierten Verbindungen.

Verbindung	Methode/Basis	Min./TS	SCF (Hartree)	ZPE (Hartree)
$(i\text{-PrLi})_6$	B3LYP/6–31+G(d)	Globales Min.	–756.439578	–755.876686
TEEDA (**6**)	B3LYP/6–1+G(d)	Globales Min.	–505,012394	–504.674652
$[(i\text{-PrLi})_3\cdot(\text{TEEDA})_2]$ (**106**)	B3LYP/6–31+G(d)	Globales Min.	–1388.253929	–1387.294923
$(i\text{-PrLi}\cdot\text{TEEDA})_2$	B3LYP/6–31+G(d)	Globales Min.	–1262.175089	–1261.309030
i-PrLi·TEEDA	B3LYP/6–31+G(d)	Globales Min.	–631.084356	–630.652840
t-BuLi·TMEDA	B3LYP/6–31+G(d)	Globales Min.	–513.144622	–512.799816
t-BuLi·TMEDA Lithiierung	B3LYP/6–31+G(d)	TS	–513.101803	–512.761418
t-BuLi·TEEDA (**107**)	B3LYP/6–31+G(d)	Globales Min.	–670.400939	–669.941859
t-BuLi·TEEDA (**107**) α-Lithiierung	B3LYP/6–31+G(d)	TS	–670.349869	–669.896587
t-BuLi·TEEDA (**107**) β-Lithiierung	B3LYP/6–31+G(d)	TS	–670.361448	–669.906750

Tabelle 228 Standardorientierung von $(i\text{-PrLi})_6$ [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
H	–0.1630230135	–0.0254107751	0.0407116569

H	–0.1739806097	0.1713745157	2.4824244906
H	1.3178526867	0.0745756811	–0.9232380462
C	0.9078389318	–0.295648141	0.026996067
H	0.9042580905	–1.4008402969	–0.0381892497
H	1.5636773109	1.3462618897	1.1717109746
C	0.8878927047	–0.1316431147	2.5324204085
H	3.0460293989	2.3090368804	–1.2054648597
C	1.6822112192	0.2445348113	1.2566904812
H	0.8812537217	–1.2173328831	2.7133523749
H	1.2884926832	0.3405804239	3.4431132076
H	3.9874565901	3.8061609186	–1.2640725362
H	3.2199317571	3.3325716104	0.2275153197
C	3.7657207066	2.9202710889	–0.642713602
H	3.6796776416	–0.1208425314	–2.5576115304
H	2.547111554	2.3806948014	3.4472490192
H	1.7013998168	–3.1239304769	1.4950353984
H	4.2239635417	–1.5465833364	–3.4536426339
H	3.2140684275	–2.1831303734	–1.2869936801
Li	2.9502480677	–1.3516662063	0.4803120165
Li	3.52769596	1.4521551797	1.1733579079
H	3.7675642318	3.3477285221	2.610104622
C	4.3899768264	–0.9593721431	–2.5329816226
C	3.6218203808	2.6172748919	3.4214721801
C	2.6869651173	–3.5808929431	1.6765219865
H	3.8310129632	3.16723028	4.3573042937
H	3.0199468484	–4.0086475542	0.7186685619
H	2.4974112057	–4.4431444256	2.3416291617
C	4.2591612622	–1.807990323	–1.2428583576
C	5.0365312142	2.1253606532	–0.2472819812
Li	3.4054363534	–0.427705679	2.6234086022
H	5.3989271921	–0.5252842329	–2.6704571946
H	5.4682491067	1.8266315946	–1.2267221259
H	3.3560608599	0.0662142528	4.6856649545
H	3.2867389453	–2.2857015747	3.2419298858
H	6.2575768463	3.9840744455	–0.3264214019
H	4.9239750888	–3.6263002601	–2.3420965338
H	5.7350412036	3.5495775741	1.296539198
C	3.7184568378	–2.5844306333	2.2624897411
Li	5.3495516985	–0.0313643011	–0.6082008423
C	4.4958267898	1.3489203429	3.2580661175
C	6.0680229347	3.121822963	0.3386857734
C	5.1331676712	–3.076344872	–1.4062644202

C	4.3650112256	0.500302163	4.5481893825
H	4.9874238202	–3.8067985022	–0.5948968621
H	4.5310245103	1.0875133563	5.4688503938
H	5.5409196245	1.7240603933	3.30220144
Li	5.227292092	–1.9112251599	0.841849852
Li	5.8047399843	0.8925962262	1.5348957434
H	7.0535882352	2.6648604968	0.5201723615
H	6.2078764979	–2.8397647815	–1.4320412593
H	5.0753104103	–0.3382274487	4.5728192902
C	4.9892673454	–3.379341069	2.6579213619
H	4.7675314618	–4.2652308987	3.2792802961
H	5.5350562949	–3.7916415905	1.7876924402
H	7.4664953688	–0.799650404	–1.4279054477
H	7.8737343303	0.758262903	–0.698144615
H	5.7089586531	–2.7681068605	3.2206726196
C	7.0727768328	–0.7036047914	0.7585172787
C	7.8670953473	–0.3274268654	–0.5172126486
H	7.1913107411	–1.8053318699	0.8434967853
H	7.8507299615	0.9417703168	2.0533970096
H	7.4371353653	–0.5336456612	2.9384458061
C	7.8471491201	–0.1634218392	1.9882116929
H	8.9289686616	–0.6304444958	–0.4672167307
H	8.9180110654	–0.433659205	1.974496103

Tabelle 229 Standardorientierung von TEEDA (**6**) [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	2.7513506749	0.7278695562	0.7037699901
N	1.5196476154	0.1547526985	0.1546534773
C	3.5956771967	1.4908726138	–0.3196927657
C	1.7173238697	–0.7908495405	–0.9515372952
H	3.3817309858	–0.0374442239	1.2016847113
H	2.4482223057	1.4277351588	1.4933534992
C	0.6541409042	–0.3321544365	1.2260407967
C	2.478996119	–2.0916624128	–0.632405148
H	2.2403367683	–0.2568818587	–1.7526596349
H	0.5127986341	0.4999008465	1.9272848936
H	1.1284858477	–1.1402674028	1.8213558977
C	–0.718550399	–0.8738325614	0.7922119131
H	–0.5911492226	–1.8570776422	0.3218839221

N	–1.4636014374	–0.0418869259	–0.1489035725
H	–1.2769008885	–1.0564593481	1.7337048657
H	0.7266477989	–1.0256464761	–1.3525590987
C	–2.6297563756	–0.7373260115	–0.7060714209
C	–3.8057752682	–1.0254258311	0.2481357868
H	–2.2661497469	–1.6865786929	–1.1217309829
H	–2.9960476768	–0.1552542026	–1.5590538615
H	–4.2392593751	–0.1028707033	0.6521861982
H	–3.5056163146	–1.6544071469	1.0943040065
H	–4.6003154442	–1.5547139045	–0.2927815408
H	2.9839253982	2.2268905267	–0.8542314773
H	4.0601413174	0.8293637882	–1.0594101382
H	4.4054456593	2.0227723035	0.1940880749
H	1.9748572875	–2.6869039258	0.1384830067
H	3.5011975237	–1.8961865882	–0.2869681164
H	2.5482687472	–2.7113039118	–1.5353886517
C	–1.7233065575	1.3101848046	0.3506016002
H	–0.7563604411	1.7333417301	0.6369423067
H	–2.3519022507	1.3001331346	1.2651049957
C	–2.3530953061	2.2419086686	–0.6879632971
H	–3.3863061709	1.9704315333	–0.9324000727
H	–1.7666713786	2.2372585614	–1.6140625062
H	–2.3697317591	3.2665989403	–0.2979205911

Tabelle 230 Standardorientierung von [(*i*-PrLi)$_3$·(TEEDA)$_2$] (**106**) [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.0977698051	–0.1399915086	0.0805351329
C	–0.0622717651	1.3845386142	–0.0135450778
C	–5.9156310945	–3.1898670686	0.0039027048
C	1.1239646226	1.9207606151	2.8272080896
C	–3.4351732772	0.5415244956	–1.8922495008
C	–6.3602592413	–3.0197558376	1.455605497
C	–0.3389902843	1.6655183773	2.4277126238
C	–9.1323258801	–4.4261543427	1.3811383504
C	–3.4979152164	–0.7495748567	2.0655338057
C	–3.6700066922	1.9189114841	–1.2289102384

C	–0.5975208687	3.5524914482	0.8496384503
C	–8.7752023571	–3.0039017592	0.921183984
N	–7.6597293036	–2.318568838	1.6236632271
C	–4.2927317404	2.8543085	–2.2832845524
Li	–3.1283362263	2.0557929206	0.9633044378
C	–4.3431350097	0.5349741527	2.1605494264
Li	–5.1895512104	1.1308368046	0.1277903334
C	–7.915815196	–2.1103303851	3.0657341527
C	–8.3593931139	–0.0889324311	–1.2894242751
C	–1.3517195732	4.4469883777	1.8343142556
C	–4.3217960745	1.0123442737	3.6221642184
C	–7.2735888822	0.8522972447	–0.7194698358
Li	–7.6271888983	–0.2433905579	1.0350938843
N	–2.820287119	4.301721412	1.770053509
C	–9.1037200857	–1.1849740782	3.3445380532
C	–3.3718860527	5.1959109048	0.7240048003
C	–7.8328103792	2.2894711622	–0.729503619
N	–8.9315873881	0.1608248519	2.7469395374
C	–3.4438384675	4.5076958605	3.0973711921
C	–4.8888484732	5.1269335174	0.5708095556
C	–8.2044993231	1.0480123884	3.6924336553
C	–	0.730287304	2.2884755014
C	–3.3130284331	5.9080021835	3.719110362
C	–7.8849520366	2.4336248341	3.1356514493
C	–	1.0296443786	3.3681133119
H	0.2881442027	–0.5611176709	–0.8549014437
H	0.5244485113	–0.5287108637	0.8945033142
H	–1.1178916692	–0.5087050202	0.2184057988
H	0.989345459	1.7197211671	–0.079317341
H	–0.5472343392	1.6916726979	–0.9462336515
H	–4.8858764776	–3.5636607524	–0.0110841565
H	–6.5311293616	–3.908114154	–0.5490028489
H	–5.9324724164	–2.2339634519	–0.5307017046
H	1.8301363392	1.4272992149	2.149798382
H	1.2982441546	1.5203984992	3.8333392493
H	1.3727647687	2.9878957377	2.8513424805
H	–2.8705755297	0.5945434943	–2.8484020675
H	–2.8875129432	–0.1562556123	–1.2415714125
H	–4.3861888716	0.0441188198	–2.1491711844
H	–6.3848461603	–4.0030924351	1.9563805306
H	–5.6136889881	–2.4202123712	1.982422142
H	–0.5514178027	0.596206461	2.4993745801

H	–1.0026501965	2.1396923246	3.1575157626
H	–8.2908511736	–5.1189468318	1.2736568871
H	–9.9529542068	–4.8065690879	0.7614889266
H	–9.4667054044	–4.4601410369	2.4241657816
H	–3.5567696946	–1.2256190865	1.0755601499
H	–2.4326921421	–0.5404392505	2.2427642113
H	–3.7643960311	–1.5284935153	2.8165666734
H	–2.6503811493	2.3291823159	–1.0566215187
H	0.4687897631	3.8436719375	0.8754735672
H	–0.9432930418	3.755274565	–0.1705015148
H	–8.5219876831	–3.0188972444	–0.1416396013
H	–9.6620152147	–2.3669422516	0.9996056005
H	–3.7262527025	2.8803881413	–3.239327742
H	–5.3151381762	2.5469815759	–2.5508126994
H	–4.3664991253	3.8939501201	–1.9342303778
H	–5.3999306272	0.2093597852	1.9828706157
H	–8.0785164875	–3.0633884629	3.5977648027
H	–7.0049368094	–1.6740621434	3.4915111502
H	–7.9651020064	–1.0865139801	–1.5305126951
H	–8.8263117998	0.2988303242	–2.2169491811
H	–9.2137441126	–0.2449011168	–0.5994645117
H	–1.0250132978	4.2272599897	2.8553757969
H	–1.0460781606	5.4895354993	1.6372862414
H	–3.314022659	1.3402032283	3.9252575427
H	–4.602268598	0.2250849632	4.3599680904
H	–4.9896986658	1.8665914923	3.7984696619
H	–6.4757684583	0.8288199447	–1.4830932116
H	–	–1.6274793849	2.9453653068
H	–9.2427651222	–1.1236285715	4.4361901991
H	–2.9120240858	4.9030371955	–0.2251313295
H	–3.0651013186	6.2411447497	0.9137328219
H	–7.0781870743	3.0399078342	–0.4563059576
H	–8.2338373931	2.5955897068	–1.7174889864
H	–8.6639297492	2.4137559434	–0.0163747067
H	–3.0022066534	3.7679978175	3.7733330323
H	–4.5001574797	4.2388578766	3.0127724013
H	–5.2144995037	4.0946682692	0.4107456202
H	–5.1911053215	5.7102874467	–0.305867795
H	–5.4192653447	5.5378043865	1.4369847314
H	–7.2644998598	0.5467004146	3.9447788329
H	–8.7718190926	1.1436344332	4.6343675659
H	–	0.0213477735	1.5637712954

H	–	1.6412568226	1.7253791511
H	–2.2653721333	6.2068848429	3.8432520661
H	–3.8138151698	6.6775243248	3.1209905217
H	–3.7766088243	5.909891256	4.7132665298
H	–7.339255237	2.3646782981	2.1894219003
H	–7.2544341816	2.9690189816	3.8538287697
H	–8.7830552206	3.03888513	2.972050232
H	–	0.1375971816	3.9502685251
H	–	1.8051625516	4.0665766065
H	–	1.390961754	2.8895907232
N	–0.7649543587	2.103402564	1.0781864648

Tabelle 231 Standardorientierung von (*i*-PrLi·TEEDA)$_2$ [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–3.4433851887	2.5378666648	–3.6992898746
C	–4.3092140573	1.3885817881	–3.1856996183
C	2.4170579106	1.5371307987	–3.5189129747
C	–5.7383390679	3.11995084	–1.0009222769
C	–1.1029480959	–0.5148831416	–3.8620762385
C	2.9439010536	0.9648888716	–2.2038243059
C	–4.3939705429	2.3770852808	–0.9178442718
C	4.1248688686	–1.6287943992	–3.5158883611
N	–4.2415865207	1.1418450457	–1.722720804
C	–0.3744962938	2.397052073	–0.9499682036
C	–1.3508329669	–1.3791475414	–2.6057118676
C	–5.249123908	0.1143326422	–1.3965169122
C	2.6909098872	–1.3553564836	–3.0305018075
N	2.51783016	–0.4232975272	–1.8906057807
C	–1.0266653534	–2.8381518194	–2.9861743789
Li	–2.2126290439	–0.0148293581	–0.9536028453
C	–0.5918759485	1.1944208754	–0.0051516602
Li	0.1615281297	–0.6481540645	–1.127774707
C	3.2568885339	–0.849992905	–0.6865321829
C	–5.2051650972	–0.3966632759	0.044389051
C	–1.1649650659	1.749167179	1.3145841201
N	–4.000401064	–1.1873650851	0.3565349533
C	2.8307617129	–2.1992892722	–0.1057932994

C	–4.1814807151	–2.5778785124	–0.1193159174
N	1.4958949944	–2.1868864775	0.5167468753
C	–3.6541514063	–1.1042011211	1.7943554115
C	–2.9976208984	–3.4974579169	0.1611925827
C	1.5852294998	–1.6056460041	1.8748124543
C	0.8771597211	–3.5313489026	0.4967660086
C	–4.6639923499	–1.6924537505	2.7936180569
C	0.2602533157	–1.5502803501	2.6289056738
C	1.5876339245	–4.6442159946	1.2858779677
H	–3.4256927166	2.5045032419	–4.7946827237
H	–3.8335139725	3.5194516897	–3.4083244296
H	–2.411893139	2.4588427488	–3.3444290735
H	–5.3562263552	1.5659409113	–3.4950913394
H	–3.994277523	0.4579802689	–3.6709136778
H	2.6443916403	2.6088693126	–3.5531001003
H	2.8870396693	1.0751690938	–4.394044226
H	1.3332656431	1.4207326159	–3.6086654849
H	–5.9888670085	3.4151779175	–2.0262802373
H	–5.6788709046	4.0351317707	–0.3994863171
H	–6.5723835446	2.5262666893	–0.6094778084
H	–1.6701159405	–0.8494401958	–4.7584938957
H	–1.3458955529	0.5457310526	–3.7112730566
H	–0.0445052129	–0.5448660846	–4.161973023
H	4.0479333343	1.0343902831	–2.2039503217
H	2.593635392	1.5899950819	–1.3745647753
H	–3.5869106946	3.0521170035	–1.2108019316
H	–4.1879971311	2.121655184	0.1253440758
H	4.651937939	–0.7098279363	–3.7968956608
H	4.0850402304	–2.2710666631	–4.4039534528
H	4.7326244906	–2.1476989868	–2.7658465246
H	0.0853861599	2.1153595744	–1.9071275959
H	–1.3297951612	2.8817289941	–1.2036301215
H	0.2576168171	3.2023150418	–0.5153667988
H	–2.4593672567	–1.3756513073	–2.4694648527
H	–6.2720645099	0.4808787423	–1.598167844
H	–5.088507081	–0.7213367307	–2.086495037
H	2.0968108724	–0.9626908238	–3.8578903081
H	2.2145855474	–2.302386943	–2.7611079059
H	–1.5360937786	–3.1797063097	–3.9139748248
H	0.0496656726	–2.9767179737	–3.1791394697
H	–1.2958855978	–3.5573055608	–2.2009214406
H	0.4347954783	0.8513389457	0.2680676573

H	4.3433764661	–0.8927064449	–0.8843262639
H	3.1211884249	–0.0663919826	0.0666854577
H	–5.2547173345	0.4466031681	0.739875135
H	–6.1231428108	–0.9872191317	0.2156587395
H	–2.1824256852	2.1508155051	1.1783522633
H	–0.5743156466	2.5908602955	1.7378271035
H	–1.2353449973	0.9904264253	2.1055605485
H	2.8365028259	–2.9602800355	–0.8922047064
H	3.6050199988	–2.5053186308	0.6214575166
H	–4.3354011049	–2.5332340924	–1.2019734677
H	–5.1024879069	–3.0145354943	0.3100900868
H	–3.4904927876	–0.0452567631	2.0189146829
H	–2.6858007206	–1.59197145	1.9298737003
H	–2.0719770946	–3.0465561997	–0.2053114111
H	–3.1422784387	–4.4484892982	–0.3639299539
H	–2.8873979392	–3.7235834036	1.2275661675
H	1.9612937515	–0.5837292448	1.766128303
H	2.3344006388	–2.150978017	2.479673027
H	0.7925162433	–3.8261229756	–0.5551725536
H	–0.1465377263	–3.4286979203	0.8637245858
H	–5.6448945004	–1.2080556156	2.7243632801
H	–4.8079507767	–2.76942346	2.6508182617
H	–4.2926727522	–1.5420044371	3.8146904648
H	–0.5064416625	–1.070618693	2.015542932
H	0.3855634716	–0.9550391704	3.5407029524
H	–0.0930225838	–2.5427102909	2.9301874352
H	2.6073170877	–4.8221924979	0.9253170826
H	1.642886752	–4.4217349548	2.3576465602
H	1.0294608751	–5.5816479942	1.1725757298

Tabelle 232 Standardorientierung von *i*-PrLi·TEEDA [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–3.286447574	1.0434236131	0.982444975
C	–1.9802379682	1.8372590092	1.0130120841
C	–1.9923234973	2.7744220115	–1.9282974019
C	–1.5021128292	1.422922923	–1.3848863654
N	–0.9827581113	1.3995499221	0.0058803718
C	0.2844296173	2.1373252306	0.1702671499
C	–2.1415738616	–2.6784131059	–0.855407114

C	–1.4083630695	–2.3986173059	0.471863047
Li	–0.3697071968	–0.6206985409	0.3083579498
C	1.4848905925	1.4158997625	–0.4599461657
C	–0.611893115	–3.6545231872	0.8653475148
N	1.6535680482	0.0396142994	0.0523172598
C	2.34694315	0.0426415759	1.3629715471
C	2.2772855201	–0.8627790261	–0.9469819547
C	2.4493616124	–1.3340822053	2.0205312327
C	3.7282919946	–0.5565429202	–1.3467235252
H	–3.8885440489	1.3107463877	1.8585712077
H	–3.8900913472	1.2622700169	0.0949216204
H	–3.0905359039	–0.0339110451	1.0139827317
H	–2.1906103288	2.9171033874	0.9164607465
H	–1.5093209467	1.7003894213	1.9940637468
H	–2.8375514108	3.1671867967	–1.3528612094
H	–2.3312901365	2.6436605709	–2.9627152054
H	–1.2047490566	3.5365462217	–1.935520786
H	–2.3116952076	0.6895549454	–1.4396471196
H	–0.7114228538	1.0384113295	–2.0385576316
H	0.234179432	3.1606716451	–0.2388732443
H	0.4537260747	2.2515216221	1.2464486759
H	–2.8347559079	–1.8673986988	–1.1355489444
H	–2.7464169059	–3.6135972412	–0.8476544801
H	–1.4378077135	–2.7924552559	–1.6988576868
H	–2.1988386953	–2.2848769008	1.2426181199
H	1.3527694546	1.3587913091	–1.5455896385
H	2.3857447227	2.0305600787	–0.2902524686
H	–0.187733838	–3.5795130157	1.8791605044
H	–1.2134203473	–4.5916618734	0.8475198581
H	0.2369569462	–3.8378730271	0.1828526962
H	1.7787146452	0.7058267473	2.0249843865
H	3.3512947746	0.4917092501	1.267642394
H	1.640269671	–0.8322142857	–1.8392826752
H	2.2027572121	–1.8833328911	–0.5609379885
H	1.4753812333	–1.834353632	2.0533761165
H	2.8125175763	–1.2176266013	3.0481440725
H	3.1514046266	–1.993303819	1.499238559
H	3.8370488608	0.4522176565	–1.7625844631
H	4.4199148419	–0.6512424421	–0.5021673745
H	4.051274057	–1.2679987806	–2.1158905749

Tabelle 233 Standardorientierung von *t*-BuLi·TMEDA [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
N	–1.8140931459	0.5110228362	0.1071882052
C	–1.5842953347	1.9253877303	0.4578191011
C	–0.3466329599	2.5039095101	–0.240508306
N	0.8590686403	1.6862151173	–0.0082687319
C	1.409237205	1.8832511516	1.3421534794
C	1.8963765379	1.9576689735	–1.0150596579
C	–2.6867262645	–0.1502983015	1.0890082432
C	–2.3769776644	0.3598120509	–1.244067223
H	–1.4561871166	1.9803701655	1.5441581554
H	–2.4618060357	2.5514371717	0.2130230634
H	–0.1993115877	3.5473327892	0.0930990947
H	–0.5163398849	2.5440202114	–1.3217000719
H	2.2697957685	1.2229223702	1.4810772926
H	0.6660214073	1.6297030803	2.1036071872
H	1.732400311	2.9270039664	1.5052660938
H	2.7446123338	1.287809988	–0.849552465
H	2.2533680451	3.0019478922	–0.9721934571
H	1.5010629633	1.7639968309	–2.017005299
H	–2.7862262241	–1.2079218522	0.8297121484
H	–3.6933115014	0.3030875003	1.1214682111
H	–2.2407560727	–0.085090961	2.086192453
H	–2.47961829	–0.7040366491	–1.4753188522
H	–1.7118926432	0.8017532661	–1.9915731078
H	–3.367485981	0.8410539497	–1.3320367891
Li	0.1376227978	–0.3076967657	–0.0197936122
C	0.9593920462	–2.2015390173	–0.1061551021
C	0.9069615419	–2.8740717877	1.2735572759
C	2.428885179	–2.158925367	–0.5486653516
C	0.2001349914	–3.1003189311	–1.0928812085
H	–0.1232460385	–2.9822368653	1.6508080173
H	1.4714784608	–2.313218075	2.0363774471
H	1.3411412769	–3.9041477445	1.2630146048
H	3.056888773	–1.5662676291	0.137243855
H	2.5527575549	–1.726552387	–1.5549809846
H	2.8926695493	–3.1750618429	–0.5893850269
H	0.2262374153	–2.7103470847	–2.1234107059
H	–0.861754165	–3.2208274291	–0.8205104047
H	0.6236731595	–4.1335621089	–1.1416434385

Tabelle 234 Standardorientierung der Deprotonierung von TMEDA via *t*-BuLi·TMEDA [Übergangszustand, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
N	–1.6519726548	1.0091890158	0.5940649587
C	–0.80752	2.227267245	0.6010520488
C	0.0445515649	2.3858384206	–0.6665787955
N	0.7459012774	1.1540351235	–1.0335079199
C	1.7067910463	0.6570940259	0.020143449
C	1.3590501514	1.2717176602	–2.3553851566
C	–2.1983499738	0.7586702571	1.9366636501
C	–2.7473121224	1.111804196	–0.3834181782
Li	–0.2179850819	–0.3227268921	–0.1111659455
C	0.921934889	–2.1638063064	0.28149307
C	1.5498816442	–2.5527923386	1.6202962532
C	1.7060316945	–2.7900457719	–0.8718698779
C	–0.5333554921	–2.6698571127	0.2483573554
H	–0.1521470199	2.157090739	1.4745254794
H	–1.4282759491	3.1318259013	0.7335510069
H	0.7514577763	3.2202293285	–0.4900189308
H	–0.5921645199	2.6791609585	–1.5117393196
H	1.3254709609	–0.7329803628	0.27777187
H	1.8122524434	1.3970347028	0.8273351226
H	2.6973827871	0.5345555102	–0.4346029112
H	1.8194007611	0.3177808021	–2.6286271266
H	2.1428557738	2.0516679317	–2.3791282873
H	0.5968823266	1.5131846683	–3.1076577917
H	–2.7915968259	–0.1611555675	1.926323906
H	–2.8433944888	1.5856500593	2.2816244246
H	–1.3795805849	0.6336372058	2.6516356601
H	–3.3402494454	0.1917280241	–0.3647197888
H	–2.3452265429	1.239675955	–1.3917623205
H	–3.416235036	1.96202236	–0.1608971159
H	1.0018791432	–2.1178847571	2.470664891
H	2.587816339	–2.1964213464	1.6940316443
H	1.5710644906	–3.6489956951	1.7769622086
H	2.7410039483	–2.4186886043	–0.8979460771
H	1.2567116546	–2.5625063225	–1.8507357997
H	1.7642789353	–3.8945571368	–0.7966335902
H	–1.033450913	–2.4747158497	–0.7172083301
H	–1.1576680199	–2.2290445218	1.0453830733

H	–0.6022335191	–3.7680239331	0.3969437569

Tabelle 235 Standardorientierung von *t*-BuLi·TEEDA (**107**) [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.5767491768	–1.7660295627	–2.4553416844
C	1.3996618828	2.4674580553	–1.7973104172
C	2.2459791672	1.3305462966	–1.2242989627
C	–0.3856074721	–2.5691176816	–1.1672356302
C	–2.3805314404	2.2379316769	–1.0438416804
C	–3.3590677119	0.0974448571	–0.2879845929
C	1.7634213259	–1.679594964	–0.4142407445
N	0.3282910076	–1.8373357533	–0.0894530592
C	–2.2465293613	1.1179817525	–0.0018699367
N	1.761248261	0.7851510284	0.0711290886
Li	–0.3443552573	0.2138617676	0.0014470403
C	2.4167631811	–0.5155109882	0.3397578428
C	2.0365494898	1.7486747896	1.1681790485
C	0.1808018099	–2.5551034306	1.2035730399
C	–2.5441905774	1.7404252566	1.3715881396
C	–1.2032644934	–2.4390904207	1.843143032
C	1.2837741156	1.4576969317	2.4675220914
H	–1.1766877369	–2.3530471624	–3.1602632464
H	0.3673114796	–1.5284347728	–2.9583910555
H	–1.11607192	–0.8325713248	–2.2582412506
H	1.791587962	2.7451219031	–2.7830089758
H	0.3536192685	2.1682813437	–1.9154011488
H	1.4209151727	3.3674533713	–1.1747864151
H	2.2506847091	0.5076861688	–1.946078469
H	3.2977587426	1.6542594473	–1.1142549065
H	0.1366336397	–3.5201481812	–1.3813238942
H	–1.3740304984	–2.827682369	–0.7812214935
H	–2.2213469678	1.8795689883	–2.0744640197
H	–3.3950247154	2.7057286613	–1.0357405651
H	–1.6661652381	3.0586695609	–0.8729621313
H	–3.264471228	–0.3634640671	–1.2846624856
H	–4.3747221935	0.561342324	–0.2608319331
H	–3.3815908913	–0.7239203482	0.4454175718
H	1.8548240857	–1.5132410568	–1.4897217488
H	2.3226646937	–2.6071921333	–0.1949055084
H	3.4896282847	–0.4763776511	0.077968325
H	2.3705024817	–0.7063245619	1.4141338434

H	1.7350893486	2.737537708	0.8154108895
H	3.1249991816	1.7949871784	1.3577889973
H	0.4500537254	–3.6187558762	1.0648321065
H	0.9172950528	–2.1392400018	1.8984422744
H	–3.5618531454	2.199110143	1.4194747641
H	–1.8373490741	2.5457763713	1.6292492801
H	–2.5072247388	1.0030887773	2.1911327945
H	–1.9863510637	–2.9170477771	1.2469737868
H	–1.4891050529	–1.3921329999	1.9887770965
H	–1.1896943182	–2.9321324033	2.8224367001
H	0.2007606898	1.4450694613	2.3030170482
H	1.5785890094	0.5096124239	2.9312096419
H	1.4989977126	2.2498512171	3.1940835298

Tabelle 236 Standardorientierung der α–Lithiierung von TEEDA via *t*-BuLi·TEEDA (**107**) [Übergangszustand, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.6152568043	–2.0946538208	–2.4208881459
C	1.6346404105	1.7988641981	–2.6622122801
C	2.3718227828	1.0962714894	–1.5219975981
C	–0.3769835582	–2.8547115117	–1.1158681572
C	–2.182831543	3.0017834738	0.2605620209
C	–2.8262859277	0.6317186467	–0.1620378657
C	1.6408716055	–1.7740682214	–0.241998102
N	0.1851548357	–2.0181677991	–0.0245669001
C	–1.9440556619	1.5548654899	0.6996085213
N	1.4854370942	0.6896047872	–0.4099434523
Li	–0.4040304778	0.0910022819	–0.0748095892
C	2.0707349538	–0.4290421024	0.3515888013
C	0.978246707	1.8093243543	0.4694809337
C	0.0087813418	–2.6976490919	1.2881188335
C	1.9663158296	2.304330725	1.5304673447
C	–2.3197841889	1.3995706893	2.1744515758
C	–1.4240574328	–2.7303477374	1.8180051768
H	–1.0118897025	–2.780887469	–3.1782975171
H	0.2999307769	–1.6505650408	–2.8256717362
H	–1.3508839086	–1.2934298453	–2.2840010874
H	2.3388742595	2.0578815268	–3.4626071364
H	0.8594989477	1.1478497754	–3.0857214968

H	1.1547359083	2.7251114492	–2.3299317707
H	2.8529405555	0.1945278807	–1.9267454737
H	3.1833954728	1.7420934924	–1.1439912099
H	0.2830759939	–3.7223605973	–1.2943203951
H	–1.3340931356	–3.255235088	–0.7721957165
H	–1.9524822682	3.1492440903	–0.8049202228
H	–3.2330549723	3.3185770791	0.4116792666
H	–1.5515397483	3.7016101453	0.8271236388
H	–2.6209408494	0.7435470337	–1.2395397409
H	–3.9078981244	0.8528232305	–0.0387595756
H	–2.7214959331	–0.4376881757	0.0899023137
H	1.837842983	–1.7660929972	–1.3173235349
H	2.2319714079	–2.6018779691	0.1858581707
H	3.1709671221	–0.3723311237	0.3942090379
H	1.7259941372	–0.3642755326	1.3896409631
H	0.7809375157	2.6406757498	–0.2206261105
H	–0.4793367068	1.5787999258	0.7285438616
H	0.4089192602	–3.7259271271	1.2222877235
H	0.6342456644	–2.1671388924	2.0134429022
H	2.9682144254	2.5696967134	1.1420629437
H	2.1215721591	1.5840532646	2.3457890292
H	1.5588783851	3.2112946291	1.9957122196
H	–3.3766159027	1.6658239539	2.373412305
H	–1.6990609382	2.0460436111	2.8117485624
H	–2.1821446485	0.3698058087	2.5387057456
H	–2.1043234112	–3.3005622811	1.1770007058
H	–1.8309501539	–1.7216841227	1.9360201741
H	–1.4302877329	–3.2100083453	2.8038280431

Tabelle 237 Standardorientierung der β-Lithiierung von TEEDA via *t*-BuLi·TEEDA (**107**) [Übergangszustand, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.1070628956	0.0190148048	0.0196356133
C	0.043110191	4.9431967842	0.0332214023
C	1.4804586521	4.4248491626	0.0548202973
C	1.1634805048	–0.4730144196	0.7127004333
C	–1.8875317312	2.8756285646	2.7018709826
C	–1.0980232585	1.0219923296	4.1995209044
C	2.6731527071	1.4230625852	0.4091339813

N	1.9411693782	0.5904563562	1.3996925452
C	–0.9182087934	2.5004632851	3.8321542197
N	1.8212067088	3.6086664152	1.2386485109
Li	0.7813171757	2.1660704483	2.3718167436
C	3.0319843253	2.8037034788	0.9667555115
C	1.9915662803	4.4303211104	2.4842844145
C	2.9181812858	–0.0321975283	2.3359970684
C	–1.2569161764	3.3510451952	5.0604992243
C	2.3114113574	–0.5374615407	3.6436120614
C	1.838881681	3.5598482962	3.7324498299
H	–0.6194235016	–0.8301243195	–0.4474815019
H	0.0933220424	0.7516653363	–0.7694843533
H	–0.8016147308	0.4699481758	0.7367586798
H	–0.1251627278	5.5204859005	–0.8840880842
H	–0.6748462267	4.116550443	0.0544440143
H	–0.1762719926	5.6008312569	0.880144412
H	1.6363850352	3.801633854	–0.8344014515
H	2.1888122966	5.2704293785	–0.0285833884
H	1.813821728	–0.9955714507	–0.0122330724
H	0.8794705231	–1.2118469781	1.4669862628
H	–1.7339433966	2.2885400056	1.7802984683
H	–2.9473857973	2.7087425704	2.9891489547
H	–1.801080648	3.9352594516	2.4250670061
H	–0.9150993835	0.3384701024	3.3534102087
H	–2.1272243976	0.8019495797	4.5516300234
H	–0.4186195021	0.7197681499	5.0097774498
H	2.0353744892	1.5534369947	–0.4697006
H	3.5843851897	0.9004536707	0.0674476487
H	0.5017979791	2.9653917718	3.7754613886
H	3.7022948403	3.3209343187	0.2594604215
H	3.5968114942	2.6959429882	1.8967315524
H	1.1907669878	5.1769508836	2.4803865565
H	2.9445874913	4.9940880554	2.408119257
H	3.4474955823	–0.8506583656	1.8151054157
H	3.6727819319	0.7214402776	2.5773423965
H	–2.2933657402	3.1815386719	5.4119020685
H	–1.1594679844	4.4258614814	4.8484158142
H	–0.5880682473	3.1278962634	5.9044467677
H	1.552785509	–1.3120347342	3.4906173503
H	1.8537450032	0.2810222541	4.2073964104
H	3.1033939387	–0.9735398196	4.2639824483
H	2.7269287455	2.9274821333	3.9050753932

H	1.7539360769	4.2036163704	4.6172023385

8.3.6 Angaben zu den quantenchemischen Rechnungen der Strukturen und Deprotonierung von (*R,R*)-TECDA (Kapitel 4.2.4)

Tabelle 238 Berechnete Energien der optimierten Verbindungen.

Verbindung	Methode/basis	Min./TS	SCF [Hartree]	ZPE [Hartree]
i-PrLi·(*R,R*)-TECDA	B3LYP/6–31+G(d)	Globales Min.	–787.126986	–786.601531
$(i\text{-PrLi})_6$	B3LYP/6–31+G(d)	Globales Min	–756.439578	–755.876686
t-BuLi·(*R,R*)-TECDA	B3LYP/6–31+G(d)	Globales Min.	–826.442215	–825.888121
t-BuLi·(*R,R*)-TECDA α-Lithiierung-TS1	B3LYP/6–31+G(d)	TS	–826.397729	–825.849797
t-BuLi·(*R,R*)-TECDA α-Lithiierung-TS2	B3LYP/6–31+G(d)	TS	–826.391193	–825.843217
t-BuLi·(*R,R*)-TECDA β-Lithiierung-TS1	B3LYP/6–31+G(d)	TS	–826.402471	–825.853164
t-BuLi·(*R,R*)-TECDA β-Lithiierung-TS2	B3LYP/6–31+G(d)	TS	–826.395468	–825.847209

Tabelle 239 Standardorientierung von *i*-PrLi·(*R,R*)-TECDA (**111**) [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–2.1343180568	–3.1873182986	–1.0804056608
C	–1.7931316947	1.4756969329	–1.0293345421
C	2.0203021549	–0.5224329824	–0.9664865241
C	–2.3924870594	–1.8066449522	–0.4619997463
C	–0.9612327483	–3.8792622759	–0.378903371
C	–1.1472623365	–0.8839628121	–0.514633295
C	0.2869686505	–2.9879991042	–0.4230891023
N	–1.3642412724	0.4984893992	0.0038163072
C	0.0466209728	–1.5915802987	0.198869918
Li	0.5519371527	1.2588665563	0.4463160372
N	1.2567651068	–0.728052851	0.2963603461
C	–2.1603204146	0.5522664633	1.2523652636
C	2.1066692699	–1.0857592311	1.4556453751
C	1.4083759045	3.1474911447	0.6094642063
C	2.6964479658	3.3117082432	–0.220756767
C	0.4769057467	4.3293150734	0.2824193339

C	–3.2153760541	1.3650627685	–1.6027168155
C	3.1203478477	–1.5296879972	–1.3503778856
C	–2.128486464	1.9122431641	1.9550525524
C	3.1583935555	–0.029650504	1.8041411723
H	–1.9093309854	–3.0805657351	–2.1524704618
H	–3.0430389055	–3.7992544444	–1.0119696927
H	–1.0692947407	1.4055232256	–1.8506817895
H	–1.6552253846	2.4730270671	–0.6025919619
H	1.2895079962	–0.4634196262	–1.7805619591
H	2.4821157128	0.4705712216	–0.9064887118
H	–3.234434252	–1.3202328394	–0.9640960333
H	–2.6951252101	–1.9508027153	0.5838418035
H	–0.7446008523	–4.8481936592	–0.8469703888
H	–1.2320925503	–4.0898891376	0.6667290107
H	–0.877274011	–0.7620405805	–1.5725289969
H	0.5882471713	–2.8695317773	–1.4726096228
H	1.1209111304	–3.4777708613	0.0935809334
H	–0.2632982005	–1.752880491	1.2406152938
H	–3.2087158512	0.2637628633	1.0783411777
H	–1.7427558425	–0.2009223248	1.9307163419
H	1.4338723517	–1.2010193306	2.3138856702
H	1.7092215676	3.2836248796	1.6704588704
H	3.1706812262	4.313990857	–0.1204665026
H	2.5058685173	3.1849851752	–1.3011914321
H	3.473426657	2.578490985	0.0494528183
H	0.9639079934	5.3250511837	0.3838306403
H	–0.4158809498	4.3580035928	0.9272301309
H	0.1120498601	4.2879512911	–0.7592101738
H	–3.9805169936	1.3868108603	–0.8183886927
H	–3.3596095031	0.4563988747	–2.1967411232
H	–3.3993879184	2.2213415583	–2.26302093
H	2.746938686	–2.5458882249	–1.5009499721
H	3.9194193263	–1.5706679217	–0.6033300392
H	3.5766474315	–1.1978325049	–2.2910853156
H	–2.6773922522	2.6798591783	1.4002589502
H	–1.1041160408	2.2746458671	2.0989987419
H	–2.6033964571	1.817692598	2.9387993018
H	2.7012117069	0.9549800482	1.950508815
H	3.9246524943	0.0716994581	1.0292263033
H	3.6656598044	–0.3210978538	2.7316448355
H	2.5971655308	–2.0629682654	1.3115248056

Tabelle 240 Standardorientierung von (*i*-PrLi)$_6$ [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.7680842665	–0.2982912843	0.6568478071
C	–0.3021464482	1.1243953539	0.3416182237
C	–5.8024928765	–2.6529223643	–0.1360631617
C	0.9581642232	1.5433959523	3.1419429338
C	–3.3756406201	0.7331574639	–1.8607626396
C	–6.2739999513	–2.908844205	1.2983889232
C	–0.4984931317	1.8460839077	2.7308863259
C	–8.6982296161	–4.507157977	0.5104582221
C	–3.8017075835	–0.5122331559	2.6700664426
C	–3.6440071784	2.0537448613	–1.0847174041
C	–0.4754956539	3.5483498228	0.8058103
C	–8.7138499805	–2.9805550173	0.7338154989
N	–7.6403315654	–2.3651874624	1.5877645523
C	–4.3659466812	3.0245612698	–2.0539629659
Li	–3.0333589843	2.2042461317	1.2591419229
C	–4.4686126233	0.8693607158	2.4751313398
Li	–5.1086281383	1.2873914172	0.3085818512
C	–7.9164020991	–2.3117136469	3.0695183194
C	–8.2767665044	0.0069786525	–1.3540945334
C	–1.1204583364	4.6781609717	1.6618384407
C	–4.5371114647	1.5593736532	3.8558941359
C	–7.2222223289	0.8878520819	–0.6251961481
Li	–7.620096322	–0.2783440507	1.1309309448
N	–2.5815715609	4.4463640499	1.9540837616
C	–9.105996469	–1.3708056106	3.4215657448
C	–3.5220289134	5.0922209698	0.984247668
C	–7.738480578	2.3487148318	–0.6407059316
N	–8.9649236489	–0.0093766747	2.7729999659
C	–2.9280290406	4.7108128584	3.3819131207
C	–4.9945732105	4.7857972082	1.2724154896
C	–8.3172119159	1.0203471983	3.6553811109
C	–	0.4610861477	2.1336614487
C	–2.8507367499	6.171948667	3.8670931631
C	–8.0745232908	2.3637012116	2.9645901296
C	–	0.8191452513	3.0744839159
H	–0.456493766	–0.9644226249	–0.1559163195

H	–0.3330775772	–0.6857714445	1.5842353827
H	–1.855164234	–0.3508575519	0.7389987774
H	0.7981206234	1.1254247711	0.2820173483
H	–0.6777464847	1.4139964369	–0.6454016743
H	–4.7674299584	–2.9960794993	–0.2450120841
H	–6.4060169073	–3.1875674899	–0.8771458017
H	–5.8346338085	–1.5852148075	–0.3764560745
H	1.4055773761	0.7613806207	2.5191525892
H	0.9672161659	1.1824999997	4.1781635383
H	1.605535085	2.4231467961	3.0936146037
H	–2.8706582334	0.8864182266	–2.8384644216
H	–2.7594790663	0.0248260231	–1.2898868983
H	–4.3186633905	0.2118752283	–2.0985115653
H	–6.2241594087	–3.9880262806	1.5127249907
H	–5.5880359181	–2.4158661182	1.9920776793
H	–1.1126602702	0.9772219371	2.9878469402
H	–0.8817569116	2.6702007092	3.335599404
H	–7.7782713505	–4.8388052533	0.019283408
H	–9.5324476756	–4.769370817	–0.1516884657
H	–8.8124864842	–5.0807039248	1.4332325148
H	–3.7871788233	–1.1080851981	1.746125175
H	–2.7535111966	–0.4075119825	2.9883661548
H	–4.282480349	–1.1377011993	3.4576520946
H	–2.6406019703	2.5038792393	–0.9061166203
C	1.0450887185	3.8362507903	0.6298483082
H	–0.9338983762	3.5894981689	–0.1936752358
H	–8.6569274659	–2.4991937941	–0.2467343377
H	–9.6788674465	–2.6894143502	1.1595752027
H	–3.8299637922	3.1641297168	–3.0170778456
H	–5.3664990049	2.6509241239	–2.3184811946
H	–4.5113834943	4.0268265294	–1.6253841446
H	–5.5364798789	0.6509872796	2.2079750871
C	–8.120614111	–3.7044072881	3.7238737486
H	–7.0097151052	–1.8643470284	3.502947211
H	–7.8838533285	–0.9891402183	–1.6005528412
H	–8.6197746618	0.4552363927	–2.3077286507
H	–9.1990110771	–0.1403877152	–0.7599210908
H	–0.6167456522	4.6743935509	2.6384731507
C	–0.8206742453	6.0601277386	1.0118241199
H	–3.5328670181	1.8312992862	4.2178272013
H	–4.9757666844	0.921107538	4.6570390173
H	–5.1278096401	2.4850651901	3.8301680814

H	–6.3427867728	0.8606662269	–1.2989035169
H	–	–1.8121698739	2.9948417187
C	–9.3117373231	–1.3252204128	4.9622076432
H	–3.2683584967	4.7105585518	–0.0082858701
H	–3.3934568359	6.1855244937	0.9575869009
H	–7.0033330804	3.061892487	–0.2430834832
H	–8.0046405523	2.7021850778	–1.6567813722
H	–8.6489105604	2.4630645428	–0.030431767
H	–2.2639803892	4.0935207984	3.9967371637
H	–3.9342674474	4.3254268336	3.5513299675
H	–5.1494195626	3.7140343902	1.4330708113
H	–5.6014307089	5.088990563	0.4133064231
H	–5.3665236537	5.3260888824	2.1500755872
H	–7.3525980726	0.6095071653	3.9711828401
H	–8.9104011985	1.1920563008	4.5648899051
H	–	–0.3286816266	1.4434612007
H	–9.9886085168	1.3269765971	1.5140219693
H	–1.8295043771	6.5664831218	3.8259151519
H	–3.4950375763	6.8341526804	3.2776685061
H	–3.1844305202	6.2296185877	4.9104703717
H	–7.5167930007	2.2364438799	2.0334845344
H	–7.4848219893	3.0024369721	3.6302451256
H	–9.0065085872	2.8934868736	2.7408358512
H	–	–0.0497986798	3.6421456702
H	–	1.6034796991	3.7867274726
H	–	1.1929159955	2.4856860211
N	–0.7955026261	2.1616803837	1.300163701
H	–8.4346243575	–0.8663381191	5.4354230269
C	–9.5108608161	–2.7211926665	5.5783800774
H	–	–0.6842829753	5.1963483103
H	–7.2691752137	–4.3507100778	3.4821625417
H	–9.0136256968	–4.1739085932	3.2904285718
C	–8.3134718895	–3.6249230813	5.2479435476
H	1.5043312388	3.0466254366	0.0263324833
H	–7.4058265083	–3.2199725855	5.7195530457
H	–8.460887662	–4.6315080131	5.6592114674
H	1.535946668	3.8124530607	1.6108927757
H	–	–3.1770410112	5.1882787286
H	–9.640759264	–2.6285180328	6.6640713302
C	1.3171670129	5.2058879365	–0.015939334
H	–1.3027186885	6.1105757232	0.0270962811
C	0.6836388201	6.3220611986	0.8269930084

H	–1.2658444685	6.8532257709	1.6224785033
H	0.894216707	5.228410407	–1.0314871206
H	2.3985387784	5.3621887517	–0.1207546494
H	1.1795022057	6.3663688084	1.808762455
H	0.8336772174	7.301176643	0.3540010411

Tabelle 241 Standardorientierung von *t*-BuLi·(*R,R*)-TECDA (**112**) [globales Minimum; B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–2.3247594855	3.4647905335	–0.4143138417
C	–1.7534453901	–0.6327126306	1.7417031727
C	1.9425897217	1.1301742907	0.4849305205
C	–2.539019929	1.9498375422	–0.2935236129
C	–1.2145856829	3.7705775802	–1.4246706289
C	–1.2484445677	1.193705365	0.1174440366
C	0.0741297113	3.0327878734	–1.0394357637
N	–1.4192193438	–0.272713327	0.33936841
C	–0.1263968608	1.5025081525	–0.921043633
Li	0.5092761703	–1.140138805	0.1428821354
N	1.1202454337	0.7193737564	–0.688896565
C	–2.2787867343	–0.9329634357	–0.6719448342
C	1.9053885088	0.5587628274	–1.9358702868
C	1.429164641	–2.8986921224	0.8660165046
C	2.8104138537	–2.5869229139	1.4639280534
C	0.5908012338	–3.5272849068	1.9897930835
C	1.6264590903	–3.9798590924	–0.2078409065
C	–3.1380322496	–0.2532359652	2.2925467904
C	2.9950896236	2.2414793711	0.3147475106
C	–2.2355190916	–2.4626745135	–0.6273135404
C	3.0082361235	–0.4969646362	–1.8493102424
H	–2.0529274543	3.8829279606	0.56674341
H	–3.2641789018	3.9489752975	–0.7106721494
H	–0.980839858	–0.1810520526	2.376263833
H	–1.615695607	–1.7125236585	1.8362761554
H	1.247949489	1.4148858494	1.2827023756
H	2.4608137928	0.2332102818	0.8446276435
H	–3.3363562407	1.7380243771	0.4249325593
H	–2.8882595583	1.5744192921	–1.2647295156
H	–1.0246257488	4.8502633669	–1.4792019017

H	–1.5366504438	3.4578056872	–2.4293620125
H	–0.9284086917	1.6008076735	1.0862385193
H	0.4217974955	3.426487966	–0.0749888841
H	0.8626423014	3.243117595	–1.7715078678
H	–0.4955480661	1.1494986167	–1.8939487279
H	–3.3263229704	–0.6037810069	–0.591959097
H	–1.9262194046	–0.6017855492	–1.6558529784
H	1.1964181386	0.2564011796	–2.7158646927
H	2.3392261877	1.5173975783	–2.2648192988
H	3.3075463045	–3.4967845726	1.8789829947
H	2.7545883072	–1.866173568	2.2967029583
H	3.5121031793	–2.1719567816	0.7230171675
H	1.066956319	–4.4467226208	2.4079489207
H	–0.4115970969	–3.8359469734	1.6508292652
H	0.4495393765	–2.8443284749	2.8434676223
H	2.1085201806	–4.9006420958	0.2012863088
H	2.2698347304	–3.6461621722	–1.0378264544
H	0.6748048572	–4.3097084262	–0.6555251662
H	–3.9527172533	–0.6366535011	1.6677696125
H	–3.2668873326	0.8291719079	2.3982860842
H	–3.2546856432	–0.6955999675	3.2894219324
H	2.5685110728	3.2046940324	0.0239313574
H	3.7599061041	1.9749310185	–0.4215628021
H	3.5070786382	2.3784843611	1.2750725141
H	–2.7313288789	–2.8672773718	0.2609949056
H	–1.2089483725	–2.8458099127	–0.6398559307
H	–2.7611214404	–2.8606560789	–1.503313444
H	2.6096822175	–1.466025452	–1.5337192183
H	3.8033898987	–0.2205782331	–1.1500029041
H	3.4673041347	–0.6174220787	–2.8377867046

Tabelle 242 Standardorientierung der α–Lithiierung von (*R*,*R*)–TECDA über *t*-BuLi·(*R*,*R*)–TECDA (**112**) [Übergangszustand; B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	0.2346852805	4.2803251137	2.4680901208
C	–3.0066576197	1.1786695696	1.4072547385
C	0.7064159533	–0.0528243232	0.0898414094
C	–1.0293621402	3.8649222382	1.6969153222

C	1.4743137177	4.2414158633	1.5658428922
C	–0.871875045	2.4519924559	1.0822489205
C	1.6198354136	2.875185317	0.8791049285
N	–2.0994667457	1.8654819314	0.4516444356
C	0.3431408028	2.4726802843	0.1028263236
Li	–1.248839455	0.2465261484	–0.6478298014
N	0.4537406734	1.2300248347	–0.6881360557
C	–2.787861931	2.809604158	–0.4578486228
C	1.2681814729	1.3955109591	–1.900632201
C	–1.2590516289	–2.0218030838	–0.9616402231
C	–0.3421981415	–3.0946829476	–1.5535022941
C	–1.8928292906	–2.557278685	0.3267166081
C	–2.3659561891	–1.7031728251	–1.9813881719
C	–3.8447240343	2.0113028931	2.3926461295
C	2.1461496096	–0.5607285962	0.1230147107
C	–3.835954806	2.1604389745	–1.3643785675
C	0.9180873666	0.395388056	–3.0038608781
H	0.3804562787	3.6000035791	3.3207548067
H	0.0979617433	5.2844056922	2.8906881563
H	–2.3897450208	0.4708822635	1.9729066444
H	–3.693519523	0.5668867385	0.8109863132
H	0.4022536372	0.1536359643	1.125443363
H	–0.2519585052	–1.0780693467	–0.4839992334
H	–1.8972544617	3.900159121	2.3617172561
H	–1.2146678613	4.5988423789	0.9000104232
H	2.3774243199	4.4716217508	2.1463306755
H	1.3880035204	5.0275213801	0.8000832095
H	–0.6240756599	1.7684635692	1.9038539833
H	1.8414241112	2.1043667177	1.6294735529
H	2.4698943382	2.8937808432	0.1864029654
H	0.1465454471	3.2713360946	–0.6298549207
H	–3.2599128517	3.6336093959	0.0994688267
H	–2.0160052015	3.2629725867	–1.0877446925
H	1.0927185735	2.4111117325	–2.2790141297
H	2.3466856975	1.327792937	–1.6829544552
H	–0.8862142601	–4.0375380766	–1.7606556046
H	0.4828750028	–3.3429910721	–0.8706146889
H	0.1070257785	–2.77216649	–2.5033829814
H	–2.4572637501	–3.4961249917	0.1614114455
H	–2.6035738027	–1.8449302085	0.7763598443
H	–1.1286696713	–2.7718728066	1.088385606
H	–2.9577623834	–2.6050232191	–2.2501178761

H	–1.9639799967	–1.3071344676	–2.9257035008
H	–3.1094144472	–0.9778743089	–1.6049313759
H	–4.4373611037	2.7823971506	1.8877672388
H	–3.2336040513	2.4957861152	3.1596817987
H	–4.5468131772	1.3436379754	2.9070323105
H	2.8961843598	0.1684211302	0.4796925103
H	2.4941043129	–0.923161954	–0.8540493907
H	2.1896346683	–1.4211763266	0.8036391544
H	–4.6915810242	1.7664470992	–0.8057026414
H	–3.41256345	1.3419811483	–1.9583488917
H	–4.2220778739	2.9104244616	–2.0643967798
H	–0.1216124972	0.5199076305	–3.3322405968
H	1.0435284045	–0.6373139044	–2.6684248348
H	1.567850117	0.5521183803	–3.8740722139

Tabelle 243 Standardorientierung der α-Lithiierung von (*R*,*R*)-TECDA via *t*-BuLi·(*R*,*R*)-TECDA (**112**) [Übergangszustand; B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–2.05032243	–3.209412557	–1.2981952453
C	–1.6747050666	1.4663525015	–0.3592219512
C	2.1118174105	–0.8411954048	–0.9395540881
C	–2.3708082773	–1.9016212763	–0.5649251342
C	–0.9677013662	–3.9844877286	–0.5413439333
C	–1.1351626225	–0.9930741211	–0.3482794566
C	0.3064581073	–3.1366497198	–0.4350801004
N	–1.4056098842	0.226178385	0.4619060635
C	0.0716348333	–1.7722683428	0.251531088
Li	0.3862066133	1.0435242138	0.2795149182
N	1.2887944816	–0.8837701923	0.3043831422
C	–2.2854811333	0.0218543851	1.6293144022
C	2.090470561	–1.110215615	1.5282252733
C	0.6954785315	3.1991164246	–0.448448656
C	2.0628118502	2.9334101253	–1.0897266354
C	–0.029489022	4.2630575905	–1.2796401417
C	0.8791528288	3.7308715379	0.9802434498
C	–2.7042625927	1.3338394358	–1.4849335496
C	3.2295132306	–1.8817367171	–1.1399394996
C	–2.0007633992	1.0016951303	2.7717584333

C	3.1186927937	–0.0122562691	1.8102517972
H	–1.7030744764	–2.9988352279	–2.3212790154
H	–2.9633448955	–3.8110711001	–1.3961297567
H	–0.4094061222	2.2333541605	–0.577603092
H	–2.0676125693	2.1995977743	0.3589007587
H	1.418684789	–0.881411849	–1.7861006947
H	2.5775957421	0.1485682277	–0.9905745194
H	–3.1349108676	–1.3331031152	–1.104317901
H	–2.8091382373	–2.1658252481	0.4056359797
H	–0.7363012007	–4.931579731	–1.0460748063
H	–1.33630778	–4.2456774831	0.4623133951
H	–0.8253773306	–0.6291917234	–1.3384621698
H	0.6797660152	–2.9769702589	–1.4541334046
H	1.0860756687	–3.6873497552	0.1064373238
H	–0.1818005337	–1.9748772903	1.2997621167
H	–3.3491019414	0.0897634508	1.344732233
H	–2.1262924101	–0.9919108049	2.018339962
H	1.3864869612	–1.1448808196	2.3665586729
H	2.5968012559	–2.0893290459	1.5031468248
H	2.6476319245	3.8669776177	–1.2272367891
H	1.9684636605	2.4764402643	–2.0868479049
H	2.7008359159	2.2723054671	–0.4815912774
H	0.5345138542	5.2147375239	–1.3174431912
H	–1.0232392104	4.4925948735	–0.8684406281
H	–0.1780298596	3.9315589638	–2.3176220808
H	1.4313702737	4.6937307073	1.0043853559
H	1.4499192853	3.0433137418	1.6282055163
H	–0.0868767937	3.9114406066	1.4736873074
H	–3.6958671388	0.962410289	–1.1643465107
H	–2.3649621366	0.6842556253	–2.3037748263
H	–2.8652396749	2.3257805446	–1.9267041512
H	2.8703085126	–2.9131852754	–1.1441705923
H	4.0102528852	–1.800190468	–0.3764232964
H	3.7068072065	–1.6896312714	–2.1088065481
H	–2.1575363923	2.0429673939	2.4732543743
H	–0.9655205394	0.9019824507	3.1232345597
H	–2.6681464591	0.7952593513	3.6181045414
H	2.6421551165	0.9701148594	1.9123002321
H	3.8827330754	0.0659657575	1.0304778442
H	3.6327669827	–0.2292054506	2.7538206501

Tabelle 244 Standardorientierung der β-Lithiierung von (*R*,*R*)-TECDA via *t*-BuLi·(*R*,*R*)-TECDA (**112**) [Übergangszustand; B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–2.0658968316	–3.4998219691	–0.7009241139
C	–1.6056437382	0.7740604111	–2.4711948499
C	2.0066008964	–0.7640866519	–1.6844327561
C	–2.2891774997	–1.9853049447	–0.5764969203
C	–0.8272197461	–3.9376237582	0.088790948
C	–1.0536723119	–1.1720670786	–1.0393400581
C	0.4021156128	–3.1181814477	–0.3305914114
N	–1.24702321	0.3021629123	–1.1173812225
C	0.164793718	–1.5984658753	–0.1595382949
Li	0.4130068572	1.1273315144	–0.2384627888
N	1.3697269201	–0.7315879997	–0.3399233306
C	–2.0700285059	0.9403318306	–0.0274829502
C	2.331652804	–0.9024074505	0.7744712969
C	0.575955716	3.3650776746	0.1368865346
C	1.5208309424	3.2580135245	–1.0740168223
C	–0.5356814006	4.3626574828	–0.2019066205
C	1.3555510255	3.8725889357	1.3513168567
C	–2.9924511491	0.4009738687	–3.0212456457
C	3.0505250722	–1.8532644474	–1.9914342214
C	–1.2142137132	1.2880659069	1.1954882345
C	3.3943693454	0.1945422264	0.8518844854
H	–1.9378223523	–3.769739484	–1.76043291
H	–2.9561589635	–4.036674735	–0.3484058552
H	–0.8362172852	0.4111441719	–3.1664642114
H	–1.5152983638	1.8666155551	–2.4579304256
H	1.201536136	–0.8208168575	–2.4225407908
H	2.4876488527	0.209782514	–1.8417540665
H	–3.1674054	–1.6853815248	–1.1573056879
H	–2.5105159533	–1.7476749054	0.4723244049
H	–0.6317698293	–5.0076634766	–0.0594182225
H	–1.01055975	–3.7984625667	1.1646102174
H	–0.8352733102	–1.4907486815	–2.0683102135
H	0.6256301651	–3.3370075105	–1.3836065254
H	1.2760660091	–3.4310372092	0.2527831033
H	–0.1286615576	–1.4319610676	0.8843675677
H	–2.4407727752	1.880457609	–0.4527777347

H	–2.9657457735	0.3351106708	0.1824313847
H	1.746378977	–0.8878387045	1.7008297021
H	2.8284888311	–1.8845917115	0.7331723609
H	2.9431007039	1.1841325492	0.9740456939
H	1.9572533695	4.2414224555	–1.351669164
H	1.0083187136	2.895181042	–1.9811535872
H	2.3838597617	2.5967092893	–0.8920772066
H	–0.1411402341	5.3802927485	–0.3953824469
H	–1.2614846555	4.4515144921	0.6195273937
H	–1.0972250984	4.0668757887	–1.101133415
H	1.7923852895	4.8774467438	1.1842242669
H	2.1900536038	3.2079132206	1.6218236712
H	0.7079561902	3.9469369976	2.2372843091
H	–3.7930748925	0.7202484701	–2.3446628628
H	–3.0945787903	–0.6769342244	–3.1895967911
H	–3.1503778583	0.901023777	–3.9852354655
H	2.6515863356	–2.8672126406	–1.9075235424
H	3.9282024162	–1.7809679971	–1.3406965305
H	3.4008168739	–1.7165449182	–3.0220524399
H	–1.7955718599	1.9265057076	1.874028464
H	–0.2294933627	2.2693493084	0.7306105289
H	–0.938220107	0.3933255705	1.7796637692
H	4.0399960977	0.2201876112	–0.0322687058
H	4.0368690422	0.0133872572	1.7214056136

Tabelle 245 Standardorientierung der β-Lithiierung von (*R*,*R*)-TECDA via *t*-BuLi·(*R*,*R*)-TECDA (**112**) [Übergangszustand; B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.2766364831	4.290554598	0.3144947278
C	–2.9747482846	0.5817566249	–0.3598227892
C	1.4837360602	–0.3341935795	0.071044414
C	–1.260896694	3.4396512673	–0.5006333483
C	1.1486976969	4.1307865028	–0.222896761
C	–0.8814886204	1.9379633194	–0.489675308
C	1.5638031202	2.6528622988	–0.2393672612
N	–1.8406439812	1.0341279476	–1.2051980295
C	0.5739518052	1.7613498119	–1.0250539827
Li	–0.6709450077	–0.8220423525	–1.5799365256

N	0.9326387573	0.3343833945	–1.1262697754
C	–2.259082882	1.5407003633	–2.5332483984
C	1.5680702686	–0.0949097044	–2.4161057384
C	–0.9477028215	–3.1641919498	–1.6006569242
C	–0.1570831549	–3.9403011847	–0.5431395936
C	–2.3590544003	–2.8863892057	–1.0603756077
C	–1.0766511711	–4.0148726297	–2.8687697556
C	–4.0305166224	1.5996656899	0.1084832233
C	3.0067606353	–0.3018503109	0.2949526922
C	–2.8535183731	0.4656329304	–3.44768953
C	1.214047759	–1.5465003579	–2.7499523301
H	–0.3084210602	3.9851029551	1.3715384479
H	–0.5849581185	5.3437115828	0.2850715365
H	–2.5379929896	0.0990534622	0.5229395208
H	–3.4864627692	–0.2119030243	–0.9100265588
H	0.9740704933	0.0797287046	0.9501165898
H	1.1917633339	–1.3908574617	0.016953174
H	–2.2781817016	3.5810023811	–0.1257291588
H	–1.2581395019	3.8079631887	–1.5359333442
H	1.8583730887	4.7103776764	0.3817189915
H	1.2002186904	4.5407686791	–1.2429274781
H	–0.8910201414	1.5944367306	0.5548718579
H	1.6379973343	2.2973398721	0.797603029
H	2.5604697355	2.5470246286	–0.6833773071
H	0.5766675166	2.1384635431	–2.0562781995
H	–2.9732671451	2.3740695544	–2.4454431952
H	–1.3677827643	1.9492036038	–3.0197707571
H	1.1504653965	0.5662564496	–3.1859672033
H	2.6526934355	0.119821085	–2.3918602666
H	0.046291805	–2.2282343214	–2.1449658346
H	–0.6102834753	–4.9267598654	–0.3205119182
H	–0.1010251703	–3.3995413258	0.4146471626
H	0.8754606577	–4.1295221979	–0.8703513395
H	–2.907563007	–3.8277167478	–0.8418157583
H	–2.987090203	–2.3364549718	–1.7792086718
H	–2.3533076177	–2.3205235779	–0.1154071645
H	–1.5952846035	–4.9743051926	–2.6780351439
H	–0.0921841995	–4.2563673332	–3.2934170426
H	–1.6451828695	–3.4917781556	–3.6529200833
H	–4.4509348764	2.1808076045	–0.7200440552
H	–3.6407600747	2.2983171356	0.8550290609
H	–4.8585063484	1.0523827722	0.5757315688

H	3.403366415	0.7117762001	0.4025290631
H	3.5408011133	–0.7928622142	–0.5249587926
H	3.2406969555	–0.8549680902	1.2134887683
H	–3.7973466964	0.0620662773	–3.0674802852
H	–2.1619887747	–0.3727854798	–3.5985386907
H	–3.0584919896	0.9007425151	–4.4327647561
H	2.0013979062	–2.2334535289	–2.4062372442
H	1.142772614	–1.6718845869	–3.8388659201

8.3.7 Angaben zu den quantenchemischen Rechnungen der Deprotonierung von Monoaminen (Kapitel 4.2.5)

Tabelle 246 Berechnete Energien der optimierten Verbindungen.

