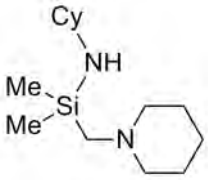
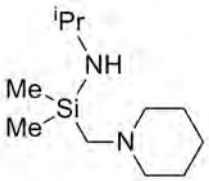
8 Anhang

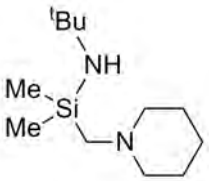
8.1 Übersicht zentraler Verbindungen



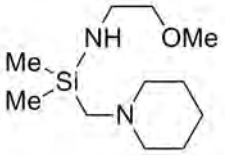
64



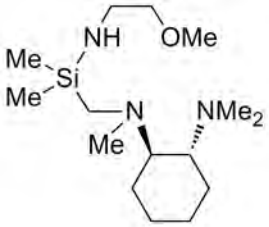
65



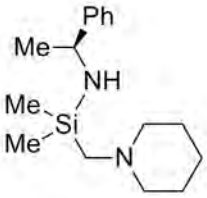
66



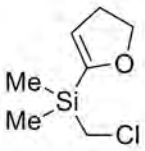
67



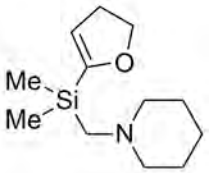
(*R*,*R*)-**68**



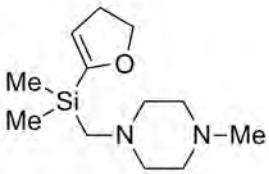
(*S*)-**69**



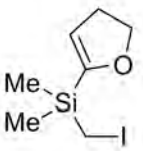
70



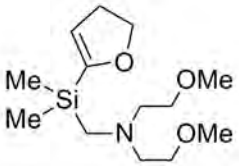
71



72

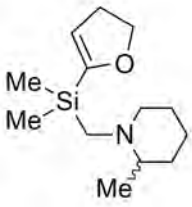


73

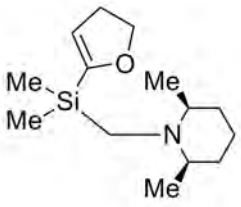


74

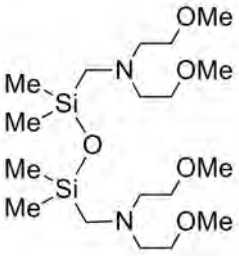
(*S*)-**75**



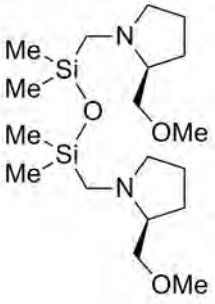
rac-**76**



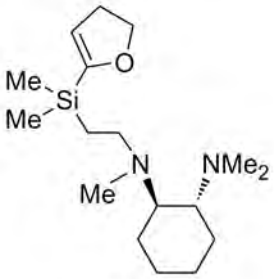
77



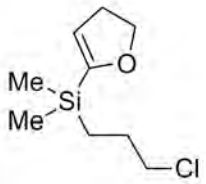
78



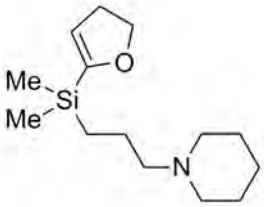
(*S*,*S*)-**79**



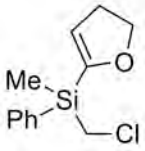
(*R*,*R*)-**80**



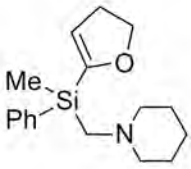
82



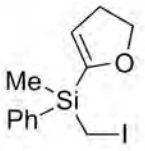
83



rac-**85**

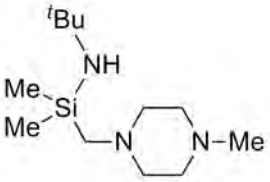


rac-**86**

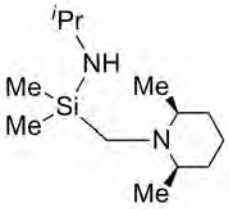


rac-**87**

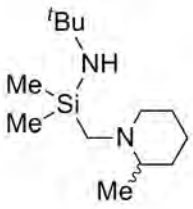
(R_{Si},*S*)-**88**
(S_{Si},*S*)-**88**



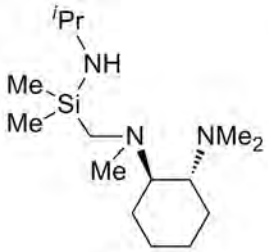
89



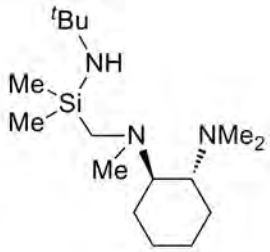
90



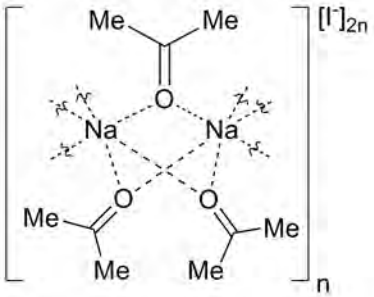
rac-**91**



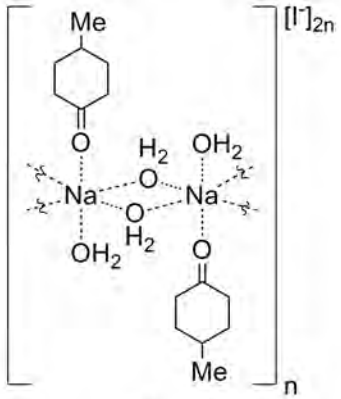
(*R*,*R*)-**93**



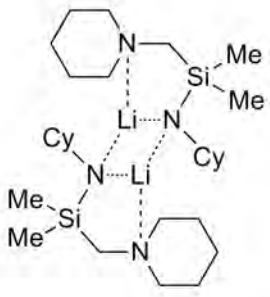
(*R*,*R*)-**94**



95

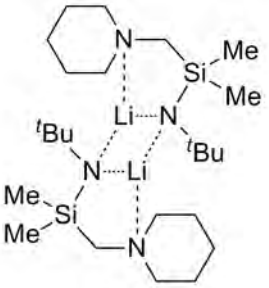


96

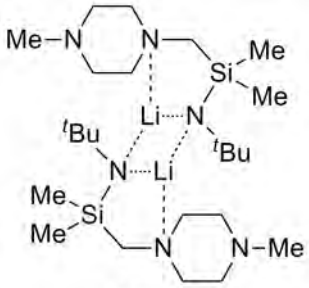


97

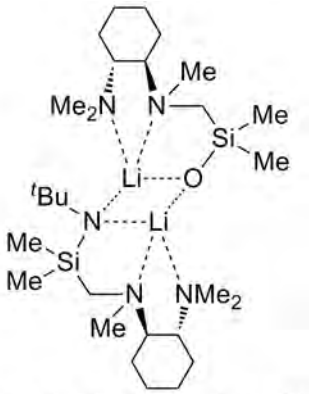
98



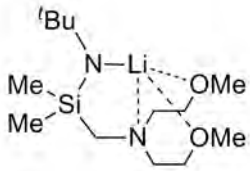
99



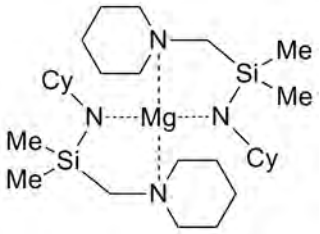
100



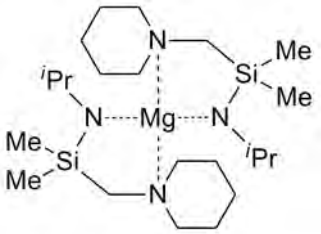
$(R_C,R_C,R_N,R_{C'},R_{C'},S_{N'})$-**101**



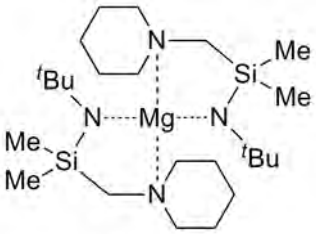
102



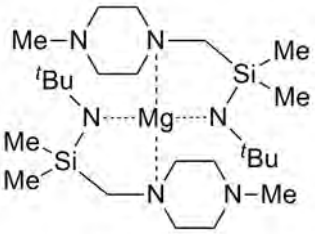
103



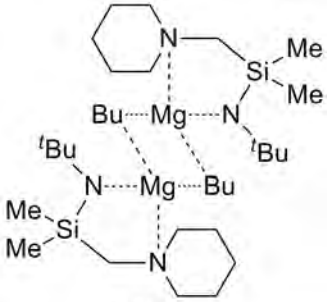
104



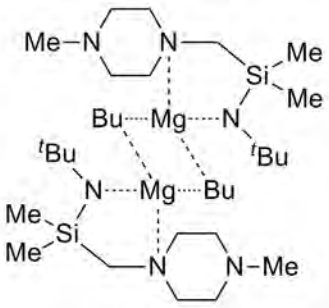
105



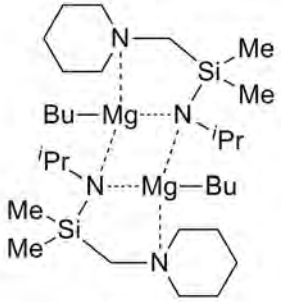
106



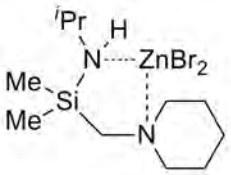
107



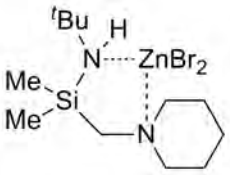
108



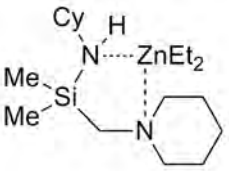
109



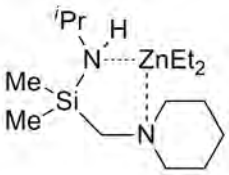
117



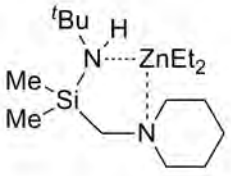
118



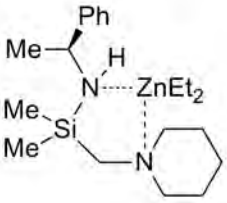
119



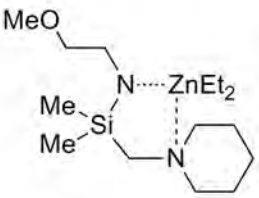
120



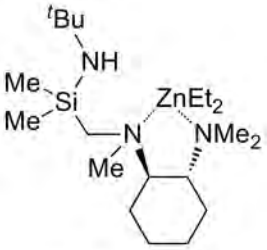
121



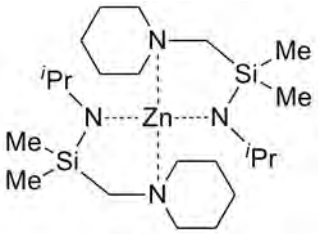
(*S*)-**122**



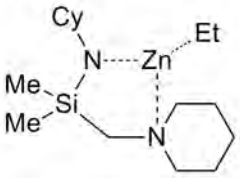
123



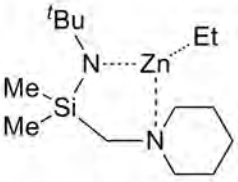
(R_C,R_C,R_N)-**124**



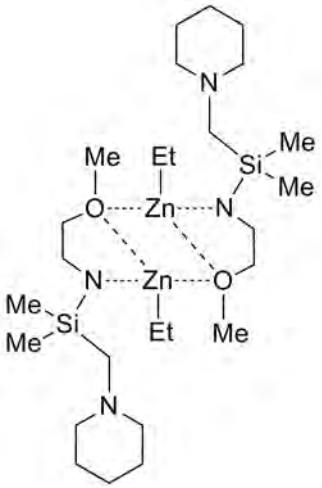
125



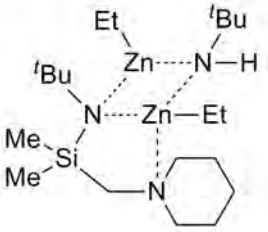
126



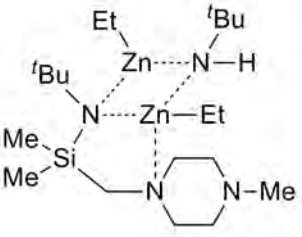
127



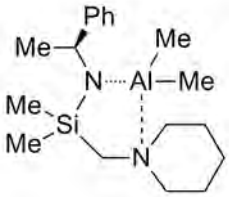
128



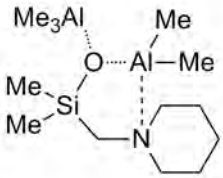
129



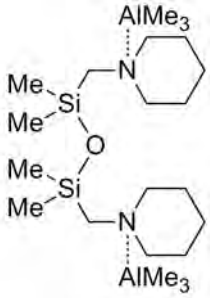
130



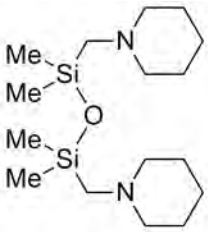
(*S*)-**131**



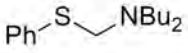
132



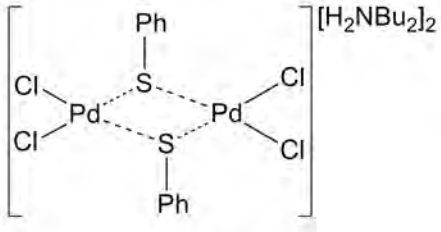
133



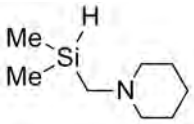
134



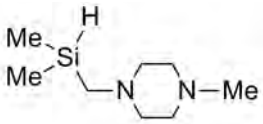
135



136



137



138

8.2 Angaben zu den Kristallstrukturen

8.2.1 Kristallstrukturen aus Kapitel 4.1.4

8.2.1.1 Verbindung 95

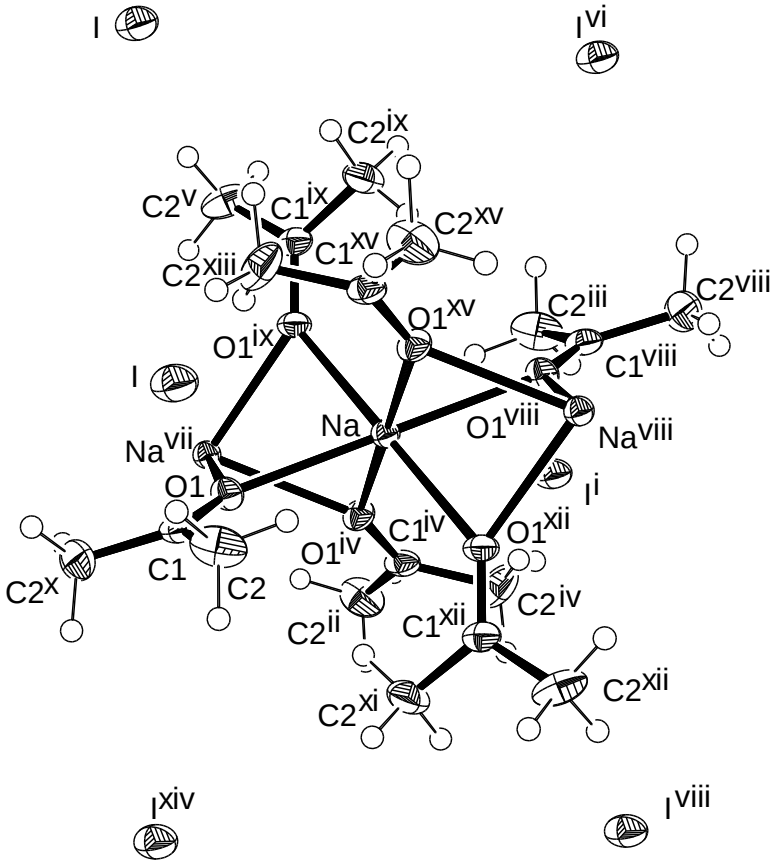


Abb. 8.1 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **95** im Kristall (Ortep−Darstellung).

Tabelle 8.1 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **95**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
I	6667	3333	2500	31(1)
Na	10000	10000	0	17(1)
O(1)	8415(2)	9922(2)	2500	22(1)
C(1)	7305(2)	9864(2)	2500	23(1)
C(2)	6617(2)	9845(2)	565(3)	39(1)

Tabelle 8.2 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **95**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
I	23(1)	23(1)	48(1)	0	0	11(1)
Na	17(1)	17(1)	18(1)	0	0	9(1)
O(1)	16(1)	25(1)	27(1)	0	0	12(1)

C(1)	17(1)	14(1)	37(1)	0	0	8(1)
C(2)	32(1)	41(1)	52(1)	−12(1)	−18(1)	24(1)

Tabelle 8.3 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **95**.

	x	y	z	U(eq)
H(2A)	7169	9840	−588	61(7)
H(2B)	6521	10663	487	57(7)
H(2C)	5707	9020	515	64(8)

8.2.1.2 Verbindung 96

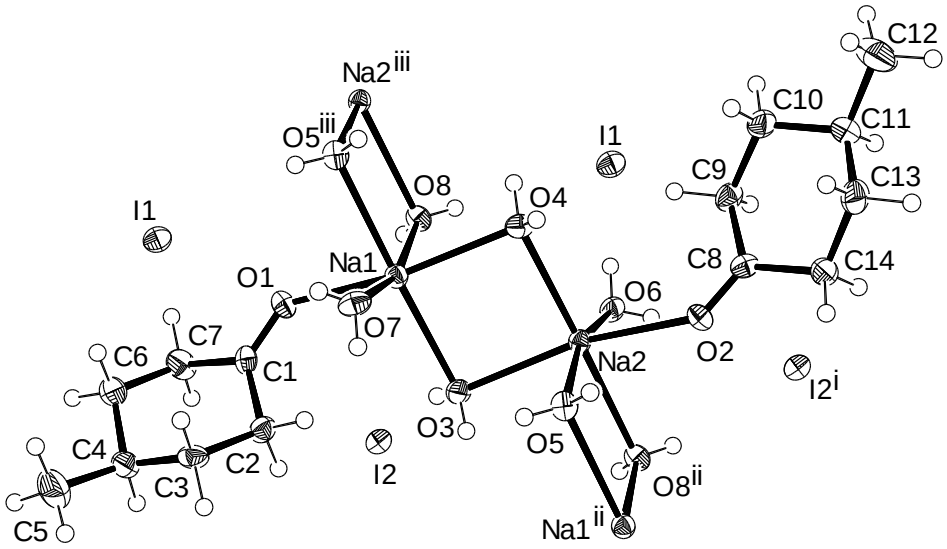


Abb. 8.2 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **96** im Kristall (Ortep−Darstellung).

Tabelle 8.4 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **96**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	4017(7)	7356(3)	2170(2)	20(1)
C(2)	6372(7)	7831(3)	2472(2)	25(1)
C(3)	6316(5)	8611(2)	3094(2)	25(1)
C(4)	4889(6)	8180(3)	3705(2)	30(1)
C(5)	4793(7)	9003(3)	4294(2)	53(1)
C(6)	2529(6)	7731(3)	3361(2)	32(1)
C(7)	2516(7)	6921(3)	2737(2)	31(1)
C(8)	11223(7)	7524(3)	−2146(2)	21(1)
C(9)	8994(6)	7032(3)	−2513(2)	26(1)
C(10)	8230(5)	7549(3)	−3218(2)	30(1)
C(11)	10057(6)	7743(3)	−3755(2)	35(1)
C(12)	9234(8)	8285(4)	−4431(2)	72(2)
C(13)	12157(6)	8382(3)	−3345(2)	34(1)
C(14)	13002(6)	7854(3)	−2662(2)	29(1)
I(1)	1740(1)	9953(1)	1824(1)	22(1)
I(2)	6825(1)	4953(1)	1886(1)	22(1)
Na(1)	5277(2)	7882(1)	448(1)	19(1)
Na(2)	9684(2)	7087(1)	−443(1)	18(1)
O(1)	3388(4)	7352(2)	1508(1)	23(1)
O(2)	11659(4)	7601(2)	−1482(1)	23(1)

O(3)	8605(6)	7072(3)	798(2)	23(1)
O(4)	6396(5)	7882(2)	−788(2)	22(1)
O(5)	11919(5)	8656(2)	59(2)	22(1)
O(6)	8367(6)	5342(2)	−887(2)	24(1)
O(7)	6549(7)	9656(3)	847(2)	25(1)
O(8)	3051(5)	6307(3)	−62(2)	21(1)

Tabelle 8.5 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **96**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	27(2)	12(2)	23(2)	−2(2)	6(2)	6(2)
C(2)	19(2)	26(2)	28(2)	−4(2)	2(2)	3(2)
C(3)	23(2)	23(2)	27(2)	−5(2)	−7(2)	3(1)
C(4)	34(2)	34(2)	22(2)	−2(2)	−2(2)	14(2)
C(5)	66(3)	59(3)	35(2)	−17(2)	1(2)	22(2)
C(6)	30(2)	45(2)	23(2)	7(2)	6(2)	8(2)
C(7)	28(2)	34(2)	26(2)	4(2)	5(2)	−8(2)
C(8)	19(2)	17(2)	26(2)	5(2)	0(2)	2(2)
C(9)	19(2)	26(2)	32(2)	7(2)	6(2)	1(2)
C(10)	20(2)	39(2)	29(2)	−7(2)	−1(2)	1(2)
C(11)	32(2)	52(3)	21(2)	2(2)	−1(2)	12(2)
C(12)	55(3)	126(5)	33(3)	27(3)	−2(2)	13(3)
C(13)	28(2)	39(2)	34(2)	12(2)	12(2)	1(2)
C(14)	21(2)	39(3)	23(2)	2(2)	2(2)	−4(2)
I(1)	19(1)	21(1)	25(1)	1(1)	1(1)	2(1)
I(2)	20(1)	19(1)	28(1)	0(1)	2(1)	3(1)
Na(1)	19(1)	19(1)	19(1)	0(1)	2(1)	3(1)
Na(2)	17(1)	18(1)	19(1)	0(1)	3(1)	2(1)
O(1)	30(2)	23(2)	18(2)	−1(1)	3(1)	4(1)
O(2)	26(2)	24(2)	17(1)	3(1)	2(1)	3(1)
O(3)	17(2)	29(2)	21(2)	5(1)	3(2)	0(2)
O(4)	18(2)	22(2)	24(2)	7(1)	0(1)	−1(2)
O(5)	25(2)	16(2)	24(2)	0(2)	4(2)	1(2)
O(6)	17(2)	26(2)	26(2)	−1(1)	3(2)	0(2)
O(7)	18(2)	24(2)	32(2)	0(1)	−4(2)	1(2)
O(8)	27(2)	17(2)	20(2)	−2(2)	1(1)	3(2)

Tabelle 8.6 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **96**.

	x	y	z	U(eq)
H(2A)	7185	8170	2067	30
H(2B)	7201	7286	2661	30
H(3A)	5706	9207	2884	30
H(3B)	7877	8859	3312	30
H(4)	5588	7617	3943	36
H(5A)	3878	9498	4090	79
H(5B)	6325	9357	4448	79
H(5C)	4116	8685	4724	79
H(6A)	1785	8294	3159	38
H(6B)	1633	7414	3755	38
H(7A)	3046	6306	2946	37
H(7B)	960	6710	2502	37
H(9A)	7843	7036	−2154	31
H(9B)	9069	6307	−2640	31
H(10A)	6885	7109	−3473	36
H(10B)	7785	8211	−3078	36
H(11)	10436	7070	−3920	42
H(12A)	8949	8965	−4278	108
H(12B)	7835	7881	−4666	108
H(12C)	10386	8361	−4786	108

H(13A)	13366	8503	−3686	40
H(13B)	11802	9057	−3192	40
H(14A)	13614	7243	−2825	34
H(14B)	14254	8328	−2386	34
H(31)	9790(70)	7230(30)	1000(20)	44(14)
H(32)	8080(80)	6750(40)	1010(20)	38(16)
H(51)	12320(80)	9060(30)	−220(20)	44(16)
H(52)	11630(70)	8920(30)	410(20)	32(15)
H(61)	7170(90)	5220(40)	−1180(30)	80(20)
H(62)	9250(70)	5250(30)	−1130(20)	26(13)
H(71)	7650(60)	9750(30)	1094(19)	11(11)
H(72)	5710(100)	9780(50)	1020(30)	100(30)
H(81)	2790(80)	5860(40)	180(20)	55(19)
H(82)	3230(70)	5970(30)	−405(19)	25(14)
H(41)	5110(60)	7680(30)	−1034(19)	26
H(42)	6920(70)	8360(30)	−960(20)	26

8.2.2 Kristallstrukturen aus Kapitel 4.3.1

8.2.2.1 Verbindung 97

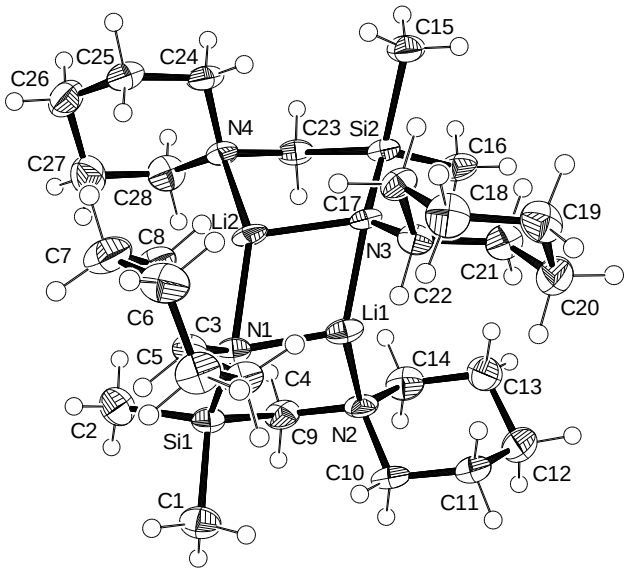


Abb. 8.3 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **97** im Kristall (Ortep−Darstellung).

Tabelle 8.7 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **97**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	7277(10)	1225(8)	5572(6)	40(2)
C(2)	4769(9)	3230(8)	4963(6)	43(2)
C(3)	8695(8)	3197(7)	4019(5)	27(2)
C(4)	10333(9)	2439(7)	4005(6)	33(2)
C(5)	11262(10)	3029(8)	4290(6)	39(2)
C(6)	11197(11)	4190(8)	3715(6)	46(2)
C(7)	9563(12)	4985(8)	3751(7)	49(2)
C(8)	8672(10)	4399(7)	3452(6)	39(2)
C(9)	5998(10)	1242(7)	3875(6)	36(2)
C(10)	8130(11)	−526(7)	3810(6)	43(2)
C(11)	9405(12)	−1283(8)	3190(6)	53(3)
C(12)	8847(13)	−1726(8)	2542(7)	57(3)

C(13)	7845(12)	−663(8)	1995(6)	50(3)
C(14)	6628(10)	95(8)	2637(6)	40(2)
C(15)	9128(10)	3868(7)	−484(5)	37(2)
C(16)	7824(10)	1917(7)	66(6)	37(2)
C(17)	11590(9)	2721(7)	1231(6)	31(2)
C(18)	13217(10)	2031(8)	1364(7)	44(2)
C(19)	13906(10)	1035(8)	830(6)	43(2)
C(20)	12916(10)	236(8)	1073(6)	44(2)
C(21)	11315(9)	941(7)	929(6)	36(2)
C(22)	10600(8)	1916(7)	1502(5)	28(2)
C(23)	6190(9)	3939(7)	1077(5)	30(2)
C(24)	6575(11)	5757(7)	1103(6)	40(2)
C(25)	6418(12)	6628(8)	1695(6)	47(2)
C(26)	4842(11)	7083(8)	2233(7)	47(2)
C(27)	4310(11)	6035(9)	2803(7)	50(2)
C(28)	4525(10)	5183(8)	2181(6)	42(2)
Li(1)	8518(14)	1617(11)	2724(9)	29(3)
Li(2)	7666(15)	3634(11)	2422(8)	30(3)
N(1)	7846(7)	2645(5)	3681(4)	27(2)
N(2)	7231(8)	485(5)	3255(4)	31(2)
N(3)	8977(7)	2560(5)	1501(4)	24(1)
N(4)	6068(7)	4769(5)	1673(4)	30(2)
Si(1)	6575(2)	2128(2)	4495(1)	28(1)
Si(2)	8188(2)	3019(2)	574(1)	25(1)

Tabelle 8.8 Anisotrope Auslenkungsparameter ($Å^2 \times 10^3$) für die Verbindung **97**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	44(6)	44(5)	36(5)	4(4)	−10(4)	−23(5)
C(2)	34(5)	52(6)	41(5)	−11(4)	−2(4)	−13(5)
C(3)	24(4)	32(5)	27(4)	0(3)	−6(3)	−13(4)
C(4)	30(5)	32(5)	40(4)	2(4)	−13(4)	−14(4)
C(5)	28(5)	45(6)	49(5)	−3(4)	−16(4)	−14(4)
C(6)	56(6)	54(6)	43(5)	2(4)	−18(4)	−36(5)
C(7)	67(7)	35(5)	56(6)	7(4)	−29(5)	−23(5)
C(8)	41(5)	30(5)	46(5)	3(4)	−18(4)	−10(4)
C(9)	37(5)	30(5)	40(5)	4(4)	−1(4)	−21(4)
C(10)	56(6)	29(5)	33(4)	13(4)	−14(4)	−10(5)
C(11)	70(7)	29(5)	37(5)	7(4)	−3(5)	−3(5)
C(12)	82(8)	28(5)	51(6)	−4(5)	0(5)	−18(6)
C(13)	80(8)	38(5)	39(5)	−9(4)	−7(5)	−28(6)
C(14)	43(5)	39(5)	49(5)	−1(4)	−10(4)	−27(5)
C(15)	51(6)	32(5)	32(4)	4(4)	−9(4)	−22(5)
C(16)	52(6)	30(5)	39(4)	5(4)	−18(4)	−26(5)
C(17)	26(4)	25(4)	40(4)	0(3)	−7(3)	−11(4)
C(18)	36(5)	50(6)	53(5)	−8(5)	−7(4)	−21(5)
C(19)	28(5)	53(6)	44(5)	−6(5)	−1(4)	−15(5)
C(20)	48(6)	33(5)	47(5)	−7(4)	−4(4)	−12(5)
C(21)	31(5)	36(5)	41(5)	−2(4)	−10(4)	−11(4)
C(22)	24(4)	34(5)	29(4)	−1(3)	−5(3)	−17(4)
C(23)	29(4)	32(5)	30(4)	8(3)	−18(3)	−10(4)
C(24)	57(6)	27(5)	33(4)	9(4)	−10(4)	−18(5)
C(25)	71(7)	28(5)	39(5)	5(4)	−12(5)	−16(5)
C(26)	58(6)	29(5)	52(5)	−5(4)	−19(5)	−5(5)
C(27)	42(6)	52(6)	48(5)	−14(5)	−6(5)	−2(5)
C(28)	30(5)	46(6)	49(5)	−4(4)	−6(4)	−13(5)
Li(1)	24(7)	28(7)	36(7)	10(6)	−12(6)	−12(6)
Li(2)	36(8)	21(7)	30(6)	10(5)	−20(6)	−5(6)
N(1)	28(4)	27(4)	28(3)	4(3)	−8(3)	−13(3)
N(2)	43(4)	23(4)	29(3)	7(3)	−7(3)	−20(3)
N(3)	27(4)	18(3)	25(3)	7(3)	−9(3)	−9(3)

N(4)	36(4)	23(4)	27(3)	5(3)	−11(3)	−4(3)
Si(1)	28(1)	28(1)	27(1)	3(1)	−6(1)	−13(1)
Si(2)	31(1)	22(1)	26(1)	6(1)	−12(1)	−12(1)

Tabelle 8.9 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **97**.

	x	y	z	U(eq)
H(1A)	8272	665	5390	61
H(1B)	6565	804	5937	61
H(1C)	7357	1739	5947	61
H(2A)	4994	3745	5270	64
H(2B)	4098	2827	5412	64
H(2C)	4273	3693	4451	64
H(3)	8192	3305	4677	33
H(4A)	10343	1699	4432	40
H(4B)	10815	2247	3371	40
H(5A)	10870	3124	4952	47
H(5B)	12327	2527	4219	47
H(6A)	11695	4086	3063	55
H(6B)	11758	4565	3943	55
H(7A)	9090	5156	4391	59
H(7B)	9557	5732	3334	59
H(8A)	9087	4314	2789	47
H(8B)	7611	4906	3508	47
H(9A)	5463	744	4351	43
H(9B)	5266	1788	3501	43
H(10A)	7473	−987	4210	51
H(10B)	8543	−252	4217	51
H(11A)	9989	−1956	3578	63
H(11B)	10091	−831	2817	63
H(12A)	8256	−2255	2904	68
H(12B)	9716	−2164	2107	68
H(13A)	8480	−202	1566	60
H(13B)	7379	−937	1618	60
H(14A)	6041	785	2264	48
H(14B)	5930	−344	3017	48
H(15A)	9389	4461	−290	56
H(15B)	8433	4247	−911	56
H(15C)	10049	3335	−798	56
H(16A)	8789	1404	−224	56
H(16B)	7209	2322	−402	56
H(16C)	7285	1452	561	56
H(17A)	11152	3349	1620	37
H(17B)	11615	3086	574	37
H(18A)	13848	2561	1158	53
H(18B)	13199	1733	2033	53
H(19A)	14914	582	970	51
H(19B)	14046	1338	157	51
H(20A)	12875	−143	1729	53
H(20B)	13359	−381	674	53
H(21A)	11356	1271	264	43
H(21B)	10681	416	1101	43
H(22)	10650	1547	2160	33
H(23A)	5693	4384	553	36
H(23B)	5613	3402	1443	36
H(24A)	5964	6140	621	48
H(24B)	7645	5464	785	48
H(25A)	7106	6257	2136	57
H(25B)	6735	7290	1293	57
H(26A)	4160	7546	1802	57
H(26B)	4818	7594	2655	57

H(27A)	4897	5645	3296	60
H(27B)	3229	6315	3105	60
H(28A)	4216	4506	2562	51
H(28B)	3853	5558	1731	51

8.2.2.2 Verbindung 98

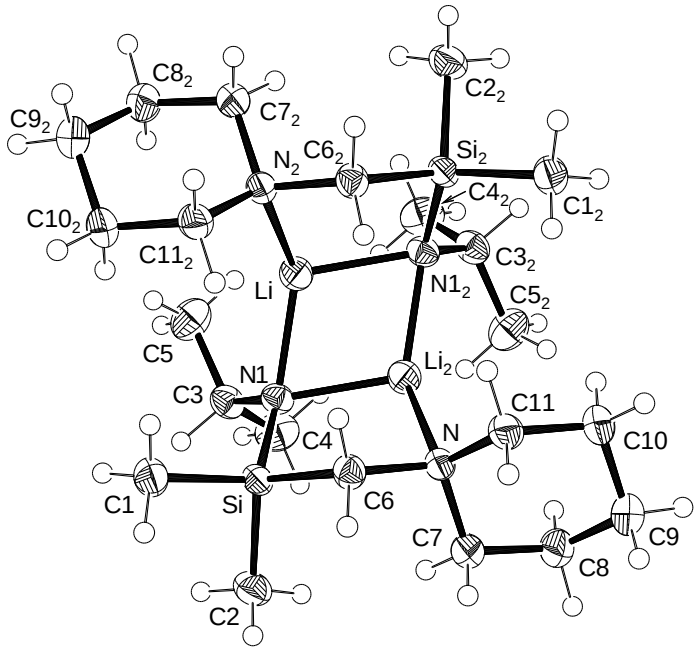


Abb. 8.4 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **98** im Kristall (Ortep−Darstellung).

Tabelle 8.10 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **98**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	3355(1)	1109(3)	5198(1)	34(1)
C(2)	4106(1)	3202(3)	4633(1)	36(1)
C(3)	3910(1)	5200(2)	6109(1)	30(1)
C(4)	4316(1)	6642(2)	6059(2)	43(1)
C(5)	3605(1)	5647(3)	6667(2)	43(1)
C(6)	4949(1)	844(2)	6254(1)	26(1)
C(7)	5896(1)	2006(2)	6140(1)	31(1)
C(8)	6650(1)	2683(3)	6612(2)	37(1)
C(9)	7191(1)	1486(3)	7287(2)	43(1)
C(10)	6959(1)	959(3)	7909(1)	36(1)
C(11)	6196(1)	311(2)	7388(1)	30(1)
Li	4560(2)	3458(4)	7677(2)	29(1)
N(2)	5685(1)	1532(2)	6763(1)	23(1)
N(1)	4362(1)	3746(2)	6446(1)	25(1)
Si	4191(1)	2356(1)	5665(1)	24(1)

Tabelle 8.11 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **98**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	27(1)	41(1)	31(1)	−6(1)	13(1)	−2(1)
C(2)	36(1)	43(1)	24(1)	3(1)	13(1)	5(1)
C(3)	31(1)	28(1)	25(1)	2(1)	12(1)	6(1)

C(4)	56(1)	33(1)	48(1)	10(1)	33(1)	5(1)
C(5)	44(1)	37(1)	57(1)	2(1)	33(1)	9(1)
C(6)	24(1)	26(1)	26(1)	−4(1)	12(1)	−2(1)
C(7)	26(1)	39(1)	25(1)	2(1)	13(1)	0(1)
C(8)	27(1)	49(1)	34(1)	2(1)	16(1)	−5(1)
C(9)	25(1)	63(1)	37(1)	−1(1)	14(1)	2(1)
C(10)	24(1)	49(1)	29(1)	3(1)	10(1)	7(1)
C(11)	28(1)	33(1)	26(1)	4(1)	13(1)	7(1)
Li	28(2)	31(2)	27(2)	5(1)	14(1)	3(1)
N(2)	21(1)	26(1)	21(1)	0(1)	10(1)	1(1)
N(1)	27(1)	24(1)	22(1)	1(1)	12(1)	2(1)
Si	21(1)	28(1)	19(1)	−2(1)	8(1)	1(1)

Tabelle 8.12 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **98**.

	x	y	z	U(eq)
H(1A)	3383	455	5669	51
H(1B)	3309	407	4732	51
H(1C)	2939	1817	4950	51
H(2A)	3657	3796	4291	53
H(2B)	4111	2323	4273	53
H(2C)	4507	3925	4800	53
H(3)	3501	4965	5497	35
H(4A)	4709	6928	6656	65
H(4B)	3991	7555	5794	65
H(4C)	4508	6363	5696	65
H(5A)	3307	4767	6654	64
H(5B)	3315	6620	6427	64
H(5C)	3996	5842	7278	64
H(6A)	4876	212	6665	31
H(6B)	4918	92	5807	31
H(7A)	5558	2822	5727	37
H(7B)	5866	1059	5789	37
H(8A)	6670	3690	6917	44
H(8B)	6774	2937	6172	44
H(9A)	7224	541	6977	51
H(9B)	7668	1993	7631	51
H(10A)	6986	1881	8274	43
H(10B)	7285	115	8312	43
H(11A)	6177	−652	7053	36
H(11B)	6055	−12	7804	36
H(1A)	3383	455	5669	51
H(1B)	3309	407	4732	51
H(1C)	2939	1817	4950	51
H(2A)	3657	3796	4291	53
H(2B)	4111	2323	4273	53
H(2C)	4507	3925	4800	53
H(3)	3501	4965	5497	35
H(4A)	4709	6928	6656	65
H(4B)	3991	7555	5794	65
H(4C)	4508	6363	5696	65
H(5A)	3307	4767	6654	64
H(5B)	3315	6620	6427	64
H(5C)	3996	5842	7278	64
H(6A)	4876	212	6665	31
H(6B)	4918	92	5807	31
H(7A)	5558	2822	5727	37
H(7B)	5866	1059	5789	37
H(8A)	6670	3690	6917	44
H(8B)	6774	2937	6172	44
H(9A)	7224	541	6977	51

H(9B)	7668	1993	7631	51
H(10A)	6986	1881	8274	43
H(10B)	7285	115	8312	43
H(11A)	6177	−652	7053	36
H(11B)	6055	−12	7804	36
H(1A)	3383	455	5669	51
H(1B)	3309	407	4732	51
H(1C)	2939	1817	4950	51
H(2A)	3657	3796	4291	53
H(2B)	4111	2323	4273	53
H(2C)	4507	3925	4800	53
H(3)	3501	4965	5497	35
H(4A)	4709	6928	6656	65

8.2.2.3 Verbindung 99

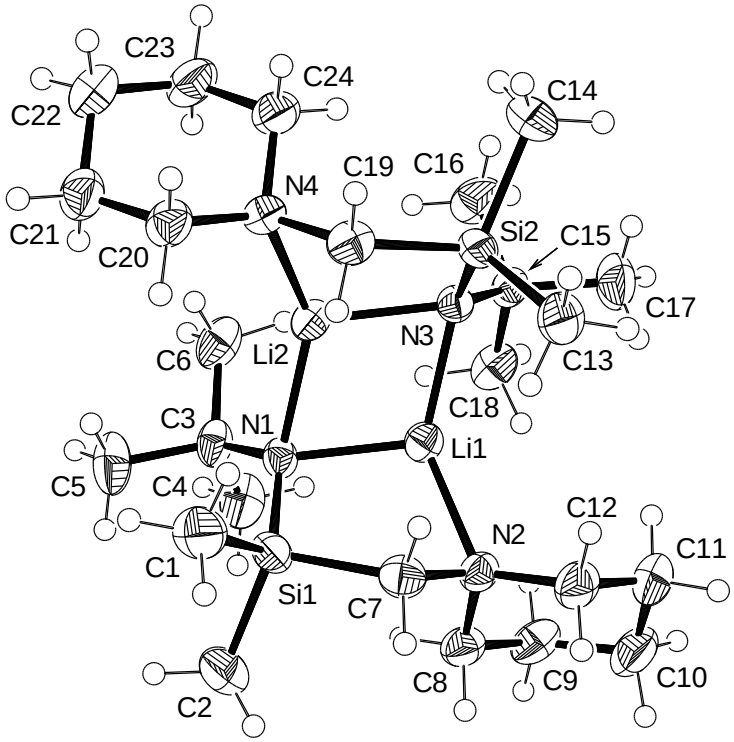


Abb. 8.5 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **99** im Kristall (Ortep−Darstellung).