Verbindung		Min./TS	ZPE [Hartree]	SCF [Hartree]
i-PrLi-(*R,R*)-TMCDA NMe_3	Edukt	Globales Min.	–803.829274	–804.363340
i-PrLi-(R,R)-TMCDA NMe_3	Deprotonierung NMe_3	TS	–803.801185	–804.330240
i-PrLi-(R,R)-TMCDA NMe_3	Deprotonierung TMCDA	TS	–803.797488	–804.326190
i-PrLi-(*R*,*R*)-TMCDA Et_2NMe	Edukt	Globales Min.	–882.397357	–882.988697
i-PrLi-(*R*,*R*)-TMCDA Et_2NMe	Deprotonierung Et_2NMe	TS	–882.369509	–882.955881
i-PrLi-(*R*,*R*)-TMCDA Et_2NMe	Deprotonierung TMCDA	TS	–882.365251	–882.950554
MeLi-(*R,R*)-TMCDA NMe_3	Edukt	Globales Min.	–725.271199	–725.747521
MeLi-(*R,R*)-TMCDA NMe_3	Deprotonierung NMe_3	TS	–725.236581	–725.7084317
MeLi-(*R,R*)-TMCDA	Edukt	Globales Min.	–550.906244	–551.2600206
MeLi-(*R*,*R*)-TMCDA	Deprotonierung TMCDA	TS	–550.86552	–551.2140353
i-PrLi-(*R,R*)-TMCDA *N*-Methylpiperidin	Edukt	Globales Min.	–920.466634	–921.0613562
i-PrLi-(*R,R*)-TMCDA *N*-Methylpiperidin	Deprotonierung Piperidin	TS	–920507417	–921.1060427

Tabelle 247 Standardorientierung von *i*-PrLi-(*R*,*R*)-TMCDA NMe_3 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–2.2531519467	–3.8211807102	–0.294186934
C	–1.2371267234	–4.0464095312	–1.4188734584
C	–1.6583046209	–2.9083708684	0.7860396281
C	–0.7906347498	–2.7019166641	–2.00803748
C	–1.1844730765	–1.5438871548	0.2284611113
C	–0.1924938609	–1.7483521588	–0.9455391496
N	0.2831225	–0.4478531326	–1.498361658
N	–0.6321899637	–0.6265605393	1.2657155351
C	1.5871089477	–0.5821957389	–2.1562869593
C	–0.6656641571	0.201534076	–2.4200945962
C	0.3826371098	–1.2365164078	2.1332184929
C	–1.6944748124	–0.0267775761	2.0876818451
Li	0.2417632492	1.0784542575	0.1624305727
C	–1.0599745898	2.7768231976	–0.0612364386
N	2.359592309	1.6768867568	0.8782656305
C	2.689184501	2.6767153829	–0.1488652338
C	3.4731069545	0.7390535343	1.0466276953
C	2.074375979	2.3570402655	2.1498390215
C	–0.8591499682	3.7724271584	–1.2189303346
C	–1.3970345961	3.6042509978	1.1932591849
H	–3.1644833517	–3.3654607767	–0.7093422206
H	–2.5565824267	–4.7769058954	0.1525098192
H	–0.3668278402	–4.5921562285	–1.023615981
H	–1.6665508572	–4.6742427395	–2.210346454
H	–2.390462958	–2.7430787469	1.5856509293
H	–0.8075350379	–3.4314902706	1.244155426
H	–0.0584384243	–2.8633862062	–2.809240815
H	–1.6633686897	–2.225590525	–2.4736342023
H	–2.0650169111	–1.0236582897	–0.171098214
H	0.7037923913	–2.2356770589	–0.5373612028
H	1.5561867578	–1.216774347	–3.0598250954
H	2.3165381614	–1.0093647629	–1.4604709233
H	1.93963445	0.4085220747	–2.4608643085
H	–1.6501390367	0.2926931046	–1.9563959539
H	–0.7644352345	–0.3364975028	–3.3776388797
H	–0.315731453	1.2149743082	–2.6266038773
H	1.1695249055	–1.7072396927	1.5369795258

H	–0.0297754548	–1.9901733361	2.8248634477
H	0.8443145321	–0.4510776472	2.7391936771
H	–2.2383351438	–0.7701741693	2.6962607331
H	–2.4016478658	0.5046323486	1.4462539087
H	–1.2506166724	0.7067413688	2.7666325573
H	–1.991395811	2.2149244049	–0.3083922311
H	1.8299959194	3.3337744278	–0.3008367852
H	3.570062511	3.2811301987	0.1381707034
H	2.9135650327	2.1738157119	–1.0953634799
H	3.677763987	0.2292536733	0.0996517438
H	3.218006308	–0.0143293581	1.7991300753
H	4.4003181897	1.2483120633	1.3703972318
H	1.8306791612	1.6181578805	2.9207716898
H	1.2181628447	3.0227066024	2.0211999497
H	2.9423193949	2.9456970125	2.5015629612
H	–0.7371034471	3.2810909714	–2.1975551231
H	0.0428222384	4.3927876651	–1.0720841184
H	–1.6932800048	4.5003002634	–1.3420617976
H	–0.5452474542	4.2351040156	1.5036599981
H	–1.6552457651	2.9819774879	2.0649013386
H	–2.2440129507	4.31458079	1.0556993076

Tabelle 248 Standardorientierung von *i*-PrLi-(*R,R*)-TMCDA NMe_3; Deprotonierung von NMe_3 [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	1.1984268416	–2.751080586	2.927057796
C	–0.3041852749	–2.9347082263	3.1711235777
C	1.4651488956	–2.4913769957	1.4392827855
C	–1.0727450448	–1.6902003123	2.7062630981
C	0.6946182673	–1.2689538436	0.8894268987
C	–0.8186926816	–1.3554661906	1.2197324305
N	–1.5407007802	–0.1225275555	0.7459818375
N	0.9063658482	–1.0278824565	–0.5617687172
C	–2.9015053023	–0.4425448454	0.2997780583
C	–1.6013287228	0.969716157	1.7323122211
C	0.8471262458	–2.2327164212	–1.3951962122
C	2.1087438732	–0.1720272363	–0.8091338871
Li	–0.0959587687	0.6945831794	–0.7742137916
C	1.2950532496	2.457560989	0.1698241782

N	–0.9185474308	1.3294039505	–2.6789482869
C	–1.552752466	2.6439966942	–2.4899765501
C	–1.9011178058	0.3658346634	–3.19653379
C	0.2035277882	1.4421057074	–3.6278539439
C	2.0585168097	3.3886505524	–0.7779865077
C	1.9679694305	2.4571151551	1.5462950733
H	1.5665408059	–1.908083338	3.5310334889
H	1.7542888028	–3.6387683192	3.2569894936
H	–0.6579205855	–3.8235407341	2.626411484
H	–0.5079356823	–3.1172749515	4.2344856716
H	2.5360835019	–2.344941044	1.2548125128
H	1.1713524878	–3.3916665219	0.8826414031
H	–2.1495793031	–1.8188102418	2.8800776574
H	–0.7527700204	–0.8477224983	3.332849411
H	1.0974887178	–0.3789526829	1.3899898208
H	–1.2318641761	–2.1784851099	0.6212947376
H	–3.5389623415	–0.8328191876	1.1132123367
H	–2.8694079827	–1.1879671966	–0.5006747102
H	–3.3818126635	0.462868355	–0.0887070082
H	–0.6056951078	1.1929006098	2.1179615025
H	–2.271157225	0.7486629052	2.5795599835
H	–1.9741910573	1.8730492394	1.2372974501
H	–0.049450483	–2.831846112	–1.1781935427
H	1.7362503566	–2.8761881606	–1.2851445734
H	0.7973133628	–1.9281233975	–2.4463274426
H	3.0242405853	–0.6420919027	–0.4022329201
H	1.6658274355	1.1695552137	–0.3066700223
H	2.2457646119	–0.1097432414	–1.8998241519
H	0.2574890105	2.8318018194	0.2790207825
H	–0.823409471	3.3520021943	–2.0877054613
H	–1.9518902849	3.0468749774	–3.4382263171
H	–2.3807667911	2.5558126011	–1.7786033277
H	–2.7468082772	0.288121545	–2.5080325994
H	–1.4367604876	–0.620611103	–3.2912314224
H	–2.2860219136	0.6679313071	–4.1871386263
H	0.6720921143	0.4629170146	–3.7607301204
H	0.955053465	2.1302069329	–3.2355915877
H	–0.1379704748	1.8064105598	–4.613227108
H	1.5098037098	3.5881402748	–1.709831889
H	3.0211028397	2.9354182931	–1.068118736
H	2.2936147337	4.3731911952	–0.3350553891
H	2.9537701713	1.9679850394	1.4845392488

H	1.393593561	1.9029230089	2.3033488008
H	2.1399322819	3.4687239815	1.955037352

Tabelle 249 Standardorientierung von *i*-PrLi-(*R,R*)-TMCDA NMe_3; Deprotonierung von TMCDA [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.1572570835	–4.3800963103	0.6395073321
C	0.1967918306	–4.3757046799	–0.8516045582
C	0.413257656	–3.1342295104	1.3319316539
C	–0.3025536222	–3.0855331746	–1.5149546302
C	–0.0664215605	–1.8157483112	0.6789210916
C	0.260459632	–1.8147871194	–0.8359571792
N	–0.1467439141	–0.5386750311	–1.4943471646
N	0.4363435877	–0.582109873	1.350574692
C	0.6590829681	–0.2743845948	–2.6960798476
C	–1.5778286694	–0.4660378849	–1.8417414516
C	1.8962857622	–0.5406660766	1.533429
C	–0.2275172205	–0.3495067737	2.6424528964
Li	0.0116281627	1.0573297576	–0.022678595
C	–2.0448244099	2.1413090782	0.5780241884
N	1.4323962395	2.58285622	–0.2191811448
C	0.2474859159	3.1129085678	–0.9590959494
C	2.6833861818	2.6315802195	–0.9818436009
C	1.602023357	3.3229720329	1.032722674
C	–3.1628451824	2.6309677899	–0.3487014989
C	–2.0535691388	2.9500098419	1.8789104227
H	–1.2512519339	–4.4030047258	0.7555725098
H	0.2277744573	–5.2847767417	1.1274079054
H	1.2875983546	–4.4599640001	–0.9703064877
H	–0.2408056827	–5.2467027345	–1.3560527647
H	0.1437125938	–3.138075683	2.3948466874
H	1.5097959378	–3.1851626273	1.2860108425
H	–0.0389297193	–3.0809593062	–2.5798517831
H	–1.3993428036	–3.073284996	–1.4634979589
H	–1.1593006731	–1.769745627	0.7828704335
H	1.3534695138	–1.8531055042	–0.9340702558
H	0.5063297551	–1.0271284802	–3.4884497501
H	1.721711591	–0.2525911954	–2.4352676998
H	0.3875804832	0.7034092345	–3.103887362
H	–2.1981918518	–0.6918983937	–0.9706379514

H	–1.8525348275	–1.1493956629	–2.6611332359
H	–1.8093360974	0.5548065086	–2.1553659515
H	2.4108121671	–0.7255736299	0.5868182331
H	2.2564648636	–1.2684216035	2.278690568
H	2.1783021625	0.4601703722	1.871847266
H	0.0188994651	–1.115625065	3.3968432902
H	–1.3120035644	–0.3219816359	2.5045858714
H	0.0857032395	0.6221598434	3.0354487642
H	–2.2328834984	1.0752225003	0.8171945837
H	–0.9133529394	2.599673492	–0.2012583041
H	0.2922475808	4.2164938657	–1.0274764254
H	0.2891739577	2.7236036378	–1.9882965372
H	2.5680156192	2.0793781137	–1.9191938597
H	3.5038526541	2.1753673338	–0.407766046
H	2.9666406615	3.6709217558	–1.2329810503
H	2.4200865853	2.8936461829	1.6255004307
H	0.6794194917	3.2888549957	1.6174019425
H	1.8402039314	4.3877016654	0.8416512479
H	–3.2683111552	2.0060039033	–1.2470519092
H	–2.9465958922	3.6522428203	–0.7023324079
H	–4.1550476286	2.6671265	0.1363392452
H	–1.7358723364	3.9883201355	1.6885151004
H	–1.3681259129	2.54279713	2.6366248187
H	–3.0505029291	3.014690572	2.353895849

Tabelle 250 Standardorientierung von *i*-PrLi-(*R*,*R*)-TMCDA Et_2NMe [Globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	0.0816468452	3.4568414814	–1.0030935119
C	0.8345623273	4.2952758502	–2.04092684
C	–1.0599646422	2.6774719508	–1.6695050811
C	1.3536724671	3.3959322806	–3.1696598549
C	–0.5781490326	1.7682409219	–2.827531002
C	0.2244336206	2.5973096744	–3.86399638
N	0.6900260373	1.7697424715	–5.0158397363
N	–1.6739470855	0.9826722827	–3.4696417785
C	0.8020465423	2.5804032265	–6.2328060985
C	1.9681018393	1.0728789762	–4.7821726054
C	–2.7828321197	1.79690966	–3.98470453
C	–2.2042568245	–0.0530671146	–2.567994096

Li	–0.6580700584	–0.1853915712	–5.0293745242
H	0.7807413619	2.7562503762	–0.5226907636
H	–0.3207611908	4.0944472748	–0.2051543537
H	0.1617855966	5.06377384	–2.4513179822
H	1.6729307181	4.8292121343	–1.5749912091
H	–1.5841857606	2.0716836097	–0.9213181002
H	–1.7908687322	3.4021122128	–2.054955442
H	1.8893065238	3.9958279195	–3.9163326479
H	2.0864185227	2.6985439833	–2.7436745428
H	0.0994075934	1.0136250195	–2.4068640376
H	–0.4656876926	3.3346127534	–4.294910772
H	1.5601249688	3.3806031061	–6.1518529043
H	–0.1613083076	3.0433821834	–6.4704041512
H	1.091801984	1.939273361	–7.071177928
H	1.9282926331	0.4976616306	–3.856155325
H	2.8262756786	1.764689526	–4.7438000928
H	2.1353350092	0.3600054277	–5.5935619327
H	–2.4170237168	2.5681767943	–4.6676397526
H	–3.3703386668	2.2841761748	–3.1887450089
H	–3.4622580869	1.1490035696	–4.5458783739
H	–2.7754680072	0.365018079	–1.7213231754
H	–2.8749942528	–0.7105723006	–3.1299630068
C	0.4075246748	–1.9872147813	–4.4934259924
C	–0.1155229467	–3.3722337247	–4.9194010708
C	0.828429849	–2.1059292068	–3.0160960523
H	1.354299362	–1.8430132307	–5.0608169514
H	–0.2555958718	–3.459261979	–6.0088414492
H	–1.0912733122	–3.6046279118	–4.4581919147
H	0.5557011414	–4.2141413413	–4.6334721198
H	–0.0359496794	–2.3259905275	–2.3658466114
H	1.2905357303	–1.1871304388	–2.6151146247
H	1.5547228745	–2.9258491231	–2.8154231605
N	–1.7460371215	–0.409266122	–7.1259214776
C	–0.5344911845	–0.7511847881	–7.8898774003
C	–2.4078691452	0.7994147398	–7.6638888209
C	–2.6269167299	–1.5985385601	–7.0772464835
C	–2.9815203436	0.7247147067	–9.0896542695
C	–3.8981578153	–1.4233787596	–6.2492288505
H	0.0214398058	–1.5245481966	–7.3527023306
H	–0.758433067	–1.1211954098	–8.9050237442
H	0.1046312793	0.1325898313	–7.9833575936
H	–1.6682086525	1.6071252921	–7.6202027541

H	–3.2083034241	1.0782586399	–6.9706779854
H	–2.0306681501	–2.4032952909	–6.6405352325
H	–2.8977696741	–1.9198256699	–8.0995595947
H	–3.7763744537	–0.0240853341	–9.1781840524
H	–2.2120564274	0.4905318109	–9.83333584
H	–3.4138693533	1.6967336749	–9.3571692526
H	–4.5928627324	–0.6932233511	–6.6801778126
H	–3.6621196698	–1.1162215398	–5.2251415163
H	–4.425622467	–2.3825360927	–6.1936471994
H	–1.3851805878	–0.6643970815	–2.1861803005

Tabelle 251 Standardorientierung von *i*-PrLi-(*R,R*)-TMCDA Et_2NMe; Deprotonierung von Et_2NMe [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	2.5917546893	3.6502730485	0.8910793585
C	1.9742792172	4.1405308241	–0.4235300094
C	1.5960891785	2.7746784274	1.6642600776
C	1.4969747869	2.9503976538	–1.2673692531
C	1.0937783942	1.5690799821	0.834020135
C	0.4886109542	2.0585923396	–0.5067855623
N	–0.0681228359	0.9303082076	–1.3104975574
N	0.1528537677	0.6726659753	1.5635803673
C	–1.2032304324	1.3691740834	–2.1344948457
C	0.9210631516	0.2520715485	–2.1678227251
C	–1.043895936	1.3450776798	2.091958944
C	0.8194323563	–0.0698940575	2.6440972606
H	3.5032664439	3.0733124743	0.6742642135
H	2.9010448585	4.499642258	1.5137476204
H	1.1266827198	4.8073677098	–0.2043009756
H	2.6996416516	4.7339846378	–0.9947920317
H	2.0565155003	2.4187172533	2.5934550818
H	0.7389752687	3.3972426313	1.9567697816
H	1.0408093314	3.3050649924	–2.2003093103
H	2.3740970245	2.3552219663	–1.5530179608
H	1.9616706769	0.9370588442	0.5982596332
H	–0.3725648671	2.6936513973	–0.2622447212
H	–0.9181993273	2.1226474537	–2.8898012704
H	–1.9875555507	1.7934953798	–1.4992792059
H	–1.6213167677	0.5067978782	–2.6617315341
H	1.7964522357	–0.0429525299	–1.5846458019

H	1.2498688248	0.8772195329	–3.0137665376
H	0.4695081026	–0.6593189315	–2.5672523059
H	–1.5519419139	1.9078372985	1.3048221201
H	–0.8205153322	2.0310074004	2.9255212029
H	–1.7408364072	0.5849407276	2.4539789342
H	1.1296779569	0.5754569905	3.4830142347
H	1.6982839128	–0.5886657764	2.2515671475
H	0.1306159288	–0.8234024208	3.0380953685
Li	–0.5363923574	–0.75774557	0.0832672575
N	–2.4320503353	–1.6827954033	0.2481248253
C	–1.7616607438	–2.2798158741	–0.9513030173
C	–3.7070530389	–0.9861592737	–0.0373762853
C	–2.5643158566	–2.7256827195	1.2816020622
C	–4.8775259181	–1.8492770174	–0.5342918189
C	–3.0734286034	–2.2428388175	2.6412824019
H	–2.2018536651	–3.2561545867	–1.2187953505
H	–1.9318272392	–1.6088488996	–1.8080650213
H	–3.4831671885	–0.2254310256	–0.7944883353
H	–4.0156927942	–0.4389901139	0.8646975287
H	–1.5743478891	–3.1721222784	1.4044150801
H	–3.2188259239	–3.5413877944	0.9205444022
H	–5.2299730197	–2.5505758767	0.2309281085
H	–4.5915573736	–2.4282372147	–1.4192311082
H	–5.7237633124	–1.2057365428	–0.8060623182
H	–4.1054415592	–1.8752951648	2.6020057278
H	–2.4440410442	–1.4410090525	3.0450931246
H	–3.0511477059	–3.0751398945	3.355291179
C	1.0293206194	–2.5817687986	–0.08682556
C	1.5902845053	–3.2737285776	–1.3349178891
C	1.062691999	–3.5551758755	1.0967607563
H	1.6837454986	–1.7179299068	0.1500263866
H	1.6980054308	–2.5869093597	–2.186131488
H	0.9117820329	–4.0767473686	–1.6659178025
H	2.5778870492	–3.7426001872	–1.1723303244
H	0.3524105887	–4.3828424134	0.9381959441
H	0.7871066709	–3.0790326345	2.0490224958
H	2.0514660319	–4.0283693767	1.2505193008
H	–0.3515764211	–2.4124952613	–0.5485881352

Tabelle 252 Standardorientierung von *i*-PrLi-(*R,R*)-TMCDA Et_2NMe; Deprotonierung von TMCDA [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	0.0004449758	0.0029063837	–0.0012682861
C	1.0340726337	–1.1271880775	–0.0638808085
C	–0.441511902	0.2339157172	1.4486073064
C	2.2446847869	–0.7876602056	0.8166840179
C	0.7359248983	0.5561849227	2.3987389934
C	1.8558362188	–0.5099728239	2.2867641783
N	3.0269984644	–0.1620377732	3.1625158517
N	0.3222781269	0.7580690984	3.8115612665
C	3.707711043	–1.3725016194	3.6355884804
C	4.016792649	0.7278019718	2.5314918106
C	–0.6234597425	–0.2431946177	4.3176532867
C	–0.0997586335	2.1742674896	4.0518737048
Li	2.036727651	1.3357140006	4.6824720627
H	0.4383394135	0.9237174429	–0.4150154778
H	–0.87133857	–0.2367191868	–0.6245159425
H	0.5708316388	–2.065985188	0.2765094042
H	1.3660288455	–1.2978709787	–1.0965316048
H	–1.1747362566	1.0468224321	1.5070119704
H	–0.9530793814	–0.6748675854	1.7942868966
H	2.9855380635	–1.597306938	0.7738267036
H	2.7277746842	0.1014927299	0.391273785
H	1.154263084	1.5205085117	2.0821540839
H	1.4541319204	–1.4430350028	2.7045554598
H	4.152923174	–1.9635124617	2.8152800645
H	3.0055441325	–2.0132929919	4.1780484796
H	4.5205434339	–1.0958075318	4.3166191509
H	3.5273560603	1.6050940611	2.1067897638
H	4.6029296965	0.2294611496	1.7415426193
H	4.7186052652	1.0783339957	3.2961378923
H	–0.2806367888	–1.2664207359	4.1057592317
H	–1.6399260381	–0.1192669968	3.9086498773
H	–0.6959471598	–0.1372963684	5.4051774227
H	–0.9237009534	2.4665130423	3.3739655885
H	–0.5049808696	2.2279251969	5.0733926478
C	2.4194451985	3.6407330209	3.9685209212
C	2.1458645702	4.7445423402	4.9951791504
C	2.3526864534	4.2237524603	2.5532570406

H	3.4362640335	3.235017217	4.13996229
H	2.361734192	4.4266627983	6.0250397997
H	1.0819910822	5.0331061501	4.970540255
H	2.7287644517	5.6664712003	4.8192359007
H	1.3160469156	4.5100378835	2.3118967757
H	2.6664755976	3.507988296	1.7789947613
H	2.971875699	5.1284810087	2.4195786409
N	2.6945125405	1.0124411301	6.7876729333
C	4.1242780939	1.3559214259	6.6849859422
C	2.4992954982	–0.4298515504	7.0833550709
C	2.0638894675	1.9014895372	7.7964660993
C	3.0053523096	–0.9505988372	8.4384425748
C	0.5701866592	1.670259402	8.0142559937
H	4.2245826193	2.3873509186	6.3331612197
H	4.6558457373	1.2707766119	7.6467187071
H	4.614211883	0.6947619126	5.9625527556
H	2.9953497512	–0.9840980588	6.280915065
H	1.42964815	–0.6425879471	6.988181055
H	2.2187868876	2.9263355245	7.4468053027
H	2.5955505842	1.8151868951	8.7603634629
H	2.4892913027	–0.4832326736	9.2839459533
H	4.0817418807	–0.7934951089	8.5689024077
H	2.8214519588	–2.0300212489	8.4981460355
H	0.356745836	0.7052629913	8.4874927053
H	0.0152543673	1.7271078035	7.0732781947
H	0.1815164432	2.4515783745	8.6773550415
H	1.2108852716	2.9007494604	4.0066930625

Tabelle 253 Standardorientierung von MeLi-(*R,R*)-TMCDA NMe_3 [Globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–1.7874677994	–3.7506427856	0.0856874368
C	–1.2458880677	–3.7212918533	–1.3477465116
C	–0.9373591968	–2.8545818486	0.9957982507
C	–1.2056636191	–2.2791640594	–1.8693192279
C	–0.8545005354	–1.391174407	0.497769924
C	–0.3624666126	–1.3411845268	–0.9740265384
N	–0.2710630944	0.0594244968	–1.4807152791
N	–0.0466669401	–0.5008705484	1.3790852223

C	0.7734361978	0.1989554274	–2.5001478305
C	–1.5409569841	0.6069981409	–1.9937409754
C	1.2989054074	–0.9976236686	1.6851339718
C	–0.754287948	–0.1655644095	2.6251945018
Li	–0.0622019322	1.3741784751	0.2891592348
C	–1.705109964	2.5994963323	0.7338238538
N	1.8203624989	2.6145744428	0.4006660546
C	1.481500888	3.714198326	–0.5150822723
C	3.1540648649	2.0898509064	0.0967990517
C	1.762125779	3.0940083695	1.7888796212
H	–2.8318145805	–3.4043199468	0.0888885949
H	–1.7965275648	–4.7764044624	0.4768210973
H	–0.2356520896	–4.1580248275	–1.3675557147
H	–1.8664970897	–4.3387137446	–2.0102236613
H	–1.3338467393	–2.8706460196	2.0180920951
H	0.074576022	–3.2807075439	1.0461355377
H	–0.8131830967	–2.2556315398	–2.8940620784
H	–2.236219221	–1.9049216425	–1.9204421572
H	–1.8665602634	–0.9659704156	0.5210988652
H	0.6668779064	–1.7243891579	–0.9867091856
H	0.5698399352	–0.385630427	–3.4156241012
H	1.7396714096	–0.1196459755	–2.0946767183
H	0.8541997576	1.2513997134	–2.7920729537
H	–2.3343328008	0.4858103181	–1.2544973861
H	–1.8476592974	0.1416287132	–2.9458280427
H	–1.423020226	1.6823158549	–2.1491607516
H	1.8332278951	–1.2645261046	0.7687813354
H	1.3008851558	–1.8735093064	2.3560297426
H	1.8627951691	–0.2011772228	2.1819701023
H	–0.9029181489	–1.0401203377	3.2827234306
H	–1.7180447832	0.2895288494	2.3873964001
H	–0.1703746101	0.5769726516	3.1781427011
H	–2.6513055704	2.0177677726	0.7841883534
H	–1.9212858146	3.3976816881	–0.0074804515
H	–1.6630192538	3.1300628393	1.7084894714
H	0.4630056177	4.0509591447	–0.3066609228
H	2.1827235899	4.5633061615	–0.4103024433
H	1.5266558307	3.3582645766	–1.5500979362
H	3.1841638997	1.7242688238	–0.9350335654
H	3.3891224777	1.2563052199	0.7670831915
H	3.9413243293	2.8584567396	0.2130356785
H	2.0159870006	2.2770002501	2.473378422

H	0.7455746439	3.4304180717	2.0080445866
H	2.4718145954	3.9240774596	1.9652592397

Tabelle 254 Standardorientierung von MeLi-(*R,R*)-TMCDA NMe_3; Deprotonierung von NMe_3 [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–4.0533553354	–0.8411961933	0.0656212329
C	–4.0654559251	0.5425935464	–0.5945824285
C	–2.7207061382	–1.5542231931	–0.2008628778
C	–2.8735024774	1.3788565805	–0.1086125367
C	–1.4990342266	–0.7314828898	0.2724730969
C	–1.518544883	0.6817591712	–0.3691120484
N	–0.3250653192	1.487613079	0.0243640129
N	–0.1887482898	–1.4088641232	0.0653388722
C	0.0341682939	2.4615352901	–1.0168482737
C	–0.4571198983	2.1814468593	1.3197307599
C	0.0585639361	–1.865786713	–1.310406878
C	0.0198506049	–2.5244702331	1.0007181454
Li	1.2957660142	0.1020339511	0.4443998069
C	1.8827601411	0.0404435457	2.6881398501
N	3.1052044809	–0.0487241521	–0.5847335001
C	3.2820373383	1.0993402189	0.354801418
C	3.447699078	0.2509909338	–1.9770289222
C	3.8927400316	–1.192519244	–0.1209566789
H	–4.2061281813	–0.730137988	1.1496451549
H	–4.8844482681	–1.4545408946	–0.3057117673
H	–4.0207071213	0.4274294362	–1.688150231
H	–5.0030355105	1.0689232519	–0.3738497403
H	–2.7153027917	–2.5356484839	0.2885241613
H	–2.6371430819	–1.7415246415	–1.2804425964
H	–2.8777272593	2.3634371271	–0.5930379246
H	–2.9930825178	1.5584124812	0.9679657753
H	–1.5824769805	–0.6020345225	1.3605757165
H	–1.430342504	0.5475470527	–1.4552089169
H	–0.7543999034	3.2144228072	–1.1909675414
H	0.2356572849	1.9435833362	–1.9602511019
H	0.9439228521	2.9888847472	–0.7170985634
H	–0.7875176205	1.486808017	2.0954548585
H	–1.1621218172	3.0274235921	1.2762491146
H	0.5248351642	2.5606790357	1.6161957331

H	–0.1102141053	–1.0558744332	–2.0250516251
H	–0.5701122474	–2.7243514243	–1.5986964505
H	1.1071025467	–2.165789346	–1.3946387593
H	–0.6526258363	–3.3779192278	0.8090817807
H	–0.1238206695	–2.1817962657	2.0287788975
H	1.0507943041	–2.8803179028	0.9072496112
H	0.7970536388	–0.1530040548	2.7688140306
H	2.1156210625	0.7910671319	3.4591863224
H	2.3969235523	–0.8896437113	2.9791429626
H	2.5490112195	0.6431371871	1.5889781004
H	4.354069698	1.2603057831	0.5792185257
H	2.9143691254	2.0074652918	–0.1473162309
H	2.8441986916	1.0917912488	–2.3338508929
H	3.2449780666	–0.6187198985	–2.6199797054
H	4.513795254	0.5260562559	–2.085517012
H	3.6892921856	–2.0758316005	–0.740439305
H	3.6427135518	–1.4197595186	0.9185941618
H	4.9792308311	–0.980481427	–0.1698748123

Tabelle 255 Standardorientierung von MeLi-(*R*,*R*)-TMCDA [Globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–1.9525198438	–0.888793868	2.3960858034
C	–2.9115217015	–0.5606792363	1.2440891666
C	–0.5888434495	–1.3456192101	1.8569717607
C	–2.2962471026	0.4864530913	0.3039866731
C	0.0447251088	–0.2982727823	0.9142096762
C	–0.9262693797	0.0367642873	–0.2510114547
N	–0.3057444653	0.9778308902	–1.2219404132
N	1.3989857921	–0.65022342	0.4087128568
C	–0.8947628438	0.8846011525	–2.5651269957
C	–0.2651994683	2.3833408017	–0.7866067952
C	1.5212697577	–2.0067132548	–0.1495910137
C	2.4581340289	–0.4177854284	1.4006253473
Li	1.7360146358	0.517131854	–1.2971376957
C	3.3080063117	0.9801424912	–2.4912464205
H	–1.8212627982	0.0030529839	3.0271890492
H	–2.3781123529	–1.6677834119	3.0414888415
H	–3.1331877899	–1.4794610545	0.6805201714

H	–3.870121205	–0.1946027237	1.633422389
H	0.0966765785	–1.5555018545	2.6875560485
H	–0.7247146226	–2.2916862456	1.31498142
H	–2.9793109979	0.697120564	–0.5284189654
H	–2.1760191137	1.4278022431	0.8577509876
H	0.1877095201	0.6219857142	1.4974257265
H	–1.0917508372	–0.8902499077	–0.8173346027
H	–1.9400578885	1.2375819998	–2.6027861612
H	–0.8629968104	–0.1525826827	–2.9140852241
H	–0.30071848	1.4900055886	–3.2563583885
H	0.1494766961	2.4618583488	0.2228634602
H	–1.2572822895	2.863927068	–0.7933327487
H	0.3914928624	2.9403865354	–1.4626976522
H	0.7224459567	–2.199050095	–0.87207271
H	1.4891087147	–2.7933174991	0.622075478
H	2.4767578315	–2.0828221369	–0.6786906394
H	2.3975419549	–1.1026373302	2.2642938315
H	2.4051493178	0.6125611168	1.7669069054
H	3.4313992031	–0.5537806339	0.9194997876
H	3.3539661877	2.0516486276	–2.766611212
H	3.2987886314	0.433972162	–3.4543344167
H	4.2936600273	0.7562965059	–2.0395598801

Tabelle 256 Standardorientierung von *i*-PrLi-(*R*,*R*)-TMCDA; Deprotonierung von TMCDA [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–3.1318041969	0.329902925	–0.613482753
C	–3.0058072821	–1.1070986183	–0.0893241967
C	–2.0610541908	1.2446312572	0.0049685173
C	–1.5850058377	–1.6559142182	–0.2912708877
C	–0.6440715561	0.6909512469	–0.2557851011
C	–0.5138276885	–0.7377355416	0.3406030165
N	0.8747910062	–1.2234743777	0.254735573
N	0.4824994012	1.5853548079	0.166481652
C	1.148743328	–2.3760162265	1.1047173439
C	1.4861415858	–1.3875730645	–1.1113952551
C	0.4318664762	1.988792502	1.5817065638
C	0.5977907989	2.7737626198	–0.6931036385
Li	2.0971123631	0.2845288724	–0.0054888735

C	4.1221285737	–0.3086329251	–0.4155671365
H	–3.020892057	0.3306133649	–1.7081295895
H	–4.1314023144	0.7309400672	–0.4008919898
H	–3.2560923014	–1.1232295825	0.9826647417
H	–3.7360839257	–1.7585014418	–0.5873066884
H	–2.1559826411	2.2576339963	–0.4059115557
H	–2.2396471577	1.3228796473	1.0867210328
H	–1.5065914405	–2.6587042569	0.1464363733
H	–1.3736191329	–1.7666322226	–1.3632122204
H	–0.5258455374	0.6008657112	–1.3434007125
H	–0.73865864	–0.6696535431	1.4174358267
H	0.6616708783	–3.3019113405	0.7464210612
H	0.8149649013	–2.1806874477	2.1320225419
H	2.2280329416	–2.5570882194	1.1198961475
H	0.8563974321	–0.9033018809	–1.8700600727
H	1.5548210126	–2.4518146211	–1.3799159724
H	2.890210786	–0.8639048194	–0.8964396643
H	0.3605140697	1.1072649847	2.2238542845
H	–0.4132782723	2.6591656437	1.8061493833
H	1.3561358277	2.5206182329	1.835215652
H	–0.2531262062	3.4670067815	–0.5907707835
H	0.6729015043	2.4664143344	–1.741094893
H	1.5093727153	3.3217675787	–0.430134022
H	4.7625758154	–0.7834952454	–1.1714016177
H	4.4760511697	–0.6585528469	0.5681958322
H	4.3446005685	0.7751377576	–0.4807958867

Tabelle 257 Standardorientierung von *i*-PrLi-(*R,R*)-TMCDA *N*-Methylpiperidin [Globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–1.8547763745	4.2867856759	0.8681463524
C	–1.7097777911	3.1653436206	1.9040766567
C	–2.6806364601	3.8101815708	–0.3361090012
C	–3.0875321105	2.6454791309	2.3396042899
C	–4.071376888	3.2822231085	0.0818776193
C	–3.9327671352	2.15700227	1.1413993788
N	–5.2598351027	1.5876071534	1.5071671866
N	–4.9415988508	2.8557023806	–1.0489716144
C	–5.1571178298	0.2269166192	2.0599866919

C	–6.0700569766	2.4325109823	2.3995101172
C	–4.29344003	1.9703529298	–2.0313695014
C	–5.5775424589	3.9874236068	–1.7378725144
H	–2.3451960069	5.1544618711	1.3346308502
H	–0.8685832862	4.6302044841	0.5304085324
H	–1.1221431758	2.3418050108	1.4713941382
H	–1.1517430169	3.5202870998	2.7799557481
H	–2.7994068893	4.6249992108	–1.0613224571
H	–2.1242094691	3.0125650297	–0.8467027041
H	–2.9723366805	1.8311649772	3.0654739884
H	–3.6183154545	3.4562862601	2.8574210945
H	–4.6070141563	4.1164578266	0.5554857915
H	–3.3880032577	1.3259535424	0.673227247
H	–4.6689483619	0.2064317329	3.0498928542
H	–4.5972352848	–0.4174414003	1.3743421257
H	–6.1649961841	–0.1859818362	2.1686269953
H	–6.1355274084	3.4541047806	2.0129139511
H	–5.6732278616	2.4745318207	3.4269757373
H	–7.0851427862	2.0245085239	2.4437395551
H	–3.7947593479	1.1367732683	–1.5278634089
H	–3.5515834123	2.4940707539	–2.6563499638
H	–5.063688585	1.5547414577	–2.6888249616
H	–4.8545359589	4.625977704	–2.2743890276
H	–6.1204691494	4.6059127176	–1.0157916841
H	–6.2997494596	3.6020964347	–2.4639341488
Li	–6.3758046111	1.5525335013	–0.2545260297
C	–8.074738302	0.6502393718	–0.9992762989
C	–8.1322323846	0.6080911065	–2.5368487149
C	–9.3710886414	1.2928221056	–0.4707478598
C	–0.9765128979	–2.7707680806	–0.8356752667
C	–1.9550331966	–1.9071917546	–1.6439185631
C	–1.4929925454	–2.9572126828	0.5978798377
C	–3.3792362793	–2.4652037914	–1.5574368891
C	–2.9357919916	–3.4732871616	0.5986521945
N	–3.8235523039	–2.5923835628	–0.1658515827
C	–5.2104173319	–3.0426893074	–0.0940703731
H	–8.0932621606	–0.4062532332	–0.6601308258
H	–5.8618983696	–2.3383310878	–0.621511525
H	–7.2959289842	0.0360341176	–2.9715030193
H	–8.0847683587	1.6188642254	–2.9805727971
H	–9.065301212	0.1537580378	–2.9426760717
H	–9.4372978564	2.3632854924	–0.7327632689

H	–9.4489805998	1.2352335617	0.6271508143
H	–	0.8305807969	–0.8754890101
H	0.0252273517	–2.3218744871	–0.8314982349
H	–0.8798355585	–3.7553049014	–1.3175152973
H	–1.6487000519	–1.8541289582	–2.6968270894
H	–1.9492664668	–0.8800358787	–1.2520607785
H	–0.8557235321	–3.6588647069	1.1517946919
H	–1.4583247092	–1.9970974248	1.131477425
H	–4.0817789394	–1.8058608088	–2.0807490237
H	–3.417815662	–3.4496294702	–2.0724489383
H	–3.3165095868	–3.5336117079	1.6256451202
H	–2.957846406	–4.5055018871	0.1859705823
H	–5.5319311416	–3.0850778618	0.9525090241
H	–5.3525522683	–4.0483748811	–0.5372681462

Tabelle 258 Standardorientierung von *i*-PrLi-(*R,R*)-TMCDA *N*-Methylpiperidin; Deprotonierung von *N*-Methylpiperidin [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–3.4079310258	5.2446456663	1.1193861549
C	–3.0719865496	4.6485736436	2.4910343969
C	–3.1969660432	4.2044919559	0.0105229359
C	–3.9081080367	3.3868007343	2.743844773
C	–4.0212783301	2.9154654526	0.2397083782
C	–3.7151018097	2.3224789944	1.6392065842
N	–4.4580696357	1.046877059	1.8754769451
N	–3.8636682373	1.8881328225	–0.8330689769
C	–3.6909089453	0.1376490586	2.7395808453
C	–5.8076052734	1.2317330745	2.4414907367
C	–2.4742429808	1.45987557	–1.0617750988
C	–4.4522130558	2.3219420842	–2.1111193751
H	–4.4541255133	5.5852896374	1.1152362486
H	–2.7903728236	6.1297934881	0.9198754765
H	–2.0000448637	4.4026693234	2.5323390687
H	–3.2557319008	5.3812045399	3.2873356012
H	–3.4541243491	4.6387997373	–0.9626320028
H	–2.1280709555	3.9531972088	–0.0296516045
H	–3.6536673825	2.951097949	3.7183805131
H	–4.9651045777	3.67791602	2.7965231849

H	–5.0856199699	3.1880180355	0.217305762
H	–2.6529440591	2.0470223718	1.6505846466
H	–3.5082483275	0.558912391	3.7435834257
H	–2.7263771051	–0.0960763538	2.2776656552
H	–4.2448206111	–0.7971802561	2.8638943547
H	–6.3643704136	1.9706876284	1.8637081574
H	–5.7831964138	1.5494861269	3.4963766955
H	–6.3503244481	0.2844631688	2.3770447336
H	–2.0147994181	1.1121568741	–0.1332870311
H	–1.8448040707	2.2565004694	–1.4902942001
H	–2.4793799998	0.6195183547	–1.7599427614
H	–3.8883788648	3.1413006863	–2.5873244457
H	–5.4840198118	2.6452458646	–1.9562282716
H	–4.4643254932	1.4754484674	–2.8049368148
Li	–4.9532320298	0.1780234975	–0.0919565104
C	–7.5876253085	0.209672475	–0.8324306322
C	–7.6889982254	0.0281214557	–2.3525389936
C	–7.9959625593	1.6372366789	–0.4414563686
C	–2.2615021082	–3.1198758992	–2.1746139525
C	–3.3331602848	–2.2195377928	–2.805063098
C	–2.0742976782	–2.7634643744	–0.693357665
C	–4.6213159295	–2.2174667662	–1.9737568268
C	–3.4203130018	–2.7667966759	0.0415215918
N	–4.3977920517	–1.8444697929	–0.5663611795
C	–5.7041347979	–1.8140248009	0.1517107735
H	–8.3535188124	–0.4548067113	–0.3866392066
H	–6.5334952355	–0.699025413	–0.2829090161
H	–7.5033873084	–1.0139361814	–2.6512393841
H	–6.9624169564	0.6530149239	–2.8977353844
H	–8.6844018779	0.2969992511	–2.7585030457
H	–7.2623671722	2.397544837	–0.7571805277
H	–8.1262804303	1.7475120104	0.6440284494
H	–8.9579666063	1.9495081483	–0.8982798601
H	–1.3123045476	–3.0361611483	–2.7203735884
H	–2.5801569904	–4.1700259155	–2.2540548824
H	–3.5672395007	–2.5525273012	–3.8250465038
H	–2.9483540881	–1.1935574053	–2.8899833856
H	–1.3921328997	–3.4739029822	–0.2071674782
H	–1.6158262031	–1.7677538343	–0.6061011244
H	–5.3550209149	–1.527580147	–2.4002352537
H	–5.079823644	–3.2279097415	–2.0154034749
H	–3.2834169258	–2.4752386303	1.0885642114

H	–3.8365910981	–3.794536161	0.048416035
H	–5.4975372498	–1.8146233534	1.2338642498
H	–6.2907622668	–2.7276790983	–0.0590926595

8.3.8 Angaben zu den quantenchemischen Rechnungen der Konformer und Isomere des Zinkbromidadduktes (*R,R*)-**143** des Dimethylphenylsilans (*R,R*)-**141** (Kapitel 4.4.1)

Tabelle 259 Berechnete Energien der optimierten Verbindungen.

	Methode/Basis	Min./TS	ZPE [Hartree]	SCF [Hartree]
R–Konf–1	B3LYP/6–31+G(d	Global Min.	–8026.55802	–8027.038081
R–Konf–2	B3LYP/6–31+G(d)	Global Min.	–8026.55783	–8027.03756
R–Konf–3	B3LYP/6–31+G(d)	Global Min.	–8026.54737	–8027.027463
R–Konf–4	B3LYP/6–31+G(d)	Global Min.	–8026.54795	–8027.028266
S–Konf–1	B3LYP/6–31+G(d	Global Min.	–8026.55605	–8027.035973
S–Konf–2	B3LYP/6–31+G(d)	Global Min.	–8026.55604	–8027.035537
S–Konf–3	B3LYP/6–31+G(d)	Global Min.	–8026.54238	–8027.022129
S–Konf–4	B3LYP/6–31+G(d)	Global Min.	–8026.54139	–8027.021815

Tabelle 260 Standardorientierung von *R*-Konf-1 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
H	1.5445391988	–0.6815091787	–3.6355973659
H	3.2840963666	–0.6181137883	–3.3574419737
C	2.324914335	–0.8760475765	–2.8907770288
H	2.3330042923	–1.954772229	–2.6896494319
H	–0.5229716977	0.3496024541	–2.7362366522
H	1.1170495461	2.2382070776	–2.3948977792
H	–2.1475255963	–0.224695352	–2.4265587804
H	–0.7957127674	–1.3929518181	–2.4798602106
H	2.886563622	2.2411450184	–2.3261784506
Br	–1.8713295506	3.0654230208	–2.1976681285
C	–1.0984479097	–0.3844427021	–2.1723605756
C	1.9776352209	1.9813193958	–1.7669507775
H	–2.3244452729	–2.4915761544	–1.2887770492

Si	2.057348822	0.1512729379	–1.3186659075
H	4.5553086658	–1.57050236	–1.3687713815
H	1.9396314158	2.6172038517	–0.8767934911
H	–4.7354567928	–2.590313407	–0.4884489006
H	–4.3284684792	1.938706079	–0.968958546
H	–3.6207229617	–0.1847330334	–0.8563367463
N	–0.8763140792	–0.1644967113	–0.7226744681
C	4.5394115378	–1.0470614089	–0.415206012
C	–1.9846065602	–2.4134135236	–0.2481863649
H	–3.0204195203	–4.2285987258	0.3091392554
H	–0.9991240366	–2.8892149725	–0.2016967213
C	3.4804855793	–0.1714140841	–0.1105953723
C	0.5281319186	–0.520126432	–0.3412546166
Zn	–1.2728424611	1.9076436124	–0.2464912355
H	6.394281004	–1.9468878481	0.2221753521
H	0.648599644	–1.6156161196	–0.3618400538
C	–4.3620388674	–2.5285244832	0.5445994721
C	–4.2897262176	1.997327074	0.1195454432
C	–3.2536157928	–0.2402521324	0.1759697944
C	5.5877817116	–1.2659461769	0.4847283122
C	–1.8599663842	–0.924342889	0.1442746527
H	–5.245726478	1.663622855	0.5482473145
C	–2.9795716444	–3.1804867638	0.6305957394
H	–4.1316488629	3.0438674412	0.3916497025
H	–5.0869603753	–3.0607730008	1.1730168004
H	–5.2596217208	–0.5871754481	0.9268723231
N	–3.1553518444	1.1910005241	0.6319668259
C	–4.2749463491	–1.0649922276	0.991855751
H	0.6640343319	–0.21035256	0.699472633
C	3.5115635914	0.4812078541	1.1396937574
H	2.7152094514	1.1699732405	1.4154819401
C	5.5978981305	–0.6084703663	1.7170260119
H	–1.4361005824	–0.8737503959	1.154731447
H	–2.6364268826	–3.1836731905	1.6758895719
C	4.5555730266	0.2649620577	2.0424810871
H	6.4119395255	–0.7743624093	2.4187483251
Br	0.081043023	2.5445266718	1.5757687634
H	–3.9896822802	–1.0562396098	2.0511687735
H	4.5569862949	0.7818243504	2.999310863
C	–3.0936897081	1.3517277304	2.1056578386
H	–2.8332843486	2.3874468048	2.3300941138
H	–4.0574159817	1.1156337847	2.5760154145

H	–2.3119082499	0.7205952422	2.5306467422

Tabelle 261 Standardorientierung von *R*-Konf-2 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
H	0.834891912	–3.6559130875	0.0633056509
H	1.7069544859	–3.7879220366	1.6002116695
C	0.8857467482	–3.2699701647	1.0868703035
H	–0.0490103431	–3.5447229002	1.5865448983
H	–1.4283621609	–1.5025143124	2.2809308034
H	2.7033969781	–1.4332196898	–0.9537698312
H	–2.931523692	–0.6404269735	2.0199787948
H	–1.4376709463	0.2711684315	2.388208125
H	3.6747700562	–1.563821305	0.5246084723
Br	–3.070272242	–3.8393196705	1.1044190873
C	–1.8534275546	–0.5929402144	1.8574837455
C	2.8089544313	–1.0637300724	0.0737387848
H	–2.7139614504	1.8003379949	1.3829864752
Si	1.2390887856	–1.4202727775	1.0698926585
H	0.8935925012	–2.6196100409	3.8299970167
H	3.0384551829	0.0081539841	0.0234360568
H	–5.0298438381	2.3973278932	0.5249305061
H	–5.2649157262	–2.1228179598	0.0500622515
H	–4.2632535944	–0.1618997012	0.4191646659
N	–1.5519083041	–0.5453834741	0.4042101134
C	1.2291995801	–1.5937425083	3.9657618738
C	–2.3160483857	1.8883731256	0.3643206751
H	–3.0672405052	3.9069683611	0.1621329846
H	–1.2761296558	2.2188063556	0.4614805046
C	1.4707489162	–0.7801282388	2.8427824323
C	–0.0875646728	–0.3354936883	0.1734948437
Zn	–2.1766446866	–2.397271851	–0.5182269879
H	1.2180908056	–1.7699666264	6.1153034068
H	0.1782966809	0.7034354395	0.4283566501
C	–4.5980036658	2.4973977866	–0.4820088257
C	–5.1446985079	–1.9814062041	–1.0247746665
C	–3.8232214363	0.0496245064	–0.5628989137
C	1.412148817	–1.1165574939	5.2678801481
C	–2.3585869164	0.5079522331	–0.3281323101
H	–6.013685702	–1.4445265116	–1.4320568509

C	–3.1402994619	2.9515094012	–0.3720821306
H	–5.0965723152	–2.9702992259	–1.4873683611
H	–5.2031156584	3.2441233683	–1.0110835093
H	–5.7115178648	0.8216236205	–1.3022236254
N	–3.8811952816	–1.2577978594	–1.3052402962
C	–4.6709075393	1.1588720286	–1.2259444858
H	0.0901176295	–0.4571088413	–0.9005811424
C	1.9091799653	0.5373460627	3.0835476786
H	2.120977849	1.20145372	2.246348318
C	1.8442128883	0.1950991867	5.4786522571
H	–1.8719844568	0.6029047554	–1.3068688844
H	–2.728815869	3.1195678171	–1.378541764
C	2.0954440552	1.0232588285	4.380373577
H	1.9892287205	0.5680970214	6.4896558814
Br	–0.7999762275	–2.8405144444	–2.3773367907
H	–4.3179361603	1.3258848777	–2.2513036674
H	2.43899012	2.0437206765	4.5341866706
C	–3.7342152606	–1.1259304539	–2.77547238
H	–3.6034471535	–2.1223431237	–3.2008757868
H	–4.618652153	–0.6581888172	–3.2281374677
H	–2.8425777204	–0.5489472073	–3.0242293036

Tabelle 262 Standardorientierung von *R*-Konf-3 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
H	–2.3701536064	–1.5144691516	0.425022259
H	–3.2497487657	–0.0030338379	0.7387158375
C	–2.458900043	–0.4611746171	0.1324538321
H	–2.7867962154	–0.429122722	–0.9141659518
H	1.7714767638	–1.5210138287	–2.8350987134
H	–0.0783798637	–0.7684377138	2.4454671188
H	3.2994976735	–0.7240968478	–2.4905107824
H	1.8874021403	0.2470602924	–3.0103981678
H	–1.1482450119	0.5920295503	2.8308291774
Br	3.6438927345	–3.6643467192	–1.6148009276
C	2.2162281298	–0.6160174887	–2.4175144775
C	–0.3043401218	0.2745636184	2.203953542
H	3.1883528295	1.7485886844	–1.9822764051
Si	–0.8103416683	0.4281708053	0.3906577937
H	–1.6576938823	1.9304328562	–2.0759770261

H	0.5562380205	0.8922704069	2.4851337924
H	5.3510693674	2.4003238154	–0.7492761574
H	5.5224398954	–1.9927778283	0.0027192861
H	4.5133757894	–0.1104381767	–0.6712532813
N	1.7914909809	–0.4885207592	–0.9965674095
C	–1.4587745776	2.676384373	–1.307608446
C	2.624245971	1.9226609208	–1.0572166153
H	3.3930861688	3.9367349645	–0.8852282669
H	1.6199290654	2.2483683785	–1.349338312
C	–1.0193565645	2.2717789345	–0.0305558365
C	0.2928578879	–0.3781344314	–0.9806477067
Zn	2.4350878482	–2.3554906176	–0.0793029421
H	–2.0086637574	4.3014605655	–2.6143856031
H	–0.0934193722	–1.396583773	–1.1023957285
C	4.7358755784	2.5686575869	0.1471353716
C	5.1718122743	–1.8333612595	1.0233265975
C	3.9228511637	0.1402957408	0.2192235434
C	–1.6639078971	4.0220432673	–1.6215243912
C	2.5181388556	0.6043658183	–0.2605499066
H	5.9173890347	–1.2611011863	1.5930399075
C	3.3359520805	3.030098897	–0.2702975356
H	5.0502879908	–2.8128905124	1.4925652397
H	5.2435896601	3.3443285832	0.7341101602
H	5.6514022409	0.9438988305	1.2592632659
N	3.8579606999	–1.1438552781	1.0049155188
C	4.6476693157	1.2772984984	0.9709073284
H	–0.0199592416	0.1669606628	–1.886994331
C	–0.79816784	3.284492841	0.9220688637
H	–0.4703829804	3.0221683366	1.9254848283
C	–1.430254004	5.0080062669	–0.657572574
H	1.9180075643	0.7998896463	0.6330193158
H	2.7498932338	3.2947122471	0.6219086648
C	–0.9971414115	4.6354503095	0.6167442912
H	–1.5903499784	6.0563567691	–0.8972260499
Br	0.7778526988	–3.219698484	1.3503990012
H	4.1095546103	1.5018116802	1.9011370997
H	–0.8186296043	5.3940836955	1.3754313909
C	3.3859757643	–0.9890810997	2.4017517985
H	3.2143409756	–1.982765623	2.8201595211
H	4.1252753308	–0.4638514953	3.0210229337
H	2.4371060689	–0.4540843921	2.4313162645

Tabelle 263 Standardorientierung von *R*-Konf-4 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
H	–0.9299167828	0.9528710343	–3.3459520229
H	0.7528414455	0.9738666653	–3.8758356736
C	0.0648175506	0.5384736104	–3.1390889233
H	0.033509591	–0.5427237524	–3.3008428572
H	–1.0495698014	–1.1883577495	2.2112275595
H	–0.52027354	3.1831660156	–1.3316336184
H	–2.7229581216	–0.6692669811	2.0654003161
H	–1.4337509362	0.5443636183	2.3371589595
H	1.1123030357	3.3886513554	–1.9599041912
Br	–2.6541175003	–3.6665237401	1.3907435086
C	–1.6935190055	–0.3940137775	1.8306687125
C	0.5200462817	2.8607170696	–1.2015270778
H	–3.1228303255	1.724465421	1.4580991818
Si	0.7016277116	0.9829616559	–1.4148440133
H	2.1703527447	–1.6167624635	–1.580582008
H	0.855800822	3.209475759	–0.2169902319
H	–5.5092021572	1.9288594793	0.5407610559
H	–5.0099251202	–2.4630071413	–0.0315522939
H	–4.2579651292	–0.4001868135	0.4247173902
N	–1.4957217653	–0.2858767007	0.3586806861
C	2.9167019787	–0.8465101059	–1.3945011743
C	–2.7287002119	1.9408563731	0.4576099269
H	–3.8574577695	3.7835518152	0.3329900027
H	–1.7673026908	2.4471623007	0.6005891852
C	2.5255764759	0.5030471842	–1.2664350117
C	–0.0569050105	0.0864608375	0.126766756
Zn	–1.9247712241	–2.2942229978	–0.3753258493
H	4.5361084567	–2.2663523345	–1.4055863146
H	0.5231731745	–0.8341047294	0.2510278483
C	–5.0663640379	2.1466928509	–0.4423856307
C	–4.8331875407	–2.3081800358	–1.0969505779
C	–3.8528250004	–0.107404321	–0.5522615546
C	4.2595852437	–1.2199431543	–1.3013035253
C	–2.4989929548	0.6167586099	–0.3027428177
H	–5.7381071587	–1.9072539938	–1.5747736519
C	–3.7262066166	2.8649480329	–0.2523128875
H	–4.604673571	–3.2792174156	–1.5433686528
H	–5.7804984708	2.7885192477	–0.9730605758
H	–5.8250415964	0.3280722459	–1.3521627145
N	–3.6711410379	–1.4063547189	–1.291394271

C	–4.8656445309	0.8431866274	–1.2267777718
H	0.2668307095	0.7440528906	0.9515708118
C	3.5339044048	1.4572690926	–1.0356485889
H	3.2751967861	2.5084861993	–0.9276944578
C	5.2449864781	–0.2540642817	–1.0748358173
H	–2.0726000347	0.855916423	–1.2821572373
H	–3.3305380984	3.1710727287	–1.2323695967
C	4.8796324053	1.0874889024	–0.9421491244
H	6.2900560058	–0.5457278445	–1.0025575647
Br	–0.3934605981	–3.0067042514	–2.017507828
H	–4.5123573299	1.1022808272	–2.2334048592
H	5.6389295224	1.8456719208	–0.7644902473
C	–3.4225337775	–1.2568520895	–2.7453264394
H	–3.1453989458	–2.2318634494	–3.1505727231
H	–4.3139382587	–0.8912553308	–3.272344532
H	–2.5867841732	–0.58073662	–2.9244569921

Tabelle 264 Standardorientierung von *S*-Konf-1 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
H	1.0423221203	2.8814190523	–0.4625127603
H	1.7371946553	3.3596994794	–2.0189233206
C	0.8179457282	3.0139506861	–1.5271386851
H	0.0722345791	3.8099195301	–1.6134346064
H	2.0861151606	0.02034292	–1.3454965742
H	–2.185178794	1.0927715199	–2.067806063
H	–1.2932832226	–0.4262102525	–2.0946181165
H	2.5330694469	0.5580784792	–2.9624755248
Br	–2.9069496246	3.7901175074	–1.0829735366
C	–1.3215932401	0.5751319677	–1.6403250872
C	1.6983866985	0.1807517593	–2.358134527
H	–3.4149942962	–1.0029266776	–1.7717466281
Si	0.2617647456	1.422168455	–2.3718679265
H	–1.7769595352	3.1991900468	–3.6657651832
H	1.4115819066	–0.7977803632	–2.7635534165
H	–5.8839481185	–1.0045244976	–0.9761054623
H	–5.0501677817	2.9030033498	0.703428697
H	–4.3019457578	1.036825267	–0.3473962612
N	–1.5493251537	0.4558665393	–0.1626989311
C	–1.2621598204	2.6772621735	–4.4694971473

C	–3.1362391203	–1.4699709428	–0.8197850232
H	–4.5350106021	–3.0920589009	–1.1177509976
H	–2.2582727088	–2.0973605887	–1.0161119876
C	–0.2391363044	1.7535063866	–4.1694250479
C	–0.3532735616	–0.1140940501	0.5038850563
Zn	–1.9385598923	2.4563063842	0.6057095002
H	–2.4224463456	3.6624595178	–5.993797008
H	–0.1322071425	–1.1253650729	0.1307595882
C	–5.5348112656	–1.4814514045	–0.0486067905
C	–4.738302683	2.5617207871	1.6914664335
C	–4.0113039318	0.484790971	0.5560363895
C	–1.6321746941	2.9436138218	–5.7901222908
C	–2.7719537103	–0.3829316724	0.2113395122
H	–5.6029156284	2.1626701363	2.2396100334
C	–4.3060998727	–2.34493332	–0.347608917
H	–4.3437288108	3.4212521811	2.2402895265
H	–6.3639960332	–2.0997193909	0.3174259308
H	–6.0719250529	0.2167898204	1.1880178871
N	–3.6627406567	1.54927813	1.5574258829
C	–5.1931287695	–0.4081083205	0.9928151725
H	–0.5070590263	–0.1455786744	1.583999663
C	0.3942841479	1.1103928123	–5.2498306465
H	1.1889495931	0.3908495165	–5.0655318807
C	–0.9865346183	2.2945315886	–6.8468736173
H	–2.4828538681	–0.9075573262	1.1288767018
H	–4.0183052369	–2.9031224326	0.5558838583
C	0.0284263372	1.3746127792	–6.5738272061
H	–1.2720153141	2.5050544109	–7.8748949229
Br	–0.4058795363	2.9807984692	2.2998690796
H	–4.9440060423	–0.9094148205	1.9377839591
H	0.5373086507	0.8646060222	–7.3887019244
C	–3.3115861789	1.0481150955	2.9062476955
H	–2.9805364108	1.8957229052	3.5092160621
H	–4.1689053997	0.5705273938	3.3996547795
H	–2.4797709644	0.3442544959	2.8593645151
H	0.5085009577	0.5290563499	0.3269320942

Tabelle 265 Standardorientierung von *S*-Konf-2 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
H	2.3597472214	–1.1922351614	1.016763791
H	3.4292649195	–1.859881182	–0.2332250743
C	2.5770956554	–1.1918622194	–0.058369076
H	2.8921253697	–0.1785889053	–0.3383623858
H	0.4581784961	–3.5764362699	0.5724130319
H	–0.0726334715	–0.0580600551	0.3541107787
H	0.1216035998	0.4601915183	–1.3233582547
H	1.409280942	–4.1975334848	–0.7848051292
Br	–0.9792963642	–1.7994290742	2.5276964247
C	–0.2248124104	–0.3658886928	–0.6848231365
C	0.5885878413	–3.5198893989	–0.5129290791
H	–0.9693292783	2.1151913117	–0.2084632843
Si	1.0619221507	–1.770961499	–1.0331416763
H	2.2330107523	0.2808187128	–2.895083718
H	–0.3275318081	–3.9031953808	–0.9746526112
H	–2.596733406	3.3917938812	1.3638322723
H	–3.5308076657	–0.4875325901	3.0687614358
H	–2.4489399478	0.7514505286	1.4944016172
N	–1.6940129664	–0.5763349374	–0.8861572392
C	2.0306940024	–0.606237505	–3.4942220811
C	–1.793947992	2.0034929378	–0.9227797619
H	–2.1447194753	4.1374738093	–0.9687541745
H	–1.3492018288	1.9829666008	–1.9250651186
C	1.4722314579	–1.7500342529	–2.8894041147
C	–1.9613833256	–1.0993468301	–2.2493735006
Zn	–2.3435202625	–2.0069307522	0.615370776
H	2.7858791411	0.3183199634	–5.2912110275
H	–1.6584947517	–0.375939818	–3.0201381295
C	–3.3719785308	3.2519550204	0.5962707085
C	–4.3709337167	–0.7109472992	2.4094522358
C	–3.2309424522	0.7015817359	0.7255255295
C	2.3507758448	–0.5775896757	–4.8540826654
C	–2.5391238004	0.6788527799	–0.6646135099
H	–5.2130163316	–0.0423527019	2.6364219744
C	–2.7203548245	3.2207204122	–0.7896713004
H	–4.687381845	–1.7415416729	2.5929453186
H	–4.0575950085	4.1040803619	0.6835045183
H	–4.5791427942	1.9704313097	1.860453208
N	–3.9439383111	–0.5920090778	0.9941390911
C	–4.1337107615	1.9468291647	0.8594872948
H	–3.0222937149	–1.3334109402	–2.3558145061

C	1.2496860163	–2.8699761294	–3.7124684291
H	0.8248661149	–3.7770814791	–3.2884092722
C	2.1146468893	–1.7025526715	–5.6503193315
H	–3.333805802	0.618599437	–1.4166859051
H	–3.5014802604	3.1845361449	–1.5636999467
C	1.5643346747	–2.8505682756	–5.0753019021
H	2.3630675462	–1.6854433425	–6.7087558521
Br	–3.3543125771	–3.8709029235	–0.3852615952
H	–4.9646104847	1.8786467045	0.1441850612
H	1.3812273023	–3.7320198923	–5.6854403207
C	–5.1126386749	–0.8514341693	0.1225506944
H	–5.4878553697	–1.8525540801	0.3424495741
H	–5.9164538102	–0.1223939893	0.2925167346
H	–4.8275501801	–0.8400743716	–0.9299428103
H	–1.4100417332	–2.0258616336	–2.4068661508

Tabelle 266 Standardorientierung von *S*-Konf-3 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
H	–0.0515375107	1.4627282476	–3.7986363479
H	1.7085732931	1.503309405	–3.9637856773
C	0.8778639242	0.9807039023	–3.4714129342
H	0.8779726145	–0.0492346657	–3.844829857
H	0.4430525097	3.4870464446	–1.4397314348
H	0.380978152	–0.7726684312	–0.1795272845
H	–0.2087440571	0.6986338071	0.4725742343
H	2.191741753	3.3438222728	–1.5810582731
Br	–0.7051090338	–1.3259106081	2.6613352342
C	–0.1443072569	0.1437022245	–0.4693260336
C	1.3063848374	2.8989869357	–1.1097664287
H	–1.4205488764	2.4854343646	–0.4072296401
Si	1.1492983315	1.0725967087	–1.5941170752
H	2.013631096	–1.8088898083	–1.5335975579
H	1.4090346405	3.0289369064	–0.0252470944
H	–3.3238923313	3.5276155834	1.0193970455
H	–3.4694135674	–0.3003550859	3.0495259488
H	–2.643618057	1.0003847195	1.3893076682
N	–1.5373260125	–0.3057745052	–0.8242325488
C	2.8853794961	–1.2091904163	–1.2761395844
C	–2.1794133216	2.1495717994	–1.1226291428

H	–2.9551668304	4.1572382917	–1.3606889646
H	–1.7062337517	2.1322522343	–2.1112458623
C	2.782746241	0.1941159177	–1.1933587245
C	–1.5581756105	–0.9954846225	–2.1343184099
Zn	–1.9899234888	–1.7853883063	0.7477972681
H	4.135945992	–2.9553129537	–1.1004683648
H	–1.4220304836	–0.293049107	–2.9647985553
C	–4.0271299701	3.1675056797	0.254174373
C	–4.2363205633	–0.7429781035	2.4119132488
C	–3.3702714968	0.7224267141	0.6141724825
C	4.090334702	–1.8712825044	–1.0312488507
C	–2.6345364737	0.7262075095	–0.7547084574
H	–5.1992085569	–0.2397667832	2.5759782027
C	–3.3365544147	3.1587731148	–1.1125784046
H	–4.3427058044	–1.7955644051	2.6879317643
H	–4.8751114138	3.8636120904	0.2552749275
H	–4.9952806478	1.7728942212	1.6026564823
N	–3.8138510437	–0.6633873845	0.9922825276
C	–4.5145953491	1.7586692977	0.6179636996
H	–2.5032203427	–1.5286798846	–2.2566291686
C	3.9465482262	0.9054257848	–0.8460253881
H	3.9176847645	1.9891844023	–0.7623753507
C	5.2309866657	–1.1407113284	–0.6862986143
H	–3.3640065886	0.4179621298	–1.5131533254
H	–4.0668232207	2.8988958328	–1.8933941278
C	5.1561320242	0.2506567268	–0.5931142813
H	6.1690381971	–1.6532290343	–0.4877915837
Br	–2.4780622087	–3.8605384892	–0.2245152878
H	–5.2847940495	1.4597763912	–0.1060021214
H	6.0367168579	0.8275154228	–0.3201900717
C	–4.8831770078	–1.2309473304	0.1394147694
H	–5.0448999362	–2.2682919	0.4386238885
H	–5.8251749292	–0.6760758881	0.2450899235
H	–4.5810856535	–1.2429832618	–0.9087637108
H	–0.7616944575	–1.7426902753	–2.1616791483

Tabelle 267 Standardorientierung von *S*-Konf-4 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
H	–1.0568620741	0.0464256059	3.4937910073
H	0.2812001488	1.176268363	3.7558411775
C	–0.4381982393	0.8086746773	3.0115674315
H	–1.0732980439	1.656350847	2.7339287646
H	1.2461689978	–1.9737989936	2.8808276219
H	0.4843533544	–1.003468755	–0.5849888871
H	–0.1578002958	–2.0629676379	0.6513778965
H	2.4643373644	–0.6886578126	3.0294477838
Br	–2.2325180054	–2.4879870481	2.9794291677
C	–0.2662327042	–1.0610315476	0.2222587659
C	1.7809569276	–1.1890540263	2.3326966675
H	–0.3558737578	1.3211619007	–0.9995552563
Si	0.5545959247	0.0491656625	1.5947492854
H	0.6675707742	3.0753978062	1.8550946841
H	2.3941270421	–1.6729622098	1.5619861308
H	–1.6017693866	3.4478173973	–0.2205704627
H	–3.3072665519	0.480882463	2.8791766069
H	–2.1877067371	1.1590493252	1.0271789349
N	–1.626828337	–1.0874755446	–0.4235551738
C	1.4001548948	2.7891243722	1.1036994938
C	–1.2064685958	1.1002874724	–1.6519466101
H	–1.0381769832	3.0295753755	–2.613878051
H	–0.8078888491	0.5478766465	–2.5111501478
C	1.5557774004	1.4338987185	0.7556442587
C	–1.5301748509	–2.0458182608	–1.5626928645
Zn	–3.1352882274	–1.8965988281	0.8894621696
H	2.0342649395	4.8300454968	0.8061692571
H	–0.8135676144	–1.6926386552	–2.3171290686
C	–2.4043344584	3.1909471534	–0.9265740552
C	–4.2312006099	0.5200757844	2.302928912
C	–2.928910325	0.9728170258	0.2456726649
C	2.1769220715	3.7922415145	0.513660274
C	–2.2170897631	0.2126954455	–0.9022085931
H	–4.6571875676	1.5327169246	2.3536344014
C	–1.8120073651	2.4311168996	–2.1179829094
H	–4.9407870437	–0.1777715017	2.7546602829
H	–2.8515149053	4.1381736377	–1.2533488204
H	–3.9006893889	2.8779402028	0.6206078752
N	–3.9782867427	0.1074703665	0.901078626
C	–3.4729427731	2.3361626681	–0.2318061282
H	–2.5119159711	–2.1903995537	–2.0156196992

C	2.5371474032	1.1272480524	–0.2089772813
H	2.7072219622	0.0918776229	–0.5010615326
C	3.1372799733	3.460579974	–0.4445367825
H	–2.9939879474	–0.0885698108	–1.6166112251
H	–2.5988509809	2.2493861809	–2.8655867396
C	3.3181603854	2.1210706524	–0.8034773824
H	3.7450893433	4.2368209569	–0.9028720579
Br	–4.6099859274	–3.2768925857	–0.3229925
H	–4.2906104614	2.1756817474	–0.9453759201
H	4.0697197602	1.8516114075	–1.5418989745
C	–5.2743057221	0.0830933167	0.1780949196
H	–5.8962006105	–0.7065544553	0.6024765486
H	–5.8009342416	1.0423599045	0.2684417433
H	–5.1234247434	–0.1556272775	–0.8756776154
H	–1.1882618653	–3.0128150641	–1.1864086146

8.3.9 Angaben zu den quantenchemischen Rechnungen der Deprotonierung des Dimethylphenylsilans (*R,R*)-**141** (Kapitel 4.4.2)

Tabelle 268 Berechnete Energien der optimierten Verbindungen der Deprotonierung von Dimethylphenylsilan (*R,R*)-**141** mit *tert*-Butyllithium.

Verbindung	Methode/Basis	Min./TS	ZPE [Hartree]	SCF [Hartree]
S_N-Ed-1	B3LYP/6–31+G(d)	Globales Min.	–1269,010862	–1269,605832
S_N-Ed-2	B3LYP/6–31+G(d)	Globales Min.	–1269,009403	–1269,604365
S_N-Ed-3	B3LYP/6–31+G(d)	Globales Min.	–1269,009392	–1269,604365
S_N-Ed-4	B3LYP/6–31+G(d)	Globales Min.	–1269,007990	–1269,603091
R_N-Ed-1	B3LYP/6–31+G(d)	Globales Min.	–1269,008803	–1269,604015
R_N-Ed-2	B3LYP/6–31+G(d)	Globales Min.	–1269,005434	–1269,600006
R_N-Ed-3	B3LYP/6–31+G(d)	Globales Min.	–1269,009848	–1269,604410
S_N-TS-1 *S*si	B3LYP/6–31+G(d)	TS	–1268,986526	–1269,578197
*S_N-TS-2 R*si	B3LYP/6–31+G(d)	TS	–1268,983227	–1269,575260
S_N-TS-3 *S*si	B3LYP/6–31+G(d)	TS	–1268,968109	–1269,578251
S_N-TS-4 *R*si	B3LYP/6–31+G(d)	TS	–1268,976905	–1269,567560
R_N-TS-1 *S*si	B3LYP/6–	TS	–1268,986835	–1269,578373

R_N-*TS-2 R*si	B3LYP/6–	TS	–1268,987728	–1269,578944
R_N-TS-3 *S*si	B3LYP/6–	TS	–1268,986835	–1269,578372
S_N-Ed-1	M052X/6–31+G(d)	Globales Min.	–1268,839044	–1269,443561
S_N-Ed-2	M052X/6–31+G(d)	Globales Min.	–1268,835820	–1269,440157
S_N-Ed-3	M052X/6–31+G(d)	Globales Min.	–1268,833663	–1269,438438
R_N-Ed-1	M052X/6–31+G(d)	Globales Min.	–1268,835594	–1269,440141
R_N-Ed-2	M052X/6–31+G(d)	Globales Min.	–1268,829732	–1269,434141
R_N-Ed-3	M052X/6–31+G(d)	Globales Min.	–1268,835223	–1269,440152
S_N-TS-1 *S*si	M052X/6–31+G(d)	TS	–1268,817690	–1269,418546
S_N-TS-2 *R*si	M052X/6–31+G(d)	TS	–1268,812047	–1269,413428
R_N-TS-1 *S*si	M052X/6–31+G(d)	TS	–1268,815541	–1269,416441
R_N-TS-2 *R*si	M052X/6–31+G(d)	TS	–1268,814886	–1269,415620

Tabelle 269 Standardorientierung von S_N-Ed-1 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	0.0499185965	0.0022060671	0.0215059746
C	0.026835001	–0.0331002668	2.4276930115
C	0.9881215384	–0.133291455	5.2703922208
C	–2.5350614218	–1.204506917	0.9471725934
N	–0.6517932461	0.5018854186	1.2228464002
Li	–0.3730097215	2.5339042977	0.8609356368
C	–2.3359907711	–1.3678751871	4.9230114986
Si	–0.3737479447	0.6198600302	4.1907656071
C	–4.0572524156	–1.3994614487	1.0060676413
C	–2.1243673055	0.2640382975	1.200127504
C	–3.5576011099	–1.8350918704	5.4142059907
C	–2.0564315738	0.0103180782	4.8267198509
C	–4.7640053516	–0.4760159659	0.0060838671
C	–2.8404521784	1.1960883657	0.1840619952
C	–0.2855188256	2.503407658	4.2760874249
C	–4.5381664857	–0.9274769736	5.8274447549
C	–4.3703023245	0.9884127737	0.249230515
N	–2.3985413495	2.6133615368	0.3308301017
C	–3.0588115484	0.9020793218	5.2542018503
C	–2.5316221869	3.3776806433	–0.919698997
C	–4.2849649666	0.4439744492	5.7482321752
C	–3.0497389414	3.3441133084	1.4305589526
H	0.116402889	–1.0972259651	–0.0037365375
H	1.0660802246	0.4078970935	0.0132064202

H	–0.4500193149	0.3391853861	–0.8913853797
H	1.0943708017	0.1972201874	2.3041959805
H	–0.0246742468	–1.1392633341	2.4524233853
H	0.9914021085	–1.2295333822	5.2249755155
H	1.9805758322	0.2158372677	4.9586231916
H	0.8490964018	0.150484608	6.3207561892
H	–2.1775537841	–1.5201780381	–0.0425492195
H	–2.0471503943	–1.8557556848	1.6818789803
H	0.6512055765	2.8620109397	3.8336024862
H	–1.5867187683	–2.096273136	4.6159079348
H	–4.3050503489	–2.4489463947	0.8010436346
H	–4.4157293362	–1.1846639046	2.0228926951
H	–2.478940738	0.532758717	2.2021013622
H	–3.74317051	–2.9047333288	5.4792102797
H	–4.4909191311	–0.7673251934	–1.019273034
H	–5.8533393416	–0.5855771459	0.0827624735
H	–2.5177582376	0.9001323515	–0.8226144071
H	–0.3110974817	2.8422093934	5.3197790668
H	–1.103022143	3.0081762477	3.749345915
H	–5.4886065211	–1.2875227304	6.213637273
H	–4.8615435158	1.6397944165	–0.4847151595
H	–4.740016371	1.2898403062	1.2383169264
H	–2.8829999056	1.9749956594	5.2111157212
H	–1.9816782977	2.8779567612	–1.7228487953
H	–3.5821254515	3.5034129316	–1.2333932066
H	–2.0922652728	4.3698738056	–0.7805284635
H	–5.038026297	1.1573092687	6.0751966296
H	–3.0221375838	2.7550166776	2.3513873293
H	–2.5080237156	4.2802046132	1.6035425479
H	–4.1011642305	3.5937359199	1.2144184045
C	1.2637978334	3.771557731	0.5426627465
C	1.5259224917	3.8317372012	–0.9703466072
C	2.5532735217	3.2761536572	1.211343721
C	1.0110308482	5.2065583007	1.0263654566
H	0.6638963708	4.2269473719	–1.5327358557
H	1.762592899	2.8430928722	–1.3980638055
H	2.3898708971	4.4922510312	–1.2282752097
H	2.8335137719	2.2594087227	0.8880283182
H	2.4779291304	3.2543834492	2.3109460922
H	3.432338521	3.9255130551	0.9778218316
H	0.8509986564	5.2611345323	2.1152126146
H	0.1278703961	5.6631257177	0.5488329775

H	1.8670723535	5.8900347013	0.8039639843

Tabelle 270 Standardorientierung von S_N-Ed-2 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.1210504971	0.0694288794	0.1237168413
C	–2.146204688	1.3121030122	0.4833205477
C	–3.173588658	4.1709106133	1.4289253259
C	0.5025620785	3.0309392262	0.3033429781
N	–0.8194861634	0.9776150666	1.0574946746
Li	–0.8702551559	–0.2908446624	2.7069091909
C	–5.7706377922	2.8792662412	–0.2036074327
Si	–3.4725699308	2.2975142905	1.4702469807
C	1.2927989866	4.2553280853	0.7880956022
C	–0.0085177347	2.1570225207	1.4720049129
C	–6.9582061667	2.5724656545	–0.8760048555
C	–5.0847300357	1.9116788747	0.5541509546
C	2.4623121715	3.8323224886	1.6852084909
C	1.1772772361	1.7410765711	2.3869027382
C	–3.5967988133	1.7035325878	3.2614338645
C	–7.4889647163	1.2824516535	–0.8030616925
C	1.9604597675	2.9843915314	2.8629300519
N	0.7329131195	0.8280481389	3.4791610687
C	–5.6406029758	0.6171680984	0.6121392607
C	1.7958185447	–0.0936221559	3.9116760818
C	–6.8267903308	0.3035175105	–0.0558389859
C	0.1621446712	1.50862251	4.6536493308
H	–0.0122548814	0.4991943516	–0.8847534504
H	–0.6983581835	–0.8561796676	0.0386923645
H	0.8726336893	–0.192765795	0.4979645137
H	–2.6343057342	0.3508849541	0.2746076196
H	–2.0399913783	1.7956529569	–0.5069232127
H	–4.0311698818	4.7038386253	1.8591146082
H	–2.2909706921	4.4585649925	2.0126306577
H	–3.0295442687	4.5464664471	0.4081748924
H	1.1523519007	2.4271796451	–0.3449131251
H	–0.3449826329	3.3518062852	–0.3136878791
H	–3.5903546152	0.6095466709	3.3366271898
H	–5.3796765662	3.8919891397	–0.2745888354
H	1.6560715139	4.8280947264	–0.0746971365

H	0.6266297784	4.9271248434	1.3501318797
H	–0.6843844399	2.7758337738	2.0763442918
H	–7.4673962634	3.3402038889	–1.4540869117
H	3.1874671775	3.2534405997	1.0938759539
H	2.9980095031	4.7130734958	2.061579873
H	1.8690881894	1.1448832334	1.7785601793
H	–4.5311393045	2.0625752654	3.7108951759
H	–2.7742900924	2.0826833419	3.879261811
H	–8.4126174414	1.0408896102	–1.3234662621
H	2.8036954315	2.6683024876	3.4899246213
H	1.3158261093	3.6104366932	3.4947029267
H	–5.1470736955	–0.1636488812	1.1884796401
H	2.1641918456	–0.6679269443	3.0560720819
H	2.6472944201	0.4276187692	4.3820297148
H	1.3818845029	–0.8003714816	4.6368711913
H	–7.2332338194	–0.7029307464	0.0081690873
H	–0.5805268058	2.2484764827	4.3440444969
H	–0.3383136373	0.7665991907	5.2843990473
H	0.9246912431	2.0194976466	5.2635995907
C	–1.6799269923	–2.1456371409	3.1788479035
C	–0.7037293735	–3.2105382446	2.6541535012
C	–3.0524300254	–2.4354635401	2.5577066082
C	–1.8056308158	–2.3403380081	4.6966296198
H	0.305030971	–3.1102734141	3.0883166373
H	–0.5871850299	–3.1726171815	1.5582943017
H	–1.0376920978	–4.2503385977	2.8917182047
H	–3.0440398911	–2.353395224	1.4581479863
H	–3.8342018016	–1.7518522576	2.9277135899
H	–3.4157891315	–3.467144302	2.7868878195
H	–2.5257900534	–1.6415820677	5.1520605834
H	–0.8452209544	–2.199034257	5.2205503089
H	–2.1543296921	–3.3666391023	4.9691854099

Tabelle 271 Standardorientierung von S_N-Ed-3 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	0.7899828263	–2.963018265	1.4391382457
C	0.7399450636	–0.5617292191	1.3595929572
C	1.752639941	2.2609727163	1.4358344885
C	–2.0425832018	–1.9742284127	1.874792364

N	0.2305469065	–1.7996123578	0.7193490127
Li	1.0307740354	–2.2109321673	–1.1573586104
Si	0.4340559878	1.1831527905	0.6071385748
C	–3.5617700602	–1.9734438107	1.6497178183
C	–1.2495573034	–1.8474051247	0.5535409925
C	–1.2818631739	1.8729737339	1.0321232609
C	–3.9717582648	–3.0849384167	0.6760727331
C	–1.6769770644	–2.9671635173	–0.4362200438
C	0.6864247263	1.1910598879	–1.2670782633
H	–1.495625803	1.8225379562	2.1070601592
C	–3.2068308644	–2.9518933206	–0.6487108493
N	–0.8725892309	–2.9257526443	–1.6913400271
H	–2.0817736213	1.3323664999	0.512154025
C	–0.7291307065	–4.2518157151	–2.3136447162
H	–1.3558255624	2.9253661622	0.7296068652
C	–1.3499534598	–1.95917257	–2.6944656413
H	0.549956042	–2.9524951796	2.5142290354
H	1.8789663138	–2.9490288475	1.3334102249
H	0.4274533088	–3.9023772894	1.0120754895
H	1.8339154334	–0.6561077477	1.3681429873
H	0.4519093166	–0.5194447382	2.4277313598
C	1.4304401737	3.2487854956	2.3852015788
C	2.4202619633	4.0312966093	2.9889262531
C	3.7626156093	3.841532546	2.652401459
H	–1.7622543779	–2.9093680506	2.3786976676
H	–1.763198944	–1.1577393395	2.5510363475
H	1.586224859	0.6403700733	–1.5664893573
H	–4.079422497	–2.0917412783	2.6101779258
H	–3.8754519824	–0.9996532004	1.2443661334
H	–1.5212951389	–0.887361804	0.0959252174
H	–3.7612992322	–4.0653429338	1.1289995257
H	–5.0523779335	–3.0532715359	0.4873668543
H	–1.4316462016	–3.9298177322	0.0298707223
H	0.7923245108	2.2224524843	–1.6261504896
H	–0.1642927961	0.7492448109	–1.7991214735
H	–3.4896851547	–3.7612466955	–1.3335612337
H	–3.5056861625	–2.0118187279	–1.1320010907
H	–0.2906480972	–4.9550995815	–1.5990112038
H	–1.6895151857	–4.6616600954	–2.670889134
H	–0.0495178133	–4.173647036	–3.1673159699
H	–1.5295640417	–0.9849962712	–2.2323675154
H	–0.5789452555	–1.8354711606	–3.4620307345

H	–2.279484829	–2.2824103785	–3.1904591708
C	2.9209991505	–2.4082921949	–1.9981686404
C	3.3937706156	–3.8425788842	–1.7126022968
C	3.985430626	–1.4546460379	–1.4404004076
C	2.8864712579	–2.2268626815	–3.5223673247
H	2.7095220367	–4.6033279669	–2.1239509938
H	3.491130452	–4.0477248246	–0.6335417711
H	4.3958191688	–4.0587677613	–2.1579428024
H	4.102774542	–1.5454762386	–0.3477795965
H	3.7569296191	–0.3976908094	–1.6549721317
H	4.9974812295	–1.642474385	–1.8756047456
H	2.5985031545	–1.2050583436	–3.8178269225
H	2.1775099738	–2.9151837575	–4.0127047368
H	3.8788348301	–2.4196256216	–3.9990652867
C	4.108459485	2.8670317916	1.7111962187
C	3.114384015	2.0886468563	1.1132445561
H	0.3923316376	3.4181636329	2.6629573004
H	2.1424158023	4.7878141473	3.7192382796
H	4.5344836586	4.4489676156	3.1188228976
H	5.1505469008	2.7132521159	1.4416841825
H	3.4115887865	1.3386267463	0.3821194674

Tabelle 272 Standardorientierung von S_N-Ed-4 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.0095745459	–2.3214938595	0.1607999461
C	–0.0579676747	0.1002448243	0.3767134367
C	2.5345097967	–0.5872371743	2.1153086839
C	–2.7372966	–1.3838685118	–0.4694918124
N	–0.1976190965	–1.0460620412	–0.5600724646
Li	1.2954001952	–1.5620383493	–2.0179533501
Si	1.6766529871	0.6670696934	0.9931818512
C	–4.0460929417	–1.1571210141	–1.2399393746
C	–1.5000025643	–0.9745281689	–1.2995018427
C	2.7553098465	1.114318801	–0.4906937009
C	–4.0267250524	–1.9105653796	–2.5753243149
C	–1.4729824245	–1.7544940021	–2.6382802481
C	1.2711001907	2.2304114754	1.9929746032
H	2.265573599	1.845434614	–1.1468130847
C	–2.7954787658	–1.5199120655	–3.4063637826

N	–0.2388079437	–1.4669759337	–3.4223870304
H	2.9954178033	0.2256668415	–1.0884781473
C	–0.0223565323	–2.4428073194	–4.5027779296
H	3.7052738252	1.5539012568	–0.1617958179
C	–0.1499504409	–0.1005407795	–3.9628150644
H	–0.6671291051	–2.4111472198	1.0405575996
H	1.0267622638	–2.401165457	0.4965708201
H	–0.2036982618	–3.1696865294	–0.5032669695
H	–0.7059880769	–0.037532065	1.2626733215
H	–0.4499635719	0.9914708855	–0.1319615101
H	3.3765268632	–0.1159165783	2.6380685267
H	1.8587106517	–0.9981374261	2.8756292099
H	2.9421712843	–1.4228025625	1.5366169116
H	–2.6677016977	–2.4464143539	–0.2003256319
H	–2.7506615138	–0.8195684227	0.4708000226
C	1.2420653768	2.2236695367	3.4008091771
H	–4.8988815713	–1.4785087993	–0.6284865779
H	–4.18317731	–0.0814844636	–1.4273616657
H	–1.6231199115	0.085912894	–1.5521424702
H	–4.0124747112	–2.9938759388	–2.3830058837
H	–4.9411341553	–1.7074966745	–3.1471895513
H	–1.4143657476	–2.8276303637	–2.4066544857
C	0.9188668635	3.3708406249	4.1326658727
C	0.6145457005	4.5615392484	3.468426605
H	–2.7825549045	–2.0862485818	–4.3449537625
H	–2.8755769422	–0.4584901097	–3.6791145421
H	–0.0724858828	–3.4584591978	–4.1004246418
H	–0.7570232632	–2.3466330555	–5.3192670321
H	0.9776843669	–2.2965972242	–4.9205302841
H	–0.2847191814	0.6395133387	–3.1689845252
H	0.8478952544	0.0415157993	–4.3912315103
H	–0.8884277086	0.0992255454	–4.7560197031
C	3.1483155961	–2.5408541831	–2.1641865705
C	2.8203779748	–4.0007056046	–2.5223911523
C	4.0746418722	–2.5845042958	–0.9429333825
C	3.9529372888	–1.9483714714	–3.331986286
H	2.2175767681	–4.0918843718	–3.4397693974
H	2.2683499194	–4.517533592	–1.7195920531
H	3.7397519329	–4.6087213244	–2.7025621126
H	3.5932912952	–3.0519418304	–0.0680328095
H	4.4172990819	–1.5862484237	–0.6300101718
H	4.9993218186	–3.1799597761	–1.1359786728

H	4.2806538371	–0.915173285	–3.1350531253
H	3.3803133666	–1.9285738564	–4.2746425602
H	4.8804957494	–2.5311781574	–3.550936196
C	0.63783747	4.596824073	2.0711296553
C	0.9624764407	3.4453343742	1.3488825984
H	1.4803960249	1.3113794534	3.9435801793
H	0.9081075257	3.3346726756	5.2195924342
H	0.3657426547	5.4561276671	4.0341850533
H	0.408746623	5.5208832269	1.5452292273
H	0.9835379905	3.5041329452	0.2617874664

Tabelle 273 Standardorientierung von R_N-Ed-1 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.0331025302	–0.7911640195	–1.3322059443
C	–0.1441297101	1.6385978873	–1.2777690682
C	–1.8893648583	–3.1091376395	–1.7698452506
C	2.6009140338	0.3327856057	–2.14787872
N	0.4934702112	0.4427044701	–0.6953502283
Li	0.1494484593	0.6416734044	1.3744459215
Si	–1.8162047544	–1.4034327745	–0.942273723
C	4.1315038535	0.4487292154	–2.1549891608
C	1.9914019734	0.5471946259	–0.74298043
C	–2.0564962447	–1.5939525981	0.9205805354
C	4.7485113966	–0.5431464852	–1.1624156755
C	2.6514308347	–0.3920271231	0.3009568028
C	–3.1507126755	–0.3021992564	–1.7070611606
H	–3.0481584998	–2.0068389108	1.1449350578
C	4.1930606735	–0.2988744746	0.2468924869
N	2.0733816725	–0.1703127013	1.6605522338
H	–1.9642010875	–0.6497572375	1.4726579695
C	2.0673429641	–1.3951761372	2.4728938827
H	–1.3169113054	–2.2961549638	1.3281707163
C	2.7010211989	0.9263172249	2.4215183079
H	0.0586533816	–0.7315625366	–2.4326548071
H	–1.2214279099	1.6019239162	–1.1050625897
H	0.6045974771	–1.6318970735	–1.0298538604
H	0.02158195	1.7211347912	–2.3648686443
H	0.2440686761	2.5384594308	–0.7908856517
H	–2.8764412786	–3.5646511004	–1.6236548414
H	–1.7125627079	–3.0543736138	–2.8513143443

C	–3.2877167685	–0.2130551082	–3.1074657937
H	2.3317803769	–0.6670087068	–2.5129988857
H	2.1632637496	1.0514743119	–2.8512964474
C	–4.2746560397	0.5815859071	–3.6952658062
H	4.5110544054	0.2689628006	–3.1690019131
H	4.4327940482	1.4718630276	–1.8846993049
H	2.2135304883	1.5804360714	–0.4396649848
H	4.5239868019	–1.5715549518	–1.48326613
H	5.8420401376	–0.4506263825	–1.1507005143
H	2.3811062022	–1.4215548021	0.0325608302
C	–5.1570320606	1.3083873778	–2.8896007523
H	4.626498556	–1.012969958	0.9589200361
H	4.5125432459	0.700109621	0.5709837717
H	1.5263413011	–2.1896314194	1.948246222
H	3.0825826272	–1.7598802797	2.7076143458
H	1.5513391456	–1.1970740518	3.4176030386
H	2.7384831746	1.8385764268	1.8197298907
H	2.0883542986	1.1374233711	3.3013583876
H	3.7220402828	0.6825372752	2.7559317217
C	–0.9539936903	1.8971168784	2.6485373832
C	–0.9003706542	1.4138335689	4.1055589038
C	–2.4324529331	2.1018931031	2.2916785665
C	–0.2872009409	3.281886863	2.5918893426
H	–1.3958265317	2.125027156	4.8103449241
H	0.1308045841	1.2936457872	4.4785198851
H	–1.4045791918	0.4439787446	4.2428785364
H	–2.931066527	2.840088184	2.965657014
H	–3.0197121488	1.1732818057	2.3770999038
H	–2.5711255033	2.480922797	1.2668340177
H	–0.3294321035	3.7277999008	1.5842408555
H	0.7736610459	3.2605962085	2.8904321122
H	–0.7794431513	4.0181609397	3.2729464358
H	–1.1424044548	–3.7927272562	–1.3456540484
C	–5.0435013067	1.2341235259	–1.4995019425
C	–4.0514594082	0.4376948539	–0.9180898473
H	–2.6179749727	–0.7743537216	–3.7575530909
H	–4.3577287639	0.6316925755	–4.7785476489
H	–5.9274676782	1.9270630593	–3.3434016125
H	–5.7225804933	1.7978230258	–0.8645689352
H	–3.9781543431	0.4069895443	0.1657717184

Tabelle 274 Standardorientierung von R_N-Ed-2 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.1852350842	–0.4149620531	0.7839515874
C	–0.3785487361	–0.1836881547	–1.6697641215
C	–1.7936271115	–3.2398199587	0.7142547188
C	1.4050250333	–2.6543931223	–0.6606449151
N	0.5271455174	–0.2553860099	–0.5171007273
Li	1.3078617194	1.6217221182	–0.0643874859
Si	–1.8391824546	–1.3829959828	1.0881692837
C	2.6354431414	–3.5104434801	–0.9961443684
C	1.6960996123	–1.1407007557	–0.7532095326
C	–2.0981163748	–1.1516017615	2.9528060521
C	3.8203575793	–3.1405470694	–0.0958293206
C	2.9007463089	–0.7699933013	0.1547916556
C	–3.28452557	–0.587640258	0.1599338499
H	–2.1382627498	–0.0913326523	3.2312104448
C	4.1286916224	–1.6395922383	–0.1962429123
N	3.1566087425	0.6968714142	0.1530798484
H	–1.2926652196	–1.618392373	3.534795525
C	3.8464135223	1.1545830845	1.3686012449
H	–3.0441039026	–1.6079855521	3.2692525377
C	3.8564533645	1.2001502702	–1.0417016723
H	0.5295102473	–0.7949380863	1.524005112
H	–1.1313506517	0.5887105639	–1.4940234329
H	–0.4398951705	0.5991990974	1.1395040649
H	–0.9051419556	–1.1300631409	–1.875683191
H	0.1907709935	0.0958164194	–2.5630434885
H	–1.0051714343	–3.739187844	1.2900629811
H	–2.7471865757	–3.6978479489	1.0070783749
C	–4.093881544	–1.3221911619	–0.727299537
H	1.0710957997	–2.8972168968	0.3564021682
H	0.5766282471	–2.9075663094	–1.3322438154
C	–5.1712413511	–0.7299258254	–1.3938724229
H	2.3886022206	–4.5747366935	–0.8914968732
H	2.9155294705	–3.3571401703	–2.0492408316
H	1.9941074267	–0.9321885461	–1.7906468109
H	3.5834278442	–3.4008603437	0.9468843753
H	4.7093119716	–3.723347628	–0.3687762076
H	2.6210955722	–1.0089773536	1.1898889121
C	–5.4635591371	0.6206122076	–1.1875600524
H	4.9651058493	–1.3791104891	0.4642710071
H	4.4557914116	–1.4163167875	–1.2209783528

H	3.2886036959	0.8346195992	2.2546390421
H	4.878785556	0.7730032027	1.4459836935
H	3.8820522416	2.247738522	1.368678202
H	3.3672879371	0.8428655055	–1.9528840588
H	3.8099764477	2.2937856341	–1.0417160933
H	4.916443219	0.9006432741	–1.0756633061
C	0.6976112219	3.6055855846	0.040616825
C	1.6951531464	4.4318684966	0.8645794787
C	–0.6924978813	3.8103436282	0.6568839555
C	0.6663410912	4.194843306	–1.3781103441
H	1.4292310827	5.5170303937	0.8934886486
H	2.7197352972	4.3850010224	0.4581985253
H	1.7488487112	4.101554239	1.9146122785
H	–0.9916856217	4.8870237209	0.6851693457
H	–0.7478124731	3.4515960343	1.6980673177
H	–1.4812938146	3.2903320912	0.0901932422
H	–0.0630126435	3.6852216133	–2.0282567258
H	1.6449550395	4.1332750067	–1.8828201871
H	0.3850392286	5.276703574	–1.3845354355
H	–1.6266638884	–3.4686985071	–0.3439752956
C	–4.67596967	1.3715323749	–0.3099558713
C	–3.6035269655	0.7714445954	0.3545513597
H	–3.8871632416	–2.3750680656	–0.9071375044
H	–5.7798475254	–1.3224776562	–2.0731238705
H	–6.2985665141	1.0852634463	–1.7062169986
H	–4.8924451349	2.4239546477	–0.1445059048
H	–3.0066149152	1.3837085643	1.0277072799

Tabelle 275 Standardorientierung von R_N-Ed-3 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	0.8135349897	0.6269575764	–0.7819163412
C	0.781504464	3.0555224495	–0.8957485882
C	–2.1498164854	–0.3541544249	–0.9897529674
C	2.9688907071	1.7097895019	0.9547630106
N	0.606979046	1.8846440943	–0.0175444351
Li	–1.3096969343	2.1097195388	0.7946009136
Si	–0.5622835592	–0.028028302	–1.9620833036
C	3.8184431554	1.8429155815	2.2262361966

C	1.4705202034	1.9943732109	1.2059860372
C	–0.9167471257	1.1061527505	–3.4331449154
C	3.2872027145	0.9157718176	3.3252376015
C	0.9216466635	1.1175277474	2.3619678855
C	0.1641939582	–1.6626067833	–2.596795267
H	–0.0010808662	1.4510394553	–3.9289539751
C	1.8135963047	1.2283626863	3.6190812074
N	–0.523878944	1.4012914465	2.6092289197
H	–1.4943286612	1.9874668016	–3.1322926218
C	–1.2438790299	0.2320981156	3.1339089907
H	–1.5117581296	0.5659592015	–4.1805161478
C	–0.7827339378	2.5695204288	3.4719804393
H	1.7567466689	0.6713472488	–1.3567317882
H	0.0432635254	3.0261106728	–1.6989208481
H	0.9497980589	–0.1951876747	–0.0682864952
H	1.7850199308	3.0976928254	–1.3525505731
H	0.6137121056	3.974890565	–0.3268640113
H	–2.6019228488	0.5846265705	–0.6415209706
H	–2.8958072493	–0.8497138887	–1.6240422145
C	–0.244021802	–2.9078688039	–2.0818875267
H	3.0865766079	0.6894866377	0.5671331861
H	3.3442268372	2.385307647	0.1765509501
C	0.3089029913	–4.1072069469	–2.5422060048
H	4.8662593582	1.6108031016	1.9966810656
H	3.7991884706	2.8832171914	2.5845094897
H	1.3816177288	3.0432263407	1.5225808804
H	3.3935974513	–0.1316125788	3.0051467633
H	3.878720979	1.0241192809	4.2432942343
H	0.9597819901	0.0722159852	2.0281724746
C	1.2922544336	–4.0882172593	–3.5344400397
H	1.429059392	0.5596073316	4.3996135986
H	1.7545198317	2.2478032494	4.0224280829
H	–1.1187134005	–0.6186975143	2.4563832128
H	–0.9008118145	–0.0672928881	4.1391798161
H	–2.3113789801	0.4660765287	3.1952893833
H	–0.2295044887	3.4427843399	3.1149452549
H	–1.8475597898	2.8122956795	3.4226965925
H	–0.5139379246	2.389564271	4.5252678904
C	–2.9519053596	3.3492720548	0.4009199541
C	–4.1897056913	2.9329415159	1.2090703973
C	–3.3780158507	3.4619135436	–1.0689463718
C	–2.5526287231	4.7617226419	0.8606054946

H	–5.0366792608	3.6521834451	1.0937091337
H	–3.9903024069	2.8753766467	2.2926677503
H	–4.5790547069	1.9487073906	0.9035150062
H	–4.2087658875	4.193868912	–1.2150844755
H	–3.7403482391	2.5068945405	–1.481440098
H	–2.5561107919	3.8041551473	–1.7194361633
H	–1.6984117451	5.1644252898	0.2909972411
H	–2.2765001345	4.8032202849	1.9271045846
H	–3.3809008246	5.500461619	0.7325073096
H	–1.9849609293	–0.9961884349	–0.115006896
C	1.7153062383	–2.8652872045	–4.0634073162
C	1.1556637607	–1.6721741738	–3.5983222672
H	–1.013646976	–2.9505919651	–1.314029275
H	–0.0308748411	–5.0543005951	–2.1294039407
H	1.722306195	–5.0188368261	–3.896694282
H	2.4765947151	–2.8412273273	–4.8396981536
H	1.4962448627	–0.7341373118	–4.0337926752

Tabelle 276 Standardorientierung von S_N-TS-1 *S*si [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	0.0471590162	–0.0508960006	0.0581206718
C	–1.4812113472	1.8311591374	0.087278064
C	–4.1691786906	3.1753479435	–0.1648561185
C	1.6507780457	2.3682996224	0.580383672
N	–0.5046987338	1.0376143968	0.8859567062
Li	–1.599729916	0.3297807025	2.4818144684
C	–1.2836698883	5.3118674107	0.5416744482
Si	–2.7733793269	2.8720975797	1.0874489406
C	2.7070854433	3.2328626984	1.2818067538
C	0.5418088207	1.8816114032	1.542165754
C	–0.7491916303	6.5711685096	0.8281318099
C	–1.9935923466	4.5688483208	1.5069930737
C	3.3343397814	2.4671009631	2.4522249771
C	1.1581396158	1.1558820362	2.7678349211
C	–3.327044485	1.87199346	2.5517920065
C	–0.9124136205	7.1267049429	2.1014101487
C	2.2476287694	2.0206614659	3.4395158197
N	0.0991610204	0.6697042726	3.7136431084
C	–2.1493802415	5.1562951155	2.7768593357

C	0.5418253226	–0.5309281823	4.4423884375
C	–1.6174007229	6.4158199857	3.0758403016
C	–0.3532347003	1.6852405267	4.685091497
H	0.4943327845	0.3129610349	–0.8802631115
H	–0.7613737813	–0.7407064212	–0.2019411439
H	0.8062627101	–0.6171472883	0.6071540218
H	–2.1002476072	1.0982525419	–0.4484273001
H	–0.9704413962	2.4125161116	–0.7014900137
H	–3.8002382034	3.6241458893	–1.0962683853
H	–4.6760375445	2.235980254	–0.4204502417
H	–4.9202389519	3.8563445821	0.2541597923
H	2.1573076129	1.5015534996	0.1344764599
H	1.1951791707	2.926206578	–0.2461548137
H	–3.2512653185	0.4730892372	2.4994685382
H	–1.146909064	4.9066993486	–0.460258327
H	3.477244281	3.534135153	0.560076549
H	2.2443965039	4.1584403929	1.6537061892
H	0.0159564488	2.7709444094	1.9097366438
H	–0.2100777884	7.1206935839	0.0592547568
H	3.878785653	1.5902313531	2.0700154575
H	4.0720812092	3.0908436937	2.9730648583
H	1.6476409869	0.2460996149	2.39669863
H	–4.4186044108	1.9452141777	2.6523430493
H	–2.9153052813	2.2235047616	3.5089913013
H	–0.499701694	8.1069885699	2.3281554701
H	2.6972561974	1.4660917828	4.2732228062
H	1.7896306042	2.9203656489	3.8698631191
H	–2.7072288332	4.6230367935	3.5444639608
H	0.7905215757	–1.3286792489	3.7361949375
H	1.4192105242	–0.3394221157	5.08256693
H	–0.2710441314	–0.8857471842	5.0835178506
H	–1.7581289364	6.842800792	4.0666239037
H	–0.6186568207	2.6151215604	4.1766039544
H	–1.2473201441	1.3122898384	5.1946816738
H	0.4069059157	1.9075225879	5.450251102
C	–3.3635644926	–1.059140151	2.4825327584
C	–2.2745812184	–2.1462542282	2.5202038879
C	–4.1761821915	–1.2176994846	1.1959166484
C	–4.2772214717	–1.2433745195	3.6965759834
H	–1.689928937	–2.1270862873	3.4527989048
H	–1.563092349	–2.0784007301	1.6802851442
H	–2.7073246529	–3.1679828211	2.4596472086

H	–3.546523979	–1.1334594026	0.295941681
H	–4.9577046493	–0.4475042625	1.1150855206
H	–4.6863821273	–2.1996171865	1.1339517188
H	–5.0727285397	–0.4846349475	3.7234009024
H	–3.721964111	–1.1599859271	4.643903849
H	–4.7760567367	–2.2332978955	3.7051803767

Tabelle 277 Standardorientierung von S_N-TS-2 *R*si [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–0.0763876201	0.059887629	–0.0137409428
C	–2.0871509562	1.3558898633	0.423869842
C	–3.165300264	3.7737905208	2.1347576034
C	0.7359442841	2.8782647184	0.0770768737
N	–0.7356083222	0.9806166782	0.9320613033
Li	–1.0857777306	0.0405481112	2.7318065332
C	–5.5753788436	2.7675001974	0.053140522
Si	–3.3868123961	1.9147543537	1.7527178445
C	1.5683064885	4.1035938326	0.4773826469
C	0.0996570034	2.1646963845	1.2926351647
C	–6.7847409758	2.6262000914	–0.6349318927
C	–5.0446890863	1.7253050599	0.8384462717
C	2.6618466991	3.7018140433	1.47368037
C	1.1855604888	1.7957874248	2.3395074921
C	–3.2133486737	0.7906157977	3.22779846
C	–7.4990064762	1.427993731	–0.5537797716
C	2.0412834238	3.0298528301	2.7061442233
N	0.5966180469	1.0873338062	3.5227702258
C	–5.7861327555	0.5293211407	0.9040790438
C	1.5846433035	0.2058436766	4.1679563093
C	–6.9955843579	0.378046606	0.2196527914
C	0.0179176377	1.9870901706	4.5391313462
H	–0.020701178	0.4651902126	–1.0359594467
H	–0.6474107814	–0.8722683024	–0.0537633307
H	0.9374584395	–0.183342852	0.3206623431
H	–2.5229950064	0.4383776018	0.0078861952
H	–2.0159678487	2.0565406501	–0.4275053483
H	–4.0558843747	4.153686492	2.6514192659
H	–2.3115572708	3.9600358828	2.7988883419
H	–3.0185373708	4.3843437181	1.2331888859
H	1.3933617035	2.1782805941	–0.4557678867

H	–0.0520477509	3.1665712537	–0.6286684049
H	–2.6081020879	–0.4762152131	3.1276299423
H	–5.0435123518	3.7140978478	–0.0224334719
H	2.0093977162	4.5617240995	–0.4171040242
H	0.9195934173	4.8665132931	0.9330758435
H	–0.5879494413	2.8756775112	1.7650231167
H	–7.1696385382	3.451359243	–1.2303897371
H	3.367531447	3.0125164574	0.9859946715
H	3.2447959602	4.5779286299	1.7852646888
H	1.8535587954	1.0601392823	1.8721336294
H	–4.2036877707	0.4378512222	3.5458010042
H	–2.8065464282	1.3298401765	4.0977709901
H	–8.4408833764	1.3144693532	–1.0854922517
H	2.8270307723	2.7382742649	3.4145367213
H	1.4144336964	3.7709683874	3.2194473246
H	–5.4181162175	–0.3011096735	1.5022468299
H	1.9586928058	–0.5283356063	3.4485864535
H	2.4408560836	0.7610842569	4.5857578973
H	1.1035542834	–0.336605276	4.9874525919
H	–7.5452192731	–0.5578135268	0.2924828126
H	–0.6747023107	2.695004797	4.0782211082
H	–0.5463926897	1.3886071015	5.2610161969
H	0.7840477945	2.5536207703	5.0911722227
C	–2.1060644964	–1.9291829476	3.0938631147
C	–0.6711179874	–2.4766123662	2.992161198
C	–2.9300363789	–2.488950184	1.9324060139
C	–2.7076706603	–2.3962529211	4.4215044866
H	–0.0426206607	–2.1701444599	3.8416294355
H	–0.1521146417	–2.1734411183	2.0668939296
H	–0.6531557859	–3.5875788864	2.9895266905
H	–2.5223663698	–2.1984943348	0.9513055333
H	–3.9694644242	–2.1319415252	1.9652826171
H	–2.9736075737	–3.5966439058	1.9404721733
H	–3.737900915	–2.0340159834	4.5493111902
H	–2.1297279464	–2.0303434052	5.2840440694
H	–2.7418049253	–3.5010392787	4.5035071126

Tabelle 278 Standardorientierung von S_N-TS-3 *S*si [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–1.8067621311	–1.2656742289	–2.6202102182
C	–0.9672043728	0.8354166562	–1.7534855667
C	–1.5713958104	1.3115360327	1.2261253597
C	1.1350421354	–1.490892641	–2.3626319332
N	–1.1002696831	–0.6256530213	–1.4950631197
Li	–2.1353913376	–0.7384428639	0.2890608368
C	1.8667331211	1.9032470715	1.3246958039
Si	–0.5975577652	1.9558923426	–0.2174994618
C	2.4580454924	–2.1676247265	–1.9814671968
C	0.1977182033	–1.2843331154	–1.1508542968
C	3.2489512865	1.9867295756	1.5277700058
C	1.2975494021	2.0234408228	0.0427427092
C	2.1909803109	–3.5134703385	–1.298234251
C	–0.0348442352	–2.6221852591	–0.3990841655
C	–1.1651745879	3.6810875355	–0.7730960285
C	4.1038634384	2.1974773962	0.4431005574
C	1.3043112008	–3.3149740385	–0.0611586008
N	–0.9430184622	–2.4366810134	0.7809636757
C	2.1835170126	2.2429338771	–1.0318282452
C	–1.7393538312	–3.6464259879	1.0456792252
C	3.5655979955	2.3292944431	–0.841165521
C	–0.2504456234	–2.0301472307	2.0191165615
H	–1.3232365491	–1.0742127344	–3.5909933545
H	–2.8246854485	–0.8687864868	–2.6688809079
H	–1.8782539194	–2.3482349528	–2.4762862577
H	–1.9568271761	1.1729035077	–2.0920412182
H	–0.2872501809	1.0298810902	–2.6027539
H	–0.9636660096	0.7405157838	1.942800501
H	–1.9922405238	2.1527894599	1.7934285341
H	–2.771056777	0.6281548604	0.9952362282
H	0.6333723818	–2.1165857061	–3.1135132457
H	1.3305928649	–0.5229339198	–2.8380376472
H	1.2157286027	1.7518779564	2.1837528833
H	3.0759038096	–2.3053389147	–2.8781714028
H	3.0281571303	–1.5166211965	–1.3030351209
H	0.7035841211	–0.5986871402	–0.4597063129
H	3.6561284445	1.8923338896	2.5323070057
H	1.6992990643	–4.1960898339	–2.0079272078
H	3.1327863588	–3.9934865032	–1.0030030998
H	–0.5805684091	–3.2897759701	–1.078232936
H	–0.9022291322	4.4343380581	–0.0202198544

H	–2.2541559803	3.7098781819	–0.9071858769
H	5.1784174479	2.2653655769	0.5962170521
H	1.1060124294	–4.2795545987	0.4239837531
H	1.8625796352	–2.7069704889	0.6622542739
H	1.7918800123	2.3557990518	–2.042128575
H	–2.3287621249	–3.9083801815	0.1615698249
H	–1.1156395763	–4.513335131	1.3223224371
H	–2.4321310001	–3.4509715892	1.8700173334
H	4.2219292399	2.5028341015	–1.6914040422
H	0.4048287459	–1.176469758	1.8298199381
H	–0.9981942108	–1.7256436024	2.7581662616
H	0.3503080259	–2.8431980993	2.4560120071
C	–4.15012388	–0.0657245801	0.9468807529
C	–4.6612325272	–1.0946674627	–0.075637579
C	–4.952314499	1.2246894332	0.7689067105
C	–4.3566015399	–0.6058820819	2.3644003574
H	–4.136414591	–2.0647719646	–0.0251590788
H	–4.575415911	–0.7286134422	–1.1098584676
H	–5.7357043684	–1.3347931663	0.0751877707
H	–4.828244216	1.6446491935	–0.2410492633
H	–4.6366361652	2.0007901886	1.4810619531
H	–6.0390352864	1.070540365	0.9215021588
H	–3.9804232934	0.0979396522	3.1214326945
H	–3.8357687268	–1.5634873603	2.5289167951
H	–5.4249637518	–0.7902815961	2.5993266175
H	–0.6998242992	3.9849668222	–1.7197546257

Tabelle 279 Standardorientierung von S_N-TS-4 *R*si [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.7938597648	–0.7768257581	–1.5396130928
C	1.150825967	0.6548721916	–1.2507780728
C	–0.8350585781	2.0704632273	0.6666328334
C	1.6213689051	–2.3602982948	–2.2209276563
N	0.463160105	–0.5959504369	–0.7894806665
Li	–0.5336962689	–0.4274585269	1.060360838
Si	0.8511175519	2.1673542086	–0.081383554
C	2.6422529046	–3.5059042172	–2.1947424501
C	1.3602689126	–1.7828867589	–0.8123113225

C	2.1971964408	2.1064052106	1.2677101169
C	2.1840218526	–4.611625132	–1.2368564202
C	0.8874356231	–2.8949596885	0.1540973098
C	1.2333985067	3.6924803442	–1.1670104123
H	3.2090573521	2.1158836906	0.8419960935
C	1.9194692737	–4.0489311372	0.168098815
N	0.5384435917	–2.3528555787	1.505406966
H	2.1116300435	1.2176573733	1.9063703554
C	–0.182391777	–3.3551209097	2.3099261851
H	2.1111338251	2.9822614805	1.923380894
C	1.6938950512	–1.8635889331	2.2796845777
H	–0.6380764196	–0.817527869	–2.6292462772
H	–1.4556656808	0.0686744062	–1.3281691256
H	–1.3052884638	–1.6930358866	–1.2269228392
H	0.8547901997	0.8887537525	–2.2854677537
H	2.2312891797	0.4659155369	–1.2949098862
H	–0.9006772279	2.7853258569	1.5008674833
H	–1.5989489727	2.3758915299	–0.065856492
H	–1.522529767	0.9946483543	1.204677474
H	0.6812898559	–2.7373049522	–2.646225277
H	1.9647817926	–1.5537295342	–2.880853301
C	0.2888455386	4.719667954	–1.3469499778
H	2.7828447091	–3.9067881777	–3.2066946685
H	3.6217260534	–3.1228218075	–1.8709619412
H	2.3231458008	–1.4189058151	–0.4325680869
H	1.2655563796	–5.0754300184	–1.6271328078
H	2.9352270658	–5.4097292246	–1.1793155721
H	–0.0573212354	–3.301590506	–0.2334932838
C	0.5605046741	5.8349638502	–2.1470747047
C	1.7942189443	5.9490684498	–2.7927284915
H	1.5740323866	–4.8533146911	0.8278188399
H	2.8689233907	–3.6851404761	0.5848405022
H	–1.0246525428	–3.7573041304	1.7400759707
H	0.4622957331	–4.1924936817	2.6210941796
H	–0.5790678403	–2.882284283	3.2122088974
H	2.2626253813	–1.1272259379	1.7071198728
H	1.3271263293	–1.3753037397	3.1891503308
H	2.3779904565	–2.6703062735	2.5878446995
C	–2.5316131594	0.0751829695	1.9394660686
C	–3.1183891085	–1.229536514	1.3807609333
C	–3.6449476579	1.1268835835	1.9305393135
C	–2.0545304793	–0.1145340914	3.3836496694

H	–2.3968524148	–2.0595700892	1.3394350361
H	–3.5085389982	–1.091201986	0.3616500726
H	–3.9682038663	–1.6020628411	1.9924584805
H	–4.0140071861	1.3182017697	0.9123184112
H	–3.3015177669	2.0889591853	2.334966707
H	–4.5167982416	0.8120083448	2.537258119
H	–1.6647080449	0.8267950044	3.7986942802
H	–1.251003217	–0.8629005187	3.4852801822
H	–2.8665811747	–0.4500315011	4.0616651304
C	2.7523342885	4.9433158627	–2.630523885
C	2.4708851742	3.8345092502	–1.8273698556
H	–0.6766767399	4.6479619398	–0.8498807756
H	–0.190147348	6.6136043314	–2.2648299533
H	2.0095377136	6.8143247005	–3.4155037882
H	3.7170310562	5.0248403777	–3.1271426488
H	3.2382719326	3.0691051817	–1.7142805989

Tabelle 280 Standardorientierung von R_N-TS-1 *S*si [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	1.4118583211	0.1833649449	–1.2726467989
C	2.6277024461	–0.190968927	0.7999171409
H	–1.1066415394	–0.0912441745	1.2688539099
C	–1.3132040518	0.5602868281	0.0576527776
C	3.4918943249	–1.9334154567	–1.6813489241
N	1.7420756896	–0.8033709331	–0.2045647044
Li	–0.092055734	–1.2627739498	0.6626159017
Si	0.0315861769	1.4707677477	–0.8433088292
C	4.0291649246	–3.2744667035	–2.1996449426
C	2.2966157789	–2.0954112779	–0.7140027417
C	0.7644387066	2.8923023908	0.1852910861
C	2.9105692057	–4.0782440401	–2.8719686993
C	1.1814971553	–2.9642289355	–1.3510775513
C	–0.4127753749	2.1972468582	–2.5500847232
C	1.8384422648	3.6602092009	–0.3089634684
C	1.750212787	–4.2958746437	–1.8911133694
N	0.0166284535	–3.1244365094	–0.4210543974
C	2.3806755995	4.7204008623	0.422039583
C	–1.2441751543	–3.3288072305	–1.155423869
C	1.8531868569	5.0456120852	1.6759393258
C	0.1892864789	–4.2095617522	0.5626421943

H	2.3252043125	0.687064277	–1.6359589084
H	2.1341980979	0.6788384768	1.2398665546
H	1.0150151124	–0.3658174234	–2.1357378104
H	3.5848865667	0.1507838618	0.3720252982
H	2.8373769396	–0.9100720904	1.5985424134
H	–2.0981070475	1.2528341542	0.3916010714
H	–1.8172140953	–0.1368470378	–0.6362966308
H	–0.833832403	1.4260058871	–3.2087374802
H	3.1795935606	–1.3270446535	–2.5414061474
H	4.2916226453	–1.3749285904	–1.1803246188
H	0.4536485517	2.6389128237	–3.061846412
H	4.8540480409	–3.0966354718	–2.9014831461
H	4.447943766	–3.8589976157	–1.3665104111
H	2.6590325262	–2.627052814	0.1778506818
H	2.553750966	–3.5382895263	–3.7618310488
H	3.2857384239	–5.0480507996	–3.2229721451
H	0.7861636933	–2.4111659791	–2.2122487601
H	–1.1680642917	2.9857239098	–2.4433612727
C	0.7842793688	4.3048537979	2.1860103379
H	0.9481468809	–4.8704423798	–2.3714674118
H	2.1190402164	–4.9076040656	–1.0572549609
H	–1.415751325	–2.4941713259	–1.8421519073
H	–1.2543082267	–4.2683598646	–1.7330679387
H	–2.0748046366	–3.3597880966	–0.4435466734
H	1.1442059781	–4.1049734519	1.0849964958
H	–0.6092908395	–4.1474096982	1.3063946792
H	0.1486633388	–5.2095235371	0.1031828793
C	–1.1266661159	–0.8554496144	2.629599354
C	–2.3332085364	–1.7983559748	2.574424542
C	–1.5054980223	0.3665557064	3.4705222672
C	0.0564736205	–1.5512873364	3.3234674419
H	–2.6796598144	–2.1039708663	3.583482465
H	–2.1252708697	–2.732212739	2.0280487769
H	–3.190333951	–1.3219224152	2.0758552201
H	–1.8226545594	0.0837823581	4.4943848734
H	–2.3392102819	0.928749531	3.0241738077
H	–0.6616309978	1.0622401083	3.5810998261
H	0.9289235344	–0.8869933678	3.4096014954
H	0.3931897168	–2.4677635385	2.8118579556
H	–0.1955893517	–1.8668745253	4.3591879774
C	0.2504855298	3.242870684	1.4475075017
H	2.2633772551	3.4329139825	–1.285996614

H	3.210139421	5.2940727441	0.0140526143
H	2.270814732	5.870974285	2.2478762816
H	0.3650951736	4.5509336246	3.159120727
H	–0.5769459193	2.676608203	1.8659178589

Tabelle 281 Standardorientierung von R_N-TS-2 *R*si [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–2.5821292395	0.0875551266	0.4939938645
C	–1.9219139963	2.3857890542	0.0535304536
C	–3.0783046504	–0.8438590798	–2.360479348
C	–3.8240092919	1.9088283166	2.5196518134
N	–3.0579350512	1.4536515405	0.1259783892
Li	–3.9426412409	1.16783553	–1.7443037735
Si	–1.8820008285	–0.9933110403	–0.9522656207
C	–4.9576117163	2.4553663545	3.3980926003
C	–4.1432353929	1.9855527603	1.0085738616
C	–0.1324266553	–0.451545102	–1.4620465284
C	–6.270545083	1.7239611815	3.0984190914
C	–5.5018502535	1.3078754772	0.6928021852
C	–1.71329664	–2.7074336073	–0.1261608567
H	0.5313593309	–0.3129861342	–0.5989923661
C	–6.621785258	1.8497991775	1.6094107136
N	–5.8188497427	1.3776908944	–0.7703888967
H	–0.1409912509	0.4807599933	–2.03854887
C	–6.7084836013	0.2814591234	–1.1926295422
H	0.3202557407	–1.2205018839	–2.1013457672
C	–6.3962650705	2.6659722434	–1.1963565282
H	–1.8773048167	0.133589482	1.34269064
H	–1.2070329709	2.0338804109	–0.6934844118
H	–3.4406119028	–0.4904864608	0.8570102575
H	–1.384803064	2.4784860846	1.0125710725
H	–2.2703997378	3.3783190919	–0.2495095882
H	–3.1879452196	0.3894021482	–2.991819558
H	–2.7324514131	–1.4147348723	–3.2329795307
C	–2.5373580178	–3.7842056243	–0.5028735876
H	–3.6397589425	0.8632628824	2.7979318389
H	–2.8945204183	2.4539926984	2.7238478068
C	–2.4327437046	–5.0380331918	0.1092316585
H	–4.6888485326	2.350546488	4.4570128562

H	–5.0899163734	3.5323877159	3.2140409632
H	–4.2363129492	3.0484032597	0.7425115133
H	–6.1717647622	0.6631341864	3.3729563775
H	–7.0887365712	2.1299957792	3.7068910587
H	–5.3935077878	0.2377196786	0.9100532003
C	–1.4930997998	–5.2454366795	1.1223301203
H	–7.5599958945	1.3228597857	1.3944980099
H	–6.7993868255	2.9106491884	1.3883810129
H	–6.262301546	–0.6827485425	–0.9312231464
H	–7.7095145033	0.343151359	–0.7342471639
H	–6.8304455306	0.3168038423	–2.2796970418
H	–5.7743789608	3.4976091463	–0.8540108691
H	–6.4287490145	2.6965613193	–2.2889926463
H	–7.4205970273	2.8172668238	–0.8215901151
C	–3.3538458837	1.6654113413	–3.8648443548
C	–4.6239690582	1.4564605505	–4.6954667075
C	–2.135388046	1.3599280298	–4.7409270961
C	–3.2571473192	3.1352174459	–3.4215606095
H	–4.6374559289	2.0769247269	–5.6154600156
H	–5.5425873364	1.710851368	–4.1419924125
H	–4.7249096479	0.4093274591	–5.0175647556
H	–2.0879462557	2.0149786508	–5.6335689382
H	–2.1441614447	0.3227804911	–5.1061329682
H	–1.1920262237	1.4998354129	–4.1921086301
H	–2.3398413094	3.3330160536	–2.8472805106
H	–4.108161882	3.4679477718	–2.8043692743
H	–3.2323425503	3.8298761527	–4.2890203977
H	–4.0752898589	–1.2439945123	–2.1081162245
C	–0.6592525654	–4.1935325924	1.5146181123
C	–0.7713302162	–2.9453211063	0.8953490828
H	–3.2684294188	–3.6411457109	–1.296639975
H	–3.0809862213	–5.8524679444	–0.207334387
H	–1.4067306336	–6.2190309424	1.5992982934
H	0.0791289739	–4.3471306212	2.2988056129
H	–0.1034809954	–2.1461679502	1.2147505534

Tabelle 282 Standardorientierung von S_N-Ed-1 [globales Minimum, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	1.4302715915	0.5773601079	–2.401427034
C	0.1117186978	–1.2331679423	–1.5521864175
C	–0.8851730036	–3.9667079937	–0.7589017397
C	–1.3594899046	1.5266031955	–1.7883040055
N	0.6621775669	0.0950266897	–1.2469315632
Li	2.1443919353	0.0605287488	0.1420892517
C	–3.3726357133	–1.4331836969	–0.5993353432
Si	–0.6626659157	–2.212120892	–0.1109343748
C	–2.4065576456	2.450655462	–1.1643764521
C	–0.3372449268	1.0593696006	–0.742535783
C	–4.6191492202	–0.8929509721	–0.291174781
C	–2.352559054	–1.5101119938	0.3601625379
C	–1.7285040839	3.6651044994	–0.5308562199
C	0.3428040957	2.2773313022	–0.0885531182
C	0.4977805159	–2.1875231903	1.3689547805
C	–4.8713181157	–0.4171123229	0.9948121567
C	–0.7128561792	3.2115636119	0.5192427972
N	1.3974797195	1.8490643612	0.8581404236
C	–2.630576178	–1.0319196855	1.6477871579
C	2.4991587242	2.810066176	0.9355813748
C	–3.8753115651	–0.4893658748	1.9660826546
C	0.9066136259	1.5605284202	2.2080609421
H	0.8232752315	0.6239252858	–3.3149627051
H	2.2633217383	–0.1069605711	–2.5690423406
H	1.8490417836	1.5649460079	–2.2037805966
H	0.9555239847	–1.8546159409	–1.875543871
H	–0.5835054791	–1.2014065373	–2.4081793792
H	–1.5162331932	–3.9837747538	–1.6512352419
H	0.0808082205	–4.4078844626	–1.0176423266
H	–1.3581993093	–4.5979639178	–0.0033076712
H	–0.8401814879	2.0667734285	–2.5884993688
H	–1.8456118707	0.6591990723	–2.2416568181
H	1.510355288	–2.4563846746	1.0555876281
H	–3.1950029136	–1.8010399612	–1.606199606
H	–3.1263206371	2.7658015414	–1.9241424421
H	–2.966467177	1.8990395828	–0.3994796419
H	–0.8891679633	0.5369647199	0.0460449235
H	–5.3919196242	–0.8443469957	–1.0491977238
H	–1.221851588	4.2475850311	–1.3093914244
H	–2.4693256907	4.3229907101	–0.0698243199
H	0.8566472747	2.8400576676	–0.875249655

H	0.1741056198	–2.9077481225	2.1255670215
H	0.5568796053	–1.2100795628	1.8528211156
H	–5.8397237474	0.0026435571	1.2387107122
H	–0.2200746516	4.0745445164	0.9770588892
H	–1.2542244086	2.6862256376	1.3131209051
H	–1.8683301913	–1.086079313	2.4189106592
H	2.9436363555	2.9434472811	–0.0514649542
H	2.1731944775	3.7869227774	1.3212291738
H	3.2694101598	2.4114798715	1.5971968248
H	–4.0683853148	–0.1289329849	2.9695209655
H	0.016082145	0.9322877075	2.1621320601
H	1.6835207897	1.0227458139	2.7562349647
H	0.6571492272	2.4733978517	2.7651054817
C	3.9994517397	–0.8356881619	0.1767505239
C	5.0186261317	0.1288269153	–0.4313387966
C	4.0785533815	–2.1319880082	–0.6272542102
C	4.467430154	–1.1497241288	1.5968832435
H	5.084783988	1.0723075917	0.1265054601
H	4.784777113	0.3832721385	–1.4743493873
H	6.0440829214	–0.3033571527	–0.437246828
H	3.8109700941	–1.9865156404	–1.6831566614
H	3.4192360596	–2.9163645481	–0.2308802076
H	5.1058841501	–2.5595929138	–0.6221939773
H	3.8151008252	–1.8742298385	2.1022782
H	4.5057292829	–0.2521499454	2.229431111
H	5.4913565124	–1.5854529885	1.6090769117

Tabelle 283 Standardorientierung von S_N-Ed-2 [globales Minimum, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	–1.1853265088	0.1292822646	–2.3895080526
C	0.6913581827	–0.5552138486	–1.0718672939
C	1.4109559661	–2.7133726122	1.1256553722
C	–1.6046059594	–2.6265915407	–1.1162897872
N	–0.7441704154	–0.2415773554	–1.0392645639
Li	–1.2367682582	1.4901782335	–0.0989301823
C	4.3614058068	–1.5962004155	0.1195855829
Si	1.5906216778	–0.9141402065	0.5754486437
C	–2.4377172539	–3.6564087862	–0.3497867786
C	–1.5769480342	–1.2734517982	–0.3916502399

C	5.6955383255	–1.3128382947	–0.1714201966
C	3.4026319855	–0.5779618601	0.1889060728
C	–3.8613951077	–3.1448023024	–0.1322223108
C	–3.0153691029	–0.7662120331	–0.1653533591
C	1.0023598844	0.2726424466	1.9188948406
C	6.0928435151	0.0025437283	–0.3971409776
C	–3.8326946337	–1.8079359985	0.6106736905
N	–3.0081400405	0.5862029396	0.4302629227
C	3.8234972851	0.7409744189	–0.042297187
C	–4.1742035174	1.3798730561	0.042135416
C	5.1541454301	1.0314396959	–0.3321429785
C	–2.87558283	0.5978989179	1.8904482037
H	–1.0568630153	–0.6856103877	–3.1135029009
H	–0.5865872566	0.9790240414	–2.7212382179
H	–2.2302072539	0.4427130176	–2.3885900165
H	1.1955566902	0.3374346211	–1.4591813098
H	0.9176286877	–1.3606776064	–1.7904655823
H	2.0694106155	–2.9138032756	1.975189851
H	0.3897699193	–2.9439695923	1.4384238298
H	1.6777729438	–3.4050917543	0.3221303825
H	–2.0353400191	–2.4948600664	–2.1151196444
H	–0.5835172232	–2.9930710981	–1.2483693618
H	0.719470225	1.2478984318	1.5069017357
H	4.0719069059	–2.6266734157	0.2961355515
H	–2.4484598626	–4.6047539613	–0.8923283046
H	–1.9713229246	–3.851425269	0.6235361495
H	–1.1319349305	–1.433755892	0.5988959078
H	6.4215123383	–2.1157485874	–0.2196661263
H	–4.3540904963	–3.0163348495	–1.1029762874
H	–4.4491751456	–3.8733487501	0.431278421
H	–3.4890396063	–0.6615348979	–1.1470863402
H	1.8073527125	0.4370218728	2.6396712274
H	0.1482985636	–0.1292188129	2.4689408446
H	7.128870836	0.2264361926	–0.6212249864
H	–4.8480323901	–1.4328219761	0.7686105508
H	–3.3890853395	–1.9663920769	1.5993748097
H	3.1071047278	1.5562968534	0.0070994526
H	–4.2271704383	1.4545180398	–1.0449903154
H	–5.1146066957	0.9528870637	0.4190197941
H	–4.062727579	2.3875338342	0.4446626806
H	5.4574734104	2.0569689556	–0.5047830015
H	–2.0639781901	–0.0586316525	2.2027202725

H	–2.6343151992	1.6130546591	2.2119927715
H	–3.7972049494	0.2775745349	2.3942059823
C	–0.6170419137	3.4504025378	–0.0654124941
C	–1.3331135226	4.1224477748	–1.2390991207
C	0.8777479192	3.7012421967	–0.2489800382
C	–1.047999127	4.1813976708	1.2048622455
H	–2.4262859966	4.0336528934	–1.1703366112
H	–1.0330430412	3.7011613565	–2.2080111523
H	–1.1111249524	5.2114689909	–1.2893544179
H	1.2710749581	3.234047658	–1.1624202478
H	1.4690129751	3.3229510583	0.5956961314
H	1.1078487511	4.786967497	–0.3261339279
H	–0.550150444	3.7881324733	2.1010913524
H	–2.131435899	4.1142955248	1.3775589373
H	–0.8077431646	5.2667325226	1.1595056869

Tabelle 284 Standardorientierung von S_N-Ed-3 [globales Minimum, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.0150079014	–2.3236728549	0.1031526496
C	–0.1231053056	0.0647252904	0.4138381512
C	2.51095927	–0.6569532649	2.0504230163
C	–2.7449284598	–1.4350421199	–0.4952135893
N	–0.2343230438	–1.0322599889	–0.5640989422
Li	1.2622886696	–1.4895172306	–1.9476833241
Si	1.633562088	0.5954955114	0.9558525106
C	–4.0352992445	–1.1783357692	–1.2770094314
C	–1.52018623	–0.9752839745	–1.2983704954
C	2.6274349755	1.0161244563	–0.585081492
C	–3.9891989065	–1.887259672	–2.630341728
C	–1.4644738791	–1.7354252004	–2.6347074163
C	1.3029637309	2.1639682368	1.9557575976
H	2.0703793259	1.6870374115	–1.2461711989
C	–2.7536471496	–1.4558782661	–3.424526311
N	–0.212779935	–1.4559004419	–3.3639721185
H	2.8850799001	0.1099538056	–1.1435442545
C	0.0026860493	–2.3807605814	–4.4772322311
H	3.5608119898	1.5157064432	–0.3126083443
C	–0.0801978811	–0.0765149244	–3.8378274698

H	–0.6847373801	–2.4635460845	0.9618846375
H	1.016756246	–2.3794770987	0.450672899
H	–0.1653144602	–3.1455638229	–0.6003793871
H	–0.7417193057	–0.1269271695	1.3057790091
H	–0.5300045927	0.9722230258	–0.0471574194
H	3.355251645	–0.1819334712	2.5577557084
H	1.8430336107	–1.0677106411	2.8124158712
H	2.9089393018	–1.4813604079	1.4572567846
H	–2.6663731373	–2.5070729059	–0.2844389495
H	–2.77130145	–0.9144880804	0.4658977432
C	1.3755741697	2.1788818782	3.3547887903
H	–4.897713214	–1.5163874162	–0.697280083
H	–4.1584212078	–0.1004275958	–1.4348747057
H	–1.6733970307	0.0823746986	–1.5369678788
H	–3.9562927916	–2.9711984251	–2.469728755
H	–4.8944690033	–1.6771699664	–3.2049656657
H	–1.4378739895	–2.8103278474	–2.4162749486
C	1.0965778921	3.3349622374	4.0829217191
C	0.7366955896	4.5052549548	3.4194367048
H	–2.7237206768	–1.9770252844	–4.3844071649
H	–2.8246742805	–0.3833888315	–3.638148907
H	–0.1221262665	–3.4065392705	–4.1298264622
H	–0.684674592	–2.1979265991	–5.3137843789
H	1.0258869296	–2.2678867722	–4.8366733841
H	–0.2050416315	0.6263096629	–3.0124759199
H	0.9258359932	0.0535223691	–4.2432969405
H	–0.8014878438	0.1709831995	–4.6277070914
C	3.1009998565	–2.4562810402	–2.0691589251
C	2.7624200915	–3.8999207739	–2.4498362984
C	4.0497026176	–2.5377099446	–0.8772543622
C	3.8930165415	–1.8560444518	–3.2320507346
H	2.1522350819	–3.9662509803	–3.3591943695
H	2.2188047728	–4.4237348591	–1.6515651789
H	3.6786523346	–4.4982211731	–2.6486665142
H	3.5919335719	–3.0485296599	–0.0194037192
H	4.3888485883	–1.5522996152	–0.5322724795
H	4.9670453365	–3.1144230986	–1.1262207977
H	4.2334290729	–0.8339031007	–3.0211500565
H	3.3109614691	–1.8175974267	–4.1637573078
H	4.8051602089	–2.4500030312	–3.4606090477
C	0.6589708416	4.5148943927	2.0278341464
C	0.9395758333	3.3549746414	1.309595658

H	1.6581062924	1.2784886151	3.8898147493
H	1.1624792929	3.3224100697	5.1644153865
H	0.5221766578	5.405675124	3.9822223422
H	0.385427338	5.4239194164	1.5054490035
H	0.8825276139	3.3851956941	0.2252511013

Tabelle 285 Standardorientierung von R_N-Ed-1 [globales Minimum, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.0331025302	–0.7911640195	–1.3322059443
C	–0.1441297101	1.6385978873	–1.2777690682
C	–1.8893648583	–3.1091376395	–1.7698452506
C	2.6009140338	0.3327856057	–2.14787872
N	0.4934702112	0.4427044701	–0.6953502283
Li	0.1494484593	0.6416734044	1.3744459215
Si	–1.8162047544	–1.4034327745	–0.942273723
C	4.1315038535	0.4487292154	–2.1549891608
C	1.9914019734	0.5471946259	–0.74298043
C	–2.0564962447	–1.5939525981	0.9205805354
C	4.7485113966	–0.5431464852	–1.1624156755
C	2.6514308347	–0.3920271231	0.3009568028
C	–3.1507126755	–0.3021992564	–1.7070611606
H	–3.0481584998	–2.0068389108	1.1449350578
C	4.1930606735	–0.2988744746	0.2468924869
N	2.0733816725	–0.1703127013	1.6605522338
H	–1.9642010875	–0.6497572375	1.4726579695
C	2.0673429641	–1.3951761372	2.4728938827
H	–1.3169113054	–2.2961549638	1.3281707163
C	2.7010211989	0.9263172249	2.4215183079
H	0.0586533816	–0.7315625366	–2.4326548071
H	–1.2214279099	1.6019239162	–1.1050625897
H	0.6045974771	–1.6318970735	–1.0298538604
H	0.02158195	1.7211347912	–2.3648686443
H	0.2440686761	2.5384594308	–0.7908856517
H	–2.8764412786	–3.5646511004	–1.6236548414
H	–1.7125627079	–3.0543736138	–2.8513143443
C	–3.2877167685	–0.2130551082	–3.1074657937
H	2.3317803769	–0.6670087068	–2.5129988857
H	2.1632637496	1.0514743119	–2.8512964474
C	–4.2746560397	0.5815859071	–3.6952658062

H	4.5110544054	0.2689628006	–3.1690019131
H	4.4327940482	1.4718630276	–1.8846993049
H	2.2135304883	1.5804360714	–0.4396649848
H	4.5239868019	–1.5715549518	–1.48326613
H	5.8420401376	–0.4506263825	–1.1507005143
H	2.3811062022	–1.4215548021	0.0325608302
C	–5.1570320606	1.3083873778	–2.8896007523
H	4.626498556	–1.012969958	0.9589200361
H	4.5125432459	0.700109621	0.5709837717
H	1.5263413011	–2.1896314194	1.948246222
H	3.0825826272	–1.7598802797	2.7076143458
H	1.5513391456	–1.1970740518	3.4176030386
H	2.7384831746	1.8385764268	1.8197298907
H	2.0883542986	1.1374233711	3.3013583876
H	3.7220402828	0.6825372752	2.7559317217
C	–0.9539936903	1.8971168784	2.6485373832
C	–0.9003706542	1.4138335689	4.1055589038
C	–2.4324529331	2.1018931031	2.2916785665
C	–0.2872009409	3.281886863	2.5918893426
H	–1.3958265317	2.125027156	4.8103449241
H	0.1308045841	1.2936457872	4.4785198851
H	–1.4045791918	0.4439787446	4.2428785364
H	–2.931066527	2.840088184	2.965657014
H	–3.0197121488	1.1732818057	2.3770999038
H	–2.5711255033	2.480922797	1.2668340177
H	–0.3294321035	3.7277999008	1.5842408555
H	0.7736610459	3.2605962085	2.8904321122
H	–0.7794431513	4.0181609397	3.2729464358
H	–1.1424044548	–3.7927272562	–1.3456540484
C	–5.0435013067	1.2341235259	–1.4995019425
C	–4.0514594082	0.4376948539	–0.9180898473
H	–2.6179749727	–0.7743537216	–3.7575530909
H	–4.3577287639	0.6316925755	–4.7785476489
H	–5.9274676782	1.9270630593	–3.3434016125
H	–5.7225804933	1.7978230258	–0.8645689352
H	–3.9781543431	0.4069895443	0.1657717184

Tabelle 286 Standardorientierung von R_N-Ed-2 [globales Minimum, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	0.3635972283	0.9801858414	–0.4440069238
C	0.8071658809	3.3716588467	–0.1825918093
C	2.996975106	0.9088002114	–2.3550823812
C	2.9931406985	1.3941044843	1.0449693772
N	0.616783833	2.0929303282	0.49520098
Li	–1.2190172795	1.9331142418	1.3472056038
Si	1.1152408882	0.8670275312	–2.2166842208
C	3.9882676684	1.2615815672	2.2004961734
C	1.6111717635	1.8326915059	1.5458923297
C	0.4950453012	–0.8126033997	–2.8143577859
C	3.4671302259	0.2840731	3.2538614318
C	1.0921095912	0.8173262323	2.5845834571
C	0.3770039296	2.2165156428	–3.3008601062
H	–0.5942748523	–0.8766899218	–2.7511448795
C	2.0867117272	0.7198773394	3.7510557232
N	–0.2995516655	1.1097579767	2.9701933978
H	0.9169677903	–1.6280671462	–2.2205362822
C	–0.9894048843	–0.0457238226	3.5407152557
H	0.776960991	–0.9706050577	–3.8579167551
C	–0.4501944459	2.2670186707	3.8568666895
H	0.5805598893	0.0322096589	0.0567163774
H	–0.0495740121	3.5648204951	–0.8294584549
H	–0.7200886301	0.9552664442	–0.6521509704
H	1.7170885325	3.4028625107	–0.7989581162
H	0.8572313571	4.1691193883	0.5612074611
H	3.453486256	0.1191865865	–1.7545865741
H	3.2745719538	0.7331963374	–3.3984630781
C	1.1751270991	3.1332431575	–3.9967483078
H	2.9029258154	0.4282889748	0.5357367579
H	3.3599695117	2.1129698892	0.3090055729
C	0.6061527918	4.1349433802	–4.7819247546
H	4.9603626636	0.9358903235	1.8221204938
H	4.1382695773	2.2439997227	2.6633959451
H	1.74165553	2.7927040682	2.0602271979
H	3.397262255	–0.7188147148	2.8162166252
H	4.1641726278	0.2183196349	4.0927321289
H	1.060576014	–0.1677871332	2.1037397429
C	–0.7795210461	4.2390348886	–4.8790872167
H	1.7125661434	0.0176962615	4.5011390058
H	2.1774244342	1.6970647434	4.2380696053
H	–0.9077904156	–0.8944070689	2.8599453732

H	–0.5885001965	–0.3357333878	4.5219227278
H	–2.0462607501	0.1995570499	3.6557329894
H	0.0701483217	3.1329083549	3.4438364468
H	–1.5109100704	2.5160835828	3.924194459
H	–0.0683835421	2.0724323101	4.8677757452
C	–3.1066043444	2.6818835006	1.0204972253
C	–4.1636433881	1.9760034756	1.8674581773
C	–3.5565787152	2.5982585863	–0.4367480748
C	–3.1227872945	4.1597001066	1.4113659458
H	–5.1723043833	2.4243708996	1.7261111145
H	–3.9483650465	2.0399932342	2.9435214278
H	–4.2559334963	0.9116608462	1.6163136191
H	–4.5691748504	3.037206699	–0.5816776552
H	–3.6126316705	1.5617751193	–0.7970255858
H	–2.88147268	3.1449340052	–1.1079912161
H	–2.4237386701	4.7560428164	0.8104314808
H	–2.8612209431	4.3169083205	2.4668003551
H	–4.1288994175	4.6134762856	1.2687730791
H	3.4303767252	1.8622923864	–2.047513819
C	–1.5922110715	3.3367595597	–4.1949926292
C	–1.0155115563	2.3343123649	–3.4191520731
H	2.2561617461	3.0719816018	–3.9268025724
H	1.2421217835	4.8335871088	–5.3124290504
H	–1.2245916099	5.0206487098	–5.4827220378
H	–2.6707278239	3.4165297189	–4.2574417548
H	–1.6690149001	1.6477450241	–2.8897724141

Tabelle 287 Standardorientierung von R_N-Ed-3 [globales Minimum, M052X /6-31+G(d)].

Atomsymbol	x	y	z
C	0.8135349897	0.6269575764	–0.7819163412
C	0.781504464	3.0555224495	–0.8957485882
C	–2.1498164854	–0.3541544249	–0.9897529674
C	2.9688907071	1.7097895019	0.9547630106
N	0.606979046	1.8846440943	–0.0175444351
Li	–1.3096969343	2.1097195388	0.7946009136
Si	–0.5622835592	–0.028028302	–1.9620833036
C	3.8184431554	1.8429155815	2.2262361966
C	1.4705202034	1.9943732109	1.2059860372

C	–0.9167471257	1.1061527505	–3.4331449154
C	3.2872027145	0.9157718176	3.3252376015
C	0.9216466635	1.1175277474	2.3619678855
C	0.1641939582	–1.6626067833	–2.596795267
H	–0.0010808662	1.4510394553	–3.9289539751
C	1.8135963047	1.2283626863	3.6190812074
N	–0.523878944	1.4012914465	2.6092289197
H	–1.4943286612	1.9874668016	–3.1322926218
C	–1.2438790299	0.2320981156	3.1339089907
H	–1.5117581296	0.5659592015	–4.1805161478
C	–0.7827339378	2.5695204288	3.4719804393
H	1.7567466689	0.6713472488	–1.3567317882
H	0.0432635254	3.0261106728	–1.6989208481
H	0.9497980589	–0.1951876747	–0.0682864952
H	1.7850199308	3.0976928254	–1.3525505731
H	0.6137121056	3.974890565	–0.3268640113
H	–2.6019228488	0.5846265705	–0.6415209706
H	–2.8958072493	–0.8497138887	–1.6240422145
C	–0.244021802	–2.9078688039	–2.0818875267
H	3.0865766079	0.6894866377	0.5671331861
H	3.3442268372	2.385307647	0.1765509501
C	0.3089029913	–4.1072069469	–2.5422060048
H	4.8662593582	1.6108031016	1.9966810656
H	3.7991884706	2.8832171914	2.5845094897
H	1.3816177288	3.0432263407	1.5225808804
H	3.3935974513	–0.1316125788	3.0051467633
H	3.878720979	1.0241192809	4.2432942343
H	0.9597819901	0.0722159852	2.0281724746
C	1.2922544336	–4.0882172593	–3.5344400397
H	1.429059392	0.5596073316	4.3996135986
H	1.7545198317	2.2478032494	4.0224280829
H	–1.1187134005	–0.6186975143	2.4563832128
H	–0.9008118145	–0.0672928881	4.1391798161
H	–2.3113789801	0.4660765287	3.1952893833
H	–0.2295044887	3.4427843399	3.1149452549
H	–1.8475597898	2.8122956795	3.4226965925
H	–0.5139379246	2.389564271	4.5252678904
C	–2.9519053596	3.3492720548	0.4009199541
C	–4.1897056913	2.9329415159	1.2090703973
C	–3.3780158507	3.4619135436	–1.0689463718
C	–2.5526287231	4.7617226419	0.8606054946
H	–5.0366792608	3.6521834451	1.0937091337

H	–3.9903024069	2.8753766467	2.2926677503
H	–4.5790547069	1.9487073906	0.9035150062
H	–4.2087658875	4.193868912	–1.2150844755
H	–3.7403482391	2.5068945405	–1.481440098
H	–2.5561107919	3.8041551473	–1.7194361633
H	–1.6984117451	5.1644252898	0.2909972411
H	–2.2765001345	4.8032202849	1.9271045846
H	–3.3809008246	5.500461619	0.7325073096
H	–1.9849609293	–0.9961884349	–0.115006896
C	1.7153062383	–2.8652872045	–4.0634073162
C	1.1556637607	–1.6721741738	–3.5983222672
H	–1.013646976	–2.9505919651	–1.314029275
H	–0.0308748411	–5.0543005951	–2.1294039407
H	1.722306195	–5.0188368261	–3.896694282
H	2.4765947151	–2.8412273273	–4.8396981536
H	1.4962448627	–0.7341373118	–4.0337926752

Tabelle 288 Standardorientierung von S_N-TS-1 *S*si [globales Minimum, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	0.4720760012	–2.6475124387	2.0427645518
C	0.616501261	–0.2421684122	2.047940934
C	1.751331188	2.5401104179	2.0218913506
C	–2.2540893224	–1.5212108951	2.1621943949
N	0.1266710595	–1.4257690445	1.3106318168
Li	0.9771902439	–1.3225825094	–0.524320313
C	–1.8261638133	2.1926691849	2.3042790663
Si	0.6301821496	1.3894349838	1.0268284559
C	–3.7151034744	–1.3258871612	1.7594241775
C	–1.3106587816	–1.3277547538	0.966329115
C	–3.1354201112	2.6649521524	2.3689696146
C	–1.138141799	2.0977109407	1.0848767211
C	–4.0860336104	–2.3231500285	0.6634198344
C	–1.6889059404	–2.288078332	–0.1752737699
C	1.2703185536	1.0175366334	–0.6664462191
C	–3.7922470896	3.0542501966	1.2019939952
C	–3.1714295405	–2.1235878028	–0.5457077406
N	–0.764042345	–2.1363241299	–1.3315702395
C	–1.8144377213	2.5082133923	–0.0712642468
C	–0.6092845167	–3.4020258418	–2.0513529679
C	–3.1269825804	2.9796015576	–0.0195525411

C	–1.1727652998	–1.0925241703	–2.2813409847
H	0.0861682532	–2.6406309405	3.069910799
H	1.5588156266	–2.7283209837	2.0899223072
H	0.090630669	–3.5304618905	1.5266515104
H	1.6736028582	–0.4275706893	2.2691353265
H	0.1154933423	–0.1416118912	3.0237185521
H	1.4219299141	2.6198790439	3.0617948588
H	2.7799608738	2.169381282	2.0172016026
H	1.7480806471	3.5432986931	1.5895247158
H	–2.1357238263	–2.5345170773	2.5628855385
H	–1.9832337532	–0.8212761654	2.9559055576
H	2.0758928967	–0.1111245601	–0.7978904052
H	–1.3322249655	1.893481722	3.2247495568
H	–4.3625489849	–1.4513651236	2.630991439
H	–3.858460437	–0.3022975969	1.3936432762
H	–1.4633675092	–0.3099786402	0.5927297717
H	–3.6428737132	2.7298594887	3.3246860314
H	–3.9813572717	–3.3447087846	1.0478290812
H	–5.1286847108	–2.1987316782	0.3611973688
H	–1.5523021779	–3.3137440986	0.184066928
H	2.0107733382	1.7727067068	–0.9502914931
H	0.5071351898	1.0221960339	–1.4511457586
H	–4.8112198271	3.4199808689	1.2469365406
H	–3.4301106448	–2.8229223693	–1.3464455542
H	–3.3397257068	–1.1124365709	–0.9293854446
H	–1.3026693495	2.4660143108	–1.0277267377
H	–0.1744991359	–4.1538773949	–1.3914097648
H	–1.5671336252	–3.7752655687	–2.4397781594
H	0.0671052801	–3.2556088577	–2.8942275167
H	–3.6265824712	3.2925249829	–0.9291867341
H	–1.4099459899	–0.1692366937	–1.7527256179
H	–0.3410254716	–0.8916930953	–2.9597755194
H	–2.0436464596	–1.3923241707	–2.8780860129
C	3.0927429518	–1.2294024334	–0.9577843328
C	2.902089448	–2.7385908883	–1.1423257473
C	3.9555353331	–0.9768048705	0.2708653539
C	3.7906356562	–0.6724096178	–2.1908946718
H	2.3453357331	–2.9737371587	–2.0579167931
H	2.3744327074	–3.2145042779	–0.3008928791
H	3.8705486036	–3.2654834091	–1.2256351614
H	3.5440166059	–1.4578326732	1.1673549037
H	4.0337329456	0.0977480808	0.4833926554

H	4.9836994121	–1.3589036325	0.1471340351
H	3.9480337744	0.4086956641	–2.1024634808
H	3.1994937391	–0.8408389658	–3.0993003429
H	4.7801857209	–1.1340580487	–2.352354588

Tabelle 289 Standardorientierung von S_N-TS-2 *R*si [globales Minimum, M052X /6-31+G(d)].

Atomsymbol	x	y	z
C	–0.5924576921	–3.0823059363	–1.266912391
C	–0.6521093133	–0.6710685864	–1.2011938258
C	1.348605736	1.7499840306	–1.3426674749
C	1.4133555542	–2.1374866134	–3.1372534955
N	0.1731333262	–1.8720595309	–0.9502792647
Li	0.6864831884	–1.7611568025	1.0105761648
C	–1.777206264	2.814990869	–1.6508056846
Si	–0.0474063999	0.9391739332	–0.3283869628
C	2.7772302596	–2.0016641814	–3.813503388
C	1.4828686613	–1.8113321798	–1.6369729831
C	–2.8994244343	3.6294348874	–1.7930761797
C	–1.555973234	2.0718254569	–0.4824147246
C	3.7842808876	–2.9298184694	–3.1368646197
C	2.5256864167	–2.7093638901	–0.9440922515
C	0.3996588578	0.5207691358	1.4199835032
C	–3.8303269285	3.7151641199	–0.7600907428
C	3.8857862234	–2.5896257233	–1.6499377042
N	2.5828358328	–2.4486060367	0.5176862683
C	–2.5055525771	2.1746503668	0.5432184669
C	3.0266092112	–3.6379288971	1.249279169
C	–3.631693347	2.9851779463	0.4100416849
C	3.4439410529	–1.3162599496	0.8822120875
H	–0.991815025	–3.0652864704	–2.2886750831
H	–1.4325098188	–3.1531796201	–0.5756205105
H	0.0242042006	–3.9746147096	–1.1414275206
H	–1.6290511391	–0.8590048618	–0.742762623
H	–0.8446807137	–0.5259774146	–2.2761808711
H	1.3657449291	2.8232711396	–1.1353712736
H	2.3324040523	1.3553156065	–1.0742317853
H	1.2147205582	1.6145200369	–2.4207916616
H	1.067196405	–3.168436489	–3.2691665171
H	0.6784612378	–1.4867614549	–3.6178364904

H	–0.0595025208	–0.668227263	1.9847903672
H	–1.0599563073	2.7662078938	–2.4645808308
H	2.6912283361	–2.2352757418	–4.8774685551
H	3.128148782	–0.9655767971	–3.7383875478
H	1.8251506434	–0.7760867743	–1.5404834486
H	–3.0454263513	4.1973658142	–2.7045068391
H	3.4600792014	–3.9699576874	–3.2597352314
H	4.7678871533	–2.8424754226	–3.6048105484
H	2.1894436556	–3.7476434242	–1.045270556
H	–0.1094503032	1.205112265	2.1070409659
H	1.4712924031	0.6501242909	1.6098769276
H	–4.7029474939	4.3487669508	–0.8649748554
H	4.6180242847	–3.2359968155	–1.1576940344
H	4.2517774477	–1.561291769	–1.5614756038
H	–2.364589608	1.6180193892	1.463385604
H	2.3290496351	–4.4588810277	1.0801148022
H	4.0354338483	–3.9553727311	0.9524329581
H	3.0397334476	–3.4158392483	2.3168152418
H	–4.3503010622	3.0492665205	1.2186889233
H	3.1884570053	–0.4370276093	0.2908646579
H	3.2759670035	–1.0739874807	1.9328305695
H	4.5087438649	–1.5423416631	0.7441271932
C	–0.6618173395	–1.865485097	2.7040865274
C	–0.3106548252	–3.3561029534	2.6444121067
C	–2.1300878247	–1.6855545415	2.3429071947
C	–0.4274130452	–1.3708832248	4.1250735174
H	0.7126962803	–3.551282712	2.9860587726
H	–0.4129871286	–3.7865545074	1.6362931898
H	–0.9739801883	–3.9550282053	3.2957262509
H	–2.3654946354	–2.0903413592	1.3505031129
H	–2.4079154743	–0.6247143152	2.332271972
H	–2.8003636472	–2.1890387042	3.0612322606
H	–0.667503232	–0.3054542343	4.2192623087
H	0.6194172804	–1.4950240313	4.4276896835
H	–1.0479389899	–1.9115574952	4.8605216272

Tabelle 290 Standardorientierung von R_N-TS-1 *S*si [globales Minimum, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	1.1417883512	–0.7514397893	0.441552583

C	1.0916510413	1.6545458988	0.3411046145
H	–2.188695627	0.269382733	0.2978566006
C	–1.8354510652	–1.0227265414	–0.0476092625
C	3.0393040913	0.3459117449	2.4184677318
N	0.8331488654	0.4868312072	1.1892374857
Li	–1.1655506816	0.3950794116	1.6062405067
Si	–0.1895156143	–1.2668552218	–0.8471579647
C	3.7139868051	0.4656819085	3.7849984982
C	1.5246000189	0.5893446362	2.4948643018
C	–0.0163744276	–0.2049848487	–2.3999179997
C	3.0823409286	–0.5206005835	4.7654091398
C	0.8758342619	–0.3486988044	3.5281619656
C	0.3224655779	–3.0327365509	–1.3131166639
C	1.1682794967	–0.2082078966	–3.1506160105
C	1.5846515962	–0.2376644556	4.886950402
N	–0.5956696293	–0.1395477062	3.5923408085
C	1.3120616189	0.5927198411	–4.2813374021
C	–1.2893785453	–1.3712329101	3.9813860466
C	0.2625977642	1.4170023595	–4.6864981358
C	–0.9833951164	0.9371472174	4.5122580143
H	2.1390809102	–0.6927569749	–0.0225015215
H	0.4139337357	1.6386054863	–0.512478879
H	1.1788335807	–1.5889513979	1.1459374349
H	2.1204118692	1.66861107	–0.0450100556
H	0.9093498267	2.5678413342	0.9092750047
H	–2.6590372231	–1.26568622	–0.7271225302
H	–1.9469371839	–1.696835614	0.8166929062
H	0.2422196273	–3.6989843323	–0.4495204321
H	3.2199466471	–0.6615366579	2.0305943423
H	3.4839097191	1.0469929467	1.707376544
H	1.3515461131	–3.0778462484	–1.6828083477
H	4.7866392916	0.2812450457	3.6876786519
H	3.5972726995	1.4851761051	4.171388853
H	1.3616940692	1.6193605803	2.8389666381
H	3.2422365352	–1.5442944211	4.4073863074
H	3.5539800904	–0.4466065158	5.7482600721
H	1.0141146955	–1.3759957635	3.1753141308
H	–0.3319678135	–3.420250014	–2.0974361939
C	–0.9248166506	1.4316777595	–3.9584554525
H	1.1198072731	–0.9223829061	5.6021901566
H	1.4636943497	0.7749622839	5.2847945085
H	–1.0675183613	–2.1624713742	3.2638762575

H	–1.0037748205	–1.7107009904	4.9868305248
H	–2.3658389908	–1.1939157922	3.9732448453
H	–0.4134784366	1.8418793849	4.2997655099
H	–2.039912474	1.1643546415	4.3712295679
H	–0.82837566	0.6590933865	5.5623065282
C	–2.84488304	1.5484399692	0.8580751769
C	–3.8459501329	0.9553746145	1.845978166
C	–3.6012917469	1.9678331906	–0.3939653267
C	–2.1885438759	2.7929889136	1.4597892657
H	–4.6273084842	1.6788956849	2.1386066469
H	–3.3744809803	0.6126776914	2.7782241281
H	–4.3508705028	0.0849196408	1.4110337488
H	–4.4228958767	2.6688656496	–0.1614921089
H	–4.0513402878	1.1039096561	–0.8996076333
H	–2.9435590886	2.469565803	–1.1119496606
H	–1.5285318514	3.2829054432	0.7367519116
H	–1.5863024791	2.5858739952	2.3572531153
H	–2.9395825094	3.5445587018	1.7696684687
C	–1.0586255236	0.627089382	–2.8271927521
H	1.9957714777	–0.8455754926	–2.8515076411
H	2.2368500358	0.5746623138	–4.8461066776
H	0.3703008699	2.0415423391	–5.5654937781
H	–1.7452400306	2.0686034772	–4.2681195729
H	–1.983209103	0.6536325746	–2.2624961083

Tabelle 291 Standardorientierung von R_N-TS-2 *R*si [globales Minimum, M052X /6-31+G(d)].