Tabelle 8.13 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **99**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	7140(3)	1274(3)	10026(2)	57(1)
C(2)	9265(3)	−1318(2)	9054(2)	61(1)
C(3)	6873(2)	182(2)	7618(2)	40(1)
C(4)	8012(3)	−989(2)	6935(2)	56(1)
C(5)	6079(3)	−371(3)	8517(2)	62(1)
C(6)	5804(3)	1081(3)	7058(2)	52(1)
C(7)	9587(2)	1292(2)	8452(2)	42(1)
C(8)	11390(2)	−243(2)	7154(2)	43(1)
C(9)	12295(2)	−389(3)	6100(2)	52(1)
C(10)	13175(3)	385(3)	5903(2)	61(1)
C(11)	12234(3)	1834(3)	6228(2)	59(1)

C(12)	11329(3)	1915(2)	7279(2)	48(1)
C(13)	7936(3)	5452(2)	7744(2)	50(1)
C(14)	5723(3)	6860(2)	6731(2)	60(1)
C(15)	7835(2)	3657(2)	5571(2)	39(1)
C(16)	6614(3)	4146(3)	5128(2)	61(1)
C(17)	8712(3)	4446(3)	5118(2)	62(1)
C(18)	8793(3)	2188(3)	5264(2)	48(1)
C(19)	5375(2)	4984(2)	8479(2)	41(1)
C(20)	3588(2)	4246(2)	9403(2)	45(1)
C(21)	2559(2)	3721(3)	9391(2)	51(1)
C(22)	1553(3)	4648(3)	8821(2)	55(1)
C(23)	2380(3)	4895(3)	7809(2)	55(1)
C(24)	3428(2)	5385(2)	7870(2)	47(1)
Li(1)	8644(4)	1916(4)	6997(3)	36(1)
Li(2)	6157(4)	2859(4)	7596(3)	37(1)
N(1)	7493(2)	970(2)	7880(1)	33(1)
N(2)	10461(2)	1181(2)	7420(1)	36(1)
N(3)	7316(2)	3748(2)	6651(1)	32(1)
N(4)	4404(2)	4440(2)	8413(1)	35(1)
Si(1)	8278(1)	523(1)	8785(1)	39(1)
Si(2)	6667(1)	5175(1)	7287(1)	38(1)

Tabelle 8.14 Anisotrope Auslenkungsparameter ($Å^2 \times 10^3$) für die Verbindung **99**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

	U11	**U22**	**U33**	**U23**	**U13**	**U12**
C(1)	54(2)	66(2)	37(1)	2(1)	−9(1)	−18(1)
C(2)	62(2)	46(2)	67(2)	15(1)	−18(2)	−20(1)
C(3)	39(1)	36(1)	45(1)	−9(1)	−1(1)	−21(1)
C(4)	57(2)	47(2)	63(2)	−20(1)	−1(1)	−26(1)
C(5)	66(2)	63(2)	64(2)	−4(1)	−1(1)	−45(2)
C(6)	44(2)	59(2)	63(2)	−17(2)	−12(1)	−28(2)
C(7)	43(1)	43(1)	39(1)	−1(1)	−15(1)	−15(1)
C(8)	37(1)	37(1)	55(2)	−4(1)	−16(1)	−12(1)
C(9)	34(1)	55(2)	60(2)	−14(1)	−10(1)	−11(1)
C(10)	36(1)	82(2)	61(2)	−1(2)	−8(1)	−26(2)
C(11)	48(2)	71(2)	72(2)	11(2)	−20(1)	−38(2)
C(12)	44(1)	45(1)	64(2)	−3(1)	−20(1)	−23(1)
C(13)	53(2)	43(1)	66(2)	−4(1)	−19(1)	−27(1)
C(14)	59(2)	36(1)	83(2)	13(1)	−26(2)	−18(1)
C(15)	34(1)	53(2)	32(1)	8(1)	−12(1)	−21(1)
C(16)	50(2)	87(2)	44(2)	8(1)	−25(1)	−23(2)
C(17)	59(2)	78(2)	53(2)	16(1)	−9(1)	−43(2)
C(18)	42(2)	66(2)	32(1)	−9(1)	−6(1)	−20(1)
C(19)	40(1)	36(1)	46(1)	−7(1)	−13(1)	−14(1)
C(20)	39(1)	52(2)	38(1)	−4(1)	−7(1)	−16(1)
C(21)	43(1)	56(2)	48(2)	−4(1)	−3(1)	−22(1)
C(22)	39(1)	65(2)	58(2)	−9(1)	−8(1)	−21(1)
C(23)	37(1)	73(2)	54(2)	0(1)	−17(1)	−21(1)
C(24)	38(1)	51(2)	43(1)	0(1)	−12(1)	−13(1)
Li(1)	36(2)	39(2)	34(2)	−2(2)	−9(2)	−16(2)
Li(2)	32(2)	38(2)	41(2)	−6(2)	−9(2)	−16(2)
N(1)	35(1)	30(1)	36(1)	−2(1)	−7(1)	−16(1)
N(2)	32(1)	35(1)	42(1)	−2(1)	−13(1)	−15(1)
N(3)	31(1)	35(1)	32(1)	2(1)	−12(1)	−15(1)
N(4)	31(1)	37(1)	35(1)	−3(1)	−10(1)	−11(1)
Si(1)	41(1)	35(1)	37(1)	4(1)	−9(1)	−14(1)
Si(2)	38(1)	30(1)	48(1)	4(1)	−16(1)	−16(1)

Tabelle 8.15 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **99**.

	x	y	z	U(eq)
H(1A)	6686	2258	9971	85
H(1B)	7723	1018	10473	85
H(1C)	6417	939	10281	85
H(2A)	8619	−1630	9541	92
H(2B)	10031	−1439	9310	92
H(2C)	9658	−1842	8449	92
H(4A)	8500	−636	6350	84
H(4B)	7574	−1466	6740	84
H(4C)	8691	−1612	7278	84
H(5A)	6738	−992	8876	93
H(5B)	5660	−851	8302	93
H(5C)	5334	377	8946	93
H(6A)	5010(30)	1760(20)	7473(17)	51(7)
H(6B)	5460(30)	590(30)	6795(18)	66(8)
H(6C)	6240(30)	1550(20)	6430(18)	62(8)
H(7A)	9054	2260	8625	51
H(7B)	10228	866	8870	51
H(8A)	10809	−739	7248	51
H(8B)	12003	−648	7592	51
H(9A)	11684	−56	5660	62
H(9B)	12925	−1355	5953	62
H(10A)	13671	356	5194	73
H(10B)	13892	−33	6264	73
H(11A)	12824	2311	6167	71
H(11B)	11620	2289	5794	71
H(12A)	11943	1530	7717	58
H(12B)	10707	2871	7461	58
H(13A)	8358	4687	8152	76
H(13B)	7432	6281	8133	76
H(13C)	8680	5531	7184	76
H(14A)	6418	7124	6254	91
H(14B)	5153	7541	7249	91
H(14C)	5111	6788	6401	91
H(16A)	6066	3625	5403	91
H(16B)	6984	4026	4415	91
H(16C)	6006	5103	5282	91
H(17A)	8112	5411	5240	93
H(17B)	9102	4283	4410	93
H(17C)	9483	4151	5414	93
H(18A)	9690(20)	1840(20)	5448(16)	49(7)
H(18B)	9070(20)	2080(20)	4564(18)	52(7)
H(18C)	8280(20)	1580(20)	5590(16)	48(7)
H(19A)	5928	4390	8921	49
H(19B)	4796	5881	8795	49
H(20A)	3066	5117	9757	54
H(20B)	4245	3605	9766	54
H(21A)	2018	3637	10073	61
H(21B)	3082	2813	9090	61
H(22A)	931	5515	9173	65
H(22B)	956	4235	8762	65
H(23A)	1721	5576	7464	66
H(23B)	2891	4049	7426	66
H(24A)	3975	5502	7199	56
H(24B)	2908	6274	8199	56

8.2.2.4 Verbindung 100

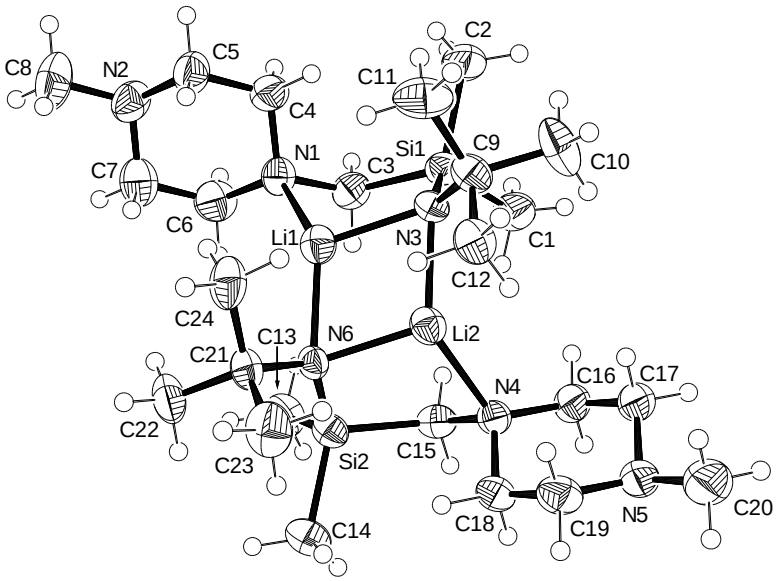


Abb. 8.6 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **100** im Kristall (Ortep–Darstellung).

Tabelle 8.16 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **100**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	−932(4)	5597(3)	2093(2)	56(1)
C(2)	−325(4)	4861(3)	863(2)	60(1)
C(3)	1450(4)	6266(3)	1605(2)	46(1)
C(4)	2700(4)	5802(3)	753(2)	48(1)
C(5)	4033(4)	5732(3)	528(2)	53(1)
C(6)	3449(5)	7034(3)	1407(2)	57(1)
C(7)	4787(5)	6945(3)	1176(2)	59(1)
C(8)	5943(5)	6515(3)	306(3)	76(2)
C(9)	1578(4)	3580(3)	2077(2)	45(1)
C(10)	187(5)	3202(3)	2017(3)	72(2)
C(11)	2217(5)	3288(3)	1478(2)	67(2)
C(12)	2364(4)	3172(3)	2692(2)	48(1)
C(13)	3339(4)	7407(3)	3335(2)	55(1)
C(14)	4438(5)	6423(3)	4486(2)	58(1)
C(15)	1721(4)	5959(3)	3762(2)	43(1)
C(16)	62(4)	4872(3)	3915(2)	45(1)
C(17)	−197(4)	3930(3)	4083(2)	48(1)
C(18)	2164(4)	4788(3)	4538(2)	45(1)
C(19)	1898(4)	3856(3)	4704(2)	51(1)
C(20)	243(5)	2809(3)	4894(2)	66(2)
C(21)	5333(4)	5217(3)	3147(2)	40(1)
C(22)	6268(4)	5997(3)	3190(2)	58(1)
C(23)	5782(4)	4598(3)	3720(2)	63(2)
C(24)	5479(4)	4735(3)	2505(2)	55(1)
N(1)	2790(3)	6176(2)	1416(2)	40(1)
N(2)	4667(4)	6578(2)	533(2)	53(1)
N(3)	1607(3)	4540(2)	2135(2)	33(1)
N(4)	1463(3)	5026(2)	3901(2)	37(1)
N(5)	507(4)	3708(2)	4711(2)	45(1)
N(6)	3953(3)	5480(2)	3149(2)	32(1)
Si(1)	511(1)	5210(1)	1704(1)	40(1)
Si(2)	3482(1)	6257(1)	3651(1)	40(1)

Li(1)	3219(7)	5329(5)	2197(4)	42(2)
Li(2)	2332(7)	4703(4)	3093(3)	40(2)

Tabelle 8.17 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **100**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	46(3)	75(4)	47(3)	4(3)	0(2)	12(3)
C(2)	57(3)	81(4)	38(3)	3(3)	−5(2)	−2(3)
C(3)	49(3)	46(3)	43(3)	6(2)	6(2)	4(2)
C(4)	56(3)	48(3)	40(3)	1(2)	8(2)	−5(2)
C(5)	53(3)	51(3)	56(3)	2(3)	17(3)	−8(2)
C(6)	77(4)	38(3)	58(3)	1(2)	11(3)	−8(3)
C(7)	61(3)	41(3)	76(4)	8(3)	14(3)	−11(2)
C(8)	69(4)	69(4)	99(5)	12(3)	40(4)	−14(3)
C(9)	48(3)	37(3)	50(3)	−7(2)	2(2)	−2(2)
C(10)	56(3)	53(3)	104(5)	5(3)	−6(3)	−21(3)
C(11)	93(4)	50(3)	56(3)	−16(3)	5(3)	13(3)
C(12)	54(3)	31(2)	58(3)	0(2)	7(3)	−1(2)
C(13)	55(3)	41(3)	67(3)	−4(3)	4(3)	1(2)
C(14)	62(3)	58(3)	51(3)	−15(3)	−3(3)	−8(3)
C(15)	43(3)	47(3)	37(3)	−4(2)	2(2)	8(2)
C(16)	32(2)	60(3)	44(3)	5(2)	5(2)	4(2)
C(17)	36(3)	65(3)	42(3)	2(2)	5(2)	−2(2)
C(18)	35(3)	59(3)	39(3)	4(2)	−6(2)	0(2)
C(19)	52(3)	54(3)	43(3)	4(2)	−6(2)	3(2)
C(20)	79(4)	61(3)	55(3)	10(3)	0(3)	−8(3)
C(21)	28(2)	42(3)	51(3)	0(2)	6(2)	−1(2)
C(22)	39(3)	58(3)	77(4)	−8(3)	13(3)	−15(2)
C(23)	43(3)	66(4)	79(4)	18(3)	3(3)	17(3)
C(24)	38(3)	52(3)	79(4)	−1(3)	22(3)	4(2)
N(1)	43(2)	33(2)	45(2)	7(2)	7(2)	−1(2)
N(2)	66(3)	43(2)	51(3)	6(2)	19(2)	−7(2)
N(3)	34(2)	30(2)	34(2)	−3(2)	1(2)	1(2)
N(4)	29(2)	45(2)	36(2)	−1(2)	3(2)	3(2)
N(5)	48(2)	48(2)	39(2)	6(2)	1(2)	−5(2)
N(6)	25(2)	36(2)	36(2)	−3(2)	5(2)	−1(2)
Si(1)	35(1)	50(1)	35(1)	0(1)	3(1)	3(1)
Si(2)	39(1)	37(1)	42(1)	−6(1)	1(1)	0(1)
Li(1)	41(4)	40(4)	47(5)	0(4)	8(4)	−1(3)
Li(2)	39(4)	35(4)	47(5)	−5(3)	6(4)	−2(3)

Tabelle 8.18 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **100**.

	x	y	z	U(eq)
H(1A)	−1458	5094	2196	85
H(1B)	−1473	5986	1792	85
H(1C)	−618	5913	2496	85
H(2A)	299	4535	637	90
H(2B)	−621	5380	608	90
H(2C)	−1084	4491	913	90
H(3A)	919	6628	1271	55
H(3B)	1523	6590	2022	55
H(4A)	2125	6174	445	58
H(4B)	2297	5215	751	58
H(5A)	4591	5328	818	63
H(5B)	3936	5489	81	63
H(6A)	3556	7288	1851	69
H(6B)	2893	7435	1113	69
H(7A)	5206	7527	1174	71
H(7B)	5356	6567	1482	71

H(8A)	6333	7097	297	115
H(8B)	5836	6266	−135	115
H(8C)	6520	6138	601	115
H(10A)	−267	3432	2368	109
H(10B)	236	2564	2049	109
H(10C)	−300	3366	1594	109
H(11A)	1750	3557	1083	100
H(11B)	2167	2652	1438	100
H(11C)	3140	3471	1532	100
H(12A)	3260	3407	2751	71
H(12B)	2396	2537	2640	71
H(12C)	1934	3313	3074	71
H(13A)	4214	7627	3279	82
H(13B)	2958	7777	3648	82
H(13C)	2773	7418	2915	82
H(14A)	4707	5856	4677	87
H(14B)	3884	6724	4767	87
H(14C)	5220	6777	4449	87
H(15A)	1465	6314	4125	51
H(15B)	1139	6129	3362	51
H(16A)	−431	5015	3483	54
H(16B)	−256	5261	4242	54
H(17A)	−1151	3844	4089	57
H(17B)	85	3541	3746	57
H(18A)	1884	5177	4875	54
H(18B)	3120	4870	4535	54
H(19A)	2221	3465	4379	61
H(19B)	2382	3714	5138	61
H(20A)	−704	2731	4894	99
H(20B)	703	2689	5331	99
H(20C)	554	2407	4580	99
H(22A)	6018	6386	2819	86
H(22B)	7169	5791	3183	86
H(22C)	6215	6315	3597	86
H(23A)	5766	4908	4133	94
H(23B)	6678	4396	3690	94
H(23C)	5188	4095	3701	94
H(24A)	4846	4254	2443	82
H(24B)	6373	4502	2526	82
H(24C)	5311	5142	2138	82

8.2.3 Kristallstrukturen aus Kapitel 4.3.2

8.2.3.1 Verbindung 101

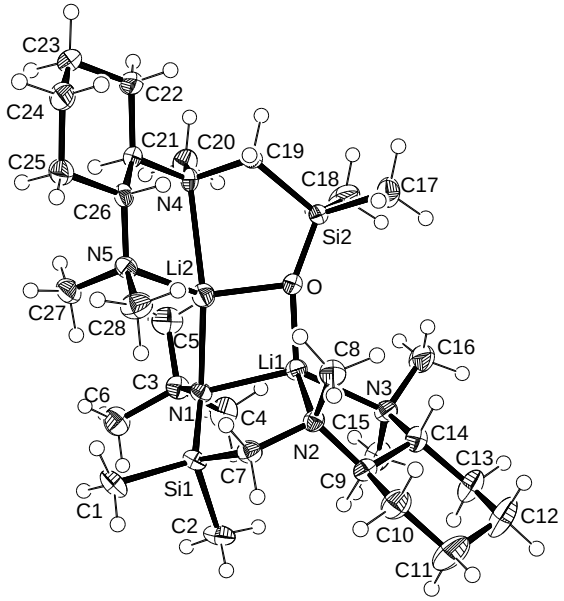


Abb. 8.7 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **101** im Kristall (Ortep−Darstellung).

Tabelle 8.19 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **101**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	3805(3)	3556(1)	4007(2)	34(1)
C(2)	1956(3)	4953(1)	4212(2)	34(1)
C(3)	−330(2)	3408(1)	5014(2)	24(1)
C(4)	−1491(2)	4078(1)	5022(2)	36(1)
C(5)	−1044(3)	2748(1)	5583(2)	38(1)
C(6)	−331(3)	3186(1)	3753(2)	35(1)
C(7)	4354(2)	4353(1)	6239(2)	24(1)
C(8)	4817(2)	4334(1)	8313(2)	28(1)
C(9)	3648(2)	5469(1)	7295(2)	22(1)
C(10)	5261(3)	5880(1)	7613(2)	36(1)
C(11)	5060(3)	6735(1)	7652(2)	53(1)
C(12)	3959(3)	6938(1)	8490(3)	53(1)
C(13)	2311(3)	6565(1)	8149(2)	39(1)
C(14)	2438(2)	5705(1)	8066(2)	25(1)
C(15)	−215(2)	5725(1)	6800(2)	35(1)
C(16)	5(3)	5210(1)	8680(2)	41(1)
C(17)	2137(3)	3393(1)	10694(2)	44(1)
C(18)	−1254(3)	3188(1)	9492(2)	45(1)
C(19)	1446(2)	2011(1)	9270(2)	20(1)
C(20)	−780(2)	1500(1)	7949(2)	29(1)
C(21)	1903(2)	1018(1)	7868(2)	21(1)
C(22)	2071(3)	398(1)	8790(2)	28(1)
C(23)	3079(3)	−266(1)	8493(2)	34(1)
C(24)	4740(3)	−1(1)	8312(2)	36(1)
C(25)	4564(3)	584(1)	7364(2)	30(1)
C(26)	3571(2)	1264(1)	7632(2)	20(1)
C(27)	2847(3)	1605(1)	5602(2)	32(1)
C(28)	4993(2)	2243(1)	6773(2)	34(1)
Li(1)	1471(4)	4179(2)	7203(3)	22(1)

Li(2)	1688(4)	2765(2)	6994(3)	26(1)
N(1)	1293(2)	3589(1)	5644(1)	21(1)
N(2)	3809(2)	4636(1)	7291(1)	20(1)
N(3)	854(2)	5321(1)	7709(1)	23(1)
N(4)	940(2)	1681(1)	8116(1)	19(1)
N(5)	3439(2)	1871(1)	6755(1)	21(1)
O	1355(2)	3414(1)	8206(1)	25(1)
Si(1)	2673(1)	4064(1)	5035(1)	21(1)
Si(2)	917(1)	3045(1)	9330(1)	21(1)

Tabelle 8.20 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **101**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	**U22**	**U33**	**U23**	**U13**	**U12**
C(1)	35(1)	49(1)	18(1)	0(1)	8(1)	0(1)
C(2)	34(1)	37(1)	32(1)	16(1)	10(1)	4(1)
C(3)	20(1)	29(1)	23(1)	1(1)	−2(1)	−1(1)
C(4)	20(1)	40(1)	45(1)	−5(1)	−2(1)	2(1)
C(5)	27(1)	45(1)	37(1)	3(1)	−6(1)	−10(1)
C(6)	34(1)	41(1)	26(1)	−4(1)	−7(1)	−3(1)
C(7)	19(1)	25(1)	28(1)	2(1)	8(1)	−1(1)
C(8)	27(1)	28(1)	26(1)	2(1)	−1(1)	6(1)
C(9)	20(1)	20(1)	24(1)	1(1)	1(1)	−1(1)
C(10)	29(1)	32(1)	46(1)	−2(1)	6(1)	−7(1)
C(11)	41(2)	33(1)	85(2)	−3(1)	9(1)	−17(1)
C(12)	48(2)	26(1)	84(2)	−19(1)	7(2)	−7(1)
C(13)	37(1)	24(1)	56(2)	−9(1)	7(1)	0(1)
C(14)	24(1)	24(1)	27(1)	−3(1)	2(1)	2(1)
C(15)	25(1)	32(1)	45(1)	−3(1)	0(1)	5(1)
C(16)	51(2)	27(1)	51(2)	−5(1)	28(1)	4(1)
C(17)	72(2)	30(1)	27(1)	−6(1)	−2(1)	8(1)
C(18)	45(1)	29(1)	66(2)	6(1)	29(1)	9(1)
C(19)	22(1)	20(1)	19(1)	3(1)	6(1)	2(1)
C(20)	25(1)	28(1)	36(1)	−3(1)	7(1)	−2(1)
C(21)	26(1)	17(1)	21(1)	−2(1)	5(1)	0(1)
C(22)	35(1)	23(1)	30(1)	2(1)	13(1)	1(1)
C(23)	53(2)	19(1)	30(1)	3(1)	11(1)	6(1)
C(24)	46(2)	30(1)	32(1)	2(1)	7(1)	19(1)
C(25)	36(1)	29(1)	27(1)	2(1)	10(1)	8(1)
C(26)	20(1)	22(1)	17(1)	−2(1)	1(1)	6(1)
C(27)	42(1)	34(1)	21(1)	3(1)	6(1)	8(1)
C(28)	28(1)	32(1)	45(1)	7(1)	12(1)	2(1)
Li(1)	22(2)	21(2)	22(2)	1(1)	4(1)	0(1)
Li(2)	26(2)	26(2)	24(2)	0(1)	3(2)	4(1)
N(1)	20(1)	24(1)	17(1)	2(1)	2(1)	0(1)
N(2)	20(1)	18(1)	22(1)	1(1)	2(1)	3(1)
N(3)	21(1)	21(1)	30(1)	1(1)	10(1)	1(1)
N(4)	17(1)	20(1)	21(1)	−5(1)	4(1)	3(1)
N(5)	19(1)	24(1)	21(1)	0(1)	6(1)	0(1)
O	37(1)	18(1)	23(1)	−1(1)	10(1)	1(1)
Si(1)	20(1)	27(1)	17(1)	4(1)	4(1)	1(1)
Si(2)	28(1)	18(1)	18(1)	0(1)	7(1)	2(1)

Tabelle 8.21 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **101**.

	x	**y**	**z**	**U(eq)**
H(1A)	4337	3108	4383	50
H(1B)	4625	3893	3778	50
H(1C)	3041	3402	3326	50
H(2A)	1332	4816	3464	51
H(2B)	2897	5257	4098	51

H(2C)	1269	5246	4648	51
H(4A)	−1629	4188	5814	53
H(4B)	−2545	3953	4567	53
H(4C)	−1040	4522	4692	53
H(5A)	−369	2300	5543	56
H(5B)	−2147	2648	5184	56
H(5C)	−1077	2871	6387	56
H(6A)	28	3617	3337	53
H(6B)	−1430	3040	3398	53
H(6C)	410	2761	3721	53
H(7A)	5070	3912	6446	28
H(7B)	5012	4750	5947	28
H(8A)	5955	4463	8300	42
H(8B)	4698	3785	8329	42
H(8C)	4478	4553	8998	42
H(9)	3181	5624	6496	26
H(10A)	5804	5701	8374	43
H(10B)	5969	5753	7045	43
H(11A)	6133	6975	7886	64
H(11B)	4596	6924	6879	64
H(12A)	3825	7492	8508	64
H(12B)	4450	6769	9269	64
H(13A)	1788	6767	7397	47
H(13B)	1612	6694	8722	47
H(14)	2877	5519	8855	30
H(15A)	−1177	5417	6533	52
H(15B)	366	5822	6158	52
H(15C)	−547	6205	7101	52
H(16A)	−278	5701	8973	61
H(16B)	708	4935	9288	61
H(16C)	−987	4918	8433	61
H(17A)	3294	3342	10655	66
H(17B)	1876	3094	11338	66
H(17C)	1881	3924	10806	66
H(18A)	−1437	3722	9650	67
H(18B)	−1503	2880	10129	67
H(18C)	−1960	3039	8782	67
H(19A)	2633	1949	9495	24
H(19B)	913	1731	9831	24
H(20A)	−991	1147	8546	44
H(20B)	−1101	1268	7193	44
H(20C)	−1406	1963	7995	44
H(21)	1322	788	7143	25
H(22A)	2585	614	9533	34
H(22B)	977	216	8877	34
H(23A)	3194	−641	9122	40
H(23B)	2521	−513	7785	40
H(24A)	5379	−434	8103	43
H(24B)	5325	221	9032	43
H(25A)	4032	350	6638	36
H(25B)	5655	757	7253	36
H(26)	4155	1486	8362	24
H(27A)	2602	2038	5086	48
H(27B)	1860	1306	5602	48
H(27C)	3678	1291	5337	48
H(28A)	5778	1881	6557	52
H(28B)	5387	2435	7546	52
H(28C)	4864	2663	6226	52

8.2.4 Kristallstrukturen aus Kapitel 4.3.3

8.2.4.1 Verbindung 102

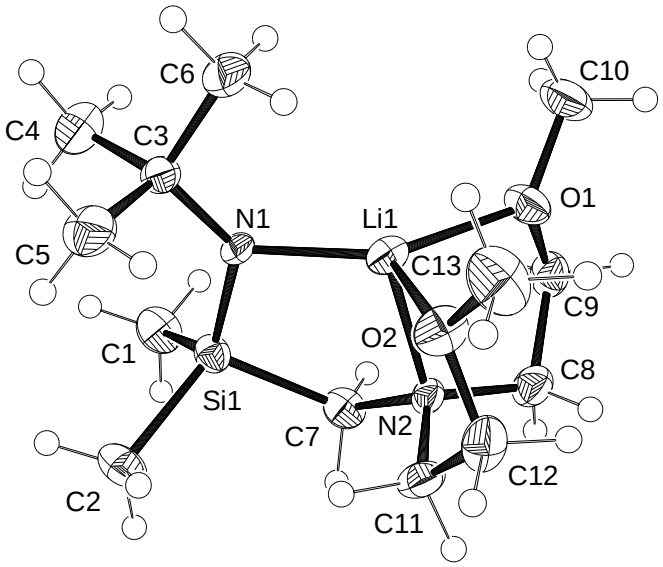


Abb. 8.8 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **102** im Kristall (Ortep−Darstellung).

Tabelle 8.22 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **102**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	4356(3)	12180(3)	3814(2)	37(1)
C(2)	5709(3)	11228(3)	1533(2)	35(1)
C(3)	764(3)	12742(3)	2250(2)	24(1)
C(4)	291(3)	14348(3)	2861(2)	42(1)
C(5)	1334(3)	12963(3)	1061(2)	39(1)
C(6)	−960(3)	12518(3)	2392(2)	38(1)
C(7)	5141(3)	8831(3)	3153(2)	28(1)
C(8)	4474(3)	6452(3)	3402(2)	31(1)
C(9)	2752(3)	7091(3)	4244(2)	32(1)
C(10)	−383(3)	8204(3)	4402(2)	42(1)
C(11)	5378(3)	7211(3)	1618(2)	31(1)
C(12)	4277(3)	6691(3)	1081(2)	36(1)
C(13)	1381(3)	7626(3)	732(2)	48(1)
Li(1)	1953(5)	9296(5)	2598(3)	26(1)
N(1)	2089(2)	11335(2)	2614(1)	19(1)
N(2)	4494(2)	7762(2)	2720(1)	21(1)
O(1)	1305(2)	7909(2)	3731(1)	32(1)
O(2)	2515(2)	7993(2)	1228(1)	33(1)
Si(1)	4126(1)	11000(1)	2731(1)	24(1)

Tabelle 8.23 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **102**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	38(2)	45(2)	39(2)	1(1)	−14(1)	−26(2)
C(2)	27(1)	49(2)	36(2)	7(1)	−6(1)	−23(2)
C(3)	21(1)	22(2)	25(2)	0(1)	−4(1)	−8(1)
C(4)	43(2)	31(2)	49(2)	3(2)	−15(1)	−12(2)
C(5)	35(2)	40(2)	36(2)	11(1)	−13(1)	−10(2)
C(6)	26(2)	30(2)	56(2)	9(2)	−16(1)	−8(1)

C(7)	27(1)	34(2)	27(2)	3(1)	−10(1)	−16(1)
C(8)	31(2)	23(2)	32(2)	5(1)	−6(1)	−7(1)
C(9)	40(2)	28(2)	27(2)	7(1)	−4(1)	−15(2)
C(10)	30(2)	52(2)	44(2)	−1(2)	4(1)	−23(2)
C(11)	24(2)	26(2)	28(2)	3(1)	−2(1)	0(1)
C(12)	56(2)	29(2)	21(2)	−4(1)	1(1)	−20(2)
C(13)	57(2)	63(2)	43(2)	−4(2)	−16(1)	−40(2)
Li(1)	23(2)	22(3)	28(2)	−2(2)	−6(2)	−6(2)
N(1)	16(1)	15(1)	23(1)	3(1)	−6(1)	−4(1)
N(2)	24(1)	16(1)	20(1)	3(1)	−2(1)	−6(1)
O(1)	27(1)	41(1)	29(1)	7(1)	−2(1)	−17(1)
O(2)	34(1)	34(1)	31(1)	−5(1)	−12(1)	−12(1)
Si(1)	24(1)	26(1)	24(1)	5(1)	−8(1)	−13(1)

Tabelle 8.24 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **102**.

	x	y	z	U(eq)
H(1A)	3947	13330	3648	55
H(1B)	5612	11722	3868	55
H(1C)	3618	12106	4489	55
H(2A)	5618	10740	900	53
H(2B)	6944	10673	1632	53
H(2C)	5389	12389	1441	53
H(4A)	−66	14243	3620	63
H(4B)	−700	15244	2626	63
H(4C)	1341	14578	2728	63
H(5A)	2391	13183	943	58
H(5B)	350	13880	835	58
H(5C)	1632	11964	646	58
H(6A)	−705	11511	2002	57
H(6B)	−1869	13449	2124	57
H(6C)	−1411	12444	3145	57
H(7A)	6462	8361	2917	33
H(7B)	4852	8848	3934	33
H(8A)	5519	6045	3739	37
H(8B)	4559	5535	2975	37
H(9A)	2623	6176	4628	38
H(9B)	2769	7855	4759	38
H(10A)	−452	7165	4533	63
H(10B)	−1352	8914	4061	63
H(10C)	−506	8737	5076	63
H(11A)	6568	6284	1588	37
H(11B)	5561	8108	1240	37
H(12A)	4826	6436	319	44
H(12B)	4223	5697	1392	44
H(13A)	1868	7444	−30	72
H(13B)	177	8538	874	72
H(13C)	1308	6637	1016	72

8.2.5 Kristallstrukturen aus Kapitel 4.4.1

8.2.5.1 Verbindung 103

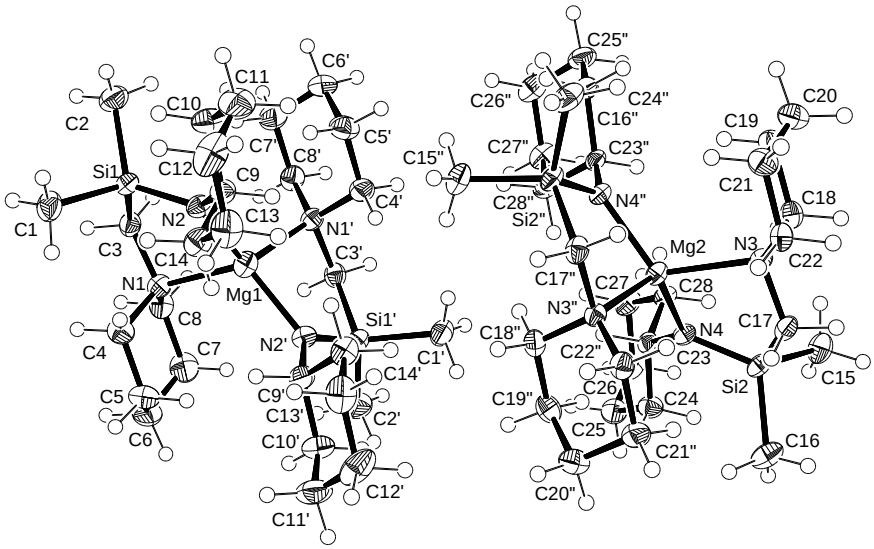


Abb. 8.9 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **103** im Kristall (Ortep−Darstellung).