Atomsymbol	x	y	z
C	0.9400818732	0.7613961207	–0.7672560924
C	0.9034731656	3.1673062903	–0.8290600572
C	–2.0411324206	0.2759727716	–0.7817231549
C	3.0354247623	1.8098477304	1.0242708517
N	0.717674606	1.9924243751	0.0243253959
Li	–1.221865036	1.828978855	0.6654510619
Si	–0.5479834256	0.2201741589	–1.8611462967
C	3.8465038292	1.9315596222	2.3143548529
C	1.5399992327	2.0766909499	1.2540560926
C	–0.7516212519	1.3174348596	–3.3916914595
C	3.3052662729	0.9623036402	3.3631020174
C	0.9883074771	1.1458417359	2.3493891312

C	0.0149250896	–1.4842770891	–2.477045382
H	0.2080892555	1.560195574	–3.8564952677
C	1.8296657791	1.2610560455	3.6299562474
N	–0.46655999	1.36524305	2.5595957578
H	–1.2667438555	2.2489731871	–3.1473759039
C	–1.1236808633	0.1587798141	3.0724748071
H	–1.3576265057	0.7902831864	–4.1333541397
C	–0.7596215333	2.486560923	3.4600212726
H	1.8711473605	0.8297332416	–1.3513987945
H	0.166379364	3.1476566665	–1.6309668873
H	1.07076691	–0.0822930057	–0.0821601308
H	1.9027843326	3.1971452041	–1.2853634128
H	0.7503845619	4.0765329106	–0.2462075802
H	–2.4109287	1.5662981231	–0.4366578751
H	–2.9473139845	–0.0158429734	–1.321804732
C	–0.6339917054	–2.6567487861	–2.070227191
H	3.1630828011	0.7971833694	0.6288171289
H	3.4171187565	2.4993372739	0.2667242535
C	–0.2107000721	–3.9107426947	–2.5109250716
H	4.901036373	1.730738199	2.1102867522
H	3.7834657087	2.955977058	2.7005162633
H	1.4318855601	3.1081756023	1.614438976
H	3.4188919173	–0.0663900295	3.0020088549
H	3.8733203604	1.0408531909	4.2932792522
H	1.0831211077	0.1164610764	1.9873166007
C	0.8797462304	–4.014220295	–3.3713489266
H	1.4327239146	0.5866824859	4.3942115354
H	1.7557876925	2.2786790987	4.0276756148
H	–0.9507671553	–0.6741254863	2.3902970155
H	–0.7642457998	–0.1182171587	4.0730413393
H	–2.1987827951	0.3363493928	3.1307187494
H	–0.2271346862	3.3822483963	3.1392314959
H	–1.828401662	2.6981748323	3.4256503621
H	–0.4870368071	2.2649738207	4.4993015326
C	–3.028972712	2.8855099163	0.0260148896
C	–4.0238706621	2.4237894585	1.086440123
C	–3.7846336842	3.1394559229	–1.2720346753
C	–2.3810467732	4.2016494833	0.4633833297
H	–4.8383257383	3.1533476557	1.2417856323
H	–3.5532676782	2.2686100226	2.0673203768
H	–4.488484268	1.47254616	0.7995719471
H	–4.5835569558	3.8904657834	–1.1430599054

H	–4.2580929612	2.2245410018	–1.6475751323
H	–3.1183083692	3.5090953427	–2.0600616448
H	–1.7147248357	4.5995270838	–0.3096012419
H	–1.7941697591	4.1155318237	1.3894390323
H	–3.1402357053	4.9826734503	0.658785642
H	–1.960182677	–0.3876915775	0.0911410585
C	1.5412635711	–2.8605810633	–3.7905860232
C	1.1087448062	–1.6128926935	–3.346538798
H	–1.4894521975	–2.5840053788	–1.4059930407
H	–0.73252743	–4.8039517539	–2.1874231533
H	1.2100984386	–4.9863732196	–3.7176864906
H	2.3873392493	–2.9345754259	–4.4639427241
H	1.6305902963	–0.7246373068	–3.6918840611

8.3.10 Angaben zu den quantenchemischen Rechnungen der Deprotonierung der Trimethylphosphorverbindungen **158**, **159** und **160** (Kapitel 4.5.1)

Tabelle 292 Berechnete Energien der optimierten Verbindungen.

Verbindung	Methode/Basis	Min./TS	ZPE [Hartree]	SCF [Hartree]
158 TS	B3LYP/6–31+G(d)	TS	–882,568976	–882,971111
158 ED	B3LYP/6–31+G(d)	Globales	–882,589818	–882,995486
159 TS	B3LYP/6–31+G(d)	TS	–1254,16134	–1254,53441
159 ED	B3LYP/6–31+G(d)	Globales Min.	–1254,17706	–1254,55442
160 TS	B3LYP/6–31+G(d)	TS	–931,205226	–931,579633
160 ED	B3LYP/6–31+G(d)	Globales Min.	–931,220814	–931,599075
158	B3LYP/6–31+G(d)	Globales Min.	–487,628844	–487,773377
159	B3LYP/6–31+G(d)	Globales Min.	–859,212827	–859,328955
160	B3LYP/6–31+G(d)	Globales Min.	–536,246679	–536,364228
TMEDA (**5**)	B3LYP/6–31+G(d)	Globales Min.	–347,534956	–347,758211
$(MeLi{\cdot}Me_2O)_4$	B3LYP/6–31+G(d)	Globales Min.	–809,552552	–810,021393
Me_2O	B3LYP/6–31+G(d)	Globales Min.	–154,953668	–155,033689

Tabelle 293 Standardorientierung von **158** TS [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–2.3681796223	–1.5428538498	–2.280693123
C	–2.5217657136	0.8459941743	–2.0803325587
N	–1.5971924082	–0.292214994	–2.1862880021
C	–0.7006054752	–0.1192825896	–3.3460330645
C	0.5662190639	–0.9745197933	–3.2491527704
C	2.327002538	–1.7472662762	–1.772235922
N	1.3594549911	–0.6736463255	–2.0428811141
C	2.0744997888	0.6069597192	–2.1687158469
H	–3.0389069688	–1.5385208304	–3.1590961189
H	–2.9662192622	–1.6689495277	–1.374687018
H	–1.6998858478	–2.4033333946	–2.3534450837
H	–3.1508590045	0.9528267986	–2.9825907507
H	–3.1793817439	0.7014166504	–1.2185712458
H	–1.9571900198	1.7703126761	–1.9283771744
H	–0.4262429008	0.9390230842	–3.3990982642
H	–1.2232026097	–0.3566883038	–4.2910366232
H	1.1654990321	–0.8306939129	–4.1678341658
H	0.2966850303	–2.0355478697	–3.2141323721
H	1.803470597	–2.6970099161	–1.6317513068
H	2.8706536877	–1.5188612481	–0.850740984
H	3.0592646784	–1.860688963	–2.5921020787
H	1.3728598307	1.4318109304	–2.3102731528
H	2.6243404989	0.8047496577	–1.2458779612
H	2.7835758722	0.5910019458	–3.0164092393
Li	–0.1887427517	–0.5176320996	–0.50139216
C	–1.9816473036	–0.1809301848	1.7661235126
C	–1.5941409246	2.5699992613	3.0469368168
P	–0.8187799208	1.0457099636	2.3350051498
B	0.4296712905	1.4488046321	0.9018506121
C	0.0417987192	0.3039139606	3.7821340746
H	–2.6676903087	0.257282739	1.0301833867
H	–2.562193074	–0.6380474185	2.5770541736
H	–0.82140293	3.2523934049	3.4211684229
H	–2.2799312743	2.3140538561	3.8623592821
H	–2.1585885138	3.085777007	2.2630483194
H	1.0790509428	0.4212263065	0.7669415329
H	–0.2482450283	1.6731062297	–0.0911072061
H	1.1472091267	2.3829721801	1.1788325708
H	–0.6664690686	0.087963377	4.5898873928
H	0.5200082493	–0.6302246531	3.4726159265
H	0.8124351054	0.9872929007	4.1537592385

C	–0.5702191982	–2.4120280865	0.5745908948
H	0.2295833614	–2.6349868161	1.3003027583
H	–0.1816932029	–2.7164437078	–0.4175234399
H	–1.3943581949	–3.1107971038	0.7859100936
H	–1.2536781337	–1.1991715906	1.0971935884

Tabelle 294 Standardorientierung von **158** Ed [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–2.0969403332	–1.8111899249	–2.869443132
C	–2.5086053449	0.5129315716	–2.4028184673
N	–1.4755299583	–0.5245651345	–2.521651622
C	–0.4392158477	–0.1300314442	–3.4925008572
C	0.8575388909	–0.9278019416	–3.3178907425
C	2.335848418	–1.8918633666	–1.6502675814
N	1.4361699363	–0.7740817121	–1.9692735216
C	2.1518836509	0.5021703916	–1.8301381261
H	–2.6249313632	–1.7594495202	–3.8397799817
H	–2.8090387311	–2.089605094	–2.0885642879
H	–1.3460409942	–2.603135309	–2.9201483696
H	–3.0351816653	0.6860475019	–3.3593871688
H	–3.2457290438	0.2035946964	–1.65551435
H	–2.0579883854	1.4506181168	–2.0670957431
H	–0.237635925	0.9363843333	–3.347369014
H	–0.7970563265	–0.2471478814	–4.5328659328
H	1.5775970432	–0.6226584319	–4.0997782368
H	0.6592011258	–1.9928192997	–3.4766611564
H	1.7797430964	–2.8329409197	–1.6705679746
H	2.7319862974	–1.7603221631	–0.6393250396
H	3.1846741026	–1.9556589833	–2.3556822171
H	1.4842528847	1.3436212409	–2.0266547023
H	2.5135397434	0.6072738736	–0.8036601519
H	3.0147185786	0.5622725123	–2.519147588
Li	–0.346057853	–0.9046908873	–0.7301306566
C	–2.3689890601	0.2257657154	2.4697740645
C	–1.1451638675	2.5863253174	3.6767520594
P	–0.8684271272	1.2755628362	2.4163727047
B	–0.4707593254	2.0345371717	0.6743273473
C	0.4705983639	0.2270987721	3.1032770403

H	–3.2263405884	0.7969587128	2.0985446462
H	–2.5793427308	–0.120936465	3.4875307953
H	–0.2536206434	3.2175805737	3.7489663572
H	–1.3633297191	2.1570998405	4.6606938274
H	–1.9845426906	3.2169987857	3.36641943
H	–0.298065511	1.1070420374	–0.0929750328
H	–1.4375378772	2.7050127059	0.372075019
H	0.5379250098	2.694771723	0.822008027
H	0.2302410218	–0.1183500016	4.1147342474
H	0.5939932489	–0.6409800308	2.4475739086
H	1.4051620751	0.7969674998	3.1284084904
C	–0.7828191511	–2.4560901368	0.5645666317
H	–0.3184602181	–2.5303444108	1.567130768
H	–0.4347894419	–3.3695099047	0.0372683926
H	–1.8633158512	–2.6388871197	0.7369629121
H	–2.2012489131	–0.6388378473	1.8175049849

Tabelle 295 Standardorientierung von **159** TS [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–2.3616615461	–1.9491828599	–2.3840847313
C	–2.4122479822	0.4539923115	–2.3410469562
N	–1.5405659874	–0.7304548447	–2.3200325322
C	–0.5624675236	–0.6743238521	–3.4232835544
C	0.6486518674	–1.5817047075	–3.1848337878
C	2.2478656592	–2.3408024088	–1.5268921605
N	1.3849917288	–1.2303311681	–1.9554979163
C	2.2028975002	–0.0209149296	–2.1411750973
H	–2.9765959223	–1.9766473859	–3.3023142028
H	–3.0205152728	–1.9877584559	–1.5126766847
H	–1.7327295415	–2.8419290776	–2.358484957
H	–2.9740585233	0.5364135413	–3.2893203136
H	–3.131632273	0.3878007539	–1.5195985759
H	–1.8141858776	1.3572545232	–2.1944037927
H	–0.2309943067	0.3643329109	–3.5207174938
H	–1.0324519612	–0.947333669	–4.3863172481
H	1.3087456641	–1.5398046667	–4.0713727532
H	0.318771399	–2.621727147	–3.0900608759
H	1.6442398888	–3.2323756125	–1.3362058615

H	2.7533110086	–2.0672735126	–0.5959091434
H	3.01633805	–2.5839566314	–2.2831082991
H	1.5786439055	0.8296208873	–2.4236581084
H	2.6907662493	0.2338405445	–1.1973048394
H	2.973921984	–0.1702806943	–2.9191495127
Li	–0.2644847683	–0.8074313939	–0.5594236889
C	–2.0771049681	–0.169005205	1.7318826567
C	–1.54681597	2.6883163519	2.6901813564
P	–0.8743884599	1.0958135939	2.0420026279
S	0.2403119795	1.4617733154	0.3867930153
C	0.1631264342	0.4744988138	3.4257484726
H	–2.834373196	0.177875852	1.0193841795
H	–2.5586010471	–0.5216219641	2.6526325799
H	–0.7304152855	3.3917778015	2.8880772859
H	–2.1143268588	2.5122409186	3.6112171443
H	–2.2112722013	3.1252585426	1.9389859182
H	–0.4476235214	0.3139088132	4.3219114189
H	0.6136469393	–0.4751980355	3.1242066032
H	0.958534173	1.1920012769	3.6479307623
C	–0.747913701	–2.5336587508	0.734158631
H	0.0636204171	–2.7162498305	1.4593331881
H	–0.4071773083	–2.965512164	–0.227607799
H	–1.5933520228	–3.1671451685	1.0450733224
H	–1.4005088217	–1.2397926166	1.1473027236

Tabelle 296 Standardorientierung von **159** Ed [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–2.2146311349	–2.2162259086	–2.6236463503
C	–2.5023197512	0.1639623816	–2.8066080869
N	–1.5308119059	–0.9153696133	–2.5973871169
C	–0.4426581477	–0.8489320952	–3.5875251937
C	0.8151320071	–1.5946794196	–3.1301989433
C	2.2644146915	–2.0270515162	–1.2370014504
N	1.3713252702	–1.0531456353	–1.8778431063
C	2.0830346942	0.2114156586	–2.0970975043
H	–2.6997349156	–2.4005132475	–3.6008277452
H	–2.9722215283	–2.2420261078	–1.8366466458
H	–1.5115920534	–3.0255061918	–2.4169656863
H	–2.9894989791	0.1006572242	–3.7977495208

H	–3.2773378952	0.107041958	–2.0365382037
H	–2.0079209468	1.1351019872	–2.7142853174
H	–0.2046523091	0.2072635046	–3.7516980991
H	–0.7642650199	–1.2543668523	–4.565751773
H	1.5640034436	–1.5699286849	–3.944910465
H	0.5747584649	–2.6485502368	–2.9569674099
H	1.706256184	–2.9343927055	–0.9932256256
H	2.6466176716	–1.6066313324	–0.3019031957
H	3.1259634022	–2.2875248714	–1.8802883068
H	1.419205884	0.9581068558	–2.5395995633
H	2.4238823127	0.6073550925	–1.1368975201
H	2.9575285816	0.0791232598	–2.7619475199
Li	–0.4638682092	–0.8862988792	–0.6615666727
C	–2.4543294421	0.2343792996	2.3350844344
C	–1.0886452457	2.6962191069	3.1118064074
P	–0.9076025487	1.1795028239	2.0913713905
S	–0.5085398536	1.6163664212	0.1815586764
C	0.4012597563	0.1958069591	2.9103907293
H	–3.2940467574	0.801415282	1.9217787504
H	–2.6287643323	0.0431233789	3.4003257305
H	–0.1650826645	3.28060333	3.0611315962
H	–1.3012465469	2.4404892178	4.1561745361
H	–1.9060111176	3.3046519064	2.7133451472
H	0.15152239	0.0128899591	3.9620030852
H	0.479288918	–0.7576172602	2.3786706185
H	1.3524612736	0.7328450713	2.8469542068
C	–0.9311495116	–2.4868085306	0.6137360613
H	–0.5330519639	–2.6006964871	1.6418050716
H	–0.5506563152	–3.3846223698	0.0807195268
H	–2.0204723671	–2.6795137288	0.7122848879
H	–2.3496464828	–0.7136190041	1.7964711656

Tabelle 297 Standardorientierung von **160** TS [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–2.3600497772	–1.9686675982	–2.3520549054
C	–2.4133506439	0.4225314812	–2.0938096618
N	–1.548142481	–0.7629383023	–2.1427897122
C	–0.5066820911	–0.6117218708	–3.174706172
C	0.6828680347	–1.5516950076	–2.9530389116

C	2.1503854461	–2.4947730924	–1.2698255
N	1.3488147293	–1.3272142677	–1.6573517974
C	2.1932600197	–0.1238806649	–1.6795060148
H	–2.9220117011	–1.9240829404	–3.3035034608
H	–3.0683556802	–2.0747477937	–1.5259423601
H	–1.7313715553	–2.8621413191	–2.3606411194
H	–2.9359766799	0.5966153132	–3.0525644081
H	–3.1663527465	0.2871346752	–1.3111768841
H	–1.8151743741	1.3021171106	–1.8420146652
H	–0.1629571796	0.4271231078	–3.1475254494
H	–0.917330459	–0.7843741134	–4.187556554
H	1.3931740836	–1.4353709649	–3.7934812508
H	0.3403292099	–2.5915623228	–2.9760049906
H	1.5081985643	–3.3757442293	–1.1829045473
H	2.6066873043	–2.3132560651	–0.2920832286
H	2.9559532004	–2.7078269191	–1.9966834012
H	1.5956564827	0.7627271314	–1.899426765
H	2.6334193471	0.025952487	–0.6905508297
H	3.0043968864	–0.2114009307	–2.4262451189
Li	–0.3394012627	–0.8794836977	–0.3333907489
C	–1.8261748939	–0.1661991634	2.1841454339
C	–1.2269485585	2.8143461754	1.9344486135
P	–0.6347649227	1.0780508903	1.7940105921
O	–0.0812221472	0.8614822205	0.3689806388
C	0.7018072605	0.9544291258	3.0450791752
H	–2.8056756428	0.0452090918	1.737884341
H	–1.9344690449	–0.3584014032	3.257074783
H	–0.4223121506	3.5122815976	1.673717701
H	–1.5822926725	3.0285390634	2.9481363284
H	–2.0552957176	2.9631708216	1.2336288622
H	0.3346453466	1.1952498659	4.0488120459
H	1.0888809421	–0.069806223	3.0480060641
H	1.516535942	1.638554111	2.7849273134
C	–0.8516062956	–2.6166639173	0.9731105656
H	0.040991794	–2.8897280837	1.5635853513
H	–0.6894590173	–3.024197136	–0.0455470976
H	–1.6873051402	–3.2051656138	1.3835816864
H	–1.3389417584	–1.2878696292	1.527663059

Tabelle 298 Standardorientierung von **160** Ed [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–2.2118064827	–2.2665332948	–2.336860523
C	–2.538816981	0.1186451749	–2.3125076042
N	–1.5489118185	–0.9595284095	–2.2569328507
C	–0.5213545031	–0.7948801559	–3.2963068359
C	0.7704647416	–1.5518488738	–2.9692133448
C	2.3125956407	–2.1266469397	–1.193010483
N	1.3783842224	–1.116893385	–1.7022425427
C	2.0483269924	0.1802319326	–1.830114442
H	–2.7605524817	–2.3895779638	–3.2903845835
H	–2.9116079912	–2.3684774882	–1.5037455139
H	–1.4822018574	–3.0733808603	–2.240739341
H	–3.080723761	0.1440079777	–3.2772154809
H	–3.2716749963	–0.0224425999	–1.5117917183
H	–2.0449573496	1.0816985473	–2.1538425766
H	–0.3075117299	0.2751905005	–3.3884473479
H	–0.8903504485	–1.1282134399	–4.2857355635
H	1.4768959263	–1.438076191	–3.8147088333
H	0.5561509181	–2.6220346496	–2.8829269353
H	1.7785917477	–3.0626451573	–1.0095654265
H	2.728549185	–1.7881023725	–0.2392938006
H	3.1490452736	–2.3132966244	–1.8932400537
H	1.3377103065	0.9540281533	–2.1292239181
H	2.4553176508	0.4733282814	–0.8584348085
H	2.8746873521	0.1478497518	–2.5662472608
Li	–0.3943249017	–0.9552110192	–0.3727262704
C	–2.2298487693	0.3823094147	2.3878345687
C	–0.7081299031	2.8687895696	2.228056399
P	–0.6564740231	1.090008258	1.7943626333
O	–0.4154897634	0.8950112818	0.3033907376
C	0.648460513	0.3624371418	2.8440829764
H	–3.0645006221	0.846290699	1.8513402698
H	–2.3593728742	0.5441538696	3.4640474906
H	0.2400942497	3.3391217605	1.9477827229
H	–0.8784132552	3.0161132008	3.3002837312
H	–1.512838028	3.3560684407	1.6677272825
H	0.4481166142	0.5334463419	3.9078971167
H	0.6774995391	–0.7126222156	2.6409629981
H	1.6160256281	0.8054648967	2.5849225414
C	–0.8162824609	–2.5579919376	0.9424404462
H	–0.3954583535	–2.6237972974	1.9673370268
H	–0.4540234623	–3.4831620004	0.4457378838

H	–1.9055803999	–2.7348519988	1.0760648671
H	–2.2132252836	–0.6900093199	2.167228367

Tabelle 299 Standardorientierung von **158** [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
P	–0.0830923445	–0.0096688546	0.0486505605
C	0.6582145689	1.6415725992	–0.6668937344
B	–2.0313152942	–0.2116070907	–0.4209303737
H	–2.4243888925	0.9075421142	–0.2160573025
C	0.2515620088	–0.0174350126	1.6950667938
H	–1.9286815313	–0.4624994458	–1.6588668652
C	1.0120762347	–1.4264617589	–0.7398719083
H	1.7215329403	1.7189472186	–0.4346613452
H	0.0859474432	2.4526721065	–0.2034314936
H	0.4776561214	1.5963679416	–1.7420201277
H	–2.4498638149	–1.1013047184	0.2796509902
H	0.8176151522	–1.3543598032	–1.811363049
H	0.6276124273	–2.3675269037	–0.3313584016
H	2.0681249502	–1.2876169113	–0.5013222645
H	–0.1136760005	–0.9689320077	2.1174440437
H	–0.3156472013	0.7931957702	2.1802458712
H	1.3056131704	0.0905279448	1.9668264987

Tabelle 300 Standardorientierung von **159** [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
P	–0.1602371039	0.004164179	0.0555081509
C	–0.3323405261	–0.0391245684	1.8868518727
S	1.7057714006	–0.0479561748	–0.5888688768
C	–1.0957667618	1.506386784	–0.4482691201
C	–1.2047099591	–1.3928691341	–0.529887192
H	–1.3854068348	–0.0117419458	2.1904787822
H	0.1930469087	0.8197863373	2.3151775002
H	0.1339455776	–0.9524378229	2.2684623692
H	–0.7575863598	–2.3359187998	–0.2013628894
H	–1.2287975278	–1.3866345967	–1.623781
H	–2.227200546	–1.3180390475	–0.1415558687

H	–1.1150259134	1.5661690514	–1.5406296176
H	–0.5821842767	2.3930337292	–0.0644898652
H	–2.1226733979	1.4842607175	–0.0651930091

Tabelle 301 Standardorientierung von **160** [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
P	0.1737295091	–0.0062968742	–0.0596247993
C	0.0162487899	–0.0429421376	1.7684222397
O	1.5970568199	–0.0578480907	–0.5481387354
C	–0.7342608252	1.5021921827	–0.577847073
C	–0.8623917361	–1.4019985121	–0.6481557946
H	–1.0301013463	–0.0127248262	2.0926856287
H	0.5487500752	0.815310521	2.1914360213
H	0.4847881651	–0.9561686605	2.1500442633
H	–0.4131248939	–2.3450352452	–0.319540181
H	–0.8817690286	–1.3973760661	–1.7430069524
H	–1.8890704578	–1.3413540118	–0.2697889281
H	–0.7447850651	1.5564454627	–1.6714712282
H	–0.2091509792	2.3849491536	–0.1982844948
H	–1.7655110375	1.5096823119	–0.207108488

Tabelle 302 Standardorientierung von TMEDA (**5**) [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	0.0200276805	0.1027737708	–0.7675662115
C	0.010175661	0.1042113808	0.7675662115
N	1.3749320814	0.0930560443	–1.3260275069
N	–1.2910093399	0.4820710945	1.3260275069
C	1.3577019783	0.429284239	–2.7451967615
C	2.0681458972	–1.172237353	–1.1052939886
C	–1.1784184244	0.7993557635	2.7451967615
C	–2.3168831246	–0.5323724738	1.1052939886
H	–0.4733132042	1.0239968566	–1.0971397605
H	–0.5713971385	–0.7464444565	–1.1663704733
H	0.7461905421	0.8460464683	1.0971397605
H	0.3342701561	–0.8785997264	1.1663704733

H	2.3846058178	0.4758422078	–3.1242119847
H	0.8960786088	1.4120229398	–2.8888569828
H	0.7991805151	–0.3088089647	–3.3572558316
H	2.1697115172	–1.3751342384	–0.0355496603
H	3.0755091657	–1.1146060754	–1.5316019829
H	1.5442591162	–2.0321519795	–1.5725310839
H	–2.1491985847	1.1374164395	3.1242119847
H	–0.4552200495	1.6092048851	2.8888569828
H	–0.8541006369	–0.0675616344	3.3572558316
H	–3.2657732433	–0.1892840576	1.5316019829
H	–2.0605670531	–1.5061345576	1.5725310839
H	–2.4721927272	–0.6977860421	0.0355496603

Tabelle 303 Standardorientierung von $(MeLi{\cdot}Me_2O)_4$ [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
Li	–0.7149761636	0.5189403863	–1.1138737065
Li	–0.7127826017	0.5252846515	1.3444214906
Li	1.4316453282	0.5102575236	0.115800921
Li	0.0109805555	–1.4974950919	0.1241139585
C	1.029455554	–0.7106420895	1.9599438966
C	0.0587516188	2.2497369097	0.0583627191
C	1.0383861654	–0.7941593715	–1.7029785645
C	–2.1195787428	–0.6893146292	0.1259815392
O	–1.6332164695	1.3989612952	2.8944799147
O	–1.6023973988	1.112984457	–2.8174276425
O	–0.1270137346	–3.502465483	0.2304568777
O	3.3846765125	0.9876650253	0.0550826362
C	–2.8958770791	2.0201710269	2.6738235057
C	–0.8405392721	2.0746968232	3.8657713275
C	–2.3628493493	0.1575488306	–3.5497352765
C	–0.942704508	2.0577300189	–3.6537414474
C	–0.4308299122	–4.250988424	–0.9410007318
C	–0.7196203955	–4.043782974	1.4084286238
C	3.857106282	1.996766784	–0.8296535441
C	4.311440935	–0.0820561007	0.224119606
H	1.5367270688	–1.6909904062	1.8612167807
H	0.365087033	–0.8508480591	2.8367885761
H	1.8256979439	–0.0416264697	2.3427687628

H	0.5011718289	2.7065568814	0.9654701872
H	–0.9467282793	2.7104303371	–0.00764799
H	0.6182699794	2.7274218866	–0.7714290682
H	1.8225926027	–1.5559462079	–1.520855507
H	1.5665552195	–0.0053975374	–2.2749630547
H	0.3815374889	–1.2673865787	–2.4604592809
H	–2.503433041	–0.9739221054	1.125936311
H	–2.2915029591	–1.5983577371	–0.4842597207
H	–2.8753501369	0.0278017545	–0.2530266337
H	–3.4768114455	2.0468046059	3.6067848265
H	–3.4226469322	1.4176700969	1.9314255798
H	–2.7648100177	3.0434468503	2.2947744677
H	–1.361191961	2.0993780834	4.8336395922
H	–0.6201449362	3.1015120292	3.5418091333
H	0.0905434721	1.513376504	3.9648456061
H	–3.1365612448	0.6612510138	–4.1465869801
H	–2.8357971338	–0.5011581572	–2.8189758431
H	–1.7139478904	–0.4304996389	–4.214301815
H	–1.6741773675	2.5990918552	–4.270533155
H	–0.2136098679	1.5571522637	–4.3067848008
H	–0.4274975865	2.7609600607	–2.996857052
H	–0.0642962394	–5.282752176	–0.8419039272
H	0.0768978627	–3.7601647595	–1.7737082918
H	–1.5147638228	–4.2662393139	–1.1253378066
H	–0.3779172326	–5.0764499369	1.5672034169
H	–1.8159620891	–4.0268160798	1.3342440907
H	–0.397712468	–3.4185024388	2.2430943082
H	4.798258946	2.4242909525	–0.4552895331
H	3.0919599104	2.7746913952	–0.8656789424
H	4.0177876207	1.5882830903	–1.8377074032
H	5.2609813379	0.2968073873	0.6280923806
H	4.4961496745	–0.5905563389	–0.7323972873
H	3.8648042534	–0.7816786973	0.9325578717

Tabelle 304 Standardorientierung von Me_2O [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
O	–0.4545166482	0.0095900677	0.3721805661
C	0.1980428174	1.1726697981	–0.0970709409

C	0.1045184179	–1.1790523405	–0.1506791891
H	0.1297948392	1.2576461799	–1.1942416804
H	1.2623244278	1.1810682739	0.1908539827
H	–0.303282084	2.0293569738	0.3602058922
H	1.1642201158	–1.2850536913	0.1347429035
H	0.0318375528	–1.2082880225	–1.2504641551
H	–0.4641290946	–2.0131549996	0.2679592875

8.3.11 Angaben zu den quantenchemischen Rechnungen der Deprotonierung des Dimethyl(*tert*-Butyl)phosphinoborans (**76**) (Kapitel 4.5.2)

Tabelle 305 Berechnete Energien der optimierten Verbindungen.

Verbindung	Methode/Basis	Min./TS	ZPE [Hartree]	SCF [Hartree]
pro-*S*-1	B3LYP/6–31+G(d)	Globales Min.	-1308,83515	-1309,45668
pro-*S*-2	B3LYP/6–31+G(d)	Globales Min.	-1308,83524	-1309,45704
pro-*S*-3	B3LYP/6–31+G(d)	Globales Min.	-1308,82893	-1309,45168
pro-*S*-4	B3LYP/6–31+G(d)	Globales Min.	-1308,82948	-1309,45102
pro-*R*-1	B3LYP/6–31+G(d)	Globales Min.	-1308,83514	-1309,45681
pro-*R*-2	B3LYP/6–31+G(d)	Globales Min.	-1308,83643	-1309,45815
pro-*R*-3	B3LYP/6–31+G(d)	Globales Min.	-1308,82969	-1309,45135
pro-*R-4*	B3LYP/6–31+G(d)	Globales Min.	geht über in pro-*R*-2 über	
S-1	B3LYP/6–31+G(d)	TS	-1349,25741	-1349,92113
S-2	B3LYP/6–31+G(d)	TS	-1349,2589	-1349,92312
S-3	B3LYP/6–31+G(d)	TS	-1349,2543	-1349,91776
S-4	B3LYP/6–31+G(d)	TS	-1349,25485	-1349,91937
R-1	B3LYP/6–31+G(d)	TS	-1349,25689	-1349,9205
R-2	B3LYP/6–31+G(d)	TS	-1349,25749	-1349,92182
R-3	B3LYP/6–31+G(d)	TS	-1349,25431	-1349,91841
R-4	B3LYP/6–31+G(d)	TS	-1349,25531	-1349,91995

Tabelle 306 Standardorientierung von pro-*S*-1 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	2.8909066005	–1.8758368867	–4.0715133929
C	2.8578707061	–0.3404956839	–4.0851227345
C	1.4618694631	–2.4342074847	–4.0689524096
C	1.9987250976	0.2268000773	–2.9301915145
C	1.9330634761	1.770925229	–2.9569849171
C	–2.3593171647	–2.9603856717	3.0263210473
C	0.6691758879	–1.8346359212	–2.8980389111
H	–2.0598589695	–3.9653526215	2.7047779572
C	1.0715847731	2.2571871646	–4.1313496043
N	0.6265360035	–0.3544963016	–2.8653733469
C	–1.605821411	–1.1815952708	0.0976920411
C	1.3901842359	2.40121504	–1.6601970519
C	–0.3227686689	0.2025908262	–3.854685873
C	–1.1639628126	–1.9939814391	3.0945591985
C	–0.3499100194	1.7442543505	–3.8675729241
C	–0.0802969583	–2.5553335217	4.0351286822
Li	–0.1613301304	0.0390151987	–0.9387043424
P	–0.4489625039	–1.6976054601	1.345578693
C	–1.6429044795	–0.6301719806	3.6300248572
N	–0.0484710078	2.1434017443	–1.4043111207
C	–0.8921243564	2.434239257	–2.594073466
B	1.0469535666	–0.4349624938	1.3522460818
C	0.1452975931	–3.3676387056	0.8250164273
C	–0.4754036863	2.9829627224	–0.2589036626
C	–2.362428625	2.1180689592	–2.2827164989
C	–1.9438772586	2.7695504415	0.1121438647
C	–2.8629464649	2.9608452766	–1.1012130497
H	–2.2480802348	–0.3792685903	0.4874780671
H	3.4581962552	–2.2521905206	–4.9323521338
H	3.4172910385	–2.2237402185	–3.1699231421
H	3.8748348522	0.0646876935	–3.9936915121
H	2.4735083858	–0.0020655293	–5.0562344317
H	1.4695652093	–3.5277094773	–3.9701357703
H	0.9696717673	–2.2101056031	–5.0258943191
H	2.4854245581	–0.0752439616	–1.9908144744
H	0.8011343662	–1.9062459571	4.0686482366
H	2.9641180028	2.1332705715	–3.067751182
H	–3.1280029898	–2.5971767284	2.3339784455
H	1.1381584318	–2.1599564706	–1.9604937279
H	–0.3632478883	–2.1987365974	–2.8786020246
H	0.2466140942	–3.5579499495	3.7350400294

H	1.4494632138	1.8915547568	–5.0930086488
H	1.0824600295	3.3541634512	–4.1821144287
H	–2.2492629166	–2.0017056026	–0.24530122
H	1.9481690528	2.0358997137	–0.7901065012
H	1.5620213732	3.4931113604	–1.7227899959
H	–0.0876058703	–0.1285193139	–4.881047094
H	–1.3121668754	–0.2035304598	–3.6135819812
H	–1.0154376768	2.0424528904	–4.6895585078
H	–0.4797082951	–2.6366725143	5.0565775528
H	1.465845201	–0.4745543168	0.1943493697
H	–2.0741075189	–0.7539493988	4.6334766285
H	–0.8331105344	3.5240167594	–2.8025195776
H	0.58546092	0.666124076	1.5960085193
H	1.9282173762	–0.7490527451	2.1214325394
H	–0.6713845089	–4.0967697431	0.8076677818
H	0.5587883653	–3.2902960215	–0.1836212677
H	0.9353428828	–3.7241859898	1.4917876059
H	0.1691779506	2.7371807911	0.5909383437
H	–0.30716422	4.0495005568	–0.5083981894
H	–2.4745827354	1.0519261582	–2.0444285411
H	–2.9647905264	2.3174243308	–3.1794155548
H	–2.0704991333	1.7594658479	0.5165627383
H	–2.2083857133	3.4702066767	0.914539333
H	–2.8751116181	4.0219902975	–1.3926308743
H	–3.8956334774	2.6904922816	–0.847740945
H	–2.418813522	–0.1953794844	2.9881049129
H	–0.8180388826	0.0868911468	3.7010394644
H	–2.8190110749	–3.0595110103	4.0199424472

Tabelle 307 Standardorientierung von pro-*S*-2 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	2.1176158786	3.8943568537	–0.0609468031
C	3.0903834251	2.9282052398	–0.7527516814
C	1.7569993067	3.3694585007	1.3349141453
C	2.538035661	1.4836905059	–0.7864825719
C	–4.6828259247	–1.1312143781	0.9245787999
C	3.5299698879	0.4968650158	–1.4483252807
C	–4.4352810006	–0.4246382857	–1.4865789959
C	1.2057742931	1.9397901321	1.2314653421

C	–3.7701162037	1.1405338842	0.3602034932
C	4.736279608	0.2445106397	–0.5331406437
N	2.1033981177	0.9755244894	0.5488353594
C	–0.8987473294	–0.1855428571	–1.196513629
C	2.9115023124	–0.8636961236	–1.824797481
C	3.2111210116	0.5327631916	1.4238076206
C	–3.8223944357	–0.3372087331	–0.077338052
C	4.1882654503	–0.4355617408	0.7277127482
H	–3.170691221	1.7436755036	–0.3322907563
Li	0.8232891224	–0.6252009591	0.0003816712
P	–2.0271987408	–0.9975637637	–0.0928056245
H	–3.3475463673	1.2521460685	1.3648681884
N	2.5179625324	–1.6952794587	–0.6611571788
C	3.6161996401	–1.8172613886	0.3351307866
B	–1.2453950832	–1.0580181475	1.7038738683
C	–2.198119244	–2.7127402983	–0.7586949371
C	2.1009460722	–3.0316689957	–1.1430151054
C	3.1600492527	–2.6641873183	1.5317607427
C	1.6443207669	–3.9453915775	–0.0027533136
C	2.723245906	–4.0636666159	1.0799318685
H	–0.912409562	0.9010749513	–1.0253089703
H	2.5566948141	4.8984803412	–0.0018758559
H	1.2001783799	3.985620794	–0.6618639757
H	3.2820063892	3.2510567127	–1.7852865629
H	4.0558056751	2.9633270917	–0.2311544568
H	0.9998251381	4.0072819177	1.8092438674
H	2.6426518392	3.3986871284	1.9853163353
H	1.6238116188	1.5039179536	–1.3979950056
H	–4.7861677678	1.5596579418	0.3720560539
H	3.8584899636	0.9580069009	–2.3896938019
H	–3.8045434663	0.0759575951	–2.2314059407
H	0.2659193421	1.9653435567	0.6663704245
H	0.9633051388	1.5288551426	2.2165279254
H	5.2584674681	1.1748950701	–0.2820772976
H	5.4663189956	–0.4037173803	–1.0361447785
H	–1.1267675826	–0.375091559	–2.253085127
H	2.0155434705	–0.7214668776	–2.440417843
H	3.6516341096	–1.4130275678	–2.4385091476
H	3.8053844832	1.385687936	1.7949656788
H	2.7569803207	0.0643193008	2.3045753111
H	5.0053763355	–0.6273727877	1.4367131182
H	–1.2149561054	0.0735126965	2.1456225291

H	–5.419835712	0.0644499802	–1.4987754511
H	4.4561358832	–2.3631235557	–0.1452991771
H	–1.8520401746	–1.8240882705	2.4210597858
H	–0.0993150318	–1.4808888798	1.5324323784
H	–2.5253991726	–2.702462001	–1.803528563
H	–1.2242047767	–3.2065710323	–0.7077541463
H	–2.9065583704	–3.2955874334	–0.1632883881
H	1.2901737598	–2.8834567264	–1.865344423
H	2.9428270103	–3.5074343046	–1.6844641281
H	2.3233923941	–2.1719000335	2.0437518952
H	3.9875906259	–2.7317093658	2.2506306044
H	0.7279062054	–3.5434692293	0.4458874301
H	1.3960986494	–4.930964012	–0.4174340491
H	3.5924547583	–4.6084506019	0.6813845845
H	2.3484632254	–4.6424906736	1.9328931048
H	–4.5846153958	–1.4625743087	–1.8070926839
H	–4.7870011808	–2.1840101337	0.6359363921
H	–5.6955837447	–0.7041640889	0.9663663341
H	–4.260280645	–1.0985915714	1.9340934402

Tabelle 308 Standardorientierung von pro-*S*-3 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	1.4397405321	3.8660618538	–0.7070187422
C	0.284181318	4.5303324632	0.0562690314
C	0.8882405107	2.9443150441	–1.8024830409
C	–0.7125965225	3.4870304218	0.6125441364
C	–1.8981256261	4.1566796759	1.3510777172
C	–2.242239989	–3.0147310497	3.0016940729
C	–0.080733848	1.9257770398	–1.1854446565
H	–2.0197860078	–3.9248059561	2.4315682276
C	–2.8473054283	4.8401474563	0.3553779359
N	–1.2084836214	2.5242320457	–0.4201961273
C	–1.5194125043	–1.1073258092	0.4634973744
C	–2.7297451755	3.1968874691	2.2216784142
C	–2.2498204338	3.0811298191	–1.309408066
C	–0.9890306875	–2.1461226573	3.2200534073
C	–3.4146972115	3.7281502413	–0.5360026724
C	0.0413906018	–2.93416674	4.05545511
Li	–1.9733219185	0.9168614602	0.6855659398

P	–0.2152342338	–1.6338285667	1.5635907207
C	–1.3762035633	–0.8729566127	3.9966840667
N	–3.4797678245	2.1749880093	1.45079348
C	–4.2657333322	2.7739937109	0.3334705757
B	1.1594144159	–0.2641715494	1.7999267924
C	0.5952289856	–3.1982589775	0.9621640152
C	–4.3877302243	1.4415355819	2.363779432
C	–4.9670977705	1.6639146328	–0.4643202157
C	–5.1209407552	0.3057025978	1.6475931051
C	–5.8949029578	0.8337380933	0.4332912123
H	–2.2795761867	–1.8894849782	0.332838831
H	2.099108384	4.6319415648	–1.1350549538
H	2.0482981882	3.2732683229	–0.0097664905
H	0.6717444248	5.1205460706	0.8976866602
H	–0.2267801777	5.236882339	–0.6113545999
H	1.7018738716	2.398423321	–2.2969719712
H	0.3904617883	3.5404505325	–2.5809269428
H	–0.1565610159	2.873205715	1.3360971584
H	0.9799113292	–2.3806086293	4.1670471395
H	–1.4680555587	4.899884686	2.0357212532
H	–3.0251274074	–2.4653803179	2.4684050104
H	0.4762637658	1.2826407491	–0.4953819693
H	–0.5142303852	1.2760945296	–1.9550271189
H	0.2690388151	–3.9100400983	3.6128091734
H	–2.3297998864	5.5962334589	–0.245724021
H	–3.6538654925	5.3574500891	0.8922426425
H	–1.0392330327	–0.9611745366	–0.5198818113
H	–2.0842498888	2.6678309817	2.9342904249
H	–3.4362070666	3.8045070659	2.818759135
H	–1.8434568427	3.8449015699	–1.9938098811
H	–2.6081393054	2.2609666175	–1.9430782648
H	–4.0972049878	4.156326566	–1.2830414662
H	–0.3650259377	–3.1172341158	5.0601051671
H	1.7289052409	–0.1803463897	0.7246605303
H	–1.8573640039	–1.1468857222	4.946553415
H	–5.0618152652	3.4060972699	0.7794298512
H	0.5797551768	0.7770375176	2.0827413952
H	1.921991368	–0.6084824082	2.6821596957
H	–0.111006278	–4.0356855414	0.9280377906
H	0.9503388175	–3.0053912874	–0.0556685803
H	1.458113509	–3.4723168943	1.5782276847
H	–3.7886921936	1.0490814219	3.1918948607

H	–5.1203485692	2.1487924399	2.7994212124
H	–4.2199840957	1.0030023759	–0.924049988
H	–5.5348365752	2.1237668932	–1.2842234559
H	–4.3863827098	–0.4431310811	1.3248639343
H	–5.7982367815	–0.185555537	2.3577890565
H	–6.7306973606	1.4636824281	0.7727597932
H	–6.3340236281	0.0040992518	–0.1343012959
H	–2.083685873	–0.2619500783	3.4264719359
H	–0.4983920632	–0.2584632227	4.2201908485
H	–2.6522128384	–3.3278926369	3.9726569647

Tabelle 309 Standardorientierung von pro-*S*-4 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	–3.3594430468	1.7480707393	2.0229788359
C	–3.0977879794	2.4542619526	0.6848583195
C	–2.0823116838	1.7406764397	2.8729060157
C	–1.8881853621	1.8443436334	–0.0638180671
C	–1.6017659816	2.5790684537	–1.3938526915
C	0.1711561683	–4.6147975549	1.0002787004
C	–0.9281032822	1.1167476789	2.0748066864
H	0.8732904517	–5.275390362	0.4795233455
C	–1.0237541902	3.9769637088	–1.1265589034
N	–0.6520613352	1.7580783037	0.7668760407
C	0.5418104739	–1.7216532355	–0.7896596422
C	–0.6430153596	1.8289134729	–2.3375598154
C	0.0728499851	3.0398715809	0.9158992468
C	0.8825041563	–3.4208303117	1.6670591
C	0.3228441065	3.7596142721	–0.4242297198
C	1.9219595852	–3.9463179899	2.6779197463
Li	0.579184969	0.3310175889	–0.2294985816
P	1.7514944454	–2.3325199755	0.3769162792
C	–0.1587223182	–2.5687123701	2.4171821133
N	0.7551865676	1.7410486182	–1.8546518546
C	1.2847850452	3.0580272778	–1.4098135049
B	2.7258368528	–0.8206281216	1.1557094504
C	3.0028340944	–3.4749939046	–0.3955835489
C	1.5967393729	1.2005798963	–2.947549822
C	2.7172964997	2.8948365817	–0.8827979337
C	3.0563081472	1.0204483021	–2.5274989003

C	3.6409913877	2.3239312611	–1.9682372378
H	–0.2700648352	–2.4367952108	–0.9678805637
H	–4.1840988146	2.2378397382	2.5563797435
H	–3.6766466894	0.7110778886	1.8356535638
H	–3.9808586578	2.3844039527	0.035100441
H	–2.933373213	3.5228206866	0.8740708624
H	–2.2287274051	1.162128242	3.7943692728
H	–1.8320673093	2.7649029101	3.1833257819
H	–2.1508369611	0.8015462479	–0.3009807935
H	2.4715018301	–3.1286542079	3.1545535716
H	–2.5591011402	2.6595622307	–1.9265891601
H	–0.5873323747	–4.2911445763	0.2799876377
H	–1.1742187814	0.0681929136	1.869788995
H	0.0041426924	1.1168604755	2.6491334095
H	2.6494579696	–4.6167976474	2.2069610327
H	–1.6964065979	4.5845845322	–0.510534687
H	–0.8829455787	4.5180682271	–2.0718210862
H	1.0556107879	–1.5710422988	–1.7534125939
H	–0.9949174372	0.8032861962	–2.5063315326
H	–0.6656365347	2.345779828	–3.3164903761
H	–0.4724478482	3.7434667947	1.5681677965
H	1.0190040728	2.8155345008	1.4210277055
H	0.7804172393	4.728520201	–0.1813843177
H	1.4102880479	–4.5189031093	3.4641057019
H	3.5091231925	–0.4677120898	0.2923397103
H	–0.6442501268	–3.1767532477	3.1938129196
H	1.3380391307	3.7248960056	–2.2966817699
H	1.9007681915	0.0655863899	1.3727711817
H	3.3043503775	–1.1245796516	2.1767470878
H	2.5352850615	–4.3711813841	–0.8160945359
H	3.4833451909	–2.9225210629	–1.2099728647
H	3.7817746531	–3.764604591	0.3183654365
H	1.1665799188	0.2421307035	–3.2574468362
H	1.5410003219	1.8818946332	–3.8198239924
H	2.7263312138	2.2272232732	–0.0123166475
H	3.0824796192	3.874456814	–0.5454435023
H	3.1245717842	0.2365448831	–1.7650093786
H	3.6329271511	0.6773417281	–3.3964911927
H	3.750363056	3.0609326586	–2.7784805087
H	4.6433051101	2.1471505434	–1.5600311771
H	–0.9367518498	–2.2022249095	1.7393453449
H	0.3082342786	–1.7075817525	2.9070530088

H	–0.3340405059	–5.2159933955	1.7693536546

Tabelle 310 Standardorientierung von pro-*R*-1 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	6.0712124357	–3.7010339289	–0.2166523505
C	5.8561706129	–2.9093597523	–1.5148665111
C	4.941890984	–4.7221154821	–0.0274450267
C	4.4519941997	–2.2623227409	–1.5701487975
C	4.2181309051	–1.4940991392	–2.8919976335
C	3.581588022	–4.0120365461	–0.0861104783
C	4.0470076033	–2.4692360522	–4.0659379046
N	3.3404643044	–3.2247625204	–1.3178891256
C	1.304528639	–0.6792796748	0.8088187769
C	3.0001996577	–0.5514663063	–2.8632982512
C	2.9928994338	–4.0798859085	–2.4754539136
C	1.3890723324	–2.5957576205	2.9602918714
C	2.7772192941	–3.2798266592	–3.7759410876
H	1.9925236085	–1.8534743487	3.4931153105
Li	1.6991460307	–2.013792801	–0.7997017514
P	0.2700001194	–1.7909728413	1.7291291683
H	2.0597421443	–3.2782961461	2.4324698581
N	1.6926472421	–1.2450509688	–2.7823287045
C	1.5627769323	–2.3218603749	–3.8005396278
B	–0.4813196521	–3.1611386604	0.5431215615
C	–1.0830116447	–0.981843289	2.8141979481
C	0.6136960489	–0.2437079664	–2.9511259639
C	0.2051805939	–3.0250605682	–3.6548280791
C	–0.7801387872	–0.862374739	–2.834547936
C	–0.9514929603	–2.0289577987	–3.8153477388
H	1.9625772088	–0.0780051555	1.4480371481
H	7.0505209163	–4.1961707687	–0.2309317848
H	6.0800390094	–3.0085809087	0.6387178358
H	6.6094238884	–2.1151386538	–1.6080884852
H	6.0048394659	–3.581588422	–2.3700007009
H	5.0347985485	–5.2332852214	0.9396862001
H	5.0062219937	–5.5008465412	–0.8003489703
H	4.3990194671	–1.5380307596	–0.7423685866
H	0.8155556723	–3.1821638014	3.684022314
H	5.0991050086	–0.8579622664	–3.0530142937

C	–1.9428821001	–2.0638976626	3.4950694598
H	3.5190698746	–3.3093061159	0.7553133501
H	2.7535038105	–4.7202122142	0.025017881
C	–1.9769783252	–0.1337481268	1.8882299495
H	4.916189984	–3.127409412	–4.1785545339
H	3.9444987077	–1.9141627011	–5.0079602331
H	0.6854000486	0.0000279905	0.2033993904
H	3.06256311	0.1304682369	–2.0061444439
H	3.033714524	0.0707769651	–3.7784971409
H	3.775706896	–4.8305334496	–2.6797208645
H	2.088482125	–4.6357287892	–2.20333486
H	2.6098356935	–4.0143474489	–4.575682202
C	–0.4425274724	–0.066916212	3.8732147519
H	–1.3983665411	–2.6811623538	–0.0936147051
H	–2.4482267852	–0.7450138413	1.1107136288
H	1.5783726607	–1.8496953444	–4.806117489
H	0.4435557867	–3.4774442891	–0.2086602863
H	–0.8270650699	–4.127300206	1.1897899346
H	–1.4058104882	0.6639746715	1.3986692395
H	–2.7758696528	0.3403956317	2.4757016995
H	–1.3601007844	–2.6799634117	4.1902155503
H	0.7551931481	0.5289582741	–2.1873895199
H	0.7228932626	0.2480603069	–3.9383170909
H	0.132620185	–3.5067417548	–2.6715667582
H	0.1375068379	–3.8180733536	–4.4118815982
H	–0.9420097743	–1.2205141349	–1.8113069036
H	–1.528295918	–0.0817642079	–3.0242177259
H	–0.965551592	–1.648045824	–4.8479816377
H	–1.9117117889	–2.5311270892	–3.6470248704
H	–2.4053226788	–2.7320699686	2.7612747017
H	–2.7465097289	–1.5898070363	4.0774560343
H	0.218685653	0.6779917927	3.4134794994
H	0.1398854275	–0.6330923455	4.6099049836
H	–1.224678314	0.4759087562	4.4231285195

Tabelle 311 Standardorientierung von pro-*R*-2 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z

C	–2.9972921156	1.0702051868	–4.2224579728
C	–1.9853376853	–0.0527900764	–4.4919681591
C	–2.3012332902	2.2513803574	–3.5339843533
C	–1.2385485023	–0.4761383055	–3.2049056778
C	–0.1902081421	–1.5806975162	–3.4847100822
C	–1.5925685351	1.7685058254	–2.259627331
C	1.0152160409	–1.0087957032	–4.2450598901
N	–0.6188005525	0.6673783044	–2.4674124796
C	–0.4820225553	1.1659511976	1.2319962769
C	0.3288074622	–2.2951541593	–2.2231306123
C	0.6524781544	1.1502793728	–3.0470238342
C	–0.7868217114	–1.0171026403	3.0942926069
C	1.6660466886	0.0191886034	–3.3111430676
H	–0.1615213298	–0.4736757184	3.8105895519
Li	–0.2514280365	–0.0508243441	–0.5067930378
P	–1.7149753648	0.1368154571	1.9890695817
H	–0.1397695092	–1.6452055153	2.475410486
N	1.1311379998	–1.4299122629	–1.3258376665
C	2.2103033126	–0.7151715393	–2.0624974872
B	–2.6237131252	–0.9078704778	0.6054213396
C	–2.9418209269	1.0125464239	3.1647684762
C	1.7081505263	–2.2583416865	–0.2427079434
C	2.9966840803	0.1903669478	–1.1031789175
C	2.5100176698	–1.4223130514	0.7576081463
C	3.6077586725	–0.6193527176	0.0487069501
H	0.2483425157	1.5584041435	1.9506318099
H	–3.4721732285	1.3869858636	–5.1598810529
H	–3.7992852833	0.6935572286	–3.5709898742
H	–2.4946719629	–0.9354781951	–4.90205904
H	–1.2765657978	0.2832790578	–5.2604688012
H	–3.0273850625	3.0286070106	–3.2619563043
H	–1.5853063201	2.7189758249	–4.2248689273
H	–1.9924161519	–0.8864046138	–2.5184786882
H	–1.4734464137	–1.6720076025	3.6383444938
H	–0.6908969486	–2.3481060466	–4.0903829675
C	–3.9303724613	–0.0011020904	3.773033156
H	–2.3474985961	1.4025036318	–1.5533230019
H	–1.0618093616	2.5903418421	–1.7660912999
C	–3.7248631334	2.0430389178	2.3268712864
H	0.716878933	–0.5437193442	–5.1917189087
H	1.7237104206	–1.8102780752	–4.4939161778
H	–0.9594120164	2.0126683802	0.7175964881

H	–0.5069476127	–2.6934792947	–1.6368377168
H	0.9412824428	–3.1579191849	–2.5497292081
H	0.494829847	1.679679908	–4.0026783629
H	1.0646824567	1.8886233061	–2.3490719974
H	2.5346184567	0.4782136821	–3.8032997847
C	–2.1782412545	1.7445837099	4.2825263222
H	–3.2517325346	–0.1477603206	–0.1080156865
H	–4.2892231039	1.5623996973	1.5201414948
H	2.9210143195	–1.4759844561	–2.4492509159
H	–1.7008567579	–1.4257337733	–0.0244465506
H	–3.322534573	–1.7715861773	1.0899541991
H	–3.0571250795	2.7894864731	1.8798318665
H	–4.4395807171	2.5775754046	2.9685507872
H	–3.4287293841	–0.7297603029	4.4211212892
H	0.8799617509	–2.7713886228	0.2599493253
H	2.3573580293	–3.0410767307	–0.6827232283
H	2.3338249621	0.9605616998	–0.6878331061
H	3.7819670888	0.7071396086	–1.6713235296
H	1.8315562744	–0.7310483007	1.2724613649
H	2.9401129199	–2.0900818698	1.5153097865
H	4.3740127056	–1.3024426639	–0.3479199571
H	4.1139549304	0.0475985505	0.7575829469
H	–4.4686355317	–0.554649388	2.9967393196
H	–4.6718161866	0.5262408744	4.3908024962
H	–1.4340012265	2.4375035305	3.8717978594
H	–1.6621291042	1.0473132605	4.953473842
H	–2.8788914744	2.3293534849	4.8955200506

Tabelle 312 Standardorientierung von pro-*R*-3 [globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	2.9927867898	–3.5931095484	0.3088194066
C	3.4440984319	–2.2872372853	0.9779176389
C	2.5210183086	–3.3126161712	–1.1235265869
C	2.3454406596	–1.1988256574	0.9193946901
C	2.8167451957	0.1294050309	1.5580172658
C	1.4255173333	–2.236159271	–1.1130091815
C	3.8634692116	0.816622505	0.6694772811
N	1.8056074059	–0.9626456405	–0.4528585852

C	–1.5156809389	–1.1386764688	1.0378386515
C	1.6844783168	1.136162042	1.8414528148
C	2.6802111057	–0.1373740325	–1.3150071169
C	–3.5807884068	–2.7662400321	–0.5126070784
C	3.1506092155	1.1677705528	–0.6420103687
H	–4.1179372811	–3.125910969	0.3717011193
Li	–0.0701952013	0.0142787463	–0.0387657096
P	–2.7839358452	–1.1079851336	–0.2207072618
H	–2.7772516908	–3.4749395844	–0.7392132886
N	1.0499466523	1.7018161836	0.6257463828
C	2.0553130081	2.2153212133	–0.3431345362
B	–1.9863003824	–0.5107490845	–1.9067956315
C	–4.2194898019	–0.0155379059	0.3659925858
C	0.1273099338	2.7874491153	1.0285918217
C	1.3576838486	2.7622157229	–1.5960267139
C	–0.5992948055	3.409053388	–0.1666428592
C	0.3898487642	3.8957613508	–1.2320347041
H	–0.978083431	–2.0968955404	0.9487708354
H	3.8092787248	–4.326508228	0.317512728
H	2.1652868735	–4.035345441	0.8838980365
H	3.7012319758	–2.4648002584	2.0312036153
H	4.3619275089	–1.9375950637	0.4873702888
H	2.1182650943	–4.2216948079	–1.5889018156
H	3.3725457953	–2.9957123749	–1.7418766421
H	1.4917377164	–1.5723136315	1.5041833622
H	–4.2599271727	–2.7413508709	–1.3719685863
H	3.2544563037	–0.1238675603	2.5332709406
C	–5.3690660554	–0.0892243328	–0.6603871725
H	0.5532824658	–2.631524454	–0.5785589291
H	1.0859124471	–1.9973417446	–2.125468214
C	–3.7333876053	1.4424908454	0.462329374
H	4.7289339721	0.1699159048	0.4856281865
H	4.2418921871	1.7240595052	1.1587666241
H	–1.9252199565	–1.0979044273	2.0537997156
H	0.8906358097	0.6661968457	2.4344758517
H	2.1103788566	1.956549646	2.4512443842
H	3.585646299	–0.6874317443	–1.624864661
H	2.1192052069	0.0757645878	–2.232121054
H	3.8555646603	1.6454607901	–1.3364554659
C	–4.7371442174	–0.4705411612	1.7442826362
H	–1.255476184	0.4422100096	–1.6336897187
H	–3.4123967031	1.8184398742	–0.5143097145

H	2.5823199616	3.0702368057	0.1319033162
H	–1.3229782426	–1.4549894201	–2.2964673724
H	–2.8200817807	–0.1816382776	–2.7231139426
H	–2.8985745337	1.5420503223	1.1639057574
H	–4.5530408244	2.0832928942	0.8173901015
H	–5.8281268259	–1.0835480033	–0.6930355139
H	–0.5936901065	2.3638661166	1.7369691109
H	0.6960298172	3.5713787554	1.5672448056
H	0.804442911	1.9590716257	–2.0993077164
H	2.1239307387	3.1185215556	–2.297646328
H	–1.2699230313	2.6650707415	–0.6098168813
H	–1.2271116673	4.2347076159	0.1924053814
H	0.9606791416	4.755164425	–0.848940202
H	–0.1475376981	4.2427891805	–2.1230617238
H	–5.0273613495	0.1639859524	–1.6694202576
H	–6.1557236743	0.624910492	–0.3795063694
H	–3.9739191397	–0.3691786773	2.5224620419
H	–5.0747033144	–1.5131451424	1.7357563342
H	–5.595810781	0.1502306039	2.0367418169

Tabelle 313 Standardorientierung von *S*-1 [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	3.5984041568	–1.0452184131	–3.1069237538
C	3.5947188744	0.489666231	–3.0944085368
C	2.157678175	–1.5698630558	–3.1265844585
C	2.7428583956	1.0553364466	–1.9332224858
C	2.7144280404	2.6017738951	–1.939891166
C	–2.4006616421	–3.9597606539	0.3987425112
C	–2.0865680913	–4.1445169327	2.8856325971
C	1.3678319518	–0.9811461872	–1.9489270067
C	1.8825173278	3.1194110197	–3.1222015912
N	1.3567251493	0.5031995288	–1.878393325
C	0.331669536	–2.0087044188	1.5565803291
C	2.1681308505	3.234296016	–0.6445344737
C	0.4244530992	1.1022208917	–2.8646290573
C	–2.5341655237	–3.2156002541	1.7422953716
C	0.4450301986	2.6452471004	–2.8731646487
H	–2.2033197485	–3.6749839208	3.8697023689
Li	0.6264344846	0.8758147784	0.064244481

P	–1.4144321069	–1.6774144153	1.6577016565
C	–4.0029653458	–2.7961795113	1.9509371619
N	0.7218408405	2.9979151341	–0.403023783
C	–0.0884344538	3.3493207396	–1.6043165559
B	–1.9221625181	–0.4402256782	0.2383861172
C	–1.625375154	–0.8413786865	3.2891257388
C	0.2953565229	3.8243541553	0.7518181683
C	–1.5831371934	3.1190690849	–1.3434426059
C	–1.1846767692	3.6354769425	1.0891660077
C	–2.06859898	3.9260363283	–0.1306407415
C	1.9143830386	0.3942070656	1.7878342586
H	4.1649647537	–1.4172709871	–3.9700911098
H	4.10958457	–1.4199236219	–2.207445941
H	4.6182517017	0.8753988582	–2.9924026987
H	3.220090272	0.8508503262	–4.0605898255
H	2.1381246362	–2.6649194167	–3.0513642763
H	1.6790330461	–1.3135656347	–4.0820506492
H	3.224131158	0.726687114	–1.0005601825
H	–4.1574829601	–2.3043247873	2.9186006515
H	3.7558415479	2.9393302723	–2.0310535048
H	–1.0384386573	–4.4453484096	2.7735333479
H	1.8134200086	–1.3424825904	–1.0131991738
H	0.3270834203	–1.3187643267	–1.9571984261
H	–4.6476934191	–3.6864820217	1.9321077878
H	2.261526078	2.7485162285	–4.0811792975
H	1.9252298138	4.2158208835	–3.1671438495
H	0.5849437077	–2.5270044665	0.6250982184
H	0.718847818	–2.5748342099	2.4127935406
H	1.0205963084	–0.7333341145	1.556623407
H	2.7167046056	2.85955804	0.2275909194
H	2.3547457076	4.3239024772	–0.7009398693
H	0.653278779	0.768824135	–3.8910465002
H	–0.5762377493	0.7245878431	–2.6284994737
H	–0.2044928534	2.9632164784	–3.7002283584
H	–4.3462636794	–2.1149697406	1.1652749649
H	–1.2066683121	0.5305038986	0.456442153
H	–2.6991004911	–5.0570671349	2.8847452059
H	0.0417487074	4.4366090185	–1.7909227938
H	–1.6687142177	–0.9440457404	–0.8373425232
H	–3.0828990335	–0.1060688429	0.3379261942
H	–1.3213447371	–1.4872149532	4.1192008153
H	–0.9832884301	0.0446193319	3.291014929

H	–2.6601827383	–0.5210709348	3.4395930267
H	0.9237600519	3.5555660939	1.60830361
H	0.4911787299	4.8918664645	0.5288008014
H	–1.7816457348	2.0554255678	–1.1741525605
H	–2.139645508	3.413485762	–2.2435669997
H	–1.3565809687	2.6077733092	1.4301618676
H	–1.442707124	4.3001680742	1.923852243
H	–2.0289769158	5.0009164456	–0.3649861176
H	–3.1158788647	3.6864208267	0.0892954006
H	1.6612618232	1.4666363783	1.894784734
H	2.8565009357	0.3320889077	1.2158635511
H	2.1630187419	0.068036724	2.8076044755
H	–3.0262776147	–4.8631064756	0.4116218864
H	–1.3662734173	–4.2736243131	0.2142154799
H	–2.7231366112	–3.3366399667	–0.442547658

Tabelle 314 Standardorientierung von *S*-2 [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	2.836524011	–2.1709154438	–4.6592042403
C	2.8270084379	–0.6359593733	–4.6382365714
C	1.3978417696	–2.7020981435	–4.6716142138
C	1.9841098883	–0.0790546573	–3.4660405966
C	1.9458635561	1.4679262831	–3.4715550107
C	0.5907798437	–1.5715880764	4.6796946511
C	0.617002057	–2.1251563754	–3.4817042197
C	1.0838429852	1.9860296629	–4.63181308
N	0.6008368047	–0.6423955406	–3.3998937074
C	–0.8434466472	–0.7364838855	1.622698234
C	1.4266668622	2.0965542788	–2.1648023448
C	–0.3450485795	–0.0428365385	–4.369313744
C	1.5581109575	–1.1579258885	3.5561170388
C	–0.3438938183	1.4998728393	–4.3534042664
H	0.3873701877	–2.6490555016	4.6740564665
Li	–0.0858237583	–0.2658818487	–1.3960336299
P	0.7677345255	–1.4585187835	1.8502741152
C	1.8529985229	0.3513113957	3.6675799538
C	2.8775788182	–1.9452198927	3.6795939951
N	–0.0076033989	1.8291276842	–1.885488344

C	–0.8547742057	2.1780597915	–3.0609725891
B	1.8890719737	–0.8673571804	0.370180903
C	0.4914148499	–3.2801217076	1.760151436
C	–0.4182595378	2.6243433579	–0.7034649826
C	–2.3387072391	1.9219664212	–2.7620995675
C	–1.8889666279	2.4081541766	–0.3400078974
C	–2.8008282471	2.7165634946	–1.5334156634
C	–1.9383142769	–1.4405335008	–0.9435966396
H	3.3974443478	–2.5359306172	–5.5291398714
H	3.356067091	–2.5482151314	–3.765886083
H	3.8502972428	–0.2482941751	–4.5419038658
H	2.4440443999	–0.2707647843	–5.6002556744
H	1.3831181257	–3.7979572251	–4.6061277201
H	0.9098329297	–2.4378750275	–5.6203661137
H	2.4734962986	–0.4055312262	–2.5379036133
H	–0.3667351204	–1.0437602324	4.6014127748
H	2.983127176	1.8106080655	–3.5866909435
H	1.0300903106	–1.3274406806	5.6570165594
H	1.0727032733	–2.4931101171	–2.5532093368
H	–0.4226405823	–2.4698068944	–3.4861463228
H	3.573688486	–1.6991873966	2.870620103
H	1.4409898085	1.6206009258	–5.6014440598
H	1.1187107643	3.0828876245	–4.6723782613
H	–0.8004150724	0.3527013576	1.7397981298
H	–1.612818094	–1.1490124949	2.2867463414
H	–1.2539631401	–1.0049263735	0.2575715629
H	2.0039577323	1.7338329677	–1.3085755103
H	1.5869665318	3.1901511521	–2.2312814857
H	–0.1231098646	–0.3561170023	–5.4039090288
H	–1.3411401446	–0.4356024562	–4.1345616548
H	–1.0159373519	1.8239885841	–5.1601293198
H	2.7130394697	–3.0291246685	3.6711667648
H	1.3554083376	–1.3783859594	–0.6064128762
H	3.3672532112	–1.6985749594	4.6324775856
H	–0.7486791023	3.2695524372	–3.2385123815
H	1.8006835923	0.3457243423	0.3367814771
H	3.0364331207	–1.2438653458	0.4598477412
H	–0.1548547214	–3.6322148759	2.5706966175
H	–0.0017269532	–3.4939036458	0.8071832618
H	1.4396623516	–3.8243573144	1.7909402254
H	0.2327640504	2.3389206404	0.1301153562
H	–0.2403469596	3.6991702125	–0.9051401958

H	–2.5121059485	0.8537729523	–2.5882786515
H	–2.9251985353	2.2054344828	–3.6465378246
H	–2.0389950652	1.37023551	–0.0217247166
H	–2.137400679	3.0473301174	0.5171824684
H	–2.7666676498	3.7933058066	–1.7587978834
H	–3.8436423835	2.4752801154	–1.2932795664
H	–1.8961478951	–2.5349265908	–0.8244281945
H	–1.8548806393	–1.2583193412	–2.0328865843
H	–2.9597639079	–1.1311928585	–0.6737127985
H	2.3059118932	0.5690319026	4.6447908464
H	0.9364678176	0.9478176598	3.5859882223
H	2.5485217337	0.6860434902	2.8903990159

Tabelle 315 Standardorientierung von *S*-3 [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
P	–2.8466772035	0.5564802237	–0.4649523171
C	–3.2479976882	2.3932991635	–0.6746887626
C	–4.5066716738	–0.2706676921	–0.3510169969
C	–1.9028234598	0.0327425495	–1.8847508344
B	–1.8488623383	0.1462569307	1.1620621452
C	0.7588173917	1.0651700853	–2.2657480116
Li	0.8325554787	0.1993324718	–0.231994855
C	3.6493517525	3.7372120907	1.3700360067
C	2.3327944016	3.5177758283	2.1259845083
C	1.4741949767	2.4721083389	1.3999345688
C	4.3712252975	2.3964305045	1.1765266301
C	3.4630676883	1.3517861171	0.4859287715
N	2.1413139882	1.1681121414	1.1556963277
C	2.1958291002	0.3341551955	2.3816619043
C	4.1711128837	–0.0096198535	0.3041642771
C	4.3590870915	–0.70182451	1.661478041
C	3.4423872838	–0.9795837436	–0.6477559886
C	2.9489380432	–0.9993854294	2.1866412879
N	2.143671033	–1.4921190542	–0.1381782867
C	2.2878424658	–2.0317162728	1.2446664389
C	1.6626666872	–2.5548824887	–1.0540507242
C	0.9519121013	–2.5816623152	1.7602040153
C	0.3254934459	–3.1469594428	–0.6051936023
C	0.4063430588	–3.6746617555	0.8320604212

H	1.3477402472	0.2892385143	–2.7838781367
H	0.3706271284	1.7243913471	–3.0551095524
C	–1.9393643189	3.1958330778	–0.5322854304
C	–4.23414115	2.8371354097	0.4248358098
H	–3.8597679878	2.5980531355	1.4260836598
H	–5.2189130659	2.3713673919	0.3067829946
C	–3.8648143283	2.6675696805	–2.0604900733
H	–5.1515872187	–0.0113013747	–1.1971933197
H	–5.0144341711	–0.0195689864	0.5868499555
H	–4.3331556815	–1.3514076027	–0.3665994725
H	–1.7629734609	–1.0548228217	–1.8279918831
H	–2.3793163467	0.2704081525	–2.8433074843
H	–0.5422000447	0.5689945557	–1.8957673729
H	–0.6891905927	0.4914116987	0.9656461369
H	–2.3037172334	0.7344849311	2.1208792249
H	–1.9274321378	–1.0605452354	1.2889535778
H	1.4685728579	1.6979381764	–1.699488569
H	4.2963521499	4.443929203	1.9051577391
H	3.4352177254	4.1861827694	0.3883696052
H	1.7621098582	4.4527442369	2.1995943253
H	2.5419311313	3.197989709	3.156437021
H	1.1866297797	2.8768509851	0.4200685285
H	0.5473465934	2.2710920508	1.9455124532
H	5.2736534243	2.5307763619	0.5646517265
H	4.7084770828	2.0321529864	2.1552578977
H	3.233952229	1.7490560234	–0.5137215193
H	2.689921538	0.867085356	3.2113612514
H	1.1608066088	0.1569526342	2.6937259134
H	5.1468944167	0.196615137	–0.1564874628
H	4.9192464194	–0.0742408366	2.3636357856
H	4.9302830405	–1.6318076946	1.5403738878
H	3.2549072435	–0.4988533146	–1.6146820414
H	4.1205092466	–1.8337711537	–0.835577832
H	3.0082345573	–1.4742402315	3.1755283129
H	2.9935031896	–2.8878764991	1.1973729367
H	1.5731902431	–2.1185243126	–2.0550477103
H	2.4223345883	–3.358906878	–1.1122634226
H	0.2127836115	–1.7772927193	1.8436039029
H	1.1097599738	–2.981875068	2.7708776633
H	–0.4549196452	–2.3800970438	–0.6680806387
H	0.0432820146	–3.9466118613	–1.302081994
H	–0.5819130201	–4.0040341497	1.1745850965

H	1.0673792371	–4.5539996429	0.8672920533
H	–4.3778408233	3.9249843743	0.3687770161
H	–4.7884758041	2.099690806	–2.224608288
H	–4.1178238753	3.7337552184	–2.144693032
H	–3.167634349	2.4271664967	–2.8695081069
H	–1.1888994113	2.8862488167	–1.2669649264
H	–1.5102543664	3.0771987892	0.4680723889
H	–2.1454489089	4.2644003179	–0.6865735604

Tabelle 316 Standardorientierung von *S*-4 [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
P	–1.2935735119	–1.1390573257	–2.4789094996
C	–1.3337599309	0.6391485909	–2.3475825967
C	–3.0381008018	–1.7451301538	–2.883013712
C	–0.2271936195	–1.7463021862	–3.8734659136
B	–0.6044029227	–1.8390226928	–0.7968297971
C	–3.4784082429	–1.2624701587	–4.2791518281
H	–2.8509585377	–1.6773474471	–5.0760928773
C	–4.0092400931	–1.1880591789	–1.8225516252
C	–3.0648050453	–3.2863062172	–2.8371957807
C	–2.2616311696	1.6479707523	0.1902475808
Li	–0.7394934483	0.1037383177	0.8351020761
C	3.7965132377	1.5613989349	0.3115023446
C	2.7162013188	2.648812011	0.2497230217
C	1.3212869033	2.0066513185	0.2839210186
C	3.5749841942	0.6701832463	1.5417485899
C	2.1428053386	0.0850632146	1.5748500366
N	1.0698330799	1.1146793403	1.4430727821
C	0.8126882199	1.8761366728	2.6878207875
C	1.8994735789	–0.7914856411	2.8242429563
C	1.8424833486	0.0784564356	4.0881958462
C	0.6199921261	–1.6484445793	2.7575507255
C	0.61205158	0.981172156	3.9303980563
N	–0.6485628012	–0.8773547806	2.8100057845
C	–0.6499428106	0.0875419297	3.9443847754
C	–1.7707231898	–1.8351072711	2.9577547695
C	–1.9723778949	0.8652456101	3.9977493714
C	–3.1288437651	–1.133336473	2.9972553629
C	–3.1725470175	–0.0840384451	4.1149512607

H	–2.6171506003	2.5361030361	–0.3539771211
H	–3.1654538508	1.1439013195	0.5710587757
H	–1.7270508358	1.027341477	–1.0200235595
H	–1.9581530675	1.1285072551	–3.1047080369
H	–0.310423733	1.0288880804	–2.4306706257
H	–0.2392646906	–2.839995517	–3.9426711216
H	–0.5263263184	–1.3124387987	–4.8325340712
H	0.7999209745	–1.4326588332	–3.6584178735
H	0.3936321848	–1.1645383643	–0.5881436301
H	–1.46019186	–1.609808597	0.0412080536
H	–0.3365870975	–3.018698008	–0.8434406302
H	–3.4572902261	–0.1704409849	–4.3610300107
H	–4.5096364412	–1.5894581516	–4.4712473451
H	–2.7461692618	–3.6664109096	–1.86102175
H	–2.4200361367	–3.7340183108	–3.602451484
H	–4.087795518	–3.6413399353	–3.0230469657
H	–1.7243480467	2.0637180943	1.0638186466
H	4.7998380985	2.0055405829	0.3377786335
H	3.7460517696	0.9478239483	–0.600691579
H	2.8096912943	3.2422627771	–0.6692432918
H	2.8414545898	3.3489525923	1.0876925143
H	1.1944274201	1.4002322613	–0.6222083719
H	0.5313941792	2.7640794113	0.2672704404
H	4.2900684972	–0.163769024	1.5447923382
H	3.7776692291	1.2577248876	2.4463463946
H	2.0416604588	–0.5554560094	0.6879081212
H	1.6408910512	2.5677447008	2.9188697819
H	–0.0706695827	2.4994342979	2.5096161725
H	2.7387553981	–1.497563382	2.8869984144
H	2.7543111757	0.6729471084	4.2146438802
H	1.7467303659	–0.5517509852	4.9823689441
H	0.6043488166	–2.2470866862	1.8402630065
H	0.6504507798	–2.3554015044	3.6089979992
H	0.5265171087	1.6555849286	4.793556823
H	–0.5869570474	–0.4975478906	4.8868905163
H	–1.7230129294	–2.5359438665	2.1188841457
H	–1.6310361572	–2.4207200195	3.8880604551
H	–2.0875662814	1.4841934485	3.1008167507
H	–1.9396587135	1.5474862158	4.8580092837
H	–3.3216298805	–0.6548914412	2.028992999
H	–3.9125524723	–1.8882658947	3.1417008461
H	–4.1111308278	0.4824737799	4.0761703461

H	–3.1456603826	–0.5892883019	5.0922326303
H	–4.0244052446	–0.0940094355	–1.8175075898
H	–3.7429892358	–1.5242205895	–0.8153897511
H	–5.0263150756	–1.5433547423	–2.0393056203

Tabelle 317 Standardorientierung von *R*-1 [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
P	–2.2003775376	0.9151468479	–0.8079631022
C	–2.0737623862	2.7575572815	–0.7966457181
C	–4.0713267416	0.5550429345	–0.8291533238
C	–1.3147208761	0.4273599408	–2.272192664
B	–1.3270416328	0.1843011183	0.7783476571
C	–4.2516426943	–0.9721720657	–0.9377990656
H	–3.7970927726	–1.4945244005	–0.0892397652
H	–3.8054520244	–1.3647881232	–1.8591342444
C	–4.7372817509	1.2322654687	–2.040830794
C	–4.7212686246	1.0555369982	0.47577334
H	–2.5746929699	3.1839041457	0.077406464
H	–2.4952560579	3.1968457302	–1.7064833502
H	–1.011950466	3.0189650292	–0.7521055668
H	–1.2793811081	–0.6633294345	–2.3727650206
H	–1.7165531387	0.8684253522	–3.1931535524
H	–0.1436263503	0.4730865719	0.6332761784
H	–1.7527471021	0.7146653732	1.7829455178
H	–1.4758238678	–1.0201182241	0.7824169154
H	–5.3225960968	–1.2179999397	–0.9535806054
H	–4.646898692	2.1444296872	0.5809547095
H	–4.2610969224	0.5981053153	1.3575516964
H	–5.7905576012	0.8001667132	0.4787541498
H	–4.2722336712	0.9211118018	–2.983716024
C	1.3331997126	1.5406234335	–2.4303553405
H	1.8973527037	0.8961479021	–3.1252291732
H	0.9162015568	2.3552354156	–3.0395097857
H	2.0727667046	2.0379679262	–1.773492099
Li	1.3944981001	0.4166152283	–0.5299221007
C	4.0610319211	3.7668026065	1.6198589155
C	2.7272610798	3.4254011021	2.2956559231
C	1.9145076322	2.4678330024	1.4108086368
C	4.8209751598	2.4782090153	1.2750678987

C	3.9572456085	1.5205427068	0.4207136435
N	2.6222815871	1.2226252706	1.0181456783
C	2.66611588	0.2335789412	2.1229508956
C	4.6991279075	0.2091278586	0.0746135497
C	4.8668442264	–0.6599109475	1.3286385339
C	4.0144833712	–0.6350377272	–1.0201219983
C	3.4507176603	–1.0490736169	1.7710760571
N	2.7163830546	–1.2363599706	–0.6193924142
C	2.8317111449	–1.9553215463	0.6820099768
C	2.2764314834	–2.16934423	–1.6846148379
C	1.4901996148	–2.5836251052	1.0800675747
C	0.9349136297	–2.8286458089	–1.3584132339
C	0.983997529	–3.54504076	–0.0036459346
H	4.6737210946	4.4097080413	2.2645531874
H	3.866607513	4.3366324363	0.6986594415
H	2.1337844606	4.3319161134	2.4724925582
H	2.911583214	2.9760548655	3.2814136424
H	1.6487096095	2.9931684604	0.4824652734
H	0.9756994042	2.1778193132	1.8924192949
H	5.7382175833	2.7110445787	0.7172102627
H	5.1365932502	1.9921182354	2.2069197508
H	3.7482699485	2.0489748783	–0.52086659
H	3.13070941	0.6592948227	3.0284199167
H	1.6282639764	–0.0010164275	2.3824638952
H	5.6815718463	0.4936850882	–0.3259227738
H	5.3981496873	–0.1256105723	2.1244328313
H	5.4591065164	–1.5552478119	1.0973824864
H	3.8368678095	–0.029666617	–1.9164971531
H	4.7160192179	–1.4413754309	–1.3072201022
H	3.4954365403	–1.6516997811	2.6885638829
H	3.5509674343	–2.7897631015	0.5422315745
H	2.2082710059	–1.6012250472	–2.6189068912
H	3.0490415882	–2.9497276728	–1.8294950127
H	0.7379784613	–1.8057348176	1.2522131201
H	1.6271054792	–3.1166340356	2.0307345102
H	0.1469394574	–2.0667448525	–1.341955336
H	0.6822905385	–3.530201407	–2.163919888
H	–0.0085896308	–3.9275995401	0.2626241592
H	1.6555048959	–4.4146574384	–0.0695282144
H	0.0518252877	0.9314955917	–2.1684964423
H	–4.6898581264	2.3259495248	–1.9804649435

H	–5.799453656	0.9537077849	–2.0852006382

Tabelle 318 Standardorientierung von *R*-2 [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
P	–2.0884017784	2.2718381979	–0.9677545789
C	–2.0093494777	4.1133784072	–1.0354382899
C	–3.9446938692	1.8521786055	–0.8997893092
C	–1.2217972427	1.7253133575	–2.4228864689
B	–1.1025240782	1.6176092848	0.5817892149
C	–4.0611963513	0.3251939041	–0.7249412367
H	–3.5910045604	–0.0101313264	0.2059904983
C	–4.5997499702	2.5575603758	0.3035583633
C	–4.6434235096	2.2735073957	–2.2044062349
C	1.5953931407	2.2908763696	–2.2370928284
Li	1.2445082994	1.1451867992	–0.3238729392
C	0.7034197672	–3.5407559273	–1.0353154909
C	1.3488700199	–2.7504902895	–2.180580648
C	1.3227960092	–1.2476820548	–1.862829366
C	1.3913576414	–3.196414879	0.2933937379
C	1.3939910478	–1.6718999768	0.5570728698
N	1.948919285	–0.8681173046	–0.5715441042
C	3.4294564469	–0.8797802177	–0.6458528376
C	2.1056959765	–1.3078050488	1.8802806793
C	3.6186578016	–1.539127534	1.7589661391
C	1.8671517779	0.1415947094	2.3493299612
C	4.1188274341	–0.5527116633	0.6961820916
N	2.4928247139	1.1816144625	1.4929639837
C	3.9288268835	0.8831711355	1.2382769468
C	2.3601147295	2.4909697063	2.1740330088
C	4.5712563789	1.9731473875	0.3688824441
C	2.9476981511	3.6325253159	1.3431369631
C	4.4191186053	3.361856657	1.0048442518
H	–2.3946700475	4.5603618664	–0.1144829825
H	–2.5652561238	4.5116589829	–1.8905680575
H	–0.9571554569	4.3928425213	–1.1443750323
H	–1.322941643	0.6423751015	–2.5624023676
H	–1.5228140321	2.2468196271	–3.3394417166
H	0.1730750769	1.9372826172	–2.1865380371

H	–0.1007201236	2.3163399911	0.5908742807
H	–1.7062309498	1.7251111738	1.6257587852
H	–0.8200737964	0.4556443951	0.3384523924
H	–3.5926265738	–0.213035327	–1.557814059
H	–5.1202226498	0.0337383704	–0.6948340437
H	–4.6075316335	3.6473574856	0.1849199921
H	–4.0865527735	2.3193982759	1.2416041903
H	–5.6457509015	2.2334226868	0.4006076795
H	1.627694227	2.2968971296	–3.3373541646
H	1.7186058682	3.3401830847	–1.9193351526
H	2.5196412783	1.7572877238	–1.9421286972
H	0.7578158136	–4.6205210294	–1.2243116699
H	–0.364880905	–3.2838605111	–0.9738167672
H	0.8148574632	–2.9212251252	–3.1245424884
H	2.3803434109	–3.0958721165	–2.3381354753
H	0.2768174903	–0.9178072968	–1.8226831385
H	1.8045139239	–0.6618779244	–2.6521555411
H	0.8799380251	–3.6919696269	1.1298598294
H	2.4150171013	–3.5919563735	0.2751296297
H	0.3421868917	–1.3654181806	0.6434906052
H	3.8112114712	–1.8617908676	–0.9740668125
H	3.7194056755	–0.1598508704	–1.4193200119
H	1.683308131	–1.9567993889	2.6595050894
H	3.8506139817	–2.572896957	1.4788453696
H	4.1123697999	–1.3518804048	2.7217794467
H	0.7947288634	0.3590099425	2.4008897726
H	2.2685251961	0.2279648767	3.3775766568
H	5.1977669438	–0.6869791258	0.5369815955
H	4.4577250813	0.9036076632	2.2152556606
H	1.2964433361	2.6616543775	2.3647500262
H	2.8715070915	2.4463866595	3.1562245555
H	4.1188242579	1.9811492905	–0.6292458924
H	5.6339045699	1.7282339544	0.2367071754
H	2.3666226959	3.7472802394	0.4193417059
H	2.8439071382	4.5699720533	1.9046430744
H	4.8093094157	4.1335733272	0.3298374348
H	5.020429838	3.4107104863	1.9252899541
H	–4.1855768586	1.7950847571	–3.0778136673
H	–4.6138791106	3.3589576294	–2.3571623495
H	–5.70116975	1.9768289864	–2.1733935977

Tabelle 319 Standardorientierung von *R*-3 [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
C	3.1099284263	–1.9044676096	–3.5390657579
C	3.2356580457	–0.3753111631	–3.5660841128
C	1.6300518002	–2.3046870316	–3.557730231
C	2.4291451524	0.2915992233	–2.4257498786
C	2.532246753	1.833071892	–2.4740907836
C	0.8873768792	–1.6194657168	–2.401274595
C	1.7576929031	2.3848529356	–3.6795746522
N	1.0000250427	–0.1385824074	–2.3668455615
C	–0.2875277362	–2.4530493021	1.0946829039
C	2.0323303608	2.5462555277	–1.2022963738
C	0.1273642126	0.5099788818	–3.3769039933
C	–4.0240518019	–1.353654071	2.9654181254
C	–3.1099306256	–3.5074136218	0.7093198644
C	0.2831129487	2.0444295848	–3.4318365088
H	–2.9910150563	–4.322429575	1.4308563376
Li	0.269791016	0.3492513195	–0.4308422379
P	–2.0258300673	–2.054918386	1.113893437
H	–2.8076477463	–3.8749151817	–0.2769020483
N	0.5685663832	2.4486642324	–0.9698239405
C	–0.1966717165	2.831177529	–2.1906021719
B	–2.3475068574	–0.6423763347	–0.190736885
C	–2.4982351217	–1.5691844727	2.8784151132
C	0.2125275037	3.3540054284	0.1500207197
C	–1.7070533544	2.743473608	–1.9381282606
C	–1.2824930898	3.3305606664	0.4740366257
C	–2.1249349773	3.6469199494	–0.7688072318
C	1.547390514	–0.2281362179	1.2850686889
H	3.6478647763	–2.3455819181	–4.3879225586
H	3.5820952966	–2.2981539967	–2.6264453365
H	4.2874388641	–0.0740451849	–3.4675023589
H	2.8963269611	–0.010188697	–4.5436337174
H	1.5162352167	–3.3916357917	–3.4535897972
H	1.1806462832	–2.0341129361	–4.5234381886
H	2.8752893418	–0.0517549122	–1.4813567063
H	–4.1647689353	–3.2165518965	0.6541719908
H	3.5993208604	2.0784914195	–2.5635041005
C	–1.7801817675	–0.2503632792	3.2304349806
H	1.2982708263	–1.9926784979	–1.4546740021
H	–0.1781680752	–1.8690318978	–2.4082463417
H	–2.113010836	0.5699368719	2.5862154358
H	2.1107677279	1.9547306795	–4.6235384071

H	1.8946400507	3.4717305828	–3.755697659
H	–0.0492567265	–2.9253828385	0.1333147862
H	0.0202185713	–3.128482676	1.901119733
H	0.5260356356	–1.2500191524	1.1131755559
H	2.5379143712	2.147842422	–0.3149264942
H	2.3170974239	3.6127640578	–1.285827379
H	0.3300931052	0.1264862533	–4.3911444392
H	–0.9035908213	0.2287447192	–3.1356116615
H	–0.3295064893	2.3921472935	–4.2749880637
H	–2.0086484063	0.0236393118	4.2700073382
H	–1.5649362048	0.2503830547	0.0989382197
H	–4.5823626291	–2.2855409435	2.8191529964
H	0.0303012866	3.8964762566	–2.4092851717
H	–2.0827849574	–1.1274451814	–1.2763847578
H	–3.4854692551	–0.2272913337	–0.1466051132
C	–2.078355627	–2.6596037581	3.8850986138
H	–0.6936747747	–0.3393033794	3.1329578269
H	–0.9925547582	–2.7977526042	3.9108197702
H	0.8003075262	3.0542580593	1.0250763178
H	0.518633507	4.3872572753	–0.107701922
H	–2.0003528995	1.710256147	–1.7233633928
H	–2.2293089247	3.0444868084	–2.8564011605
H	–1.5580580818	2.3432850844	0.8608945118
H	–1.4792882281	4.0574405597	1.2728360523
H	–1.9819088212	4.7011190001	–1.0519649736
H	–3.19190218	3.5177755704	–0.5507137498
H	1.4210548466	0.8698817337	1.3511466523
H	2.4616488526	–0.4226373632	0.6978541571
H	1.7836862613	–0.5391425179	2.3128195747
H	–2.5409190594	–3.6285695135	3.6641173593
H	–2.3992019493	–2.3660285496	4.8942548034
H	–4.3745907424	–0.6255509498	2.225863003
H	–4.2808962333	–0.9719330781	3.9630811826

Tabelle 320 Standardorientierung von *R*-4 [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z

C	2.7735562455	–1.5135301625	–4.1558451959
C	2.804640067	0.0189118032	–4.0742558283
C	1.32126278	–2.0060574611	–4.1815218539
C	1.9834051759	0.5488807225	–2.874470687
C	1.9893862275	2.0948689164	–2.813671169
C	0.5574201007	–1.4544181886	–2.968757091
C	1.1427070866	2.6868945775	–3.9493928091
N	0.5844231631	0.0230585246	–2.8260032216
C	–0.9547825228	–0.4879795587	2.1718866986
C	1.4895692391	2.6805793684	–1.4794937731
C	–0.3440343607	0.6900786311	–3.7680935931
C	1.4381441714	–0.4674115512	4.0373008522
C	–0.2975848362	2.2296198355	–3.6891810722
H	0.8475168147	–0.8184591678	4.8894141316
Li	–0.0983461642	0.3296727114	–0.7993552062
P	0.7230000013	–1.0395819266	2.4211365168
H	1.4169199841	0.6274322427	4.0312417985
N	0.0473433567	2.4477694443	–1.2094311607
C	–0.7878399742	2.8702093703	–2.3690628645
B	1.8011377358	–0.3186051873	0.9676537969
C	0.7350321504	–2.9273723753	2.5212739346
C	–0.3368375428	3.2148750818	–0.0007453643
C	–2.2796572368	2.649144783	–2.080336042
C	–1.8099057936	3.0213640652	0.3635550418
C	–2.7195542371	3.3966540949	–0.8134136404
C	–2.0556137786	–0.7603063181	–0.4675339782
H	3.3203319201	–1.8592293444	–5.0425016317
H	3.2869283048	–1.9393070795	–3.2809192327
H	3.8381606749	0.376315589	–3.9705132213
H	2.4240799246	0.4318055692	–5.0177205064
H	1.2785489536	–3.1029165269	–4.1560343904
H	0.8378771942	–1.6963756939	–5.1188920187
H	2.4671256513	0.1702038583	–1.9632806006
H	2.4800187522	–0.7860094319	4.1548026338
H	3.0361425382	2.4121878298	–2.915397839
C	2.1828763717	–3.4169073237	2.7294922033
H	1.0016210539	–1.8733597787	–2.0562637807
H	–0.49153808	–1.768623323	–2.9856346015
H	0.1959136208	–4.593706707	1.2404756222
H	2.2044585175	–4.515114726	2.7087666994
H	1.4892693185	2.3541905146	–4.9344583391
H	1.2081133808	3.7830641225	–3.9421720766

H	–0.9984552678	0.5908237838	2.3735178837
H	–1.692495455	–0.9919075732	2.8073547071
H	–1.3456555308	–0.588243925	0.7707645359
H	2.0549313582	2.2637900976	–0.6398772225
H	1.6845925441	3.7702492999	–1.4984054413
H	–0.1313472234	0.4123873199	–4.8147573179
H	–1.3510904147	0.3176524394	–3.548251905
H	–0.9607938458	2.6055517046	–4.4807792104
H	2.590290839	–3.101673017	3.6969722047
H	1.3572077795	–0.798855627	–0.0649431211
H	–0.646876587	3.9640085463	–2.5021567904
H	1.5853050054	0.8805174308	1.020028935
H	2.9808927535	–0.5668126525	1.084066692
C	0.1932570699	–3.4958430453	1.194382051
C	–0.1492748908	–3.4240463609	3.68209133
H	0.2056749086	–3.0671427316	4.6554895923
H	2.8512596654	–3.0502793627	1.9431524531
H	0.8128679249	–3.1925033392	0.3443220413
H	0.3108935922	2.8877657998	0.8197430732
H	–0.1343139951	4.2909288886	–0.1701203252
H	–2.4905105042	1.5805640918	–1.9627134912
H	–2.8553431303	2.9970115004	–2.948878426
H	–1.9831127053	1.9763816753	0.6461057953
H	–2.0395074718	3.6352165957	1.2441857872
H	–2.6644340102	4.4814518991	–0.9909393863
H	–3.7663442958	3.1663058258	–0.5800157014
H	–2.2281456396	–1.8464265094	–0.4262888254
H	–1.8732951973	–0.539666641	–1.5368237221
H	–3.0138894001	–0.2767465863	–0.2219026303
H	–1.1922817727	–3.1123688069	3.5631813542
H	–0.831184613	–3.1657292136	0.9991617552
H	–0.1328574399	–4.5223713311	3.7105861851

8.3.12 Angaben zu den quantenchemischen Rechnungen der Dilithiierung des Dimethylphenylphosphinoborans **120** (Kapitel 4.5.3)

Tabelle 321 Berechnete Energien der optimierten Verbindungen.

Verbindung	Methode/Basis	Min./TS	ZPE [Hartree]	SCF [Hartree]
cis-**173**	B3LYP/6-31+G(d)	Globales Min.	–1356,2409	–1356,601041
trans-Ph **173**	B3LYP/6-31+G(d)	Globales Min.	–1356,24621	–1356,607332
trans-BH_3 **173**	B3LYP/6-31+G(d)	Globales Min.	–1356,23802	–1356,598079
Mono-TS **120**	B3LYP/6-31+G(d)	TS	–1192,09638	–1192,637763
Mono-Ed **120**	B3LYP/6-31+G(d)	Globales Min.	–1192,11962	–1192,664354
Dilithiierung-Ed **120**	B3LYP/6-31+G(d)	Globales Min.	–1546,63584	–1547,395194
Dilithiierung-TS **120**	B3LYP/6-31+G(d)	TS	–1546,60066	–1547,356733

Tabelle 322 Standardorientierung von *cis*-**173** [Globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
P	–1.9207179918	0.5325103892	–1.8351065211
C	–0.2258911012	1.2787658584	–1.7945730896
C	–1.561450976	–1.2772938693	–1.9970246449
B	–3.0300973189	1.2273549764	–3.2678705726
C	–2.615959835	0.7641999427	–0.1490296829
H	–0.3375036965	2.3593929545	–1.6488990362
H	0.1702644129	1.1505656743	–2.808699363
C	0.7473526068	0.6972444067	–0.7508001665
H	1.7136959084	1.2111052743	–0.8214189172
C	–2.3912896766	1.9577791164	0.5570376935
H	0.3688268847	0.8555038231	0.2650024203
H	–2.5174367963	–1.8133017606	–1.9803173582
C	–0.5955114889	–1.8748172774	–0.9553203592
H	–1.1638945563	–1.4021865357	–3.0110315603
H	–0.4561180601	–2.9445195276	–1.1531651159
H	–1.0067823861	–1.7823955134	0.0558109271
P	1.0926223878	–1.1071278199	–1.0101275352
C	1.918241123	–1.6607193184	0.5280407196
C	1.344324979	–1.4589577835	1.7954243639
B	2.0623444192	–1.4842425621	–2.6467120295
C	2.0021550502	–1.8941952753	2.9467119306
C	3.240881518	–2.5361574716	2.8449375404
C	3.8179049449	–2.740674697	1.5897648099

C	3.1612845843	–2.3056482327	0.4347881722
H	0.3818556449	–0.961783968	1.8942906174
H	1.5488273371	–1.7325816627	3.9213230235
H	3.7524897321	–2.8747603129	3.7422311561
H	4.7800885021	–3.238930281	1.5054514526
H	3.6113101561	–2.4651590001	–0.5404700306
C	–2.9985591316	2.1796550169	1.7951630639
C	–3.8470174811	1.214926518	2.3445523062
C	–4.0891382915	0.0297140567	1.6454215552
C	–3.4814910868	–0.1921468071	0.4073343187
H	–1.7499425562	2.7298769853	0.140948404
H	–2.8130369207	3.1100539209	2.3255790809
H	–4.32229073	1.3890304453	3.3062777908
H	–4.7564541904	–0.7220909335	2.0588110636
H	–3.6986170726	–1.1133885493	–0.1262223514
H	–2.4031209798	0.9763531737	–4.276355407
H	–3.1348635911	2.4139391995	–3.0381220133
H	–4.0780336535	0.622972616	–3.1783358326
H	3.120513734	–0.8999529204	–2.5451101177
H	1.3654017177	–1.0414031746	–3.5350689054
H	2.1714339256	–2.6915090941	–2.6937218

Tabelle 323 Standardorientierung von *trans*-Ph-**173** [Globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
P	–1.6269073627	0.7268505463	–0.2428692176
C	–0.0331457761	1.5105909764	–0.7810258108
C	–1.2220687638	–1.0837718307	–0.203117633
C	–2.7743993942	0.9390228232	–1.6521937782
B	–2.2676153862	1.4003861692	1.4615770845
H	–3.2786956541	0.7781306828	1.7103349369
H	–1.3731091347	1.1669300306	2.2499140519
H	–0.2057121154	2.5931349323	–0.7999975362
H	0.209607328	1.196006403	–1.8010574024
C	1.1342387441	1.1883656746	0.1736957703
C	–0.0547754565	–1.4058492474	0.7518682212
H	–0.9967350787	–1.4363717749	–1.2147173632
H	–2.1277447507	–1.6013262475	0.1344212849
P	1.5390052919	–0.6222893232	0.2137177706
H	0.909006922	1.5409916181	1.1852629747

H	2.0400376823	1.7056705176	–0.1638928943
H	–0.2977203216	–1.0910523041	1.771773028
C	–2.4447092005	0.5002297284	–2.946592062
H	0.1177147389	–2.4884033238	0.7711033225
H	–2.4499082569	2.5894692195	1.3060525048
C	–3.3425708658	0.6770277423	–4.000327466
C	2.6863534119	–0.8339699257	1.6232777949
C	2.3564813108	–0.3949224969	2.9175604443
C	3.2542195258	–0.571465885	3.9714337328
C	4.4893183906	–1.1876113804	3.7439069888
C	4.8239389916	–1.6263542533	2.4608474007
C	3.9274146291	–1.4513340222	1.4027428708
H	1.4004332095	0.0860192172	3.1116049281
H	2.9896101111	–0.2284867689	4.968260717
H	5.1873002487	–1.3242594487	4.5659864809
H	5.7825077453	–2.1055246337	2.2798462789
H	4.1885670008	–1.7928224292	0.4055913873
C	–4.5776262327	1.2931346504	–3.7725117694
C	–4.9120954731	1.7315808131	–2.4893016115
C	–4.0154336006	1.5563624118	–1.4313621432
H	–1.4887013723	0.0192791689	–3.140867555
H	–3.0780776231	0.3342473322	–4.9972540213
H	–5.2757171928	1.429957005	–4.5944689082
H	–5.8706341825	2.21072698	–2.3080821308
H	–4.2764699352	1.897610472	–0.4340990727
B	2.1798540449	–1.2959158864	–1.4907881149
H	2.3606582851	–2.4852601605	–1.3358533337
H	3.1915470541	–0.6744403327	–1.7389284638
H	1.2857584638	–1.0608934396	–2.2791716866

Tabelle 324 Standardorientierung von *trans*-BH_3-**173** [Globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
P	–1.6366229491	0.7390737929	–0.4812949646
C	0.1125792544	1.310974981	–0.2682494972
C	–1.4426821903	–1.0775102935	–0.7798971824
B	–2.5423352224	1.6481297491	–1.9371139162
C	–2.4249458108	0.9211613262	1.167577902
H	0.0814282971	2.3767127299	–0.0128545236

H	0.560004291	1.2551810902	–1.2680051152
C	0.9567546844	0.5413849683	0.7602196977
H	1.9575806942	0.9824039725	0.8365796765
C	–2.2704745206	2.1241905887	1.8775531918
H	0.5199389191	0.6137902816	1.7636086457
H	–2.4466817569	–1.515323188	–0.833402327
C	–0.5705689466	–1.8583852576	0.2200596082
H	–1.03622435	–1.1460133789	–1.7956723787
H	–0.5316196135	–2.9191942634	–0.0551004651
H	–1.0029900779	–1.830301776	1.2269907785
P	1.1704440366	–1.272200299	0.4483732999
B	2.083053348	–2.1727670748	1.9051628964
H	1.3814342834	–1.9451275557	2.8706750055
C	1.9897428207	–1.4035235036	–1.1902156941
H	3.1765435649	–1.6509257883	1.9650923052
H	2.1206675177	–3.3433804356	1.5922043076
C	3.1158728273	–0.6089986585	–1.4653874115
C	3.8070235188	–0.7464604918	–2.6704393866
C	3.3899346755	–1.6870135587	–3.6161963395
C	2.2828825213	–2.4942524629	–3.3462687412
C	1.5892744694	–2.3554086764	–2.1412777723
H	3.4693277192	0.113758555	–0.7348049442
H	4.674395521	–0.1217577981	–2.866803567
C	–2.9241671173	2.3214310075	3.0951188874
C	–3.7508338736	1.3234823402	3.6183971803
C	–3.9258963872	0.1310125167	2.9131327538
C	–3.2698487928	–0.0679312576	1.6955783854
H	–1.6489919105	2.9211909751	1.4780177925
H	–2.7910143636	3.2574184327	3.6311611094
H	–4.2593827434	1.4771684242	4.5663755377
H	–4.5733781643	–0.647606673	3.307669415
H	–3.431156965	–0.999584505	1.1608991904
H	–1.8492724269	1.4056035534	–2.9051772369
H	–2.5481068812	2.8203109757	–1.6247735046
H	–3.6485288415	1.1550004563	–1.9909676696
H	3.9279662896	–1.7935917153	–4.5543151255
H	1.9559108927	–3.234381053	–4.0718272739
H	0.738163759	–3.0027410525	–1.9503025302

Tabelle 325 Standardorientierung von Mono-TS **120** [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
P	0.6676328939	1.6210508282	0.6460277386
C	0.6677577079	3.4625440159	0.6465561083
B	–1.1346548619	0.9092484342	0.7754909194
C	1.7436084735	1.1941158617	2.0859386151
C	1.3535637926	1.1224496109	–0.9316252797
C	1.1694064126	0.8130852182	3.3091649876
C	1.9785928736	0.4963833616	4.4048179508
C	3.3699892877	0.5561062676	4.290899627
C	3.9513998485	0.9301632844	3.0747026141
C	3.1429313779	1.2421833192	1.9796337864
H	0.2354621958	3.830899512	1.5819483516
H	0.0602276193	3.819586683	–0.1904060159
H	1.6855715699	3.853169626	0.5442022765
H	–1.0397782206	–0.2974746164	0.6492198065
H	–1.6912691702	1.4130978597	–0.185048442
H	–1.6881941589	1.2195465973	1.8053246691
H	2.2517795877	1.685636934	–1.2089926539
H	1.6016944825	0.054981142	–0.9069348902
H	0.0881469131	0.7605565882	3.4018179493
H	1.5206057863	0.2010785313	5.345870357
H	3.998972636	0.3085938498	5.1425117672
H	5.0336752962	0.9743282399	2.9782203861
H	3.6026241535	1.5147829231	1.0320553765
Li	–1.0888727441	0.1132471147	–1.7257928857
N	–0.3717657126	–2.0691624299	–1.8916501294
N	–3.1676422621	–0.8398943276	–1.8997512083
C	–2.8471367706	–2.2406651413	–1.5571357473
C	0.1254413383	–2.6036968532	–0.6115181193
C	–1.6132632847	–2.7623295929	–2.2944985066
C	0.6695707259	–2.2533986259	–2.9164037983
C	–4.0791245032	–0.2705655823	–0.8905443116
C	–3.8149871326	–0.7589223174	–3.220011242
H	–3.7050976043	–2.9033957721	–1.7751905943
H	–2.6799123506	–2.2875366262	–0.4766881834
H	0.3845493683	–3.6739896397	–0.7009868233
H	–0.6210568646	–2.4850831526	0.1752675746
H	1.0189081587	–2.0541276078	–0.3041493088
H	–1.5254819919	–3.8514571937	–2.1266250013
H	–1.7406176799	–2.6246394877	–3.3728887566
H	0.3287501965	–1.8507646517	–3.8726231078

H	0.928324649	–3.3192074042	–3.0495447214
H	1.5729295007	–1.7122943886	–2.6208155205
H	–5.0341422825	–0.8245136987	–0.8495292369
H	–4.292539095	0.7725865901	–1.1401644281
H	–3.6066034803	–0.2924372895	0.093434141
H	–3.1666470552	–1.1634609993	–4.0005182647
H	–4.018532218	0.2864516742	–3.4656576359
H	–4.7690140078	–1.3162255914	–3.2343366273
C	–0.3800376462	1.7841768784	–3.2174434452
C	–1.7013228038	2.5283908214	–2.9754436427
C	–0.5168036134	0.8600288489	–4.4346495812
C	0.6868154049	2.8325902734	–3.5577949883
H	–2.007486891	3.1300902764	–3.8579787255
H	–1.6271763463	3.2247515377	–2.1285498674
H	–2.5466405373	1.8591894235	–2.7555195857
H	–1.2716586487	0.0689206446	–4.3035765104
H	0.4351399534	0.3641612061	–4.6724649211
H	–0.8183434286	1.4152611486	–5.348914019
H	1.661586513	2.3695457217	–3.7708521967
H	0.842302504	3.5434515221	–2.7327574761
H	0.4103293904	3.4306218412	–4.4482105212
H	0.4432607555	1.327411779	–1.9465890817

Tabelle 326 Standardorientierung von Mono-Ed von **120** [Globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
P	2.3573264953	0.4024786319	–0.1439910267
C	2.099983086	1.6059052201	1.2209660066
H	1.3161218667	–1.7550374756	–1.0820686739
B	1.0932597882	–1.0684009148	–0.106667663
C	4.1177700223	–0.1023484325	–0.030361343
C	2.244888215	1.4119912721	–1.6770010733
C	4.4411013345	–1.4663733548	0.0287931663
C	5.7769324602	–1.8726174372	0.1047129604
C	6.8000087592	–0.9222741378	0.1235083536
C	6.4867601837	0.4398979839	0.0665939594
C	5.1539248119	0.8466382334	–0.010177051
Li	–2.5330557598	0.2248527717	–0.0074969098
N	–3.2521148993	–1.1972717366	–1.4603176484

N	–2.9670354941	–1.2355367917	1.4849364679
C	–3.1526214467	–2.4648776294	0.6916018558
C	–2.129489473	–1.7790100327	–2.2138277944
C	–3.9157613449	–2.2079635185	–0.6123180245
C	–4.2056455508	–0.5746264091	–2.390715704
C	–1.9247745902	–1.4222196359	2.505939698
C	–4.2159481636	–0.7954136945	2.1252393179
C	–2.6223670925	2.3132894027	0.0911691935
C	–2.2562915337	2.8157557092	1.4937406368
C	–4.0568938857	2.7753894959	–0.2030974279
C	–1.6991127855	3.0170156202	–0.9104783622
H	2.2086798419	1.0901121951	2.179826592
H	1.0838365082	2.0072296833	1.1521718927
H	0.0095619665	–0.5183901337	–0.161080784
H	2.9587288771	2.2416718918	–1.6687295369
H	1.2302957078	1.8135343532	–1.7642723292
H	2.4480918629	0.7737578594	–2.5422493759
H	3.6478117812	–2.2076295436	0.0152327441
H	6.0151773431	–2.9321673679	0.1495078099
H	7.8381433792	–1.2390992897	0.1826357593
H	7.2790910526	1.1838855067	0.0817866651
H	4.9273563855	1.9094085838	–0.0543277422
H	–3.6845419104	–3.2415743628	1.2728005641
H	–2.1581007672	–2.8636791117	0.4659437951
H	–2.4747379388	–2.5605311118	–2.915100282
H	–1.3892982663	–2.2118380231	–1.5380491406
H	–1.6303627459	–0.9919700351	–2.7864544269
H	–4.0406657759	–3.1641316023	–1.1523221387
H	–4.9237712716	–1.8456573047	–0.386232449
H	–5.0109085256	–0.0891208737	–1.8322221084
H	–4.6463215261	–1.3113817794	–3.0865647223
H	–3.6913511327	0.1936115094	–2.9749039312
H	–2.1980415909	–2.2085597254	3.2327152714
H	–1.7815424064	–0.4829054269	3.0483920203
H	–0.9796568441	–1.6904726061	2.0272849013
H	–4.9838614212	–0.5809835122	1.3774982415
H	–4.0296251154	0.1285539722	2.6787429966
H	–4.6077568532	–1.5577618155	2.8233427576
H	–2.3335630124	3.9277444357	1.5870387364
H	–1.2233634167	2.5561578661	1.7796999186
H	–2.9144242568	2.400813239	2.2748619995
H	–4.7913884604	2.3456009071	0.4983606134

H	–4.3860883842	2.5047783301	–1.2195254062
H	–4.1737843603	3.8849863944	–0.1276669882
H	–1.9161369729	2.7363240352	–1.9539349193
H	–0.6363782236	2.7851221237	–0.7301945264
H	–1.7825373281	4.1318027907	–0.8645508912
H	2.8150319348	2.4333348766	1.1763900587
H	1.2662361195	–1.6547404971	0.9419928629

Tabelle 327 Standardorientierung von Dilithiierung-TS von **120** [TS, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
Li	–0.6910559121	–2.166605223	–0.6488768948
P	–0.7178919635	1.0497344052	–0.6532961362
B	0.9082515772	–0.0245158122	–0.6326342794
C	–2.0739085794	–0.1051792874	–0.9965117214
C	–2.3834084392	–2.2224880515	1.0131174066
C	–0.6420969677	2.320023032	–2.0021540099
C	–0.7925676069	1.9809762232	0.864457784
C	0.355217185	2.2742347494	–2.9905331608
C	0.3782284139	3.2064824243	–4.0348917028
C	–0.596997495	4.2041350543	–4.1082160851
C	–1.597391821	4.2611045662	–3.1300630588
C	–1.6192859965	3.3275216213	–2.0923543884
Li	1.2781872818	2.2005268868	0.9996737868
N	2.4861076949	1.8568417783	2.7253699288
N	2.5898530592	3.8180513479	0.5148550658
C	3.665445514	2.7077110309	2.4776070468
C	3.2939653405	4.0287018452	1.7943319378
C	2.8737497927	0.4519045619	2.9161710001
C	1.7057031882	2.3217157458	3.882566307
C	1.8289352888	5.0156748229	0.1236107892
C	3.5179638575	3.4436406025	–0.5631193887
C	–3.5741542882	–1.4203961083	1.5503866282
C	–1.3245254311	–2.2910630539	2.120805775
C	–2.8819024127	–3.629638881	0.6671806976
N	0.9932253885	–3.8779694058	–0.533556051
N	–0.9612822616	–3.0553898862	–2.7388933745
C	0.640329139	–5.1055631162	0.196076003
C	2.2458211711	–3.34136166	0.0208829306
C	–2.3781810772	–3.3446582768	–3.0149439636

C	–0.181415328	–4.308600711	–2.700928298
C	–0.4431521752	–2.1544216146	–3.7831264257
C	1.1548014162	–4.1509077335	–1.9743394077
H	1.0786711199	–0.6027818082	–1.6910822809
H	0.7156336649	–0.8245140072	0.2717133323
H	1.8911227512	0.6595792837	–0.3632838207
H	–2.1168336008	–1.183069689	–0.09704987
H	–3.0495142947	0.37043508	–0.8371548554
H	–2.0298022833	–0.4475965767	–2.0397507315
H	–1.5519027683	2.7719836576	0.8289981086
H	–1.0587703689	1.2888963782	1.6781114089
H	1.1174848858	1.5006361617	–2.9434947437
H	1.1585054411	3.1508846561	–4.7914463383
H	–0.581867659	4.9283371139	–4.9193286983
H	–2.3627481072	5.0327514946	–3.1787670831
H	–2.4070072611	3.3802471564	–1.3443109362
H	4.3529460461	2.1434703239	1.8387902281
H	4.2102069709	2.9246101615	3.4149352917
H	2.6323867848	4.6084552286	2.4466790487
H	4.2082899682	4.6346184951	1.6548089826
H	3.3926221812	0.0875921125	2.0249973044
H	1.9753031199	–0.1557171644	3.0554432592
H	3.5303934095	0.3191923833	3.7949506079
H	0.8128617029	1.7003565245	3.9891329508
H	1.3734642905	3.3524557329	3.7346843179
H	2.293267928	2.2705160912	4.8173068427
H	1.0910122003	5.2520664854	0.895576449
H	1.2916964128	4.8156106025	–0.8070429573
H	2.4862347119	5.8912509569	–0.0257540724
H	2.95073128	3.2577263125	–1.4788020334
H	4.0537740725	2.5250914293	–0.3100141661
H	4.2575917715	4.2415207336	–0.7582963068
H	–4.3849674659	–1.3509552132	0.8103299831
H	–3.2866551045	–0.3916561994	1.8094558702
H	–4.0048514998	–1.8798576717	2.4623823609
H	–0.9639556975	–1.2885901827	2.3916203337
H	–0.4398799574	–2.883022473	1.8408228842
H	–1.7230207704	–2.7507905416	3.0515227741
H	–2.0913526121	–4.2899531575	0.2793585438
H	–3.6809442206	–3.5993222001	–0.0878620982
H	–3.3082150561	–4.1522593192	1.5513635676
H	–0.2906128592	–5.5330158263	–0.1825851926

H	0.4923038067	–4.8748299619	1.2541470416
H	1.4356713317	–5.8689401189	0.1087177433
H	2.1096384458	–3.1300115366	1.0854845655
H	2.5029185866	–2.4059835128	–0.4800554721
H	3.0800863618	–4.0587079818	–0.0905290316
H	–2.9466857915	–2.4107970335	–3.0151599863
H	–2.7844013894	–3.9905520577	–2.2331111882
H	–2.5107982531	–3.8392902665	–3.9940857111
H	0.0050871979	–4.6844660407	–3.7240984381
H	–0.7896463924	–5.06693552	–2.1978652692
H	0.6003622731	–1.8992049045	–3.5895976984
H	–1.0151314046	–1.223412682	–3.7841477657
H	–0.5203354087	–2.6176536824	–4.7836097923
H	1.7629728135	–5.0612657336	–2.1356410671
H	1.7146911421	–3.3174533693	–2.4096609364

Tabelle 328 Standardorientierung von Dilithiierung-Ed von **120** [Globales Minimum, B3LYP/6–31+G(d)].

Atomsymbol	x	y	z
Li	–4.3189988494	–0.0761007581	0.3408491908
P	2.3913499092	–1.5751366109	–1.2164080578
B	0.7575956424	–1.0266472509	–0.3050375239
C	2.1433433499	–3.2230462906	–2.0521480283
C	–5.0295102112	1.8737982768	0.2171838014
C	3.7458782932	–1.9624644609	–0.0233769749
C	2.9482067662	–0.2398635854	–2.2282515985
C	3.4465584109	–2.2741180758	1.3123678474
C	4.4639298364	–2.5978100366	2.2166230428
C	5.7966446066	–2.6150809726	1.7974741035
C	6.1071228674	–2.3073664164	0.4688552242
C	5.0896595839	–1.9841983638	–0.4325659311
Li	2.3074904838	1.2459152457	–0.8593373025
N	1.2664304381	3.0232190683	–1.341548145
N	3.3233536101	2.3369245495	0.6675084301
C	1.574097579	3.9017115377	–0.1950648352
C	3.0161910502	3.7336262351	0.2948425112
C	–0.189194688	2.8560633823	–1.4973827247
C	1.8433931685	3.5387508256	–2.5934377624
C	4.7745646325	2.0941292435	0.6562883462

C	2.7727221074	1.9959350852	1.9895309289
C	–6.0072620886	2.0569330998	–0.9508920372
C	–3.8891046873	2.8831114662	0.0324653318
C	–5.7713188046	2.2423839457	1.5097410712
N	–3.4417648458	–1.2357278249	1.8745913874
N	–4.348764182	–1.8344037337	–0.8448354618
C	–4.5122866219	–1.4768688735	2.8531372937
C	–2.2965529717	–0.5907861612	2.5358590919
C	–5.6281508116	–2.0691085906	–1.5292696917
C	–4.052567942	–2.9084403966	0.1241860128
C	–3.2710263878	–1.6788539476	–1.8364069309
C	–3.030018937	–2.4726493292	1.1808487231
H	1.3491202605	–3.1141484639	–2.7990538399
H	0.3714940926	–1.8795433072	0.4691906828
H	–0.0460191157	–0.813501374	–1.1948394689
H	1.0238549297	0.0125929968	0.2949339548
H	3.0619347516	–3.5416489771	–2.5570076545
H	1.8443061642	–3.9897971793	–1.3276965956
H	3.9394111631	–0.3843643336	–2.6711074189
H	2.2150390935	–0.0753380536	–3.031694936
H	2.4121546091	–2.2621670413	1.6443451055
H	4.2134677605	–2.8368609705	3.2476301394
H	6.5880348629	–2.867706713	2.4990057492
H	7.1416784725	–2.3202520609	0.1337189289
H	5.3471273072	–1.7439395873	–1.4607448336
H	0.8768586071	3.650526366	0.610657504
H	1.3973881967	4.9638233756	–0.443736303
H	3.7129670553	4.0273617269	–0.4973407802
H	3.1945031892	4.4213127187	1.1412354435
H	–0.6162561934	2.4244326764	–0.5891179478
H	–0.3879037749	2.1695173831	–2.3251276861
H	–0.6960596592	3.8136899982	–1.703594116
H	1.6252920933	2.8401263317	–3.4057149175
H	2.9305818426	3.6243588772	–2.5140501114
H	1.43001795	4.5290175745	–2.8556143837
H	5.1740688282	2.2889700576	–0.3433994618
H	4.9703331809	1.0466009028	0.9007599037
H	5.3060307313	2.7336801738	1.3835586635
H	2.9758069515	0.9438191975	2.2059874169
H	1.6890038201	2.1359233554	2.0031137352
H	3.2190800275	2.6169726071	2.7869564558
H	–6.8836708373	1.3932743468	–0.873242092

H	–5.5363397248	1.8558091674	–1.9270741206
H	–6.4115707148	3.0979757498	–1.011027669
H	–3.3341087801	2.7176657978	–0.9050969154
H	–3.1552740803	2.8432562404	0.8547464277
H	–4.254911946	3.940093188	–0.0054445217
H	–5.1228314095	2.1792725598	2.3996190818
H	–6.6402811415	1.5906734807	1.6974075354
H	–6.167725024	3.2881302693	1.4920399234
H	–5.3901183674	–1.9145091147	2.3686155272
H	–4.8166432062	–0.5257905993	3.2994038868
H	–4.18407769	–2.159358043	3.6581052152
H	–2.6208937771	0.3605424366	2.9685055661
H	–1.5063162187	–0.3958838023	1.8058870827
H	–1.8784043861	–1.2205319321	3.3417302669
H	–5.8399360864	–1.2310081471	–2.1991559345
H	–6.4382450897	–2.1305979012	–0.7957253354
H	–5.6173855967	–3.0015435825	–2.1220236417
H	–3.6811262735	–3.8168557993	–0.3837881672
H	–4.9951364143	–3.1853217726	0.608837882
H	–2.3150529003	–1.4721654785	–1.3488932745
H	–3.5063426324	–0.8364938145	–2.4939154089
H	–3.1551753901	–2.5866564754	–2.4558971844
H	–2.8779503369	–3.3024525601	1.8955155729
H	–2.0605864849	–2.2828814211	0.7105051656

8.3.13 Angaben zu den quantenchemischen Rechnungen der Lithiierung und Carbolithiierung von Stilben **177** (Kapitel 4.6.2)

Tabelle 329 Berechnete Energien der optimierten Verbindungen.

Verbindung	Methode/Basis	Min./TS	ZPE [Hartree]	SCF {Hartree]
cis-Stilben·(MeLi·TMEDA)	B3LYP/6-31+G(d)	Globales Min.	–935.460802	–935.936700
cis-Stilben Carbolithiierung	B3LYP/6-31+G(d)	TS	–935.437770	–935.915410
cis-Stilben Lithiation	B3LYP/6-31+G(d)	TS	–935.440231	–935.912339
trans-Stilben·(MeLi·TMEDA)	B3LYP/6-31+G(d)	Globales Min.	–935.470552	–935.946138
trans-Stilben Carbolithiierung	B3LYP/6-31+G(d)	TS	–935.448767	–935.926206
trans-Stilben Lithiatiierung	B3LYP/6-31+G(d)	TS	–935.443653	–935.916164
cis-Anion	B3LYP/6-31+G(d)	Globales Min.	–539.905127	–540.104636
*trans-A*nion	B3LYP/6-31+G(d)	Globales Min.	–539.911808	–540.110865
E-Z-TS	B3LYP/6-31+G(d)	TS	–539.899622	–540.097637

Tabelle 330 Standardorientierung von *cis*-Stilben·(MeLi·TMEDA) [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.0171015423	–0.0007296033	–0.0386827024
C	–0.0546506715	–0.0175570393	1.3128679766
C	1.0283183084	–0.0513610134	2.3167352342
C	1.1187596649	–0.1443135949	–0.971906993
C	2.2644257047	0.5987216344	2.1367122801
C	3.2366469938	0.5784698938	3.1365769622
C	2.9995537583	–0.0883604116	4.3437877387
C	1.7709099231	–0.7226631008	4.5467279634
C	0.7954665697	–0.6932135717	3.5484321337
C	2.2294999084	–0.9744877735	–0.7244073254
C	3.2486054906	–1.1082142519	–1.6680102029
C	3.184200846	–0.4164881253	–2.8831759493
C	2.0795919227	0.397505802	–3.1515951052
C	1.0531338918	0.5205327144	–2.2126394353
C	–3.1141929719	0.3156618176	–2.1954284875
Li	–2.7080358283	–1.6778050746	–2.2452886321

C	–2.1524947285	–2.7197236281	–5.018297066
C	–0.4180570679	–3.1254107	–3.3971345624
N	–1.8720276616	–3.0802329025	–3.6211641942
C	–2.5256912779	–4.349386537	–3.2511268539
C	–2.6701427705	–4.5047660503	–1.7322434644
N	–3.3698849459	–3.3598055526	–1.1210359595
C	–4.8218407646	–3.4096395322	–1.3513199656
C	–3.0938091223	–3.2660383372	0.3191820189
H	–0.9779368354	0.1306782785	–0.5399085147
H	–1.0529310398	0.026918344	1.7504421173
H	2.4560046779	1.1351023716	1.2127076329
H	4.1806451882	1.0939999282	2.9765793654
H	3.758902815	–0.1009645504	5.1215753248
H	1.5676549377	–1.2327654856	5.4853025119
H	–0.164164905	–1.177296126	3.719666579
H	2.2898936177	–1.5232710428	0.2105730648
H	4.0955894451	–1.7565241497	–1.4552806486
H	3.9828366119	–0.5175386978	–3.6139856347
H	2.0127594205	0.934064262	–4.0951540029
H	0.1852482408	1.1370546469	–2.4336666004
H	–3.2693054916	0.7663983255	–1.1963410085
H	–4.0530941736	0.5209204454	–2.7469232685
H	–2.3531658061	0.9508339358	–2.6891045602
H	–1.6974182111	–1.7503319418	–5.2392313307
H	–1.7566561333	–3.4674961847	–5.7290044704
H	–3.232499373	–2.6286103615	–5.1694853281
H	0.0678110895	–3.8893046204	–4.0306306118
H	0.0179733282	–2.1491131846	–3.624327466
H	–0.1938486799	–3.3518292707	–2.3514293557
H	–3.515572824	–4.3628343189	–3.7195250342
H	–1.9758970196	–5.2202262347	–3.653093893
H	–1.6788795883	–4.5716242659	–1.2716633826
H	–3.1843922563	–5.4586107902	–1.5133142055
H	–5.2805919143	–4.2986128127	–0.8816918938
H	–5.2834715154	–2.5097599065	–0.9357601896
H	–5.0430733845	–3.4319767061	–2.4222166433
H	–3.4518719666	–4.153952532	0.8708512713
H	–2.0176677286	–3.1589613076	0.4860870763
H	–3.5903078105	–2.3792757883	0.7232570324

Tabelle 331 Standardorientierung der Carbolithiierung von *cis*-Stilben mit (MeLi·TMEDA) [TS, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.9391034814	–1.0173495892	–1.3036248826
C	0.3820287317	0.2742369558	–1.4235472212
C	0.6485992832	1.5071963625	–0.6964872959
C	2.3021304376	–1.2636902646	–0.7067758665
C	–0.0149735578	2.694603544	–1.1149451831
C	0.1798304993	3.9192992704	–0.4822702239
C	1.0545180125	4.0283601607	0.6071130386
C	1.7278978809	2.8785807035	1.0335497883
C	1.53157706	1.6477931009	0.4068483135
C	2.5391268727	–1.7788568769	0.5744042854
C	3.8415500781	–1.9732782207	1.0454072908
C	4.9380508413	–1.6631440066	0.2377303592
C	4.718240245	–1.1519608024	–1.0449727477
C	3.4157551749	–0.9527323684	–1.5072853484
C	–1.2508063448	0.9116228623	2.4414209155
C	–2.0136299624	–1.3584531366	2.6167260611
N	–1.9479430788	–0.1798441837	1.737451626
C	–3.2980699411	0.264278	1.3371466139
C	–0.2310565352	–2.7101170848	–0.3479234751
Li	–1.0518989637	–0.7827058252	–0.189365704
C	–3.9305691512	–0.6326037996	0.2721240087
N	–3.1438056852	–0.6823372955	–0.9761752356
C	–3.3012139396	0.5561430833	–1.7555113432
C	–3.5616896628	–1.829372466	–1.7960672498
H	0.7729666251	–1.6297435465	–2.1880049386
H	–0.3070037484	0.3984702655	–2.2609373511
H	–0.6829870954	2.642595559	–1.9735965445
H	–0.3476568034	4.7986562467	–0.8474957053
H	1.21458548	4.983759758	1.0997778489
H	2.4226613523	2.9375369368	1.8695161724
H	2.0783260364	0.7864205918	0.7707445636
H	1.6931652075	–2.0313894121	1.2048325272
H	3.9968851797	–2.3725758641	2.0452927672
H	5.950783407	–1.8176884885	0.6019879736
H	5.5609293015	–0.9036278519	–1.6861065885
H	3.2524231837	–0.5385233265	–2.4995781917
H	–0.2485451548	0.5819155185	2.7255351449
H	–1.7943883012	1.2158934282	3.3536582937

H	–1.1429987521	1.7759185107	1.7823853199
H	–2.573384985	–1.1414933304	3.5444234315
H	–0.9997830112	–1.666737502	2.8862379933
H	–2.4929863859	–2.1995695593	2.1095909809
H	–3.2103304601	1.2874490391	0.9582871554
H	–3.973204687	0.309661783	2.2117672266
H	0.5905189001	–3.3872845398	–0.5850818412
H	–1.0705316965	–2.9447428393	–1.0203281096
H	–0.5369007408	–2.9059888384	0.6939778482
H	–4.0161747211	–1.6562793252	0.6513649832
H	–4.9611467591	–0.2825421239	0.0762527803
H	–2.720564951	0.4792227282	–2.678608625
H	–2.9256140584	1.4172394837	–1.1981376363
H	–4.3586106068	0.7374728999	–2.0209951537
H	–4.6219974192	–1.7561868956	–2.0976584808
H	–3.4185785489	–2.7593255462	–1.238829177
H	–2.9471655633	–1.8758408827	–2.7001501917

Tabelle 332 Standardorientierung der Lithiierung von *cis*-Stilben mit (MeLi·TMEDA) [TS, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.2947852243	0.9091318645	0.3964734877
C	1.0822141056	0.8359166823	1.49321037
C	2.550498339	0.785268218	1.6593412754
C	0.6973705434	0.8529495983	–1.0124937624
C	3.4688025616	1.1911820581	0.6695648164
C	4.843467823	1.1324549515	0.8983548862
C	5.3443090485	0.6680650163	2.1199008245
C	4.4493749972	0.2754890936	3.1192702291
C	3.0742070346	0.3426073021	2.8910705573
C	1.3656528668	–0.2664960186	–1.5649742426
C	1.6413817412	–0.3491180291	–2.9291936479
C	1.2591763058	0.6823854268	–3.7970347794
C	0.5930888777	1.7959976009	–3.2734915016
C	0.3056763868	1.8760875623	–1.9085055357
C	–2.2716772713	2.0087513644	1.1326937801
Li	–1.7769164227	0.0277417665	0.3561660102
C	–3.8422762612	0.4405446315	–1.771814349
C	–2.1895052601	–1.2035933294	–2.365930914

N	–2.9862999526	–0.6426735434	–1.260634675
C	–3.7949058553	–1.6793480686	–0.5886550164
C	–2.9521888873	–2.5620036409	0.3375410975
N	–2.2619045624	–1.7774795024	1.3833603272
C	–3.1689853239	–1.4418435873	2.4938225341
C	–1.0920005255	–2.5032271039	1.9032102332
H	–0.9377400699	1.4145802836	0.7226179471
H	0.5552083248	0.8420040978	2.4556612208
H	3.101462368	1.5674572334	–0.278638254
H	5.5290283711	1.4578714653	0.1191012695
H	6.4167360097	0.6233892698	2.2930116877
H	4.8217258018	–0.0754272027	4.0791717173
H	2.3844999285	0.0476964685	3.6802925364
H	1.6802370822	–1.0691252435	–0.9014367828
H	2.1667942781	–1.2192340405	–3.318217425
H	1.4812460008	0.6205953967	–4.8593690542
H	0.2949599358	2.6095076659	–3.9319323508
H	–0.2120149226	2.7478042782	–1.5149510511
H	–1.9341106544	2.5781543186	2.0095766503
H	–3.2102887649	1.5051199905	1.4337626153
H	–2.5339450538	2.7363034488	0.3496981406
H	–3.2152362307	1.2017225052	–2.2436657477
H	–4.5704673078	0.0720744404	–2.5158791144
H	–4.3832132809	0.9097544762	–0.9452763732
H	–2.8370604198	–1.632607624	–3.1515268825
H	–1.5702883876	–0.417583678	–2.8045951052
H	–1.5189941248	–1.9859852646	–2.0023994126
H	–4.5730760543	–1.1709026227	–0.0089288163
H	–4.3159236942	–2.3195926029	–1.3237539781
H	–2.1877331505	–3.0838817317	–0.2469128405
H	–3.5951251286	–3.3421408123	0.783138356
H	–3.5232761311	–2.3486002986	3.0156379476
H	–2.645746138	–0.8032444079	3.2107558278
H	–4.0380303617	–0.8881183885	2.1294720111
H	–1.3758523664	–3.4605108887	2.3750860377
H	–0.3879460262	–2.7049614586	1.0910063093
H	–0.5808273659	–1.8848113871	2.6458409092

Tabelle 333 Standardorientierung von *trans*-Stilben·(MeLi·TMEDA) [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–1.4440717544	1.4477216462	0.379645714
C	–0.7765081019	2.3598128625	–0.361442045
C	0.5824369614	2.8603206352	–0.12180818
C	–2.8097522972	0.958748241	0.1504270213
C	1.1127941394	3.8280153086	–0.9987444549
C	2.3948000928	4.3496045344	–0.8174624492
C	3.1814879979	3.9149685401	0.2525038089
C	2.6707943418	2.9520214961	1.132461069
C	1.3922162383	2.4272239766	0.9506739122
C	–3.3817681741	0.0971033967	1.1086342252
C	–4.6794968433	–0.3944717322	0.9575382056
C	–5.4389330038	–0.0419281721	–0.1612566366
C	–4.8844877195	0.8081935807	–1.1262491895
C	–3.589794117	1.3005512163	–0.9740420258
C	–1.2346880733	–2.8370753552	–0.7265383384
C	0.1286408366	–4.3081226864	0.6050886079
N	0.1316891424	–3.1207550016	–0.26356626
C	1.0630405432	–3.2666366835	–1.397661309
C	0.6231844537	–0.9045701869	2.8361832636
Li	1.0200449191	–1.6106352683	0.9625309229
C	2.5230689221	–3.054871228	–0.9801803363
N	2.7277832672	–1.7606851401	–0.3030824129
C	2.7218533528	–0.6362753754	–1.2527361431
C	3.9780434305	–1.7555915043	0.4704372085
H	–0.9538419068	1.0116378086	1.2487109572
H	–1.2700637192	2.8033001665	–1.2263907321
H	0.5043535506	4.1777609181	–1.8308183081
H	2.7756626819	5.0981597139	–1.5081904026
H	4.1777972686	4.3230109754	0.4033771493
H	3.2708538426	2.6089412827	1.972060538
H	1.0298014491	1.6732225871	1.6437271282
H	–2.7949071561	–0.1810568421	1.9811920599
H	–5.098049435	–1.050926609	1.7167349368
H	–6.4502993351	–0.4217615015	–0.2817748335
H	–5.4657051865	1.0884896338	–2.001678549
H	–3.1822906297	1.9559846401	–1.7389759717
H	–1.8878942148	–2.6888479799	0.1373113669
H	–1.6429729946	–3.6591072048	–1.341457934

H	–1.2454934457	–1.9172846241	–1.3186624694
H	–0.2324293828	–5.2051045563	0.0699702941
H	–0.5187337689	–4.1228584322	1.4664691588
H	1.1339675223	–4.5131897826	0.983921505
H	0.7838915458	–2.5250611533	–2.1532976278
H	0.9643210694	–4.2572680861	–1.8784109847
H	1.3328938521	–0.1411387809	3.209836953
H	0.7035292164	–1.7379852792	3.5626704661
H	–0.3837866494	–0.4790658633	3.0128287495
H	2.8273402603	–3.8446581536	–0.2848056822
H	3.1718305491	–3.1519900025	–1.8701823579
H	3.5462591066	–0.7160744227	–1.9843495483
H	2.8264907463	0.3042718849	–0.7055628806
H	1.7769751767	–0.5990586558	–1.8018334896
H	4.8653787311	–1.8934595729	–0.1733370957
H	3.9563017939	–2.5554447287	1.2168325693
H	4.0719586239	–0.8028271864	0.9984070477

Tabelle 334 Standardorientierung der Carbolithiierung von *trans*-Stilben mit (MeLi·TMEDA) [TS, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.0727716321	–0.8277686901	–1.936384034
C	–0.1172561983	0.5835842128	–1.9136327574
C	1.0494973297	1.4419260838	–1.9357981271
C	–1.2288992593	–1.6277336935	–2.4310351131
C	0.8974336888	2.8487185253	–2.0809181187
C	1.9904817078	3.7082438745	–2.1229947024
C	3.2982364167	3.2109741097	–2.0194966838
C	3.476291271	1.8306047078	–1.8775209937
C	2.3837459287	0.9639928239	–1.8277248811
C	–2.5563999948	–1.1649928243	–2.4106747612
C	–3.6036471421	–1.9373312928	–2.9172875829
C	–3.352384316	–3.1974945903	–3.4677228283
C	–2.0377196111	–3.6704437683	–3.5079554304
C	–0.9962118432	–2.8955096874	–2.9961136939
C	0.3235108576	–1.9659011087	–0.0344453695
Li	–0.1988674109	0.0739175446	0.1857749722
H	0.8784536502	–1.2694802807	–2.2206925463
H	–1.0752680824	1.0832421875	–2.0435869785

H	–0.1078508393	3.2559439342	–2.1830113296
H	1.8247703434	4.7768732758	–2.2473243217
H	4.1526602276	3.8812837585	–2.0598427409
H	4.4817258492	1.4195383411	–1.8042129053
H	2.5668907632	–0.1014132863	–1.7154695307
H	–2.7779339976	–0.1800790279	–2.0109426208
H	–4.619230153	–1.5481307265	–2.8910712315
H	–4.1669287051	–3.7969254643	–3.8662371017
H	–1.8206580275	–4.6433812861	–3.9426673252
H	0.0224295068	–3.2751225771	–3.0379701182
H	1.3670592345	–1.8110796334	0.2747487859
H	0.2452315457	–2.9127256793	–0.5672128568
H	–0.3233952974	–2.0316102767	0.8573389297
C	1.8293174798	2.058613776	1.5480207591
C	1.4594819713	–0.0086024997	2.7131065271
N	0.822772636	1.0406105549	1.8996510472
C	–0.2975264103	1.6704088553	2.6252655095
C	–1.5509473128	0.7952167069	2.6563675691
N	–2.0616757286	0.4783122987	1.3074272258
C	–2.7446241515	1.6381410614	0.7123401329
C	–2.9928835026	–0.6603433476	1.3723891926
H	2.6517137663	1.5887085394	1.005160476
H	2.2320406967	2.5570561792	2.447830513
H	1.3881383754	2.8104126428	0.8890225072
H	1.8646495501	0.4011393664	3.6559076472
H	2.2791251912	–0.4587509751	2.1473337393
H	0.7490168256	–0.8033589438	2.9538746253
H	–0.5199513231	2.6220360875	2.1317690618
H	–0.0079250043	1.9167388298	3.6635974828
H	–1.3277088804	–0.1525232753	3.1569275866
H	–2.3263360205	1.2973141974	3.264003746
H	–3.1213976383	1.3705122655	–0.2780374833
H	–2.0534707449	2.4760937141	0.5906141146
H	–3.5970852117	1.9710909113	1.3318390329
H	–3.8728200686	–0.4361850568	2.0016791475
H	–2.4815360724	–1.534521809	1.7850375292
H	–3.335063233	–0.9146645651	0.3662613076

Tabelle 335 Standardorientierung des Übergangszustandes der Lithiierung von *trans*-Stilben mit (MeLi·TMEDA) [TS, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.7203269852	–1.106100706	0.1259065304
C	0.0719115295	–2.1967384643	–0.3514256114
C	–1.2530918192	–2.7063842961	0.0402584195
C	2.059158323	–0.7837082096	–0.3987202194
C	–1.8586947605	–3.7131767159	–0.7392215591
C	–3.1080838062	–4.2410370615	–0.4080385668
C	–3.7834818886	–3.7860064609	0.7278480491
C	–3.1898950457	–2.7992231259	1.5248584379
C	–1.947078957	–2.2638458746	1.1866334869
C	3.1085311844	–0.4500021936	0.4883218833
C	4.3841225711	–0.1333115166	0.0171037676
C	4.6504637296	–0.1174426592	–1.3566478731
C	3.6226282651	–0.4311411837	–2.2530518425
C	2.3495251469	–0.7579505408	–1.7821910368
C	1.8664937993	2.8904428211	–0.6894658338
C	0.7079505079	3.6454683403	1.2766837409
N	0.5849860937	2.8593373502	0.0369266708
C	–0.502685906	3.3686961584	–0.8220596989
C	0.236393347	0.2489224735	2.6557802507
Li	–0.1528758278	0.9240504398	0.6258221318
C	–1.8917443363	3.0007162821	–0.2953364248
N	–2.0661177829	1.544496976	–0.1202144892
C	–2.2720718382	0.8646861405	–1.4123933561
C	–3.2097473672	1.2708536273	0.7662012144
H	0.422786908	–0.4890482324	1.3397299769
H	0.5628618011	–2.8236373985	–1.1082121806
H	–1.334881044	–4.0848499131	–1.6180170948
H	–3.5499335263	–5.0138810288	–1.0329654945
H	–4.7518889646	–4.2008548349	0.9961487008
H	–3.6951769039	–2.4531005006	2.4242872752
H	–1.4907979465	–1.5162650503	1.8279574574
H	2.9170826425	–0.4680675265	1.5581230406
H	5.1762483197	0.097970973	0.7264254894
H	5.6432733358	0.1321684984	–1.7227820742
H	3.8151002735	–0.4248499096	–3.3241998728
H	1.5579221836	–0.9940111237	–2.4902905669
H	2.6559593362	2.4793848609	–0.0562973992
H	2.1426040019	3.9186416399	–0.9833473739

H	1.8029494394	2.2696704381	–1.5867243788
H	0.9297347317	4.7063658666	1.0630113736
H	1.5154257318	3.2329236379	1.8866210518
H	–0.2114393394	3.5931301203	1.8657759683
H	–0.359886172	2.9437202638	–1.8210279355
H	–0.439887927	4.4667175126	–0.9343955683
H	–0.7056280309	0.7422844481	2.9625491578
H	1.0631429887	0.9266268577	2.9253313968
H	0.336827072	–0.635550274	3.3003819679
H	–2.0567984546	3.4739343177	0.6783319108
H	–2.6565074123	3.4123843981	–0.978789092
H	–3.1828960862	1.2297500163	–1.9197400111
H	–2.3643363291	–0.2109292834	–1.2447034485
H	–1.4169832089	1.0278435048	–2.0738597454
H	–4.1493146984	1.6874503944	0.3621932886
H	–3.0271240052	1.7082523143	1.7526605179
H	–3.3285598638	0.1911844125	0.8832375912

Tabelle 336 Standardorientierung von *cis*-Stilben [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.1002582204	–1.7820393319	0.8144080488
C	1.0807455113	–1.5923644534	–0.0879929996
C	–0.9874786803	–0.8749055343	1.2534238615
C	1.4424112574	–0.5148925013	–0.9281589086
C	–1.1769328502	0.4337243555	0.7525170079
C	–2.2209775526	1.2396743712	1.2063870581
C	–3.120305046	0.7776894748	2.1775626568
C	–2.9515683315	–0.5144912679	2.6872961064
C	–1.9057924498	–1.3191489744	2.2313498894
C	2.4116365832	0.4709793663	–0.5377958377
C	2.849737916	1.4605364746	–1.4103906346
C	2.3702915906	1.5454635806	–2.7297057772
C	1.4235792674	0.5900520197	–3.1404471699
C	0.9738699052	–0.4065052242	–2.281891275
H	0.0508492856	–2.7468925047	1.3403765551
H	–0.4922453285	0.8105930927	0.0005306231
H	–2.3351112319	2.2426488859	0.7969248557
H	–3.9331172148	1.4114486362	2.5277418425
H	–3.6376126215	–0.89668406	3.4430990737

H	–1.7848393182	–2.3239080043	2.6361443419
H	2.8126252007	0.4259283038	0.4732679893
H	3.5828576273	2.1869897936	–1.056105081
H	2.7229435379	2.3183537567	–3.4093213813
H	1.0271572676	0.6271303687	–4.1564156061
H	0.2496407498	–1.1382424	–2.6356153707

Tabelle 337 Standardorientierung von deprotoniertem *trans*-Stilben [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.65213894	–0.1213605608	0.0579457384
C	0.6709304133	0.1111257095	–0.0443667235
C	–1.6197524283	–0.0299626277	–1.0509851123
C	1.5962393778	0.0232738645	1.039304311
C	–1.2335949884	0.3265028357	–2.3629782613
C	–2.1628090931	0.4083134153	–3.3966549071
C	–3.5212604652	0.13708558	–3.1661520462
C	–3.9242743934	–0.2178341629	–1.8747968465
C	–2.9885819555	–0.2988106565	–0.8392040748
C	2.3282662103	–1.1717623781	1.3192585752
C	3.2862824487	–1.2306354138	2.3280350343
C	3.5836027662	–0.1081195572	3.1179681784
C	2.8761975225	1.0784903786	2.8664518371
C	1.9150557325	1.1481979624	1.8610236139
H	–1.1252010231	–0.4096119954	1.0181522444
H	–0.1797005465	0.5340837455	–2.5315799025
H	–1.8300248706	0.6865269121	–4.3966268425
H	–4.2460101176	0.2017002862	–3.9760327334
H	–4.9731144027	–0.4332796322	–1.6716095218
H	–3.3158027458	–0.5765437835	0.1626792831
H	2.1266789247	–2.0526332481	0.7124484048
H	3.8124079283	–2.1697313666	2.5051007128
H	4.3387657259	–0.15654285	3.9000458795
H	3.0771054174	1.9650040069	3.4696163386
H	1.3899224651	2.0840015919	1.6787102376

Tabelle 338 Standardorientierung des Übergangszustandes der *E-Z* Isomerisierung von deprotoniertem Stilben [TS, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.7154527282	–1.3590193115	–0.2418593071
C	0.5356630365	–0.94336911	–0.1717722646
C	–1.9382215243	–0.5271592238	–0.0821530798
C	1.7949507296	–0.4415761195	–0.0907193703
C	–1.8761467674	0.8577796193	0.1768975278
C	–3.0345142668	1.6182485141	0.3226987065
C	–4.300566403	1.0228195134	0.2149857002
C	–4.3811484416	–0.3497157121	–0.0415801769
C	–3.216627852	–1.1085983664	–0.1869770092
C	2.5408333142	–0.3791390999	1.1593484258
C	3.8298380916	0.124600154	1.2167609417
C	4.5062936335	0.6067648158	0.0768273603
C	3.8085642289	0.5575424013	–1.1480872005
C	2.5191656494	0.0621411697	–1.2504339203
H	–0.9666288919	–2.4225374051	–0.4360722808
H	–0.892526548	1.3152074119	0.2594566869
H	–2.9543304336	2.6861905205	0.5224587543
H	–5.2042155997	1.6188984615	0.3291845997
H	–5.3549027205	–0.8312470529	–0.1288853735
H	–3.287220641	–2.1780951147	–0.3868117637
H	2.0581458467	–0.7418302369	2.0649647675
H	4.3327826464	0.144420818	2.1857792719
H	5.5190253184	0.9977253149	0.1392862965
H	4.2946612361	0.9209129854	–2.0558383829
H	2.0194255855	0.0424388305	–2.2171405776

8.3.14 Angaben zu den quantenchemischen Rechnungen Carbolithiierung von *E*-benzyl-(2-propenylaryl)amin (**180**) (Kapitel 4.6.3)

Tabelle 339 Berechnete Energien der optimierten Verbindungen.

Verbindung	Methode/Basis	Min./TS	ZPE [Hartree]	SCF {Hartree]
MeLi TMEDA Addition ED	M052X/6-31+G(d)	Globales Min.	–1423,689465	–1424,46883
MeLi TMEDA Addition TS	M052X/6-31+G(d)	TS	–1423,678244	–1424,45871
*trans-S*2	M052X/6-31+G	Globales Min.	–1377,292314	–1377,98695
*trans-S*1	M052X/6-31+G	Globales Min.	–1377,295156	–1377,99018
*cis-R*2	M052X/6-31+G	Globales Min.	–1377,289621	–1377,98467
*cis-R*1	M052X/6-31+G	Globales Min.	–1377,289004	–1377,98377
*trans-R*2	M052X/6-31+G	Globales Min.	–1377,291953	–1377,98686
*trans-R*1	M052X/6-31+G	Globales Min.	–1377,293259	–1377,98855
*cis-S*2	M052X/6-31+G	Globales Min.	–1377,289161	–1377,98435
*cis-S*1	M052X/6-31+G	Globales Min.	–1377,289268	–1377,98419
*trans-S*2	M052X/6-31+G(d)	Globales Min.	–1377,645493	–1378,33719
*trans-S*1	M052X/6-31+G(d)	Globales Min.	–1377,64751	–1378,33994
*trans-R*2	M052X/6-31+G(d)	Globales Min.	–1377,645835	–1378,33781
*trans-R*1	M052X/6-31+G(d)	Globales Min.	–1377,646569	–1378,33874
trans-S-TS1	M052X/6-31G	TS	–2120,736463	–2121,88195
trans-S-TS2	M052X/6-31G	TS	–2120,741146	–2121,8867
trans-S-TS3	M052X/6-31G	TS	–2120,73574	–2121,88152
trans-S-TS4	M052X/6-31G	TS	–2120,742342	–2121,88803
cis-R-TS1	M052X/6-31G	TS	–2120,723641	–2121,86913
cis-R-TS2	M052X/6-31G	TS	–2120,730674	–2121,87703
trans-R-TS1	M052X/6-31G	TS	–2120,732847	–2121,87869
trans-R-TS2	M052X/6-31G	TS	–2120,740592	–2121,88603
trans-R-TS1	M052X/6-31G	TS	–2120,738348	–2121,88456
trans-R-TS2	M052X/6-31G	TS	–2120,741808	–2121,88795

Tabelle 340 Standardorientierung von MeLi TMEDA Addition ED [globales Minimum, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	1.6015617315	3.9857081784	–0.2280699995
C	0.3882980839	2.9734198014	1.5601177355

C	2.7868465691	2.8322724449	1.5332743501
N	1.575909017	2.8553503722	0.7083692132
C	3.9766436365	2.2502074228	0.7780100907
C	–2.5376058952	2.6831108768	–1.299400084
C	–1.3808991727	2.3810245159	–2.0055014227
C	–2.9060313266	1.9593651529	–0.1614589301
C	0.9429797213	1.5065620859	–3.5216444415
C	–0.5003094618	1.3334517048	–1.6014580336
Li	1.7322556512	1.1980144134	–0.5716163192
N	3.6832065126	0.9238280981	0.2161631728
N	0.6737413324	0.9985456779	–2.1881466252
C	–2.0786393957	0.9166138709	0.252000232
C	4.8079005086	0.4876223546	–0.6116664536
C	–0.8989926324	0.5975928671	–0.4265402691
C	3.4703807607	–0.0629725817	1.2788815806
C	–0.0776869531	–0.5487343812	0.0025119796
C	–0.0124349142	–1.0314620434	1.2602184506
C	0.7362609398	–2.2638427762	1.6712785216
C	–2.9613963649	–2.3731263889	1.9395945044
Li	–2.0251494594	–2.1403206775	0.091490141
H	1.6283167874	4.9424501823	0.3159366348
H	0.7061063727	3.9500125116	–0.8481846376
H	2.4689307574	3.9280422168	–0.8859488675
H	0.4501462757	3.8666631262	2.2000848113
H	–0.5010694617	3.0399902797	0.9351563012
H	0.2955832869	2.0866022123	2.1893742075
H	3.0443676805	3.8437413783	1.8838975253
H	2.5806366054	2.2338102212	2.4226113025
H	4.2462375587	2.9051279614	–0.0536592087
H	4.8450154254	2.199180182	1.4547285016
H	–3.1633798153	3.4992504995	–1.6453996354
H	–1.1327675001	2.9818514912	–2.8692880268
H	–3.8187022442	2.1854953454	0.3750696061
H	0.0269520169	1.7475916041	–4.07491418
H	1.4433863167	0.7113271733	–4.0863201222
C	1.8700620535	2.709285507	–3.5239137619
H	–2.376375705	0.2989875154	1.0942869255
H	5.0184065776	1.2393497952	–1.3708972458
H	4.5559338743	–0.4511610427	–1.1063539924
H	5.7142160662	0.3372433577	–0.0061483851
H	4.3276589821	–0.0965998596	1.9685845434
H	2.5656512454	0.1642193194	1.8414571447

H	3.3404955057	–1.0477036123	0.829490154
H	0.4829478984	–1.0468363018	–0.7893263422
H	–0.5503444762	–0.5203784703	2.0542495179
H	1.4840335018	–2.0367170419	2.4383817944
H	1.2428521208	–2.7249177711	0.8196990879
H	0.0408128255	–2.9857108924	2.1054944526
H	–3.5281760006	–1.4880520993	2.2744116674
H	–2.2994934105	–2.6343838915	2.7827790878
H	–3.708766666	–3.1869076041	1.8990775578
C	–4.5527164987	–1.6631149661	–1.041527761
C	–2.9997890523	–0.8371966343	–2.6579171781
C	–3.1970336076	–3.2042154559	–2.3072287057
N	–3.2446431581	–1.8862751194	–1.6667812769
C	–2.8006642293	–4.2972447297	–1.3240865081
N	–1.4879237824	–4.0518665789	–0.7156756682
C	–1.2704421908	–5.0407807942	0.3404391726
C	–0.4141910423	–4.1309669599	–1.7015155181
H	–5.353131274	–1.6664859668	–1.7991576581
H	–4.5437160317	–0.6993421791	–0.532641373
H	–4.7507317107	–2.4281031588	–0.2923568605
H	–3.7130897994	–0.9076024218	–3.4946616871
H	–3.1037765451	0.1391739443	–2.1882243839
H	–1.9824360711	–0.9222232652	–3.0449964796
H	–4.169299538	–3.4566701789	–2.7580892378
H	–2.4760602044	–3.1632649337	–3.1256967415
H	–3.5271850632	–4.3426910513	–0.5092833712
H	–2.8111151797	–5.2733973072	–1.8389294125
H	–2.0200850107	–4.9007656603	1.1189862525
H	–0.2843271704	–4.8938064949	0.7803644151
H	–1.3274571892	–6.0675774462	–0.0549579436
H	–0.4317978448	–5.0874471296	–2.249142018
H	–0.4824984739	–3.3113573952	–2.4166810089
H	0.5448748821	–4.0449037083	–1.1896930744
C	3.2274562672	2.508188908	–3.2506880716
C	4.1174576655	3.5766889345	–3.1819020977
C	3.6589922605	4.8783101562	–3.3915995418
C	2.3140711594	5.0908264105	–3.685710558
C	1.4300899042	4.0132808425	–3.7564601642
H	3.5780775637	1.4910816091	–3.1086313867
H	5.1690689472	3.3987894193	–2.9838460408
H	4.3461216249	5.7142694699	–3.3424544932
H	1.9518857291	6.0960109675	–3.8663500271

H	0.38830132	4.1928945917	–3.9967274046

Tabelle 341 Standardorientierung von MeLi TMEDA Addition TS [TS, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	2.0369474058	3.1573964867	–0.4307158812
C	0.9574817551	2.4852581565	1.587864874
C	3.3409279454	2.2549791496	1.3877747075
N	2.0642090594	2.1912708074	0.6730943828
C	4.4319534043	1.4734359368	0.6652940602
C	–2.0980064309	1.9209515955	–0.9571549507
C	–1.0004754486	1.44818343	–1.6794671767
C	–2.4275413333	1.3707904711	0.2772986239
C	1.0973563139	0.1948930256	–3.2334083625
C	–0.1710652697	0.4004366402	–1.2018306926
Li	2.0163511332	0.2786103935	–0.2481088549
N	4.0414003145	0.0793107354	0.4180473507
N	0.9085282618	–0.1313875238	–1.8337189353
C	–1.6193933859	0.3461462435	0.7898064246
C	5.0780155036	–0.5818016759	–0.3732021584
C	–0.4947700795	–0.1337967854	0.1098247233
C	3.8699252286	–0.6522008126	1.6755349822
C	0.3455792722	–1.1966257333	0.6732772018
C	0.1589787765	–1.7238702218	1.9466988496
C	1.126891628	–2.7576373167	2.4735558006
C	–1.8642659884	–2.8657645645	2.3699715617
Li	–1.2429211072	–2.5832450891	0.3715405271
H	2.1209949611	4.1870496864	–0.0487300828
H	1.0962431285	3.0490874228	–0.9695466615
H	2.8513141797	2.9714500147	–1.1303012059
H	1.1010773473	3.4603463008	2.0791993915
H	0.0211755946	2.4978543808	1.0318957394
H	0.8901836407	1.7040341346	2.3473342059
H	3.6701213101	3.2980009517	1.5166005007
H	3.1938449049	1.8464792792	2.3893419405
H	4.6388151107	1.9330934849	–0.3039081274
H	5.3602683663	1.5143993174	1.2594285659
H	–2.6941846651	2.727086192	–1.3718871659
H	–0.7713445038	1.9125860198	–2.6288911009
H	–3.2835319487	1.7257619087	0.8381992383

H	0.1498512125	0.4063089255	–3.748596057
H	1.5267223229	–0.6868202448	–3.724714387
C	2.0620523439	1.3449219143	–3.4724450028
H	–1.8725871141	–0.0908181057	1.7485698136
H	5.2704764024	–0.0100006009	–1.2798734318
H	4.7434322874	–1.5815255254	–0.6530219674
H	6.0189938025	–0.6672863105	0.1916262577
H	4.7607627128	–0.5587169344	2.3166366894
H	2.9942661103	–0.2934165622	2.2157106569
H	3.7045583628	–1.7056257028	1.4518613675
H	0.9702280904	–1.7416597902	–0.0322028381
H	–0.285164311	–1.086853682	2.7031138874
H	1.8701610969	–2.2854533132	3.1248388769
H	1.6648936394	–3.2331898679	1.6494668637
H	0.6265423216	–3.5330310661	3.05304684
H	–2.7324438674	–2.1996990356	2.4180003439
H	–1.47411983	–2.9926648924	3.3797559899
H	–2.2098068163	–3.8525730973	2.0238538953
C	–4.0146604423	–2.6158915643	–0.3286763511
C	–2.8221257691	–1.4591814434	–2.0437082664
C	–2.605191075	–3.843941942	–1.8560822322
N	–2.7797556065	–2.5919469142	–1.1153322085
C	–1.9402896586	–4.9144322695	–1.0026018638
N	–0.6560005334	–4.4675605844	–0.4527097588
C	–0.1480526527	–5.5002282032	0.4478124712
C	0.3200853286	–4.2034826326	–1.5114597028
H	–4.8966695883	–2.7017445483	–0.9824299238
H	–4.0862018106	–1.6924590752	0.2467680322
H	–4.0077250979	–3.4516495926	0.371521927
H	–3.6341123441	–1.5817935109	–2.7781025336
H	–2.9794266602	–0.5381271523	–1.485255396
H	–1.8685613638	–1.3784044239	–2.5669818894
H	–3.5696401094	–4.2216352343	–2.2295340786
H	–1.9880555572	–3.6387487124	–2.7323110235
H	–2.5849005455	–5.1734435979	–0.1583160463
H	–1.8066187353	–5.8282254356	–1.6065679113
H	–0.8535536436	–5.6510581959	1.2652518844
H	0.8028544721	–5.183293493	0.8725283872
H	0.0007322071	–6.4556749511	–0.0797288428
H	0.406345992	–5.0565207035	–2.2035962961
H	0.0572850985	–3.3040636159	–2.0689571503
H	1.2943748859	–4.0237733958	–1.0558610544

C	3.4207307669	1.1407998707	–3.2083461381
C	4.3512355651	2.1628393168	–3.371636773
C	3.9324938479	3.4216889431	–3.8067445265
C	2.5855922477	3.6337755264	–4.0905835778
C	1.660964671	2.6002275294	–3.9307363884
H	3.7359409657	0.1543899362	–2.8850746498
H	5.402535525	1.9798442918	–3.1758528707
H	4.6508138272	4.2222055969	–3.9365282071
H	2.252803041	4.6033944818	–4.4420812569
H	0.6174496001	2.7754571476	–4.1678258772

Tabelle 342 Standardorientierung von *trans*-*S*2 [globales Minimum, M052X/6-31+G].