Tabelle 8.25 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **103**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	10373(1)	2859(2)	3375(1)	36(1)
C(2)	9600(2)	1298(2)	4331(1)	38(1)
C(3)	9048(1)	598(2)	2888(1)	27(1)
C(4)	9058(2)	1698(2)	1835(1)	31(1)
C(5)	8617(2)	1940(2)	1114(1)	37(1)
C(6)	8398(2)	649(2)	734(1)	40(1)
C(7)	7866(2)	−201(2)	1108(1)	42(1)
C(8)	8323(1)	−391(2)	1834(1)	31(1)
C(9)	8237(1)	4277(2)	3514(1)	28(1)
C(10)	8597(2)	4453(2)	4265(1)	36(1)
C(11)	8418(2)	5813(3)	4518(1)	47(1)
C(12)	8767(2)	6880(2)	4130(1)	49(1)
C(13)	8409(2)	6741(2)	3383(1)	43(1)
C(14)	8589(2)	5375(2)	3133(1)	32(1)
C(15)	−318(1)	5665(2)	1420(1)	35(1)
C(16)	639(2)	7185(2)	554(1)	37(1)
C(17)	962(1)	7924(2)	1999(1)	25(1)
C(18)	871(1)	6840(2)	3044(1)	26(1)
C(19)	1280(2)	6618(2)	3779(1)	31(1)
C(20)	1451(2)	7919(2)	4152(1)	34(1)
C(21)	2000(1)	8790(2)	3804(1)	31(1)
C(22)	1595(1)	8946(2)	3064(1)	25(1)
C(23)	1867(1)	4219(2)	1474(1)	21(1)
C(24)	1587(1)	4032(2)	714(1)	27(1)
C(25)	1763(2)	2642(2)	490(1)	34(1)
C(26)	1334(2)	1614(2)	856(1)	35(1)
C(27)	1636(2)	1765(2)	1611(1)	31(1)
C(28)	1449(1)	3151(2)	1833(1)	26(1)
Mg(1)	7500	2136(1)	2500	30(1)
Mg(2)	2500	6392(1)	2500	22(1)
N(1)	8529(1)	873(2)	2199(1)	26(1)

N(2)	8380(1)	2973(2)	3258(1)	25(1)
N(3)	1430(1)	7673(2)	2703(1)	20(1)
N(4)	1704(1)	5543(2)	1708(1)	21(1)
Si(1)	9309(1)	2068(1)	3471(1)	24(1)
Si(2)	787(1)	6440(1)	1417(1)	24(1)

Tabelle 8.26 Anisotrope Auslenkungsparameter ($Å^2 \times 10^3$) für die Verbindung **103**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	**U22**	**U33**	**U23**	**U13**	**U12**
C(1)	26(1)	43(2)	37(2)	−9(1)	2(1)	−4(1)
C(2)	39(1)	43(2)	31(2)	5(1)	1(1)	7(1)
C(3)	23(1)	28(1)	31(1)	3(1)	5(1)	3(1)
C(4)	34(1)	31(1)	28(1)	−6(1)	7(1)	−7(1)
C(5)	47(2)	38(2)	27(2)	2(1)	10(1)	−3(1)
C(6)	44(2)	50(2)	25(2)	−10(1)	6(1)	−4(1)
C(7)	42(2)	45(2)	39(2)	−18(1)	6(1)	−6(1)
C(8)	31(1)	24(1)	37(2)	−8(1)	7(1)	0(1)
C(9)	28(1)	30(1)	25(1)	−2(1)	3(1)	2(1)
C(10)	47(2)	36(2)	24(2)	−2(1)	3(1)	3(1)
C(11)	55(2)	51(2)	32(2)	−16(1)	4(1)	5(1)
C(12)	45(2)	29(2)	65(2)	−22(2)	−9(2)	4(1)
C(13)	40(2)	29(2)	59(2)	3(1)	10(1)	1(1)
C(14)	32(1)	29(1)	35(2)	3(1)	3(1)	−1(1)
C(15)	23(1)	37(2)	41(2)	−3(1)	−2(1)	−2(1)
C(16)	38(1)	37(2)	31(2)	4(1)	−8(1)	−3(1)
C(17)	20(1)	26(1)	28(1)	7(1)	0(1)	2(1)
C(18)	21(1)	26(1)	32(2)	−2(1)	8(1)	−2(1)
C(19)	34(1)	31(2)	33(2)	6(1)	14(1)	−3(1)
C(20)	42(2)	36(2)	27(1)	−1(1)	10(1)	0(1)
C(21)	35(1)	30(1)	28(1)	−6(1)	7(1)	−2(1)
C(22)	22(1)	23(1)	32(2)	−2(1)	6(1)	2(1)
C(23)	16(1)	26(1)	20(1)	−2(1)	−1(1)	0(1)
C(24)	28(1)	30(1)	23(1)	−2(1)	3(1)	−5(1)
C(25)	35(1)	39(2)	25(1)	−11(1)	2(1)	1(1)
C(26)	34(1)	26(1)	40(2)	−10(1)	−4(1)	7(1)
C(27)	33(1)	23(1)	33(2)	2(1)	−1(1)	2(1)
C(28)	26(1)	28(1)	20(1)	2(1)	0(1)	1(1)
Mg(1)	28(1)	28(1)	33(1)	0	3(1)	0
Mg(2)	19(1)	23(1)	23(1)	0	0(1)	0
N(1)	26(1)	24(1)	26(1)	−3(1)	2(1)	−2(1)
N(2)	27(1)	22(1)	23(1)	−1(1)	2(1)	3(1)
N(3)	20(1)	20(1)	20(1)	2(1)	2(1)	−1(1)
N(4)	21(1)	21(1)	19(1)	−1(1)	−1(1)	−2(1)
Si(1)	23(1)	25(1)	22(1)	1(1)	1(1)	0(1)
Si(2)	20(1)	24(1)	23(1)	1(1)	−4(1)	−1(1)

Tabelle 8.27 Wasserstoffkoordinaten ($x\ 10^4$) und isotrope Auslenkungsparameter ($Å^2 \times 10^3$) für die Verbindung **103**.

	x	**y**	**z**	**U(eq)**
H(1A)	10286	3300	2936	54
H(1B)	10828	2179	3404	54
H(1C)	10557	3508	3735	54
H(2A)	9810	1983	4667	57
H(2B)	10064	639	4340	57
H(2C)	9078	871	4433	57
H(3A)	9611	183	2846	33
H(3B)	8721	−55	3103	33
H(4A)	9631	1261	1849	37
H(4B)	9176	2557	2069	37
H(5A)	9009	2472	893	44

H(5B)	8069	2449	1097	44
H(6A)	8058	827	273	48
H(6B)	8948	187	699	48
H(7A)	7765	−1073	885	51
H(7B)	7285	215	1089	51
H(8A)	7942	−926	2065	37
H(8B)	8876	−887	1852	37
H(9)	7585	4405	3438	34
H(10A)	8330	3782	4514	43
H(10B)	9241	4300	4363	43
H(11A)	7776	5931	4471	56
H(11B)	8699	5889	5001	56
H(12A)	9417	6833	4223	59
H(12B)	8599	7753	4282	59
H(13A)	8685	7414	3140	51
H(13B)	7767	6903	3283	51
H(14A)	8314	5304	2648	39
H(14B)	9232	5259	3182	39
H(15A)	−441	4976	1074	52
H(15B)	−778	6343	1324	52
H(15C)	−309	5275	1863	52
H(16A)	1215	7430	467	56
H(16B)	267	7972	528	56
H(16C)	357	6540	217	56
H(17A)	1296	8596	1803	30
H(17B)	379	8308	2009	30
H(18A)	773	5976	2812	31
H(18B)	290	7270	3007	31
H(19A)	1842	6133	3818	38
H(19B)	882	6071	3987	38
H(20A)	885	8359	4160	41
H(20B)	1764	7759	4623	41
H(21A)	2596	8404	3854	37
H(21B)	2062	9669	4021	37
H(22A)	1031	9428	3016	30
H(22B)	1992	9486	2851	30
H(23)	2518	4074	1596	26
H(24A)	950	4224	571	33
H(24B)	1908	4672	486	33
H(25A)	1532	2557	−2	40
H(25B)	2406	2485	580	40
H(26A)	1487	721	720	42
H(26B)	686	1712	730	42
H(27A)	2275	1585	1743	37
H(27B)	1327	1114	1842	37
H(28A)	804	3291	1742	31
H(28B)	1675	3233	2325	31

8.2.5.2 Verbindung 104

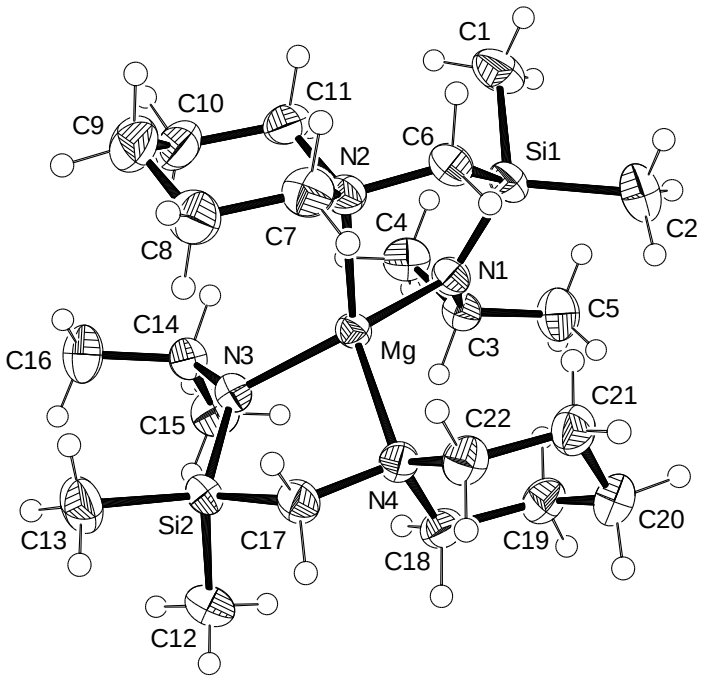


Abb. 8.10 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **104** im Kristall (Ortep–Darstellung).

Tabelle 8.28 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **104**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	−151(1)	2622(2)	3984(1)	54(1)
C(2)	1002(1)	4821(2)	4383(1)	50(1)
C(3)	1195(1)	2983(1)	2450(1)	34(1)
C(4)	518(1)	2050(2)	2026(1)	45(1)
C(5)	867(1)	4340(2)	2284(1)	52(1)
C(6)	1659(1)	2274(1)	5007(1)	37(1)
C(7)	2659(1)	630(2)	5581(1)	43(1)
C(8)	3048(1)	−653(2)	5470(1)	53(1)
C(9)	2372(1)	−1670(2)	5235(1)	59(1)
C(10)	1738(1)	−1234(2)	4489(1)	51(1)
C(11)	1382(1)	68(2)	4625(1)	42(1)
C(12)	4431(1)	612(2)	2225(1)	53(1)
C(13)	4587(1)	−1245(2)	3586(1)	52(1)
C(14)	2337(1)	−562(1)	2455(1)	34(1)
C(15)	2244(1)	−67(2)	1585(1)	49(1)
C(16)	2564(1)	−1974(2)	2483(1)	52(1)
C(17)	4317(1)	1446(1)	3988(1)	38(1)
C(18)	3792(1)	3350(1)	3245(1)	37(1)
C(19)	3300(1)	4585(1)	3225(1)	42(1)
C(20)	3605(1)	5373(2)	3990(1)	47(1)
C(21)	3564(1)	4566(2)	4738(1)	43(1)
C(22)	4051(1)	3337(1)	4724(1)	39(1)
Mg	2490(1)	1578(1)	3699(1)	27(1)
N(1)	1482(1)	2682(1)	3317(1)	31(1)
N(2)	2056(1)	1049(1)	4835(1)	33(1)
N(3)	2922(1)	213(1)	3048(1)	30(1)
N(4)	3746(1)	2564(1)	3977(1)	31(1)
Si(1)	989(1)	3100(1)	4079(1)	34(1)
Si(2)	3978(1)	210(1)	3156(1)	34(1)

Tabelle 8.29 Anisotrope Auslenkungsparameter ($Å^2 \times 10^3$) für die Verbindung **104**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	33(1)	69(1)	61(1)	−12(1)	14(1)	4(1)
C(2)	50(1)	44(1)	51(1)	−12(1)	−1(1)	14(1)
C(3)	31(1)	37(1)	32(1)	3(1)	4(1)	4(1)
C(4)	38(1)	54(1)	40(1)	−2(1)	0(1)	−4(1)
C(5)	56(1)	44(1)	51(1)	9(1)	1(1)	13(1)
C(6)	39(1)	41(1)	33(1)	−4(1)	11(1)	3(1)
C(7)	45(1)	51(1)	34(1)	7(1)	5(1)	4(1)
C(8)	56(1)	55(1)	51(1)	17(1)	13(1)	14(1)
C(9)	81(1)	43(1)	58(1)	16(1)	24(1)	7(1)
C(10)	70(1)	37(1)	49(1)	3(1)	19(1)	−8(1)
C(11)	44(1)	42(1)	42(1)	3(1)	14(1)	−8(1)
C(12)	48(1)	57(1)	62(1)	−3(1)	28(1)	4(1)
C(13)	42(1)	43(1)	67(1)	−2(1)	2(1)	15(1)
C(14)	36(1)	34(1)	32(1)	−2(1)	4(1)	2(1)
C(15)	54(1)	57(1)	33(1)	1(1)	4(1)	1(1)
C(16)	66(1)	36(1)	49(1)	−7(1)	−1(1)	4(1)
C(17)	26(1)	37(1)	47(1)	1(1)	3(1)	4(1)
C(18)	38(1)	36(1)	39(1)	2(1)	11(1)	−5(1)
C(19)	45(1)	34(1)	44(1)	7(1)	7(1)	−3(1)
C(20)	54(1)	31(1)	54(1)	−1(1)	10(1)	−4(1)
C(21)	49(1)	36(1)	44(1)	−6(1)	8(1)	−3(1)
C(22)	38(1)	38(1)	37(1)	−3(1)	−1(1)	−4(1)
Mg	25(1)	28(1)	28(1)	1(1)	6(1)	2(1)
N(1)	27(1)	34(1)	31(1)	1(1)	4(1)	4(1)
N(2)	34(1)	36(1)	30(1)	2(1)	8(1)	1(1)
N(3)	31(1)	30(1)	30(1)	−1(1)	6(1)	2(1)
N(4)	28(1)	30(1)	35(1)	0(1)	3(1)	0(1)
Si(1)	29(1)	38(1)	37(1)	−5(1)	7(1)	5(1)
Si(2)	30(1)	33(1)	41(1)	0(1)	9(1)	7(1)

Tabelle 8.30 Wasserstoffkoordinaten ($x\ 10^4$) und isotrope Auslenkungsparameter ($Å^2 \times 10^3$) für die Verbindung **104**.

	x	y	z	U(eq)
H(1A)	−503	3135	3561	80
H(1B)	−325	2758	4505	80
H(1C)	−215	1723	3835	80
H(2A)	1566	5172	4403	75
H(2B)	855	4895	4922	75
H(2C)	591	5291	3984	75
H(3)	1692	2889	2183	41
H(4A)	726	1180	2124	67
H(4B)	394	2218	1439	67
H(4C)	4	2157	2245	67
H(5A)	359	4456	2512	78
H(5B)	731	4489	1694	78
H(5C)	1300	4942	2539	78
H(6A)	2111	2863	5261	44
H(6B)	1299	2113	5410	44
H(7A)	2359	582	6042	52
H(7B)	3113	1268	5719	52
H(8A)	3430	−900	5984	64
H(8B)	3387	−590	5040	64
H(9A)	2637	−2475	5113	71
H(9B)	2082	−1821	5694	71
H(10A)	1272	−1855	4367	61
H(10B)	2016	−1198	4013	61
H(11A)	984	330	4125	50

H(11B)	1064	12	5072	50
H(12A)	4363	−114	1853	80
H(12B)	5031	813	2394	80
H(12C)	4133	1346	1947	80
H(13A)	4378	−1543	4063	78
H(13B)	5186	−1033	3745	78
H(13C)	4513	−1913	3171	78
H(14)	1770	−492	2604	41
H(15A)	2094	834	1570	73
H(15B)	1800	−543	1225	73
H(15C)	2778	−173	1401	73
H(16A)	3084	−2095	2276	78
H(16B)	2106	−2452	2145	78
H(16C)	2647	−2277	3047	78
H(17A)	4372	1021	4524	45
H(17B)	4883	1761	3945	45
H(18A)	3566	2855	2748	44
H(18B)	4389	3547	3243	44
H(19A)	2694	4392	3178	50
H(19B)	3365	5082	2739	50
H(20A)	3246	6133	3983	56
H(20B)	4191	5656	4007	56
H(21A)	3804	5049	5237	52
H(21B)	2969	4372	4751	52
H(22A)	4655	3537	4758	46
H(22B)	4003	2828	5210	46

8.2.5.3 Verbindung 105

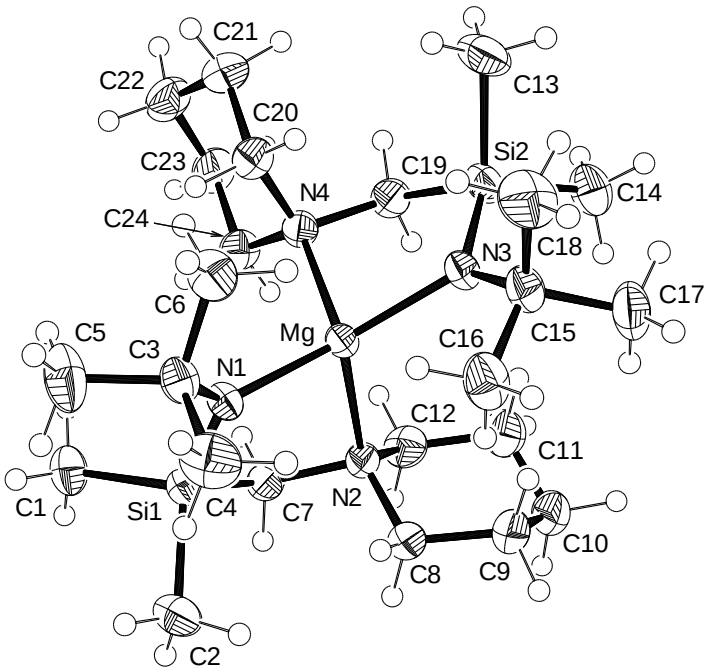


Abb. 8.11 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **105** im Kristall (Ortep−Darstellung).

Tabelle 8.31 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **105**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	4780(3)	1077(1)	9859(2)	44(1)
C(2)	7319(3)	2016(2)	10475(1)	50(1)
C(3)	5080(3)	2757(1)	8572(1)	35(1)
C(4)	6058(3)	3398(1)	8988(2)	56(1)
C(5)	3817(3)	2729(2)	8926(2)	60(1)
C(6)	4480(3)	2959(1)	7681(1)	44(1)
C(7)	7271(2)	711(1)	9316(1)	35(1)
C(8)	9410(3)	1310(2)	9221(1)	39(1)
C(9)	10517(3)	1402(2)	8774(2)	48(1)
C(10)	11048(3)	660(2)	8559(2)	54(1)
C(11)	9803(3)	194(2)	8104(2)	52(1)
C(12)	8740(3)	114(1)	8585(2)	42(1)
C(13)	5571(3)	1492(2)	5126(1)	55(1)
C(14)	8262(3)	696(2)	5780(2)	50(1)
C(15)	8063(3)	2543(1)	6786(1)	37(1)
C(16)	8376(3)	2988(1)	7578(2)	48(1)
C(17)	9479(3)	2392(2)	6603(2)	54(1)
C(18)	7175(3)	3045(2)	6122(2)	58(1)
C(19)	5974(3)	431(1)	6561(1)	36(1)
C(20)	3904(2)	1133(1)	6722(1)	37(1)
C(21)	2748(3)	694(2)	6137(2)	48(1)
C(22)	2291(3)	29(2)	6555(2)	51(1)
C(23)	3563(3)	−437(1)	6991(2)	46(1)
C(24)	4687(3)	53(1)	7544(1)	38(1)
Mg	6663(1)	1533(1)	7836(1)	25(1)
N(1)	5840(2)	2034(1)	8658(1)	29(1)
N(2)	8195(2)	846(1)	8777(1)	30(1)
N(3)	7322(2)	1841(1)	6866(1)	30(1)
N(4)	5171(2)	688(1)	7131(1)	31(1)
Si(1)	6240(1)	1545(1)	9529(1)	31(1)
Si(2)	6844(1)	1205(1)	6114(1)	35(1)

Tabelle 8.32 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **105**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	45(2)	47(2)	47(1)	5(1)	25(1)	−3(1)
C(2)	55(2)	64(2)	32(1)	−8(1)	12(1)	−8(2)
C(3)	39(1)	32(1)	36(1)	−2(1)	17(1)	3(1)
C(4)	70(2)	39(2)	57(2)	−11(1)	15(2)	2(2)
C(5)	66(2)	58(2)	71(2)	15(2)	45(2)	22(2)
C(6)	51(2)	35(2)	46(1)	5(1)	16(1)	12(1)
C(7)	32(1)	41(1)	30(1)	9(1)	8(1)	−1(1)
C(8)	32(1)	50(2)	33(1)	1(1)	8(1)	−5(1)
C(9)	34(2)	68(2)	43(1)	4(1)	13(1)	−8(1)
C(10)	34(2)	85(2)	44(2)	6(2)	14(1)	10(2)
C(11)	44(2)	61(2)	54(2)	−4(1)	18(1)	17(2)
C(12)	39(2)	40(2)	45(1)	4(1)	8(1)	10(1)
C(13)	67(2)	68(2)	28(1)	−3(1)	10(1)	4(2)
C(14)	59(2)	51(2)	49(2)	−10(1)	29(1)	6(1)
C(15)	43(2)	36(1)	37(1)	2(1)	19(1)	−4(1)
C(16)	59(2)	38(2)	55(2)	−7(1)	29(1)	−14(1)
C(17)	52(2)	62(2)	59(2)	−3(1)	34(2)	−11(2)
C(18)	72(2)	43(2)	59(2)	19(1)	18(2)	−2(2)
C(19)	35(1)	36(1)	37(1)	−10(1)	10(1)	0(1)
C(20)	35(1)	35(1)	41(1)	−2(1)	10(1)	0(1)
C(21)	38(2)	56(2)	43(1)	−2(1)	3(1)	−4(1)
C(22)	36(2)	57(2)	56(2)	−10(1)	7(1)	−12(1)

C(23)	43(2)	40(2)	54(2)	−6(1)	14(1)	−15(1)
C(24)	38(2)	35(1)	39(1)	1(1)	10(1)	−4(1)
Mg	27(1)	26(1)	23(1)	0(1)	9(1)	−1(1)
N(1)	32(1)	30(1)	26(1)	−1(1)	11(1)	2(1)
N(2)	26(1)	35(1)	29(1)	3(1)	8(1)	1(1)
N(3)	35(1)	30(1)	27(1)	1(1)	13(1)	−2(1)
N(4)	30(1)	31(1)	31(1)	−4(1)	9(1)	−2(1)
Si(1)	32(1)	40(1)	25(1)	0(1)	11(1)	−4(1)
Si(2)	40(1)	39(1)	28(1)	−4(1)	14(1)	2(1)

Tabelle 8.33 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **105**.

	x	y	z	U(eq)
H(1A)	4232	1457	10051	66
H(1B)	5187	724	10296	66
H(1C)	4160	807	9403	66
H(2A)	8148	2252	10371	76
H(2B)	7625	1642	10903	76
H(2C)	6745	2398	10643	76
H(4A)	6388	3302	9568	83
H(4B)	5539	3872	8892	83
H(4C)	6871	3428	8767	83
H(5A)	3207	2306	8692	90
H(5B)	3279	3197	8800	90
H(5C)	4155	2667	9512	90
H(6A)	5235	2936	7412	65
H(6B)	4089	3467	7634	65
H(6C)	3733	2603	7424	65
H(7A)	7867	518	9836	41
H(7B)	6589	312	9072	41
H(8A)	9849	1076	9750	46
H(8B)	9061	1811	9320	46
H(9A)	10112	1692	8275	58
H(9B)	11321	1691	9113	58
H(10A)	11572	395	9055	65
H(10B)	11696	742	8220	65
H(11A)	10135	−309	7996	62
H(11B)	9347	434	7580	62
H(12A)	7938	−194	8274	50
H(12B)	9187	−153	9094	50
H(13A)	4841	1817	5230	82
H(13B)	5129	1044	4835	82
H(13C)	6083	1762	4800	82
H(14A)	8565	1004	5389	76
H(14B)	7888	219	5530	76
H(14C)	9070	601	6249	76
H(16A)	7486	3118	7693	72
H(16B)	8890	3446	7527	72
H(16C)	8951	2682	8019	72
H(17A)	10047	2049	7008	81
H(17B)	9990	2865	6616	81
H(17C)	9303	2166	6067	81
H(18A)	7041	2800	5599	87
H(18B)	7661	3524	6124	87
H(18C)	6254	3134	6218	87
H(19A)	5320	154	6115	43
H(19B)	6714	76	6849	43
H(20A)	4200	1549	6426	44
H(20B)	3511	1356	7138	44
H(21A)	3094	514	5684	57
H(21B)	1927	1025	5914	57

H(22A)	1799	210	6947	61
H(22B)	1624	−286	6152	61
H(23A)	3963	−685	6591	55
H(23B)	3265	−830	7312	55
H(24A)	4307	255	7975	45
H(24B)	5512	−264	7803	45

8.2.5.4 Verbindung 106

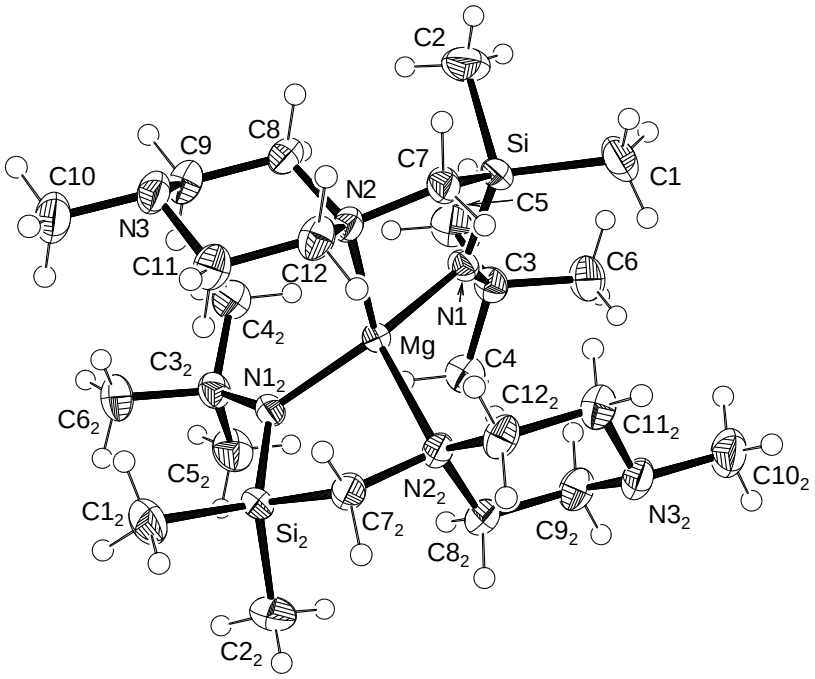


Abb. 8.12 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **106** im Kristall (Ortep−Darstellung).

Tabelle 8.34 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **106**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	6614(1)	1078(2)	6227(1)	52(1)
C(2)	7066(1)	2765(2)	7791(1)	49(1)
C(3)	6095(1)	−594(1)	8068(1)	31(1)
C(4)	6162(1)	−1828(2)	7438(1)	45(1)
C(5)	6739(1)	−426(2)	8677(1)	43(1)
C(6)	5618(1)	−1114(1)	8580(1)	37(1)
C(7)	5817(1)	3561(1)	6789(1)	31(1)
C(8)	5050(1)	2497(1)	5648(1)	31(1)
C(9)	4364(1)	2384(1)	5201(1)	36(1)
C(10)	4806(1)	4736(1)	6296(1)	32(1)
C(11)	4120(1)	4565(1)	5861(1)	35(1)
C(12)	3417(1)	3715(2)	4611(1)	46(1)
Mg	5000	1714(1)	7500	21(1)
N(1)	5875(1)	814(1)	7637(1)	26(1)
N(2)	5129(1)	3280(1)	6467(1)	26(1)
N(3)	4074(1)	3843(1)	5051(1)	34(1)
Si	6333(1)	1880(1)	7152(1)	31(1)

Tabelle 8.35 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **106**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	44(1)	72(1)	45(1)	3(1)	23(1)	8(1)
C(2)	26(1)	67(1)	52(1)	8(1)	3(1)	−12(1)
C(3)	28(1)	29(1)	34(1)	1(1)	5(1)	7(1)
C(4)	45(1)	39(1)	52(1)	−9(1)	10(1)	13(1)
C(5)	33(1)	47(1)	46(1)	6(1)	−3(1)	10(1)
C(6)	42(1)	28(1)	41(1)	7(1)	9(1)	2(1)
C(7)	29(1)	35(1)	28(1)	6(1)	3(1)	−8(1)
C(8)	35(1)	35(1)	23(1)	0(1)	4(1)	0(1)
C(9)	39(1)	36(1)	29(1)	−3(1)	−2(1)	−2(1)
C(10)	39(1)	25(1)	28(1)	4(1)	−1(1)	−2(1)
C(11)	37(1)	33(1)	32(1)	2(1)	0(1)	4(1)
C(12)	37(1)	56(1)	39(1)	4(1)	−6(1)	−2(1)
Mg	20(1)	22(1)	21(1)	0	4(1)	0
N(1)	21(1)	28(1)	27(1)	2(1)	6(1)	2(1)
N(2)	28(1)	27(1)	21(1)	3(1)	2(1)	−2(1)
N(3)	35(1)	38(1)	26(1)	5(1)	−2(1)	−2(1)
Si	21(1)	42(1)	29(1)	3(1)	7(1)	−2(1)

Tabelle 8.36 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **106**.

	x	y	z	U(eq)
H(1A)	6962	389	6427	78
H(1B)	6760	1880	5910	78
H(1C)	6266	550	5863	78
H(2A)	6997	3012	8350	74
H(2B)	7162	3671	7511	74
H(2C)	7421	2074	7844	74
H(4A)	5754	−1997	7058	68
H(4B)	6303	−2743	7743	68
H(4C)	6473	−1527	7112	68
H(5A)	7062	−188	8359	65
H(5B)	6848	−1356	8983	65
H(5C)	6715	373	9076	65
H(6A)	5604	−398	9027	55
H(6B)	5746	−2084	8828	55
H(6C)	5199	−1192	8213	55
H(7A)	5863	4261	7265	37
H(7B)	5984	4059	6341	37
H(8A)	5230	1488	5744	38
H(8B)	5288	3033	5285	38
H(9A)	4336	1869	4659	43
H(9B)	4130	1790	5545	43
H(10A)	5026	5340	5940	39
H(10B)	4831	5270	6832	39
H(11A)	3896	3967	6215	42
H(11B)	3917	5552	5778	42
H(12A)	3397	3229	4069	69
H(12B)	3230	4705	4520	69
H(12C)	3184	3125	4949	69

8.2.6 Kristallstrukturen aus Kapitel 4.4.2

8.2.6.1 Verbindung 107

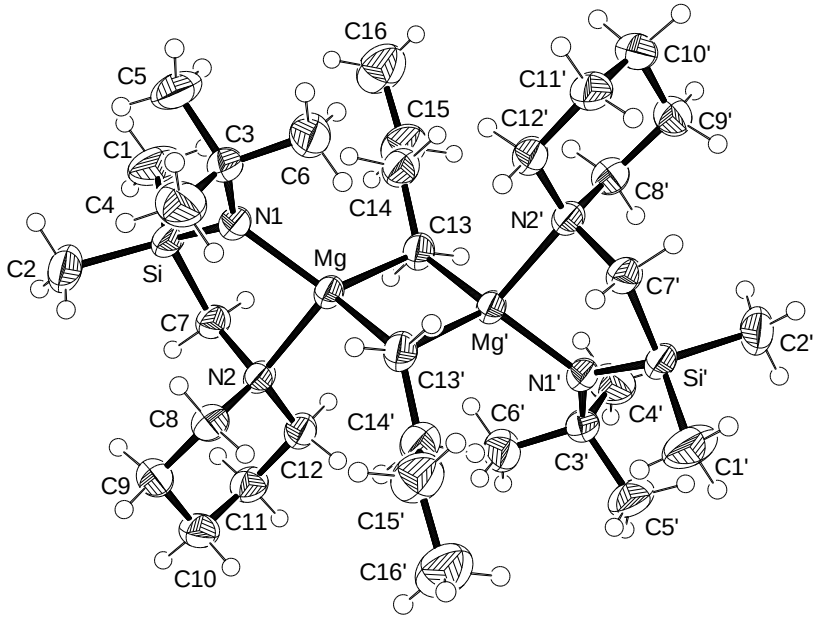


Abb. 8.13 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **107** im Kristall (Ortep–Darstellung).

Tabelle 8.37 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **107**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	1032(3)	6096(3)	1923(3)	78(1)
C(2)	2671(4)	6843(3)	−6(2)	70(1)
C(3)	5333(3)	6500(2)	2946(2)	43(1)
C(4)	6423(3)	6665(3)	2091(3)	65(1)
C(5)	4622(3)	5076(2)	2647(3)	69(1)
C(6)	6216(3)	6704(3)	4313(2)	57(1)
C(7)	1787(2)	8954(2)	1919(2)	40(1)
C(8)	3802(2)	10249(2)	1313(2)	43(1)
C(9)	2878(3)	10701(2)	149(2)	48(1)
C(10)	2211(3)	11994(2)	495(2)	51(1)
C(11)	1355(3)	11864(2)	1527(2)	48(1)
C(12)	2325(3)	11361(2)	2650(2)	43(1)
C(13)	3337(3)	9534(2)	5526(2)	43(1)
C(14)	2876(3)	8128(2)	5749(2)	50(1)
C(15)	1332(3)	7930(3)	6047(3)	69(1)
C(16)	908(4)	6514(3)	6165(3)	84(1)
Mg	4424(1)	9259(1)	3830(1)	34(1)
N(1)	4210(2)	7477(2)	2791(2)	38(1)
N(2)	2966(2)	10087(2)	2316(2)	36(1)
Si	2574(1)	7272(1)	1699(1)	44(1)

Tabelle 8.38 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **107**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	63(2)	45(2)	110(3)	16(2)	−13(2)	−14(1)
C(2)	98(2)	51(2)	45(2)	−11(1)	−14(1)	18(2)
C(3)	54(1)	32(1)	39(1)	4(1)	3(1)	7(1)

C(4)	78(2)	60(2)	67(2)	16(1)	27(2)	25(1)
C(5)	79(2)	32(1)	85(2)	7(1)	−7(2)	6(1)
C(6)	64(2)	52(1)	50(2)	3(1)	−2(1)	17(1)
C(7)	39(1)	35(1)	43(1)	4(1)	0(1)	−4(1)
C(8)	41(1)	39(1)	46(1)	4(1)	9(1)	0(1)
C(9)	53(1)	51(1)	40(1)	8(1)	10(1)	0(1)
C(10)	57(2)	44(1)	50(1)	15(1)	3(1)	2(1)
C(11)	52(1)	38(1)	53(1)	7(1)	3(1)	10(1)
C(12)	49(1)	36(1)	40(1)	−1(1)	4(1)	5(1)
C(13)	48(1)	40(1)	37(1)	−1(1)	1(1)	3(1)
C(14)	54(1)	44(1)	51(1)	2(1)	11(1)	−3(1)
C(15)	69(2)	62(2)	79(2)	2(1)	33(2)	−7(1)
C(16)	89(2)	70(2)	96(2)	−1(2)	40(2)	−20(2)
Mg	37(1)	29(1)	32(1)	0(1)	2(1)	0(1)
N(1)	46(1)	29(1)	36(1)	1(1)	2(1)	3(1)
N(2)	37(1)	29(1)	37(1)	1(1)	3(1)	0(1)
Si	52(1)	29(1)	43(1)	−1(1)	−7(1)	−2(1)

Tabelle 8.39 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **107**.

	x	y	z	U(eq)
H(1A)	1264	5185	1694	116
H(1B)	75	6260	1384	116
H(1C)	954	6231	2809	116
H(2A)	3472	7412	−189	105
H(2B)	1706	6978	−550	105
H(2C)	2886	5916	−166	105
H(4A)	5870	6525	1208	98
H(4B)	7176	6017	2216	98
H(4C)	6927	7559	2297	98
H(5A)	3884	4960	3166	104
H(5B)	5408	4466	2832	104
H(5C)	4120	4890	1752	104
H(6A)	6743	7590	4516	86
H(6B)	6951	6040	4428	86
H(6C)	5522	6615	4875	86
H(7A)	1115	9087	1115	48
H(7B)	1171	8955	2563	48
H(8A)	4192	9394	1062	51
H(8B)	4678	10899	1666	51
H(9A)	2056	10016	−263	58
H(9B)	3521	10825	−458	58
H(10A)	3028	12711	790	61
H(10B)	1523	12227	−261	61
H(11A)	448	11246	1186	58
H(11B)	1022	12736	1806	58
H(12A)	3161	12037	3049	51
H(12B)	1711	11243	3280	51
H(13A)	2380(30)	9790(20)	4990(30)	60(7)
H(13B)	3100(30)	10000(30)	6190(30)	65(8)
H(14A)	2907	7507	4986	60
H(14B)	3637	7888	6457	60
H(15A)	1317	8495	6847	82
H(15B)	569	8220	5370	82
H(16A)	974	5942	5393	127
H(16B)	−124	6433	6289	127
H(16C)	1598	6248	6889	127

8.2.6.2 Verbindung 108

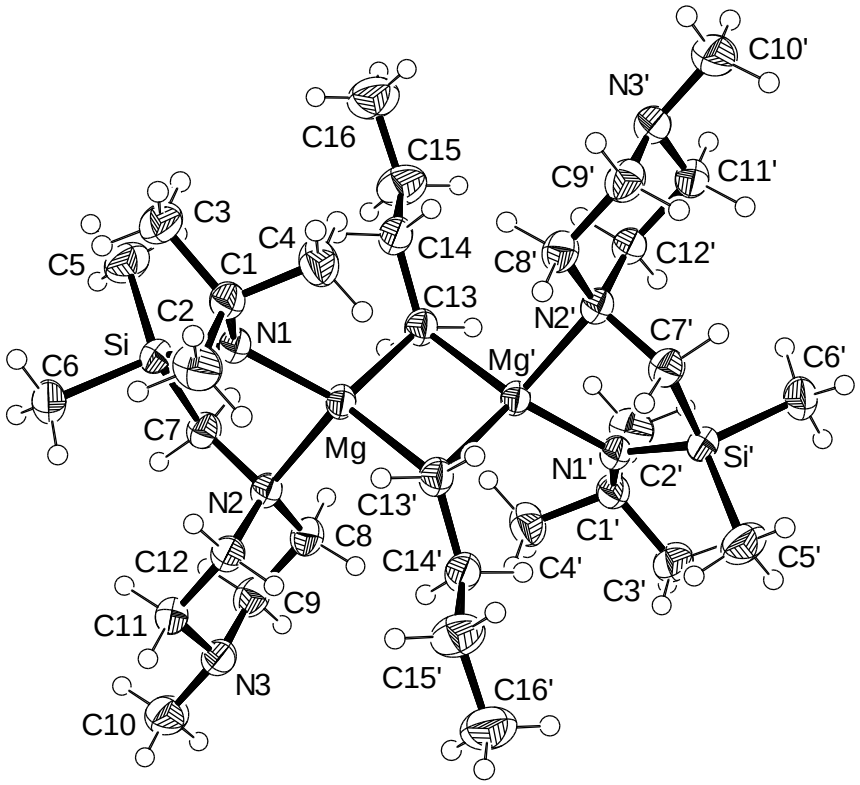


Abb. 8.14 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **108** im Kristall (Ortep−Darstellung).

Tabelle 8.40 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **108**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	5318(2)	7631(2)	1810(2)	34(1)
C(2)	6618(3)	7152(2)	2485(2)	49(1)
C(3)	4493(3)	8869(2)	2149(2)	49(1)
C(4)	6092(3)	8087(2)	487(2)	47(1)
C(5)	787(3)	7267(2)	3013(2)	51(1)
C(6)	2791(3)	5954(2)	4705(2)	45(1)
C(7)	1925(2)	4448(2)	3096(2)	35(1)
C(8)	2695(2)	2374(2)	2465(2)	37(1)
C(9)	2001(2)	1310(2)	3616(2)	40(1)
C(10)	2515(3)	−118(2)	5440(2)	55(1)
C(11)	3660(2)	2093(2)	4588(2)	37(1)
C(12)	4365(2)	3152(2)	3447(2)	32(1)
C(13)	3103(2)	5585(2)	−347(2)	34(1)
C(14)	2592(2)	7085(2)	−591(2)	37(1)
C(15)	1062(3)	7433(2)	−991(2)	56(1)
C(16)	597(3)	8911(3)	−1171(3)	67(1)
Mg	4473(1)	5195(1)	1102(1)	29(1)
N(1)	4210(2)	6518(1)	2045(1)	30(1)
N(2)	3267(2)	3609(1)	2638(1)	31(1)
N(3)	3161(2)	908(2)	4341(1)	39(1)
Si	2579(1)	6150(1)	3157(1)	32(1)

Tabelle 8.41 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **108**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	41(1)	32(1)	31(1)	−11(1)	−8(1)	−1(1)
C(2)	52(1)	50(1)	53(1)	−15(1)	−23(1)	−5(1)
C(3)	62(1)	33(1)	51(1)	−16(1)	−6(1)	−1(1)
C(4)	56(1)	46(1)	36(1)	−11(1)	−2(1)	−12(1)
C(5)	41(1)	49(1)	62(1)	−20(1)	−8(1)	14(1)
C(6)	55(1)	47(1)	32(1)	−16(1)	−5(1)	0(1)
C(7)	31(1)	37(1)	36(1)	−13(1)	−6(1)	2(1)
C(8)	40(1)	37(1)	37(1)	−18(1)	−9(1)	−2(1)
C(9)	40(1)	36(1)	45(1)	−17(1)	−4(1)	−5(1)
C(10)	59(1)	42(1)	50(1)	−5(1)	1(1)	2(1)
C(11)	40(1)	40(1)	32(1)	−14(1)	−7(1)	6(1)
C(12)	31(1)	35(1)	33(1)	−13(1)	−8(1)	2(1)
C(13)	34(1)	40(1)	33(1)	−15(1)	−9(1)	3(1)
C(14)	37(1)	42(1)	37(1)	−17(1)	−10(1)	6(1)
C(15)	47(1)	53(1)	74(2)	−21(1)	−26(1)	12(1)
C(16)	66(2)	59(2)	79(2)	−20(1)	−29(1)	22(1)
Mg	31(1)	32(1)	26(1)	−12(1)	−6(1)	2(1)
N(1)	33(1)	31(1)	29(1)	−12(1)	−6(1)	1(1)
N(2)	32(1)	32(1)	31(1)	−13(1)	−7(1)	1(1)
N(3)	44(1)	33(1)	36(1)	−10(1)	−2(1)	1(1)
Si	32(1)	32(1)	31(1)	−13(1)	−5(1)	5(1)

Tabelle 8.42 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **108**.

	x	y	z	U(eq)
H(2A)	6143	6866	3335	74
H(2B)	7364	7895	2306	74
H(2C)	7186	6385	2250	74
H(3A)	3666	9198	1708	73
H(3B)	5275	9588	1958	73
H(3C)	4013	8612	2998	73
H(4A)	6669	7324	253	71
H(4B)	6833	8829	324	71
H(4C)	5269	8401	39	71
H(5A)	937	8106	3195	77
H(5B)	−155	6793	3565	77
H(5C)	643	7485	2204	77
H(6A)	3694	5359	4862	67
H(6B)	1818	5557	5273	67
H(6C)	2969	6845	4785	67
H(7A)	1371	3925	3900	41
H(7B)	1155	4618	2585	41
H(8A)	3592	1967	2004	44
H(8B)	1875	2643	1997	44
H(9A)	1047	1683	4054	48
H(9B)	1675	507	3442	48
H(10A)	1585	250	5888	82
H(10B)	3323	−380	5908	82
H(10C)	2202	−915	5264	82
H(11A)	4459	1819	5075	44
H(11B)	2735	2482	5040	44
H(12A)	4681	3948	3637	39
H(12B)	5336	2776	3033	39
H(13A)	3020(30)	5310(30)	−1010(20)	64(7)
H(13B)	2190(30)	5070(20)	250(20)	52(6)
H(14A)	2492	7352	140	45
H(14B)	3449	7639	−1202	45

H(15A)	202	6864	−397	67
H(15B)	1168	7210	−1743	67
H(16A)	467	9135	−426	100
H(16B)	−406	9071	−1427	100
H(16C)	1429	9481	−1775	100

8.2.6.3 Verbindung 109

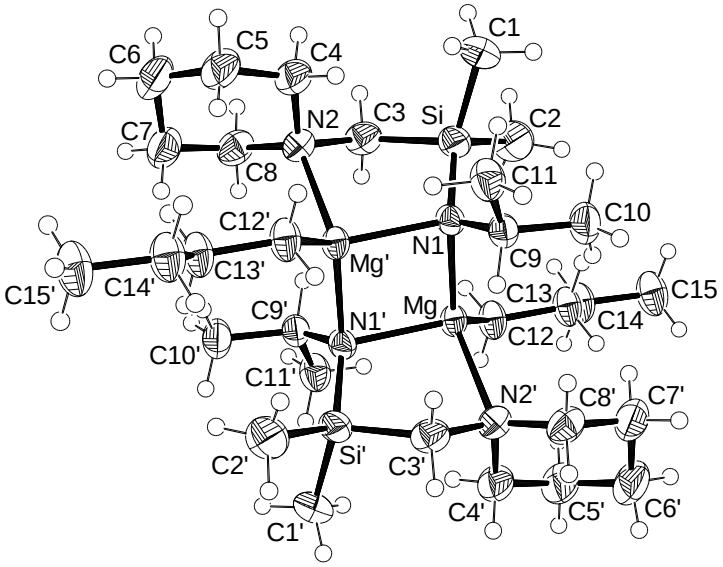


Abb. 8.15 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **109** im Kristall (Ortep−Darstellung).

Tabelle 8.43 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **109**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	2093(3)	6555(3)	7939(2)	62(1)
C(2)	3231(3)	6305(3)	5379(3)	68(1)
C(3)	3305(2)	8858(2)	6332(2)	44(1)
C(4)	2575(3)	9694(2)	8314(2)	51(1)
C(5)	2133(3)	10873(3)	9089(2)	61(1)
C(6)	3185(4)	11847(3)	8809(2)	68(1)
C(7)	3177(3)	12273(3)	7411(2)	57(1)
C(8)	3703(2)	11031(2)	6722(2)	48(1)
C(9)	−1309(2)	8148(2)	6150(2)	38(1)
C(10)	−1220(3)	6754(2)	5752(2)	52(1)
C(11)	−1828(3)	8188(2)	7516(2)	48(1)
C(12)	1670(3)	8307(2)	2538(2)	42(1)
C(13)	1784(3)	6853(2)	2255(2)	44(1)
C(14)	3140(3)	6260(2)	1393(2)	50(1)
C(15)	3144(3)	4840(2)	1093(2)	60(1)
Mg	−26(1)	9322(1)	3844(1)	31(1)
N(1)	177(2)	8615(2)	5837(1)	32(1)
N(2)	2609(2)	10118(2)	6943(1)	39(1)
Si	2032(1)	7594(1)	6367(1)	42(1)

Tabelle 8.44 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **109**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	75(2)	42(1)	61(2)	9(1)	−24(1)	−6(1)
C(2)	62(2)	50(2)	79(2)	−26(1)	−9(1)	14(1)
C(3)	35(1)	48(1)	46(1)	−10(1)	−2(1)	−1(1)
C(4)	65(1)	55(2)	37(1)	−6(1)	−5(1)	−21(1)
C(5)	88(2)	67(2)	35(1)	−14(1)	−2(1)	−29(1)
C(6)	90(2)	72(2)	56(1)	−20(1)	−13(1)	−36(2)
C(7)	63(1)	60(2)	57(1)	−12(1)	−5(1)	−31(1)
C(8)	39(1)	61(2)	49(1)	−7(1)	−3(1)	−21(1)
C(9)	46(1)	31(1)	38(1)	−6(1)	−1(1)	−13(1)
C(10)	71(2)	40(1)	53(1)	−12(1)	−1(1)	−23(1)
C(11)	59(1)	43(1)	45(1)	−8(1)	10(1)	−21(1)
C(12)	48(1)	36(1)	44(1)	−16(1)	14(1)	−15(1)
C(13)	54(1)	36(1)	45(1)	−16(1)	16(1)	−15(1)
C(14)	60(1)	42(1)	53(1)	−18(1)	16(1)	−17(1)
C(15)	76(2)	43(1)	65(2)	−23(1)	21(1)	−18(1)
Mg	35(1)	28(1)	31(1)	−11(1)	5(1)	−7(1)
N(1)	38(1)	26(1)	32(1)	−7(1)	1(1)	−4(1)
N(2)	40(1)	44(1)	35(1)	−8(1)	−1(1)	−12(1)
Si	45(1)	31(1)	45(1)	−8(1)	−7(1)	2(1)

Tabelle 8.45 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **109**.

	x	y	z	U(eq)
H(1A)	1449	7126	8536	93
H(1B)	3215	6221	8231	93
H(1C)	1647	5780	7866	93
H(2A)	2605	5662	5237	101
H(2B)	4245	5809	5805	101
H(2C)	3472	6767	4576	101
H(3A)	4355	8380	6736	53
H(3B)	3531	9137	5449	53
H(4A)	3653	9106	8579	61
H(4B)	1785	9142	8484	61
H(5A)	2238	10512	9984	73
H(5B)	989	11376	8929	73
H(6A)	4304	11398	9098	82
H(6B)	2766	12659	9254	82
H(7A)	2076	12803	7140	68
H(7B)	3921	12863	7213	68
H(8A)	3736	11328	5816	58
H(8B)	4810	10515	6990	58
H(9)	−2204	8807	5651	45
H(10A)	−910	6747	4871	79
H(10B)	−2279	6561	5868	79
H(10C)	−413	6056	6262	79
H(11A)	−1031	7501	8045	71
H(11B)	−2887	7993	7622	71
H(11C)	−1898	9093	7758	71
H(13A)	1915	6249	3054	53
H(13B)	748	6844	1881	53
H(14A)	4186	6214	1784	60
H(14B)	3046	6879	604	60
H(15A)	3313	4206	1862	90
H(15B)	4016	4530	503	90
H(15C)	2104	4872	722	90
H(12A)	2700(30)	8340(20)	2811(19)	41(6)
H(12B)	1530(30)	8850(20)	1810(20)	43(6)

8.2.7 Kristallstrukturen aus Kapitel 4.5.1

8.2.7.1 Verbindung 117

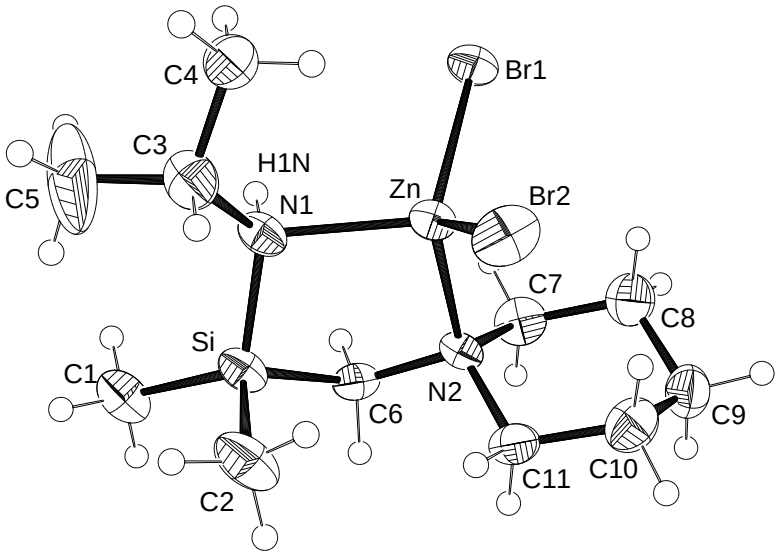


Abb. 8.16 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **117** im Kristall (Ortep−Darstellung).

Tabelle 8.46 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **117**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
Br(1)	9669(1)	8417(1)	10755(1)	37(1)
Br(2)	6257(1)	7199(1)	9665(1)	48(1)
C(1)	7329(5)	11537(8)	7090(5)	50(2)
C(2)	5552(5)	9465(9)	7226(5)	56(2)
C(3)	6587(5)	10816(8)	9421(5)	47(2)
C(4)	6927(6)	10635(8)	10478(5)	50(2)
C(5)	6510(14)	12167(13)	9184(11)	128(6)
C(6)	8307(4)	8916(6)	7639(4)	34(1)
C(7)	9636(4)	7219(7)	8426(4)	40(2)
C(8)	9782(5)	5944(8)	8895(5)	46(2)
C(9)	8933(5)	4970(8)	8276(5)	47(2)
C(10)	7661(5)	5488(8)	8050(5)	46(2)
C(11)	7543(4)	6771(7)	7598(4)	38(1)
N(2)	8387(3)	7717(5)	8199(3)	30(1)
N(1)	7446(3)	10138(6)	8975(3)	33(1)
Si	7115(1)	10054(2)	7710(1)	35(1)
Zn	7915(1)	8276(1)	9428(1)	30(1)

Tabelle 8.47 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **117**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

	U11	U22	U33	U23	U13	U12
Br(1)	33(1)	47(1)	28(1)	1(1)	2(1)	−2(1)
Br(2)	41(1)	56(1)	54(1)	−10(1)	25(1)	−14(1)
C(1)	45(3)	56(6)	44(4)	15(4)	7(3)	2(3)
C(2)	38(2)	72(6)	48(4)	17(5)	−2(2)	2(3)
C(3)	45(3)	56(5)	47(4)	6(4)	23(3)	16(3)
C(4)	59(3)	50(5)	42(4)	−1(4)	18(3)	15(3)
C(5)	207(12)	95(10)	135(11)	66(8)	134(11)	105(10)
C(6)	36(2)	38(4)	27(3)	−6(3)	8(2)	−6(2)

C(7)	30(2)	50(4)	44(4)	−3(3)	19(2)	0(2)
C(8)	43(3)	45(5)	52(4)	0(3)	15(3)	4(3)
C(9)	59(3)	35(4)	49(4)	2(4)	18(3)	6(3)
C(10)	47(3)	43(4)	52(4)	−6(4)	20(3)	−6(3)
C(11)	37(2)	42(4)	32(3)	−7(3)	6(2)	−1(2)
N	29(2)	36(3)	22(2)	4(2)	6(2)	2(2)
N(1)	26(2)	44(3)	29(2)	6(3)	6(2)	4(2)
Si	28(1)	44(1)	30(1)	7(1)	4(1)	0(1)
Zn	26(1)	36(1)	26(1)	1(1)	7(1)	−1(1)

Tabelle 8.48 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **117**.

	x	y	z	U(eq)
H(1N)	8200(50)	10420(90)	9260(50)	60(20)
H(1A)	6620	12071	6988	74
H(1B)	7446	11328	6470	74
H(1C)	8032	11986	7484	74
H(2A)	5407	8809	7651	82
H(2B)	5438	9115	6587	82
H(2C)	4992	10161	7191	82
H(3)	5774	10444	9136	57
H(4A)	7716	10993	10774	75
H(4B)	6941	9729	10621	75
H(4C)	6335	11047	10733	75
H(5A)	7260	12586	9523	191
H(5B)	5850	12550	9374	191
H(5C)	6360	12278	8491	191
H(6A)	8183	8695	6959	40
H(6B)	9093	9350	7865	40
H(7A)	10190	7813	8857	47
H(7B)	9868	7157	7829	47
H(8A)	9622	6006	9524	56
H(8B)	10617	5649	9014	56
H(9A)	9143	4821	7678	57
H(9B)	8993	4161	8624	57
H(10A)	7104	4901	7611	54
H(10B)	7430	5538	8648	54
H(11A)	7695	6694	6969	46
H(11B)	6712	7063	7486	46

8.2.7.2 Verbindung 118

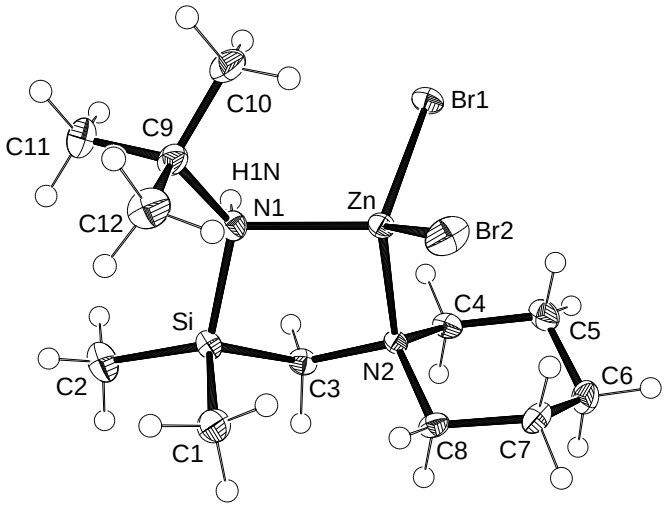


Abb. 8.17 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **118** im Kristall (Ortep−Darstellung).

Tabelle 8.49 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **118**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
Br(1)	343(1)	3430(1)	4254(1)	20(1)
Br(2)	3697(1)	2172(1)	5463(1)	27(1)
C(1)	4378(2)	4264(2)	8068(2)	25(1)
C(2)	2739(2)	6418(2)	8098(2)	30(1)
C(3)	1646(2)	3884(2)	7421(2)	17(1)
C(4)	342(2)	2212(2)	6567(2)	18(1)
C(5)	203(2)	941(2)	6079(2)	23(1)
C(6)	1025(2)	−26(2)	6740(2)	25(1)
C(7)	2285(2)	459(2)	7025(2)	22(1)
C(8)	2398(2)	1747(2)	7487(2)	18(1)
C(9)	3229(2)	5977(2)	5693(2)	20(1)
C(10)	2842(2)	5668(2)	4614(2)	27(1)
C(11)	2945(2)	7356(2)	5816(2)	28(1)
C(12)	4546(2)	5736(2)	6159(2)	28(1)
N(1)	2554(2)	5136(2)	6172(1)	17(1)
N(2)	1579(1)	2698(2)	6845(1)	13(1)
Si	2903(1)	4963(1)	7462(1)	17(1)
Zn	2086(1)	3273(1)	5658(1)	14(1)

Tabelle 8.50 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **118**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
Br(1)	18(1)	25(1)	15(1)	0(1)	2(1)	0(1)
Br(2)	27(1)	28(1)	34(1)	7(1)	19(1)	11(1)
C(1)	22(1)	24(2)	25(2)	2(1)	2(1)	−4(1)
C(2)	29(2)	30(2)	31(2)	−11(1)	11(1)	−6(1)
C(3)	18(1)	20(1)	15(1)	−1(1)	8(1)	2(1)
C(4)	14(1)	24(1)	16(1)	1(1)	6(1)	−3(1)
C(5)	20(1)	28(2)	21(1)	−3(1)	5(1)	−11(1)
C(6)	31(2)	17(1)	26(2)	−1(1)	12(1)	−8(1)
C(7)	25(1)	15(1)	25(1)	5(1)	10(1)	2(1)
C(8)	15(1)	18(1)	18(1)	5(1)	3(1)	2(1)
C(9)	18(1)	19(1)	22(1)	3(1)	7(1)	−4(1)
C(10)	35(2)	23(2)	27(2)	6(1)	14(1)	−3(1)

C(11)	28(2)	20(2)	35(2)	−1(1)	12(1)	−6(1)
C(12)	18(1)	35(2)	34(2)	5(1)	11(1)	−2(1)
N(1)	14(1)	19(1)	19(1)	−1(1)	6(1)	−4(1)
N(2)	10(1)	14(1)	12(1)	−1(1)	2(1)	−1(1)
Si	17(1)	18(1)	16(1)	−3(1)	5(1)	−2(1)
Zn	14(1)	17(1)	13(1)	−1(1)	5(1)	0(1)

Tabelle 8.51 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **118**.

	x	y	z	U(eq)
H(1A)	4537	3636	7637	38
H(1B)	4397	3863	8679	38
H(1C)	4980	4924	8209	38
H(2A)	3418	6969	8175	44
H(2B)	2703	6207	8742	44
H(2C)	2011	6850	7714	44
H(3A)	1720	3654	8098	20
H(3B)	894	4349	7138	20
H(4A)	−202	2816	6117	21
H(4B)	116	2148	7159	21
H(5A)	380	1013	5465	28
H(5B)	−625	656	5912	28
H(6A)	809	−159	7331	29
H(6B)	954	−837	6394	29
H(7A)	2824	−132	7490	26
H(7B)	2522	504	6437	26
H(8A)	2232	1680	8107	21
H(8B)	3222	2043	7646	21
H(10A)	3038	4793	4529	41
H(10B)	3250	6223	4295	41
H(10C)	1987	5790	4320	41
H(11A)	2090	7489	5533	41
H(11B)	3349	7893	5481	41
H(11C)	3214	7569	6511	41
H(12A)	4815	6038	6835	42
H(12B)	4973	6182	5792	42
H(12C)	4701	4833	6152	42
H(1N)	1857(18)	5440(20)	5961(15)	24(7)

8.2.8 Kristallstrukturen aus Kapitel 4.5.2

8.2.8.1 Verbindung 119

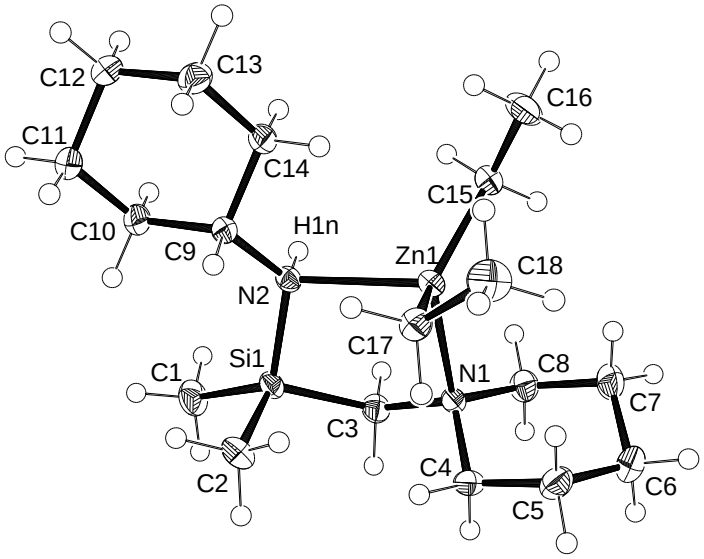


Abb. 8.18 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **119** im Kristall (Ortep−Darstellung).

Tabelle 8.52 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **119**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	10387(2)	397(2)	2981(2)	30(1)
C(2)	9679(2)	2547(2)	4452(1)	29(1)
C(3)	9269(2)	2493(2)	1857(1)	22(1)
C(4)	9250(2)	4787(2)	2527(1)	23(1)
C(5)	8367(2)	5826(2)	2360(1)	28(1)
C(6)	8042(2)	6063(2)	1175(2)	31(1)
C(7)	7100(2)	4670(2)	313(1)	30(1)
C(8)	8011(2)	3654(2)	533(1)	24(1)
C(9)	6078(2)	−174(2)	3188(1)	18(1)
C(10)	6639(2)	−1388(2)	3429(2)	27(1)
C(11)	5707(2)	−2226(2)	4096(2)	31(1)
C(12)	3827(2)	−2751(2)	3477(1)	26(1)
C(13)	3253(2)	−1541(2)	3263(1)	26(1)
C(14)	4189(2)	−685(2)	2604(1)	22(1)
C(15)	4043(2)	1365(2)	437(1)	21(1)
C(16)	2305(2)	1285(2)	430(1)	32(1)
C(17)	5807(2)	3340(2)	3435(1)	22(1)
C(18)	4349(2)	3855(2)	3282(2)	34(1)
N(1)	8285(1)	3427(1)	1691(1)	17(1)
N(2)	6920(2)	606(1)	2492(1)	17(1)
Si(1)	9072(1)	1507(1)	2983(1)	19(1)
Zn(1)	5826(1)	2330(1)	1967(1)	17(1)

Tabelle 8.53 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **118**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	24(1)	38(1)	37(1)	17(1)	11(1)	19(1)
C(2)	24(1)	33(1)	21(1)	5(1)	−1(1)	8(1)
C(3)	17(1)	26(1)	26(1)	10(1)	10(1)	9(1)

C(4)	19(1)	21(1)	22(1)	4(1)	3(1)	2(1)
C(5)	32(1)	19(1)	29(1)	5(1)	10(1)	6(1)
C(6)	36(1)	24(1)	36(1)	14(1)	12(1)	12(1)
C(7)	35(1)	31(1)	24(1)	13(1)	6(1)	13(1)
C(8)	28(1)	27(1)	20(1)	8(1)	9(1)	10(1)
C(9)	18(1)	18(1)	16(1)	5(1)	4(1)	6(1)
C(10)	21(1)	26(1)	35(1)	15(1)	6(1)	10(1)
C(11)	26(1)	27(1)	37(1)	18(1)	4(1)	7(1)
C(12)	24(1)	20(1)	31(1)	9(1)	7(1)	4(1)
C(13)	22(1)	24(1)	32(1)	10(1)	12(1)	7(1)
C(14)	18(1)	24(1)	26(1)	9(1)	7(1)	9(1)
C(15)	20(1)	24(1)	19(1)	6(1)	4(1)	9(1)
C(16)	18(1)	48(1)	28(1)	13(1)	2(1)	9(1)
C(17)	24(1)	22(1)	21(1)	5(1)	10(1)	8(1)
C(18)	34(1)	32(1)	40(1)	1(1)	15(1)	16(1)
N(1)	15(1)	19(1)	17(1)	6(1)	4(1)	6(1)
N(2)	17(1)	19(1)	14(1)	4(1)	4(1)	6(1)
Si(1)	15(1)	23(1)	20(1)	8(1)	4(1)	8(1)
Zn(1)	15(1)	20(1)	16(1)	4(1)	4(1)	6(1)

Tabelle 8.54 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **119**.

	x	y	z	U(eq)
H(1A)	10426	−56	3618	45
H(1B)	11523	980	3062	45
H(1C)	9903	−317	2262	45
H(2A)	8914	3056	4480	43
H(2B)	10824	3213	4683	43
H(2C)	9622	1922	4971	43
H(3A)	10464	3061	2050	26
H(3B)	8927	1810	1125	26
H(4A)	10362	5169	2450	27
H(4B)	9423	4643	3307	27
H(5A)	7290	5478	2494	33
H(5B)	9061	6724	2923	33
H(6A)	9117	6523	1067	37
H(6B)	7375	6681	1064	37
H(7A)	5967	4274	357	36
H(7B)	6974	4811	−464	36
H(8A)	7352	2750	−29	29
H(8B)	9105	4018	426	29
H(9)	6364	484	3934	22
H(10A)	7853	−1026	3867	32
H(10B)	6456	−2011	2698	32
H(11A)	5977	−1632	4860	37
H(11B)	6075	−3030	4201	37
H(12A)	3543	−3411	2742	32
H(12B)	3242	−3255	3942	32
H(13A)	3438	−933	4001	31
H(13B)	2039	−1902	2826	31
H(14A)	3891	−1262	1830	26
H(14B)	3833	130	2525	26
H(15A)	4317	1872	−135	26
H(15B)	4039	407	211	26
H(16A)	2024	783	994	49
H(16B)	1486	788	−328	49
H(16C)	2285	2231	619	49
H(17A)	5757	2706	3957	27
H(17B)	6865	4147	3795	27
H(18A)	4416	4515	2792	51
H(18B)	4392	4324	4026	51

H(18C)	3296	3061	2929	51
H(1N)	6620(20)	120(20)	1905(16)	25(5)

8.2.8.2 Verbindung 120

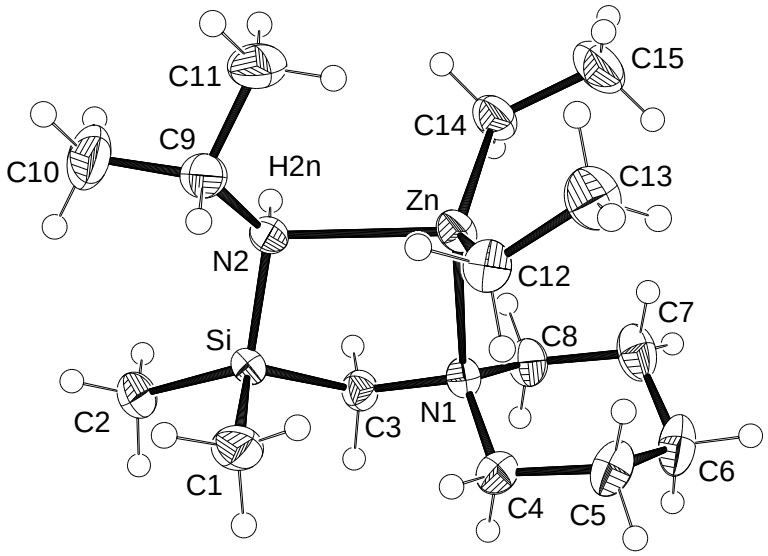


Abb. 8.19 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **120** im Kristall (Ortep−Darstellung).

Tabelle 8.55 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **120**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	3198(2)	−1268(2)	3767(1)	41(1)
C(2)	3171(2)	−3137(2)	1240(2)	44(1)
C(3)	4078(2)	−93(1)	1609(1)	29(1)
C(4)	5217(2)	1914(1)	3320(1)	33(1)
C(5)	5341(2)	3452(2)	3954(1)	42(1)
C(6)	5845(2)	4318(2)	3135(2)	47(1)
C(7)	4695(2)	3748(2)	1994(2)	45(1)
C(8)	4609(2)	2206(2)	1414(1)	35(1)
C(9)	−554(2)	−1783(2)	2425(1)	34(1)
C(10)	−1115(2)	−3329(2)	1770(2)	58(1)
C(11)	−1947(2)	−1064(2)	2389(2)	48(1)
C(12)	1249(2)	1913(2)	4375(1)	34(1)
C(13)	514(2)	3192(2)	4806(2)	46(1)
C(14)	335(2)	1763(2)	1233(1)	38(1)
C(15)	−101(3)	3175(2)	1540(2)	57(1)
N(1)	4066(1)	1385(1)	2217(1)	26(1)
N(2)	862(1)	−1127(1)	1938(1)	26(1)
Si	2793(1)	−1432(1)	2166(1)	27(1)
Zn	1401(1)	1368(1)	2610(1)	28(1)

Tabelle 8.56 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **120**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	41(1)	46(1)	39(1)	23(1)	−6(1)	5(1)
C(2)	42(1)	27(1)	63(1)	10(1)	2(1)	14(1)
C(3)	31(1)	24(1)	30(1)	6(1)	5(1)	8(1)
C(4)	32(1)	31(1)	32(1)	7(1)	0(1)	4(1)
C(5)	45(1)	32(1)	38(1)	2(1)	5(1)	−2(1)
C(6)	51(1)	25(1)	56(1)	5(1)	19(1)	0(1)

C(7)	55(1)	30(1)	55(1)	21(1)	20(1)	11(1)
C(8)	42(1)	31(1)	33(1)	14(1)	11(1)	7(1)
C(9)	31(1)	38(1)	36(1)	18(1)	5(1)	7(1)
C(10)	52(1)	35(1)	83(1)	21(1)	19(1)	−2(1)
C(11)	29(1)	56(1)	62(1)	22(1)	7(1)	11(1)
C(12)	38(1)	34(1)	30(1)	11(1)	8(1)	7(1)
C(13)	57(1)	45(1)	38(1)	7(1)	13(1)	19(1)
C(14)	46(1)	36(1)	37(1)	14(1)	−2(1)	17(1)
C(15)	66(1)	48(1)	65(1)	21(1)	−6(1)	29(1)
N(1)	31(1)	22(1)	26(1)	8(1)	4(1)	6(1)
N(2)	27(1)	27(1)	25(1)	11(1)	0(1)	7(1)
Si	27(1)	22(1)	32(1)	10(1)	−1(1)	7(1)
Zn	35(1)	28(1)	26(1)	10(1)	4(1)	12(1)

Tabelle 8.57 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **120**.

	x	y	z	U(eq)
H(1A)	2892	−428	4260	61
H(1B)	4355	−1202	3961	61
H(1C)	2559	−2087	3922	61
H(2A)	2493	−3896	1455	66
H(2B)	4318	−3147	1386	66
H(2C)	2900	−3261	395	66
H(3A)	5214	−198	1672	35
H(3B)	3719	−308	752	35
H(4A)	6304	1768	3116	40
H(4B)	4855	1377	3865	40
H(5A)	6147	3768	4667	50
H(5B)	4278	3592	4221	50
H(6A)	5815	5302	3536	56
H(6B)	6968	4282	2949	56
H(7A)	5070	4260	1434	54
H(7B)	3598	3890	2173	54
H(8A)	3847	1859	675	42
H(8B)	5694	2073	1194	42
H(9)	−220	−1666	3278	40
H(10A)	−1409	−3472	924	87
H(10B)	−2061	−3718	2109	87
H(10C)	−236	−3797	1853	87
H(11A)	−1581	−70	2830	72
H(11B)	−2848	−1477	2754	72
H(11C)	−2310	−1180	1559	72
H(12A)	571	1123	4567	41
H(12B)	2347	2116	4803	41
H(13A)	1191	3979	4627	69
H(13B)	464	3428	5667	69
H(13C)	−583	2987	4398	69
H(14A)	1073	1696	603	46
H(14B)	−667	1032	901	46
H(15A)	−858	3245	2147	85
H(15B)	−611	3282	822	85
H(15C)	886	3910	1848	85
H(2N)	590(20)	−1224(17)	1263(16)	30(4)

8.2.8.3 Verbindung 121

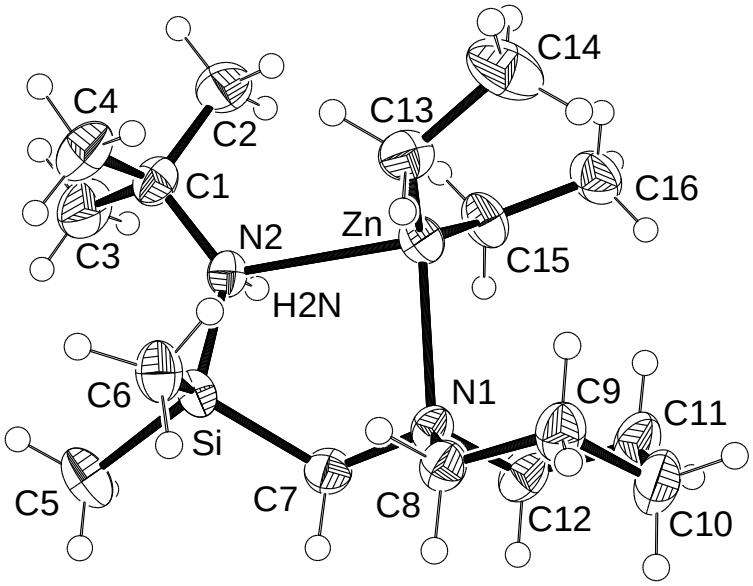


Abb. 8.20 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **121** im Kristall (Ortep−Darstellung).

Tabelle 8.58 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **121**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	3283(1)	11256(2)	596(1)	37(1)
C(2)	2986(2)	10762(2)	−326(1)	50(1)
C(3)	2913(2)	12631(2)	571(2)	58(1)
C(4)	4582(2)	11157(2)	1019(1)	53(1)
C(5)	2869(2)	11807(2)	2816(1)	51(1)
C(6)	4408(1)	9625(2)	2728(1)	40(1)
C(7)	1708(1)	9330(1)	2277(1)	35(1)
C(8)	2451(1)	7218(2)	2592(1)	34(1)
C(9)	2375(2)	5848(2)	2328(1)	42(1)
C(10)	1144(2)	5366(2)	2159(1)	51(1)
C(11)	333(2)	6200(2)	1488(1)	51(1)
C(12)	451(1)	7558(2)	1771(1)	42(1)
C(13)	3708(1)	7393(2)	815(1)	39(1)
C(14)	3687(2)	6303(2)	201(1)	64(1)
C(15)	675(2)	8471(2)	−254(1)	42(1)
C(16)	195(2)	7334(2)	−804(1)	49(1)
N(1)	1655(1)	8029(1)	1937(1)	31(1)
N(2)	2656(1)	10486(1)	1091(1)	30(1)
Si	2961(1)	10339(1)	2209(1)	30(1)
Zn	2169(1)	8196(1)	668(1)	33(1)

Tabelle 8.59 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **121**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	38(1)	31(1)	45(1)	4(1)	14(1)	−2(1)
C(2)	63(1)	49(1)	42(1)	9(1)	20(1)	−3(1)
C(3)	73(1)	31(1)	77(1)	9(1)	33(1)	−1(1)
C(4)	38(1)	62(1)	62(1)	9(1)	17(1)	−9(1)
C(5)	59(1)	41(1)	47(1)	−16(1)	7(1)	3(1)
C(6)	32(1)	38(1)	43(1)	−2(1)	−1(1)	−3(1)

C(7)	33(1)	34(1)	38(1)	−1(1)	13(1)	2(1)
C(8)	32(1)	35(1)	31(1)	3(1)	4(1)	−4(1)
C(9)	46(1)	33(1)	43(1)	6(1)	8(1)	−3(1)
C(10)	55(1)	41(1)	52(1)	6(1)	9(1)	−18(1)
C(11)	43(1)	55(1)	49(1)	3(1)	2(1)	−22(1)
C(12)	28(1)	50(1)	46(1)	7(1)	7(1)	−7(1)
C(13)	42(1)	34(1)	43(1)	5(1)	17(1)	7(1)
C(14)	85(2)	54(1)	56(1)	−4(1)	26(1)	28(1)
C(15)	44(1)	37(1)	35(1)	−5(1)	−2(1)	4(1)
C(16)	48(1)	57(1)	36(1)	−11(1)	3(1)	−6(1)
N(1)	26(1)	32(1)	32(1)	1(1)	7(1)	−3(1)
N(2)	27(1)	27(1)	34(1)	0(1)	6(1)	−1(1)
Si	30(1)	27(1)	31(1)	−6(1)	5(1)	−1(1)
Zn	32(1)	32(1)	31(1)	−1(1)	4(1)	3(1)

Tabelle 8.60 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **121**.

	x	y	z	U(eq)
H(1N)	1972(16)	10604(16)	874(11)	34(5)
H(2A)	3233	9889	−318	75
H(2B)	3382	11266	−656	75
H(2C)	2151	10815	−593	75
H(3A)	2084	12697	282	87
H(3B)	3339	13123	256	87
H(3C)	3079	12951	1161	87
H(4A)	4776	11508	1601	80
H(4B)	4989	11623	676	80
H(4C)	4815	10276	1050	80
H(5A)	3470	12391	2769	76
H(5B)	2979	11605	3424	76
H(5C)	2110	12192	2574	76
H(6A)	4550	8953	2361	60
H(6B)	4424	9283	3291	60
H(6C)	5006	10267	2802	60
H(7A)	1723	9281	2890	41
H(7B)	986	9763	1964	41
H(8A)	2265	7297	3145	41
H(8B)	3251	7514	2685	41
H(9A)	2902	5347	2791	50
H(9B)	2621	5753	1801	50
H(10A)	1092	4494	1948	61
H(10B)	922	5379	2700	61
H(11A)	513	6119	933	61
H(11B)	−472	5922	1399	61
H(12A)	−74	8077	1319	51
H(12B)	214	7645	2303	51
H(13A)	4251	8035	727	46
H(13B)	4006	7086	1415	46
H(14A)	3206	5629	318	96
H(14B)	4473	5994	287	96
H(14C)	3368	6589	−395	96
H(15A)	93	8761	22	50
H(15B)	786	9149	−637	50
H(16A)	794	6976	−1029	73
H(16B)	−466	7586	−1285	73
H(16C)	−51	6709	−453	73

8.2.8.4 Verbindung 122

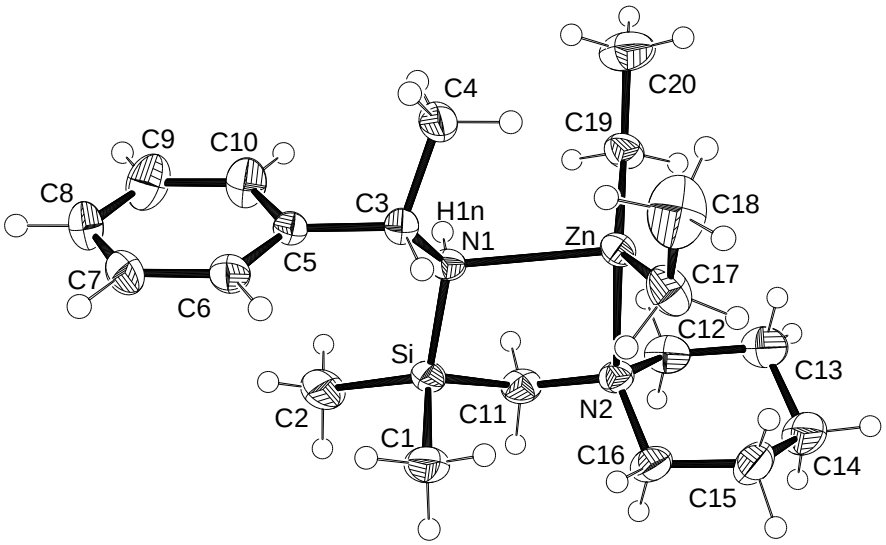


Abb. 8.21 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **122** im Kristall (Ortep−Darstellung).