Atomsymbol	x	y	z
C	–0.0412450704	0.1880299271	0.0364506212
C	0.0195446955	0.1221939177	1.5667613647
C	1.3797427428	0.1840411489	–0.5364083567
C	0.8581394145	1.280503561	2.137843742
C	4.5397661626	7.9030397108	1.463174139
C	0.9225530066	1.2311510774	3.6771503593
C	4.605234235	6.6495361889	0.8690293925
C	3.4243659489	8.2905604087	2.2169162581
C	2.1772997327	1.3491271429	0.0565369843
C	4.5611012553	4.0136887765	–0.4298223866
C	3.560471324	5.6933831216	1.0256333234
C	1.8369765191	0.0962886973	4.1526990561
Li	2.871911819	3.2134908657	1.9346594524
N	2.2225679284	1.3470409133	1.539886034
N	3.6091764081	4.3859656513	0.618523389
C	1.4126445518	2.5380195278	4.3097553852
C	2.349400636	7.4093805131	2.3081615125
C	3.193490332	0.3742647394	2.0887591407
C	2.3800911741	6.1418505607	1.7130066242
C	3.2395072313	0.4114534266	3.6231067755
C	1.1723202901	5.3085554604	1.6429441768
C	0.1390351087	5.2963088511	2.5062248976
C	–1.1541902226	4.5674790849	2.2630525053
N	2.8109109384	2.8668646482	3.9491683757
C	3.7338591202	1.7349874192	4.2404827239
C	3.2308658491	4.0950457242	4.6717874901

C	5.1522548371	2.1056215168	3.8100199797
C	4.6471101898	4.5114127599	4.288653277
C	5.6312102678	3.3646769127	4.5399523847
H	–0.6241544746	–0.6480176672	–0.3592657262
H	–0.5507070215	1.1118582331	–0.2683776648
H	–0.9868015096	0.173365103	1.9957428403
H	5.3698598552	8.5894128036	1.3395512867
H	0.449725883	–0.8400479593	1.8661960039
H	5.4929355443	6.3860772261	0.3086370947
H	1.3609996681	0.2778431545	–1.6262246587
H	3.3765057866	9.2702094164	2.6730603575
H	1.8679512433	–0.7698053775	–0.3042611773
H	0.3628871788	2.2186906379	1.8481593189
C	5.7830132984	3.2522550602	0.056830892
H	4.8915197342	4.8913382949	–1.0033782309
H	4.0430673973	3.3691456957	–1.1516092241
H	–0.101247324	1.064501583	4.0326532652
H	1.4359102181	7.731427527	2.7960075575
H	1.7307100801	2.3001421721	–0.2574809279
H	3.2091121325	1.3503350543	–0.2994891739
H	1.4978052149	–0.8780803098	3.7902382124
H	1.8399401551	0.0571073691	5.2474428823
H	1.1097689491	4.6970449624	0.7412146124
H	0.7891404567	3.3780053352	3.9991530166
H	0.20329854	5.8713238756	3.4286495699
H	1.3331480463	2.4418802989	5.4084088588
H	–1.3716637517	3.8345653563	3.0499813984
H	2.9458861138	–0.6565163182	1.7887716346
H	–1.1310916506	4.0436765196	1.3037831212
H	4.1702038313	0.6102144956	1.6573596799
H	–1.9985404953	5.2639017006	2.2392099516
H	3.9459794063	–0.3620970105	3.9460612325
H	3.7378228831	1.5810222011	5.3403322201
H	2.5210855305	4.8865811363	4.4200394843
H	3.1729029863	3.9081655557	5.7603810379
H	5.1752278797	2.2928982066	2.7308433862
H	5.8202511547	1.2601520757	4.0071292764
H	4.661414821	4.7915164185	3.2309356416
H	4.925288779	5.4016706056	4.8595282942
H	5.6958339944	3.1610388681	5.6169637074
H	6.6328162741	3.6384125417	4.199701174
C	6.0984993534	1.998801842	–0.4806760763

C	7.2172931728	1.2841674418	–0.042612183
C	8.0491147375	1.824345509	0.9378816649
C	7.7481221863	3.0774654017	1.4793703395
C	6.619809079	3.7774797493	1.0531306508
H	5.4659229255	1.5833969579	–1.2582154794
H	7.4405671154	0.3149720964	–0.4713633144
H	8.9225205957	1.2801506222	1.2738815192
H	8.3915586159	3.5058620175	2.2382675174
H	6.3777208334	4.7342955598	1.4986593105

Tabelle 343 Standardorientierung von *trans*-*S*1 [globales Minimum, M052X/6-31+G].

Atomsymbol	x	y	z
C	0.0853355658	0.0851483509	–0.1647186666
C	0.0665345575	0.009589593	1.3661520651
C	1.5348607725	0.1226744884	–0.6584565069
C	0.8372396095	1.1896888779	1.9857627432
C	2.4812716884	5.3607736545	–2.5545039049
C	0.8027240132	1.1459955439	3.5250750812
C	2.298321384	5.5133925423	–1.184857269
C	3.4904958062	4.5330257172	–3.0597808267
C	2.2725840467	1.2989006277	–0.012882826
C	2.1483284385	5.925850323	1.6966259245
C	3.1113039744	4.8230905218	–0.2428913111
C	1.6925552823	0.018173917	4.0620654162
Li	2.9004816002	3.1401345701	1.9785869497
N	2.2376583421	1.2870709755	1.4749856484
N	2.9128158367	4.8259521375	1.1153610826
C	1.2358260108	2.4608413936	4.1809514127
C	4.3373302915	3.8914566614	–2.1565579756
C	3.1634516081	0.2978785908	2.0716637765
C	4.1825210365	4.0299294423	–0.7725917912
C	3.121905289	0.329986248	3.6082842898
C	5.1705691372	3.4664588887	0.1577683997
C	5.8813087057	2.3363410038	–0.015620384
C	7.0131093304	1.8987466515	0.8729575708
N	2.6639502054	2.7806049171	3.9462476842
C	3.5795994743	1.6505691997	4.2589496458
C	3.0413701734	3.9904812004	4.7147946716
C	5.0047418236	2.0456957297	3.8681539061

C	4.4551527463	4.4447606278	4.3630502974
C	5.4556270403	3.3094714308	4.6089656787
H	–0.4529927386	–0.7630601687	–0.5964718867
H	–0.4306846628	0.9977062616	–0.4915703353
H	–0.96176979	0.0295769383	1.7427669994
H	1.8261368354	5.8903926198	–3.2370066256
H	0.5070279493	–0.9429155925	1.6813081849
H	1.4876775694	6.1391156863	–0.8322297244
H	1.5752286292	0.2336686212	–1.7456597352
H	3.6364985268	4.4237356535	–4.1260401288
H	2.0323665764	–0.8229422686	–0.4123039053
H	0.3395538851	2.1126240926	1.664159336
C	0.7020265891	5.5945392765	2.0328823859
H	2.6364911597	6.2329988175	2.6323369793
H	2.1682886522	6.8166046099	1.0497329704
H	–0.2402255297	0.9731346992	3.8139538429
H	5.1771365244	3.3143160536	–2.5277912895
H	1.8191059211	2.2395128991	–0.3454172699
H	3.3191257307	1.3320393601	–0.3180671712
H	1.3745562246	–0.9592392334	3.6895691187
H	1.6361306541	–0.0131823234	5.1558639654
H	5.3597826244	4.0794837072	1.0392472982
H	0.6396193388	3.2956081298	3.8002457358
H	5.6679659169	1.6994815178	–0.8727267853
H	1.0522875774	2.3834974543	5.2681060065
H	6.8298514164	0.9132665768	1.316551117
H	2.9184903997	–0.728129618	1.7553591345
H	7.1723598748	2.6141866038	1.6837339411
H	4.1653979476	0.5216022045	1.6941713843
H	7.9476626475	1.8245998849	0.3076164986
H	3.8085889071	–0.4454058942	3.9684193151
H	3.5551135706	1.4832415707	5.3560093614
H	2.3122801453	4.7695304152	4.4814653279
H	2.9700573676	3.7705312857	5.7963443101
H	5.0444107125	2.2301743658	2.7885635559
H	5.6796806692	1.2083007723	4.0763412447
H	4.4738771339	4.7450347523	3.3085845943
H	4.7141367664	5.3225436881	4.9621468138
H	5.5145044792	3.0975794093	5.6842428837
H	6.4566834999	3.6040641671	4.2817312506
C	0.0877765859	6.1530167239	3.1613220165
C	–1.2313497221	5.8374440465	3.4928210323

C	–1.961442073	4.9563517174	2.6917841071
C	–1.3612591588	4.3998856382	1.5595516428
C	–0.0384878435	4.7116920643	1.237662193
H	0.6536254088	6.8358755012	3.787105615
H	–1.6861277569	6.2739293357	4.3733414122
H	–2.9851338597	4.7106666716	2.9440657733
H	–1.9233888547	3.722335692	0.9274425198
H	0.4342788668	4.2730559062	0.3667679289

Tabelle 344 Standardorientierung von *cis*-*R*2 [globales Minimum, M052X/6-31+G].

Atomsymbol	x	y	z
C	0.1030575782	0.0956070361	–0.0021287519
C	0.10921457	0.0576694747	1.5303463492
C	1.5449258875	0.1095292937	–0.5216646919
C	0.90306353	1.2448012955	2.1061624509
C	5.4749345259	7.460601379	1.6559257906
C	0.9082399105	1.2409784931	3.6454307393
C	5.1579680419	6.309132433	0.9492739543
C	4.5893829929	7.9941144007	2.6008023913
C	2.303679519	1.2946926057	0.0835456068
C	4.4144411504	3.9594174357	–0.5604585031
C	3.9328091043	5.6053398373	1.1539366964
C	1.7751447246	0.0927510795	4.1758396322
Li	2.9121374786	3.2154956954	1.9741443037
N	2.2903480043	1.3199645665	1.5680908992
N	3.6419032533	4.3869408739	0.604740246
C	1.4020088647	2.5553167449	4.2664033098
C	3.3585526557	7.3679605234	2.7675018923
C	3.2365922166	0.3497380488	2.1666249306
C	2.9859044677	6.2215264551	2.0463394744
C	3.2049085624	0.3709924368	3.7028984793
C	1.5933545492	5.7881446298	2.2045517306
C	0.8297259321	4.9397642081	1.4818908155
C	–0.6544609934	4.8139424273	1.7082119097
N	2.8370077321	2.8356989118	4.0071422076
C	3.6987090953	1.6726914463	4.3577030669
C	3.2544529119	4.0324908984	4.7834252018
C	5.1553389185	1.9902334965	4.0306320946

C	4.7047786671	4.4092853603	4.4980408283
C	5.6365010092	3.2300662255	4.7907340312
H	–0.4472063738	–0.7596193283	–0.4033927899
H	–0.4135710289	1.0026315227	–0.3425830474
H	–0.9122694212	0.094663038	1.9238071191
H	6.4309369466	7.9407999854	1.4804176089
H	0.5481819075	–0.8897364809	1.8605752641
H	5.8886992399	5.9067250528	0.2596110453
H	1.5653913308	0.1911489047	–1.6124831281
H	4.841981942	8.8818916537	3.1644811988
H	2.0396456404	–0.8333932032	–0.2618105667
H	0.4071424438	2.1632195376	1.7661910996
H	4.7807198125	4.8269905673	–1.130469057
H	3.7391102483	3.4283551412	–1.2423793896
C	5.5894749535	3.0336395837	–0.2829611693
H	–0.1314897002	1.1082178933	3.9668150126
H	2.6324843118	7.7963784336	3.4526233083
H	1.8498054526	2.2306856863	–0.2624389476
H	3.348118859	1.304356471	–0.2338020785
H	1.4250537416	–0.8776995103	3.815149002
H	1.735590686	0.0693834913	5.2703902008
H	1.0753737752	6.3303700778	2.9993210479
H	0.8274290207	3.4030954263	3.8830357113
H	1.2724973737	4.4100610909	0.6444950837
H	1.2374374395	2.4993919338	5.3579408495
H	–1.2109009104	5.1577632907	0.829830861
H	3.0117168018	–0.6793661112	1.8457882788
H	–0.9721450549	5.4204460354	2.5608355388
H	4.2340611101	0.5926230755	1.7885876595
H	–0.9711952436	3.7815606706	1.8952950103
H	3.8762280993	–0.4233585872	4.0498386564
H	3.6203476454	1.5173341852	5.4545952635
H	2.5886083874	4.854314457	4.5145879541
H	3.1248139674	3.8200506499	5.8613020055
H	5.2513616021	2.1674668129	2.9564064089
H	5.7726184841	1.1181332877	4.2733399053
H	4.7950946031	4.7140155403	3.450887105
H	4.9726750016	5.2822014697	5.0995107216
H	5.6399505125	3.0192652013	5.868052524
H	6.6637088869	3.4757628428	4.5059919902
C	5.9235699358	2.026809629	–1.1991502371
C	7.0017333585	1.171225246	–0.9681443257

C	7.7688691174	1.3112466426	0.190774766
C	7.4455752655	2.3106535969	1.1103074694
C	6.3616512369	3.160441691	0.8772001153
H	5.3290931468	1.9147857417	–2.1004408613
H	7.2411629651	0.3976746933	–1.6873150637
H	8.6069852024	0.6509230515	0.3733483201
H	8.035350948	2.4283619457	2.0118185173
H	6.108093392	3.9314606303	1.5945181337

Tabelle 345 Standardorientierung von *cis-R*1 [globales Minimum, M052X/6-31+G].

Atomsymbol	x	y	z
C	–0.0214150584	0.1559571386	–0.0291008356
C	–0.0106304094	0.0922348506	1.5027746171
C	1.4183615208	0.1580680575	–0.5504518753
C	0.7992676678	1.2587071067	2.0999485086
C	1.6617994731	5.6389569342	–2.3162138653
C	0.7986076714	1.2186386401	3.6401353465
C	1.8246044585	5.7212291898	–0.9394684025
C	2.4541132602	4.7768728733	–3.0807828076
C	2.1898114006	1.3253102001	0.0709873205
C	2.2237147041	5.9782794272	1.8788617367
C	2.7897159974	4.9419152789	–0.2345884999
C	1.6692394032	0.066740419	4.1560801541
Li	2.909928797	3.1888628999	2.0137159812
N	2.1895248144	1.325343311	1.5593338921
N	2.8825349783	4.9054384466	1.1343888653
C	1.2824256535	2.5198920757	4.2893096588
C	3.4431222149	4.0486238245	–2.4258949659
C	3.1068204865	0.3172681398	2.1370780708
C	3.6639664174	4.1336316417	–1.0415844331
C	3.0961576993	0.3442347417	3.6737122737
C	4.8550164153	3.433460829	–0.5467802963
C	5.5430878085	3.5596503322	0.6064875976
C	6.8832280977	2.9047167372	0.8186663535
N	2.7123927815	2.8085890487	4.0180296429
C	3.5994510092	1.6507431175	4.316554028
C	3.1369031031	3.9906925094	4.8065671951
C	5.0271000053	2.0050681484	3.9036075162
C	4.5532127521	4.4162573131	4.4332790969

C	5.5324559416	3.2538957036	4.6348202549
H	–0.5871182739	–0.6830622935	–0.4432714171
H	–0.5226414812	1.0775055434	–0.3528925181
H	–1.0302269766	0.1376588447	1.900203897
H	0.8980929307	6.2416625206	–2.7944814469
H	0.4145182727	–0.8677090518	1.8159160461
H	1.1602249941	6.3680123653	–0.3816805809
H	1.4395634313	0.261514496	–1.6389853137
H	2.3213668951	4.6951781314	–4.1510774964
H	1.9008133178	–0.7961511825	–0.3075818473
H	0.3140822953	2.1902105116	1.7857463356
H	2.2240633791	6.9194504947	1.3070251828
H	2.8189280122	6.1853746087	2.7775968744
C	0.8011820109	5.6917028101	2.3427016093
H	–0.241865081	1.0750246799	3.9531826016
H	4.104506443	3.4122676725	–3.0064149589
H	1.7431832485	2.2695688012	–0.2594435831
H	3.2297277152	1.3403183428	–0.2596318371
H	1.3187073309	–0.9012388819	3.7889189898
H	1.6345283931	0.0347694435	5.2507849318
H	5.298014614	2.7747951117	–1.2973226992
H	0.6951262081	3.371311207	3.9360774564
H	5.1774603515	4.2445390257	1.3623869219
H	1.131176695	2.4364376855	5.3811327041
H	7.6686133369	3.6606023363	0.9272729253
H	2.8375266354	–0.7029440809	1.8220008564
H	7.1465215325	2.2715996049	–0.0328453686
H	4.1061016506	0.521108519	1.7413871997
H	6.9157883784	2.2850185866	1.7209585695
H	3.7706054443	–0.4489577161	4.0182465003
H	3.5837098432	1.4846480768	5.4137735912
H	2.4213903204	4.7921490346	4.6145185824
H	3.0860993107	3.7439888373	5.8832960396
H	5.0453339686	2.1895306358	2.8243255308
H	5.6817782946	1.1485494272	4.0982969169
H	4.5587081829	4.7372012907	3.3859507507
H	4.8477686725	5.277337536	5.0401005003
H	5.6236531451	3.0342886085	5.7060660905
H	6.5280110064	3.5263217737	4.2731730119
C	–0.0344485893	4.8153326201	1.6408397874
C	–1.3309286505	4.5514751521	2.0904132635
C	–1.8089564714	5.1512562083	3.2572859069

C	–0.983498641	6.0282166955	3.9659855029
C	0.30762691	6.2945902676	3.507943331
H	0.3385098005	4.349197409	0.7368868689
H	–1.9677767551	3.878533969	1.5281601856
H	–2.8118937683	4.9433873754	3.6076096181
H	–1.3436470116	6.4999478989	4.8717413179
H	0.9472091257	6.9748881126	4.0617513495

Tabelle 346 Standardorientierung von *trans*-*R*2 [globales Minimum, M052X/6-31+G].

Atomsymbol	x	y	z
C	–3.3564241885	–0.4287884593	–2.7202152132
C	–2.9260502044	–1.7609925653	–2.0993188074
C	–2.1117635727	0.3450345199	–3.1626986202
C	–1.9684667563	–1.5371052487	–0.914108858
C	–3.0946876074	2.6211151309	0.7341885542
C	–1.5390755996	–2.8762272738	–0.2846686195
C	–1.9694282106	1.9442432979	1.2250938078
C	–2.9822221143	3.7679072694	–0.0479507126
C	–1.1855050357	0.5550653779	–1.9607228573
C	1.7330258053	2.2649583753	1.3693895461
C	–0.6490103508	2.4118317991	0.8987796321
C	–0.5738436979	–3.63145721	–1.2056735286
Li	0.0128691797	–0.1175521852	0.5437440192
N	–0.7806213107	–0.7037694579	–1.2727298533
N	0.4216257032	1.6284356589	1.244957973
C	–0.8800944638	–2.7284179688	1.0913569314
C	–1.7013867468	4.277803714	–0.3040232707
C	0.27530705	–1.4333327531	–2.0157075464
C	–0.5665936643	3.6332127508	0.168314093
C	0.6747155729	–2.7553698461	–1.3419716396
H	0.4057801188	4.0436660913	–0.0741638241
N	0.430769493	–2.0369987844	1.0485601624
C	1.3485659639	–2.6271045643	0.0365473607
C	1.0442296578	–2.0648518221	2.3988889534
C	2.6588285744	–1.8399640803	0.0042294694
C	2.3635835631	–1.3004196785	2.4281621221
C	3.3325663274	–1.8557482016	1.3798947793
H	–4.0326542153	–0.5992948456	–3.5623915098

H	–3.9024844599	0.164907208	–1.9756046516
H	–3.7958486863	–2.3209525605	–1.7391543955
H	–4.0791260109	2.2681662514	1.0203606028
H	–2.445644523	–2.3728086023	–2.8709590245
C	–2.104132512	0.8252567942	2.1674386273
C	–3.1637485532	0.0050571391	2.3024344647
H	–2.3842670791	1.3242567054	–3.5666856029
H	–3.8646038819	4.2798774779	–0.4077001985
H	–1.5990232006	–0.204188077	–3.9613320129
H	–2.5141192715	–0.959585759	–0.1560323771
C	2.6991069861	1.9285883372	0.2475042322
H	2.1948839424	1.9397802267	2.3107015653
H	1.6433309031	3.3579352331	1.4515026101
H	–2.4540235204	–3.462052378	–0.1368196219
H	–1.5903818262	5.1884080135	–0.8818485086
H	–1.6962794245	1.1861741263	–1.2279372175
H	–0.2724305907	1.0724696199	–2.2583813848
H	–1.0189325498	–3.8271816336	–2.1846359482
H	–0.3155979951	–4.6001582461	–0.7632841064
H	–1.5287998757	–2.1622159069	1.762948986
H	–0.743124403	–3.7384438503	1.5190466963
H	–0.0517016969	–1.6731639484	–3.0397040181
H	1.1351143463	–0.7629416328	–2.0995599048
H	1.4066801863	–3.2419550243	–1.9975271879
H	1.5849553044	–3.6626999906	0.3610416802
H	0.3284716288	–1.6241875695	3.0976264061
H	1.2093223389	–3.1165942171	2.6983842359
H	2.4671527791	–0.8001454713	–0.2839142623
H	3.3152845981	–2.2727918991	–0.757947856
H	2.1589581396	–0.2465314093	2.2199178547
H	2.7948046985	–1.3642966865	3.4315116192
H	3.610348246	–2.8851898138	1.6416372031
H	4.2498697981	–1.2630524308	1.3554845862
C	2.2653387324	1.9258551068	–1.0844225859
C	3.138621513	1.5948363726	–2.1207112771
C	4.4639183686	1.2503376299	–1.8388884821
C	4.9079858829	1.2538204261	–0.5156922574
C	4.0300290763	1.5928854747	0.5170608563
H	1.2360944729	2.1880603832	–1.2925266829
H	2.7887713259	1.6062194723	–3.1463014238
H	5.1415682421	0.9868825866	–2.6408600689
H	5.9331250938	0.988583479	–0.2872915451

H	4.3751505491	1.5849416319	1.545807149
C	–3.3136874605	–1.0038314591	3.4075195234
H	–4.1319536385	–0.7294560889	4.0818331259
H	–1.2577588215	0.7127333058	2.8446147102
H	–2.3997416073	–1.0654250152	4.0044683403
H	–3.5433671481	–2.0037358747	3.0228944501
H	–3.9966992055	0.080819786	1.6054489535

Tabelle 347 Standardorientierung von *trans*-*R*1 [globales Minimum, M052X/6-31+G].

Atomsymbol	x	y	z
C	–2.2542887567	–1.012562849	–3.6453631605
C	–2.4869888617	0.3642412983	–3.0133249091
C	–2.7467377567	–2.1041370271	–2.6901377606
C	–1.7948527218	0.4698588913	–1.6420008137
C	1.7221355068	–3.010859848	3.3555465186
C	–2.0128504872	1.8563840288	–1.0044561337
C	1.0546246618	–2.543327728	2.2185889404
C	3.0945769009	–2.8333111944	3.5266961781
C	–2.0370830629	–1.9648652891	–1.3401338805
C	1.772586586	–0.8547674434	–1.0239568991
C	1.7674218533	–1.8223316615	1.2021516216
C	–3.4519727943	2.0076327561	–0.4977127916
Li	–0.6771808353	–0.5831427716	0.6319462105
N	–2.1975900602	–0.628370453	–0.7122193252
N	1.0464673992	–1.2725704911	0.1733030665
C	–1.0570864989	2.1523784189	0.154925359
C	3.8141571565	–2.1997926704	2.5071703143
C	–3.5146748512	–0.4408940933	–0.0679468368
C	3.177374119	–1.7148571648	1.3706795256
C	–3.649199724	0.942729777	0.585528922
H	3.769962722	–1.2081665188	0.6197362908
N	–1.2644673378	1.2538046572	1.317550601
C	–2.6856403825	1.2231971244	1.7551520292
C	–0.3820854151	1.6746520269	2.433227017
C	–2.8402955331	0.2322186664	2.9082519791
C	–0.4811910556	0.7118267526	3.6119514013
C	–1.933729437	0.6006177498	4.0873503111
H	–2.7613698878	–1.0815402662	–4.6115019538

H	–1.1808778943	–1.1519961514	–3.8310163626
H	–2.0985606795	1.1579119917	–3.6602208559
H	1.158347742	–3.5767896819	4.0890962138
H	–3.5650338142	0.5314292804	–2.9082643064
C	–0.3544920356	–2.8850401914	1.9803397958
C	–1.3143381143	–3.0151164675	2.9150235979
H	–2.5484990716	–3.0994654815	–3.098415074
H	3.5955947718	–3.214005043	4.4065209914
H	–3.8322863888	–2.0189280111	–2.5623855184
H	–0.7164061957	0.3401316246	–1.8060403091
C	2.0963883197	0.6297062323	–1.0922905744
H	1.1577095042	–1.0923841986	–1.9038021756
H	2.70138403	–1.4315233738	–1.1530653371
H	–1.805715973	2.5978046295	–1.7845371132
H	4.887299199	–2.0778424288	2.6016310298
H	–0.9619655202	–2.136163633	–1.4641187671
H	–2.4032635442	–2.70890297	–0.6279843581
H	–4.1817740749	1.8803937404	–1.3018475402
H	–3.5947428547	3.0100714901	–0.0797584073
H	–0.0189044233	2.0522451012	–0.1674889302
H	–1.2105137634	3.1999769881	0.4730138934
H	–4.3392950198	–0.546233882	–0.7910783209
H	–3.6330145296	–1.2380779717	0.6711775517
H	–4.6632239231	1.0092706293	0.9976088314
H	–2.9445384396	2.2346974581	2.1337890917
H	0.6379861384	1.7148011326	2.0488479936
H	–0.6678423449	2.6942637008	2.7529824128
H	–2.5666019361	–0.7674961823	2.5580300385
H	–3.8913654086	0.2042423055	3.216666291
H	–0.1076164294	–0.2721346079	3.3075105412
H	0.1657915781	1.0629448329	4.4206301874
H	–2.2561230591	1.5607723246	4.5104732883
H	–2.0208038016	–0.1488058862	4.8789435511
C	2.5242666321	1.3293946816	0.0441629732
C	2.7990074728	2.6962631263	–0.0221688655
C	2.6358569448	3.3913605694	–1.2237906387
C	2.2051315438	2.7058045533	–2.3608292236
C	1.9419872003	1.3352727999	–2.2919667193
H	2.6281435902	0.795315472	0.9803100413
H	3.1348920859	3.2206684618	0.8642627915
H	2.8425131641	4.4528150062	–1.2724140707
H	2.0735355324	3.2348998192	–3.2966579774

H	1.6053135662	0.8051256417	–3.1775870573
C	–2.6910393367	–3.5577797866	2.6489603546
H	–2.8393735059	–4.5161394356	3.1576187979
H	–0.5951714824	–3.109053678	0.9404583413
H	–2.8442297082	–3.7260390503	1.5797692287
H	–3.4748440132	–2.8828171601	3.0097453368
H	–1.0877131755	–2.7496929989	3.9464535154

Tabelle 348 Standardorientierung von *cis*-*S*2 [globales Minimum, M052X/6-31+G].

Atomsymbol	x	y	z
C	1.6710849383	–0.6083368154	–2.575977349
C	0.5779952128	–1.6794783839	–2.6360654339
C	2.4172538607	–0.7263591821	–1.2452294359
C	–0.3973595572	–1.5552441401	–1.4494451186
C	–0.1797911227	2.7519788962	–0.6155065034
C	–1.4803975552	–2.6530778729	–1.5140956878
C	–0.9818846184	1.9655687259	0.2284728669
C	0.9884079284	3.370621239	–0.1805183072
C	1.4236155106	–0.5761533621	–0.089873373
C	–1.0432190177	0.7610415056	3.7714992832
C	–0.5541330291	1.7134857533	1.5827440224
C	–0.8953689487	–4.0246815053	–1.1587211759
Li	–1.2019709517	–0.7776621817	1.1288606694
N	0.2917089905	–1.5474126861	–0.1211479939
N	–1.2208686744	0.7775624058	2.3199918508
C	–2.687031886	–2.3982963002	–0.6052462559
C	1.3486984224	3.2226739558	1.166240317
C	0.7177899855	–2.8862252978	0.3552850245
C	0.600153512	2.4300892436	2.0241564553
C	–0.404057978	–3.9288098388	0.2880929954
H	0.933892443	2.315123639	3.0474632814
N	–2.3512844856	–2.4386634136	0.8402586708
C	–1.6039925517	–3.6704959256	1.2154566715
C	–3.596411609	–2.3338637002	1.6407132183
C	–1.2246275193	–3.6066949797	2.6964847766
C	–3.2911005256	–2.2675242909	3.1338806859
C	–2.4759284961	–3.4878120396	3.5718848515
H	2.3564046782	–0.7142504388	–3.4215108724

H	1.2162054971	0.3880682197	–2.6445775415
H	0.0022567593	–1.595658322	–3.5641299794
H	–0.514833675	2.9054117897	–1.6373426627
H	1.0499288294	–2.6682658869	–2.6381344553
C	–2.2711853063	1.5304823067	–0.323190377
C	–3.3665488522	1.0304196502	0.2871484548
H	3.1754086862	0.0565128199	–1.1527183425
H	1.5796456804	3.9772579646	–0.8531078678
H	2.9382867173	–1.6900692161	–1.1963763091
H	–0.8888428865	–0.5752195391	–1.5311637131
C	–0.1036799166	–0.3185951681	4.2814424222
H	–2.0226810038	0.5890747622	4.235350567
H	–0.7079062437	1.7380890823	4.1489148294
H	–1.8566814986	–2.6610969426	–2.5436609468
H	2.2330890294	3.7217967464	1.5456985631
H	1.0038091298	0.4313709493	–0.1188895816
H	1.926963953	–0.6974756002	0.8704571671
H	–0.0773323273	–4.3034750058	–1.8275910821
H	–1.6704541331	–4.7937481292	–1.2495610484
H	–3.1234125672	–1.4190451605	–0.8156955861
H	–3.4509292469	–3.1672849735	–0.8225753063
H	1.5607824223	–3.2698269402	–0.2409758453
H	1.0768650606	–2.7640701529	1.3803901683
H	0.026382669	–4.8868096445	0.6031405256
H	–2.2909240906	–4.5323604638	1.0772792212
H	–4.127749348	–1.4383276665	1.3164029671
H	–4.2371241987	–3.2086506394	1.4238892897
H	–0.5791356395	–2.739602319	2.8776032242
H	–0.6489370181	–4.5010923086	2.9576482348
H	–2.7228019754	–1.3536709633	3.3333301297
H	–4.2295400128	–2.2038534983	3.692435334
H	–3.0849449084	–4.3952286356	3.4669661216
H	–2.1920413141	–3.4011887083	4.623292153
C	1.1072530488	–0.5762492875	3.6258253145
C	1.96755301	–1.577004865	4.078168485
C	1.6241243157	–2.347526311	5.1926257165
C	0.420382455	–2.0991088042	5.8540565572
C	–0.4340823141	–1.0912562455	5.3999782847
H	1.366685601	0.0232298725	2.7633737747
H	2.9052296843	–1.7555784386	3.564883072
H	2.2875777378	–3.1282620357	5.5423628682
H	0.1445307586	–2.6914308987	6.7179755613

H	–1.3735402835	–0.906901089	5.9106908306
C	–4.678640086	0.8597621149	–0.4313129745
H	–4.5737188657	1.0716998484	–1.4990278596
H	–2.3710614843	1.7519940069	–1.3882349033
H	–5.4312552751	1.545593904	–0.0276980333
H	–5.0894199666	–0.1508478255	–0.326531455
H	–3.3236335624	0.8239146385	1.3508178993

Tabelle 349 Standardorientierung von *cis*-S1 [globales Minimum, M052X/6-31+G].

Atomsymbol	x	y	z
C	–3.9066393093	–5.6498605461	7.843714061
C	–2.7552515969	–6.4950037475	7.2910458386
C	–4.6771550522	–5.0217692483	6.6798619843
C	–1.8232699253	–5.6548834976	6.3975073739
C	0.1119288736	0.6335596682	3.4949614505
C	–0.6662395527	–6.5111619168	5.848170683
C	–0.5913352409	–0.4365947288	4.0696639498
C	0.9880765346	1.4357771239	4.2190291185
C	–3.7226510896	–4.1879186976	5.8193435442
C	–0.7673013733	–2.1618969644	7.3978094327
C	–0.3433479674	–0.8027270941	5.4405685261
C	–1.1499243303	–7.4573224439	4.7438195705
Li	–1.1969062979	–3.4631468407	4.790462687
N	–2.5513230297	–4.9430151274	5.3018912266
N	–0.8940432578	–1.9438835099	5.9577609734
C	0.496729909	–5.6840226082	5.2984337116
C	1.1606436422	1.1505377708	5.5777386244
C	–2.8911647646	–5.7939174772	4.1402876889
C	0.521184671	0.0701924591	6.1695213034
C	–1.6789759603	–6.5719589054	3.6121170659
H	0.7270746038	–0.1355633417	7.2113201798
N	0.1286854425	–4.8870505675	4.1014249705
C	–0.5262019138	–5.71520744	3.0529225087
C	1.3519666358	–4.2423318833	3.5599974226
C	–0.9410896513	–4.813638416	1.8891951193
C	1.037259226	–3.3430674694	2.3694492939
C	0.2824175571	–4.1170807136	1.2828469547
H	–4.5669728179	–6.2598257413	8.465981485

H	–3.5019967337	–4.8535483022	8.482796656
H	–2.1584880353	–6.9164801453	8.1068291886
H	–0.0745162329	0.859206096	2.4490952097
H	–3.1688371226	–7.3376560913	6.7250859229
C	–1.6057834582	–1.0617383972	3.2139971493
C	–2.7140721828	–1.756006603	3.5453008586
H	–5.4823121587	–4.3771541866	7.0444326522
H	1.5035081613	2.2623822338	3.7493470055
H	–5.1441245947	–5.8113710544	6.0795600552
H	–1.3880605888	–4.867759628	7.0260604431
C	0.4626918046	–2.9438434749	7.8404595141
H	–1.644139785	–2.7286082067	7.7380715939
H	–0.8068889124	–1.2128957311	7.9545405436
H	–0.2731898333	–7.0859446687	6.6944398913
H	1.8177154868	1.7667057986	6.1809969174
H	–3.3358604337	–3.3510583044	6.4111491041
H	–4.2467103995	–3.7645277183	4.959637847
H	–1.930923227	–8.1350432609	5.0995028847
H	–0.3152730418	–8.073568093	4.3921781822
H	0.8729876919	–4.9962634454	6.0576298208
H	1.3180570667	–6.3754379135	5.0343820534
H	–3.672862921	–6.528358719	4.3929737072
H	–3.3019902859	–5.1422121659	3.3658736725
H	–2.031734465	–7.1941522085	2.7807768565
H	0.2294238004	–6.4342944927	2.671274602
H	1.8059353996	–3.6655533623	4.3681009426
H	2.066193331	–5.0316727217	3.2600354455
H	–1.6416661506	–4.0519189352	2.2495743171
H	–1.4606140989	–5.4155619591	1.1354467358
H	0.4366330048	–2.497190228	2.713662941
H	1.9705297664	–2.931993495	1.9742211349
H	0.9447638003	–4.8716759675	0.8394238254
H	–0.0239839563	–3.4418861892	0.4791322442
C	1.6926750992	–2.8129932139	7.1819408354
C	2.8026335921	–3.5552519236	7.5906561977
C	2.6981413817	–4.4556274453	8.6537056328
C	1.4757263612	–4.5997125427	9.3129878023
C	0.3716958555	–3.8461262872	8.9084750895
H	1.7722523694	–2.1309688268	6.3456770214
H	3.7476218583	–3.4346044015	7.0751343918
H	3.5576031555	–5.0354659959	8.9648355225
H	1.3819807368	–5.296307786	10.1369607451

H	–0.5780954069	–3.963190565	9.4217966275
C	–3.7592934346	–2.1454846864	2.5342797175
H	–3.983460108	–3.2178825699	2.5443162935
H	–1.4756931221	–0.8359497728	2.1531818296
H	–3.4383921609	–1.8835712676	1.5223972484
H	–4.7032626078	–1.6255914418	2.7309218903
H	–2.9202182294	–1.9355078281	4.5947964873

Tabelle 350 Standardorientierung von *trans-R*2 [globales Minimum, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	–3.3891402134	–0.2469570852	–2.703499544
C	–3.0107065085	–1.5901443541	–2.0833573491
C	–2.1184857699	0.4556631655	–3.1733838331
C	–2.0159691921	–1.4096315357	–0.924274683
C	–2.9786528572	2.5726478338	0.7406454993
C	–1.6414493261	–2.7708162003	–0.3087329411
C	–1.8591971017	1.9236531957	1.2743666638
C	–2.8646655147	3.6934300697	–0.0730876808
C	–1.1656156741	0.6231406612	–1.9893471434
C	1.8274673696	2.2427656622	1.4127023785
C	–0.5319687381	2.3897831053	0.9609317585
C	–0.726751436	–3.5606579754	–1.2449433381
Li	–0.0196026274	–0.0536070336	0.5541820269
N	–0.8054936957	–0.6314538199	–1.2927605956
N	0.517774461	1.6295608107	1.3554074509
C	–0.9520557043	–2.6761094473	1.0548335741
C	–1.5845035157	4.2103642987	–0.3096292439
C	0.1912021628	–1.4034566244	–2.0527189046
C	–0.4536622839	3.597248611	0.2031092447
C	0.5507549509	–2.7371493338	–1.385524637
H	0.5164019179	4.0197865236	–0.0284066615
N	0.3634991318	–2.0213410726	1.0034733074
C	1.2389851974	–2.6398528887	–0.0132752164
C	0.9862803944	–2.1087933446	2.3335481513
C	2.5789363449	–1.9092926424	–0.0583994707
C	2.333107746	–1.3982352706	2.3701131638
C	3.2681165896	–1.9673012263	1.3042910191
H	–4.0904125415	–0.3898689324	–3.5293153448

H	–3.8878236736	0.3782558594	–1.9529885362
H	–3.8965028913	–2.1027558807	–1.6956482829
H	–3.9652438918	2.2166616166	1.0175188481
H	–2.5847763749	–2.2323801126	–2.8607543861
C	–2.0064609429	0.8409710268	2.2577079993
C	–3.0625492806	0.0247101583	2.4158700274
H	–2.3434229017	1.4470342205	–3.574893619
H	–3.7451430976	4.1856970108	–0.4654614881
H	–1.6501423616	–0.1214290986	–3.9783151233
H	–2.5236620058	–0.8129132432	–0.1556847735
C	2.7489914879	1.8654602199	0.2644869794
H	2.3226311466	1.9270851359	2.3396988888
H	1.7667898239	3.3378150035	1.4756566185
H	–2.5789778273	–3.3131994714	–0.1488111379
H	–1.4691802298	5.1083386062	–0.907534916
H	–1.6351599223	1.2871471403	–1.2584597361
H	–0.2351201391	1.0949351555	–2.3078166131
H	–1.1887390395	–3.7292190951	–2.2203704157
H	–0.5077576978	–4.5424557544	–0.8128212968
H	–1.5721927346	–2.1136775772	1.7552033213
H	–0.8376312311	–3.700261805	1.4514817698
H	–0.1651130422	–1.6331832788	–3.0678414409
H	1.076705389	–0.7715451284	–2.1599203991
H	1.2578330297	–3.2462919627	–2.0487594327
H	1.4370358516	–3.6838824541	0.3020281288
H	0.297141676	–1.6588572497	3.0526093916
H	1.1126335624	–3.1714641972	2.6070065761
H	2.4285967792	–0.8607265138	–0.3369518521
H	3.2050323341	–2.3633009014	–0.8325593759
H	2.1686372538	–0.3325462367	2.1898857287
H	2.7658647893	–1.5042586315	3.3683738385
H	3.5129709559	–3.0085042023	1.5470441298
H	4.2051130308	–1.4075262297	1.2766689207
C	2.2829277548	1.8722138281	–1.0543096342
C	3.1146707952	1.5069333515	–2.1097920997
C	4.4312744119	1.1160241137	–1.8632074837
C	4.9076152385	1.1068603606	–0.5543817808
C	4.0707986081	1.4810071371	0.4971533389
H	1.2589375905	2.1707004656	–1.2416915961
H	2.7368801781	1.5270874675	–3.1261309174
H	5.0779288459	0.8251272145	–2.6821753773
H	5.9278202409	0.8029391404	–0.3500760366

H	4.4442428524	1.461057639	1.5164004805
C	–3.2144656107	–0.9417139037	3.5565546886
H	–4.0373368783	–0.6445261127	4.2145599002
H	–1.168879917	0.7511077011	2.948174269
H	–2.3034397213	–0.9799774951	4.158337368
H	–3.4414768777	–1.9546535505	3.2075526
H	–3.8919086735	0.0740111023	1.7125819706

Tabelle 351 Standardorientierung von *trans*-*R*1 [globales Minimum, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	–2.2398795614	–1.0188195631	–3.6126959335
C	–2.4359974678	0.3586115571	–2.9805393292
C	–2.7787571191	–2.0893795335	–2.6665197218
C	–1.7694354749	0.4387018577	–1.5971380956
C	1.7071452157	–2.9468580868	3.3420466046
C	–1.9633687615	1.8299268784	–0.9667914851
C	1.0616230388	–2.521120368	2.1793973794
C	3.070343518	–2.7474365406	3.5390527535
C	–2.0805748977	–1.9665496798	–1.3114135599
C	1.8019568076	–0.8798900872	–1.0532968984
C	1.7806950562	–1.8140512172	1.1565563496
C	–3.4014429496	2.0148736513	–0.4821485648
Li	–0.661289503	–0.6657343825	0.6928575875
N	–2.1995610816	–0.6420934896	–0.6757093932
N	1.0698801577	–1.3059629652	0.1185395101
C	–1.0249327019	2.1088714802	0.2077098875
C	3.80035536	–2.1385385013	2.5143795959
C	–3.5148575796	–0.423434877	–0.0620921075
C	3.1868940902	–1.6941507546	1.352281146
C	–3.6262003509	0.9577478021	0.596838923
H	3.7947487832	–1.2049921756	0.6013124958
N	–1.2506617672	1.2109526272	1.352330887
C	–2.6662938303	1.2228332577	1.7714670265
C	–0.3885065338	1.6383051898	2.4651615374
C	–2.8642433818	0.2522443642	2.9326051003
C	–0.5095425813	0.6967261594	3.6559614789
C	–1.9647758474	0.6109921434	4.1157362979
H	–2.7351602927	–1.0683750689	–4.5853548014

H	–1.1704560046	–1.1935141219	–3.7834996527
H	–2.0052489396	1.1397016663	–3.6143951682
H	1.1322225241	–3.499588686	4.0779676926
H	–3.5084049716	0.5649419582	–2.9025857448
C	–0.3354499007	–2.8959778873	1.917002319
C	–1.325836286	–2.9826478237	2.8216032189
H	–2.6030886631	–3.091812039	–3.06562805
H	3.558018387	–3.0978391556	4.4395414502
H	–3.8621145355	–1.9732520217	–2.5538999774
H	–0.6932654073	0.2859832955	–1.7475290842
C	2.0969341394	0.6120405067	–1.1222356997
H	1.2099007798	–1.1271412097	–1.9454793187
H	2.7447193012	–1.4332383306	–1.171283022
H	–1.7228897704	2.5639748744	–1.7422452286
H	4.8710416938	–2.0025007945	2.6248233431
H	–1.0103252965	–2.1676441777	–1.4341321484
H	–2.4685371206	–2.7050131511	–0.6056375353
H	–4.1255658504	1.9007962663	–1.2924370454
H	–3.528587423	3.0204601128	–0.0689524868
H	0.0160552481	2.0062746188	–0.1023068154
H	–1.1761161244	3.1548256538	0.5278124658
H	–4.3303542228	–0.5018143993	–0.7967644196
H	–3.6690414741	–1.221449293	0.6693480347
H	–4.640286513	1.0408279311	1.0015910559
H	–2.9046370153	2.2421857343	2.1358997329
H	0.6380947139	1.6631465026	2.0960892991
H	–0.6643120629	2.6645766265	2.7668051684
H	–2.619210187	–0.7593941872	2.5976442705
H	–3.9185412909	0.2593489926	3.2274641582
H	–0.1408474144	–0.2941653391	3.3705203298
H	0.1328951806	1.0553797777	4.4638896306
H	–2.2748630445	1.5790707709	4.5268110427
H	–2.0742389343	–0.1281517644	4.9132980214
C	2.5340062949	1.3184214905	0.0040164139
C	2.779830278	2.6879088163	–0.063918983
C	2.5778031526	3.382392747	–1.2569758115
C	2.1370093	2.6920093231	–2.38361619
C	1.9045225966	1.3183831963	–2.3126689382
H	2.6652872952	0.7880517514	0.9394983071
H	3.1221991228	3.2165471597	0.8184240514
H	2.7615364275	4.448822932	–1.3065429406
H	1.9726965045	3.2203606836	–3.3155828602

H	1.5573263205	0.7859246025	–3.1936676879
C	–2.6806749182	–3.5704990188	2.5448906875
H	–2.826836104	–4.492824162	3.1157798318
H	–0.5421858198	–3.1842291142	0.8854249667
H	–2.7924071751	–3.8155138849	1.4863440878
H	–3.4895561979	–2.8909178289	2.8330916042
H	–1.1353809362	–2.6574292783	3.8431689542

Tabelle 352 Standardorientierung von *trans-S*2 [globales Minimum, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	–4.2456816047	–0.3539558619	–2.3323912717
C	–4.3670128274	–0.1629909353	–0.820328478
C	–3.1333444432	–1.3578808679	–2.6309696565
C	–3.0258353248	0.2739556454	–0.2077120381
C	4.2457332906	2.4374184441	–0.56469784
C	–3.1390223485	0.4743643314	1.3142065789
C	3.5154175357	1.3900109366	–1.1029782498
C	3.6188260353	3.5830852894	–0.0624334515
C	–1.8278832492	–0.8770521268	–1.9967318942
C	1.8415662578	–0.7240691498	–2.2238906584
C	2.0896314754	1.4107195874	–1.136443468
C	–3.2611385476	–0.869705382	2.0328921491
Li	–0.1781046473	0.403506122	–0.2074645265
N	–1.9078125589	–0.6353804925	–0.5459095552
N	1.2778642186	0.3798889722	–1.4735357704
C	–1.9577797247	1.2322791086	1.9268821442
C	2.2368314026	3.6764809179	–0.1803678627
C	–1.8901717532	–1.8829069613	0.2323068459
C	1.4697052855	2.6432886111	–0.7267605313
C	–1.9665252778	–1.6260171532	1.7429903281
C	0.0443445561	2.8396205995	–1.0268983593
C	–0.8212969766	3.6443394105	–0.3865162143
C	–2.2085247038	3.951054524	–0.8761223988
N	–0.6788835642	0.5183837597	1.8059100626
C	–0.7835730846	–0.8510722043	2.3513603861
C	0.3586926916	1.2788052676	2.5236792316
C	0.549283582	–1.5747598731	2.1895134867
C	1.7254396005	0.6180939458	2.4022092797

C	1.6674470134	–0.8218305035	2.9095848695
H	–5.1975346931	–0.6854697715	–2.7540343968
H	–4.0004888747	0.6064502455	–2.8023489809
H	–5.1202238583	0.5955422294	–0.5859217529
H	5.3274360995	2.3593914387	–0.5333701722
H	–4.706121283	–1.100618067	–0.3691828053
H	4.0488006433	0.5193458185	–1.4624006207
H	–2.9851903182	–1.4695835253	–3.708365558
H	4.1972321514	4.3995584511	0.350255187
H	–3.4092741565	–2.3435225759	–2.2414287548
H	–2.7659134287	1.2408673947	–0.6588644979
C	2.1157194404	–1.9782172436	–1.4080127932
H	2.7608520655	–0.4353217363	–2.7497673303
H	1.1315433911	–1.0056756542	–3.011802206
H	–4.0328514465	1.081838841	1.4906928177
H	1.7389886169	4.5995757347	0.0977859295
H	–1.5232671703	0.0639695459	–2.4694051034
H	–1.016538234	–1.5876113075	–2.1634097791
H	–4.1290499352	–1.4390754128	1.6914668013
H	–3.3790982226	–0.7062830596	3.1088277658
H	–0.3011828944	2.3102274494	–1.9160730144
H	–1.836760692	2.2059452137	1.4492514209
H	–0.5032816907	4.1555840224	0.5204980817
H	–2.1808011097	1.4072138995	2.9941905594
H	–2.9721416957	3.7146226477	–0.1258592347
H	–2.7319742927	–2.5404723936	–0.0315466384
H	–2.433895579	3.3899297443	–1.786214186
H	–0.9733568359	–2.4171161252	–0.0303436978
H	–2.3139932403	5.015659536	–1.1068075933
H	–1.98194706	–2.6039852847	2.2348976619
H	–0.9974391493	–0.7685021418	3.4357799602
H	0.3873707885	2.284228611	2.0972756463
H	0.0749932204	1.3644229037	3.5878603721
H	0.8004047192	–1.6553837455	1.1271616448
H	0.452476056	–2.5942893438	2.5756664708
H	2.041819487	0.635955744	1.3549539212
H	2.4549195519	1.2066038899	2.964147953
H	1.4721840589	–0.8254240628	3.9890296906
H	2.6237619875	–1.3245839525	2.750831879
C	1.4900386161	–3.1846053357	–1.7326141831
C	1.7212158424	–4.3448536507	–0.9921068516
C	2.6036586291	–4.3187155771	0.0837985113

C	3.2416424712	–3.1228536214	0.4154336174
C	2.9905213081	–1.9640485327	–0.3137026728
H	0.8163951959	–3.218718491	–2.5833057891
H	1.2200663214	–5.2669031551	–1.2628544853
H	2.7961444919	–5.2182609691	0.6560133579
H	3.9331800404	–3.0931858546	1.2497029212
H	3.4683653583	–1.0352427317	–0.0256742103

Tabelle 353 Standardorientierung von *trans*-S1 [globales Minimum, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	0.1650385703	0.2274874288	4.1985394991
C	1.4044337943	–0.3904688704	3.5514103561
C	–1.0844873429	–0.4678191881	3.6619455769
C	1.3263976903	–0.3122590721	2.017790873
C	–3.6292483934	3.1157380698	0.2206599933
C	2.5811680606	–0.9089139197	1.3581959128
C	–2.4731489817	2.8359678721	–0.4936251081
C	–4.5174152125	2.1023202653	0.5911133127
C	–1.1096655718	–0.3725244988	2.1366216715
C	–0.1739862984	2.1426819748	–2.1096328552
C	–2.1244167297	1.5049072427	–0.8606931806
C	2.5968583904	–2.4313246235	1.5003398114
Li	–0.119883927	–0.2957609075	–0.4860737369
N	0.0892982569	–0.9158123473	1.4664959392
N	–0.9607654659	1.1262605256	–1.4511517847
C	2.7209882854	–0.5621929918	–0.1263885694
C	–4.232611813	0.8004419037	0.1897132707
C	0.1119004725	–2.3862312782	1.454224971
C	–3.0787711387	0.4843334492	–0.5310731638
C	1.3637024364	–2.9426764748	0.7582893805
C	–2.8669249592	–0.8732854711	–1.0531191191
C	–3.2658862546	–2.0225505577	–0.481929387
C	–3.1931393469	–3.3707689486	–1.1417818154
N	1.6673912137	–1.1541129636	–0.9663234056
C	1.5103003756	–2.6035563525	–0.7358264777
C	1.9788177518	–0.8954967199	–2.3801394101
C	0.3464871755	–3.1200875184	–1.5791060824
C	0.8501940394	–1.3655984733	–3.2896220229

C	0.5778129374	–2.8532843046	–3.0666352276
H	0.2221681604	0.1498576807	5.2870312872
H	0.1173194	1.2952234245	3.9517927215
H	2.3116975792	0.1276317194	3.8772185765
H	–3.8390750761	4.1437757806	0.4967376588
H	1.4944215404	–1.4301946116	3.8806042858
H	–1.7990784221	3.6502059969	–0.730950575
H	–1.9925051967	–0.0041250177	4.055291047
H	–5.4248749941	2.3280823466	1.1363250358
H	–1.0928083465	–1.5148631377	3.9832423729
H	1.2816324079	0.7496264057	1.7510179062
C	0.990847186	2.6883599599	–1.294385742
H	0.2532779889	1.7159672014	–3.0272823601
H	–0.7917843422	2.9884240282	–2.4453479283
H	3.4460922623	–0.4706020022	1.8659429657
H	–4.9481861967	0.0100825054	0.3914076221
H	–1.1962811287	0.6816256953	1.849739364
H	–1.9797401226	–0.8796331568	1.7193159787
H	2.5777733532	–2.7423955121	2.5473758555
H	3.5096043478	–2.8399898799	1.0549618547
H	–2.3796395147	–0.9151272726	–2.0274498068
H	2.6929920582	0.5218183539	–0.2711098408
H	–3.7202449541	–1.9939584332	0.5070660075
H	3.7073740076	–0.9195380302	–0.469604279
H	–2.6046815168	–4.0834605113	–0.5533289871
H	0.0901345751	–2.8050558016	2.4711969872
H	–2.7481728428	–3.2970531049	–2.1366286252
H	–0.8016305143	–2.7185340045	0.9528207337
H	–4.1925580632	–3.8019794645	–1.2540874446
H	1.3089643466	–4.0344346092	0.8238759112
H	2.4337948206	–3.111202731	–1.0780026914
H	2.1432205971	0.1784001967	–2.4902873976
H	2.9199847578	–1.4088063402	–2.6464057021
H	–0.5771573656	–2.6226238741	–1.2641897413
H	0.2144024105	–4.1900522262	–1.3897283425
H	–0.0469357881	–0.777123465	–3.0671185786
H	1.1226972852	–1.1740488953	–4.3307466198
H	1.4384347637	–3.4397800196	–3.4093600601
H	–0.2874635342	–3.1782600943	–3.649818328
C	2.1958160748	3.0311189519	–1.9154310152
C	3.2751049889	3.5155371578	–1.1785744458
C	3.1634515341	3.6708324533	0.2022980929

C	1.9654373209	3.3375264088	0.8327105405
C	0.8927073025	2.8443966355	0.0910649258
H	2.2897116719	2.9088545726	–2.9905138182
H	4.2019638751	3.7672871169	–1.6804067219
H	3.998749543	4.0490783419	0.7791649013
H	1.8655648155	3.4617050297	1.9056579594
H	–0.0360078223	2.5774626338	0.5831679918

Tabelle 354 Standardorientierung von *trans*-S-TS1 [TS, M052X/6-31G].

Atomsymbol	x	y	z
C	3.1382532967	–0.6502864747	–5.4401768208
C	3.1601207809	0.8821230543	–5.4375338426
C	1.6894463866	–1.1487687018	–5.4703972484
C	2.3436231826	1.4410465972	–4.258140057
C	–0.1705860025	2.4755058715	2.0656438189
C	2.3709299745	2.9786784406	–4.2197282105
C	5.2741381646	–0.1018103176	0.9860681746
C	–0.6078906462	1.5013205866	1.1632522043
Li	3.2947347545	–0.8576000695	0.7663044764
C	1.1408160318	2.9379966719	2.0138904843
C	2.6972937671	–0.8286483399	5.5052145672
C	0.9040707109	–0.5514574925	–4.2978684837
C	1.6228468413	–0.1220206838	4.6754155147
C	–1.4296335781	–0.61104769	–0.7204476983
C	2.0449281291	–0.0647531333	3.2042141209
C	0.2342945918	0.9611430279	0.1629126129
C	2.9342084425	–2.2255093187	4.9223789565
C	1.5434139428	3.5598746695	–5.3718958866
C	3.3353957098	–2.1398810584	3.4360777913
Li	0.3533314666	1.3133582021	–2.3241846904
N	2.3592248336	–1.3879959948	2.6043809106
N	0.9415505962	0.930001136	–4.2415381715
C	1.128879127	–2.1376391181	2.2427416857
N	–0.1651909038	0.1199507876	–0.8598249036
C	3.5948675224	–3.5276142729	2.8360035335
C	1.8652002641	3.573704579	–2.8980299106
C	2.2822244131	–4.3133354261	2.7470459418
C	2.0228072559	2.3649720006	1.0897412468
C	4.2595760699	–3.4866855588	1.4524122034

C	0.0347735567	1.5733747505	–5.2174122858
C	1.4003667027	–3.5659498243	1.7423001383
C	1.629329985	1.364591715	0.1865756149
N	3.3901353141	–2.9860622884	0.3491475853
C	0.0981779152	3.1054478505	–5.1456388178
C	2.0673503071	–3.6694019054	0.3646410845
C	2.5886593732	0.690213987	–0.6950545605
C	4.0865755473	–3.2436848171	–0.9378624803
C	3.9648438839	0.9212181508	–0.6508805925
C	1.1917701093	–3.189052409	–0.7897207058
C	4.8958697442	0.5089814569	–1.7694051606
C	3.2443975005	–2.857631125	–2.1515802481
C	1.8722055936	–3.5330537425	–2.1173502665
N	0.4156340178	3.3450417574	–2.6619943678
H	5.7956564512	–0.967712142	0.5590014054
C	–0.4166565909	3.7260578146	–3.8359892559
H	5.8998539037	0.7833389121	0.8770665545
C	–0.0112131208	4.1068704814	–1.4565958943
C	–1.8848177559	3.4110548224	–3.5494807952
C	–1.4837694045	3.8731717337	–1.1380699184
C	–2.3706939493	4.2105103727	–2.337576253
H	3.7001442302	–1.0405321689	–6.2925453703
H	3.6287664914	–1.0182549933	–4.5314140882
H	4.1874855903	1.2516146305	–5.3568062665
H	–0.8664664148	2.8779478355	2.7921255284
H	2.7596138831	1.2480105932	–6.3891147529
H	–1.6440694693	1.1933354402	1.2021658815
H	1.6527054378	–2.2406477794	–5.4078131842
H	1.4878126992	3.7046686238	2.6940709763
H	1.2232608853	–0.8664626398	–6.4211731643
H	2.7954518196	1.0702082378	–3.3305703931
C	–2.5660568358	–0.0723152781	–1.5737107025
H	–1.7610037476	–0.6679231882	0.3255231356
H	5.0846668086	–0.2592164627	2.0562947225
H	–1.2558128232	–1.6465394477	–1.0418681058
H	2.4055763356	–0.8952242265	6.5566348982
H	3.4205445018	3.2776850614	–4.3205231709
H	3.6289424279	–0.2507534495	5.4610240011
H	1.4564772221	0.9008680351	5.023812572
H	3.0581506002	2.6821207376	1.1051966669
H	1.3145154212	–0.9186318742	–3.3518582583
H	0.6693888313	–0.652743126	4.7796335626

H	2.9417729651	0.5568564509	3.1125065137
H	–0.1441302538	–0.8524514154	–4.3324504971
H	1.9113847363	3.2232044359	–6.344260244
H	1.2686607556	0.3977388105	2.5994653576
H	3.7267916224	–2.7497349358	5.466814852
H	1.6016162543	4.6533444877	–5.3590549732
H	2.0177854303	–2.8120942528	5.0416545948
H	2.181356614	–0.0866133511	–1.3321035718
H	2.4062804549	3.1428316859	–2.0506968604
H	4.2695289338	–1.565535615	3.3939827567
H	4.2903963684	1.8250934261	–0.1527644813
H	0.4483892196	–2.2165553119	3.104626847
H	0.6129275696	–1.5500009264	1.4765720533
H	2.0626441068	4.6601576998	–2.9166005568
H	4.2971387269	–4.0400297563	3.503426825
H	4.8699014914	1.2530373125	–2.5764093799
H	1.7955091072	–4.3918191334	3.7210287125
H	0.2758846438	1.2766611644	–6.2504075361
H	2.472845781	–5.3323071958	2.393725353
H	4.6177375346	–0.4539842039	–2.1995194664
H	–0.9772647217	1.2172624124	–5.0048693948
H	5.1543129689	–2.8604589479	1.4830024239
H	5.9250259648	0.4368368041	–1.4189572429
H	4.5764851219	–4.516610253	1.2069383538
H	–0.5463178728	3.4918454716	–5.9435493547
H	0.4276879616	–4.0629810749	1.6534465903
H	–0.3296441611	4.8245854158	–3.9672629246
H	2.2526979652	–4.7527802088	0.1981460824
H	0.6112445389	3.7886973801	–0.6189368435
H	5.0246914313	–2.6836728653	–0.9253885245
H	0.1675731162	5.1831261437	–1.6357151984
H	4.3345050356	–4.319110233	–1.001949113
H	–2.0006610043	2.341936497	–3.3371648684
H	1.0238406012	–2.1055931403	–0.7266246966
H	–2.4807668728	3.6369654281	–4.4400049561
H	0.2175129613	–3.6829071132	–0.7132441474
H	–1.6166056338	2.8221171793	–0.8704214863
H	3.0984871368	–1.7765831012	–2.1533031294
H	–1.7535635568	4.4642872555	–0.2590361741
H	3.7945474268	–3.1196883022	–3.060775565
H	–2.3113277201	5.2837534918	–2.5587215803
H	1.2611560841	–3.2090410954	–2.9639840513

H	–3.414817339	3.9748507881	–2.1215186087
H	1.9905881473	–4.6207108415	–2.2004234744
C	–2.6983379846	–0.510075055	–2.897926742
C	–3.7058011693	–0.0165973913	–3.7274647828
C	–4.6138327035	0.9221916617	–3.2367690819
C	–4.5086313758	1.3509189764	–1.9131220709
C	–3.4932805812	0.859227556	–1.0915672662
H	–2.0150469809	–1.2677823637	–3.2628066135
H	–3.7934730094	–0.3758869217	–4.745225955
H	–5.4028083927	1.3029521309	–3.8717283827
H	–5.2221012779	2.062631291	–1.5173065008
H	–3.4268142713	1.1949315633	–0.0646386066

Tabelle 355 Standardorientierung von *trans-S*-TS2 [TS, M052X/6-31G].

Atomsymbol	x	y	z
C	2.6959235072	4.363055742	0.1666927963
C	3.4392253943	3.9336683336	–1.1029752101
C	3.0360405149	3.4080523234	1.3168925033
C	3.1094433253	2.4730627549	–1.4617020388
C	0.0753640488	–4.3209478431	–0.6076251328
C	3.8220565451	2.0189412927	–2.747177984
C	–2.8259658208	0.106992919	–3.4881755209
C	0.5179080467	–3.3033350693	0.244315942
Li	–2.1958834926	–0.2409278576	–1.4597876438
C	–0.3525195727	–4.0219250627	–1.8969301567
C	–1.2765730028	3.6338513933	1.193523776
C	2.7243201028	1.9621543864	0.9156116452
C	–2.0563588467	3.8712123051	–0.1035410521
C	1.297107923	–1.0715268548	1.9848885152
C	–2.0991124865	2.5680600276	–0.9090627007
C	0.5904910124	–1.9538778207	–0.1744535715
C	–1.915635698	2.4813924629	1.9738369662
C	5.3293457965	1.8759248205	–2.5035467553
C	–2.0134110607	1.1986057564	1.1230921189
Li	2.3616711527	–0.1643025608	–0.79180202
N	–2.6969435887	1.4226272282	–0.1848033161
N	3.3916555402	1.5363154833	–0.3400628337
C	–4.1736036445	1.5199513514	–0.1091743838
N	1.1591471328	–0.9208439205	0.5411038155

C	–2.6982029081	0.0701841349	1.9086375516
C	3.2893370311	0.6953176131	–3.3108525554
C	–4.190949181	0.3640260682	2.1015672125
C	–0.382922339	–2.681929348	–2.3087325501
C	–2.5442055662	–1.3045245666	1.2548185353
C	4.822874514	1.2017999158	–0.1536109058
C	–4.8148157381	0.3865164836	0.7029423757
N	–3.2865499049	–1.4611090258	–0.0242717024
C	0.0644057627	–1.6348835974	–1.4876902498
C	5.5029976596	0.7661089251	–1.4619312558
C	–4.7003104845	–1.0193551462	0.0942408137
C	0.0045097214	–0.2322111948	–1.9080393222
C	–3.2488187571	–2.89833681	–0.3989734816
C	–5.407672796	–1.1704366026	–1.2521398372
C	–0.5100399651	0.1823295892	–3.1353396162
C	–0.3082427831	1.6019329078	–3.6299049146
C	–3.9240566624	–3.1480560965	–1.739609494
N	3.5689305242	–0.4781495335	–2.4475589228
C	–5.3667390009	–2.6289050707	–1.7290983759
C	5.0011054444	–0.5603005371	–2.0602751888
H	–3.478451401	0.905152294	–3.1031575721
H	–2.5124579178	0.3717098198	–4.497006545
C	3.1388477274	–1.7139253223	–3.1514000872
C	5.2159542824	–1.7537011832	–1.1338078162
C	3.3262545808	–2.9473965906	–2.2755897081
C	4.779071794	–3.0614034357	–1.8025859355
H	2.9507541876	5.3927552751	0.4299140604
H	1.615448772	4.336936407	–0.0224016506
H	3.1681563622	4.5753768944	–1.9472873317
H	0.0780573699	–5.3457039435	–0.2561711464
H	4.5161446229	4.0496033183	–0.9419548392
H	0.8741635091	–3.5686142112	1.2319897401
H	2.4643611078	3.6619562669	2.2143435856
H	–0.6923387903	–4.8023207638	–2.5651141128
H	4.0966994364	3.5089936525	1.5733022085
H	2.0242482868	2.4142197255	–1.6298069011
C	2.6709185886	–1.4826103058	2.4910030039
H	–3.3741941033	–0.8395909846	–3.5322939501
H	0.557824011	–1.7882744843	2.3819167578
H	–1.2425724424	4.539905156	1.8043711223
H	1.0580291475	–0.1090970328	2.4597712661
H	3.6336544756	2.7879240462	–3.504816696

H	–0.2411157063	3.3695565159	0.9460876937
H	–1.5816069873	4.6497225944	–0.7085082959
H	–0.7771288904	–2.4494751706	–3.2911573921
H	1.645271837	1.839077103	0.7652717551
H	–3.0679442683	4.2209176448	0.1293828305
H	3.0153675216	1.2570281216	1.696832407
H	–1.0731078574	2.2829689078	–1.1492795288
H	5.7727126757	2.8113325287	–2.1537002999
H	–2.6351292086	2.6879977467	–1.8525847609
H	5.8331004464	1.6024153532	–3.4364578018
H	–1.3333280235	2.2539772046	2.872795323
H	0.2295051126	0.5102451408	–1.1467927383
H	–2.9109247102	2.7938518523	2.3066399391
H	–0.9929306665	0.8676947037	0.8758716492
H	2.2068336761	0.7388942408	–3.4432578541
H	–0.5488334546	–0.5523071669	–3.930193733
H	–4.4887765116	2.4690227467	0.3526511034
H	3.7515212461	0.5362769912	–4.3017905688
H	–4.5504376626	1.522337587	–1.1355373519
H	0.3990206432	1.6127448442	–4.4668538287
H	–2.1956189617	0.0132164359	2.8812639227
H	5.3885620695	2.060362856	0.2408154167
H	–4.3571406495	1.3120316218	2.6188253824
H	0.105456795	2.239296873	–2.8465124398
H	–4.6500011083	–0.4246531865	2.7068312522
H	–1.493621685	–1.5169956432	1.0515928425
H	4.8736712059	0.4101373239	0.5993120944
H	–2.9095438997	–2.0615858636	1.9724175943
H	–1.2356566526	2.0527846218	–3.9823616837
H	6.566366129	0.6235729359	–1.2386524245
H	–5.8860478557	0.6093969863	0.7719319659
H	5.5945364018	–0.7308497568	–2.9823951031
H	–5.2053332784	–1.7005917085	0.812071212
H	–2.2076413658	–3.2122694882	–0.4260881347
H	2.0861216054	–1.5949245992	–3.4139568671
H	–3.7635210572	–3.4804469477	0.3887673718
H	3.7245770333	–1.8184226221	–4.0831628362
H	4.6339549654	–1.6051736655	–0.221128193
H	–4.9226999568	–0.5319800811	–1.9940646773
H	6.2714895433	–1.7951413527	–0.8442751783
H	–6.4435872883	–0.8304997454	–1.1471281515
H	2.6485142157	–2.8792407074	–1.4192576383

H	–3.3448276055	–2.6499378896	–2.5199816267
H	–3.9009014015	–4.2199484958	–1.9554038948
H	3.0253513291	–3.8347653678	–2.8378156642
H	5.4307895966	–3.2648370755	–2.6616016744
H	–5.8146686852	–2.7151758736	–2.7223229817
H	–5.9661288871	–3.2447942339	–1.0467234746
H	4.8904693509	–3.8984550903	–1.1076227802
C	3.211423303	–0.8881840734	3.6376926904
C	4.4658471187	–1.262725701	4.1198116657
C	5.2026906702	–2.2454343853	3.4590704283
C	4.6755938334	–2.8436337021	2.3139662336
C	3.4233707802	–2.4616783891	1.8321810524
H	2.64080943	–0.1232037294	4.1534890484
H	4.8672228539	–0.7888827403	5.0064678569
H	6.1751305583	–2.5407586048	3.8304489848
H	5.2404907057	–3.606558861	1.7922280158
H	3.0193306254	–2.9194238609	0.9380185189

Tabelle 356 Standardorientierung von *trans*-*S*-TS3 [TS, M052X/6-31G].