Tabelle 8.61 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **122**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	−766(3)	1901(2)	9737(3)	39(1)
C(2)	−1320(3)	4062(2)	10818(3)	50(1)
C(3)	2865(2)	3094(2)	10792(2)	26(1)
C(4)	4466(2)	3465(3)	10678(2)	36(1)
C(5)	2898(3)	3221(2)	12168(2)	24(1)
C(6)	2953(3)	2326(2)	12935(3)	31(1)
C(7)	3043(4)	2437(2)	14203(3)	38(1)
C(8)	3080(2)	3451(3)	14724(2)	41(1)
C(9)	3049(4)	4342(2)	13980(3)	48(1)
C(10)	2965(4)	4234(2)	12714(3)	39(1)
C(11)	−1636(3)	4040(2)	8034(2)	34(1)
C(12)	−1746(3)	4535(2)	5886(3)	37(1)
C(13)	−1440(3)	4209(2)	4680(3)	44(1)
C(14)	−2333(3)	3169(2)	4115(3)	48(1)
C(15)	−1872(4)	2296(2)	5152(3)	44(1)
C(16)	−2110(3)	2667(2)	6371(3)	36(1)
C(17)	2197(4)	2001(2)	7469(3)	40(1)
C(18)	3978(5)	1675(3)	7942(4)	63(1)
C(19)	2225(4)	5090(2)	7475(3)	33(1)
C(20)	3997(4)	5380(3)	7862(4)	53(1)
N(1)	1487(2)	3666(2)	9826(2)	24(1)
N(2)	−1225(2)	3674(2)	6898(2)	27(1)
Si	−542(1)	3391(1)	9630(1)	27(1)
Zn	1603(1)	3543(1)	7662(1)	25(1)

Tabelle 8.62 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **122**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	37(1)	38(1)	40(2)	2(1)	11(1)	−12(1)
C(2)	39(1)	66(2)	56(2)	−15(2)	31(2)	−10(1)
C(3)	26(1)	30(1)	23(1)	−1(1)	9(1)	−1(1)
C(4)	22(1)	59(2)	26(1)	4(2)	7(1)	1(2)

C(5)	21(1)	29(1)	22(1)	0(1)	8(1)	−1(1)
C(6)	36(1)	28(1)	31(2)	−2(1)	13(1)	−7(1)
C(7)	49(2)	37(2)	29(2)	7(1)	15(1)	−10(1)
C(8)	48(1)	54(2)	26(1)	0(2)	18(1)	−2(2)
C(9)	65(2)	38(2)	40(2)	−16(1)	16(2)	6(1)
C(10)	58(2)	26(2)	34(2)	2(1)	15(2)	2(1)
C(11)	21(1)	38(1)	40(2)	−5(1)	9(1)	1(1)
C(12)	29(1)	32(1)	42(2)	13(1)	3(1)	6(1)
C(13)	43(2)	48(2)	33(2)	20(1)	1(1)	−4(1)
C(14)	48(2)	59(2)	28(2)	7(1)	1(1)	−11(1)
C(15)	60(2)	38(2)	29(2)	−4(1)	7(2)	−15(1)
C(16)	38(2)	34(1)	29(2)	3(1)	2(1)	−9(1)
C(17)	47(2)	34(2)	48(3)	3(2)	29(2)	9(2)
C(18)	62(3)	62(2)	61(3)	2(2)	18(2)	35(2)
C(19)	36(2)	26(2)	40(2)	2(1)	18(2)	−5(1)
C(20)	45(2)	49(2)	58(3)	9(2)	6(2)	−14(2)
N(1)	24(1)	22(1)	27(1)	1(1)	8(1)	−2(1)
N(2)	24(1)	28(1)	25(1)	2(1)	4(1)	−2(1)
Si	22(1)	32(1)	30(1)	−4(1)	13(1)	−4(1)
Zn	25(1)	24(1)	27(1)	3(1)	11(1)	1(1)

Tabelle 8.63 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **122**.

	x	y	z	U(eq)
H(1N)	1620(30)	4250(17)	9870(20)	16(6)
H(1A)	−256	1535	9182	59
H(1B)	−1927	1713	9451	59
H(1C)	−234	1665	10635	59
H(2A)	−740	3774	11685	75
H(2B)	−2490	3916	10583	75
H(2C)	−1139	4848	10811	75
H(3)	2743	2301	10579	32
H(4A)	4436	3355	9787	54
H(4B)	5364	3041	11271	54
H(4C)	4633	4238	10900	54
H(6)	2928	1618	12582	37
H(7)	3079	1810	14716	45
H(8)	3126	3533	15594	49
H(9)	3087	5047	14340	58
H(10)	2954	4865	12212	47
H(11A)	−2820	3926	7834	40
H(11B)	−1436	4834	8132	40
H(12A)	−1144	5215	6228	44
H(12B)	−2924	4682	5675	44
H(13A)	−254	4103	4879	53
H(13B)	−1804	4800	4032	53
H(14A)	−2030	2934	3368	58
H(14B)	−3526	3295	3811	58
H(15A)	−2547	1641	4821	53
H(15B)	−715	2093	5346	53
H(16A)	−3289	2784	6195	43
H(16B)	−1738	2085	7029	43
H(17A)	1637	1538	7924	48
H(17B)	1732	1815	6538	48
H(18A)	4608	2217	7660	94
H(18B)	4093	963	7584	94
H(18C)	4386	1636	8890	94
H(19A)	1697	5297	6555	40
H(19B)	1742	5552	7985	40
H(20A)	4547	5206	8779	80

H(20B)	4105	6159	7724	80
H(20C)	4497	4963	7337	80

8.2.8.5 Verbindung 123

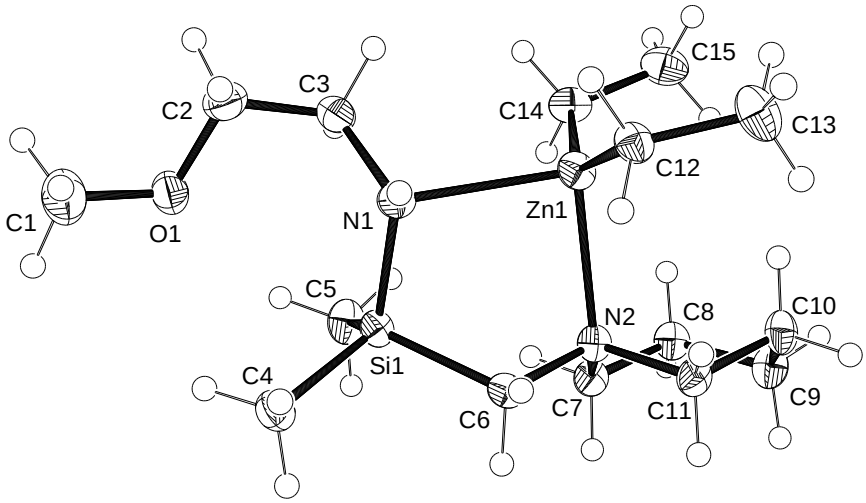


Abb. 8.22 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **123** im Kristall (Ortep−Darstellung).

Tabelle 8.64 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **123**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	2564(6)	9761(4)	4205(4)	45(1)
C(2)	625(5)	7601(4)	3684(3)	32(1)
C(3)	713(5)	6250(3)	3442(3)	31(1)
C(4)	5509(5)	7980(3)	2495(3)	27(1)
C(5)	5004(5)	6475(4)	4278(3)	30(1)
C(6)	4863(4)	5147(3)	1637(2)	21(1)
C(7)	5309(5)	3562(3)	2547(3)	24(1)
C(8)	4692(5)	2181(3)	2601(3)	25(1)
C(9)	4607(5)	1235(3)	1444(3)	28(1)
C(10)	3400(5)	1491(3)	547(3)	27(1)
C(11)	4132(5)	2897(3)	546(3)	23(1)
C(12)	−124(5)	3389(3)	291(3)	24(1)
C(13)	−962(5)	2009(3)	−486(3)	35(1)
C(14)	328(5)	2943(4)	3232(3)	28(1)
C(15)	−588(5)	1483(4)	2970(3)	36(1)
N(1)	1866(4)	5890(3)	2548(2)	23(1)
N(2)	4102(4)	3785(3)	1666(2)	20(1)
O(1)	2448(3)	8473(2)	4126(2)	30(1)
Si(1)	4302(1)	6414(1)	2779(1)	20(1)
Zn(1)	1023(1)	3562(1)	1873(1)	24(1)

Tabelle 8.65 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **123**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	49(3)	31(2)	51(3)	10(2)	2(2)	12(2)
C(2)	26(2)	36(2)	32(2)	5(2)	3(2)	12(2)
C(3)	25(2)	27(2)	33(2)	2(2)	7(2)	2(2)
C(4)	27(2)	25(2)	25(2)	4(2)	2(1)	3(2)
C(5)	37(2)	31(2)	18(2)	2(2)	−4(2)	11(2)

C(6)	20(2)	24(2)	16(2)	7(1)	0(1)	4(1)
C(7)	23(2)	28(2)	18(2)	4(1)	−3(1)	9(2)
C(8)	28(2)	29(2)	19(2)	8(2)	−2(1)	10(2)
C(9)	35(2)	27(2)	26(2)	8(2)	−1(2)	15(2)
C(10)	32(2)	24(2)	19(2)	0(1)	−4(1)	9(2)
C(11)	26(2)	26(2)	14(2)	3(1)	1(1)	8(2)
C(12)	23(2)	24(2)	24(2)	7(1)	−3(1)	7(2)
C(13)	39(2)	35(2)	24(2)	5(2)	−13(2)	4(2)
C(14)	25(2)	39(2)	22(2)	12(2)	3(1)	9(2)
C(15)	28(2)	43(2)	39(2)	18(2)	0(2)	10(2)
N(1)	22(2)	28(2)	18(1)	4(1)	1(1)	7(1)
N(2)	24(2)	23(2)	13(1)	6(1)	0(1)	8(1)
O(1)	31(1)	23(1)	34(1)	5(1)	1(1)	7(1)
Si(1)	22(1)	22(1)	12(1)	3(1)	−2(1)	4(1)
Zn(1)	24(1)	28(1)	16(1)	5(1)	−2(1)	5(1)

Tabelle 8.66 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **123**.

	x	**y**	**z**	**U(eq)**
H(1A)	2080	9814	3465	67
H(1B)	3873	10310	4417	67
H(1C)	1819	10062	4788	67
H(2A)	168	7752	2973	38
H(2B)	−250	7739	4246	38
H(3A)	1214	6133	4158	37
H(3B)	−577	5642	3210	37
H(4A)	4899	8016	1782	41
H(4B)	6823	8046	2426	41
H(4C)	5442	8702	3127	41
H(5A)	4778	7225	4802	45
H(5B)	6338	6558	4388	45
H(5C)	4267	5676	4434	45
H(6A)	4395	5200	885	25
H(6B)	6242	5369	1686	25
H(7A)	5287	4146	3304	28
H(7B)	6615	3787	2375	28
H(8A)	3441	1982	2858	30
H(8B)	5579	2075	3168	30
H(9A)	4069	332	1480	34
H(9B)	5886	1344	1234	34
H(10A)	3413	918	−217	32
H(10B)	2091	1291	715	32
H(11A)	5430	3087	359	27
H(11B)	3353	3046	−52	27
H(12A)	−1118	3811	365	29
H(12B)	851	3874	−85	29
H(13A)	43	1632	−688	53
H(13B)	−1650	2022	−1183	53
H(13C)	−1819	1483	−88	53
H(14A)	1472	3204	3786	34
H(14B)	−539	3387	3603	34
H(15A)	−1724	1209	2421	54
H(15B)	−916	1267	3677	54
H(15C)	285	1031	2644	54
H(1N)	1480(50)	5990(30)	1960(30)	29(11)

8.2.8.6 Verbindung 124

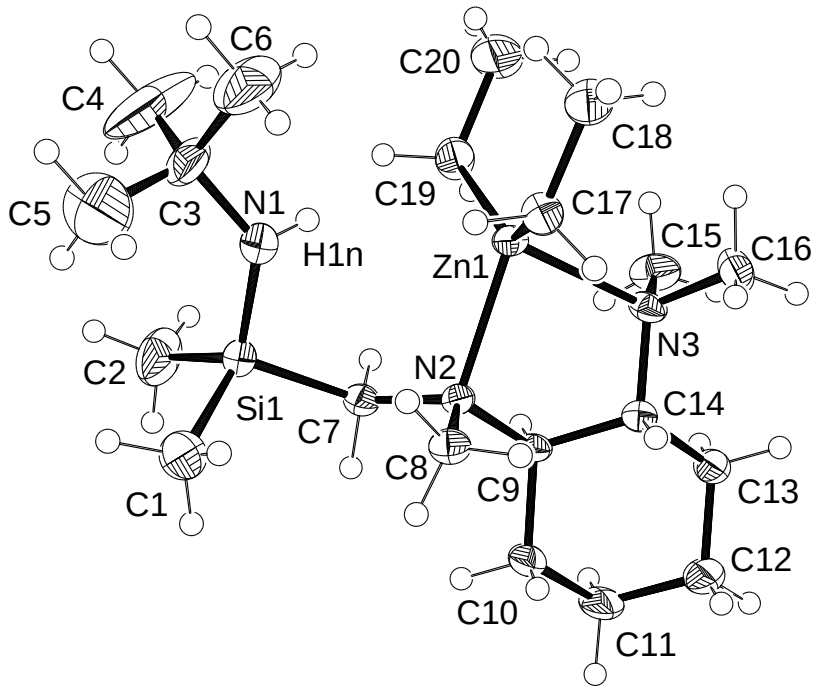


Abb. 8.23 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **124** im Kristall (Ortep–Darstellung).

Tabelle 8.67 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **124**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	2804(2)	4546(2)	8051(2)	61(1)
C(2)	3660(2)	2784(3)	9457(2)	59(1)
C(3)	995(2)	2894(3)	8870(2)	47(1)
C(4)	1286(3)	2250(6)	9701(2)	122(2)
C(5)	1050(3)	4350(4)	8938(4)	155(3)
C(6)	−8(2)	2489(4)	8422(2)	73(1)
C(7)	3196(1)	1546(2)	7870(1)	24(1)
C(8)	2225(2)	2234(2)	6541(1)	25(1)
C(9)	3203(1)	208(2)	6704(1)	22(1)
C(10)	3917(2)	957(2)	6382(1)	33(1)
C(11)	4503(2)	37(3)	6032(2)	43(1)
C(12)	3847(2)	−769(2)	5350(2)	42(1)
C(13)	3167(2)	−1557(2)	5669(1)	31(1)
C(14)	2579(1)	−681(2)	6045(1)	22(1)
C(15)	2332(2)	−2623(2)	6821(2)	39(1)
C(16)	1072(2)	−1862(2)	5688(2)	38(1)
C(17)	187(1)	742(2)	6399(1)	27(1)
C(18)	−728(1)	−20(3)	6344(1)	37(1)
C(19)	1689(2)	−1030(2)	8218(1)	36(1)
C(20)	892(2)	−1965(3)	8246(2)	60(1)
N(1)	1626(1)	2432(2)	8418(1)	33(1)
N(2)	2623(1)	1095(2)	7059(1)	20(1)
N(3)	1904(1)	−1446(2)	6354(1)	24(1)
Si(1)	2752(1)	2845(1)	8451(1)	29(1)
Zn(1)	1375(1)	−99(1)	7137(1)	22(1)

Tabelle 8.68 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **124**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	97(2)	30(2)	75(2)	−11(1)	56(2)	−13(1)
C(2)	41(2)	92(2)	40(2)	−25(2)	6(1)	−6(2)
C(3)	35(1)	68(2)	45(2)	−21(1)	22(1)	−1(1)
C(4)	67(2)	265(6)	48(2)	0(3)	37(2)	17(3)
C(5)	146(4)	88(3)	299(8)	−98(4)	169(5)	−31(3)
C(6)	41(2)	120(3)	64(2)	−15(2)	26(1)	5(2)
C(7)	20(1)	27(1)	26(1)	−1(1)	8(1)	−3(1)
C(8)	25(1)	23(1)	27(1)	6(1)	9(1)	3(1)
C(9)	20(1)	18(1)	30(1)	1(1)	13(1)	−1(1)
C(10)	31(1)	32(1)	43(1)	−10(1)	21(1)	−12(1)
C(11)	37(1)	43(1)	64(2)	−15(2)	36(1)	−15(1)
C(12)	49(2)	40(1)	53(2)	−15(1)	37(1)	−12(1)
C(13)	32(1)	27(1)	40(1)	−9(1)	21(1)	−5(1)
C(14)	23(1)	21(1)	23(1)	2(1)	8(1)	−1(1)
C(15)	47(2)	23(1)	59(2)	9(1)	32(1)	6(1)
C(16)	26(1)	39(1)	50(2)	−22(1)	14(1)	−8(1)
C(17)	21(1)	27(1)	33(1)	−2(1)	7(1)	5(1)
C(18)	22(1)	45(1)	44(1)	−6(2)	12(1)	5(1)
C(19)	52(2)	31(1)	26(1)	2(1)	12(1)	−8(1)
C(20)	85(2)	62(2)	41(2)	5(1)	30(2)	−31(2)
N(1)	35(1)	34(1)	34(1)	−8(1)	15(1)	−5(1)
N(2)	20(1)	20(1)	21(1)	1(1)	8(1)	0(1)
N(3)	18(1)	20(1)	35(1)	0(1)	11(1)	−1(1)
Si(1)	31(1)	29(1)	28(1)	−7(1)	13(1)	−5(1)
Zn(1)	20(1)	24(1)	22(1)	2(1)	8(1)	−1(1)

Tabelle 8.69 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **124**.

	x	y	z	U(eq)
H(1A)	2270	4671	7557	92
H(1B)	3407	4662	7931	92
H(1C)	2762	5199	8454	92
H(2A)	3472	3379	9825	89
H(2B)	4279	3062	9411	89
H(2C)	3709	1879	9666	89
H(4A)	1231	1287	9641	183
H(4B)	868	2564	10004	183
H(4C)	1948	2485	9991	183
H(5A)	1708	4613	9221	232
H(5B)	630	4659	9241	232
H(5C)	849	4742	8398	232
H(6A)	−194	2872	7879	110
H(6B)	−440	2807	8711	110
H(6C)	−44	1522	8382	110
H(7A)	3808	1875	7820	29
H(7B)	3347	750	8216	29
H(8A)	1744	2670	6736	37
H(8B)	1929	1930	5986	37
H(8C)	2737	2861	6555	37
H(9)	3582	−383	7147	26
H(10A)	3565	1586	5960	40
H(10B)	4352	1476	6826	40
H(11A)	4885	−563	6458	52
H(11B)	4947	561	5827	52
H(12A)	3483	−172	4913	51
H(12B)	4229	−1375	5125	51
H(13A)	3536	−2193	6078	37

H(13B)	2732	−2069	5222	37
H(14)	2188	−89	5609	26
H(15A)	2471	−3281	6459	59
H(15B)	1886	−2999	7078	59
H(15C)	2925	−2374	7235	59
H(16A)	796	−1093	5356	57
H(16B)	595	−2255	5906	57
H(16C)	1270	−2517	5356	57
H(17A)	129	1650	6592	33
H(17B)	253	814	5852	33
H(18A)	−675	−925	6162	56
H(18B)	−1272	421	5959	56
H(18C)	−824	−43	6876	56
H(19A)	2289	−1536	8312	44
H(19B)	1789	−364	8652	44
H(20A)	317	−1452	8216	90
H(20B)	1088	−2466	8752	90
H(20C)	756	−2578	7790	90
H(1N)	1500(16)	1740(20)	8291(13)	17(6)

8.2.9 Kristallstrukturen aus Kapitel 4.5.3

8.2.9.1 Verbindung 125

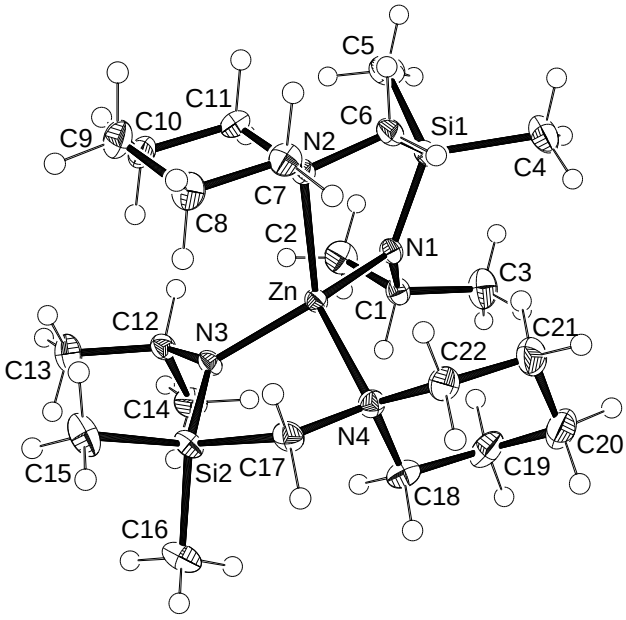


Abb. 8.24 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **125** im Kristall (Ortep−Darstellung).

Tabelle 8.70 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **125**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	7326(1)	−555(2)	7456(1)	19(1)
C(2)	7228(1)	−33(2)	6583(1)	29(1)
C(3)	7565(1)	−1964(2)	7464(1)	31(1)
C(4)	9582(1)	−1274(2)	8590(1)	32(1)
C(5)	9426(1)	585(2)	7226(1)	32(1)
C(6)	9319(1)	1437(2)	8997(1)	21(1)

C(7)	9029(1)	3326(2)	9724(1)	22(1)
C(8)	8535(1)	4558(2)	9728(1)	25(1)
C(9)	8596(1)	5364(2)	8980(1)	28(1)
C(10)	8298(1)	4569(2)	8210(1)	23(1)
C(11)	8794(1)	3331(2)	8239(1)	20(1)
C(12)	6208(1)	2964(2)	7444(1)	18(1)
C(13)	5866(1)	4319(2)	7282(1)	30(1)
C(14)	5535(1)	2017(2)	7030(1)	26(1)
C(15)	6003(1)	4830(2)	9381(1)	30(1)
C(16)	4844(1)	2626(2)	8976(1)	32(1)
C(17)	6657(1)	2259(2)	10011(1)	21(1)
C(18)	6364(1)	56(2)	9611(1)	24(1)
C(19)	6716(1)	−1250(2)	9465(1)	31(1)
C(20)	7364(1)	−1699(2)	10200(1)	36(1)
C(21)	8049(1)	−695(2)	10420(1)	33(1)
C(22)	7667(1)	599(2)	10547(1)	24(1)
N(1)	7911(1)	197(1)	8064(1)	15(1)
N(2)	8736(1)	2548(1)	8972(1)	16(1)
N(3)	6500(1)	2682(1)	8322(1)	16(1)
N(4)	7048(1)	1035(1)	9816(1)	17(1)
Si(1)	8980(1)	196(1)	8167(1)	18(1)
Si(2)	5995(1)	3101(1)	9088(1)	19(1)
Zn	7459(1)	1550(1)	8655(1)	14(1)

Tabelle 8.71 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **125**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	**U22**	**U33**	**U23**	**U13**	**U12**
C(1)	20(1)	20(1)	16(1)	0(1)	2(1)	3(1)
C(2)	31(1)	37(1)	16(1)	0(1)	1(1)	2(1)
C(3)	40(1)	21(1)	30(1)	−7(1)	−3(1)	2(1)
C(4)	26(1)	27(1)	39(1)	−2(1)	−1(1)	8(1)
C(5)	30(1)	35(1)	36(1)	−2(1)	17(1)	3(1)
C(6)	14(1)	21(1)	26(1)	2(1)	1(1)	2(1)
C(7)	22(1)	23(1)	19(1)	−1(1)	−1(1)	−3(1)
C(8)	30(1)	21(1)	23(1)	−5(1)	3(1)	−2(1)
C(9)	35(1)	16(1)	32(1)	0(1)	7(1)	−1(1)
C(10)	25(1)	19(1)	24(1)	6(1)	2(1)	−3(1)
C(11)	22(1)	19(1)	20(1)	1(1)	6(1)	−5(1)
C(12)	16(1)	21(1)	17(1)	2(1)	2(1)	3(1)
C(13)	34(1)	25(1)	28(1)	5(1)	−1(1)	8(1)
C(14)	23(1)	33(1)	19(1)	−1(1)	0(1)	−1(1)
C(15)	30(1)	28(1)	30(1)	−7(1)	−2(1)	11(1)
C(16)	19(1)	40(1)	36(1)	−6(1)	8(1)	4(1)
C(17)	24(1)	22(1)	19(1)	−3(1)	8(1)	3(1)
C(18)	25(1)	27(1)	21(1)	1(1)	7(1)	−5(1)
C(19)	45(1)	21(1)	30(1)	2(1)	13(1)	−7(1)
C(20)	50(1)	25(1)	35(1)	10(1)	16(1)	5(1)
C(21)	33(1)	36(1)	30(1)	13(1)	8(1)	11(1)
C(22)	26(1)	29(1)	17(1)	7(1)	2(1)	2(1)
N(1)	16(1)	15(1)	14(1)	−1(1)	2(1)	2(1)
N(2)	14(1)	15(1)	17(1)	0(1)	1(1)	0(1)
N(3)	13(1)	19(1)	14(1)	1(1)	1(1)	4(1)
N(4)	20(1)	18(1)	15(1)	1(1)	4(1)	1(1)
Si(1)	16(1)	18(1)	22(1)	0(1)	5(1)	4(1)
Si(2)	16(1)	22(1)	19(1)	−4(1)	3(1)	4(1)
Zn	14(1)	15(1)	14(1)	1(1)	3(1)	2(1)

Tabelle 8.72 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **125**.

	x	**y**	**z**	**U(eq)**

H(1)	6752	−503	7611	22
H(2A)	7085	878	6581	43
H(2B)	6773	−497	6221	43
H(2C)	7765	−143	6387	43
H(3A)	8104	−2062	7273	47
H(3B)	7117	−2439	7100	47
H(3C)	7627	−2297	8025	47
H(4A)	9366	−1578	9071	47
H(4B)	10189	−1070	8751	47
H(4C)	9505	−1943	8168	47
H(5A)	9340	−143	6847	49
H(5B)	10037	764	7385	49
H(5C)	9135	1337	6954	49
H(6A)	9370	1016	9539	25
H(6B)	9890	1756	8951	25
H(7A)	9641	3529	9766	26
H(7B)	8970	2815	10213	26
H(8A)	8764	5046	10233	30
H(8B)	7930	4361	9730	30
H(9A)	9192	5643	9004	33
H(9B)	8234	6134	8968	33
H(10A)	7684	4376	8158	28
H(10B)	8373	5066	7721	28
H(11A)	8572	2829	7738	24
H(11B)	9399	3528	8241	24
H(12)	6712	2877	7172	22
H(13A)	5351	4422	7514	45
H(13B)	5730	4472	6688	45
H(13C)	6298	4933	7539	45
H(14A)	5746	1143	7140	39
H(14B)	5415	2169	6436	39
H(14C)	5012	2131	7248	39
H(15A)	6576	5180	9407	45
H(15B)	5841	4915	9920	45
H(15C)	5597	5300	8970	45
H(16A)	4499	3131	8537	47
H(16B)	4651	2784	9494	47
H(16C)	4782	1717	8838	47
H(17A)	7116	2843	10272	25
H(17B)	6289	2087	10416	25
H(18A)	5960	327	9112	28
H(18B)	6047	0	10068	28
H(19A)	6987	−1214	8976	37
H(19B)	6242	−1872	9352	37
H(20A)	7080	−1848	10673	43
H(20B)	7622	−2513	10067	43
H(21A)	8381	−632	9974	39
H(21B)	8444	−951	10929	39
H(22A)	7378	551	11023	29
H(22B)	8131	1236	10677	29

8.2.9.2 Verbindung 126

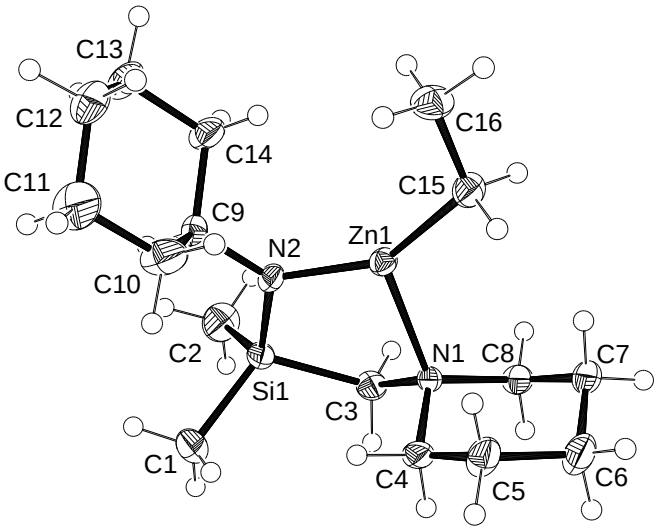


Abb. 8.25 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **126** im Kristall (Ortep−Darstellung).

Tabelle 8.73 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **126**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	15(2)	−257(2)	6730(2)	39(1)
C(2)	66(2)	1172(2)	8710(2)	42(1)
C(3)	1338(2)	1899(2)	6765(2)	25(1)
C(4)	2141(2)	1095(2)	5154(2)	28(1)
C(5)	3111(2)	930(2)	4488(2)	35(1)
C(6)	3600(2)	2018(2)	4177(2)	38(1)
C(7)	3765(2)	2701(2)	5211(2)	28(1)
C(8)	2779(2)	2808(2)	5859(2)	26(1)
C(9)	2050(2)	−893(2)	8639(2)	21(1)
C(10)	2315(2)	−1902(2)	7970(2)	41(1)
C(11)	2318(3)	−2931(2)	8674(2)	56(1)
C(12)	3055(2)	−2828(2)	9655(2)	36(1)
C(13)	2826(2)	−1831(2)	10327(2)	36(1)
C(14)	2797(2)	−804(2)	9614(2)	33(1)
C(15)	4775(2)	723(2)	7257(2)	28(1)
C(16)	5358(2)	−23(2)	8049(2)	34(1)
N(1)	2330(1)	1737(1)	6177(1)	19(1)
N(2)	2038(2)	87(1)	7950(2)	21(1)
Si(1)	892(1)	655(1)	7558(1)	22(1)
Zn(1)	3249(1)	678(1)	7325(1)	20(1)

Tabelle 8.74 Anisotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **126**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	33(2)	39(1)	45(2)	8(1)	−11(1)	−13(1)
C(2)	30(2)	51(2)	44(2)	6(1)	7(1)	5(1)
C(3)	22(1)	22(1)	30(1)	3(1)	−4(1)	3(1)
C(4)	42(2)	21(1)	20(1)	−1(1)	−8(1)	−10(1)
C(5)	55(2)	27(1)	21(1)	−5(1)	7(1)	−11(1)
C(6)	55(2)	31(1)	27(1)	5(1)	7(1)	−10(1)
C(7)	36(2)	20(1)	29(1)	8(1)	−4(1)	−6(1)
C(8)	35(2)	15(1)	27(1)	3(1)	−8(1)	−3(1)
C(9)	19(1)	20(1)	24(1)	3(1)	4(1)	0(1)

C(10)	66(2)	25(1)	32(2)	−6(1)	−14(1)	6(1)
C(11)	93(3)	17(1)	57(2)	−4(1)	−19(2)	−1(1)
C(12)	40(2)	25(1)	43(2)	9(1)	3(1)	12(1)
C(13)	54(2)	26(1)	27(1)	8(1)	−2(1)	2(1)
C(14)	55(2)	20(1)	24(1)	2(1)	−10(1)	−3(1)
C(15)	21(1)	33(1)	29(1)	6(1)	4(1)	3(1)
C(16)	26(2)	42(1)	34(2)	2(1)	−3(1)	9(1)
N(1)	22(1)	15(1)	20(1)	2(1)	−4(1)	−3(1)
N(2)	23(1)	19(1)	21(1)	5(1)	0(1)	0(1)
Si(1)	18(1)	24(1)	24(1)	3(1)	−2(1)	−1(1)
Zn(1)	19(1)	20(1)	20(1)	3(1)	0(1)	2(1)

Tabelle 8.75 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **126**.

	x	y	z	U(eq)
H(1A)	392	−541	6087	59
H(1B)	−595	157	6472	59
H(1C)	−213	−865	7196	59
H(2A)	−199	555	9140	62
H(2B)	−521	1587	8398	62
H(2C)	484	1645	9196	62
H(3A)	790	2102	6215	30
H(3B)	1419	2514	7291	30
H(4A)	1613	1473	4687	33
H(4B)	1853	374	5359	33
H(5A)	2937	518	3802	41
H(5B)	3619	494	4927	41
H(6A)	4277	1891	3811	45
H(6B)	3138	2409	3648	45
H(7A)	4310	2360	5685	34
H(7B)	4012	3435	4995	34
H(8A)	2924	3236	6542	31
H(8B)	2259	3215	5408	31
H(9)	1334	−993	8942	25
H(10A)	3012	−1807	7636	49
H(10B)	1801	−1984	7356	49
H(11A)	1605	−3072	8944	67
H(11B)	2530	−3559	8211	67
H(12A)	2992	−3482	10132	43
H(12B)	3781	−2792	9385	43
H(13A)	3368	−1748	10914	43
H(13B)	2146	−1923	10695	43
H(14A)	2590	−178	10082	40
H(14B)	3506	−657	9333	40
H(15A)	4983	539	6489	33
H(15B)	5003	1481	7405	33
H(16A)	5174	156	8816	50
H(16B)	6110	73	7952	50
H(16C)	5169	−782	7891	50

8.2.9.3 Verbindung 127

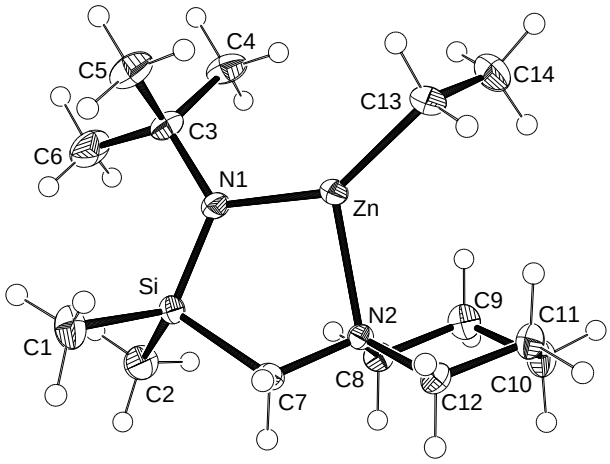


Abb. 8.26 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **127** im Kristall (Ortep−Darstellung der asymmetrischen Eiheit).

Tabelle 8.76 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **127**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	4435(2)	8943(2)	7783(2)	36(1)
C(2)	4682(2)	7338(2)	9726(1)	32(1)
C(3)	132(2)	6984(2)	8645(1)	23(1)
C(4)	−1436(2)	5783(2)	8910(1)	31(1)
C(5)	−455(2)	7776(2)	7779(2)	34(1)
C(6)	921(2)	8077(2)	9832(1)	40(1)
C(7)	4167(2)	5852(1)	7035(1)	18(1)
C(8)	3129(2)	3593(1)	7749(1)	20(1)
C(9)	1918(2)	2018(1)	7506(1)	25(1)
C(10)	2208(2)	1169(1)	6321(1)	27(1)
C(11)	2079(2)	1945(1)	5311(1)	24(1)
C(12)	3274(2)	3520(1)	5619(1)	19(1)
C(13)	−1526(2)	3415(2)	5699(1)	29(1)
C(14)	−2625(2)	2025(2)	6067(2)	41(1)
N(1)	1358(1)	6340(1)	8092(1)	20(1)
N(2)	2931(1)	4324(1)	6766(1)	15(1)
Si	3523(1)	7133(1)	8226(1)	19(1)
Zn	505(1)	4678(1)	6805(1)	18(1)

Tabelle 8.77 Anisotrope auslenkungsparameter (Å^2 x 10^3) für die Verbindung **127**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	38(1)	20(1)	46(1)	5(1)	5(1)	5(1)
C(2)	31(1)	36(1)	24(1)	−7(1)	−7(1)	13(1)
C(3)	25(1)	28(1)	22(1)	5(1)	6(1)	16(1)
C(4)	28(1)	40(1)	36(1)	16(1)	14(1)	20(1)
C(5)	39(1)	39(1)	39(1)	18(1)	12(1)	26(1)
C(6)	44(1)	48(1)	31(1)	−6(1)	7(1)	27(1)
C(7)	15(1)	19(1)	20(1)	4(1)	2(1)	4(1)
C(8)	22(1)	24(1)	15(1)	5(1)	1(1)	10(1)
C(9)	31(1)	24(1)	22(1)	11(1)	4(1)	8(1)
C(10)	33(1)	18(1)	29(1)	5(1)	1(1)	7(1)
C(11)	29(1)	21(1)	20(1)	0(1)	2(1)	9(1)
C(12)	23(1)	21(1)	14(1)	4(1)	5(1)	10(1)
C(13)	19(1)	31(1)	34(1)	2(1)	−5(1)	9(1)

C(14)	24(1)	33(1)	52(1)	−2(1)	1(1)	0(1)
N(1)	18(1)	21(1)	20(1)	1(1)	2(1)	9(1)
N(2)	15(1)	16(1)	13(1)	3(1)	2(1)	5(1)
Si	18(1)	17(1)	19(1)	0(1)	−1(1)	6(1)
Zn	15(1)	20(1)	19(1)	2(1)	0(1)	5(1)

Tabelle 8.78 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **127**.

	x	y	z	U(eq)
H(1A)	3933	8873	6974	54
H(1B)	5682	9217	7786	54
H(1C)	4166	9683	8356	54
H(2A)	4361	8010	10337	48
H(2B)	5921	7724	9676	48
H(2C)	4367	6385	9948	48
H(4A)	−1957	5066	8164	47
H(4B)	−2271	6208	9241	47
H(4C)	−1087	5304	9494	47
H(5A)	541	8555	7606	51
H(5B)	−1271	8197	8151	51
H(5C)	−1008	7082	7029	51
H(6A)	1249	7576	10408	59
H(6B)	80	8496	10161	59
H(6C)	1939	8856	9685	59
H(7A)	4281	6228	6284	22
H(7B)	5305	5851	7308	22
H(8A)	2898	4126	8513	24
H(8B)	4325	3622	7841	24
H(9A)	717	1988	7475	30
H(9B)	2107	1558	8170	30
H(10A)	3356	1085	6387	32
H(10B)	1339	174	6140	32
H(11A)	2377	1440	4560	28
H(11B)	885	1906	5173	28
H(12A)	4474	3554	5686	23
H(12B)	3135	4006	4961	23
H(13A)	−2260	3993	5597	35
H(13B)	−1138	3142	4904	35
H(14A)	−1955	1390	6091	61
H(14B)	−3634	1519	5481	61
H(14C)	−2994	2270	6864	61

8.2.9.4 Verbindung 128

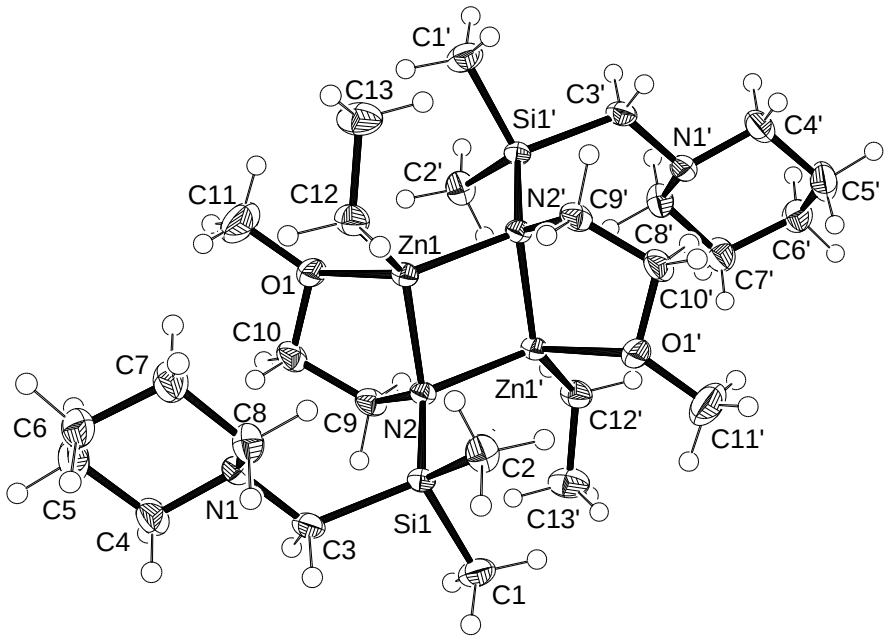


Abb. 8.27 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **128** im Kristall (Ortep−Darstellung).

Tabelle 8.79 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **128**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	5499(2)	−1434(2)	8718(2)	31(1)
C(2)	7151(2)	−1721(2)	6549(2)	28(1)
C(3)	8553(2)	1158(2)	8917(2)	24(1)
C(4)	10978(3)	3493(2)	9684(2)	34(1)
C(5)	12297(3)	4769(2)	9269(2)	41(1)
C(6)	13166(2)	4152(2)	8487(2)	34(1)
C(7)	11977(2)	2928(2)	7291(2)	34(1)
C(8)	10660(2)	1713(2)	7754(2)	29(1)
C(9)	5556(2)	1697(2)	7207(2)	23(1)
C(10)	6743(2)	3218(2)	7040(2)	26(1)
C(11)	7715(3)	4519(2)	5301(3)	53(1)
C(12)	8486(2)	1409(2)	4164(2)	27(1)
C(13)	8429(3)	1658(3)	2692(2)	36(1)
N(1)	9837(2)	2355(2)	8493(2)	22(1)
N(2)	5762(2)	418(2)	6518(1)	17(1)
O(1)	6584(2)	3169(2)	5594(1)	27(1)
Si(1)	6739(1)	−341(1)	7600(1)	19(1)
Zn(1)	6513(1)	977(1)	4792(1)	18(1)

Tabelle 8.80 Anisotrope auslenkungsparameter (Å^2 x 10^3) für die Verbindung **128**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	30(1)	35(1)	31(1)	18(1)	8(1)	14(1)
C(2)	27(1)	26(1)	33(1)	2(1)	3(1)	15(1)
C(3)	25(1)	30(1)	16(1)	6(1)	3(1)	12(1)
C(4)	35(1)	34(1)	23(1)	−4(1)	5(1)	7(1)
C(5)	38(1)	28(1)	39(1)	−6(1)	5(1)	3(1)
C(6)	23(1)	33(1)	36(1)	8(1)	1(1)	6(1)
C(7)	26(1)	36(1)	32(1)	0(1)	10(1)	7(1)

C(8)	26(1)	25(1)	31(1)	−1(1)	6(1)	9(1)
C(9)	32(1)	25(1)	17(1)	1(1)	7(1)	17(1)
C(10)	36(1)	22(1)	21(1)	−2(1)	2(1)	15(1)
C(11)	79(2)	24(1)	54(2)	12(1)	30(2)	14(1)
C(12)	20(1)	35(1)	23(1)	7(1)	5(1)	11(1)
C(13)	29(1)	56(2)	30(1)	16(1)	15(1)	22(1)
N(1)	21(1)	23(1)	18(1)	3(1)	2(1)	9(1)
N(2)	20(1)	17(1)	14(1)	3(1)	4(1)	11(1)
O(1)	38(1)	19(1)	24(1)	6(1)	8(1)	11(1)
Si(1)	20(1)	20(1)	16(1)	5(1)	2(1)	9(1)
Zn(1)	19(1)	20(1)	15(1)	4(1)	5(1)	9(1)

Tabelle 8.81 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **128**.

	x	y	z	U(eq)
H(1A)	5151	−785	9223	47
H(1B)	6135	−1763	9371	47
H(1C)	4558	−2330	8149	47
H(2A)	6137	−2556	6005	42
H(2B)	7740	−2131	7156	42
H(2C)	7793	−1202	5933	42
H(3A)	8161	1670	9541	29
H(3B)	9044	618	9470	29
H(4A)	11457	3001	10314	41
H(4B)	10411	3922	10183	41
H(5A)	11830	5308	8691	49
H(5B)	13063	5510	10100	49
H(6A)	13748	3724	9097	40
H(6B)	13956	4982	8150	40
H(7A)	12536	2457	6825	41
H(7B)	11504	3389	6622	41
H(8A)	9879	948	6943	34
H(8B)	11123	1189	8356	34
H(9A)	5677	1669	8197	28
H(9B)	4460	1564	6818	28
H(10A)	6521	4037	7445	32
H(10B)	7843	3417	7505	32
H(11A)	7527	5381	5628	79
H(11B)	7603	4410	4308	79
H(11C)	8798	4703	5765	79
H(12A)	9372	2330	4783	32
H(12B)	8753	550	4268	32
H(13A)	7571	750	2060	54
H(13B)	9456	1843	2491	54
H(13C)	8223	2540	2580	54

8.2.10 Kristallstrukturen aus Kapitel 4.5.5

8.2.10.1 Verbindung 129

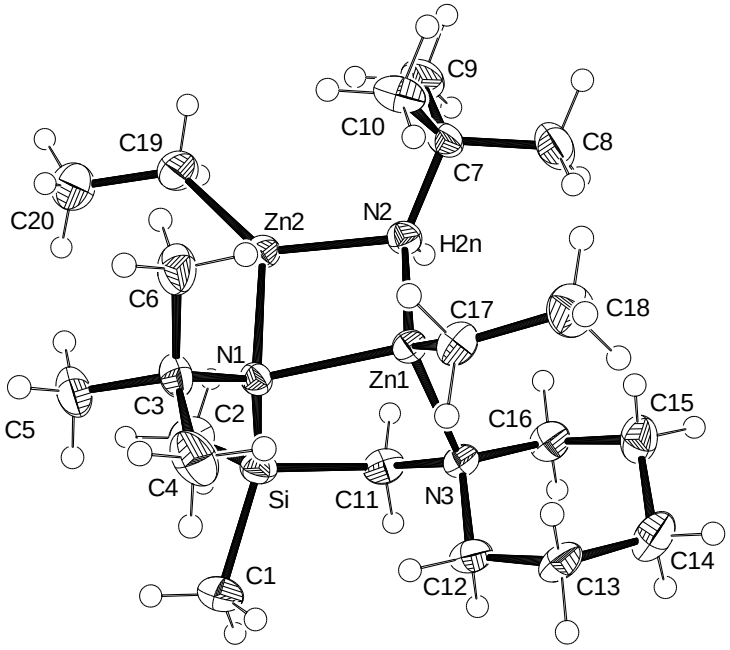


Abb. 8.28 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **129** im Kristall (Ortep−Darstellung).

Tabelle 8.82 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **129**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	1695(4)	474(1)	8048(3)	44(1)
C(2)	1842(4)	1455(1)	8817(3)	42(1)
C(3)	5869(3)	838(1)	8804(3)	29(1)
C(4)	5834(4)	334(1)	8375(3)	43(1)
C(5)	5738(4)	861(1)	10200(3)	41(1)
C(6)	7536(3)	1046(1)	8871(3)	39(1)
C(7)	5791(3)	2145(1)	5530(3)	29(1)
C(8)	5334(4)	2117(1)	4013(3)	46(1)
C(9)	5672(4)	2645(1)	5928(3)	41(1)
C(10)	7533(3)	1966(1)	6208(3)	40(1)
C(11)	1256(3)	1246(1)	5953(3)	28(1)
C(12)	1440(3)	580(1)	4636(3)	30(1)
C(13)	1873(3)	388(1)	3469(3)	33(1)
C(14)	1042(4)	658(1)	2197(3)	42(1)
C(15)	1449(4)	1165(1)	2449(3)	37(1)
C(16)	992(3)	1333(1)	3626(3)	31(1)
C(17)	6061(3)	740(1)	5149(3)	29(1)
C(18)	6230(4)	797(1)	3772(3)	40(1)
C(19)	5655(4)	2279(1)	9330(3)	40(1)
C(20)	6061(5)	2162(1)	10807(3)	55(1)
N(1)	4514(2)	1101(1)	7800(2)	22(1)
N(2)	4649(3)	1851(1)	5966(2)	24(1)
N(3)	1853(2)	1075(1)	4876(2)	23(1)
Si	2468(1)	1048(1)	7711(1)	26(1)
Zn(1)	4577(1)	1155(1)	5752(1)	21(1)
Zn(2)	5033(1)	1796(1)	7937(1)	26(1)

Tabelle 8.83 Anisotrope auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **129**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	49(2)	43(2)	44(2)	1(1)	20(2)	−19(1)
C(2)	36(2)	51(2)	45(2)	−11(1)	24(2)	−2(1)
C(3)	30(1)	33(1)	23(1)	7(1)	8(1)	5(1)
C(4)	57(2)	30(1)	45(2)	14(1)	21(2)	16(1)
C(5)	46(2)	49(2)	27(2)	10(1)	13(1)	3(1)
C(6)	26(1)	57(2)	29(2)	9(1)	5(1)	6(1)
C(7)	38(2)	23(1)	29(1)	2(1)	15(1)	−6(1)
C(8)	70(2)	39(2)	35(2)	3(1)	26(2)	−8(1)
C(9)	58(2)	24(1)	43(2)	2(1)	22(2)	−7(1)
C(10)	36(2)	36(1)	53(2)	5(1)	21(2)	−7(1)
C(11)	20(1)	29(1)	37(2)	−4(1)	10(1)	2(1)
C(12)	26(1)	23(1)	36(2)	0(1)	3(1)	−3(1)
C(13)	34(1)	24(1)	33(2)	−8(1)	2(1)	−1(1)
C(14)	45(2)	38(2)	32(2)	−8(1)	−1(1)	4(1)
C(15)	42(2)	37(1)	26(2)	4(1)	4(1)	7(1)
C(16)	29(1)	25(1)	33(2)	2(1)	2(1)	6(1)
C(17)	25(1)	30(1)	29(1)	−4(1)	6(1)	3(1)
C(18)	38(2)	48(2)	40(2)	−6(1)	20(1)	5(1)
C(19)	53(2)	35(1)	34(2)	−11(1)	17(2)	−12(1)
C(20)	76(2)	55(2)	37(2)	−14(2)	24(2)	−18(2)
N(1)	23(1)	21(1)	21(1)	3(1)	8(1)	0(1)
N(2)	25(1)	20(1)	26(1)	3(1)	7(1)	1(1)
N(3)	21(1)	20(1)	26(1)	−2(1)	5(1)	1(1)
Si	26(1)	27(1)	29(1)	−2(1)	13(1)	−5(1)
Zn(1)	22(1)	19(1)	23(1)	−2(1)	7(1)	1(1)
Zn(2)	31(1)	23(1)	25(1)	−3(1)	11(1)	−5(1)

Tabelle 8.84 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **129**.

	x	y	z	U(eq)
H(1A)	1966	240	7491	66
H(1B)	491	487	7833	66
H(1C)	2224	395	8996	66
H(2A)	2428	1376	9758	63
H(2B)	644	1432	8628	63
H(2C)	2126	1768	8645	63
H(4A)	4797	192	8370	64
H(4B)	6775	171	9008	64
H(4C)	5909	318	7475	64
H(5A)	5772	1182	10481	61
H(5B)	6667	694	10833	61
H(5C)	4692	722	10184	61
H(6A)	7623	1047	7973	58
H(6B)	8440	862	9474	58
H(6C)	7612	1360	9209	58
H(8A)	5460	1801	3753	69
H(8B)	6067	2319	3727	69
H(8C)	4182	2215	3584	69
H(9A)	4546	2759	5472	61
H(9B)	6464	2831	5668	61
H(9C)	5930	2664	6900	61
H(10A)	7822	1990	7182	60
H(10B)	8313	2149	5921	60
H(10C)	7592	1645	5959	60
H(11A)	89	1149	5740	34
H(11B)	1273	1585	5940	34
H(12A)	240	538	4459	36

H(12B)	2047	405	5456	36
H(13A)	1518	64	3325	39
H(13B)	3090	398	3684	39
H(14A)	−173	613	1905	50
H(14B)	1434	547	1475	50
H(15A)	2648	1213	2632	45
H(15B)	831	1343	1640	45
H(16A)	1279	1662	3776	37
H(16B)	−220	1303	3411	37
H(17A)	7187	766	5819	34
H(17B)	5685	422	5201	34
H(18A)	5141	761	3077	60
H(18B)	6988	563	3650	60
H(18C)	6670	1102	3704	60
H(19A)	6632	2440	9246	48
H(19B)	4737	2504	9095	48
H(20A)	5077	2034	10948	82
H(20B)	6407	2441	11347	82
H(20C)	6961	1937	11077	82
H(2N)	3790(30)	1960(9)	5660(30)	25(8)

8.2.10.2 Verbindung 130

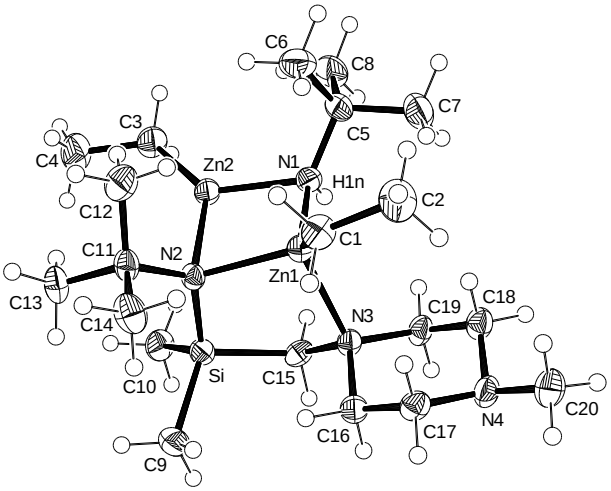


Abb. 8.29 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **130** im Kristall (Ortep−Darstellung).

Tabelle 8.85 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **130**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(1)	−1003(6)	725(2)	4176(5)	34(1)
C(2)	−1284(7)	757(2)	5467(5)	45(1)
C(3)	−446(7)	2349(2)	447(5)	39(1)
C(4)	−895(8)	2247(2)	−1036(5)	51(1)
C(5)	−683(6)	2132(2)	4139(4)	32(1)
C(6)	−2435(6)	1974(2)	3316(5)	42(1)
C(7)	−219(7)	2071(2)	5650(5)	46(1)
C(8)	−540(7)	2641(2)	3861(5)	43(1)
C(9)	3415(6)	526(2)	1870(5)	39(1)
C(10)	3364(6)	1502(2)	1107(5)	36(1)
C(11)	−717(6)	923(1)	706(4)	29(1)
C(12)	−2376(6)	1136(2)	476(5)	42(1)
C(13)	−515(7)	958(2)	−627(4)	39(1)

C(14)	−771(6)	416(2)	1051(5)	40(1)
C(15)	3843(5)	1293(1)	3936(4)	27(1)
C(16)	3715(6)	611(1)	5154(4)	29(1)
C(17)	3284(6)	407(1)	6238(4)	30(1)
C(18)	3531(6)	1132(2)	7266(4)	32(1)
C(19)	4015(6)	1340(1)	6216(4)	29(1)
C(20)	3641(7)	455(2)	8548(5)	40(1)
N(1)	439(5)	1858(1)	3737(4)	27(1)
N(2)	634(4)	1167(1)	1846(3)	24(1)
N(3)	3227(4)	1096(1)	4902(3)	24(1)
N(4)	4065(5)	658(1)	7509(3)	31(1)
Si	2668(2)	1103(1)	2111(1)	26(1)
Zn(1)	489(1)	1164(1)	3808(1)	24(1)
Zn(2)	120(1)	1850(1)	1789(1)	27(1)

Tabelle 8.86 Anisotrope auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **130**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	**U22**	**U33**	**U23**	**U13**	**U12**
C(1)	30(2)	38(2)	36(2)	5(2)	16(2)	−6(2)
C(2)	41(3)	54(3)	44(3)	0(2)	22(2)	−11(2)
C(3)	50(3)	27(2)	36(3)	6(2)	14(2)	6(2)
C(4)	79(4)	40(3)	32(3)	11(2)	21(3)	8(3)
C(5)	38(2)	27(2)	31(2)	−6(2)	14(2)	3(2)
C(6)	41(3)	38(3)	50(3)	2(2)	21(2)	10(2)
C(7)	62(4)	43(3)	36(3)	−5(2)	24(3)	6(3)
C(8)	61(3)	25(2)	45(3)	−5(2)	22(3)	7(2)
C(9)	46(3)	41(3)	36(3)	2(2)	24(2)	12(2)
C(10)	39(3)	41(3)	32(2)	8(2)	20(2)	0(2)
C(11)	33(2)	26(2)	25(2)	−7(2)	9(2)	−6(2)
C(12)	32(3)	48(3)	39(3)	−6(2)	7(2)	−6(2)
C(13)	47(3)	42(3)	24(2)	−10(2)	12(2)	−6(2)
C(14)	51(3)	30(2)	40(3)	−9(2)	21(3)	−13(2)
C(15)	24(2)	24(2)	30(2)	5(2)	8(2)	−1(2)
C(16)	36(2)	23(2)	27(2)	1(2)	12(2)	2(2)
C(17)	33(2)	23(2)	31(2)	4(2)	11(2)	0(2)
C(18)	37(3)	29(2)	24(2)	−2(2)	7(2)	−2(2)
C(19)	35(2)	24(2)	21(2)	−1(2)	4(2)	−2(2)
C(20)	49(3)	42(3)	32(2)	10(2)	19(2)	0(2)
N(1)	26(2)	24(2)	26(2)	−4(2)	7(2)	2(2)
N(2)	27(2)	20(2)	22(2)	−4(1)	8(1)	−2(1)
N(3)	31(2)	18(2)	22(2)	2(1)	10(2)	0(1)
N(4)	36(2)	33(2)	22(2)	6(2)	10(2)	2(2)
Si	32(1)	23(1)	25(1)	2(1)	14(1)	2(1)
Zn(1)	27(1)	22(1)	25(1)	1(1)	11(1)	−1(1)
Zn(2)	33(1)	21(1)	25(1)	2(1)	11(1)	3(1)

Tabelle 8.87 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **130**.

	x	**y**	**z**	**U(eq)**
H(1A)	−2096	747	3407	40
H(1B)	−579	416	4149	40
H(2A)	−1746	1056	5513	67
H(2B)	−234	718	6254	67
H(2C)	−2054	519	5465	67
H(3A)	−1382	2517	498	47
H(3B)	502	2561	753	47
H(4A)	16	2086	−1127	76
H(4B)	−1104	2533	−1545	76
H(4C)	−1886	2058	−1393	76
H(6A)	−2713	2020	2351	64

H(6B)	−3194	2149	3577	64
H(6C)	−2530	1650	3487	64
H(7A)	−295	1748	5845	69
H(7B)	−974	2247	5913	69
H(7C)	911	2177	6163	69
H(8A)	584	2745	4407	65
H(8B)	−1318	2816	4101	65
H(8C)	−795	2684	2900	65
H(9A)	3025	297	2324	58
H(9B)	4622	524	2258	58
H(9C)	2989	457	901	58
H(10A)	2804	1427	144	54
H(10B)	4556	1473	1398	54
H(10C)	3095	1815	1254	54
H(12A)	−2555	1113	1307	63
H(12B)	−3258	975	−257	63
H(12C)	−2379	1457	230	63
H(13A)	−416	1278	−831	58
H(13B)	−1478	824	−1358	58
H(13C)	479	793	−544	58
H(14A)	277	272	1187	60
H(14B)	−1670	266	304	60
H(14C)	−953	389	1879	60
H(15A)	5016	1208	4232	32
H(15B)	3786	1628	3974	32
H(16A)	4917	585	5426	35
H(16B)	3156	437	4304	35
H(17A)	2075	411	5941	35
H(17B)	3652	86	6385	35
H(18A)	4040	1306	8121	38
H(18B)	2320	1148	6956	38
H(19A)	3676	1664	6087	35
H(19B)	5227	1328	6534	35
H(20A)	4230	614	9408	60
H(20B)	3957	133	8654	60
H(20C)	2452	481	8283	60
H(1N)	1230(60)	1947(16)	4060(50)	22(14)

8.2.11 Kristallstrukturen aus Kapitel 4.6.1

8.2.11.1 Verbindung 131

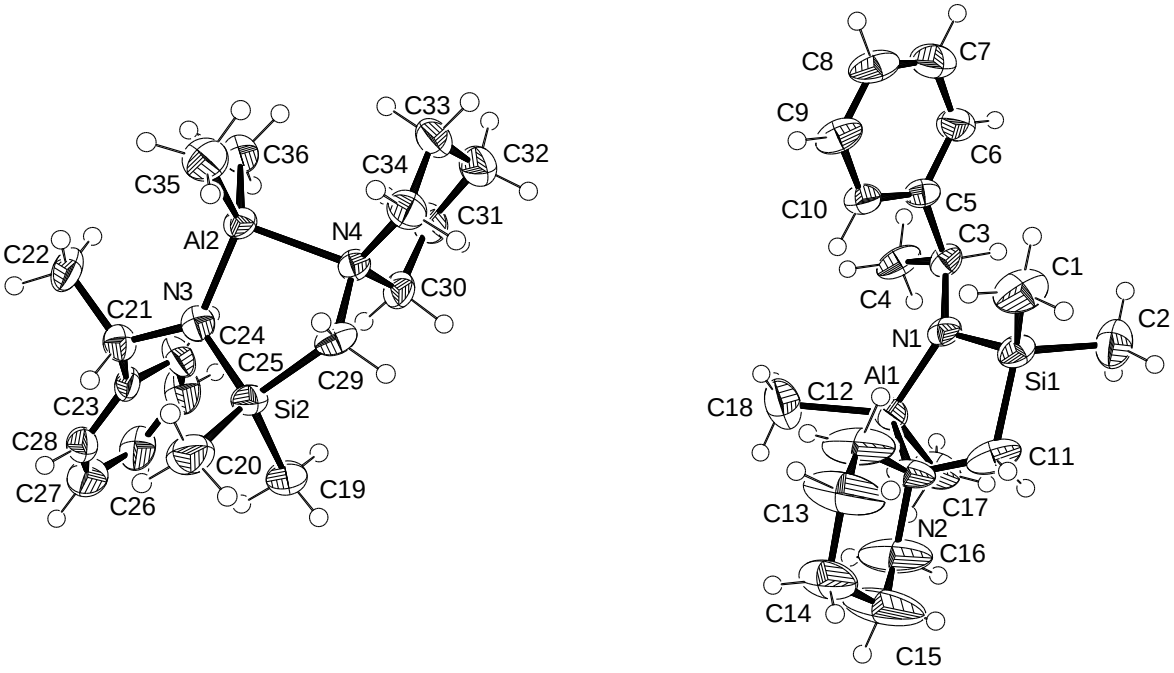


Abb. 8.30 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **131** im Kristall (Ortep−Darstellung).

Tabelle 8.88 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **131**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
Al(1)	3037(2)	1931(1)	2132(1)	40(1)
Al(2)	6354(1)	6305(1)	8934(1)	31(1)
C(1)	4218(7)	−2607(6)	4266(3)	65(2)
C(2)	3775(7)	−2472(5)	2101(4)	63(1)
C(3)	6400(5)	−656(4)	2284(3)	35(1)
C(4)	6992(6)	553(5)	1593(3)	48(1)
C(5)	7563(5)	−1453(4)	3222(3)	34(1)
C(6)	9043(6)	−2714(5)	3232(3)	47(1)
C(7)	10099(6)	−3411(5)	4076(4)	57(1)
C(8)	9662(6)	−2838(5)	4919(3)	53(1)
C(9)	8200(6)	−1598(5)	4933(3)	47(1)
C(10)	7158(5)	−890(4)	4083(3)	38(1)
C(11)	1221(6)	124(5)	2991(3)	53(1)
C(12)	1423(7)	1526(8)	4156(3)	93(2)
C(13)	135(9)	1761(9)	4826(4)	137(4)
C(14)	−1565(7)	3048(7)	4472(4)	87(2)
C(15)	−1947(8)	3103(9)	3405(5)	141(4)
C(16)	−596(7)	2848(7)	2770(4)	91(2)
C(17)	2121(6)	2563(5)	740(3)	56(1)
C(18)	3539(7)	3492(5)	2478(4)	71(2)
C(19)	1305(6)	8995(5)	7452(3)	53(1)
C(20)	971(6)	8247(6)	9741(3)	58(1)
C(21)	4269(5)	9529(4)	8844(3)	34(1)
C(22)	5882(6)	9404(5)	9319(3)	48(1)
C(23)	3928(5)	10771(4)	7823(3)	33(1)
C(36)	8510(6)	6385(5)	8193(3)	50(1)

C(24)	4876(6)	10451(4)	6947(3)	48(1)
C(25)	4612(7)	11578(5)	6034(3)	56(1)
C(26)	3413(7)	12994(5)	6013(3)	53(1)
C(27)	2460(6)	13321(5)	6870(3)	54(1)
C(28)	2746(5)	12189(4)	7770(3)	40(1)
C(29)	3433(5)	5776(4)	8766(3)	40(1)
C(30)	5222(5)	5612(4)	7220(3)	40(1)
C(31)	6966(6)	4886(5)	6730(3)	49(1)
C(32)	7748(7)	3203(5)	7157(3)	57(1)
C(33)	7764(6)	2804(5)	8319(3)	49(1)
C(34)	5976(6)	3531(4)	8744(3)	46(1)
C(35)	6893(6)	5090(5)	10349(3)	57(1)
N(1)	4554(4)	−49(3)	2539(2)	33(1)
N(2)	1101(4)	1595(4)	3077(2)	47(1)
N(3)	4419(4)	8072(3)	8732(2)	33(1)
N(4)	5253(4)	5200(3)	8359(2)	31(1)
Si(1)	3555(1)	−1279(1)	2982(1)	39(1)
Si(2)	2534(1)	7868(1)	8649(1)	36(1)

Tabelle 8.89 Anisotrope auslenkungsparameter ($Å^2 \times 10^3$) für die Verbindung **131**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
Al(1)	44(1)	38(1)	33(1)	−11(1)	−6(1)	−8(1)
Al(2)	31(1)	35(1)	24(1)	−6(1)	−4(1)	−11(1)
C(1)	68(4)	68(3)	47(3)	23(2)	−21(3)	−34(3)
C(2)	82(4)	57(3)	64(3)	−12(2)	−9(3)	−39(3)
C(3)	38(3)	46(2)	24(2)	−11(2)	−2(2)	−18(2)
C(4)	39(3)	75(3)	31(2)	2(2)	−8(2)	−31(3)
C(5)	25(2)	39(2)	33(2)	−4(2)	0(2)	−12(2)
C(6)	37(3)	48(3)	50(3)	−18(2)	−4(2)	−7(3)
C(7)	48(3)	46(3)	62(3)	−1(2)	−12(3)	−7(2)
C(8)	44(3)	60(3)	41(3)	17(2)	−18(2)	−20(3)
C(9)	40(3)	71(3)	25(2)	−2(2)	−5(2)	−24(3)
C(10)	31(3)	45(3)	34(2)	−9(2)	−5(2)	−10(2)
C(11)	38(3)	88(4)	24(2)	4(2)	−6(2)	−25(3)
C(12)	57(4)	149(6)	23(3)	−29(3)	−18(3)	18(4)
C(13)	88(5)	197(7)	56(4)	−86(4)	−33(4)	59(5)
C(14)	56(4)	122(5)	62(4)	−64(4)	−11(3)	17(4)
C(15)	73(5)	203(8)	75(4)	−86(5)	−40(4)	63(5)
C(16)	48(4)	138(5)	32(3)	−8(3)	−13(3)	13(4)
C(17)	59(3)	56(3)	30(2)	1(2)	−2(2)	−6(3)
C(18)	83(4)	56(3)	87(4)	−34(3)	20(3)	−35(3)
C(19)	48(3)	45(3)	56(3)	−11(2)	−25(2)	−1(2)
C(20)	39(3)	82(3)	53(3)	−26(3)	1(2)	−18(3)
C(21)	44(3)	28(2)	31(2)	−5(2)	−1(2)	−15(2)
C(22)	74(3)	38(2)	39(2)	−3(2)	−26(2)	−25(2)
C(23)	44(3)	30(2)	28(2)	−10(2)	−11(2)	−12(2)
C(36)	44(3)	49(3)	61(3)	−25(2)	−1(2)	−16(2)
C(24)	63(3)	29(2)	44(3)	−15(2)	1(2)	−8(2)
C(25)	87(4)	50(3)	32(2)	−8(2)	1(2)	−29(3)
C(26)	83(4)	38(3)	32(3)	5(2)	−22(2)	−23(3)
C(27)	63(3)	37(3)	54(3)	1(2)	−23(3)	−12(2)
C(28)	45(3)	38(3)	37(2)	−15(2)	−6(2)	−10(2)
C(29)	30(2)	48(3)	41(2)	−4(2)	−6(2)	−18(2)
C(30)	53(3)	35(2)	33(2)	−7(2)	−17(2)	−13(2)
C(31)	67(3)	44(3)	25(2)	−10(2)	−9(2)	−8(3)
C(32)	60(3)	53(3)	55(3)	−26(2)	−10(2)	−6(3)
C(33)	55(3)	33(2)	52(3)	−15(2)	−9(2)	−5(2)
C(34)	53(3)	30(2)	49(3)	−3(2)	−11(2)	−12(2)
C(35)	65(3)	58(3)	34(2)	−7(2)	−14(2)	−10(3)
N(1)	30(2)	44(2)	23(2)	−10(2)	−6(1)	−11(2)

N(2)	36(2)	61(3)	20(2)	−12(2)	−12(2)	10(2)
N(3)	40(2)	31(2)	26(2)	−5(1)	−1(2)	−14(2)
N(4)	33(2)	30(2)	27(2)	−5(1)	−6(1)	−10(2)
Si(1)	38(1)	44(1)	34(1)	−1(1)	−8(1)	−18(1)
Si(2)	30(1)	36(1)	37(1)	−9(1)	−7(1)	−6(1)

Tabelle 8.90 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **131**.

	x	y	z	U(eq)
H(1A)	5428	−3300	4231	97
H(1B)	3481	−3185	4476	97
H(1C)	4097	−2037	4765	97
H(2A)	3447	−1828	1410	95
H(2B)	3016	−3026	2342	95
H(2C)	4977	−3189	2090	95
H(3)	6599	−1420	1897	42
H(4A)	6295	1042	975	72
H(4B)	8214	86	1402	72
H(4C)	6848	1306	1958	72
H(6)	9349	−3117	2651	56
H(7)	11123	−4284	4072	68
H(8)	10390	−3313	5496	64
H(9)	7890	−1217	5523	56
H(10)	6151	−6	4089	46
H(11A)	664	272	2353	64
H(11B)	585	−296	3573	64
H(12A)	2315	516	4443	112
H(12B)	1936	2267	4113	112
H(13A)	519	1938	5415	164
H(13B)	−84	825	5080	164
H(14A)	−2508	2911	4948	104
H(14B)	−1506	4011	4474	104
H(15A)	−2445	2350	3456	170
H(15B)	−2834	4110	3107	170
H(16A)	−381	3787	2540	109
H(16B)	−958	2700	2162	109
H(17A)	3059	2561	235	84
H(17B)	1214	3580	626	84
H(17C)	1635	1861	670	84
H(18A)	3996	3113	3170	107
H(18B)	2472	4395	2445	107
H(18C)	4396	3745	1990	107
H(19A)	923	10071	7407	80
H(19B)	292	8752	7459	80
H(19C)	2049	8757	6860	80
H(20A)	1551	7622	10387	87
H(20B)	−13	8004	9674	87
H(20C)	558	9313	9734	87
H(21)	3266	9872	9317	41
H(22A)	6130	8614	9962	72
H(22B)	5679	10368	9452	72
H(22C)	6870	9149	8844	72
H(02A)	8226	7059	7506	75
H(02B)	9290	5372	8140	75
H(02C)	9076	6765	8567	75
H(24)	5708	9462	6971	58
H(25)	5258	11362	5435	67
H(26)	3238	13766	5394	63
H(27)	1619	14305	6847	65
H(28)	2095	12413	8366	48
H(29A)	3402	5237	9495	47

H(29B)	2688	5555	8388	47
H(30A)	4826	6721	6966	49
H(30B)	4374	5309	7006	49
H(31A)	6828	5118	5984	58
H(31B)	7765	5323	6842	58
H(32A)	8946	2794	6888	68
H(32B)	7069	2740	6937	68
H(33A)	8184	1697	8590	59
H(33B)	8566	3152	8539	59
H(34A)	6018	3258	9499	56
H(34B)	5196	3133	8555	56
H(03A)	7294	5602	10714	85
H(03B)	7802	4100	10347	85
H(03C)	5852	4963	10693	85

8.2.12 Kristallstrukturen aus Kapitel 4.6.2

8.2.12.1 Verbindung 132_monoklin

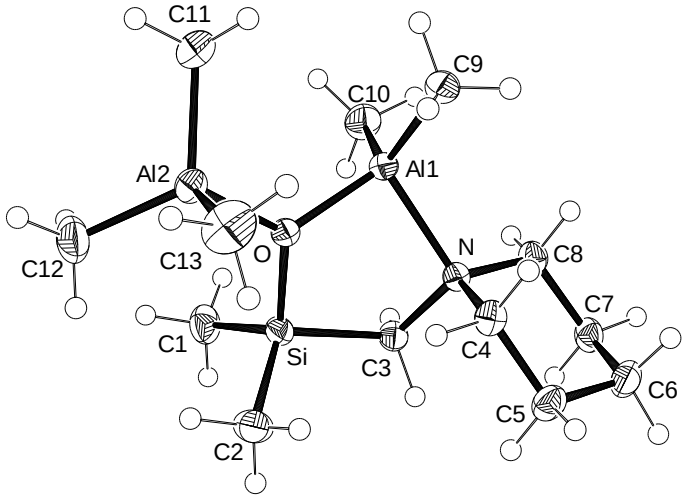


Abb. 8.31 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **132** (monoklin) im Kristall (Ortep−Darstellung).

Tabelle 8.91 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **132** (monoklin). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
Al(1)	4084(1)	1403(1)	7961(1)	20(1)
Al(2)	1222(1)	2566(1)	7073(1)	26(1)
C(1)	838(2)	1630(1)	9366(1)	33(1)
C(2)	1724(2)	4011(1)	9037(1)	33(1)
C(3)	3952(2)	2189(1)	9550(1)	22(1)
C(4)	5508(2)	3289(1)	8741(1)	23(1)
C(5)	6284(2)	3907(1)	9461(1)	28(1)
C(6)	7575(2)	3264(1)	9823(1)	31(1)
C(7)	7156(2)	2105(1)	10043(1)	26(1)
C(8)	6354(2)	1541(1)	9312(1)	23(1)
C(9)	5109(2)	1698(1)	7013(1)	30(1)
C(10)	3775(2)	−107(1)	8296(1)	34(1)
C(11)	1458(2)	1315(1)	6329(1)	39(1)
C(12)	−709(2)	2598(2)	7413(1)	44(1)
C(13)	1901(2)	3998(1)	6704(1)	47(1)
N	5064(1)	2157(1)	8961(1)	18(1)

O	2472(1)	2209(1)	8020(1)	20(1)
Si	2170(1)	2539(1)	8980(1)	22(1)

Tabelle 8.92 Anisotrope auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **132** (monoklin). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
Al(1)	20(1)	20(1)	20(1)	−3(1)	3(1)	−1(1)
Al(2)	24(1)	30(1)	22(1)	0(1)	−2(1)	2(1)
C(1)	23(1)	47(1)	30(1)	2(1)	6(1)	−2(1)
C(2)	37(1)	33(1)	28(1)	−5(1)	1(1)	9(1)
C(3)	21(1)	26(1)	18(1)	1(1)	3(1)	0(1)
C(4)	24(1)	21(1)	25(1)	5(1)	2(1)	−2(1)
C(5)	28(1)	21(1)	35(1)	−1(1)	−1(1)	−4(1)
C(6)	24(1)	31(1)	36(1)	−4(1)	−3(1)	−5(1)
C(7)	20(1)	31(1)	26(1)	2(1)	−2(1)	4(1)
C(8)	21(1)	21(1)	28(1)	3(1)	2(1)	2(1)
C(9)	26(1)	40(1)	25(1)	−8(1)	7(1)	−5(1)
C(10)	34(1)	24(1)	43(1)	−3(1)	2(1)	−2(1)
C(11)	35(1)	49(1)	30(1)	−9(1)	−4(1)	−1(1)
C(12)	26(1)	67(1)	37(1)	0(1)	−2(1)	11(1)
C(13)	59(2)	39(1)	39(1)	11(1)	−4(1)	−2(1)
N	18(1)	18(1)	19(1)	2(1)	3(1)	0(1)
O	19(1)	23(1)	18(1)	−2(1)	1(1)	2(1)
Si	19(1)	27(1)	19(1)	−2(1)	3(1)	2(1)

Tabelle 8.93 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter ($Å^2$ x 10^3) für die Verbindung **132** (monoklin).

	x	y	z	U(eq)
H(1A)	−77	1739	9037	50
H(1B)	746	1805	9946	50
H(1C)	1135	863	9322	50
H(2A)	2477	4451	8831	49
H(2B)	1629	4212	9611	49
H(2C)	827	4153	8697	49
H(3A)	4210	2748	9982	26
H(3B)	3900	1466	9823	26
H(4A)	4657	3713	8528	28
H(4B)	6132	3237	8291	28
H(5A)	5638	4026	9892	34
H(5B)	6585	4635	9271	34
H(6A)	8280	3233	9417	37
H(6B)	8017	3642	10324	37
H(7A)	8017	1676	10229	31
H(7B)	6556	2134	10505	31
H(8A)	6994	1445	8875	28
H(8B)	6065	801	9483	28
H(9A)	4860	1144	6585	45
H(9B)	6130	1671	7182	45
H(9C)	4854	2429	6792	45
H(10A)	3396	−110	8833	51
H(10B)	4676	−507	8340	51
H(10C)	3098	−463	7883	51
H(11A)	2322	1417	6057	58
H(11B)	638	1274	5910	58
H(11C)	1530	632	6649	58
H(12A)	−944	1873	7624	65
H(12B)	−1386	2786	6938	65
H(12C)	−759	3149	7848	65

H(13A)	2074	4491	7179	70
H(13B)	1183	4321	6298	70
H(13C)	2783	3892	6451	70

8.2.12.2 Verbindung 132_orthorhombisch

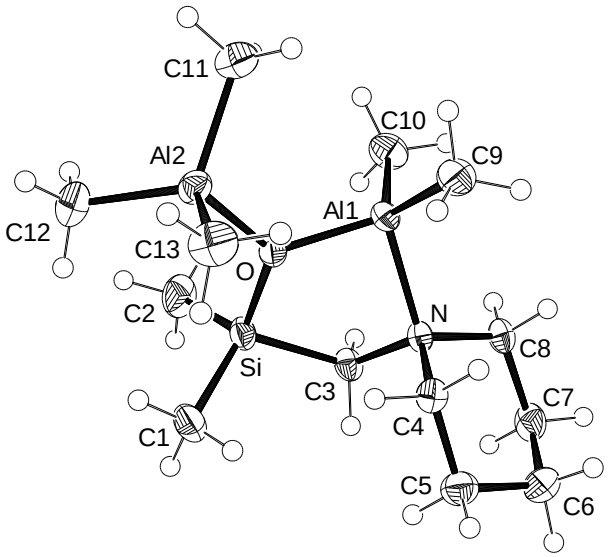


Abb. 8.32 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **132** (orthorhombisch) im Kristall (Ortep−Darstellung).