Atomsymbol	x	y	z
C	5.0344676206	–3.0863738268	–2.8603570152
C	5.8515524702	–1.9616201618	–2.2157324679
C	3.7901764438	–2.4926038444	–3.5272270112
C	5.0005858752	–1.166721455	–1.2072096223
C	–0.0991210319	–4.0001942377	–0.4894616535
C	5.8158937471	–0.0433194859	–0.5429400062
C	–2.5242817891	0.4099197951	–3.6867451404
C	0.2872466037	–3.0092486845	0.4216798482
C	–0.3892819514	–3.6674240341	–1.807774617
C	2.9738621039	–1.704885101	–2.4995356756
Li	–2.2395986835	0.247429225	–1.5670403143
C	1.163720211	–0.911566983	2.2330673178
C	0.4354387582	–1.6557920643	0.0363506133
C	–5.5195971359	–3.2421343812	–1.2386080012
C	6.1060690596	1.0809576211	–1.5444691769
C	–4.1854794798	–3.5048038976	–0.536364119
Li	2.4652258215	0.0071194425	–0.2925162591
N	3.7437242627	–0.6344930766	–1.8082944344
N	1.010341792	–0.6644155547	0.8058246158

C	–3.1961599646	–2.3835369071	–0.8657482101
C	5.1343730513	0.5607971802	0.6879875793
C	–6.0463277224	–1.8686261592	–0.8087922879
C	–0.3584079049	–2.3184330371	–2.1875463268
C	3.9331057025	0.5658573213	–2.6576670616
C	0.0184415212	–1.298504649	–1.3023942974
C	–5.0187042962	–0.7599759712	–1.1152382982
C	4.7509502573	1.6639549755	–1.9588139669
C	0.0209468061	0.1115802139	–1.6977135025
N	–3.6775656526	–1.0197852681	–0.5275266068
C	–0.3021883594	0.5130857109	–2.9930469559
C	–3.57078624	–0.7536224943	0.9277900546
C	–0.0908059378	1.923567847	–3.493613426
N	3.8984783304	1.3162198267	0.3690308572
C	4.0937531575	2.3049704114	–0.7239120404
C	–5.5311884369	0.6220085112	–0.6890046723
C	3.4017164536	1.9702987817	1.6026731042
C	2.7645574797	2.997820818	–1.0290047173
C	–5.6078117183	0.7087608898	0.8386575841
C	2.0750848451	2.6781816462	1.3571149054
C	–4.6810742246	1.7856205227	–1.2175598039
C	2.2227490159	3.6975186547	0.2222836557
H	5.6426522929	–3.6364144762	–3.5829018049
H	4.722246894	–3.7999768792	–2.0874635672
C	–4.1686186955	0.5954461195	1.3504400101
H	6.7252557323	–2.3643962121	–1.6931560496
H	–0.1527197613	–5.0310060064	–0.1597503602
N	–3.3246623235	1.902155266	–0.6094591251
H	6.2254430938	–1.2997629159	–3.0042898688
H	0.5576961698	–3.3061183244	1.4273495937
C	–3.3981043266	1.8328026697	0.8766823634
H	3.1564656913	–3.278686506	–3.9457231065
H	–0.6787110514	–4.4274662818	–2.5221324878
C	–2.7457515675	3.2037707901	–1.0307550555
H	4.0919603016	–1.8448430262	–4.3584810768
H	4.682603793	–1.8653662551	–0.4238242978
C	–2.0086101152	1.9820286924	1.4931443881
C	2.4986746562	–1.511385153	2.6586936241
H	1.0594115735	0.0452603412	2.7624496777
C	–1.3895105267	3.4817240519	–0.3877408497
C	–1.4578154437	3.3654128841	1.136231658
H	0.3543798071	–1.554271845	2.6193768291

H	6.7544340732	–0.49217971	–0.1992223953
H	–2.9291382161	1.4287495164	–3.7079552762
H	–0.6733604025	–2.0544631316	–3.1902949627
H	2.5986591065	–2.3919241891	–1.7331853705
H	2.0985333341	–1.238057335	–2.9507612698
H	–2.0929652927	0.1761542255	–4.6597215113
H	6.6536103668	0.7139050598	–2.4156900853
H	6.7221474825	1.8523694227	–1.0701941293
H	0.149171747	0.8342814485	–0.89935846
H	4.8699378113	–0.2203974509	1.4046925054
H	–0.1743676282	–0.2314052589	–3.7697449517
H	5.8548778706	1.2401835524	1.1781256417
H	0.9604146554	2.0755803119	–3.7683621436
H	4.4516269049	0.3182867215	–3.5970613157
H	–0.3427286247	2.6687267777	–2.7395206582
H	2.9345489935	0.9225849127	–2.9251625494
H	–0.6975690064	2.1183926805	–4.378037892
H	4.8960427155	2.4704213688	–2.6867483097
H	4.8015912467	3.0806669241	–0.3643012699
H	3.294102534	1.19421996	2.3626514348
H	4.1560828971	2.695910209	1.9590275335
H	2.0340696617	2.2573468619	–1.3770654229
H	2.9153611864	3.7127007541	–1.8444083442
H	–3.3257569925	–0.3148903679	–3.4859562588
H	1.3222168247	1.9226544002	1.0990909554
H	1.7564678	3.1689569129	2.2815206026
H	–6.2499648066	–4.0218500839	–1.0070948353
H	2.9241201598	4.4842860345	0.5275905804
H	1.2681077766	4.1818890781	0.0069658586
H	–5.3651839432	–3.251751465	–2.3248601202
H	–3.7455763053	–4.4529762646	–0.8569331083
C	3.0654482452	–1.168635284	3.8924970649
C	4.2953962251	–1.6920889058	4.2914620518
C	4.9799894761	–2.5785602469	3.4595239734
C	4.4246283415	–2.930669966	2.2287437551
H	–4.3457140605	–3.5774495294	0.5454140295
H	–2.9913844225	–2.3990637822	–1.9398153346
C	3.1993158165	–2.3941721254	1.8277423963
H	2.5362514151	–0.4779694858	4.5403374167
H	4.7188254414	–1.4076210387	5.24623492
H	5.9317557818	–2.9906187525	3.767802792
H	–2.2457087226	–2.5367808986	–0.3572518953

H	4.9453004572	–3.6240363303	1.5792893196
H	–6.9814429866	–1.6274039957	–1.3250408569
H	2.7694133919	–2.6638471444	0.8707681089
H	–6.2683038325	–1.9023042659	0.2624849291
H	–4.8725194371	–0.7540047534	–2.2027151963
H	–4.0824754011	–1.5350488272	1.5106693821
H	–2.5079670632	–0.8070377314	1.183426773
H	–6.5297939869	0.7433354344	–1.1240822218
H	–6.239148132	–0.0785935585	1.2550387845
H	–6.0397438038	1.6684731014	1.1419092088
H	–4.5560930199	1.7012264112	–2.2992592601
H	–5.2361263767	2.7193380143	–1.0135785213
H	–4.1563814015	0.6238156083	2.4460440844
H	–3.9925775505	2.7067298944	1.2202774806
H	–2.6629174837	3.192530649	–2.1200861903
H	–3.4448793875	4.0139368162	–0.7522895309
H	–1.3332557431	1.201276258	1.1207381363
H	–2.0902204426	1.8612266128	2.5781962172
H	–0.6608218315	2.7571903866	–0.7546140233
H	–1.0532974567	4.4763112169	–0.69685957
H	–0.4729445183	3.5231062403	1.5777858096
H	–2.1242885165	4.1373430483	1.5407885536

Tabelle 357 Standardorientierung von *trans*-S-TS4 [TS, M052X/6-31G].

Atomsymbol	x	y	z
C	4.9115324783	–3.2633585252	–2.2338017503
C	5.6408951014	–1.9538374053	–1.913500279
C	3.6513651722	–2.9594793543	–3.0500739749
C	4.7144807551	–0.9767693195	–1.164485953
C	–0.1633908015	–3.9406241716	0.1127391771
C	5.4375199278	0.3349251092	–0.8105878534
C	–3.0100626551	–0.3404397061	–3.7918133607
C	0.195825215	–2.7595747034	0.7726955365
C	–0.5541263136	–3.9081272654	–1.2217718598
C	2.7607442786	–1.9761732982	–2.2861163334
Li	–2.5650528612	–0.2255752685	–1.6936998162
C	0.8801587034	–0.2445882589	2.0866406794
C	0.2252904687	–1.5096313151	0.1110993692

C	–2.2443682847	4.2023238397	0.1379621776
C	5.693287088	1.170546056	–2.0709006648
C	–2.8812422845	4.0650984284	–1.2488106846
Li	2.1110607124	0.1960393904	–0.6117249407
N	3.4476757548	–0.7106169969	–1.9061160224
N	0.7265733195	–0.3363933633	0.6397216819
C	–2.7177771147	2.621352727	–1.7360075185
C	4.6788244286	1.1997671858	0.2022117267
C	–2.8452516482	3.1678930131	1.0956634901
C	–0.631456203	–2.6701864373	–1.8747609489
C	3.60330468	0.2189120998	–3.0494227108
C	–0.2611898244	–1.4685947151	–1.251515082
C	–2.7413010317	1.7314309032	0.54220281
C	4.3198262416	1.5201287567	–2.6535552983
C	–0.3283571364	–0.181254723	–1.9433410508
N	–3.306193957	1.6057682814	–0.832810587
C	–0.7301661368	–0.0529001515	–3.2707681371
C	–4.7867056476	1.5936129257	–0.8906383527
C	–0.5163868916	1.2336075136	–4.0379867345
N	3.4072350115	1.7474768227	–0.3295191174
C	3.5685357394	2.4131001017	–1.6491908135
C	–3.4054320641	0.7240332008	1.4928877641
C	2.8123405539	2.6722845255	0.6637155907
C	2.1979376428	2.8582324673	–2.1566770567
C	–4.9275635583	0.9131446458	1.5096355071
C	1.4343632374	3.1479898912	0.2154952306
C	–3.0920672049	–0.7350663678	1.151052847
C	1.5216185042	3.8102942436	–1.1650030388
H	5.5718539483	–3.9481720849	–2.7718014431
H	4.6225501422	–3.7579352144	–1.2978604543
C	–5.4218855947	0.6021367786	0.0936400412
H	6.5248754597	–2.1403189841	–1.295080645
H	–0.1278055256	–4.8803755806	0.6507403149
N	–3.7136270422	–1.2186884825	–0.1117283784
H	5.9912559932	–1.5053596292	–2.8492994136
H	0.5243689892	–2.8196710049	1.8029044479
C	–5.1583171862	–0.8818638219	–0.19592391
H	3.0795327495	–3.870915753	–3.2419996557
H	–0.833233073	–4.815232795	–1.7418341208
C	–3.5515828507	–2.6942065182	–0.1644341497
H	3.935286558	–2.5461925937	–4.0248132326
H	4.4147700528	–1.4617395797	–0.2287303917

C	–5.7240928149	–1.3612315302	–1.5320100897
C	2.2692060623	–0.5617552739	2.6236495282
H	0.6465534943	0.7843492843	2.3939343744
C	–4.0883875804	–3.2732765006	–1.466368088
C	–5.5546184501	–2.878966871	–1.6788608301
H	0.1499761151	–0.8853863804	2.6100826648
H	6.3885541084	0.0575081131	–0.3427643294
H	–3.7675767696	0.4417856136	–3.6340909219
H	–0.9921404906	–2.6424864647	–2.89613687
H	2.4073085799	–2.451251413	–1.3641815788
H	1.8707409127	–1.7080208961	–2.8562596821
H	–2.6239326691	–0.2504738718	–4.8058181418
H	6.2970084863	0.6256747878	–2.8003553523
H	6.2385582648	2.0836597156	–1.8092294222
H	–0.1854990964	0.7044929718	–1.332707273
H	4.4429854698	0.6236330189	1.1002626744
H	–0.6673121772	–0.9365737684	–3.8952708664
H	5.3374129564	2.0359116019	0.4992549946
H	0.4386241245	1.1896682351	–4.5761900088
H	4.1814840977	–0.2388336997	–3.8669012903
H	–0.4722528903	2.0986119361	–3.376316112
H	2.6005196897	0.418404186	–3.436630569
H	–1.3036986625	1.4063429546	–4.7710182587
H	4.439243377	2.1137486807	–3.5671378417
H	4.1933817877	3.3184713797	–1.5056617568
H	2.746616332	2.1347124772	1.6115955518
H	3.4850590362	3.5375316863	0.8063615505
H	1.5650500921	1.9759739029	–2.2971686263
H	2.3149587148	3.3318482067	–3.1369215822
H	–3.464980048	–1.3306022015	–3.6784112386
H	0.7643378319	2.2795670332	0.1849173929
H	1.0381887028	3.8482817113	0.956790718
H	–2.3812036394	5.2120199379	0.5344603804
H	2.1090017612	4.7337622364	–1.0898018781
H	0.5275410381	4.0888961396	–1.527253617
H	–1.1663434745	4.0307826458	0.0524050871
H	–2.4026749818	4.7404233213	–1.9647616116
C	2.8065715392	0.18135507	3.681797207
C	4.0858694583	–0.0827513329	4.1719991338
C	4.8509747111	–1.1058276249	3.6119558201
C	4.3255234109	–1.8563740496	2.5588594297
H	–3.9389883038	4.3453905756	–1.2059815119

H	–1.6501516707	2.3971344187	–1.7912289536
C	3.0497727412	–1.5807913443	2.0637092823
H	2.2150767668	0.9791336314	4.1179432712
H	4.4845812113	0.509124576	4.9859579937
H	5.8418171038	–1.3163813631	3.9920709176
H	–3.1371069328	2.4742921373	–2.7332914833
H	4.9099117003	–2.6568291348	2.1212744117
H	–2.3372939113	3.2021123152	2.06509557
H	2.6463264897	–2.1562213919	1.2392518054
H	–3.8934371273	3.4269138588	1.2755806086
H	–1.6772256271	1.4650945551	0.4564836661
H	–5.2046992302	2.5870677141	–0.6650822798
H	–5.06829842	1.3535216304	–1.9193184072
H	–2.9913381528	0.9101125253	2.4907019847
H	–5.2106388072	1.9243521727	1.81063522
H	–5.3806203159	0.2204263276	2.2266681931
H	–2.0139338286	–0.8864960506	1.065796986
H	–3.455207825	–1.3606166386	1.9867161575
H	–6.507309724	0.7438350666	0.0344849626
H	–5.6825646036	–1.4439006092	0.6062309866
H	–2.4942350677	–2.9206501338	–0.0485040322
H	–4.0953844798	–3.1391373865	0.6906499528
H	–5.2057225216	–0.8554998679	–2.3504335574
H	–6.7828254076	–1.0856920543	–1.5874354475
H	–3.4731352532	–2.9068921174	–2.2908051373
H	–3.9795484695	–4.3612861197	–1.4421849377
H	–5.9031466684	–3.2066367562	–2.661576542
H	–6.1766560906	–3.3821210235	–0.9278110071

Tabelle 358 Standardorientierung von *cis*-*R*-TS1 [TS, M052X/6-31G].

Atomsymbol	x	y	z
C	4.0312770364	–3.0152994044	–3.4831498562
C	4.3722376719	–3.7283990825	–2.1696240595
C	4.5592769185	–1.577389694	–3.4370581804
C	3.7936430411	–2.9597508544	–0.9668335579
C	0.2815958486	2.6228799726	2.6234606305
C	4.1018882049	–3.6618050578	0.3679541425
C	0.9393922791	2.4381282351	1.4066314213

C	–0.9814474411	–1.204989625	–2.29464476
C	–0.3152977826	1.5394068883	3.2659117806
C	3.9711821732	–0.8473294926	–2.2252352904
Li	–1.7764086984	–0.5633589786	–0.4333493879
C	2.2872334311	1.9994398849	–1.1411062899
C	1.0376763148	1.1703499627	0.7761396987
C	–4.8832267514	–3.9254800777	0.982733847
C	5.592758217	–3.539754158	0.7052606324
Li	2.8405938179	–0.6677450971	0.3054087838
C	–3.9623076363	–3.3863360065	2.0780021139
N	4.228542357	–1.534884719	–0.9336712385
N	1.8394790147	0.8893597732	–0.3068187216
C	–2.9150913173	–2.4598578505	1.4529409593
C	3.2903412379	–3.1283376869	1.5567266732
C	–0.3039142032	0.2972803667	2.6266634044
C	–5.531051747	–2.7426181966	0.2606801434
C	5.6048462657	–1.3159247023	–0.4337747526
C	–4.4781411999	–1.7767215656	–0.3238001363
C	0.2940776864	0.0788452366	1.3698368824
C	5.8787718844	–2.0457986688	0.8901895313
C	0.1498954704	–1.253651849	0.7670597423
N	–3.4719663523	–1.318755434	0.6812838402
C	0.3290982243	–1.7125571348	–0.5494576411
C	0.1974906617	–3.2161406817	–0.776706162
C	–3.9249510949	–0.2278256784	1.5831650666
N	3.6206569603	–1.7300272712	1.9250488747
C	5.0829384371	–1.5334876601	2.1036631824
C	–5.1766855897	–0.5873411534	–1.0076751336
C	2.8894640594	–1.3654161746	3.1653653214
C	5.3726650623	–0.0723358094	2.4339703082
C	–5.7906224348	0.3540641169	0.0355588096
C	3.1275293959	0.0912543916	3.5445146723
C	4.6257848255	0.3727530781	3.6961509476
C	–4.2696499455	0.2355847709	–1.9240815667
H	4.4508402501	–3.5581735582	–4.333908861
H	2.9416928002	–2.9953563752	–3.6147945594
C	–4.6240963871	0.9215245347	0.8489434491
H	3.9687920311	–4.7460474889	–2.1630505269
H	0.2665089783	3.6066633276	3.0771931629
N	–3.1918967794	0.9596081486	–1.208758138
H	5.4607653786	–3.8107561001	–2.0824891158
H	1.4533830034	3.2812174701	0.9609393537

C	–3.7326959519	1.7635546776	–0.0776405743
H	4.2901985501	–1.0339381677	–4.3468668953
C	–2.513095114	1.8573741283	–2.179560514
H	–0.7941791391	1.6560572912	4.2294552134
H	5.6538123787	–1.5896235565	–3.3826666124
C	–2.5879088548	2.4778506546	0.6372677899
H	2.7059116697	–2.9314694722	–1.099615419
H	1.5719128692	2.8378929571	–1.10532347
C	–1.3546765229	2.6033245661	–1.5311017492
H	2.2908707483	1.6659255661	–2.1866971152
C	–1.8539367568	3.4122850626	–0.3294584631
C	3.6727146116	2.5568178885	–0.849594189
H	3.8282834709	–4.7157019049	0.2424718258
H	–0.7120378002	–0.1692034146	–2.5220744332
H	–0.791357612	–0.5464985365	3.1086058694
H	2.8851339342	–0.7652117937	–2.341464406
H	4.3621451794	0.1682833371	–2.1392938172
H	–0.348435392	–1.8753811433	–2.8732959647
H	6.2209473156	–3.9628892304	–0.0823480275
H	5.8129201637	–4.0842783706	1.6294801986
H	–0.297393679	–1.9749319081	1.447732138
H	2.2188344387	–3.1540398905	1.3457953131
H	1.018368646	–1.1627192415	–1.1768736341
H	3.4838341246	–3.7879737408	2.42227302
H	0.5391244841	–3.4990654115	–1.773392262
H	6.3563037224	–1.6615208985	–1.1612392575
H	–0.8430698948	–3.5356100812	–0.6986061203
H	5.7387760112	–0.2363307063	–0.3225425752
H	0.7755188688	–3.7861868141	–0.0409359467
H	6.9378976593	–1.8933864681	1.1274295439
H	5.4032463625	–2.1509264816	2.9688496101
H	1.8277780012	–1.5392930346	2.984834218
H	3.2222396839	–2.0287917565	3.9852657987
H	5.059521993	0.5479366731	1.5919008341
H	6.4537649589	0.0575301713	2.5531622286
H	–2.0293973782	–1.4120831495	–2.558158134
H	2.691003941	0.733675529	2.7736016989
H	–5.6474056029	–4.5868253144	1.3984611733
H	2.5900951195	0.3134739089	4.4696042698
H	5.0170319162	–0.1768139161	4.561729674
H	–4.2938271299	–4.5160179367	0.2701639517
H	4.7978777801	1.4362399764	3.8841236973

H	–3.4484334055	–4.1992054954	2.5985939902
C	4.4823839995	3.010830638	–1.8987497195
C	5.7515633955	3.5339193835	–1.654441707
C	6.2348882897	3.6120869002	–0.347885284
C	5.4380973413	3.1629966958	0.7052951271
H	–4.555014901	–2.8501133499	2.8273260958
C	4.1696561642	2.6363981232	0.4552604647
H	–2.2916771251	–3.0457118422	0.7713847623
H	4.1101640205	2.9461805816	–2.9155900957
H	6.3631012306	3.875011245	–2.4800507828
H	–2.2600631162	–2.0444135904	2.2178401868
H	7.2192997479	4.0173107965	–0.1538248639
H	5.8037145551	3.2200580114	1.723522016
H	–6.1708747152	–3.087587796	–0.5576276227
H	3.5507697637	2.2865620652	1.2716147508
H	–6.1737458923	–2.2103144894	0.9697821863
H	–3.9059731411	–2.3305019556	–1.081856297
H	–4.6301134634	–0.609601493	2.3383533253
H	–3.0424518119	0.1380164322	2.1144071128
H	–5.965411148	–1.0098953596	–1.6405593863
H	–6.5030269268	–0.1629161015	0.682778053
H	–6.3316376496	1.162003706	–0.4677743236
H	–3.8018838206	–0.3991068353	–2.6786505142
H	–4.9048416805	0.968809427	–2.4548457023
H	–4.9994488538	1.6065182169	1.6176541
H	–4.3973456246	2.5420330882	–0.5093599325
H	–2.1718315217	1.2458147464	–3.0150708523
H	–3.2510400979	2.5832262175	–2.5683319952
H	–1.8736009453	1.7474647183	1.0305096957
H	–2.9869055169	3.0327896026	1.4923700972
H	–0.5985070028	1.8829627351	–1.2008717016
H	–0.8832451607	3.2541820545	–2.2733434484
H	–1.0199516977	3.8950574166	0.1806769106
H	–2.5400286423	4.1964185872	–0.6763025726

Tabelle 359 Standardorientierung von *cis*-*R*-TS2 [TS, M052X/6-31G].

Atomsymbol	x	y	z
C	2.0007761227	–1.2915157365	–5.1324775369
C	1.9115521431	0.229137046	–5.3066492212

C	0.5914592153	–1.8737801894	–4.9814209575
C	1.1602684896	0.8693864856	–4.1242605245
C	–2.7956936178	1.0905421876	2.2304672946
C	1.071257183	2.4008551009	–4.258837922
C	–2.4861501725	0.1830729494	1.2135234598
C	3.0293421027	–1.2953356848	0.4166855562
C	–1.9033800858	2.1160936672	2.5313177251
C	–0.1248059363	–1.2042851678	–3.8043090379
Li	1.847982519	–0.243302961	1.8686528613
C	–1.7915419077	–1.7433719882	–0.8421254016
C	–1.2803068391	0.2431993845	0.4708511676
C	–1.8520928966	–2.7485990403	3.3641089722
C	0.1062694589	2.7795730387	–5.3899354542
Li	–0.6304289881	0.8341217701	–1.9973389234
C	–0.7795282152	–3.5444220944	2.6135863152
N	–0.1885701427	0.2759658425	–3.9111994427
N	–1.0232255939	–0.5161163081	–0.6553912415
C	0.2776291488	–2.5941705587	2.0394636727
C	0.6226121071	3.1207145607	–2.9785702096
C	–0.6781260696	2.157102996	1.8591817012
C	–1.1978440397	–1.8811544696	4.4444740026
C	–1.2345754893	0.7414880988	–4.8487751948
C	–0.1167384625	–0.9608509847	3.8439532204
C	–0.2838557649	1.2084074469	0.8940459473
C	–1.2790917656	2.2733389816	–4.9740261336
C	1.0916294346	1.2921068698	0.3841438537
N	0.9094657259	–1.7131509077	3.0592911051
C	1.8670731793	0.3946454052	–0.3888821819
C	3.121123601	0.96144588	–1.0399743672
C	1.8940165654	–2.4382771076	3.8934636766
N	–0.7756584615	2.8204150748	–2.5832696767
C	–1.723089313	3.0304651583	–3.7093053571
C	0.5535840947	–0.1035793473	4.9316963703
C	–1.145581001	3.6694977131	–1.4208917309
C	–3.1422994488	2.6803315995	–3.2707345694
C	1.4204430886	–0.9685627015	5.8536947625
C	–2.5500158585	3.3509763707	–0.9240579407
C	–3.5718765339	3.5084150357	–2.0546082455
C	1.4200188315	1.0334275881	4.3798099716
H	2.5216830171	–1.7439875864	–5.9800065286
H	2.5842254768	–1.5202353291	–4.2314731598
C	2.5306256534	–1.5550211255	4.9762061354

H	2.9105191613	0.6723216347	–5.3690429969
H	–3.743791782	1.0122049676	2.7483906235
N	2.6357543951	0.5746088962	3.6556418333
H	1.3999060263	0.4495656208	–6.2494213858
H	–3.2282203158	–0.5561493381	0.9367823958
C	3.4131681826	–0.4043224613	4.463698725
H	0.6325445355	–2.9526576242	–4.8082754171
C	3.4749645644	1.7534780133	3.3332904014
H	–2.1415203112	2.8637899459	3.2770784778
H	0.0282767072	–1.7193081207	–5.9086589467
C	4.6428996268	–0.8745119582	3.6884130532
H	1.729405295	0.62908308	–3.2182722621
H	–2.1066706617	–2.1650213717	0.1283447605
C	4.7190031185	1.3532128862	2.548505032
H	–1.1315138181	–2.4996254414	–1.2876101899
C	5.5378813412	0.3141751272	3.3209542791
C	–3.0277235422	–1.6648900005	–1.7267406919
H	2.0811895005	2.7592588671	–4.4884629168
H	2.8695923249	–1.8185876808	–0.526891021
H	0.0330319906	2.9407461842	2.1095078788
H	0.4016069034	–1.4388630143	–2.8722557177
H	–1.1474325019	–1.570195229	–3.6975972611
H	4.0643212941	–0.9494138964	0.4809539645
H	0.4110657132	2.3420245462	–6.3435615676
H	0.0885124312	3.8669255303	–5.5179251301
H	1.625673281	2.1748344259	0.7431848408
H	1.2538871473	2.8552357176	–2.127742552
H	1.3099754435	–0.3407754937	–0.9557548714
H	0.7254736319	4.2076559323	–3.1492521851
H	3.7280357302	0.1825807104	–1.5019332393
H	–1.0793772456	0.334407369	–5.8604651025
H	3.7373408321	1.4776153385	–0.3005331871
H	–2.1884137245	0.3476937392	–4.4863186403
H	2.8725599777	1.698743024	–1.809315578
H	–2.0139238931	2.5107628389	–5.7517947867
H	–1.7025878216	4.1095716162	–3.9694014568
H	–0.4149902593	3.4853686082	–0.6313940196
H	–1.0824663637	4.7321648602	–1.7200068457
H	–3.1824068831	1.6185207836	–3.0196794373
H	–3.8224171592	2.842910567	–4.113816467
H	2.8269865477	–2.0003683822	1.2325875542
H	–2.5629219959	2.3300824948	–0.530377916

H	–2.5907656718	–3.4201341474	3.8105583623
H	–2.7903903232	4.0063741882	–0.0836241077
H	–3.6396934372	4.5651513317	–2.3423431632
H	–2.377758308	–2.0972480954	2.659461567
H	–4.5658513407	3.2009502675	–1.7177696731
H	–1.2237538488	–4.1153246228	1.7926285298
C	–3.3994940752	–2.7671682239	–2.5075861102
C	–4.5332071144	–2.7264729427	–3.3175220378
C	–5.3194715442	–1.5742660064	–3.3609595376
C	–4.9588178958	–0.4698572062	–2.5894929844
H	–0.3144809463	–4.2698053371	3.2915185068
C	–3.8204095631	–0.5146842514	–1.781965456
H	–0.1760725958	–1.9439678183	1.2860919298
H	–2.7864265551	–3.6617874458	–2.4797431601
H	–4.8003898413	–3.5879925128	–3.9160026521
H	1.0742450296	–3.1542850049	1.5450331447
H	–6.2005034094	–1.5384478405	–3.9880471164
H	–5.5632785055	0.4289373423	–2.6141317878
H	–1.9478909455	–1.2512996686	4.9331670811
H	–3.541633088	0.3398741916	–1.1789489066
H	–0.7684349164	–2.5326393313	5.2138176776
H	–0.614958224	–0.2953533636	3.1308280341
H	1.4323865879	–3.2977399158	4.4041816077
H	2.6592562099	–2.8404247383	3.2236999704
H	–0.2556478699	0.3676383477	5.5002495546
H	0.8407100739	–1.7619090298	6.3299087287
H	1.8516802679	–0.3533876008	6.6509135739
H	0.8337574378	1.6464560766	3.6959850081
H	1.730909163	1.6667290094	5.231190076
H	3.1831786172	–2.2004650097	5.5760285957
H	3.7756176867	0.1267970999	5.3695446418
H	2.8602940444	2.4489882013	2.7574217769
H	3.7706702498	2.2581203089	4.2714620277
H	4.3265767144	–1.3861403173	2.7761614041
H	5.1906524284	–1.5960777797	4.3032019506
H	4.407454212	0.9247754883	1.5934702046
H	5.3177997832	2.2434807669	2.3371982657
H	6.39142345	–0.0192207053	2.7256713329
H	5.9351600842	0.767766019	4.2374142975

Tabelle 360 Standardorientierung von *trans*-*R*-TS1 [TS, M052X/6-31G].

Atomsymbol	x	y	z
C	2.6888504996	–0.189670612	–4.2112153465
C	2.7566987356	1.3409535966	–4.2052883747
C	1.2236538269	–0.6348278336	–4.1964433891
C	2.0081427782	1.921172624	–2.9910427095
C	–1.7359004343	2.1491383971	3.2910669209
C	2.0787916676	3.4566277472	–2.9624453663
C	–4.7820465696	–1.6888633837	–0.3150698952
C	–0.6101556383	1.6013901877	2.6660010889
Li	–2.8040057382	–1.7515110586	0.4789846449
C	–2.9706264058	2.1409801416	2.6496962206
C	–4.4796367712	–2.3729766312	4.9281478669
C	0.5069112041	–0.0296530428	–2.9851365121
C	–3.460946669	–1.2485157817	4.7267228477
C	1.6924918912	0.3878370509	1.2677913072
C	–3.1574214995	–1.0752132079	3.2355689555
C	–0.6641852129	1.0481672737	1.3629829427
C	–3.9312662773	–3.6578260755	4.2992278785
C	1.179515264	4.0695534823	–4.0423523468
C	–3.6110987317	–3.4480238924	2.8052875389
Li	0.0584305872	1.8094590629	–0.9465394865
N	–2.6868258427	–2.309841704	2.556577823
N	0.5973828472	1.4465835134	–2.9047549079
C	–1.2603133525	–2.5878529464	2.8582820368
N	0.4153100224	0.6472507824	0.60154712
C	–3.0719742959	–4.7287198961	2.1554710557
C	1.6940807091	4.054728315	–1.6080213605
C	–1.6828546334	–5.0581667031	2.7133904947
C	–3.0791535396	1.5106298422	1.4035839853
C	–2.9977511386	–4.6578126646	0.6241285529
C	–0.3555001695	2.1249368798	–3.8091149236
C	–0.7595245376	–3.9171207679	2.276466511
C	–1.9780593315	0.9333025506	0.753477395
N	–1.9533832418	–3.7411339516	0.0852447458
C	–0.2568855838	3.6506211841	–3.7124547542
C	–0.6385782902	–3.9651507343	0.7487756073
C	–2.108986953	0.1879904625	–0.501976627
C	–1.8322486835	–3.9908800094	–1.373240123
C	–3.3318278543	–0.0351463339	–1.1308526358
C	0.4203664421	–3.025364703	0.1771834421
C	–3.4325783724	–0.5489117225	–2.5492904009

C	–0.7440007666	–3.1373763257	–2.0160209646
C	0.603820534	–3.3219447999	–1.3141129957
N	0.2641851684	3.8622630628	–1.2556419495
H	–4.6972954779	–2.5742741812	–0.957851416
C	–0.6611373903	4.2536162217	–2.3554989929
H	–5.5621097581	–1.035150057	–0.7038172569
C	–0.0329482255	4.6699460769	–0.0422849383
C	–2.0951843196	3.9282085523	–1.9334248217
C	–1.4649708938	4.4752043725	0.4361807691
C	–2.4758106126	4.7341383626	–0.6852220017
H	3.2120753591	–0.5950415974	–5.0807819139
H	3.1934449978	–0.5791871333	–3.3172792773
H	3.7960348046	1.6826578231	–4.1687077714
H	–1.6325499761	2.5932191561	4.2740481504
H	2.3239262644	1.7227762556	–5.1368135909
H	0.3375386689	1.6426419849	3.1858260406
H	1.1452411707	–1.7250658097	–4.1517600453
H	–3.8428636953	2.5799266152	3.1161512292
H	0.733820494	–0.3169962595	–5.1239477457
H	2.5025045446	1.5418448922	–2.0864397287
C	2.7399362402	1.4758771683	1.0938075049
H	1.5586649879	0.1874957719	2.3412474563
H	–5.059116267	–1.984036369	0.7064223564
H	2.1179304761	–0.5303794466	0.8407347347
H	–4.6953017315	–2.5267006804	5.9887174234
H	3.1248446488	3.7286647053	–3.1422595776
H	–5.4233929495	–2.0998955492	4.4396545943
H	–3.8346278399	–0.2963539024	5.1127046298
H	–4.0581075816	1.4361421527	0.9461205657
H	0.9334695015	–0.4279742729	–2.0571117667
H	–2.5440341077	–1.4788891881	5.28144468
H	–4.0667939404	–0.746313523	2.7223277331
H	–0.5532723794	–0.2837603482	–2.9939221354
H	1.4604627934	3.7306291032	–5.0430068323
H	–2.4044883757	–0.3062248285	3.0815496996
H	–4.6518733291	–4.4775193485	4.3883635302
H	1.2717204467	5.1606263731	–4.0259001508
H	–3.0319816603	–3.9577563867	4.846885111
H	–1.2077098274	–0.2970613385	–0.855703226
H	2.2939477312	3.6138471068	–0.8099546892
H	–4.5545733254	–3.1807496686	2.3125855635
H	–4.1458653687	0.6255063864	–0.8618196037

H	–1.0848304893	–2.6181472207	3.9446607751
H	–0.681479488	–1.7469884649	2.4636199281
H	1.9171756024	5.1365209239	–1.6375859783
H	–3.7760377478	–5.5331817156	2.3969864271
H	–3.1960138541	0.2526195061	–3.2599345849
H	–1.7010417876	–5.1583288951	3.8002377461
H	–0.1907605263	1.8426340673	–4.8608382396
H	–1.3260406414	–6.009033051	2.3035206964
H	–2.7436908502	–1.3735636357	–2.735479435
H	–1.3561651465	1.7823157961	–3.532931949
H	–3.9600613847	–4.3425796946	0.2134005703
H	–4.4399777996	–0.9029107274	–2.766618794
H	–2.7917709792	–5.6791609701	0.2557648696
H	–0.9494024787	4.0677911009	–4.4523989306
H	0.2498903413	–4.0794776801	2.6712976007
H	–0.5881640235	5.3536592775	–2.4811819636
H	–0.3152777415	–4.9998855744	0.5039655149
H	0.6716984105	4.3685822974	0.7342639466
H	–2.8039140238	–3.7824046505	–1.8277150769
H	0.1512997777	5.7344712865	–0.277348018
H	–1.6029023822	–5.0596788982	–1.5379831292
H	–2.1809450266	2.8567257417	–1.7120914497
H	0.1267707243	–1.9761323461	0.3126370927
H	–2.7736557081	4.1510075019	–2.7639246163
H	1.3561861523	–3.1809487931	0.724167721
H	–1.5824875045	3.4554551382	0.8014806868
H	–1.031897224	–2.0904497617	–1.931515346
H	–1.6524796284	5.138278406	1.2850584586
H	–0.6787654143	–3.3831329785	–3.0804923895
H	–2.4905135417	5.801757934	–0.9392094124
H	1.3605167946	–2.6657861521	–1.7523877106
H	–3.4785600083	4.4616111885	–0.3477967869
H	0.9543035564	–4.3535585414	–1.4435429671
C	3.8284616004	1.2684359495	0.2380780014
C	4.793275674	2.2582686944	0.0381493887
C	4.6907976928	3.4768458814	0.7077219477
C	3.6145192532	3.6964105645	1.5707395112
C	2.647347522	2.7089746343	1.7558127451
H	3.9191158704	0.3146393339	–0.2704850332
H	5.6267281458	2.0730942776	–0.6276695832
H	5.4409774192	4.2433860122	0.5651632071
H	3.5287911807	4.6373916221	2.099199521

H	1.8112299426	2.8945520489	2.4160488353

Tabelle 361 Standardorientierung von *trans*-*R*-TS2 [TS, M052X/6-31G].

Atomsymbol	x	y	z
C	0.9355051868	–2.5366918773	–3.3211051598
C	1.3340466014	–1.2660473218	–4.0779531815
C	–0.5568401439	–2.4853422917	–2.9801118382
C	0.9945587409	–0.0065038833	–3.259604586
C	0.1995361266	2.8955349432	3.3986541457
C	1.4055042568	1.2753205711	–4.0104758778
C	–5.2404486586	1.1028778108	1.8886257445
C	0.6993613243	1.9594956511	2.4865708818
Li	–3.4365508058	–0.0236163642	1.9437027007
C	–1.1159424184	3.3327415519	3.3050845234
C	–3.6178807807	–3.8001354444	–0.976299603
C	–0.8560152827	–1.2194569967	–2.170371456
C	–4.9758966774	–3.2458161325	–0.5339223798
C	1.6948937786	0.0376087845	0.5530621577
C	–4.7590082515	–1.9374898945	0.2342665829
C	–0.0824800635	1.4546696314	1.4207124769
C	–2.704342141	–3.9746213488	0.2434398635
C	0.4393410238	1.5784173104	–5.1614651719
C	–2.5652696201	–2.6676671114	1.0514232711
Li	–0.3614323769	1.345701698	–1.2613716316
N	–3.8815303152	–2.074364327	1.4200293224
N	–0.4395979033	0.0353000884	–2.8419618008
C	–4.5725253772	–2.7620922119	2.5351238399
N	0.3811279543	0.654459283	0.3969203493
C	–1.6933168056	–2.8634434415	2.3022047187
C	1.4817004709	2.507278657	–3.1070656694
C	–2.413490519	–3.7509055685	3.3242857239
C	–1.9449263242	2.7746155885	2.3223096023
C	–1.2844979681	–1.5495852322	2.9832583667
C	–1.3839508137	0.4824977582	–3.8850556778
C	–3.6723757535	–2.9918444346	3.7534736524
C	–1.4814959235	1.8314133656	1.3927004788
N	–2.4068035235	–0.8288752174	3.6493024882
C	–0.9388004325	1.7995972423	–4.5312641742
C	–3.244656611	–1.7200237579	4.4940608278

C	–2.3740923854	1.2353016826	0.3948231843
C	–1.836067386	0.24528059	4.5054641819
C	–3.7060892345	1.6321951617	0.2414207724
C	–4.4129622113	–0.9247213804	5.0781358403
C	–4.4910160098	1.2237051006	–0.9905796664
C	–2.9281002986	1.0870768948	5.154581765
C	–3.8928132155	0.2136766975	5.9623385733
N	0.1648118036	2.8814145919	–2.5396346473
H	–5.678776706	0.1365044405	2.1833287268
C	–0.8857697489	3.0160460529	–3.5858491387
H	–5.9446209013	1.613657848	1.2333647447
C	0.2946809766	4.1436555979	–1.7682149723
C	–2.2221597925	3.3062143242	–2.9060273778
C	–1.0133525187	4.5127024609	–1.074833244
C	–2.1562650598	4.6025228118	–2.0921214955
H	1.1708723898	–3.4261389221	–3.9107368932
H	1.513982676	–2.5991913772	–2.3902328895
H	2.4081490149	–1.26324097	–4.2879491449
H	0.8523345167	3.2820680083	4.1721422494
H	0.8158801904	–1.2435988519	–5.0435017597
H	1.7370844537	1.6633439315	2.5698227433
H	–0.8533312659	–3.3645025827	–2.4003814641
H	–1.5111119853	4.0644937044	3.9974892943
H	–1.1462198051	–2.495854726	–3.9045164013
H	1.571870494	–0.0532735203	–2.3270984019
C	2.8683014878	0.8149880707	–0.0300473346
H	1.9098117064	–0.1871502139	1.6110604474
H	–5.0624875878	1.7153484849	2.7790694583
H	1.6803295024	–0.9362243851	0.0434181962
H	–3.7344681313	–4.7516697401	–1.5019009916
H	2.4149161774	1.1020082643	–4.3989894034
H	–3.1606667744	–3.0968448593	–1.6827279879
H	–5.6178867667	–3.0525328063	–1.3979281984
H	–2.98714945	3.0675865037	2.2969625586
H	–0.3364687747	–1.2516542259	–1.20592155
H	–5.4933010639	–3.9826117287	0.0891737417
H	–4.277763141	–1.2202349169	–0.4316240452
H	–1.925662543	–1.1333600442	–1.9581804441
H	0.4019023294	0.761595405	–5.8873455782
H	–5.7017482669	–1.4951972262	0.5617659583
H	–1.7042599416	–4.2992937614	–0.0638553702
H	0.7688764762	2.4774158109	–5.6926368805

H	–3.1163808617	–4.7682583845	0.8746883207
H	–2.0104818023	0.3611279086	–0.1396339558
H	2.1672821609	2.3322270083	–2.2774658051
H	–2.0730411149	–1.9248376429	0.4100290401
H	–3.9632881831	2.6209352287	0.6044574751
H	–4.9580855143	–3.7443298483	2.2203562151
H	–5.4371332306	–2.1498433349	2.8049768777
H	1.8782576828	3.3500977544	–3.702010948
H	–0.766894461	–3.3462239519	1.9703433328
H	–4.6157978185	2.0852588759	–1.6549838388
H	–2.6666632935	–4.7289295366	2.9086062439
H	–1.4922769675	–0.2637232601	–4.6886606332
H	–1.7657137996	–3.9217745094	4.1903268036
H	–3.9592866776	0.4537443112	–1.5568101251
H	–2.3640495996	0.5916998584	–3.4133267488
H	–0.8307290944	–0.8671000254	2.2576522585
H	–5.4854019354	0.8501756128	–0.7477131415
H	–0.5176318192	–1.7922206333	3.7403830745
H	–1.6727800038	2.0455295003	–5.3071751892
H	–4.2471818104	–3.5915460728	4.468681721
H	–0.6227145302	3.8872198316	–4.2207176066
H	–2.6203742624	–2.0619332808	5.3464769698
H	1.0924303539	4.0011885355	–1.0376422975
H	–1.1872658336	0.8630040507	3.89031194
H	0.600682062	4.9548185025	–2.4539761645
H	–1.2152418591	–0.2252805379	5.2909365659
H	–2.4550476388	2.4831999312	–2.2231015721
H	–5.0105350814	–0.5028182622	4.2641333219
H	–3.0123263571	3.3528430712	–3.6629620138
H	–5.0553498561	–1.6026440158	5.650503997
H	–1.2489329937	3.7570058885	–0.3191659436
H	–3.4739889467	1.6161535815	4.3694780681
H	–0.8854640892	5.4626319248	–0.5493784155
H	–2.4593196751	1.8460063113	5.7862493354
H	–1.9857761422	5.4498995716	–2.7680323991
H	–4.7234565424	0.8101780855	6.3478623637
H	–3.1063790192	4.7780649498	–1.5809240141
H	–3.3674383072	–0.2124142872	6.8261299718
C	3.8449701822	0.1525618455	–0.7837173292
C	4.9137330332	0.8468758628	–1.3530676057
C	5.0282787948	2.2240946247	–1.1676557874
C	4.0630696799	2.8970073249	–0.4164047857

C	2.9874069404	2.2017656393	0.1368617926
H	3.7589033783	–0.9191773734	–0.931502971
H	5.6534074748	0.3144011469	–1.9373882492
H	5.8575317636	2.7664422585	–1.6022886229
H	4.1421555315	3.9667209826	–0.2678723268
H	2.2277268806	2.7313616996	0.6955221343

Tabelle 362 Standardorientierung von *trans*-R-TS3 [TS, M052X/6-31G].

Atomsymbol	x	y	z
C	4.4038617825	–0.7171798164	–4.4663214633
C	4.2789434412	0.7991032686	–4.2914805952
C	3.0787727446	–1.2699694925	–4.9968538171
C	3.1254055606	1.1547227371	–3.3350889703
C	1.4964056903	–3.8326970755	–1.559354959
C	2.9968947531	2.6826424367	–3.1693295117
C	4.5390968554	–0.5383244846	2.5934373269
C	0.4862340385	–2.9000146402	–1.3021778999
Li	2.4515397482	–0.7740592694	2.2308724929
C	2.830624177	–3.4959316017	–1.3520185668
C	2.6875600379	–5.30668525	3.7262679206
C	1.9528133935	–0.9160748971	–4.0212965505
C	2.0403785473	–5.0711714044	2.3592600267
C	–1.5688122897	–0.8922538289	–0.7549832054
C	2.1971811879	–3.6045612917	1.9473366182
C	0.7691283475	–1.5877683848	–0.8505352061
C	2.0548200172	–4.3540798627	4.7459888594
C	2.4222212068	3.3302333132	–4.4349053006
C	2.2076763831	–2.887531257	4.2967129238
Li	0.7332653636	0.7127772304	–1.9647598277
N	1.6650203009	–2.629740694	2.9358270266
N	1.8188882929	0.5428961306	–3.740511053
C	0.1854883157	–2.5229260039	2.8613766691
N	–0.1468706328	–0.560055675	–0.7550534562
C	1.5937878481	–1.9151974196	5.3132586477
C	2.1335595086	3.1091407517	–1.9772640422
C	0.0689749105	–2.0653507346	5.3286415817
C	3.1353783699	–2.2368141303	–0.8186492533
C	1.9562806728	–0.4456498935	5.0584832363
C	1.1260211454	1.2457816787	–4.8461160295

C	–0.4216772324	–1.6215388966	3.9476851837
C	2.1498631917	–1.2818407531	–0.524237757
N	1.3336691511	0.1541133511	3.8441206213
C	1.0135766825	2.7576530911	–4.6188649602
C	–0.1295215998	–0.1225712476	3.803206237
C	2.4684986175	–0.0002999259	0.1134673683
C	1.5766299689	1.6194495801	3.8785033575
C	3.7460815605	0.3323800885	0.562120115
C	–0.7686983059	0.5182805255	2.574842829
C	4.1434521903	1.7487032982	0.9102686774
C	0.9067618047	2.35311774	2.7195052742
C	–0.5885326602	2.0368731627	2.642128723
N	0.7030252399	2.7492837499	–2.1293026286
H	4.4409018638	0.2090085865	3.3909162799
C	0.1332452261	3.1855983034	–3.4321121792
H	5.512013519	–0.4263722428	2.1160295109
C	–0.0736263714	3.3187036521	–1.001921628
C	–1.3136974933	2.7023850735	–3.5430780611
C	–1.5352670271	2.8870675675	–1.0593672533
C	–2.1625100432	3.2717314583	–2.4023276869
H	5.2293859802	–0.9588593419	–5.1405814062
H	4.6193849378	–1.1823069559	–3.4967372467
H	5.2035934198	1.2217356631	–3.8854579421
H	1.230522101	–4.8124002691	–1.9376609411
H	4.1180783319	1.2577342746	–5.2736571362
H	–0.5389845182	–3.1750239867	–1.5173913874
H	3.1212783927	–2.3579794597	–5.0942396944
H	3.6222342046	–4.2025388543	–1.5639947362
H	2.8807357933	–0.8615633149	–5.9949767383
H	3.3607972881	0.7184665188	–2.3544137929
C	–2.2628555962	–0.7177393683	–2.0970182538
H	–1.7466653426	–1.917000951	–0.3909190868
H	4.4735662756	–1.552842586	3.0085073635
H	–2.0809446663	–0.2353485139	–0.0391644433
H	2.5700171462	–6.3453946588	4.0460253366
H	4.0071817926	3.0621192761	–2.9785203281
H	3.7642648622	–5.1062441772	3.6574200782
H	2.4996523481	–5.6950636839	1.5877605601
H	4.170944803	–2.011169423	–0.5956870283
H	2.1388857371	–1.4245352567	–3.0737512398
H	0.9803170853	–5.3467033371	2.4014553406
H	3.2608063	–3.3824384145	1.8108975238

H	0.9902621201	–1.2604251594	–4.4027422074
H	3.040252354	3.1231530547	–5.3116162304
H	1.703098204	–3.4163371185	0.9970374819
H	2.5204001257	–4.4670339388	5.7307660297
H	2.3801644764	4.4176907778	–4.3105073281
H	0.9975630897	–4.6154358897	4.8563593271
H	1.6251539436	0.647479678	0.323970096
H	2.4918424974	2.6337342941	–1.061924341
H	3.2845556693	–2.6859158513	4.2327672459
H	4.5702343079	–0.2444730541	0.1636567618
H	–0.2862680942	–3.5132182709	2.9570250914
H	–0.0570258167	–2.1453817731	1.8630242556
H	2.2263771325	4.2033766473	–1.8564608654
H	2.0085623825	–2.1727281733	6.2945925282
H	4.4466993956	2.2865030525	0.0028208142
H	–0.2305202	–3.0925148138	5.5454465919
H	1.6481211582	1.0952633488	–5.8039518407
H	–0.3668776333	–1.426699406	6.1042542363
H	3.3234381011	2.3053411453	1.3653802675
H	0.1358147356	0.7934369713	–4.9442217256
H	3.0391845224	–0.3345004022	4.9686021379
H	4.9867094853	1.7646423396	1.5999224273
H	1.6296659993	0.1331804098	5.9414447978
H	0.5481541008	3.1839598174	–5.5149629771
H	–1.5101221236	–1.7319869909	3.8826137194
H	0.1219357715	4.2953180433	–3.4409122929
H	–0.5829423468	0.3629328819	4.6943582957
H	0.3921226315	2.9764678582	–0.0753021417
H	2.6580390957	1.7760414197	3.860620805
H	–0.0028279065	4.4211877418	–1.0316116317
H	1.1905161528	2.0244725474	4.8318994504
H	–1.342846114	1.6088604036	–3.4943838577
H	–0.317888799	0.1318363501	1.6516798645
H	–1.716494834	2.9989535785	–4.5167827238
H	–1.8316977312	0.2546743536	2.5599062322
H	–1.5813247317	1.802042506	–0.926476505
H	1.3748402882	2.0397662006	1.7862710845
H	–2.0823386165	3.3493846315	–0.2325592433
H	1.0803845941	3.4275904245	2.8335112507
H	–2.2063481015	4.364820527	–2.4880921715
H	–1.0371769371	2.5184904956	1.7704236541
H	–3.1843757349	2.8926108518	–2.4683089265

H	–1.0979022879	2.4295544881	3.531192969
C	–3.5090228155	–0.0895620613	–2.1887583056
C	–4.1281194933	0.1010729319	–3.4259365654
C	–3.5075925404	–0.3390299156	–4.5943835956
C	–2.2666188261	–0.9746408584	–4.5148017278
C	–1.6494170178	–1.156003466	–3.2775270142
H	–3.9893037147	0.2651635036	–1.283247194
H	–5.0896344111	0.5963110051	–3.4766581036
H	–3.9856234212	–0.1924070529	–5.5539531929
H	–1.7816648347	–1.3308808195	–5.4157514692
H	–0.6886419289	–1.6477290463	–3.2084536841

Tabelle 363 Standardorientierung von *trans*-R-TS4 [TS, M052X/6-31G].

Atomsymbol	x	y	z
C	3.7341672931	–0.9246159411	–4.0264233134
C	3.7278491597	0.6019962689	–3.9055501382
C	2.4287105413	–1.3814886769	–4.6814422658
C	2.5095148698	1.0951341817	–3.1006514068
C	0.1024835648	–3.6946528645	–1.486641141
C	2.5015495847	2.6335748509	–3.005634656
C	2.7455553725	–0.5838231277	3.0037770985
C	–0.8296536876	–2.6525349598	–1.4733694143
Li	0.7329988851	–0.7642432138	2.2625467259
C	1.3788608069	–3.5029790026	–0.9657297559
C	–2.1232599867	2.9900008275	2.8904194321
C	1.2462589341	–0.8972006207	–3.8376298903
C	–0.8479687451	2.9646177265	3.7387350453
C	–2.7578804098	–0.4504312421	–1.2625865155
C	0.0328340612	1.7971585748	3.2808913079
C	–0.5135561468	–1.3651973554	–0.9780003028
C	–2.8380392658	1.6393475899	3.0021786109
C	2.1229423688	3.2690652114	–4.348414332
C	–1.9157472649	0.4670710546	2.6107291697
Li	–0.0761496056	0.9120689608	–2.0216172529
N	–0.6233968943	0.4718464688	3.3597246083
N	1.2083631656	0.5784295974	–3.6291540778
C	–0.703682846	–0.0276972311	4.7521200035
N	–1.3254189724	–0.2521239404	–1.0593521706
C	–2.6352393981	–0.8804482493	2.7777380735

C	1.558354107	3.1816753412	–1.9310915929
C	–2.8416284967	–1.2133777574	4.2601730763
C	1.6971034604	–2.264052772	–0.3925331939
C	–1.9050639472	–2.0460181004	2.1077216812
C	0.6934479475	1.2895581218	–4.8236947587
C	–1.4452651952	–1.3657987917	4.8712177841
C	0.7950904733	–1.1875783549	–0.3769844642
N	–0.6136008898	–2.4094043792	2.7492921564
C	0.6943340689	2.8151264216	–4.6610246913
C	–0.7517618244	–2.5719109875	4.2198481189
C	1.1347288441	0.1014918174	0.2319022136
C	–0.1505169725	–3.6879398856	2.1507203949
C	2.3508500151	0.3508650191	0.8624441286
C	0.6052482776	–2.9116445071	4.8348898917
C	2.7964632885	1.7574195937	1.1998791042
C	1.2051946284	–4.1091201667	2.700960771
C	1.1671517476	–4.2056920563	4.2310689881
N	0.1263150488	2.9326279779	–2.2217202858
H	2.3359302431	–0.1359186496	3.9216777162
C	–0.2614099834	3.3723149328	–3.5894765839
H	3.730236636	–0.1578106112	2.8177424989
C	–0.7079783529	3.5981219408	–1.1925469805
C	–1.7289482599	3.0278635061	–3.8420378001
C	–2.189077073	3.2956718948	–1.3962682764
C	–2.6308241615	3.705372398	–2.8052705668
H	4.6020961951	–1.259597656	–4.6000212059
H	3.805894781	–1.3720791433	–3.0274251037
H	4.6353665086	0.9557300749	–3.405828119
H	–0.1770871103	–4.6512961792	–1.9112336329
H	3.7228465038	1.0376409234	–4.9109736005
H	–1.8064528841	–2.8252186164	–1.9078685873
H	2.3850502114	–2.4718005304	–4.746504831
H	2.1072030464	–4.3032375017	–0.9685556751
H	2.3705457551	–0.9920932773	–5.7046750077
H	2.5943646153	0.6839920264	–2.0846096606
C	–3.2468712032	–0.205746084	–2.6803467939
H	–3.0752265196	–1.4579816871	–0.9481077681
H	2.8543332468	–1.6659554395	3.1299536487
H	–3.3043199748	0.2456532033	–0.6101837284
H	–2.7869587924	3.8010446733	3.2015489413
H	3.5159524888	2.9352294391	–2.720552217
H	–1.8552270265	3.173216417	1.8418168067

H	–0.2883021103	3.8987925987	3.6348394863
H	2.6722003148	–2.1393168282	0.0620911828
H	1.3007758162	–1.3721962127	–2.8563639138
H	–1.1089468786	2.8642106565	4.7977335863
H	0.2867687788	1.9545064196	2.2312903734
H	0.2976460877	–1.1861419479	–4.2918617046
H	2.8058791224	2.9667146764	–5.1459656439
H	0.9695764519	1.7450120417	3.8395118106
H	–3.7188569051	1.6144402961	2.3522111625
H	2.1702976262	4.36048038	–4.2704250914
H	–3.1934031511	1.516121199	4.0307032861
H	0.3346321338	0.8330462984	0.2909763447
H	1.777991697	2.719438106	–0.9688757317
H	–1.6501597501	0.5785345987	1.5484252264
H	3.1761816788	–0.3111761914	0.6318344059
H	–1.2212372846	0.6910459987	5.4070024412
H	0.3214303358	–0.1177057493	5.121753448
H	1.7304967386	4.2692852679	–1.8393644768
H	–3.6041814557	–0.7852740692	2.2738358176
H	3.4898305628	2.1196260138	0.4303663604
H	–3.411576809	–0.437818372	4.7779479516
H	1.2932216107	1.0562707239	–5.7171866923
H	–3.400372861	–2.1502705702	4.3566788337
H	1.9565355564	2.452655871	1.2322645811
H	–0.3182749343	0.9187994494	–5.0071110894
H	–1.6988687501	–1.815151754	1.0627249714
H	3.3141729074	1.8063371391	2.1573346977
H	–2.5748944196	–2.9250148881	2.1357127329
H	0.3649976479	3.2402603007	–5.6160621094
H	–1.5252282001	–1.593201286	5.9407399803
H	–0.1603666912	4.4768940912	–3.6302581451
H	–1.4231347703	–3.4389405753	4.399249405
H	–0.3720333212	3.2404342371	–0.2151419105
H	–0.1071401263	–3.5582452876	1.0711067169
H	–0.5347126149	4.6888213573	–1.2316417327
H	–0.8991931429	–4.4718486258	2.3732661717
H	–1.8716979469	1.9441779493	–3.7811043957
H	1.3044082308	–2.0920080173	4.6535657235
H	–1.9988766891	3.3371869722	–4.856697954
H	0.4866586239	–3.0139346197	5.9189821748
H	–2.3447417073	2.2218498786	–1.2562569412
H	1.9533452481	–3.3793390574	2.3840019157

H	–2.7734440208	3.822262836	–0.635870712
H	1.4845865405	–5.070155366	2.2599970956
H	–2.5576391853	4.7951520916	–2.9115571922
H	2.1647237659	–4.4080394396	4.6292251743
H	–3.6721729328	3.4253097041	–2.9757864919
H	0.5230911936	–5.0449518808	4.5229536646
C	–4.3851333851	0.5691429446	–2.9231793954
C	–4.8162706505	0.8237054954	–4.2266130948
C	–4.1132703755	0.3001388395	–5.3106575577
C	–2.980088212	–0.4835976578	–5.0805341585
C	–2.5497181882	–0.7283462599	–3.7771594225
H	–4.9279653161	0.9874148622	–2.0825978142
H	–5.695510974	1.4327807541	–4.3943624751
H	–4.4448332277	0.4963114767	–6.3217353752
H	–2.4332282694	–0.9035385023	–5.9159285115
H	–1.6697522686	–1.3291658431	–3.5915132272

8.3.15 Angaben zu den quantenchemischen Rechnungen der Carbolithiierung von Methylstyrol (Kapitel 4.6.3)

Tabelle 364 Berechnete Energien der optimierten Verbindungen.

Verbindung	Methode/Basis	Min./TS	ZPE [Hartree]	SCF [Hartree]
EtLi TS-*S*-1	B3LYP/6-31+G(d)	TS	–1131,874985	–1132,50495
EtLi TS-*S*-2	B3LYP/6-31+G(d)	TS	–1131,869845	–1132,49929
EtLi TS-*R*1	B3LYP/6-31+G(d)	TS	–1131,872007	–1132,5019
EtLi TS-*R*-2	B3LYP/6-31+G(d)	TS	–1131,873814	–1132,50346
EtLi TS-*S*-1 Dis	M052X/6-31+G(d)	TS	–1131,738514	–1132,37986
EtLi TS-*S*-2 Dis	M052X/6-31+G(d)	TS	–1131,731968	–1132,37181
EtLi TS-*R*1 Dis	M052X/6-31+G(d)	TS	–1131,733371	–1132,37391
EtLi TS-*R*-2 Dis	M052X/6-31+G(d)	TS	–1131,73358	–1132,37487
i-PrLi TS-*S*-1	B3LYP/6-31+G(d)	TS	–1171,153003	–1171,81213
i-PrLi TS-*S*-2	B3LYP/6-31+G(d)	TS	–1171,149965	–1171,80791
i-PrLi TS-*R*1	B3LYP/6-31+G(d)	TS	–1171,152515	–1171,81015
i-PrLi TS-*R*-2	B3LYP/6-31+G(d)	TS	–1171,152926	–1171,81086
i-PrLi TS-*S*-1 Dis	M052X/6-31+G(d)	TS	–1171,011164	–1171,68126
i-PrLi TS-*S*-2 Dis	M052X/6-31+G(d)	TS	–1171,00534	–1171,67431
i-PrLi TS-*R*1 Dis	M052X/6-31+G(d)	TS	–1171,006972	–1171,67576
i-PrLi TS-*R*-2 Dis	M052X/6-31+G(d)	TS	–1171,008173	–1171,6775

Tabelle 365 Standardorientierung von EtLi TS-*S*-1 [TS, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.0555651169	2.3895424068	0.4733140686
C	0.57067483	1.8598776858	–0.7162522424
C	1.8922632174	1.284384339	–0.8990842653
C	2.3371118267	0.9294762266	–2.2012179681
C	3.6036676507	0.3989472377	–2.4321668962
C	4.4967405901	0.1925760433	–1.3720456485
C	4.0873840776	0.5421027541	–0.0798359668
C	2.8187048921	1.0714445036	0.1562863715
C	–0.952970137	3.5152247527	0.3978644592
C	2.4680980689	–3.4028052901	0.4167950019
C	1.4608694374	–3.531841906	–0.734346517
C	1.7292790991	–3.0812085124	1.7220823776
C	0.5690989584	–2.2738683102	–0.8599768348
C	–0.4678525258	–2.4165816909	–1.9986867581

C	0.8634017475	–1.8252468418	1.5405515773
C	–1.5428763221	–3.4473898985	–1.6270012746
N	–0.105610561	–1.8831810153	0.4157224948
C	–1.1726894017	–1.1039266764	–2.3934032478
C	–1.2825134968	–2.7177621652	0.7504419016
C	–2.2827057096	–2.8725803762	–0.4126263879
Li	–0.6824576822	0.1976911759	0.148145797
N	–2.0905062128	–0.5540567253	–1.3625595015
C	–3.0278638389	–1.5935539279	–0.8552305355
C	–2.8585654225	0.5613990353	–1.9618064137
C	–3.9575010046	–1.0042825569	0.2147161809
C	–3.8231890418	1.2096041114	–0.9667068716
C	–4.7675322686	0.1706130895	–0.3499808304
C	–1.2166566006	1.1159648628	2.0229077655
H	0.7401626715	2.4725896683	1.3126170527
H	0.0137012244	2.054701783	–1.6352799286
H	1.6701461441	1.1015593059	–3.0451785014
H	3.9017924315	0.1525830304	–3.4496292675
H	5.4881075156	–0.2151707745	–1.5506999901
H	4.7689460278	0.407387559	0.7582801398
H	2.5477722228	1.345600588	1.1727790595
H	–1.6790416931	3.3531577076	–0.406999743
H	–0.4273318516	4.454703308	0.1698066768
H	–1.5022068734	3.6600359748	1.3327371081
H	3.052352095	–4.3267417469	0.5158786566
H	3.1795690257	–2.5959473676	0.1918538288
H	1.9865268881	–3.677611349	–1.6875641209
H	0.8499419975	–4.4296066968	–0.5725277228
H	2.4397424209	–2.9014846645	2.5397174007
H	1.113022305	–3.9391501627	2.0268209996
H	1.237491831	–1.4387275725	–1.1090713962
H	0.0831165717	–2.7463626119	–2.8898119059
H	1.5274069882	–0.9735607643	1.350592049
H	0.3004882397	–1.5995383416	2.4528490441
H	–1.1072023124	–4.4260111957	–1.3970268257
H	–2.2364598719	–3.5968591116	–2.4654374907
H	–0.4329857709	–0.3296467864	–2.6250251462
H	–1.7422674118	–1.2993451394	–3.3225603205
H	–0.9857124151	–3.734481838	1.0596083746
H	–1.7671881426	–2.2604393422	1.6211838079
H	–3.054148668	–3.5778663655	–0.0735277747
H	–3.6741274497	–1.9083991895	–1.7021804509

H	–2.1415121686	1.2998081553	–2.3372061668
H	–3.4263905935	0.187281267	–2.8366691805
H	–3.3732477164	–0.6657999964	1.0787327254
H	–4.6296309107	–1.7972610841	0.5695584042
H	–3.2507944009	1.6992337718	–0.1712694821
H	–4.3903275679	1.9940357001	–1.4844326376
H	–5.4618259295	–0.2015738214	–1.1181870524
H	–5.3804223081	0.627870886	0.4366082831
C	–0.5432163947	1.6343712277	3.2869591335
H	–1.3523650032	0.0222133926	2.1146452569
H	–2.2162611849	1.5530529986	1.8974928627
H	–0.3740135062	2.7209353749	3.2416382459
H	0.442694774	1.1694672786	3.4369500412
H	–1.1207705164	1.4527346136	4.2089761176

Tabelle 366 Standardorientierung von EtLi TS-*S*-2 [TS, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.8233735784	–1.1253594173	2.4220298455
C	0.7821737334	0.2721875721	2.4104968922
C	1.9295417469	1.1675281991	2.479194922
C	1.7233983914	2.5618869104	2.6471020364
C	2.7829052999	3.4565630589	2.7742872451
C	4.1081941986	3.003400336	2.7355893397
C	4.3391293315	1.6326014212	2.5726124918
C	3.2799460127	0.7341678968	2.4452300761
C	–0.2809109943	–1.8966057943	3.1122478571
C	–4.3535159116	–0.8474002317	–0.5967821024
C	–3.537797661	–0.6071426558	–1.8731148242
C	–3.9474337734	0.1726592907	0.4721518542
C	–2.0115115123	–0.599823167	–1.6080959655
C	–1.2277658355	–0.2922740919	–2.9045469599
C	–2.4313943555	0.0991390453	0.706085748
C	–1.3778610499	1.1854049758	–3.2935453301
N	–1.5870951367	0.3038525193	–0.4951958535
C	0.2712858554	–0.6256689703	–2.8376546368
C	–1.4924686585	1.7358371295	–0.862959539
C	–0.7161531115	1.9920291805	–2.16996493
Li	0.4059610717	–0.3685562277	0.2174965598

N	1.0516268715	0.2239772878	–1.9077783207
C	0.796234157	1.66932522	–2.1555736376
C	2.4892162628	–0.0752724465	–2.1103877078
C	1.6149878199	2.5274314887	–1.1845082317
C	3.3917078901	0.7454521292	–1.1914961494
C	3.1174184401	2.2481639273	–1.3314618918
C	0.7345441313	–2.4700997193	0.4303390481
H	1.8012555149	–1.5895863641	2.5127552526
H	–0.1812519857	0.7467147766	2.6055227304
H	0.7014297089	2.935935131	2.6974422933
H	2.5742238477	4.5159695725	2.9115059708
H	4.9372057297	3.6984443692	2.8398583594
H	5.359671534	1.2546503181	2.5498969237
H	3.5035056373	–0.323915015	2.334245223
H	–1.2588784883	–1.4263694487	2.9656865263
H	–0.0893035745	–1.8955585107	4.1961713808
H	–0.3469223512	–2.9389825509	2.7887412796
H	–5.4275105083	–0.7867708013	–0.8138406956
H	–4.1638572733	–1.8637930965	–0.2200670522
H	–3.7510520294	–1.3866356248	–2.6171276837
H	–3.854326133	0.3441653124	–2.3196794074
H	–4.4604016933	–0.0260758073	1.4223081392
H	–4.2457638421	1.1832028422	0.1600170823
H	–1.7415124704	–1.6139020952	–1.2765493958
H	–1.6507563184	–0.9342790808	–3.6891300201
H	–2.1939785718	–0.897376471	1.0981094129
H	–2.1170090453	0.8259139766	1.461627822
H	–2.4280899707	1.4728804092	–3.419477544
H	–0.8789725096	1.3776062934	–4.252670158
H	0.4167218939	–1.6707637336	–2.5412518876
H	0.6821265063	–0.5220513697	–3.8607683095
H	–2.4904443	2.1908254548	–0.9859582573
H	–1.0167164691	2.2520325809	–0.0206376073
H	–0.7998629283	3.0674560218	–2.3785528412
H	1.1552883487	1.9073665045	–3.1798413819
H	2.6365950292	–1.1470586049	–1.9349482576
H	2.7557253388	0.1206180158	–3.1680961739
H	1.3107247769	2.3286373127	–0.1498394536
H	1.4011537529	3.5865900856	–1.3822683479
H	3.2326669538	0.4423783374	–0.1510879692
H	4.439144096	0.517955025	–1.4288630099
H	3.4568971964	2.5957967077	–2.3192211662

H	3.6824533005	2.8090994291	–0.5788282936
C	1.7320021468	–3.5201505661	0.9041407679
H	–0.2934501487	–2.8654222173	0.4293422132
H	1.5551571101	–3.81678137	1.948708928
H	2.7632797749	–3.1391481199	0.8579138927
H	0.9821764052	–2.2027444647	–0.6116839904
H	1.715519216	–4.4527780303	0.3150968702

Tabelle 367 Standardorientierung von EtLi TS-*R*-1 [TS, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.0483386885	–1.2713967827	–2.5490146863
C	–0.0148963993	0.1258251902	–2.532978689
C	1.1822822007	0.9550204131	–2.5119947223
C	1.0674447076	2.3690093655	–2.5618584239
C	2.1838151504	3.2027284259	–2.5681215845
C	3.4765621968	2.664756648	–2.527166263
C	3.6179277908	1.2722227638	–2.49014079
C	2.5027230105	0.4356899118	–2.4809405786
C	–1.1966751566	–1.9924350424	–3.220745093
C	2.7490422192	–0.360427523	3.2582728749
C	1.2955981837	–0.1993592757	3.7235547298
C	3.0201945556	0.5759629842	2.0753221548
C	0.2971448973	–0.4131490799	2.5600625111
C	–1.1693858269	–0.2461200981	3.0141550047
C	1.9988938898	0.3301598347	0.9549779482
C	–1.463644153	1.2254460806	3.3350590584
N	0.5743722476	0.4302217125	1.3615151262
C	–2.2146812207	–0.7473076679	1.9967028216
C	0.1379635765	1.8392294163	1.508153831
C	–1.3134385805	1.9863365699	2.0121503906
Li	–0.4444303782	–0.4611292493	–0.3767320719
N	–2.319734876	0.0585608396	0.7518187415
C	–2.4300798536	1.5120320822	1.0577294895
C	–3.5239345362	–0.391384809	0.0131966664
C	–2.5434193213	2.3261763565	–0.2364492785
C	–3.760817537	0.3915330961	–1.2805869287
C	–3.7857290535	1.9047422965	–1.0324379189
C	–0.2052376881	–2.5912628762	–0.5571726628
H	0.9032807413	–1.7870359708	–2.6375804835

H	–0.9446810678	0.6592908864	–2.7357851565
H	0.0732319872	2.8108338417	–2.6141852625
H	2.0448072976	4.2813105885	–2.6123390608
H	4.3493507648	3.3122423998	–2.5359307282
H	4.6123600712	0.8298148208	–2.4722358442
H	2.6572045627	–0.6396903792	–2.4551868171
H	–1.2515169619	–3.0488986949	–2.9445368132
H	–1.0691962368	–1.9380488809	–4.3126047748
H	–2.1627727608	–1.5315936666	–2.9888528898
H	3.4395971453	–0.1589054749	4.0871908822
H	2.9237080127	–1.4016567366	2.9475130239
H	1.0621262936	–0.9222730876	4.517362262
H	1.1733920516	0.7983765678	4.163805169
H	4.0278175544	0.4178350172	1.6699358468
H	2.98018515	1.6219844005	2.4102690765
H	0.4322543266	–1.4521200967	2.2273781325
H	–1.2984397549	–0.8645207432	3.9129608163
H	2.1500381765	–0.6841097161	0.5598639892
H	2.1599997137	1.0187212086	0.12267079
H	–0.7840632206	1.6189328975	4.0989132997
H	–2.4827156691	1.3355472326	3.7293401282
H	–2.0039252224	–1.782994578	1.705424584
H	–3.1956720356	–0.7495040974	2.5096669723
H	0.7818400992	2.3920873602	2.2134642337
H	0.266124553	2.3202751526	0.5318453387
H	–1.4818279821	3.0598259975	2.175432768
H	–3.3784285942	1.6706637316	1.6147677408
H	–3.4044152983	–1.4592015771	–0.2030129779
H	–4.411985784	–0.2895178145	0.6679223442
H	–1.6434869366	2.1859068934	–0.8475105609
H	–2.5958609213	3.3924722954	0.0209973927
H	–2.9704820788	0.156158924	–1.9998734913
H	–4.7054745725	0.0535133669	–1.7258043733
H	–4.6883356954	2.1732527345	–0.4636684406
H	–3.8390440361	2.4477111856	–1.9842970046
C	0.7752156378	–3.6735584435	–0.9933095478
H	–1.2443570286	–2.953164427	–0.5919250968
H	0.0124675976	–2.3310344246	0.4933155687
H	1.8154714898	–3.3253751616	–0.9073315376
H	0.6288004284	–3.9634729046	–2.0447113539
H	0.7062868455	–4.6053622108	–0.4068898011

Tabelle 368 Standardorientierung von EtLi TS-*R*-2 [TS, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–1.2264879344	2.443015677	–0.4530756884
C	0.1699925261	2.4233193666	–0.4169456253
C	1.0581122691	2.4517485113	–1.568041667
C	2.4569676991	2.6105386788	–1.3788828993
C	3.3448404091	2.6819085651	–2.4493592655
C	2.8812984519	2.5957205744	–3.7689001079
C	1.5066265362	2.443061498	–3.9835789242
C	0.6140060085	2.3679909679	–2.9141849804
C	–1.9898560559	3.0959169318	0.677744182
C	1.5351365364	0.2116483461	4.0641657762
C	2.2881465671	–0.6493091308	3.040394532
C	0.0388275253	–0.1221350558	4.0269788856
C	1.6888010606	–0.5224649627	1.6190252754
C	2.4202272707	–1.432724155	0.6050894078
C	–0.4956648925	0.0428310827	2.5965741285
C	2.0901213983	–2.907562384	0.8750935706
N	0.2133780645	–0.7476820404	1.5613644077
C	2.1120967909	–1.1252473057	–0.873293714
C	–0.1894653935	–2.1735007884	1.5930718022
C	0.5888394173	–3.0646461299	0.6037476959
Li	–0.4365604297	0.2201280389	–0.2679257726
N	0.7169021363	–1.4214601051	–1.288392069
C	0.3351617867	–2.806296411	–0.8983951638
C	0.6258331697	–1.2754031616	–2.7611063884
C	–1.0905561643	–3.1453651479	–1.3557407434
C	–0.7861308945	–1.5491125305	–3.2800154473
C	–1.2580571759	–2.9495142966	–2.8690075622
C	–2.5720153554	0.4523116287	–0.3677863242
H	–1.69726859	2.561922253	–1.425225607
H	0.6511672511	2.5928583931	0.5486908849
H	2.8387613068	2.7010537798	–0.3626567096
H	4.4074777132	2.8134843251	–2.254123485
H	3.5715441383	2.655283504	–4.6060948967
H	1.1213662324	2.3847779109	–4.9999776408
H	–0.4467215894	2.2588377967	–3.1256531216
H	–3.0476905126	2.8205983326	0.6927095465
H	–1.930528819	4.1889394452	0.5646998409
H	–1.558842841	2.8524849979	1.655583456
H	1.9480848123	0.0565791557	5.0689802263
H	1.6752569603	1.2770987923	3.8265459057

H	3.3457085427	–0.3555576258	2.996438178
H	2.2694539267	–1.6938130922	3.3768587961
H	–0.5282833769	0.5392908959	4.6950330619
H	–0.1253101904	–1.1470222416	4.3878097525
H	1.8352844939	0.5218380532	1.305722148
H	3.4961468097	–1.2545727544	0.7370349304
H	–0.4049159278	1.0992382205	2.3153477528
H	–1.5595542412	–0.2100914165	2.5377134419
H	2.3394834354	–3.2025289148	1.9006223413
H	2.6719109056	–3.5559632495	0.2069165308
H	2.3149946226	–0.0740109492	–1.1026516047
H	2.8096726342	–1.7279303677	–1.4868277875
H	–0.0517696813	–2.6100382878	2.5972995126
H	–1.2654061583	–2.2068636011	1.3856182924
H	0.2770504464	–4.0996686725	0.8008889689
H	1.0120687574	–3.5040837621	–1.4370540342
H	0.9433560624	–0.2619139553	–3.0206917144
H	1.3368991362	–1.976614669	–3.2419428852
H	–1.8182904541	–2.5224432603	–0.8232989078
H	–1.3018150265	–4.1876093157	–1.0803974123
H	–1.4742234376	–0.7913717544	–2.8853810789
H	–0.7878340493	–1.4445245088	–4.3725965463
H	–0.6616175198	–3.7052890435	–3.4017913863
H	–2.3036463257	–3.1087123401	–3.1606063443
C	–3.6318538386	0.8721581068	–1.3786374147
H	–2.9357546875	0.5596037644	0.6628222888
H	–2.3440363247	–0.6186650001	–0.5132895353
H	–3.2875163594	0.7195369006	–2.4126035917
H	–3.8819443564	1.94032674	–1.2899458966
H	–4.5865852079	0.3271611528	–1.2829055766

Tabelle 369 Standardorientierung von EtLi TS-*S*-1 Dis [TS, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	0.0074223219	2.4069693358	0.4008492603
C	0.5001664642	1.8996387118	–0.786087952
C	1.787408342	1.2422196	–0.9542838681
C	2.2191735151	0.8607868448	–2.2432041468
C	3.4316383263	0.2145650427	–2.4478042387
C	4.2739125223	–0.0707335792	–1.3712445271

C	3.8793175629	0.3220915394	–0.0924856094
C	2.6632719064	0.9644534222	0.1159388308
C	–1.0432538429	3.4864869231	0.3722933971
C	2.4797233514	–3.2877266407	0.4743511553
C	1.4985937284	–3.4360522156	–0.688122336
C	1.7017594878	–3.0045755214	1.7588642303
C	0.615351336	–2.183701735	–0.8266718711
C	–0.3761702363	–2.3209668265	–1.9949778696
C	0.8291479773	–1.7618548626	1.568370778
C	–1.4375666001	–3.3736241401	–1.6761876593
N	–0.0982553886	–1.8268045174	0.4226890929
C	–1.0982741589	–1.0220486248	–2.3766284753
C	–1.2431593328	–2.7036707829	0.7135168371
C	–2.2082694717	–2.8445332188	–0.4689887549
Li	–0.7073854826	0.2036861351	0.1620547966
N	–2.0197249733	–0.5111033621	–1.3454550889
C	–2.9464375903	–1.563162968	–0.8803588237
C	–2.7979710331	0.5976830506	–1.9183131236
C	–3.8579574242	–1.0127185718	0.213238979
C	–3.7341199626	1.2173261283	–0.8872368476
C	–4.6792600708	0.1623565001	–0.3157192387
C	–1.2507441849	1.0363649313	2.0355585837
H	0.6708347745	2.4402232206	1.2551711624
H	–0.0528661469	2.1004069164	–1.7005672304
H	1.5866985679	1.0907255235	–3.0948727335
H	3.7259329594	–0.0614505652	–3.4540187381
H	5.2204007017	–0.5728467669	–1.5276871559
H	4.525704736	0.126001224	0.7560319542
H	2.3909738485	1.2591297233	1.1227000281
H	–1.7281224136	3.3460641394	–0.4664652169
H	–0.5505988747	4.455011041	0.2332598982
H	–1.6208963763	3.5277049319	1.2948487515
H	3.0881190371	–4.1899940922	0.5775821486
H	3.1587464137	–2.4534560672	0.2686707531
H	2.0360763463	–3.5837229042	–1.6298250295
H	0.887608628	–4.3285176944	–0.5219934231
H	2.3815849042	–2.8283421447	2.5971334155
H	1.0900773932	–3.8735408963	2.0235100093
H	1.2878816082	–1.3452501324	–1.0413041202
H	0.2074657022	–2.6202094184	–2.8715236324
H	1.4843925247	–0.9032373015	1.4031182411
H	0.2381299636	–1.5538480811	2.4628298946

H	–0.9933963282	–4.3476831602	–1.461919047
H	–2.1097771886	–3.5028485004	–2.5306861907
H	–0.3725020381	–0.2344278914	–2.5912344492
H	–1.6644158973	–1.2170506385	–3.3046379171
H	–0.9160694918	–3.716814647	0.9885261281
H	–1.7568253481	–2.2894031786	1.5849984822
H	–2.9788057167	–3.563181385	–0.1704942333
H	–3.5914428118	–1.8480528846	–1.7361277523
H	–2.0955648939	1.3434796537	–2.2962550208
H	–3.3823792641	0.2267365289	–2.7792363081
H	–3.2552760561	–0.6769379629	1.0613603864
H	–4.5113343361	–1.8171968979	0.5647592213
H	–3.1351981313	1.6403886742	–0.0775498166
H	–4.2919558097	2.0340185149	–1.3535133851
H	–5.3577584724	–0.1908729197	–1.1014726608
H	–5.2949377353	0.5894717328	0.4791090518
C	–0.4808461554	1.5972635963	3.222746667
H	–1.3972089837	–0.045106401	2.1873920558
H	–2.2508962802	1.4797263461	1.9769567725
H	–0.3519210644	2.683857494	3.1419076879
H	0.5268472969	1.1662826686	3.2823139973
H	–0.9599166805	1.4184500041	4.1944018438

Tabelle 370 Standardorientierung von EtLi TS-*S*-2 Dis [TS, M052X /6-31+G(d)].