Tabelle 8.94 Atomkoordinaten ($x\,10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2\,x\,10^3$) für die Verbindung **132** (orthorhombisch). U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
Al(1)	1389(1)	2146(1)	5574(1)	22(1)
Al(2)	2667(1)	3013(1)	6862(1)	27(1)
C(1)	4182(1)	1046(1)	6635(1)	38(1)
C(2)	1913(2)	709(1)	7290(1)	42(1)
C(3)	2179(1)	560(1)	5720(1)	24(1)
C(4)	3172(1)	1376(1)	4826(1)	25(1)
C(5)	3747(1)	661(1)	4470(1)	33(1)
C(6)	3029(1)	304(1)	3895(1)	38(1)
C(7)	1895(1)	98(1)	4173(1)	34(1)
C(8)	1381(1)	825(1)	4547(1)	26(1)
C(9)	1632(2)	3090(1)	4967(1)	35(1)
C(10)	−99(1)	1841(1)	5838(1)	37(1)
C(11)	1332(1)	3696(1)	6804(1)	38(1)
C(12)	2967(2)	2645(1)	7826(1)	45(1)
C(13)	3966(1)	3467(1)	6388(1)	42(1)
N	2076(1)	1155(1)	5128(1)	20(1)
O	2296(1)	2067(1)	6332(1)	22(1)
Si	2675(1)	1109(1)	6529(1)	25(1)

Tabelle 8.95 Anisotrope auslenkungsparameter ($Å^2\,x\,10^3$) für die Verbindung **132** (orthorhombisch). Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

	U11	U22	U33	U23	U13	U12
Al(1)	22(1)	20(1)	23(1)	3(1)	−2(1)	1(1)
Al(2)	26(1)	28(1)	27(1)	−6(1)	0(1)	−1(1)
C(1)	36(1)	41(1)	37(1)	−3(1)	−15(1)	8(1)
C(2)	62(1)	39(1)	25(1)	11(1)	2(1)	1(1)

C(3)	30(1)	19(1)	24(1)	5(1)	−4(1)	−1(1)
C(4)	24(1)	26(1)	24(1)	1(1)	1(1)	−4(1)
C(5)	29(1)	36(1)	35(1)	−4(1)	2(1)	2(1)
C(6)	44(1)	38(1)	33(1)	−10(1)	−1(1)	8(1)
C(7)	42(1)	29(1)	31(1)	−7(1)	−12(1)	−1(1)
C(8)	26(1)	28(1)	23(1)	0(1)	−7(1)	−3(1)
C(9)	45(1)	25(1)	33(1)	6(1)	3(1)	5(1)
C(10)	26(1)	40(1)	44(1)	2(1)	−1(1)	−1(1)
C(11)	37(1)	33(1)	42(1)	−7(1)	4(1)	2(1)
C(12)	54(1)	50(1)	31(1)	−11(1)	−7(1)	2(1)
C(13)	33(1)	38(1)	53(1)	−5(1)	4(1)	−8(1)
N	22(1)	20(1)	18(1)	3(1)	−3(1)	−3(1)
O	26(1)	20(1)	20(1)	0(1)	−3(1)	1(1)
Si	31(1)	24(1)	20(1)	3(1)	−6(1)	2(1)

Tabelle 8.96 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **132** (orthorhombisch).

	x	y	z	U(eq)
H(1A)	4538	1173	6188	57
H(1B)	4385	491	6784	57
H(1C)	4420	1443	6990	57
H(2A)	2170	984	7716	63
H(2B)	2036	116	7331	63
H(2C)	1127	816	7228	63
H(3A)	2704	120	5593	29
H(3B)	1457	302	5814	29
H(4A)	3648	1586	5206	30
H(4B)	3073	1825	4482	30
H(5A)	4449	852	4266	40
H(5B)	3913	230	4819	40
H(6A)	2963	705	3508	46
H(6B)	3376	–200	3707	46
H(7A)	1417	–70	3779	41
H(7B)	1950	–370	4501	41
H(8A)	1248	1269	4202	31
H(8B)	661	657	4739	31
H(9A)	1188	3553	5131	52
H(9B)	1420	2949	4487	52
H(9C)	2410	3241	4978	52
H(10A)	–85	1317	6090	55
H(10B)	–551	1785	5416	55
H(10C)	–411	2268	6141	55
H(11A)	1322	3988	6356	56
H(11B)	1329	4094	7189	56
H(11C)	681	3344	6839	56
H(12A)	2278	2481	8051	67
H(12B)	3300	3096	8092	67
H(12C)	3471	2177	7816	67
H(13A)	4542	3048	6368	62
H(13B)	4234	3945	6649	62
H(13C)	3767	3634	5912	62

8.2.12.3 Verbindung 133

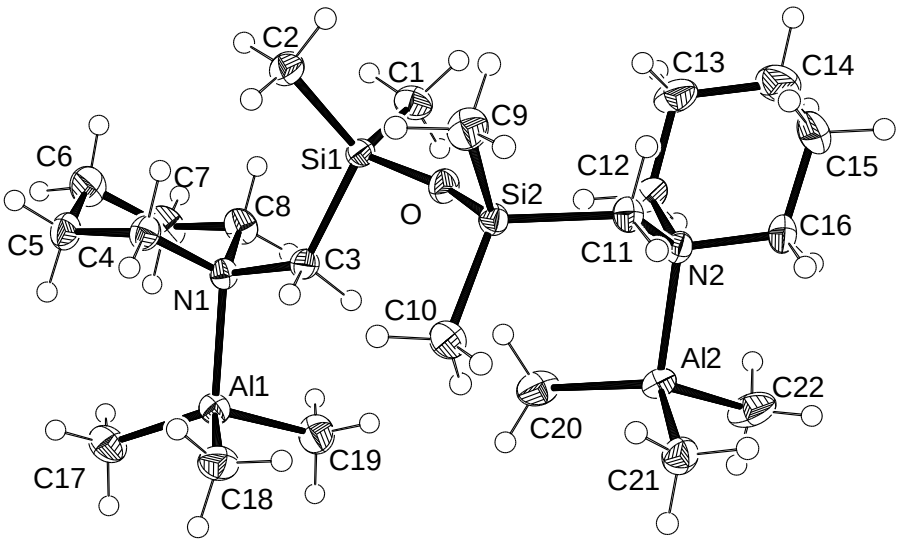


Abb. 8.33 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **133** im Kristall (Ortep−Darstellung).

Tabelle 8.97 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **133**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
Al(1)	4555(1)	2876(1)	4665(1)	23(1)
Al(2)	3862(1)	2676(1)	225(1)	23(1)
C(1)	9706(2)	3465(1)	1680(1)	31(1)
C(2)	10144(2)	1052(1)	3162(1)	30(1)
C(3)	6879(2)	2288(1)	3390(1)	22(1)
C(4)	7814(2)	1781(1)	4949(1)	25(1)
C(5)	8148(2)	2143(1)	5741(1)	29(1)
C(6)	9130(2)	3256(2)	5323(1)	38(1)
C(7)	8297(2)	4162(1)	4554(1)	36(1)
C(8)	7994(2)	3757(1)	3781(1)	27(1)
C(9)	8233(2)	−582(1)	1893(1)	32(1)
C(10)	4933(2)	139(1)	2506(1)	32(1)
C(11)	6691(2)	1170(1)	356(1)	21(1)
C(12)	7285(2)	3255(1)	−337(1)	26(1)
C(13)	8972(2)	3248(1)	−865(1)	36(1)
C(14)	8905(2)	3305(2)	−1880(1)	48(1)
C(15)	7769(2)	2361(2)	−1826(1)	42(1)
C(16)	6115(2)	2400(1)	−1272(1)	30(1)
C(17)	4209(2)	3132(1)	5877(1)	34(1)
C(18)	3479(2)	1415(1)	4882(1)	32(1)
C(19)	3898(2)	4193(1)	3562(1)	36(1)
C(20)	4099(2)	3073(1)	1329(1)	34(1)
C(21)	2518(2)	1302(1)	504(1)	29(1)
C(22)	3224(2)	4011(1)	−868(1)	41(1)
N(1)	6987(1)	2673(1)	4195(1)	20(1)
N(2)	6150(1)	2327(1)	−263(1)	21(1)
O	7755(1)	1617(1)	1905(1)	25(1)
Si(1)	8673(1)	2104(1)	2547(1)	19(1)
Si(2)	6889(1)	645(1)	1690(1)	20(1)

Tabelle 8.98 Anisotrope auslenkungsparameter ($Å^2 \times 10^3$) für die Verbindung **133**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	U22	U33	U23	U13	U12
Al(1)	25(1)	20(1)	23(1)	−9(1)	−2(1)	2(1)
Al(2)	19(1)	21(1)	28(1)	−9(1)	−6(1)	1(1)
C(1)	29(1)	28(1)	33(1)	−11(1)	1(1)	−2(1)
C(2)	27(1)	35(1)	29(1)	−14(1)	−8(1)	10(1)
C(3)	21(1)	27(1)	22(1)	−14(1)	−4(1)	0(1)
C(4)	28(1)	24(1)	25(1)	−11(1)	−7(1)	3(1)
C(5)	33(1)	34(1)	25(1)	−15(1)	−9(1)	2(1)
C(6)	39(1)	51(1)	35(1)	−26(1)	−6(1)	−12(1)
C(7)	44(1)	28(1)	39(1)	−19(1)	2(1)	−15(1)
C(8)	32(1)	21(1)	27(1)	−8(1)	1(1)	−9(1)
C(9)	36(1)	25(1)	33(1)	−9(1)	−9(1)	8(1)
C(10)	29(1)	35(1)	24(1)	−6(1)	−1(1)	−3(1)
C(11)	26(1)	19(1)	20(1)	−9(1)	−5(1)	2(1)
C(12)	26(1)	20(1)	30(1)	−4(1)	−9(1)	−2(1)
C(13)	23(1)	34(1)	39(1)	−1(1)	−6(1)	−3(1)
C(14)	32(1)	59(1)	31(1)	−2(1)	5(1)	2(1)
C(15)	42(1)	61(1)	20(1)	−14(1)	−1(1)	6(1)
C(16)	31(1)	41(1)	19(1)	−10(1)	−7(1)	0(1)
C(17)	38(1)	33(1)	33(1)	−17(1)	2(1)	4(1)
C(18)	27(1)	34(1)	37(1)	−16(1)	−1(1)	−4(1)
C(19)	41(1)	33(1)	33(1)	−11(1)	−7(1)	11(1)
C(20)	28(1)	36(1)	49(1)	−28(1)	−9(1)	6(1)
C(21)	28(1)	30(1)	29(1)	−11(1)	−6(1)	−4(1)
C(22)	26(1)	33(1)	51(1)	−2(1)	−12(1)	2(1)
N(1)	23(1)	18(1)	20(1)	−9(1)	−4(1)	−2(1)
N(2)	22(1)	21(1)	18(1)	−6(1)	−6(1)	0(1)
O	26(1)	29(1)	24(1)	−15(1)	−7(1)	2(1)
Si(1)	18(1)	21(1)	21(1)	−10(1)	−4(1)	2(1)
Si(2)	21(1)	20(1)	18(1)	−7(1)	−4(1)	2(1)

Tabelle 8.99 Wasserstoffkoordinaten ($\times 10^4$) und isotrope Auslenkungsparameter ($Å^2 \times 10^3$) für die Verbindung **133**.

	x	y	z	U(eq)
H(1A)	10312	3357	1121	46
H(1B)	10459	3714	2003	46
H(1C)	8896	4046	1455	46
H(2A)	9555	369	3662	45
H(2B)	10819	1386	3465	45
H(2C)	10837	842	2683	45
H(3A)	6164	2828	2963	26
H(3B)	6277	1542	3700	26
H(4A)	8855	1612	4634	30
H(4B)	7125	1072	5246	30
H(5A)	7103	2231	6106	35
H(5B)	8748	1541	6203	35
H(6A)	9246	3507	5848	46
H(6B)	10230	3146	5032	46
H(7A)	8987	4871	4250	43
H(7B)	7250	4335	4861	43
H(8A)	7436	4357	3291	33
H(8B)	9051	3637	3447	33
H(9A)	9292	−315	1488	48
H(9B)	7739	−1145	1719	48
H(9C)	8379	−935	2580	48
H(10A)	5132	−202	3184	47
H(10B)	4413	−434	2355	47
H(10C)	4219	785	2411	47

H(11A)	7770	1083	26	26
H(11B)	5943	613	307	26
H(12A)	7378	3182	327	32
H(12B)	6808	4001	−680	32
H(13A)	9511	2544	−487	44
H(13B)	9626	3910	−917	44
H(14A)	10009	3220	−2183	57
H(14B)	8514	4058	−2290	57
H(15A)	7647	2455	−2493	51
H(15B)	8242	1610	−1497	51
H(16A)	5606	3120	−1648	36
H(16B)	5420	1761	−1228	36
H(17A)	3053	3244	6041	52
H(17B)	4844	3812	5783	52
H(17C)	4559	2467	6408	52
H(18A)	4138	779	5235	49
H(18B)	3367	1402	4253	49
H(18C)	2401	1342	5264	49
H(19A)	3958	4003	2995	55
H(19B)	4629	4851	3405	55
H(19C)	2781	4380	3739	55
H(20A)	4081	3904	1116	51
H(20B)	5134	2798	1561	51
H(20C)	3201	2714	1857	51
H(21A)	1410	1390	782	43
H(21B)	2985	631	969	43
H(21C)	2490	1203	−101	43
H(22A)	2269	4344	−635	61
H(22B)	2961	3774	−1369	61
H(22C)	4124	4581	−1144	61

8.2.13 Kristallstrukturen aus Kapitel 4.7

8.2.13.1 Verbindung 136

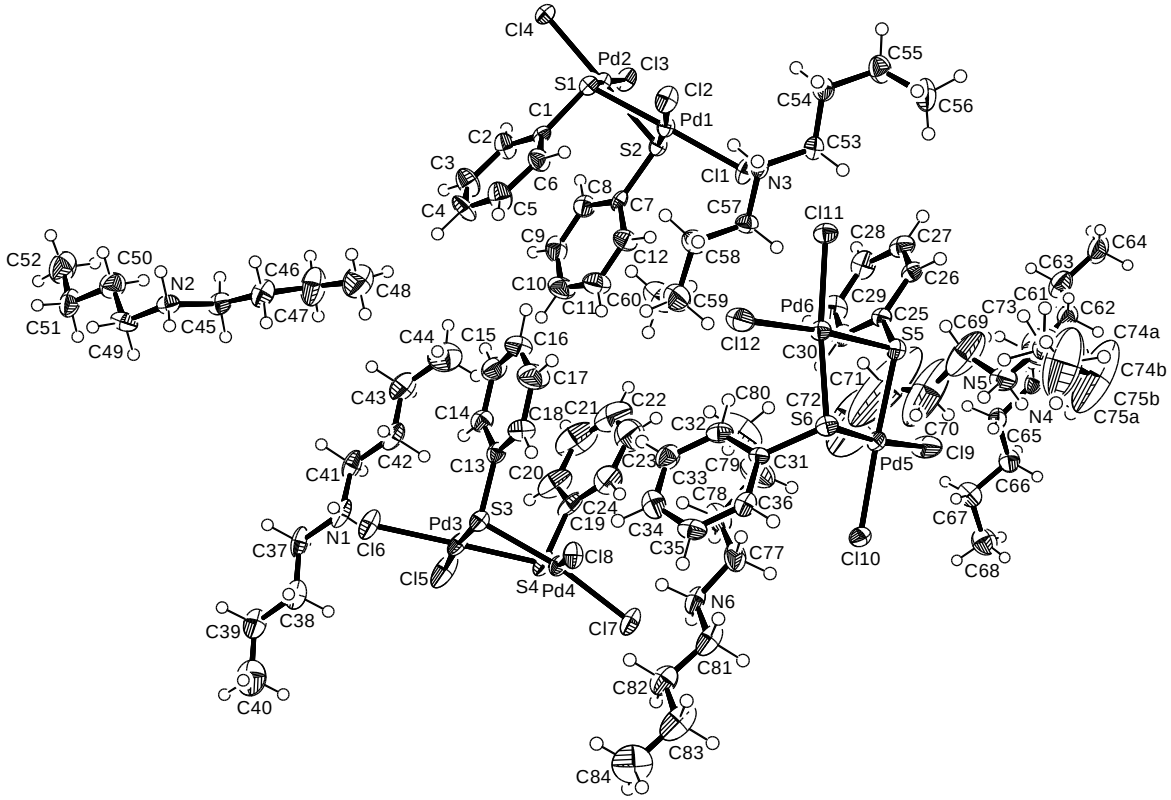


Abb. 8.34 Thermische Auslenkungsellipsoide (50% Aufenthaltswahrscheinlichkeit) der Molekülstruktur des Zinksilylamids **136** im Kristall (Ortep−Darstellung).

Tabelle 8.100 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **136**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalen U^{ij} Tensors.

	x	y	z	U(eq)
C(74A)	4393(4)	11085(4)	3843(3)	159(4)
C(75A)	4141(8)	11625(7)	3894(8)	176(9)
C(75B)	3484(4)	11648(3)	3997(3)	173(5)
C(74B)	3642(6)	11103(7)	3841(4)	97(5)
C(1)	726(2)	4320(2)	3320(1)	20(1)
C(2)	881(2)	3631(2)	3466(2)	36(1)
C(3)	902(2)	3419(2)	3952(2)	44(1)
C(4)	762(2)	3863(2)	4292(2)	41(1)
C(5)	596(2)	4543(2)	4137(2)	42(1)
C(6)	581(2)	4768(2)	3657(2)	33(1)
C(7)	2329(2)	4418(2)	3436(1)	22(1)
C(8)	2467(2)	3718(2)	3529(2)	34(1)
C(9)	2694(2)	3478(2)	4025(2)	42(1)
C(10)	2783(2)	3929(2)	4433(2)	50(1)
C(11)	2652(2)	4626(2)	4339(2)	47(1)
C(12)	2425(2)	4868(2)	3848(2)	35(1)
C(13)	2596(2)	4994(2)	6410(1)	26(1)
C(14)	2591(2)	4407(2)	6118(2)	32(1)
C(15)	2261(2)	4398(2)	5605(2)	44(1)
C(16)	1914(2)	4961(3)	5384(2)	53(1)
C(17)	1902(2)	5558(2)	5669(2)	57(2)
C(18)	2239(2)	5571(2)	6184(2)	40(1)

C(19)	4251(2)	4867(2)	6462(2)	39(1)
C(20)	4379(2)	4236(2)	6263(2)	61(2)
C(21)	4305(3)	4176(3)	5742(3)	89(2)
C(22)	4117(3)	4738(4)	5436(2)	89(2)
C(23)	3984(2)	5360(3)	5623(2)	76(2)
C(24)	4052(2)	5426(3)	6140(2)	55(1)
C(25)	2777(2)	9314(2)	4071(2)	22(1)
C(26)	2681(2)	9423(2)	3552(2)	26(1)
C(27)	2813(2)	8892(2)	3254(2)	37(1)
C(28)	3040(2)	8252(2)	3468(2)	39(1)
C(29)	3139(2)	8150(2)	3979(2)	41(1)
C(30)	3006(2)	8669(2)	4284(2)	32(1)
C(31)	2268(2)	9373(2)	5867(1)	20(1)
C(32)	2188(2)	8665(2)	5746(2)	31(1)
C(33)	2157(2)	8178(2)	6114(2)	37(1)
C(34)	2197(2)	8395(2)	6600(2)	38(1)
C(35)	2280(2)	9099(2)	6730(2)	34(1)
C(36)	2314(2)	9584(2)	6357(2)	27(1)
C(37)	3800(2)	1277(2)	7704(2)	41(1)
C(38)	4024(2)	1582(2)	8230(2)	43(1)
C(39)	4193(2)	1025(2)	8641(2)	48(1)
C(40)	4445(2)	1320(2)	9176(2)	74(2)
C(41)	3533(2)	1558(2)	6766(2)	41(1)
C(42)	3356(2)	2141(2)	6375(2)	45(1)
C(43)	3206(2)	1875(2)	5834(2)	53(1)
C(44)	3037(2)	2456(2)	5432(2)	72(2)
C(45)	835(2)	721(2)	5879(2)	36(1)
C(46)	761(2)	1466(2)	5678(2)	44(1)
C(47)	1233(2)	1608(2)	5374(2)	68(2)
C(48)	1229(2)	2334(2)	5211(2)	71(2)
C(49)	427(2)	−168(2)	6398(1)	39(1)
C(50)	334(2)	−769(2)	6052(2)	50(1)
C(51)	428(2)	−1469(2)	6336(2)	49(1)
C(52)	386(2)	−2076(2)	5967(2)	67(2)
C(53)	1291(2)	8177(2)	2804(2)	29(1)
C(54)	780(2)	8276(2)	2303(1)	34(1)
C(55)	1004(2)	8685(2)	1908(2)	40(1)
C(56)	1176(2)	9446(2)	2067(2)	51(1)
C(57)	1511(2)	7691(2)	3686(1)	28(1)
C(58)	1204(2)	7425(2)	4074(2)	36(1)
C(59)	1690(2)	7201(2)	4573(2)	55(1)
C(60)	2041(2)	6529(2)	4507(2)	69(2)
C(61)	8678(2)	6334(2)	2561(2)	32(1)
C(62)	8576(2)	6680(2)	2051(2)	42(1)
C(63)	8624(2)	6181(2)	1645(2)	57(1)
C(64)	8547(2)	6519(2)	1132(2)	69(2)
C(65)	8680(2)	6486(2)	3466(2)	36(1)
C(66)	9374(2)	6489(2)	3782(2)	40(1)
C(67)	9481(2)	6081(2)	4273(2)	43(1)
C(68)	10140(2)	6224(2)	4660(2)	58(1)
C(69)	4636(3)	9092(3)	3798(2)	102(2)
C(70)	4956(3)	8570(4)	4229(4)	204(5)
C(71)	4931(4)	7905(5)	4264(6)	318(12)
C(72)	5200(5)	7518(5)	4659(6)	232(6)
C(73)	4392(3)	10388(3)	3620(2)	106(2)
C(77)	3904(2)	8324(2)	6618(2)	44(1)
C(78)	3886(2)	7710(2)	6274(2)	49(1)
C(79)	3817(2)	7924(2)	5727(2)	68(2)
C(80)	3734(3)	7325(3)	5365(2)	101(2)
C(81)	3916(2)	8723(2)	7484(2)	43(1)
C(82)	3864(2)	8501(2)	7996(2)	45(1)
C(83)	3828(2)	9120(2)	8341(2)	62(2)

C(84)	3773(2)	8909(2)	8850(2)	76(2)
Cl(1)	2061(1)	6469(1)	2930(1)	34(1)
Cl(2)	444(1)	6325(1)	2793(1)	35(1)
Cl(3)	2064(1)	3361(1)	2049(1)	31(1)
Cl(4)	487(1)	3152(1)	1957(1)	27(1)
Cl(5)	4502(1)	3252(1)	7475(1)	56(1)
Cl(6)	2944(1)	3326(1)	7429(1)	41(1)
Cl(7)	4664(1)	6615(1)	7430(1)	37(1)
Cl(8)	3030(1)	6803(1)	7163(1)	30(1)
Cl(9)	4176(1)	9819(1)	4989(1)	50(1)
Cl(10)	3858(1)	9986(1)	6114(1)	29(1)
Cl(11)	1113(1)	9413(1)	3765(1)	29(1)
Cl(12)	817(1)	9340(1)	4895(1)	44(1)
N(1)	3654(2)	1829(2)	7296(1)	40(1)
N(2)	338(2)	527(2)	6119(1)	32(1)
N(3)	1035(1)	7829(1)	3187(1)	27(1)
N(4)	8570(1)	6808(1)	2952(1)	35(1)
N(5)	4697(2)	9834(2)	3975(1)	49(1)
N(6)	3938(1)	8120(2)	7140(1)	36(1)
Pd(1)	1304(1)	5570(1)	2812(1)	24(1)
Pd(2)	1322(1)	3933(1)	2383(1)	22(1)
Pd(3)	3694(1)	4113(1)	7271(1)	30(1)
Pd(4)	3760(1)	5879(1)	7200(1)	24(1)
Pd(5)	3248(1)	9937(1)	5248(1)	25(1)
Pd(6)	1689(1)	9667(1)	4620(1)	24(1)
S(1)	649(1)	4608(1)	2688(1)	23(1)
S(2)	2059(1)	4743(1)	2800(1)	25(1)
S(3)	2985(1)	5031(1)	7082(1)	25(1)
S(4)	4377(1)	4941(1)	7131(1)	33(1)
S(5)	2588(1)	10013(1)	4427(1)	26(1)
S(6)	2290(1)	10032(1)	5415(1)	25(1)

Tabelle 8.101 Anisotrope auslenkungsparameter ($Å^2 \times 10^3$) für die Verbindung **136**. Der Exponent des anisotropen Auslenkungsfaktors hat die Form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	**U22**	**U33**	**U23**	**U13**	**U12**
C(74A)	149(9)	74(5)	294(11)	43(7)	127(8)	5(6)
C(75A)	79(13)	52(9)	410(30)	−42(13)	104(15)	4(9)
C(75B)	164(10)	69(5)	325(12)	−11(6)	133(9)	−8(6)
C(74B)	89(12)	173(15)	18(6)	43(8)	0(6)	−87(11)
C(1)	14(2)	25(2)	24(3)	−7(2)	9(2)	−2(2)
C(2)	51(3)	28(3)	35(3)	−2(2)	24(3)	2(2)
C(3)	59(4)	33(3)	44(4)	11(3)	23(3)	11(2)
C(4)	61(4)	48(3)	22(3)	8(2)	22(3)	7(3)
C(5)	55(4)	40(3)	43(3)	−2(2)	30(3)	4(2)
C(6)	41(3)	25(3)	32(3)	4(2)	10(2)	3(2)
C(7)	13(2)	20(2)	35(3)	−4(2)	11(2)	−1(2)
C(8)	28(3)	34(3)	39(3)	3(2)	8(2)	3(2)
C(9)	33(3)	36(3)	55(4)	16(3)	11(3)	7(2)
C(10)	36(3)	67(4)	38(3)	17(3)	0(3)	8(3)
C(11)	49(4)	48(3)	35(3)	1(3)	2(3)	5(3)
C(12)	37(3)	34(3)	32(3)	5(2)	7(2)	9(2)
C(13)	20(3)	26(2)	33(3)	2(2)	8(2)	0(2)
C(14)	27(3)	32(3)	37(3)	1(2)	7(2)	2(2)
C(15)	45(4)	44(3)	42(4)	−10(3)	11(3)	−11(3)
C(16)	58(4)	69(4)	27(3)	−2(3)	5(3)	−15(3)
C(17)	59(4)	50(3)	48(4)	8(3)	−4(3)	11(3)
C(18)	38(3)	45(3)	33(3)	−4(2)	4(3)	0(2)
C(19)	18(3)	44(3)	58(4)	−22(3)	14(2)	−11(2)
C(20)	41(4)	62(4)	80(5)	−31(3)	17(3)	−2(3)
C(21)	67(5)	93(5)	112(7)	−64(5)	35(5)	−2(4)
C(22)	51(5)	156(7)	74(5)	−52(5)	41(4)	−37(5)

C(23)	79(5)	94(5)	67(5)	−11(4)	40(4)	−19(4)
C(24)	59(4)	66(4)	53(4)	−22(3)	36(3)	−11(3)
C(25)	13(2)	31(3)	23(3)	0(2)	7(2)	1(2)
C(26)	19(3)	31(3)	29(3)	−6(2)	10(2)	−4(2)
C(27)	22(3)	58(3)	34(3)	−7(3)	12(2)	−8(2)
C(28)	37(3)	34(3)	53(4)	−6(3)	25(3)	3(2)
C(29)	36(3)	38(3)	49(4)	2(3)	14(3)	10(2)
C(30)	25(3)	39(3)	33(3)	−3(2)	12(2)	−6(2)
C(31)	16(3)	28(2)	17(3)	−2(2)	5(2)	2(2)
C(32)	19(3)	41(3)	30(3)	−3(2)	2(2)	5(2)
C(33)	33(3)	29(3)	45(3)	1(3)	5(3)	−1(2)
C(34)	22(3)	48(3)	47(4)	15(3)	13(3)	8(2)
C(35)	16(3)	58(3)	27(3)	−2(3)	5(2)	8(2)
C(36)	18(3)	24(2)	39(3)	0(2)	9(2)	5(2)
C(37)	36(3)	18(3)	76(4)	7(3)	28(3)	−1(2)
C(38)	37(3)	31(3)	65(4)	2(3)	24(3)	3(2)
C(39)	35(3)	37(3)	70(4)	12(3)	15(3)	4(2)
C(40)	53(4)	76(4)	96(5)	18(3)	24(4)	9(3)
C(41)	32(3)	32(3)	68(4)	−12(3)	30(3)	−7(2)
C(42)	42(3)	30(3)	65(4)	−13(3)	19(3)	−9(2)
C(43)	37(3)	48(3)	73(4)	−8(3)	16(3)	−4(2)
C(44)	69(4)	66(4)	71(4)	−4(3)	9(3)	9(3)
C(45)	20(3)	52(3)	38(3)	−9(2)	14(2)	1(2)
C(46)	37(3)	34(3)	61(4)	−1(2)	16(3)	−2(2)
C(47)	51(4)	43(3)	115(5)	22(3)	34(3)	8(3)
C(48)	56(4)	65(4)	90(4)	0(3)	19(3)	−3(3)
C(49)	40(3)	51(3)	24(3)	2(2)	5(2)	9(2)
C(50)	54(4)	39(3)	52(3)	−3(3)	11(3)	−6(2)
C(51)	37(3)	39(3)	67(4)	20(3)	11(3)	−5(2)
C(52)	66(4)	43(3)	87(4)	7(3)	18(3)	−8(3)
C(53)	30(3)	27(2)	34(3)	0(2)	13(2)	−2(2)
C(54)	40(3)	27(2)	35(3)	3(2)	10(2)	−1(2)
C(55)	52(4)	27(3)	44(3)	4(2)	18(3)	1(2)
C(56)	53(4)	46(3)	61(3)	13(3)	28(3)	−9(2)
C(57)	29(3)	28(2)	26(3)	0(2)	3(2)	4(2)
C(58)	42(3)	36(3)	31(3)	−1(2)	13(3)	3(2)
C(59)	73(4)	50(3)	41(4)	0(3)	17(3)	−10(3)
C(60)	69(4)	85(4)	53(4)	16(3)	17(3)	15(3)
C(61)	25(3)	25(2)	46(3)	−9(2)	12(2)	3(2)
C(62)	50(4)	35(3)	44(3)	−5(3)	16(3)	−7(2)
C(63)	63(4)	50(3)	64(4)	−19(3)	29(3)	−18(3)
C(64)	107(5)	48(3)	60(4)	−16(3)	35(3)	−37(3)
C(65)	42(3)	33(3)	38(3)	1(2)	16(3)	−7(2)
C(66)	31(3)	41(3)	48(3)	8(2)	12(3)	3(2)
C(67)	40(3)	46(3)	47(3)	5(3)	19(3)	15(2)
C(68)	54(4)	58(3)	60(4)	10(3)	17(3)	9(3)
C(69)	91(6)	97(5)	149(6)	−78(5)	82(5)	−46(4)
C(70)	48(5)	71(5)	459(17)	8(9)	24(7)	6(5)
C(71)	37(7)	153(12)	720(40)	−142(18)	44(12)	8(7)
C(72)	109(10)	100(8)	470(20)	−25(9)	60(11)	36(5)
C(73)	42(4)	135(6)	121(6)	35(5)	−6(4)	8(4)
C(77)	34(3)	39(3)	56(4)	22(3)	8(3)	2(2)
C(78)	31(3)	66(4)	51(4)	23(3)	13(3)	11(3)
C(79)	59(4)	89(4)	53(4)	24(3)	11(3)	24(3)
C(80)	118(6)	123(5)	66(5)	20(4)	35(4)	51(4)
C(81)	21(3)	21(3)	80(4)	−1(3)	5(3)	4(2)
C(82)	29(3)	40(3)	62(4)	−1(3)	9(3)	2(2)
C(83)	33(3)	38(3)	107(5)	−19(3)	11(3)	7(2)
C(84)	79(5)	65(4)	85(5)	−9(3)	25(4)	20(3)
Cl(1)	37(1)	24(1)	48(1)	−9(1)	21(1)	−9(1)
Cl(2)	29(1)	26(1)	53(1)	−1(1)	16(1)	4(1)
Cl(3)	25(1)	27(1)	45(1)	−7(1)	17(1)	1(1)

Cl(4)	23(1)	24(1)	33(1)	−5(1)	7(1)	−2(1)
Cl(5)	22(1)	21(1)	116(1)	2(1)	8(1)	4(1)
Cl(6)	25(1)	26(1)	73(1)	1(1)	15(1)	−3(1)
Cl(7)	25(1)	22(1)	61(1)	3(1)	7(1)	−5(1)
Cl(8)	31(1)	20(1)	44(1)	4(1)	17(1)	5(1)
Cl(9)	22(1)	96(1)	33(1)	−7(1)	11(1)	−12(1)
Cl(10)	24(1)	31(1)	28(1)	−2(1)	4(1)	−3(1)
Cl(11)	25(1)	34(1)	26(1)	−4(1)	7(1)	2(1)
Cl(12)	23(1)	81(1)	30(1)	6(1)	10(1)	−5(1)
N(1)	29(2)	26(2)	70(3)	−10(2)	24(2)	−9(2)
N(2)	27(2)	36(2)	30(2)	−3(2)	5(2)	0(2)
N(3)	28(2)	15(2)	38(2)	5(2)	11(2)	2(2)
N(4)	23(2)	26(2)	56(3)	1(2)	12(2)	0(2)
N(5)	23(2)	87(3)	38(3)	4(2)	10(2)	−14(2)
N(6)	17(2)	24(2)	59(3)	13(2)	0(2)	0(2)
Pd(1)	25(1)	18(1)	29(1)	−1(1)	10(1)	0(1)
Pd(2)	20(1)	19(1)	26(1)	−2(1)	8(1)	0(1)
Pd(3)	18(1)	17(1)	52(1)	−3(1)	5(1)	0(1)
Pd(4)	22(1)	18(1)	31(1)	0(1)	7(1)	0(1)
Pd(5)	20(1)	27(1)	27(1)	0(1)	6(1)	−3(1)
Pd(6)	19(1)	27(1)	26(1)	0(1)	7(1)	2(1)
S(1)	21(1)	23(1)	27(1)	−3(1)	8(1)	1(1)
S(2)	24(1)	21(1)	30(1)	−2(1)	10(1)	−1(1)
S(3)	21(1)	19(1)	33(1)	−1(1)	7(1)	2(1)
S(4)	20(1)	23(1)	55(1)	−5(1)	10(1)	−2(1)
S(5)	25(1)	28(1)	27(1)	1(1)	9(1)	−3(1)
S(6)	21(1)	27(1)	27(1)	−1(1)	7(1)	3(1)

Tabelle 8.102 Wasserstoffkoordinaten (x 10^4) und isotrope Auslenkungsparameter (Å^2 x 10^3) für die Verbindung **136**.

	x	y	z	U(eq)
H(74A)	4490	11459	3626	190
H(74B)	4698	11114	4195	190
H(75A)	3596	12041	3809	256
H(75B)	3706	11695	4363	256
H(75C)	3016	11644	3939	256
H(74C)	3361	11013	3487	115
H(74D)	3570	10706	4058	115
H(2)	973	3305	3234	43
H(3)	1019	2946	4054	53
H(4)	779	3709	4626	50
H(5)	487	4864	4366	51
H(6)	468	5242	3559	40
H(8)	2405	3397	3250	41
H(9)	2790	2990	4086	51
H(10)	2934	3756	4774	60
H(11)	2720	4944	4618	57
H(12)	2332	5355	3789	42
H(14)	2821	4000	6274	39
H(15)	2277	3993	5405	53
H(16)	1674	4951	5030	64
H(17)	1660	5960	5513	68
H(18)	2224	5978	6383	48
H(20)	4518	3841	6481	74
H(21)	4386	3740	5602	107
H(22)	4078	4699	5080	107
H(23)	3845	5750	5399	91
H(24)	3959	5865	6270	66
H(26)	2522	9864	3401	31
H(27)	2748	8971	2899	44
H(28)	3125	7886	3261	47

H(29)	3304	7711	4129	49
H(30)	3072	8585	4640	38
H(32)	2154	8512	5407	37
H(33)	2109	7692	6029	45
H(34)	2170	8059	6849	46
H(35)	2312	9251	7067	41
H(36)	2370	10070	6444	32
H(37A)	3409	991	7668	49
H(37B)	4137	958	7654	49
H(38A)	3680	1886	8282	51
H(38B)	4406	1880	8260	51
H(39A)	4522	707	8578	58
H(39B)	3805	737	8616	58
H(40A)	4832	1600	9206	112
H(40B)	4552	931	9424	112
H(40C)	4115	1618	9248	112
H(41A)	3181	1208	6692	49
H(41B)	3925	1317	6739	49
H(42A)	2976	2395	6414	54
H(42B)	3717	2481	6442	54
H(43A)	2840	1542	5766	64
H(43B)	3583	1612	5799	64
H(44A)	2667	2722	5466	106
H(44B)	2932	2247	5090	106
H(44C)	3407	2774	5485	106
H(45A)	812	393	5592	42
H(45B)	1265	668	6134	42
H(46A)	843	1799	5969	52
H(46B)	315	1538	5455	52
H(47A)	1673	1482	5588	81
H(47B)	1123	1300	5067	81
H(48A)	786	2484	5040	106
H(48B)	1485	2379	4972	106
H(48C)	1417	2635	5511	106
H(49A)	867	−187	6643	47
H(49B)	117	−199	6597	47
H(50A)	645	−737	5851	59
H(50B)	−105	−751	5807	59
H(51A)	854	−1474	6601	58
H(51B)	94	−1524	6511	58
H(52A)	−50	−2100	5728	99
H(52B)	486	−2518	6160	99
H(52C)	695	−2002	5775	99
H(53A)	1643	7887	2750	35
H(53B)	1474	8642	2937	35
H(54A)	412	8529	2364	41
H(54B)	624	7808	2159	41
H(55A)	1387	8448	1859	48
H(55B)	660	8680	1576	48
H(56A)	825	9664	2170	76
H(56B)	1243	9710	1779	76
H(56C)	1572	9460	2358	76
H(57A)	1750	8130	3816	34
H(57B)	1825	7337	3642	34
H(58A)	925	7019	3926	43
H(58B)	929	7801	4146	43
H(59A)	1466	7120	4833	66
H(59B)	2007	7583	4697	66
H(60A)	1728	6154	4371	103
H(60B)	2334	6385	4840	103
H(60C)	2291	6618	4268	103
H(61A)	8383	5925	2519	38

H(61B)	9124	6150	2685	38
H(62A)	8145	6903	1944	51
H(62B)	8901	7058	2087	51
H(63A)	8291	5814	1603	68
H(63B)	9050	5945	1761	68
H(64A)	8119	6730	1004	104
H(64B)	8600	6161	890	104
H(64C)	8876	6886	1169	104
H(65A)	8523	5994	3424	43
H(65B)	8426	6748	3652	43
H(66A)	9518	6981	3865	48
H(66B)	9637	6280	3580	48
H(67A)	9442	5570	4193	52
H(67B)	9141	6205	4430	52
H(68A)	10476	6156	4493	86
H(68B)	10212	5894	4949	86
H(68C)	10154	6707	4786	86
H(69A)	4833	9044	3518	122
H(69B)	4171	8977	3655	122
H(70A)	5421	8680	4321	239
H(70B)	4822	8742	4530	239
H(71A)	5090	7729	3980	391
H(71B)	4466	7789	4160	391
H(73A)	3939	10251	3450	127
H(73B)	4610	10420	3352	127
H(77A)	4281	8621	6628	53
H(77B)	3512	8614	6473	53
H(78A)	3521	7401	6278	59
H(78B)	4288	7435	6410	59
H(79A)	3439	8241	5606	82
H(79B)	4203	8195	5722	82
H(80A)	4075	6977	5506	150
H(80B)	3760	7495	5035	150
H(80C)	3313	7105	5321	150
H(81A)	3542	9025	7311	51
H(81B)	4310	9009	7537	51
H(82A)	4241	8206	8170	53
H(82B)	3473	8206	7941	53
H(83A)	4218	9413	8390	73
H(83B)	3451	9414	8161	73
H(84A)	3412	8585	8802	114
H(84B)	3702	9331	9033	114
H(84C)	4173	8678	9048	114
H(1A)	3298	2076	7312	48
H(1B)	3995	2138	7366	48
H(2A)	−53	519	5868	38
H(2B)	320	877	6347	38
H(3A)	714	8110	3239	32
H(3B)	849	7409	3053	32
H(4A)	8152	6969	2838	42
H(4B)	8836	7192	2983	42
H(5A)	4539	9861	4251	59
H(5B)	5129	9936	4095	59
H(6A)	4314	7874	7281	44
H(6B)	3601	7821	7128	44

8.3 Angaben zu den quantenchemischen Rechnungen

8.3.1 Angaben zu den quantenchemischen Rechnungen aus Kapitel 4.1.3.1

8.103 Berechnete Energien der optimierten Verbindungen [B3LYP/6−31+G(d)].

Verbindung	SCF [Hartree]	ZPE [Hartree]
$Me_3SiN(Me)H$	−504.561838171	−504.396335
2,3−Dihydrofuran (= DHF)	−231.232563564	−231.139499
Me_3SiDHF	−639.918463273	−639.723834
$Me_3SiN(Me)^-$	−503.944166088	−503.794852
DHF^-	−230.592928411	−230.515451
$MeN(H)^-$	−95.2069936518	−95.160365
$Me_3SiN(Me)H$ in THF	−504.56523911	−504.400198
DHF in THF	−231.237572158	−231.145002
Me_3SiDHF in THF	−639.922024157	−639.72796
$Me_3SiN(Me)^-$ in THF	−504.015698551	−503.865341
DHF^- in THF	−230.683239685	−230.604831
$MeN(H)^-$ in THF	−95.3058489456	−95.257925

Tabelle 8.104 Standardorientierung von $Me_3SiN(Me)H$ in der Gasphase und in THF [Minima, B3LYP/6−31+G(d)].