Atomsymbol	x	y	z
C	0.8224657761	–0.9530130896	2.3638766064
C	0.821764793	0.4292790348	2.3351144855
C	2.0070039581	1.2843167089	2.386458539
C	1.8486245751	2.6812501688	2.4868825198
C	2.9374461188	3.538077784	2.5958371031
C	4.2375637237	3.0316483124	2.6069519253
C	4.4177563727	1.6516059337	2.511993958
C	3.3278665261	0.7941611021	2.4069974782
C	–0.2976614364	–1.6904516028	3.0546115045
C	–4.2929880907	–0.947512347	–0.6537494163
C	–3.5133247435	–0.5901150949	–1.9177114471
C	–3.8814704378	0.0011493818	0.4689813832
C	–1.9930573095	–0.6146613983	–1.6756050627

C	–1.2357343128	–0.2456885946	–2.9613662274
C	–2.3661043585	–0.074412988	0.6616475411
C	–1.3755443217	1.2455667657	–3.2720731968
N	–1.5647536536	0.2296038582	–0.5347316947
C	0.2527844047	–0.5831219582	–2.9115770481
C	–1.5308485871	1.6680469898	–0.8348897419
C	–0.7289342273	1.9860350215	–2.1046103984
Li	0.3910995545	–0.3537941653	0.1129385777
N	0.9969671308	0.187953903	–1.9078806113
C	0.7694723169	1.6388362548	–2.062967746
C	2.4267461144	–0.1159513565	–2.0656547013
C	1.5247285041	2.3883017532	–0.9718889912
C	3.2497038092	0.5732288906	–0.9905029297
C	3.0218483721	2.0837175497	–1.0149924739
C	0.6615462112	–2.421958327	0.3524407189
H	1.7803548576	–1.455835535	2.4002057116
H	–0.1185473962	0.941943986	2.5274314471
H	0.8433479503	3.0922688664	2.4877872857
H	2.7699192452	4.6061050994	2.6765885851
H	5.0886542561	3.6952085965	2.6951184369
H	5.4185489856	1.2349572063	2.5276047124
H	3.5076112507	–0.272779745	2.3484264489
H	–1.2328900817	–1.1326871906	2.998775989
H	–0.0422829485	–1.7793516981	4.1165540884
H	–0.4564602747	–2.6923294933	2.6593838696
H	–5.3684887757	–0.8971039513	–0.8397355314
H	–4.0619465802	–1.9780335727	–0.3591023008
H	–3.7436008566	–1.2912289296	–2.7255713003
H	–3.8277268179	0.4017757545	–2.2568997064
H	–4.3695663904	–0.2667164715	1.4100043285
H	–4.1911777352	1.0232833738	0.2271955891
H	–1.719895744	–1.6417167093	–1.3984459409
H	–1.6702643432	–0.8420541705	–3.7699279547
H	–2.1031553458	–1.093343104	0.9631334986
H	–2.0418678386	0.5982467278	1.4579942834
H	–2.419783783	1.5430986805	–3.3930168202
H	–0.8590839174	1.4801528031	–4.2084071749
H	0.394110301	–1.6442990867	–2.6921431401
H	0.6804755497	–0.3920753598	–3.9118255895
H	–2.5404755464	2.0821998376	–0.9766211265
H	–1.1006971027	2.1700581821	0.0365810467
H	–0.7920995763	3.0679282354	–2.2613258597

H	1.1827027506	1.9494515421	–3.0435294669
H	2.5456776027	–1.2003925265	–2.0034527492
H	2.7618491171	0.2029848031	–3.0688815417
H	1.1348264322	2.0945414795	0.0062862429
H	1.3450073752	3.4627108356	–1.0810078588
H	2.9584249016	0.1735306488	–0.015707217
H	4.3084541139	0.3378423936	–1.1282809227
H	3.4506406229	2.5006283634	–1.9345291908
H	3.5236328137	2.5562302098	–0.1682087981
C	1.6855416896	–3.3997835893	0.9117200829
H	–0.3558459156	–2.8286805358	0.4253344832
H	1.5316192894	–3.5872772911	1.9815573305
H	2.7022583909	–3.0003194304	0.8083381949
H	0.8685905742	–2.2793473324	–0.7188605917
H	1.6812421173	–4.384390393	0.4254284733

Tabelle 371 Standardorientierung von EtLi TS-*R*-1 Dis [TS, M052X /6-31+G(d)].

Atomsymbol	x	y	z
C	–0.1196869475	–1.2403664323	–2.5777196683
C	–0.0694230713	0.1366394508	–2.5806959656
C	1.1527697167	0.9269381478	–2.4538313236
C	1.075810804	2.3300370398	–2.347187945
C	2.2135773775	3.1172798272	–2.2074185122
C	3.4798545016	2.5317991837	–2.1808914365
C	3.580078461	1.1464396099	–2.3155542202
C	2.4429543596	0.358400028	–2.4501234153
C	–1.2732109847	–1.9885216221	–3.1946562014
C	2.778627906	–0.2666479717	3.1106411246
C	1.3456740408	–0.0913479901	3.6125029826
C	3.0034911631	0.6692653336	1.9257609783
C	0.3381028558	–0.361398425	2.481316037
C	–1.1135420789	–0.233512218	2.9647732006
C	1.9642020183	0.3994543399	0.8362424469
C	–1.434177368	1.2246932056	3.2911429976
N	0.5590489543	0.4720554717	1.27946147
C	–2.1583986206	–0.748475424	1.9663046475
C	0.1192114541	1.866486402	1.4472373392
C	–1.3184425157	1.9861616961	1.9728620266
Li	–0.4733774109	–0.4615658037	–0.3707310958

N	–2.271302371	0.0439740574	0.7256584683
C	–2.417656072	1.4808456664	1.0292831299
C	–3.4611088211	–0.4280372963	–0.0017267701
C	–2.5241079631	2.2811333311	–0.26427528
C	–3.6901768501	0.3410911519	–1.2970822436
C	–3.7604088311	1.8461438792	–1.0492265453
C	–0.2832737516	–2.5830866542	–0.4713445969
H	0.8162537302	–1.7821560728	–2.5787243603
H	–0.9741809748	0.6991882568	–2.796108749
H	0.0996258061	2.8040523403	–2.3791078951
H	2.1115890275	4.1933312572	–2.1238242226
H	4.3680102826	3.1419512495	–2.0745125115
H	4.555571539	0.6733429837	–2.3168832349
H	2.5594747939	–0.7135007662	–2.5497761199
H	–1.3383886997	–3.0115060718	–2.8286428324
H	–1.130466278	–2.022830681	–4.2804778856
H	–2.22763204	–1.4961398398	–3.007847415
H	3.4943146982	–0.066833008	3.9120083199
H	2.9302257243	–1.3042311383	2.7899908845
H	1.1330730655	–0.7789862236	4.4371302697
H	1.233200505	0.9236395099	4.0035400594
H	3.9985620133	0.5321406157	1.4941420751
H	2.9436960464	1.7102022209	2.2603813092
H	0.5037191243	–1.3964346554	2.1631469941
H	–1.2098563071	–0.8538031307	3.8615685341
H	2.1237503473	–0.608366698	0.4334228562
H	2.0873835974	1.1001244792	0.0119266143
H	–0.7560375803	1.6320475006	4.0436599822
H	–2.4500577029	1.3083466466	3.6905885476
H	–1.9441523965	–1.781393481	1.6822209965
H	–3.1342596762	–0.7422618174	2.4827093839
H	0.7681430744	2.4121049592	2.1482456141
H	0.2246187947	2.3557683472	0.4751251389
H	–1.5131989162	3.051557203	2.1347368999
H	–3.3726382524	1.6174534005	1.5766031724
H	–3.3230975954	–1.4915773591	–0.2102745917
H	–4.3481125602	–0.32331943	0.6482359791
H	–1.6260337633	2.1146180147	–0.867217794
H	–2.5693066092	3.3471057761	–0.0214482053
H	–2.8663028745	0.1339742533	–1.9795953203
H	–4.6061021849	–0.0236429938	–1.7693278844
H	–4.6593649056	2.0873306239	–0.4702623081

H	–3.8304815406	2.3863252866	–1.9964965144
C	0.7194536093	–3.6138287739	–0.9763591125
H	–1.3097500534	–2.9679495511	–0.535903123
H	–0.0807781774	–2.4143640319	0.5953331629
H	1.7461644375	–3.2407286178	–0.8731004008
H	0.5778148169	–3.8428892569	–2.0398743779
H	0.6788441	–4.577339311	–0.4508735645

Tabelle 372 Standardorientierung von EtLi TS-*R*-2 Dis [TS, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.853191062	2.6141431433	–0.4020307135
C	0.5020559486	2.5204646203	–0.6437095503
C	1.0991466706	2.3985830592	–1.9655279189
C	2.49847415	2.4851479915	–2.1175801344
C	3.1049711933	2.3803338019	–3.3626823905
C	2.3338763642	2.1876469065	–4.5113835789
C	0.9473927647	2.1116491659	–4.3840220377
C	0.3375245905	2.2108548406	–3.1373124405
C	–1.332448811	3.2072140474	0.8991421239
C	1.0811242997	0.2490803732	4.225182765
C	1.9766103746	–0.6023119492	3.3249275281
C	–0.3825964246	–0.0771899378	3.9326635991
C	1.6304931672	–0.3959051146	1.8400092505
C	2.522092063	–1.2522050333	0.9270756285
C	–0.6636838982	0.14491764	2.4448375353
C	2.1735733843	–2.7333956104	1.0770750266
N	0.2021720965	–0.6195146715	1.5311089877
C	2.4366683619	–0.8862316253	–0.5592947931
C	–0.1797133056	–2.0390408957	1.4898031756
C	0.7331281291	–2.8810219973	0.5921376102
Li	–0.181249875	0.3523272246	–0.3259151676
N	1.1358378624	–1.1729099216	–1.1928715867
C	0.6889135114	–2.551078432	–0.9055059832
C	1.3061035248	–1.032567475	–2.6512026321
C	–0.6718734571	–2.8025823732	–1.5505719492
C	–0.0062871558	–1.2484021489	–3.3912266927
C	–0.5882410993	–2.6238593345	–3.0672329529
C	–2.2654723367	0.5661060338	–0.6092613747

H	–1.5205591276	2.7639056065	–1.2403973163
H	1.1899776103	2.6635134785	0.1871857565
H	3.1092848855	2.6499464988	–1.2352356225
H	4.183673686	2.4544000259	–3.4398432503
H	2.8037517187	2.1075049148	–5.4835313651
H	0.3313620703	1.9665318215	–5.2643337892
H	–0.7410125894	2.1356721202	–3.0716676946
H	–2.1930005334	2.6869962361	1.3154680206
H	–1.6255691274	4.2473167004	0.7229089147
H	–0.5297953178	3.2220662806	1.6395330541
H	1.3208324632	0.0764476507	5.2771449447
H	1.2611009273	1.3120307447	4.0222263072
H	3.0312175103	–0.3513510486	3.474805392
H	1.8550233914	–1.6527555496	3.6040189232
H	–1.0506253719	0.5629612709	4.5151665733
H	–0.5988171319	–1.1105140773	4.2224234047
H	1.8212745368	0.6620249597	1.6104870611
H	3.558321232	–1.0740067015	1.2328935582
H	–0.5058388397	1.20142904	2.2212843843
H	–1.7008170212	–0.0809774307	2.1886060359
H	2.2789096349	–3.0747497094	2.1091321519
H	2.8461027607	–3.3404613776	0.4628272896
H	2.6479916823	0.175588527	–0.710289031
H	3.2260719544	–1.4531909523	–1.0828847415
H	–0.1590684914	–2.4922242287	2.4919007714
H	–1.2146713863	–2.0838212854	1.1417812381
H	0.4076541115	–3.9219663583	0.6908312727
H	1.4106867346	–3.24449535	–1.3829287994
H	1.7092750736	–0.0422297471	–2.8574663951
H	2.0485300594	–1.7747588504	–2.9955471213
H	–1.4087644292	–2.1046190713	–1.1451466885
H	–1.0000219438	–3.8159877748	–1.2982535725
H	–0.7121222515	–0.4675310887	–3.0977447011
H	0.1705835904	–1.1385310752	–4.4644176709
H	0.0594903097	–3.4026019756	–3.4872417041
H	–1.5750933299	–2.7425853103	–3.5206768498
C	–3.5742558997	1.2643275326	–0.2701213788
H	–2.2635346362	–0.4266853027	–0.1314691625
H	–2.2091112252	0.394277557	–1.6932256326
H	–3.5797285581	2.3114239004	–0.6022248102
H	–3.7515050419	1.2764417021	0.811163676

H	–4.4574047216	0.7948853695	–0.7233727662

Tabelle 373 Standardorientierung von *i*-PrLi TS-*S*-1 [TS, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.2501780889	–1.2339072289	2.2032181272
C	0.2528415542	0.1725999569	2.2181661011
C	1.4196971692	1.0356019229	2.2372360134
C	1.2658595836	2.432132153	2.4565031172
C	2.3546052301	3.2980696036	2.5116892544
C	3.6612552894	2.8169388636	2.349163138
C	3.8422496655	1.4446388534	2.1399655148
C	2.7542506622	0.5739532205	2.079627906
C	–0.9021357381	–1.9440970779	2.8799078372
C	3.1524522927	2.434038131	–2.0913492316
C	1.7298521445	2.9999348278	–2.1922222589
C	3.1482728472	0.9498989705	–2.4766956155
C	0.7198140388	2.1783228797	–1.3549228519
C	–0.7174298464	2.7282343987	–1.4940046948
C	2.1403814192	0.1864849548	–1.6051127501
C	–1.2797533388	2.4329537823	–2.8922766879
N	0.7497137714	0.7098220722	–1.6349583108
C	–1.7073705103	2.1901108472	–0.4447986282
C	0.0468395231	0.3155027604	–2.8772146581
C	–1.3720432505	0.9065150175	–3.0015516186
Li	–0.1884560215	–0.2694614422	0.0963306669
N	–2.0412936285	0.74841816	–0.5813542116
C	–2.4206530208	0.4090796078	–1.9829224121
C	–3.1736247116	0.446324417	0.3265386533
C	–2.7590862736	–1.0826725154	–2.1007265529
C	–3.5956217567	–1.0222010587	0.2695485616
C	–3.916413868	–1.4569634331	–1.1652042494
C	0.3881625019	–2.4561568213	0.1339401181
H	1.2070389231	–1.7268777853	2.3460176482
H	–0.6956768108	0.6665312116	2.4421662643
H	0.2626212498	2.8279662161	2.6109529052
H	2.1847459848	4.3578925243	2.6931026011
H	4.5128976042	3.4902463241	2.3976259441
H	4.8476410207	1.0429879414	2.0254159179
H	2.9404200127	–0.4855564548	1.9262799957

H	–1.8521615801	–1.4216069009	2.7181050526
H	–0.7263529779	–1.9475639182	3.9664457248
H	–1.0217399461	–2.9818890763	2.5634905532
H	3.8338689732	3.00444152	–2.7356925973
H	3.5197937321	2.5427690605	–1.0611885318
H	1.7057671403	4.0379996675	–1.8340684884
H	1.4315809923	3.0262975005	–3.2484801685
H	4.141549071	0.504726248	–2.3333020583
H	2.9064677024	0.8384457712	–3.5432526413
H	1.0246588149	2.2817728142	–0.3051997395
H	–0.6590665888	3.8126186752	–1.3299527863
H	2.4812698638	0.2346666974	–0.5642012722
H	2.1025834714	–0.8702969515	–1.8881756149
H	–0.6434046704	2.8470185304	–3.6821174076
H	–2.2712777233	2.8901563757	–3.0109996003
H	–1.3119792159	2.343622908	0.5657095763
H	–2.6360295132	2.7870654546	–0.5240895967
H	0.6065103915	0.6250093991	–3.7761238947
H	0.013793374	–0.7806262589	–2.8955479163
H	–1.7470634543	0.6223865953	–3.9945004775
H	–3.3511657741	0.9655311638	–2.2251390338
H	–2.8717558461	0.7188229934	1.3440421696
H	–4.035703226	1.0891855407	0.0611454854
H	–1.8788231402	–1.6912937031	–1.8594007023
H	–3.0237338851	–1.3015165948	–3.1438182507
H	–2.7908185366	–1.6466490301	0.6713816964
H	–4.4652503818	–1.1652858995	0.9239188085
H	–4.8355081953	–0.9580469787	–1.506969356
H	–4.1091816588	–2.5361367396	–1.2050660509
C	1.8208631593	–2.9511540744	0.2920554228
H	0.3147341637	–1.9418245889	–0.8446563706
C	–0.5732871821	–3.6399256761	0.1033706388
H	1.9643146235	–3.4425861803	1.2673871693
H	2.5609354798	–2.143980298	0.2306680631
H	2.1003708933	–3.7044126824	–0.4692511552
H	–1.6269908174	–3.3477869079	0.0096430739
H	–0.4897425732	–4.2468864874	1.015661722
H	–0.3580567614	–4.3319737692	–0.7346129988

Tabelle 374 Standardorientierung von *i*-PrLi TS-*S*-2 [TS, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.826619155	–1.2070659319	2.0861981181
C	0.688741699	0.1862674374	2.1213990547
C	1.7665617951	1.1520120141	2.2831470937
C	1.4571042904	2.5143715296	2.537156651
C	2.4462970187	3.4705296757	2.7523582239
C	3.8014348013	3.115718622	2.7227907635
C	4.1339036547	1.777786995	2.4793987848
C	3.1454491422	0.8182767254	2.2625051566
C	–0.2363663227	–2.0749550036	2.7190935916
C	–4.4208265186	–0.4609488289	–1.0736856075
C	–3.5608929168	–0.1259300261	–2.2982963351
C	–3.9720318692	0.3945185979	0.1155584433
C	–2.0469292485	–0.2700333018	–2.0068307141
C	–1.1993280491	0.1101546226	–3.2404791149
C	–2.4699426254	0.1949011272	0.3662718599
C	–1.2548319775	1.6248231756	–3.483092121
N	–1.5814501241	0.465810982	–0.7919606562
C	0.2752749106	–0.3236044142	–3.1592334922
C	–1.3838327985	1.9223224731	–1.0007841132
C	–0.5795677716	2.2744254099	–2.2696787293
Li	0.3761392794	–0.3539279401	–0.0834737272
N	1.0895255078	0.4042628518	–2.1556375362
C	0.9141271989	1.8768617983	–2.2801244537
C	2.5129295863	0.0528700872	–2.3802603849
C	1.7716316847	2.6100326195	–1.2423990758
C	3.4465848113	0.7389490893	–1.3851653796
C	3.2576611834	2.2604244006	–1.4043452976
C	0.9575751014	–2.4867952461	0.0002312462
H	1.8329204248	–1.5993958255	2.1968741358
H	–0.3088782593	0.5818067145	2.318721618
H	0.4099745798	2.8117690271	2.5835541729
H	2.1584015087	4.5009026199	2.9529800895
H	4.5754157946	3.8587996804	2.8957416035
H	5.1791025772	1.4740039504	2.4637079278
H	3.4458825186	–0.2124781302	2.0924786243
H	–1.247666188	–1.7814620899	2.4150035931
H	–0.1858877691	–1.9620217533	3.8130105277
H	–0.106055062	–3.1350880506	2.491518717
H	–5.483047137	–0.300107013	–1.2971313554
H	–4.3087368304	–1.5258843726	–0.8202130737

H	–3.8121623602	–0.7888097354	–3.13735041
H	–3.7971965553	0.8944555797	–2.6256216767
H	–4.5186535919	0.1214494304	1.0276735683
H	–4.195728483	1.4526862453	–0.0788635636
H	–1.8715609938	–1.3329038712	–1.7888924776
H	–1.6293338573	–0.4267900714	–4.0969849158
H	–2.3068783829	–0.8498032689	0.6620212469
H	–2.1311377482	0.8194414574	1.1977752753
H	–2.2837663064	1.981437823	–3.6049553636
H	–0.7185778016	1.8838647658	–4.4054604534
H	0.3472990318	–1.3947530881	–2.9345039863
H	0.7181310862	–0.1769176464	–4.1633076987
H	–2.3490885462	2.4519138565	–1.0725066892
H	–0.8812407689	2.3088061905	–0.10653068
H	–0.6095438164	3.368649617	–2.3630328366
H	1.2906148199	2.1810775539	–3.28022556
H	2.6080446483	–1.0362699491	–2.3084106624
H	2.7975894525	0.3353542684	–3.4133286702
H	1.4480228047	2.3554564092	–0.2269218649
H	1.6191092335	3.6911748949	–1.3623485268
H	3.2530861309	0.3604372069	–0.3752087928
H	4.4827082692	0.4716318178	–1.6305649052
H	3.6257519013	2.6650607422	–2.3596274349
H	3.8443334825	2.7283439771	–0.6063835772
C	2.1847274627	–3.2759590573	0.4314209729
H	1.2172771572	–1.974480144	–0.9436479471
C	–0.228384808	–3.411799609	–0.2646164996
H	3.0824570082	–2.6452284791	0.495869276
H	2.4259301394	–4.1078847537	–0.257880266
H	2.0449311683	–3.7360504553	1.4227714872
H	–0.4909511822	–3.9990733674	0.6249006602
H	–0.0218284317	–4.1525062586	–1.0634754452
H	–1.141166919	–2.8764163795	–0.5620904122

Tabelle 375 Standardorientierung von *i*-PrLi TS-*R*-1 [TS, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	1.2767175202	–2.9320272199	0.9229213287
C	1.479152004	–2.8582951949	–0.461964848

C	2.4598074179	–2.0227905122	–1.1398188924
C	2.6697626489	–2.1647933842	–2.5374026265
C	3.6185451347	–1.4113302023	–3.2250700973
C	4.4120340066	–0.4740278887	–2.5511021917
C	4.2335487998	–0.3217940861	–1.1707884793
C	3.2819297512	–1.0712145383	–0.4803663442
C	0.8293314941	–4.2354369231	1.5449391532
C	–0.7051737675	3.2037942816	–0.0473960348
C	–1.9799950214	2.5301638154	–0.5712777388
C	0.5186608305	2.5982124682	–0.7432921759
C	–1.9204739698	0.9907315047	–0.4224178481
C	–3.1969095198	0.3144873999	–0.9681149635
C	0.5308012414	1.0734474632	–0.5619009556
C	–3.2390133177	0.4097317646	–2.4992445902
N	–0.6980754534	0.3679153502	–1.0096214724
C	–3.3644164334	–1.1619734618	–0.5604974938
C	–0.7419484292	0.2273122585	–2.4849938766
C	–2.0464939971	–0.4092221697	–3.0073204531
Li	–0.4009170852	–1.6515134027	–0.1298085003
N	–2.3886089355	–2.1014701956	–1.1730108262
C	–2.292874833	–1.8903157956	–2.6462747647
C	–2.8536025542	–3.4849806864	–0.9074935046
C	–1.2833719132	–2.8652513361	–3.2624268839
C	–1.9277709637	–4.5476801384	–1.5023122163
C	–1.6995041712	–4.3196137147	–3.0021562935
C	–0.3386523031	–1.5337982359	2.0852437799
H	1.9641088514	–2.3673561994	1.5448134905
H	1.0395794517	–3.6450272638	–1.0769509967
H	2.0858245698	–2.9056863148	–3.0814413818
H	3.746508392	–1.5628322709	–4.2953342983
H	5.1559865948	0.1120903178	–3.0840316453
H	4.8470074145	0.3903141076	–0.6215488731
H	3.1773036142	–0.9217934596	0.591012895
H	0.5971585874	–4.1318069434	2.6072783528
H	1.6369008996	–4.9775897828	1.4527629561
H	–0.0521034727	–4.6565290891	1.0475476157
H	–0.7540690789	4.288561323	–0.2068029051
H	–0.6231747801	3.0468623852	1.038862698
H	–2.8617206747	2.8955232524	–0.027012306
H	–2.1211900086	2.81430957	–1.622018375
H	1.449950014	3.0059579232	–0.3294243577
H	0.5107520196	2.8617113852	–1.810312289

H	–1.864911844	0.7867267904	0.6573754607
H	–4.051915685	0.8483564371	–0.531125294
H	0.6584099705	0.8545118061	0.5068921026
H	1.3810105926	0.6246526599	–1.0799428213
H	–3.1816987526	1.4483049603	–2.8427537905
H	–4.1820638453	–0.0013452337	–2.8833450114
H	–3.293849128	–1.2683728068	0.5280025918
H	–4.3892804227	–1.4671478086	–0.8470940585
H	–0.6380305422	1.2039111655	–2.9880571123
H	0.1320614606	–0.365060509	–2.7786317845
H	–2.0001479107	–0.3641877797	–4.1041751283
H	–3.2831000248	–2.137698018	–3.0851282353
H	–2.9343370033	–3.613494621	0.1770717543
H	–3.8720926395	–3.6111145548	–1.3251712365
H	–0.2867765429	–2.6810144639	–2.8460188251
H	–1.2220126446	–2.672854597	–4.341864582
H	–0.967625287	–4.5297565474	–0.9761564644
H	–2.368406874	–5.536794992	–1.3223366201
H	–2.628198851	–4.5336766009	–3.5518928149
H	–0.9400520849	–5.0131329435	–3.3840630796
C	0.655350464	–1.0504615165	3.1308355398
C	–1.4962631742	–2.2865482855	2.7366598594
H	–0.7448698352	–0.6374302494	1.5818820324
H	1.4281805474	–0.3981070551	2.7006680542
H	1.1795225493	–1.8928958946	3.6100137235
H	0.177055085	–0.4829057507	3.951799118
H	–2.2314751483	–2.6667895616	2.0140707274
H	–2.0582014499	–1.6618539595	3.4598322246
H	–1.1430915543	–3.1566962305	3.3054228995

Tabelle 376 Standardorientierung von *i*-PrLi TS-*R*-2 [TS, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.3883144182	–1.1118721434	–2.513279139
C	0.3410949683	0.2855169615	–2.4504492925
C	1.4933505116	1.1702726127	–2.4401446507
C	1.3216074335	2.568833533	–2.6243872296
C	2.400463063	3.4488594683	–2.6495466975
C	3.7113067832	2.979150232	–2.4888592298

C	3.9088413582	1.6053851506	–2.3081176284
C	2.8310906518	0.7201475488	–2.2777693015
C	–0.7521907406	–1.873137975	–3.1458682279
C	–3.9746128919	2.0430905347	–0.4924878768
C	–2.930753794	2.7002713553	0.4192358402
C	–4.0997161799	0.5564098377	–0.1427689673
C	–1.5666868718	1.9683633035	0.3772035716
C	–0.5536368803	2.6178576707	1.3470408382
C	–2.7213329366	–0.114469595	–0.2349402602
C	–0.9329158585	2.3135720446	2.80294882
N	–1.6566746406	0.4914946647	0.6042500005
C	0.9125729884	2.2041821555	1.1258033915
C	–1.7950311936	0.1003075267	2.0273543723
C	–0.7918404919	0.7958481969	2.9696232034
Li	0.1860174499	–0.3288745851	–0.2819736465
N	1.2173143624	0.7865892329	1.4520934057
C	0.6995564932	0.4270057708	2.8004786229
C	2.6940329409	0.628612609	1.4343556351
C	1.0348082586	–1.0316159695	3.1398536466
C	3.1501631377	–0.7905427561	1.7767292928
C	2.5525283858	–1.2674065409	3.1080938192
C	0.5558876965	–2.5150139432	–0.5198493653
H	1.3611475317	–1.5583380809	–2.6931559122
H	–0.6241265181	0.7688095907	–2.6145147211
H	0.3142870598	2.9554862129	–2.7739347174
H	2.2193692077	4.5108687847	–2.8047612612
H	4.5546764269	3.6639738676	–2.5132423884
H	4.9182469915	1.21503589	–2.1906385428
H	3.0281475694	–0.3399028574	–2.1384670008
H	–0.6943792864	–2.9473652573	–2.9550980939
H	–0.7225418142	–1.7291557026	–4.2366816353
H	–1.7306709797	–1.5192481582	–2.8019908263
H	–4.9407709074	2.5544147693	–0.3959865762
H	–3.6668535101	2.1448452092	–1.5441215662
H	–2.7665978752	3.7454092051	0.1239163892
H	–3.3251318926	2.7246158673	1.4431073056
H	–4.7862518206	0.0450593444	–0.830179934
H	–4.5225766843	0.4427934883	0.8651397153
H	–1.1777017004	2.0788694135	–0.6446981755
H	–0.5937140171	3.7001334231	1.1639654171
H	–2.382704295	–0.0554339886	–1.2760697196
H	–2.7844199302	–1.1765781745	0.0191564177

H	–1.9503099817	2.6445777065	3.0402204042
H	–0.2589417302	2.8410625984	3.4906181777
H	1.2144123316	2.3829609744	0.0888068579
H	1.5360319255	2.8635865284	1.7601832118
H	–2.8051673884	0.3246992139	2.4107579174
H	–1.680951564	–0.9888423398	2.0752848825
H	–1.069085259	0.5017370682	3.991457269
H	1.2367819718	1.0538390844	3.5446740735
H	3.0501617468	0.9191082505	0.4416053749
H	3.137096556	1.3376187414	2.1617859179
H	0.5370636059	–1.7094731043	2.436203046
H	0.6376569646	–1.2593150747	4.1384760901
H	2.8666584327	–1.4762239648	0.9710674527
H	4.2468631227	–0.7997413624	1.8244258449
H	3.0172707847	–0.7111443473	3.9359268422
H	2.7790569706	–2.3278756008	3.2742179376
C	1.6138139438	–3.415467809	–1.1394655039
C	–0.6885404504	–3.3048587592	–0.1233448748
H	0.9943414214	–2.0848741977	0.3956242924
H	2.5690137111	–2.8930264933	–1.2914575983
H	1.3035858034	–3.8006629388	–2.1239715712
H	1.8319482757	–4.3062082997	–0.5201535575
H	–1.2720567666	–3.6369654161	–0.9934527756
H	–1.3724580462	–2.726881433	0.5123816385
H	–0.4410383594	–4.2250587736	0.443761529

Tabelle 377 Standardorientierung von *i*-PrLi TS-*S*-1 Dis [TS, M052X /6-31+G(d)].

Atomsymbol	x	y	z
C	0.1558520359	–1.1911763285	2.2205040809
C	0.1309876149	0.1993393418	2.2455898106
C	1.2840494122	1.0767932902	2.1614251556
C	1.1260700159	2.4684608839	2.3525287379
C	2.1985679884	3.3460772002	2.2679612605
C	3.4845815889	2.8735771088	1.995038535
C	3.6680348501	1.5011372462	1.8278129031
C	2.5948168337	0.6194466597	1.9075023068
C	–0.9951085558	–1.9273700157	2.8604951344
C	3.1596803151	2.2907203655	–2.0951730551

C	1.7515794438	2.8780257523	–2.1791232503
C	3.1114152423	0.8223965465	–2.5132441576
C	0.7661094325	2.0791416626	–1.3093891476
C	–0.6508966156	2.6701900905	–1.3920921194
C	2.114990438	0.0736103618	–1.6261968604
C	–1.2539380601	2.4308252306	–2.7760116063
N	0.7465496985	0.627839425	–1.6150424388
C	–1.6297091567	2.1245666435	–0.347390684
C	0.0337898565	0.3009630191	–2.859515194
C	–1.3691158305	0.9160633551	–2.9314915971
Li	–0.2006700783	–0.3163393815	0.0978521606
N	–1.9695709276	0.6996214677	–0.5141736647
C	–2.3793098478	0.3955049763	–1.9004061445
C	–3.078348705	0.3783435684	0.3970245697
C	–2.67768439	–1.0953877416	–2.0387170263
C	–3.4339095919	–1.1007892421	0.3359491636
C	–3.8025140399	–1.5075391258	–1.089187601
C	0.3409895025	–2.4318836735	0.0945871885
H	1.1157513241	–1.6812904475	2.3175251792
H	–0.812967519	0.6834541885	2.4839327336
H	0.1381007874	2.854114593	2.584678749
H	2.0330997326	4.4061950492	2.4237141218
H	4.322937067	3.5559505666	1.9302900909
H	4.6601360552	1.1087798907	1.6323228978
H	2.7734205658	–0.4409075063	1.777665764
H	–1.9129791479	–1.3376027184	2.8109314611
H	–0.7660191289	–2.076382006	3.9212759116
H	–1.1816438873	–2.9024739633	2.4173641487
H	3.8488631118	2.8561001107	–2.7277003949
H	3.5216274412	2.3636810099	–1.0634667178
H	1.7447180002	3.916983661	–1.8359851186
H	1.4337507173	2.8817633001	–3.2262251381
H	4.09219622	0.3509945402	–2.405516003
H	2.8345846568	0.7434288827	–3.5698345874
H	1.1167500034	2.1630946445	–0.274297133
H	–0.5580981993	3.7435901859	–1.1979623852
H	2.48253218	0.1132842961	–0.5977693737
H	2.0445420467	–0.9780385517	–1.9124869876
H	–0.6394991516	2.8614714321	–3.5688412363
H	–2.2431498317	2.8958513305	–2.8413707325
H	–1.2193488109	2.25029471	0.6574551591
H	–2.5531770128	2.7264866772	–0.4103500998

H	0.5859014534	0.648493726	–3.744544924
H	–0.0167513196	–0.7894035351	–2.9282732834
H	–1.7777201714	0.6683078797	–3.9169242918
H	–3.3233320562	0.9408241707	–2.1023805167
H	–2.7764546383	0.6598796451	1.4079502395
H	–3.9588417957	0.989990761	0.1318917887
H	–1.7787991875	–1.6741024272	–1.8059004168
H	–2.9486449367	–1.3069513654	–3.0776622063
H	–2.5675835819	–1.6785079451	0.6655356605
H	–4.2536863675	–1.3063332048	1.0295956469
H	–4.7317406666	–1.0079243501	–1.3871781208
H	–3.9793092358	–2.5842069404	–1.1481048765
C	1.7673866526	–2.9066842474	0.3274079628
H	0.2989565725	–1.9738980292	–0.9092231019
C	–0.5760704684	–3.6481417251	0.0793231407
H	1.8706069565	–3.3526676213	1.3258928246
H	2.5035157783	–2.1016073298	0.2582960905
H	2.0739481674	–3.6898528196	–0.3852961657
H	–1.6322960406	–3.4049069819	–0.0687181841
H	–0.5019063299	–4.2065676748	1.0190035207
H	–0.2968944749	–4.3631225481	–0.7128575559

Tabelle 378 Standardorientierung von *i*-PrLi TS-*S*-2 Dis [TS, M052X /6-31+G(d)].

Atomsymbol	x	y	z
C	0.889830743	–1.1017223049	2.2056816075
C	1.0248059177	0.2755561281	2.2287534687
C	2.2904051058	1.007348447	2.25332158
C	2.2771627023	2.4036847211	2.4463600376
C	3.4489820825	3.1449334935	2.5372772249
C	4.6916155367	2.5180866902	2.43799096
C	4.72913291	1.1359492111	2.2529149906
C	3.5563098119	0.3940340924	2.1631381184
C	–0.2428013708	–1.7564585071	2.9509107646
C	–4.4247545969	–0.2139488382	–0.4723821158
C	–3.6820918471	0.144548487	–1.7580609489
C	–3.8242571294	0.5807504352	0.6841448697
C	–2.1689704646	–0.1037445183	–1.6255573423
C	–1.441207434	0.2619491996	–2.9286867617
C	–2.3251728121	0.2904406548	0.7688187417

C	–1.3952922171	1.7773482874	–3.1226082287
N	–1.5578085649	0.574497006	–0.4563231339
C	–0.012004484	–0.2738236753	–2.9984400896
C	–1.3409193122	2.0165494636	–0.6532125704
C	–0.5859495929	2.3307577563	–1.9525687029
Li	0.3223896261	–0.3203241723	0.0418928345
N	0.8893571482	0.3156280695	–1.9997120863
C	0.8517860703	1.7904065792	–2.0459492471
C	2.253450316	–0.1579752184	–2.2792675656
C	1.7717379698	2.3568578132	–0.9713787889
C	3.2236064985	0.3354120626	–1.2194718054
C	3.2077406835	1.8608404193	–1.1405034744
C	0.5380624471	–2.4509403381	0.0660008415
H	1.7951186255	–1.6919908594	2.1582744606
H	0.1538233856	0.8647506335	2.5096670741
H	1.3190380623	2.9072994151	2.5350634785
H	3.3920736235	4.2166299371	2.6908161643
H	5.6075057376	3.090949233	2.5114081076
H	5.6833912578	0.626239698	2.1827999818
H	3.6280598012	–0.6791633971	2.0299597802
H	–1.1588136027	–1.1673862534	2.8919403088
H	0.033834693	–1.8106017366	4.0103603603
H	–0.4477535209	–2.7648953132	2.6029700312
H	–5.4935836219	–0.0130850157	–0.5774551856
H	–4.3134587885	–1.2861173846	–0.270610353
H	–4.054405878	–0.4486576773	–2.5985674086
H	–3.8781337378	1.1943450694	–1.9967064273
H	–4.2888323332	0.3065950304	1.6350656951
H	–4.0047379742	1.6503725554	0.5350793752
H	–2.0295287057	–1.1775705951	–1.4493385221
H	–1.9967890672	–0.207762974	–3.7466893586
H	–2.1905933433	–0.7739848346	0.9850529374
H	–1.8669187705	0.8517108256	1.5852775923
H	–2.3951946171	2.2165900058	–3.1504440544
H	–0.9073876113	2.0172725006	–4.0726563113
H	–0.0056151666	–1.3583326717	–2.8583862083
H	0.3798780792	–0.0697638085	–4.0105747262
H	–2.2909072286	2.5706702835	–0.6859431512
H	–0.7891565401	2.3820102946	0.2176983415
H	–0.5139783806	3.4209271808	–2.0250770235
H	1.236319018	2.114411576	–3.0340805764
H	2.2320545067	–1.2503935135	–2.3012937183

H	2.5664905059	0.192368915	–3.2788607279
H	1.4101242483	2.0493427799	0.0129645015
H	1.7333411413	3.4503469233	–1.003298909
H	2.9303496032	–0.0833407631	–0.2531028728
H	4.2291243849	–0.0341231136	–1.4373925175
H	3.6311825331	2.2766927279	–2.0630758851
H	3.8217164795	2.2057132012	–0.3063522193
C	1.7959413883	–3.2658106856	0.318113581
H	0.619693713	–2.0412586923	–0.9529591532
C	–0.6809503422	–3.367997848	0.0868009803
H	2.7073089855	–2.6668121268	0.2030592858
H	1.8900551992	–4.1351440293	–0.3542216521
H	1.804047717	–3.6722416443	1.3392539117
H	–1.6347932357	–2.8329192618	0.0151045743
H	–0.7199178174	–3.9553813698	1.0098127125
H	–0.6647681494	–4.1076446614	–0.7325394522

Tabelle 379 Standardorientierung von *i*-PrLi TS-*R*-1 Dis [TS, M052X /6-31+G(d)].

Atomsymbol	x	y	z
C	0.4018962816	–2.7339518258	0.6863946299
C	0.6195983564	–2.4610323197	–0.6465555752
C	1.74142628	–1.6797428787	–1.161872868
C	1.8418784846	–1.421718463	–2.5436525185
C	2.8817607487	–0.6670404268	–3.0749225242
C	3.8765922991	–0.1495370079	–2.2448640856
C	3.8132806004	–0.4196144208	–0.8772376812
C	2.7694270955	–1.1666607185	–0.3440770082
C	–0.4659049154	–3.8816923581	1.1408071219
C	0.1915003552	3.7551065779	0.7683860975
C	–1.2376258132	3.5430142205	0.2709981317
C	1.1453620679	2.9655947574	–0.1244890144
C	–1.5893693391	2.0450468877	0.260068855
C	–3.0335983651	1.7987608684	–0.1952640529
C	0.748276406	1.4881488476	–0.1438272154
C	–3.185898312	2.1436362001	–1.6750966007
N	–0.6500935486	1.2184263806	–0.5291394001
C	–3.5260658469	0.3626960636	0.0297621233
C	–0.8382422203	1.3531081934	–1.9836648928

C	–2.2940370986	1.1598072144	–2.4272318739
Li	–0.8897088527	–0.8625944118	0.0735348657
N	–2.8760887357	–0.6618902152	–0.8149135494
C	–2.8709383999	–0.2482249375	–2.2341270814
C	–3.6477067136	–1.9109515092	–0.6866508252
C	–2.1808099313	–1.3080675543	–3.0852620538
C	–3.0667704329	–3.0426853868	–1.5266643963
C	–2.9333179111	–2.6344295197	–2.9923458352
C	–0.7902185692	–1.0816724481	2.2377694757
H	1.1726253765	–2.4456085062	1.3857784571
H	–0.0004844621	–2.9450668737	–1.3961938253
H	1.0872438157	–1.8297832028	–3.2085556932
H	2.9190597333	–0.4875879454	–4.1434040619
H	4.6890188432	0.4367434429	–2.6554954957
H	4.5849543865	–0.0421868124	–0.2158952273
H	2.7502315259	–1.3446806271	0.7238281461
H	–0.4399458082	–3.9752845611	2.224789285
H	–0.0976932868	–4.8186616107	0.7096063232
H	–1.5098444266	–3.7615512018	0.8496656244
H	0.4444755486	4.8181875817	0.7726237009
H	0.2769108336	3.3955458215	1.8008980014
H	–1.956736908	4.0620236276	0.9126251473
H	–1.3292286393	3.976498237	–0.7293063849
H	2.175892434	3.0398188271	0.2329512457
H	1.1316445661	3.3807552161	–1.1379375199
H	–1.4971850643	1.7017522592	1.2968135893
H	–3.6766291807	2.4425770331	0.4133957849
H	0.8944118656	1.0708096022	0.8596524993
H	1.3910035693	0.9295333788	–0.8223144364
H	–2.8975725552	3.1762693375	–1.8797614891
H	–4.2287730457	2.0274398598	–1.9874033362
H	–3.3842546953	0.0736933807	1.0740958953
H	–4.6112808938	0.3540267234	–0.1723829547
H	–0.5206959346	2.3439828417	–2.3399258084
H	–0.1820699143	0.6213293792	–2.4621814373
H	–2.3305183498	1.3643676896	–3.502440504
H	–3.9251196208	–0.1910728592	–2.5728341198
H	–3.6654138522	–2.1911079666	0.3681535772
H	–4.6906493185	–1.723726702	–0.9987427864
H	–1.153787797	–1.436340496	–2.7330903515
H	–2.1352352296	–0.9584444642	–4.1211819168
H	–2.0846857709	–3.3112933609	–1.1372682199

H	–3.7074055321	–3.9225365434	–1.4231982162
H	–3.9290417899	–2.5142867134	–3.4344435057
H	–2.4193736809	–3.4136620005	–3.5604231193
C	0.3956545362	–1.0797742622	3.1896755736
C	–2.0077376244	–1.6653249236	2.9476783256
H	–1.0120841094	–0.0282713798	2.0054837105
H	1.2673544135	–0.5664393977	2.7675546689
H	0.7146339425	–2.1029506968	3.4341690819
H	0.1701736298	–0.5968590212	4.1551557796
H	–2.9120928213	–1.6682769868	2.330793371
H	–2.2576056903	–1.1199509387	3.8752417849
H	–1.8355469886	–2.7034639949	3.2480885886

Tabelle 380 Standardorientierung von *i*-PrLi TS-*R*-2 Dis [TS, M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	0.3075580072	–1.1737032033	–2.5022785021
C	0.2258491571	0.2001744343	–2.4616036118
C	1.3690867452	1.092047242	–2.3451393125
C	1.2040506423	2.4809056713	–2.5383310336
C	2.2744245377	3.3607882997	–2.4501440311
C	3.5581779778	2.8890716213	–2.1640661997
C	3.7423831776	1.5207909749	–1.9738716166
C	2.6707830802	0.6355019861	–2.0539745318
C	–0.8220288919	–1.9983512629	–3.0546564336
C	–3.8354351094	1.8581232968	–0.5319818528
C	–2.834025022	2.5365329648	0.4018044058
C	–3.9461220798	0.382602009	–0.154326808
C	–1.4613125435	1.8409960647	0.3627611544
C	–0.4693261197	2.5253414036	1.3175117751
C	–2.5584932041	–0.256864084	–0.2219304823
C	–0.8508781172	2.2522197174	2.7722883416
N	–1.5307024926	0.3817471106	0.6208812555
C	0.9932026553	2.1138828117	1.1206595807
C	–1.7159452314	0.0410895232	2.0404934082
C	–0.7167982366	0.7438608903	2.965991432
Li	0.2545485803	–0.4465427382	–0.2132954478
N	1.2786353922	0.7040326965	1.4473493307
C	0.7586700286	0.3589970974	2.7866942447

C	2.7439041401	0.5458664345	1.4682759411
C	1.0483762183	–1.1051615596	3.1062740182
C	3.161728371	–0.891251205	1.7427527828
C	2.5522365903	–1.3896260787	3.0553031896
C	0.5403717199	–2.6042428752	–0.3704604844
H	1.2860844151	–1.6232390967	–2.6035085531
H	–0.7357095078	0.6741742594	–2.642830336
H	0.2151442317	2.8603666749	–2.7762509765
H	2.110202151	4.4201064243	–2.6112225384
H	4.3955134582	3.5722886683	–2.0993442529
H	4.7317363626	1.1348807639	–1.7540728276
H	2.8468550305	–0.4217378722	–1.8877309056
H	–0.7567953109	–3.039282491	–2.7470518727
H	–0.7770063333	–1.9687754494	–4.1488592553
H	–1.7972041027	–1.6107325893	–2.7560886971
H	–4.8071206057	2.3548657646	–0.47710405
H	–3.486858944	1.9406860505	–1.5688961796
H	–2.6952430412	3.5864998057	0.1267249147
H	–3.2418803262	2.5235937543	1.4169119592
H	–4.6109010717	–0.1507367052	–0.8392591613
H	–4.3761780593	0.2859940678	0.8477625747
H	–1.0739057492	1.942098995	–0.6587246664
H	–0.5188344176	3.5987191393	1.106938949
H	–2.2070464993	–0.189099402	–1.253151173
H	–2.591922265	–1.3157927376	0.0370488528
H	–1.8638655146	2.5892506628	3.0022160309
H	–0.1702517042	2.7849618238	3.4438290893
H	1.3122408574	2.2916321541	0.0911306661
H	1.6042281515	2.7643630022	1.7712542551
H	–2.7239168781	0.3090219108	2.3899404001
H	–1.6285809843	–1.0443133926	2.1273366123
H	–0.9856952971	0.4698603082	3.9916793303
H	1.313720572	0.9713626572	3.5267521648
H	3.1314929758	0.8870436825	0.5096802539
H	3.1608473332	1.205545219	2.2507713433
H	0.5204541003	–1.7491140493	2.3994574026
H	0.6571144942	–1.3286679626	4.1039369342
H	2.8495572819	–1.5243373171	0.9095847619
H	4.2531496655	–0.9377829992	1.7918680014
H	3.0363499019	–0.8698439211	3.8906282924
H	2.7417481797	–2.4574752997	3.1865603169
C	1.5306466997	–3.4932459618	–1.1042075249

C	–0.7095285642	–3.3843686751	0.0266458604
H	1.0356557292	–2.2960082074	0.5575395689
H	2.4979705318	–2.9967635283	–1.2484549345
H	1.174365259	–3.7856149412	–2.100945669
H	1.7304387753	–4.4350836125	–0.5672165166
H	–1.4202634642	–3.5095961418	–0.7986108522
H	–1.2570266317	–2.8934178978	0.838755893
H	–0.4713008584	–4.4022147809	0.3832960019

8.3.16 Angaben zu den quantenchemischen Rechnungen der Lithiierung des Ferrocenderivats (*R*)-**186** (Kapitel 4.6.4)

Tabelle 381 Berechnete Energien der optimierten Verbindungen der Lithiierung von (*R*)-**186**

Verbindung	Methode/Basis	Min./TS	SCF [Hartree]	ZPE [Hartree]
(*R*)-**186**-K1	B3LYP/6-31+G(d)	Globales Min.	–1.901.435372	–1.901.127449
(*R*)-**186**-K2	B3LYP/6-31+G(d)	Globales Min.	–1.901.424474	–1.901.116005
(*R*)-**186**-K3	B3LYP/6-31+G(d)	Globales Min.	–1.901.428051	–1.901.120103
(*R*)-**186**-K4	B3LYP/6-31+G(d)	Globales Min.	–1.901.430142	–1.901.122286
(*R,R,S*$_N$)-Ed	B3LYP/6-31+G(d)	Globales Min.	–2.258.964624	–2.258.457822
(*R,R,S*$_N$)-TS	B3LYP/6-31+G(d)	TS	–2.258.930784	–2.258.428326
(*R,S,R*$_N$)-Ed	B3LYP/6-31+G(d)	Globales Min.	–2.258.961311	–2.258.454256
(*R,S,R*$_N$)-TS	B3LYP/6-31+G(d)	TS	–2.258.924261	–2.258.421609

Tabelle 382 Standardorientierung von (*R*)-**186**-K1 [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–2.0291121048	–0.8478345017	–0.9668470229
C	–2.0460782382	–0.7820738017	2.6365293944
C	–0.6158483486	–0.855880668	–1.1638898502
C	–1.6173191308	–2.0426081985	2.1185731288
C	–0.0907356087	0.4130819254	–0.7566959149
C	–0.1954320561	–2.0046124955	1.9846629195
H	–0.0378436659	–1.6877885211	–1.5452633528
H	–2.2596468234	–2.8721527178	1.8504411909
H	–2.7019838939	–1.6747585916	–1.1576898546

H	–3.0707692011	–0.4878216505	2.826064297
H	1.2781401259	–0.3722967444	2.4249445724
H	–1.1345947613	2.2074409338	0.0892871703
C	–2.3935498696	0.4264904958	–0.4344540473
C	–0.8898431527	0.0357497446	2.8218992038
C	1.3329045304	0.8950926499	–0.879100025
H	0.4289562601	–2.8014921923	1.600531696
Fe	–1.0644554777	–0.5164720756	0.8326522779
H	–3.3905497498	0.7379196354	–0.1487343301
H	–0.8834927137	1.0577365801	3.179658982
C	0.2535094097	–0.7203485417	2.4204452402
C	–1.2010301789	1.2003814651	–0.3052866754
H	1.4464422307	1.775852119	–0.211449327
N	1.6678506262	1.2907291491	–2.2637597949
C	2.4412002287	–0.1324568972	–0.5321849628
C	0.9747484894	2.4719890071	–2.7470782259
H	2.0742774733	–1.1547194878	–0.6574409455
C	3.1231865706	1.414493431	–2.2814855897
H	1.1930180584	3.3716993836	–2.1342940173
H	2.746318501	–0.0269455518	0.5131872448
C	3.6018627205	0.17035297	–1.518402924
H	4.5549682412	0.3456519072	–1.0086017163
H	–0.1061406528	2.304838915	–2.7403341499
H	3.7466184516	–0.6655266942	–2.2107948005
H	1.281973433	2.6793769527	–3.7781419967
H	3.4533772909	2.3394168491	–1.7613362059
H	3.491039866	1.4658392892	–3.3127830086

Tabelle 383 Standardorientierung von (*R*)-**186**-K2 [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–2.0020802152	–1.0982390569	–1.316567873
C	–2.0197433896	–1.0978128265	2.3007109871
C	–0.5862652017	–1.0872938141	–1.4877192938
C	–1.5903391029	–2.3406293129	1.7421292585
C	–0.0721390482	0.1844786291	–1.0624574866
C	–0.1702482408	–2.2890888952	1.5914879216
H	0.0164052384	–1.9090038813	–1.8565172515
H	–2.2321234472	–3.1641875491	1.4548595486
H	–2.6636970766	–1.9302438703	–1.5223550593

H	–3.0430528788	–0.8150065007	2.5139185611
H	–1.1787872898	1.9685343385	–0.2457374747
H	1.2994456905	–0.6534815868	2.0256346086
C	–2.3829936897	0.1700821539	–0.7849301379
C	–0.8636641832	–0.2809565708	2.4963750483
C	1.3677355266	0.5859441877	–1.265615321
H	0.4530585344	–3.0673115525	1.1691329995
Fe	–1.0584323004	–0.7774704337	0.4939112425
H	–3.3865898817	0.4747224754	–0.5147480635
H	–0.8611675718	0.728481339	2.8884735095
C	–1.2029956088	0.9593967634	–0.6345270911
C	0.2800342546	–1.0162021501	2.0573840312
H	1.9015702124	–0.3352140032	–1.5384226854
N	2.1476212537	1.1356769808	–0.1265872271
C	1.5781783456	1.5980923454	–2.4378157962
C	1.5078675708	2.2266262531	0.6119901598
H	0.7966723708	2.3659335131	–2.4207915226
C	3.3859866209	1.576265739	–0.792137796
H	1.510859342	1.0949255954	–3.4083592267
C	2.9770282719	2.2040973148	–2.1594384092
H	3.7033901304	1.958628446	–2.9421638099
H	2.9295478128	3.2970541781	–2.0974939422
H	4.0159353219	0.6927165534	–0.9613799506
H	3.9447175273	2.2592906181	–0.1449580508
H	0.6323694572	1.8461390167	1.1411649519
H	1.193689651	3.0858781219	–0.0101202166
H	2.2154764307	2.5980725995	1.3610721497

Tabelle 384 Standardorientierung von (*R*)-**186**-K3 [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–2.0391177292	–0.852397855	–0.9401092129
C	–2.030024043	–0.8272324274	2.6614965739
C	–0.6247962826	–0.8572509513	–1.13810052
C	–1.5749352339	–2.0733792311	2.1305902402
C	–0.1023996684	0.4136620077	–0.7283210519
C	–0.1555724677	–1.9998359977	1.9855998879
H	–0.0475737305	–1.6947940653	–1.5079652069
H	–2.199798792	–2.9142345381	1.8568432417

H	–2.7095040787	–1.6819109005	–1.1277512616
H	–3.0597494935	–0.5589822846	2.8618891183
H	–1.1493404995	2.2068080791	0.1101034105
H	1.282809712	–0.3354758499	2.4285564964
C	–2.4048572839	0.4220919211	–0.4096116719
C	–0.891670088	0.0161764909	2.8466714528
C	1.3159884673	0.9132706925	–0.7954794726
H	0.4847231747	–2.7753995758	1.5842885341
Fe	–1.0671604744	–0.5242788941	0.8540929699
H	–3.4029919098	0.7318917562	–0.1259105471
H	–0.9072565825	1.0349805596	3.2131574289
C	–1.2150174744	1.1978790814	–0.278033031
C	0.2662087456	–0.70846963	2.428814858
H	1.498949981	1.5066739564	0.1118441786
N	1.564643567	1.8564119891	–1.9206921423
C	2.443341091	–0.1555039634	–0.8866508504
C	1.0715674165	1.3940853651	–3.2209845402
H	2.1296704055	–1.0058792076	–1.5010156092
C	3.0279740591	2.000871218	–1.8934765501
H	2.6967071576	–0.5512144	0.1022947285
C	3.622359745	0.6000664812	–1.5549848074
H	4.4912157993	0.6867782816	–0.8930275513
H	3.960572483	0.0815435958	–2.4589119099
H	3.2871937211	2.7169169736	–1.1020632458
H	3.3897347085	2.4124238475	–2.8408916772
H	–0.0168973731	1.2988099701	–3.1882504343
H	1.4887871579	0.4254160235	–3.5543871568
H	1.3221200034	2.1478158888	–3.9749025848

Tabelle 385 Standardorientierung von (*R*)-**186**-K4 [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.	0.	0.
C	0.	0.	3.62470557
C	1.4132176657	0.	–0.1942023948
C	0.3818011139	–1.2620346031	3.0742819577
C	1.9474675108	1.2528250881	0.2620515986
C	1.8026275676	–1.2624580505	2.9189354194
H	1.9822890245	–0.8182394649	–0.61537848
H	–0.2896493998	–2.0654842843	2.7982724575

H	–1.0119985628	0.3215255673	3.8372237001
H	–0.6711171052	–0.8205028084	–0.2216063046
H	0.8766740266	3.0200482682	1.1483881685
H	3.3286379192	0.3289293586	3.3257844608
C	–0.3631627989	1.2560591858	0.5702033876
C	1.1849321352	0.7777599932	3.8075282227
C	3.3661133008	1.7614772763	0.0892319422
H	2.3955209538	–2.0693064239	2.5064635172
Fe	0.9617005323	0.2736384079	1.8133690558
H	–1.3601316445	1.5629769351	0.8608961311
H	1.227070712	1.7926844812	4.1828821231
C	2.2994642489	–0.0016499591	3.370823625
C	0.8287040363	2.0244076346	0.7281438102
H	3.576805445	1.7211870279	–1.0033999286
N	4.4460379235	1.0411627226	0.7963385852
C	3.5896158606	3.213288417	0.5597916335
C	4.6743321207	–0.3344519309	0.3859211521
H	3.0694204321	3.3767034259	1.5085529168
C	5.6315106763	1.8812641286	0.5961318908
H	4.8584382254	–0.4286552177	–0.7045216359
H	3.1990006141	3.9348273464	–0.1651040861
C	5.1223583882	3.3261733584	0.7665274729
H	5.591049677	3.9975450025	0.0395483981
H	3.820972636	–0.9605770078	0.6542206197
H	5.3542482972	3.7134906045	1.7638046399
H	5.5546658867	–0.7236062124	0.9100874172
H	6.0464880726	1.7394760574	–0.4234792464
H	6.4151246454	1.6039358646	1.3105301552

Tabelle 386 Standardorientierung von (R,R,S_N)-Ed [globales Minimum, B3LYP/6-31+G(d)].

Atomic symbol	x	y	z
C	0.0213424406	–0.051067165	0.0798194481
C	–0.0097138423	0.0965894314	3.6467570126
C	1.4344721498	–0.0739921306	–0.1192815672
C	0.5499129523	–1.1359738001	3.1891801157
C	1.9595687475	1.217403848	0.213734944
C	1.9644955522	–0.9678346058	3.0830719619
H	2.0160165256	–0.9201136574	–0.4617872158
H	–0.0035973984	–2.0321179652	2.9379991845

H	–0.6511785216	–0.8896177678	–0.0541951281
H	–1.0620335574	0.2985156885	3.8031860751
H	3.2644279532	0.8149773663	3.4885766198
H	0.9169904413	3.0591690308	0.9629567022
C	–0.3435824085	1.2528228671	0.5390226138
C	1.0591361527	1.0276284956	3.8234819944
C	3.3882765832	1.6808929541	0.1004583712
H	2.6700213823	–1.7114333915	2.7345613027
Fe	0.9873771794	0.3849683325	1.8544765926
H	–1.3395961424	1.5798592488	0.8110966791
H	0.9600150344	2.0584380537	4.140010858
C	2.278158089	0.3692710267	3.4763886315
C	0.8498167472	2.0326221319	0.6217733645
H	3.5067340231	2.5662178745	0.7567193761
N	3.7593065805	2.08967412	–1.2902302579
C	4.4830403348	0.6537893964	0.4487219485
C	3.0836221852	3.3093158424	–1.7288175119
H	4.1904587236	–0.3388949465	0.0992592665
C	5.2241654594	2.2822377702	–1.2164087224
H	3.3034461037	4.1647673205	–1.0615566549
H	4.6431313071	0.6032911391	1.5292985746
C	5.7365298159	1.1326878102	–0.3268703949
H	6.5305601029	1.4844186064	0.340625446
H	2.0011282909	3.1581285949	–1.7441474615
H	6.1406832819	0.3165368164	–0.9304466538
H	3.4197483052	3.5715980844	–2.7376669599
H	5.4468740808	3.2606223727	–0.7494553501
H	5.6486427559	2.2881732847	–2.2250067523
Li	3.487302895	0.4097112926	–2.8172893521
O	4.5568823231	1.2560786374	–4.4392443205
O	1.5819003049	0.360425829	–3.7130468335
C	4.21108446	–1.5312702728	–2.4431167803
H	3.5774974817	–2.1535818873	–1.7761342015
H	5.2221056045	–1.5877327355	–1.9885526222
H	4.3000218794	–2.1338738474	–3.3726481894
C	5.6641651059	0.452076988	–4.8492135996
C	4.0077842598	2.0089031592	–5.5092019483
C	0.4905066186	1.267819457	–3.7581900104
C	1.1766157246	–0.9859625653	–3.9715100818
H	3.175112529	2.5913757068	–5.108862311
H	2.0656507722	–1.605907156	–3.8549022874
H	0.7717380409	–1.0701282916	–4.9910510172

H	0.4097187615	–1.2992446981	–3.2491980856
H	5.370853469	–0.2165487469	–5.6706463575
H	5.9518894633	–0.151391133	–3.9883724148
H	6.4969140733	1.0914262054	–5.1781953202
H	3.6343754581	1.3468289413	–6.3041383288
H	4.7593099023	2.6915668952	–5.9337234621
H	–0.0128704567	1.2221658623	–4.7357820021
H	0.8891788426	2.2734789163	–3.607959633
H	–0.2371220087	1.0455030047	–2.9650288851

Tabelle 387 Standardorientierung von (R,R,S_N)-TS [Übergangszustand, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–2.1608768039	–0.9862031057	0.1711611918
C	–2.2159591202	–2.9544205079	3.1494090619
C	–0.866695197	–0.3776378033	0.2828772464
C	–1.2493572548	–3.4192687374	2.2051782152
C	–0.9778456529	0.5387999467	1.3901272756
C	–0.0020680613	–2.787915327	2.4994377795
H	0.3372950551	–0.7814644069	–0.3828789904
H	–1.4370501905	–4.1050327932	1.3884083226
H	–2.4261150646	–1.7723902964	–0.5300583079
H	–3.2635866912	–3.2278400603	3.174822432
H	0.5508003266	–1.3038787438	4.0876555061
H	–2.6859791183	1.075490567	2.7671821115
C	–3.051644199	–0.4533424058	1.1631164734
C	–1.5669746559	–2.0331236159	4.0275365619
C	0.1212743662	1.492654242	1.7842847967
H	0.9169873077	–2.9083571696	1.9402333384
Fe	–1.4485779037	–1.3652228092	2.0653098626
H	–4.0809241002	–0.7473765241	1.3386033426
H	–2.0344578069	–1.4895306709	4.8393208974
C	–0.1995713418	–1.9323344695	3.6265021186
C	–2.3125612275	0.503872739	1.923254803
H	–0.2431897911	2.158907683	2.5893186786
N	0.512694292	2.3431876212	0.6123464749
C	1.471609909	0.8702844433	2.2207411919
C	–0.503866061	3.3406557398	0.2772626226
H	1.572432441	–0.1309751697	1.7983093609
C	1.7847238975	2.9645711896	1.0161594727

H	–0.6739393393	4.0476659338	1.110442939
H	1.5101206171	0.7750333741	3.3098724184
C	2.5700692261	1.8213128017	1.6751568941
H	3.2388457652	2.1946059008	2.4578430192
H	–1.4526391857	2.8454483823	0.0545276956
H	3.1900568138	1.3047094307	0.9350919499
H	–0.1902761027	3.9150576613	–0.6016531048
H	1.598155362	3.7769506888	1.7447234328
H	2.2874678701	3.4039670984	0.1479639599
Li	0.6575537485	0.821766843	–1.0848291062
O	2.2981238373	1.849254073	–2.1743212179
O	–0.556376605	1.0673519226	–2.7547218605
C	1.57772801	–1.232813965	–1.00736264
H	1.3558738093	–2.3071172255	–0.9151795869
H	2.4897691388	–1.0586722402	–0.4090847526
H	1.8438153076	–1.0744645435	–2.0684020207
C	3.6638701204	1.441355557	–2.1595597192
C	2.1066008844	3.0829112946	–2.854036216
C	–1.980388085	1.1138520976	–2.6657751972
C	–0.1205483423	0.402911609	–3.9391205357
H	1.0362968146	3.2955377829	–2.8427039187
H	0.9696661349	0.4231466099	–3.9376010927
H	–0.5026252696	0.921168045	–4.8307408027
H	–0.4661395601	–0.6395297083	–3.9464449031
H	4.0465661866	1.3401327068	–3.18572128
H	3.7059256065	0.4733377469	–1.6597360752
H	4.2811355307	2.1728763364	–1.6174747169
H	2.4526345577	3.0112511706	–3.8960746566
H	2.6534466515	3.8966826508	–2.3546603077
H	–2.3908098927	1.7040880656	–3.4979820284
H	–2.2357387609	1.5793803421	–1.7143612161
H	–2.4028582029	0.1018320017	–2.6855971938

Tabelle 388 Standardorientierung von (*R,S,R*$_N$)-Ed [globales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	2.4812160102	–0.4636038375	–2.9474911712
C	2.5599440489	3.1717258508	–2.9276743888
C	1.0614921645	–0.6140146341	–2.9031600666
C	2.145853252	2.6356933939	–4.1861319213

C	0.5935546921	–0.145162841	–1.6296470624
C	0.7238936757	2.4985474694	–4.1602134688
H	0.4468627633	–0.9887214954	–3.7118408078
H	2.7974997264	2.3563437223	–5.0046979695
H	3.1184764909	–0.7005619784	–3.790561408
H	3.581086404	3.3675546345	–2.6250983418
H	1.7072856212	0.7341195312	0.0952277526
H	–0.7648719805	2.9500133058	–2.5419716649
C	2.9032649759	0.0975886597	–1.7027216028
C	1.3951005596	3.3666608746	–2.1239971155
C	–0.8115271781	–0.1264574823	–1.0906942354
H	0.1088372856	2.0994614346	–4.9573374517
Fe	1.5782355885	1.3716890336	–2.6466881629
H	3.9189300892	0.3656508331	–1.4384406892
H	1.3752972339	3.7293138704	–1.1040655427
C	1.7439437815	0.2957512951	–0.8943270203
C	0.2613049806	2.9505013757	–2.885780594
H	–0.9113255351	0.7586037659	–0.4524659247
N	–1.120162065	–1.2710584579	–0.1599060731
C	–1.9658045893	–0.1168596203	–2.1293236679
C	–0.7742079184	–2.5873879865	–0.7196360696
H	–1.7095729243	–0.7043142761	–3.0172739846
C	–2.587431772	–1.1301214286	0.0094954169
H	–2.1690642085	0.9023644758	–2.4712591272
C	–3.1678546944	–0.7456521023	–1.3777190807
H	–4.0054262832	–0.0481109763	–1.2719686658
H	–3.5495688801	–1.6246431991	–1.9093822168
H	–2.7572017192	–0.3210293564	0.7284675375
H	–3.0090205407	–2.0478312718	0.4296108803
H	0.3045601305	–2.6464682503	–0.8833287456
H	–1.2745352457	–2.8125850833	–1.6760587304
H	–1.0625831322	–3.3612767909	0.0004508619
Li	–0.3650772296	–0.7168876982	1.8124645323
O	–1.5339474812	–1.8586003319	3.1211024856
C	–0.5223666215	1.3374200705	2.2287850491
O	1.517033954	–1.5011339338	2.2629978897
C	2.3105350052	–0.5848034519	3.0181633832
H	–1.5044869562	1.7882656988	1.9704108617
H	0.2154851499	1.9685487534	1.6897853205
H	–0.3777293443	1.6004552645	3.2983137203
C	2.270134042	–2.5926621923	1.7581807175
C	–1.2810886513	–3.1787332456	3.5708392871

H	–2.2220762348	–3.7107506169	3.7773638988
C	–2.2568974661	–1.0768918784	4.0720175224
H	–0.7406713104	–3.6978890068	2.7757265158
H	–0.6649025801	–3.1735772581	4.4823389615
H	–3.2599055583	–1.5003930929	4.2299116118
H	–2.320004492	–0.0685367449	3.6621412828
H	–1.7205973572	–1.0446235368	5.0315082473
H	2.7134750292	–1.0776247489	3.915523964
H	1.6525293004	0.2407726171	3.2927311556
H	3.1442943746	–0.2070842458	2.4087404679
H	1.5815833916	–3.2437552652	1.2149425662
H	2.7358273259	–3.1597339832	2.5784825417
H	3.0537729022	–2.2440036307	1.0702385399

Tabelle 389 Standardorientierung von (R,S,R_N)-TS [Übergangszustand, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	2.18721700	–0.79745900	–1.99318300
C	3.72354200	–1.42471300	1.22428600
C	1.78925300	0.55352500	–1.74984900
C	4.52133300	–0.58584900	0.38612700
C	0.76588000	0.51689800	–0.74130500
C	4.15294900	0.77089700	0.64155100
H	2.22204300	1.43341900	–2.21298200
H	5.25419800	–0.92087900	–0.33742400
H	2.97319100	–1.11454200	–2.67018400
H	3.74359400	–2.50720800	1.24423700
H	–0.25261700	–1.11121700	0.84893300
H	2.62741700	1.64098600	2.04019900
C	1.39635000	–1.63940600	–1.13935400
C	2.86199500	–0.58847300	1.99886500
C	–0.04270400	1.64245300	–0.16379700
H	4.56487000	1.64508300	0.15216500
Fe	2.50862600	–0.30632700	–0.02155000
H	1.51462700	–2.71726300	–1.07066000
H	2.10731200	–0.92471800	2.69738100
C	0.49382500	–0.84660500	–0.35367600
C	3.12762500	0.76799100	1.63791100
H	–0.01780500	1.54820200	0.93032200
N	–1.50518100	1.49199900	–0.50363100

C	0.29781100	3.10743200	–0.50964800
C	–1.74256800	1.42314100	–1.95925100
H	0.58788400	3.20480100	–1.56171500
C	–2.07184100	2.74240900	0.05043500
H	1.13687300	3.47314700	0.09039100
C	–1.02587900	3.86862600	–0.22123300
H	–0.93902100	4.53162500	0.64628900
H	–1.32004300	4.49487400	–1.07068900
H	–2.21008700	2.60503200	1.12909700
H	–3.05425600	2.94499600	–0.38825200
H	–1.17740100	0.58826100	–2.37905000
H	–1.44686900	2.33629200	–2.49885000
H	–2.81176900	1.25716500	–2.13321900
Li	–1.90216900	–0.52339900	0.31242700
O	–3.86510500	–0.16455800	1.09295400
C	–0.86888600	–1.23680600	2.16478400
H	–0.21884500	–2.04594700	2.53175100
O	–2.60329400	–2.16517700	–0.80658000
C	–2.51993900	–3.37059600	–0.04386100
H	–0.63983900	–0.35119800	2.78311400
C	–2.20157100	–2.36916000	–2.16108700
C	–5.04030200	–0.21738000	0.29562800
H	–5.40839600	0.79519800	0.07166700
C	–4.09042000	0.43065700	2.36681300
H	–4.77483000	–0.73211600	–0.62908900
H	–5.83351800	–0.77964500	0.81016900
H	–4.43295900	1.47008700	2.25627800
H	–3.14276200	0.40592900	2.90684100
H	–4.84436700	–0.13827100	2.92994000
H	–3.15144900	–4.14847900	–0.49661000
H	–2.87532100	–3.14459900	0.96212300
H	–1.48128400	–3.72116400	0.00967300
H	–2.35967400	–1.42903900	–2.69263400
H	–2.81587600	–3.15500400	–2.62360300
H	–1.14061600	–2.64140900	–2.21511200
H	–1.89874200	–1.54931800	2.41603400

8.4 Vollständige Gaussian-Zitate

[74a] Gaussian 98, Revision A.7, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, J. A. Pople, Gaussian, Inc., Pittsburgh PA, **1998**.

[74b] Gaussian 03 (Revision B.04), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Pittsburgh, PA, **2003**

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