Gasphase				THF			
C	0.51905700	−1.23660200	−1.43164900	**C**	−0.46726600	1.38917300	−1.28873800
H	0.39882400	−0.73483000	−2.39949600	**H**	−0.34324200	0.99924000	−2.30676800
H	−0.24624300	−2.02087100	−1.36654500	**H**	0.31140900	2.14445400	−1.12162200
H	1.49557900	−1.73851300	−1.42877800	**H**	−1.43539200	1.90501600	−1.23954300
C	0.67669600	−0.93929400	1.61967400	**C**	−0.66159000	0.75825600	1.71065000
H	1.64590400	−1.45628500	1.62398200	**H**	−1.62428200	1.28464000	1.76754000
H	0.65801300	−0.25972600	2.48170500	**H**	−0.65636600	−0.01236900	2.49294900
H	−0.09869100	−1.69941900	1.78369400	**H**	0.12428800	1.48491800	1.95651000
C	1.68526200	1.36822700	−0.18221700	**C**	−1.72737000	−1.29654100	−0.33677700
H	1.57261900	1.90238000	−1.13367400	**H**	−1.63329200	−1.72352800	−1.34297600
H	1.61027500	2.10537000	0.62815800	**H**	−1.67400500	−2.12212600	0.38543800
H	2.70094100	0.95367800	−0.14992500	**H**	−2.72726300	−0.85151000	−0.25200200
Si	0.39281900	0.00043700	−0.00599500	**Si**	−0.39009000	−0.00236200	−0.00916800
N	−1.16613900	0.79312900	−0.07932000	**N**	1.15540300	−0.82146800	−0.16904200
H	−1.20277300	1.75568200	0.23896300	**H**	1.18328300	−1.77404100	0.20012400
C	−2.45526400	0.11704500	0.03217100	**C**	2.43661700	−0.13613200	0.01815100
H	−3.24524000	0.70327400	−0.45502900	**H**	3.25892600	−0.74675200	−0.37585300
H	−2.41166000	−0.84904000	−0.48359900	**H**	2.43873000	0.80586600	−0.54208000
H	−2.76854400	−0.07597800	1.07183400	**H**	2.66828900	0.10099800	1.07020900

Tabelle 8.105 Standardorientierung von DHF in der Gasphase und in THF [Minima, B3LYP/6−31+G(d)].

Gasphase				THF			
C	1.20491000	−0.06321000	0.01031900	C	1.20827100	−0.08454600	0.01166600
C	0.56420300	1.10894500	0.04828600	C	0.58516900	1.09710400	0.05002800
O	0.39810900	−1.16736100	−0.07713500	O	0.37527700	−1.17649600	−0.08197000
H	2.26533500	−0.28490800	0.02259900	H	2.26747500	−0.32628500	0.02561200
H	1.02979200	2.08508300	0.09315400	H	1.06866400	2.06738900	0.09841300
C	−0.97047600	−0.69283100	0.08009200	C	−0.98828800	−0.67243800	0.08507400
H	−1.57992500	−1.19913500	−0.67180800	H	−1.61390100	−1.17040400	−0.65937400
H	−1.30434900	−0.99688800	1.07927900	H	−1.31699700	−0.96346400	1.08999500
C	−0.92507700	0.84816500	−0.06834600	C	−0.90882800	0.86423200	−0.07223900
H	−1.51680500	1.34454700	0.71005100	H	−1.49423900	1.37655100	0.70067000

Tabelle 8.106 Standardorientierung von Me_3SiDHF in der Gasphase und in THF [Minima, B3LYP/6−31+G(d)].

Gasphase				THF			
O	1.28570700	−1.07432200	0.09752700	O	1.29490100	−1.08065800	0.10294000
C	2.69965000	−0.79502700	−0.09880200	C	2.71144300	−0.79172500	−0.10056400
H	3.25744300	−1.39298900	0.62612300	H	3.27606700	−1.38738200	0.62134700
H	2.96091400	−1.12352900	−1.11284600	H	2.96803800	−1.11635000	−1.11709700
C	2.86801200	0.73066800	0.06809800	C	2.86919400	0.73314100	0.06874200
H	3.52068800	1.15519900	−0.70424000	H	3.51877900	1.16258700	−0.70371500
H	3.30360400	0.99929800	1.04224700	H	3.30293900	1.00325900	1.04348500
C	1.42768300	1.19142600	−0.03979200	C	1.42650900	1.18684000	−0.03816700
H	1.11697800	2.22813900	−0.08708600	H	1.11516400	2.22501300	−0.08836200
C	0.60161000	0.13230900	0.00819700	C	0.60234600	0.12605800	0.01015100
Si	−1.28602000	0.00928500	−0.00231700	Si	−1.28755700	0.00937500	−0.00282400
C	−1.84124200	−0.84446900	1.59179600	C	−1.85510500	−0.82603600	1.59711300
H	−2.93074100	−0.97769700	1.61094900	H	−2.94736500	−0.93675300	1.61369100
H	−1.37960300	−1.83484900	1.68459400	H	−1.41514800	−1.82604900	1.69764700
H	−1.55858000	−0.26098600	2.47666000	H	−1.56297000	−0.24098400	2.47827700
C	−1.99309200	1.76107200	−0.10443700	C	−1.98885700	1.76070100	−0.12278700
H	−1.67479300	2.27281800	−1.02103000	H	−1.66849100	2.26260400	−1.04432700
H	−3.09033800	1.73182400	−0.10715200	H	−3.08633300	1.72982600	−0.12609200
H	−1.68177600	2.37466100	0.74989700	H	−1.67719700	2.38155000	0.72642800
C	−1.81876400	−1.01302900	−1.50212700	C	−1.82333300	−1.02523300	−1.49361100
H	−1.36055700	−2.00906700	−1.47777800	H	−1.37926800	−2.02775100	−1.45764000
H	−2.90839500	−1.14462100	−1.52457900	H	−2.91490100	−1.14211700	−1.51620700
H	−1.51937600	−0.53130700	−2.44113400	H	−1.51592000	−0.55590700	−2.43667500

Tabelle 8.107 Standardorientierung von $Me_3SiN(Me)^-$ in der Gasphase und in THF [Minima, B3LYP/6−31+G(d)].

Gasphase				THF			
C	−0.72445200	−1.06411600	1.51014000	C	−0.56676300	1.14601300	−1.46372300
H	−0.64907500	−0.50092400	2.45205400	H	−0.58016200	0.61832200	−2.42842500
H	−0.03214100	−1.91674200	1.58572300	H	0.23570600	1.89653300	−1.51516800
H	−1.74578700	−1.47320400	1.43998200	H	−1.51820500	1.69057800	−1.36640500
C	−0.72432000	−1.06434700	−1.51001000	C	−0.55398000	1.02559100	1.55140400
H	−1.74547800	−1.47383600	−1.43963700	H	−1.50223400	1.58197700	1.50266700
H	−0.64934500	−0.50117400	−2.45196800	H	−0.56649800	0.42245900	2.47086300
H	−0.03168300	−1.91670000	−1.58568400	H	0.25386300	1.76433300	1.65864300
C	−1.60718000	1.44005300	−0.00014200	C	−1.77364500	−1.27577300	−0.04520000
H	−1.49661200	2.08138100	0.88524500	H	−1.76684700	−1.89339800	−0.95415100
H	−1.49622300	2.08155000	−0.88535600	H	−1.76265500	−1.95815700	0.81614500
H	−2.62715500	1.02577900	−0.00040000	H	−2.72361400	−0.72307800	−0.02269800

Si	−0.26344700	0.07399500	−0.00000500	**Si**	−0.27867400	−0.08699100	−0.00416200
N	1.24486800	0.77179500	−0.00002000	**N**	1.18093600	−0.94140600	−0.04355900
C	2.50531100	0.09805800	0.00003100	**C**	2.41793300	−0.18094400	−0.00921500
H	3.35104900	0.81876000	−0.00026800	**H**	3.30137500	−0.84744200	−0.04029300
H	2.70033000	−0.56037300	0.88658700	**H**	2.56098700	0.52377100	−0.86294100
H	2.70014400	−0.56089500	−0.88617900	**H**	2.56190700	0.44249600	0.90535000

Tabelle 8.108 Standardorientierung von DHF^- in der Gasphase und in THF [Minima, B3LYP/6−31+G(d)].

Gasphase				**THF**			
C	0.53517000	−1.25331100	0.01648800	**C**	0.55480500	−1.24234400	0.01806400
C	1.23673700	−0.08203900	0.07638700	**C**	1.23863100	−0.06663400	0.06968900
O	−0.85282600	−0.89761700	−0.11084800	**O**	−0.84176600	−0.91347500	−0.10568000
H	2.32291200	−0.02869200	0.12366800	**H**	2.32387900	0.00344500	0.12531700
C	−1.02101900	0.52240200	0.11750400	**C**	−1.03208300	0.51615700	0.11180100
H	−1.80777500	0.89528000	−0.55415700	**H**	−1.81096400	0.86715500	−0.57457400
H	−1.35298500	0.66944900	1.16179000	**H**	−1.38200200	0.65727100	1.14669100
C	0.35980100	1.15758800	−0.10240400	**C**	0.34422600	1.16020600	−0.09718000
H	0.55185100	1.96817800	0.61958000	**H**	0.53244300	1.96000600	0.63263000
H	0.44446200	1.60888200	−1.11194200	**H**	0.43729800	1.61561200	−1.09887200

Tabelle 8.109 Standardorientierung von $MeN(H)^-$ in der Gasphase und in THF [Minima, B3LYP/6−31+G(d)].

Gasphase				**THF**			
C	0.61268200	−0.01503600	0.00000000	**C**	0.62638700	−0.01661500	−0.00003800
H	1.08291100	−0.54693800	−0.88890800	**H**	1.05891000	−0.54961300	−0.88457500
H	1.09253400	0.98383400	0.00000000	**H**	1.10634300	0.97739000	−0.00144100
H	1.08291100	−0.54693800	0.88890800	**H**	1.05856200	−0.54675700	0.88641300
N	−0.81576000	0.14346900	0.00000000	**N**	−0.82270500	0.14602000	−0.00003800
H	−1.22412400	−0.80402500	0.00000000	**H**	−1.22320100	−0.80346800	0.00009700

8.3.2 Angaben zu den quantenchemischen Rechnungen aus Kapitel 4.2

8.110 Berechnete Energien der optimierten Verbindungen [B3LYP/6−31+G(d)].

Verbindung	**SCF [Hartree]**	**ZPE [Hartree]**
66·EtLi	−959.960717852	−959.504387
66·EtLi (ÜZ)	−959.951592925	−959.499021
66·Et_2Mg	−1231.75026078	−1231.228641
66·Et_2Mg (ÜZ)	−1231.72521522	−1231.207591
66·Et_2Zn	−2810.82637397	−2810.303943
66·Et_2Zn (ÜZ)	−2810.78027076	−2810.262282
66·Et_3Al (Koordination an N_{Si})	−1353.33042995	−1352.7405
66·Et_3Al (Koordination an N)	−1353.34030371	−1352.75162

66·Et_3Al (ÜZ)	−1353.28209197	−1352.696314
66·Me_3Al (Koordination an N_{Si})	−1235.41319151	−1234.910033
66·Me_3Al (Koordination an N)	−1235.42014054	−1234.91791
66·Me_3Al (ÜZ)	−1235.36234227	−1234.864259

Tabelle 8.111 Standardorientierung von **66·EtLi** und **66·EtLi (ÜZ)** [B3LYP/6−31+G(d)].

66·EtLi				**ÜZ**			
C	−1.75435500	3.61697800	1.10524100	**C**	0.32365300	3.54891100	−0.85744800
C	−0.56127300	3.10283500	0.26665200	**C**	−0.34906700	2.32979200	−1.53179800
C	−2.90444400	−0.15501500	0.87602800	**C**	2.99390300	−0.11623400	−1.05865100
C	−3.85786200	0.23509000	−0.25611300	**C**	3.95542700	0.69820900	−0.18783400
C	2.11159900	−0.64911400	2.73072400	**C**	−1.98560000	−1.65538000	−2.29066800
C	−0.65108400	−0.85467000	1.48363400	**C**	0.79841200	−1.17592900	−1.23445600
C	3.97018700	0.36968200	−0.47246000	**C**	−3.87216100	0.22629300	0.25772700
N	1.48493700	0.37829800	−0.08142200	**N**	−1.36925200	0.23541000	0.07238800
N	−1.56760400	−0.53990500	0.36055300	**N**	1.73216800	−0.42613200	−0.34659300
C	2.44963900	1.94357000	−1.70133200	**C**	−2.50688300	2.11617700	1.17233100
Si	1.22780600	−0.93923900	1.08223800	**Si**	−1.05084000	−1.30842500	−0.67269600
Li	−0.54919500	1.13579400	−0.32161200	**Li**	0.44436000	1.10861800	−0.00668300
C	2.56991100	0.52938000	−1.10187700	**C**	−2.52703300	0.59175800	0.92658300
C	−3.99085300	−0.89388600	−1.28610700	**C**	4.25653400	−0.02453900	1.13195200
C	−1.68812300	−1.67229500	−0.57962100	**C**	2.02063700	−1.18793900	0.88812000
C	−2.60186900	−1.33634100	−1.76332600	**C**	2.94769100	−0.41432100	1.83161100
C	1.73706400	−2.64704600	0.44874500	**C**	−1.29669400	−2.84772200	0.41753100
H	−1.74293300	4.70126500	1.33112200	**H**	0.55950900	4.38454600	−1.53883300
H	−1.81480500	3.10794000	2.08192000	**H**	1.29089800	3.29609700	−0.37741500
H	−2.71667000	3.42463100	0.60291400	**H**	−0.31083800	3.96859000	−0.06269500
H	0.36797400	3.39864600	0.79984400	**H**	0.28247700	1.99212100	−2.37607900
H	−0.51765300	3.70773700	−0.66303000	**H**	−1.28433600	2.66943400	−2.00341800
H	1.38460600	1.27834900	0.40590300	**H**	−1.08035100	1.14231000	−0.70316100
H	−2.76784400	0.68986800	1.55766600	**H**	2.73787000	0.43934000	−1.96722300
H	−3.33241400	−0.99372300	1.45895500	**H**	3.48111900	−1.05789300	−1.37601900
H	−4.83493600	0.48833000	0.17404400	**H**	4.87873900	0.88370400	−0.75103300
H	−3.47966300	1.14571600	−0.74076500	**H**	3.51059200	1.68223500	0.02033100
H	1.89787100	0.35118500	3.12796800	**H**	−1.92960600	−0.79305400	−2.96653800
H	1.79543700	−1.37938600	3.48802900	**H**	−1.56940200	−2.52471100	−2.81921300
H	3.19958800	−0.73726600	2.62228600	**H**	−3.04718500	−1.86273300	−2.10741300
H	−0.76441700	−0.04975100	2.22282500	**H**	0.78396100	−0.64774700	−2.19647500
H	−0.96985700	−1.78144600	2.00138000	**H**	1.20599100	−2.18323500	−1.44673200
H	4.11510500	1.09393400	0.33790700	**H**	−3.95395200	0.70142900	−0.72665000
H	4.11379600	−0.63604800	−0.05975400	**H**	−3.96574900	−0.85807200	0.11890600
H	4.75743300	0.53571800	−1.21844700	**H**	−4.72352200	0.55341500	0.86916100
H	2.56951700	2.71553000	−0.93223500	**H**	−2.59094100	2.67364900	0.23421600
H	3.22226300	2.10019400	−2.46306000	**H**	−3.33816800	2.41105300	1.82411400
H	1.46973000	2.09630300	−2.16658800	**H**	−1.57359500	2.42107600	1.66385600
H	−4.50711300	−1.75070600	−0.82765900	**H**	4.84138400	−0.93297900	0.92484400
H	−4.60544900	−0.57256000	−2.13621700	**H**	4.87232600	0.60482300	1.78647800
H	−2.07972100	−2.56172500	−0.04745600	**H**	2.48240200	−2.15925300	0.62512500
H	−0.68869600	−1.92909500	−0.94259300	**H**	1.07145700	−1.40569800	1.38554200
H	−2.14200800	−0.53356900	−2.35799300	**H**	2.43261700	0.49171800	2.18520300
H	−2.67307200	−2.21426400	−2.41825000	**H**	3.14660600	−1.02755400	2.71967000
H	2.82344300	−2.72910400	0.32564900	**H**	−2.36174800	−3.04502200	0.59331400
H	1.44313700	−3.38896100	1.20371100	**H**	−0.89054100	−3.72732400	−0.10140800
H	1.26869900	−2.93957400	−0.49593800	**H**	−0.80794000	−2.78314600	1.39591800
C	2.37871400	−0.50332400	−2.22606000	**C**	−2.43717300	−0.11019700	2.29861700

H	2.49783500	−1.52982700	−1.86754000	H	−2.49506300	−1.19851300	2.20062900
H	1.38251200	−0.40738100	−2.67357100	H	−1.48924600	0.13656500	2.79273700
H	3.12177800	−0.34281000	−3.01620500	H	−3.25737000	0.20871100	2.95578000

Tabelle 8.112 Standardorientierung von **66·Et_2Mg** und **66·Et_2Mg (ÜZ)** [B3LYP/6−31+G(d)].

66·Et_2Mg				**ÜZ**			
C	−1.73405000	2.33268300	2.89035400	C	0.92586100	2.86515400	2.32736100
C	−0.48472200	1.63342700	2.30752500	C	0.38200300	1.44887500	2.06136800
C	−2.48963500	−1.22527100	1.13753800	C	−2.55916900	−0.91310200	1.44593700
C	−3.72010400	−0.57700800	0.50059400	C	−3.79425300	−0.18134000	0.91686100
C	2.73725900	−2.31643800	1.61475600	C	2.59012900	−2.47612300	1.36606200
C	−0.15727400	−1.84176700	0.93924900	C	−0.32766700	−1.77862000	1.02938900
C	4.21986000	0.52864800	−0.10008800	C	3.88061300	0.80406600	0.34826600
N	1.73632500	0.24509600	0.23385500	N	1.53902800	0.06103200	−0.10051900
N	−1.28212000	−1.13916600	0.26740400	N	−1.45721900	−0.99370200	0.44282900
C	2.67938300	2.50387600	−0.00625400	C	2.36188600	2.16411600	−1.11453100
Si	1.62008400	−1.54281900	0.29602700	Si	1.37884900	−1.66639900	0.14841100
Mg	−0.52456300	1.07089700	0.20152900	Mg	−0.45651100	0.97896600	−0.08328600
C	2.81234200	1.04052500	−0.46713800	C	2.73962200	0.73004600	−0.69182700
C	−4.02897800	−1.20307200	−0.86492000	C	−4.31567500	−0.83564300	−0.36903700
C	−1.56568500	−1.76253400	−1.05153500	C	−1.96182800	−1.66560600	−0.78835100
C	−2.78003000	−1.14751400	−1.75231300	C	−3.17860600	−0.95794700	−1.39104300
C	1.98474800	−2.38327200	−1.35524600	C	1.39077000	−2.74913600	−1.41740800
C	−0.99820800	2.14951200	−1.61887600	C	−1.34858300	2.45541300	−1.35240400
C	−2.36125400	2.87661800	−1.66769000	C	−2.73688000	3.05868100	−1.05352900
H	−1.62315800	2.65465800	3.94042400	C	3.25173400	−0.01018300	−1.94246400
H	−2.62095200	1.68093700	2.86011300	H	0.69167500	3.24058100	3.33539100
H	−1.99497200	3.23178600	2.31376700	H	0.52141900	3.59772600	1.61520900
H	−0.23239500	0.77867300	2.96785400	H	2.01931300	2.89857700	2.22637900
H	0.37029100	2.32657000	2.43359900	H	−0.71355700	1.46660900	2.24742100
H	1.71554700	0.56909200	1.20686700	H	1.14556300	0.68932700	0.94980000
H	−2.24476000	−0.73524700	2.08441100	H	0.75287100	0.76649100	2.84434500
H	−2.69950500	−2.28959600	1.35273500	H	−2.16270700	−0.41037100	2.33384100
H	−4.56810600	−0.69089700	1.18770800	H	−2.83389500	−1.94041600	1.74571500
H	−3.55089400	0.50209200	0.38596200	H	−4.56370700	−0.18806100	1.69930400
H	2.60741400	−1.83207100	2.59081100	H	−3.54763700	0.87035100	0.72401600
H	2.50382500	−3.38190600	1.74424400	H	2.67939800	−1.90041000	2.29520000
H	3.79745200	−2.24374300	1.34654600	H	2.25629800	−3.48972900	1.62869800
H	−0.14446700	−1.50041500	1.98278500	H	3.59505300	−2.57125400	0.93638300
H	−0.36050000	−2.92914800	0.98245300	H	−0.16527200	−1.39322400	2.04339300
H	4.37950300	0.55503400	0.98479500	H	−0.63559800	−2.83302100	1.14950700
H	4.37968300	−0.49967900	−0.44485300	H	3.55517600	1.34325200	1.24480600
H	4.99030400	1.15326100	−0.56819900	H	4.20398200	−0.19626500	0.65612300
H	2.79880900	2.59320900	1.08096800	H	4.75316600	1.32738900	−0.06365800
H	3.45325500	3.11947600	−0.47868800	H	1.98041800	2.74552000	−0.26879300
H	1.70426900	2.91929500	−0.27901100	H	3.23890800	2.69254100	−1.50810800
H	−4.34152900	−2.24939900	−0.72636500	H	1.59640900	2.15412600	−1.89893700
H	−4.86508000	−0.68302300	−1.34799400	H	−4.71237000	−1.83554300	−0.13680800
H	−1.72844600	−2.84758400	−0.90638900	H	−5.14591900	−0.25379100	−0.78697900
H	−0.67835100	−1.64770600	−1.67933000	H	−2.22235100	−2.71003300	−0.53792200
H	−2.55451500	−0.10771700	−2.01270300	H	−1.14566800	−1.70449700	−1.51513900
H	−2.94535900	−1.68763000	−2.69358800	H	−2.88508400	0.03923500	−1.74101500
H	3.05813000	−2.37328400	−1.57925600	H	−3.50542300	−1.52375200	−2.27281700
H	1.68024500	−3.43605800	−1.28402300	H	2.41203100	−3.03223600	−1.69846600
H	1.46111500	−1.94412400	−2.20925300	H	0.83872700	−3.68058300	−1.23074200
H	−0.21121400	2.91497500	−1.75101100	H	0.93798100	−2.25942600	−2.28656100
H	−0.90521400	1.51421400	−2.51945100	H	−0.61526600	3.28073900	−1.35823300
H	−2.47393300	3.57724900	−0.82777900	H	−1.34321500	2.08597400	−2.39414400
H	−3.20795900	2.17622000	−1.59850200	H	−2.79169600	3.47563300	−0.03731700

H	−2.52247600	3.46285700	−2.58892900	H	−3.53948600	2.31040900	−1.12860500
C	2.60608000	0.97030100	−1.98861000	H	−3.01478700	3.87463000	−1.74132800
H	2.77609300	−0.03816200	−2.37660900	H	3.63670100	−1.00691000	−1.69836500
H	1.59476000	1.28621500	−2.26112600	H	2.45684100	−0.12148500	−2.68863500
H	3.31884500	1.63648800	−2.48862200	H	4.07354200	0.55067500	−2.40536100

Tabelle 8.113 Standardorientierung von **66·Et_2Zn** und **66·Et_2Zn (ÜZ)** [B3LYP/6−31+G(d)].

66·Et_2Zn				**ÜZ**			
C	1.81756600	−2.38279500	2.64901800	C	0.86732800	2.76689200	2.30259900
C	0.56931300	−1.67961900	2.07689900	C	0.30357700	1.36092100	2.03752100
C	2.44404500	1.31313000	1.23503100	C	−2.50116800	−1.00795700	1.44443200
C	3.71887200	0.71612800	0.63622700	C	−3.74182200	−0.28701900	0.91610700
C	−2.71704900	2.66064700	1.44178600	C	2.64350100	−2.56402500	1.36444100
C	0.11275100	1.86186100	0.95682700	C	−0.27474700	−1.87629100	1.03119700
C	−4.45707800	−0.34544700	0.21257700	C	3.90761900	0.74754500	0.42731400
N	−1.95626600	−0.09311300	0.28171300	N	1.58397600	−0.00779300	−0.05634100
N	1.28405000	1.22396200	0.31501700	N	−1.40152400	−1.09479400	0.44133000
C	−2.92798500	−2.33439400	0.14549700	C	2.42050100	2.10192800	−1.06847700
Si	−1.64979800	1.64620100	0.24036600	Si	1.42974700	−1.73493600	0.15935700
Zn	0.64900100	−1.21391600	0.11713300	C	2.78449500	0.66874800	−0.63307700
C	−3.09575000	−0.86827900	−0.29553400	C	−4.26219300	−0.94852700	−0.36655400
C	4.07212700	1.39886300	−0.69055100	C	−1.90480200	−1.76970500	−0.78697200
C	1.60011700	1.89297900	−0.96615900	C	−3.12632000	−1.07172100	−1.38988700
C	2.86476600	1.34448200	−1.63388300	C	1.45084200	−2.80076200	−1.42044200
C	−1.88690200	2.38658300	−1.48263100	C	3.32604500	−0.07022000	−1.87398300
C	0.81702300	−1.77334000	−1.80344800	H	0.62236000	3.14578100	3.30650700
C	2.08685400	−2.57555400	−2.15409400	H	0.48071600	3.49973600	1.58188400
H	1.70373600	−2.65898200	3.70949400	H	1.96203900	2.78523700	2.21773100
H	2.71318100	−1.74955500	2.58177100	H	−0.79017400	1.39318800	2.20133400
H	2.04498700	−3.30771100	2.10215800	H	0.65794600	0.66613200	2.81743700
H	0.34973300	−0.78834200	2.68774900	H	1.08525300	0.63824600	0.98171600
H	−0.29723100	−2.34673400	2.21412300	H	−2.10415200	−0.49720500	2.32670000
H	−1.75750100	−0.45415500	1.21534600	H	−2.77067000	−2.03452300	1.75204500
H	2.17534800	0.79107900	2.15848400	H	−4.50966400	−0.29684700	1.70022800
H	2.62313800	2.37503000	1.49594100	H	−3.49964500	0.76480600	0.72191700
H	4.53371500	0.82404400	1.36372700	H	2.72889100	−2.00683900	2.30528300
H	3.57799900	−0.36164100	0.47563900	H	2.31311600	−3.58410800	1.60620300
H	−2.64197300	2.28251500	2.46954800	H	3.64991600	−2.64718100	0.93559000
H	−2.40389300	3.71357600	1.45469700	H	−0.12271000	−1.49657400	2.04859800
H	−3.77659500	2.63822800	1.16091300	H	−0.57833900	−2.93312300	1.14192500
H	0.04946800	1.46636300	1.97996500	H	3.56619000	1.29349200	1.31378500
H	0.29748400	2.94907100	1.07859800	H	4.22248800	−0.25110300	0.74865000
H	−4.50150400	−0.36927500	1.30827100	H	4.78919300	1.26597800	0.02796500
H	−4.63322200	0.68683100	−0.11186300	H	2.00471200	2.68192700	−0.23893300
H	−5.28129400	−0.95831900	−0.17400100	H	3.31315600	2.62857700	−1.42849400
H	−2.94650300	−2.42372400	1.23964300	H	1.68607900	2.08852200	−1.88076700
H	−3.74275700	−2.95034900	−0.25208800	H	−4.65398800	−1.94912300	−0.12925200
H	−1.97917900	−2.74581800	−0.21404200	H	−5.09654500	−0.37308300	−0.78584600
H	4.34804700	2.44710700	−0.49946600	H	−2.16172100	−2.81436100	−0.53279800
H	4.94432600	0.92084700	−1.15374300	H	−1.08907500	−1.80544700	−1.51307100
H	1.72124500	2.98068200	−0.78809900	H	−2.83691700	−0.07647800	−1.74674900
H	0.74593500	1.76770000	−1.63536900	H	−3.45287800	−1.64438200	−2.26738800
H	2.68598400	0.30963600	−1.94469600	H	2.47384700	−3.07721600	−1.70209400
H	3.05548100	1.92522100	−2.54583900	H	0.90061200	−3.73595000	−1.24697300
H	−2.95204900	2.50645300	−1.71538500	H	0.99936600	−2.30104700	−2.28472700
H	−1.43863900	3.38855800	−1.50906500	H	3.71316900	−1.06409000	−1.62142300
H	−1.43361400	1.79343500	−2.28256800	H	2.54497200	−0.18830300	−2.63362300
H	−0.06048200	−2.40043200	−2.02559300	H	4.15246000	0.49499500	−2.32363900
H	0.72903600	−0.90527100	−2.47430500	Zn	−0.45110400	0.88715300	−0.11859300

H	2.16730800	−3.48679500	−1.54627300	C	−1.22752200	2.26274400	−1.35701300
H	3.00541500	−1.99871000	−1.97602200	C	−2.56983500	2.92612700	−1.00229200
H	2.11241100	−2.89196400	−3.20913100	H	−0.45734800	3.04361300	−1.42295000
C	−3.05822700	−0.80386600	−1.83225600	H	−1.28685700	1.82908300	−2.36716100
H	−3.26888200	0.20328700	−2.20384900	H	−2.55225300	3.37516600	−0.00028100
H	−2.07931300	−1.11330700	−2.21040700	H	−3.40458400	2.21322000	−1.01929500
H	−3.81936600	−1.47211100	−2.25233500	H	−2.83244500	3.72982600	−1.70764700

Tabelle 8.114 Standardorientierung von **66·Et$_3$Al** (N_{Si}) und **66·Et$_3$Al** (ÜZ) [B3LYP/6−31+G(d)].

66·Et$_3$Al				**ÜZ**			
Si	−0.42791800	−1.19885700	−0.85112700	Si	0.22688700	−1.67173800	1.21142600
C	0.57624900	−2.76449700	−0.54348800	N	1.14815200	−0.86611000	−0.10944400
C	−1.24728300	−1.51072300	−2.53567800	C	−0.21354700	−3.51397300	1.00839700
N	0.72097300	0.25383900	−0.97123600	C	1.25270000	−1.59340400	2.80426700
C	0.15729100	1.67798000	−1.11552500	C	−1.42406600	−0.76235600	1.61757200
C	1.20720700	2.52116000	−1.86086800	C	1.56491500	−1.60116500	−1.37574100
C	−0.12223400	2.25268000	0.28105400	C	0.34602300	−1.92892900	−2.25702200
C	−1.62145200	−1.02218500	0.63444800	C	2.53741900	−0.74658100	−2.22217300
N	−2.85664400	−0.23760700	0.49767100	N	−2.19499300	−0.13917200	0.53445000
C	−3.34789500	0.21579200	1.80922600	C	−2.80909900	−1.13788400	−0.34740800
C	−4.58203200	1.11256400	1.67031600	C	−3.54881300	−0.48765700	−1.52125900
C	−5.70152000	0.39648100	0.90341900	C	−4.61393300	0.49725800	−1.02197100
C	−5.16250400	−0.14497700	−0.42684400	C	−3.98802400	1.49095600	−0.03512500
C	−3.90370700	−0.99014600	−0.20557200	C	−3.22914200	0.75821400	1.07554800
Al	2.56660900	0.02496800	0.29440300	H	2.24438100	−0.19474400	0.27106200
C	3.55083900	1.77801400	0.53788500	H	−0.96952300	−3.73403900	1.77480400
C	4.61993900	1.66409900	1.65141700	H	−0.64683000	−3.79383900	0.04344100
C	3.56418200	−1.22623300	−0.95124000	H	0.63893000	−4.17345500	1.20422200
C	5.07501100	−0.93982000	−1.10348200	H	0.68143600	−2.00230000	3.64878200
C	1.95057000	−0.68707400	2.08202900	H	1.55208800	−0.57387800	3.07074100
C	2.98044500	−1.62381100	2.75578300	H	2.16675500	−2.19288700	2.70530300
H	1.13715800	−2.76550900	0.39354100	H	−1.17657800	0.02460300	2.33752400
H	−0.13449400	−3.60199100	−0.50966100	H	−2.05236800	−1.48596700	2.18443200
H	1.27941100	−2.96824800	−1.35776000	C	2.33453000	−2.89677000	−1.03189200
H	−2.00307200	−0.78154100	−2.83482800	H	0.67002200	−2.39839100	−3.19465300
H	−1.71992600	−2.50170600	−2.52050400	H	−0.33794600	−2.62541200	−1.76490600
H	−0.48044600	−1.54035500	−3.32213300	H	−0.21001900	−1.01945000	−2.50661300
C	−1.14502900	1.72038200	−1.93612700	H	2.79189900	−1.30268800	−3.13151500
H	0.84655800	3.55026600	−1.96894000	H	3.47307900	−0.54486800	−1.69350700
H	1.37581700	2.12649000	−2.87240200	H	2.10052300	0.20270000	−2.53484600
H	2.16347900	2.55220900	−1.33851500	H	−2.02586900	−1.80025800	−0.72348100
H	−0.43752300	3.29882000	0.19079500	H	−3.51905400	−1.77272900	0.22713900
H	−0.93240000	1.70808800	0.77306200	H	−4.00416900	−1.27287000	−2.13925900
H	0.76373600	2.22269600	0.91912200	H	−2.82144000	0.04113700	−2.15207300
H	−1.01954400	−0.58029200	1.43720200	H	−5.07848600	1.02596000	−1.86415700
H	−1.84494000	−2.05307100	0.98346800	H	−5.41621200	−0.06123300	−0.51626100
H	−2.54097500	0.76543000	2.30721600	H	−4.75899800	2.12914700	0.41628700
H	−3.59126300	−0.65501700	2.45442600	H	−3.29085400	2.15207000	−0.56709500
H	−4.29641400	2.02966600	1.13698300	H	−2.74269300	1.48115500	1.73885200
H	−4.92399400	1.41141900	2.66962700	H	−3.94854700	0.18244000	1.69693200
H	−6.54851200	1.07293300	0.73221100	Al	1.05367300	1.15104600	−0.04694400
H	−6.08111300	−0.43962400	1.50989200	C	0.73145500	2.11581800	−1.77109600
H	−4.91830300	0.69211400	−1.09544100	H	2.73643000	−3.34616700	−1.94817200
H	−5.92030700	−0.75531500	−0.93517600	H	1.70701900	−3.64862600	−0.55276800
H	−4.17027000	−1.90314900	0.37062100	H	3.18056200	−2.67946400	−0.36887000
H	−3.50799400	−1.32916900	−1.16675600	C	0.40911100	2.05936800	1.61538300
H	4.05890800	2.06928000	−0.39565500	C	3.22403600	0.83887400	0.59973800
H	2.89551000	2.62505400	0.78966500	C	3.95279100	1.95498300	−0.18508800
H	5.19993300	2.59165300	1.77029000	C	−0.10234200	3.41103900	−1.66057900

H	4.16493500	1.44466700	2.62605800	C	1.13097200	3.38686000	1.94514200
H	5.34274000	0.86352600	1.44666300	H	0.21404800	1.42719600	−2.45714600
H	3.44505300	−2.26450300	−0.60609700	H	1.68534500	2.35129100	−2.26647600
H	3.11604400	−1.21857600	−1.96218000	H	0.48346100	1.40772900	2.49633400
H	5.56440300	−1.62469400	−1.81240100	H	−0.66262600	2.27018900	1.49190500
H	5.26480000	0.08143900	−1.45848200	H	3.90784500	−0.02610900	0.63637000
H	5.60338800	−1.04512200	−0.14682200	H	3.11090200	1.13543900	1.65141700
H	1.78088300	0.17993300	2.74270400	H	4.94619100	2.15900600	0.23873900
H	0.98442000	−1.21028700	2.05509800	H	3.40149300	2.90308300	−0.17337300
H	2.66261900	−1.95342000	3.75650500	H	4.09989400	1.68428200	−1.23736200
H	3.95680000	−1.13721300	2.87692600	H	−0.31882400	3.84465000	−2.64764900
H	3.15239200	−2.53052200	2.15949800	H	0.41686000	4.18366300	−1.08062100
H	1.21917900	0.07611200	−1.85044500	H	−1.06680400	3.23531800	−1.16757600
H	−1.95723900	1.18480100	−1.43531100	H	0.70051200	3.87506200	2.83147200
H	−1.00033600	1.31609500	−2.94418600	H	1.06484300	4.10913500	1.12228800
H	−1.46293400	2.76429000	−2.04489900	H	2.19712000	3.23392400	2.15544000

Tabelle 8.115 Standardorientierung von **66·Me$_3$Al** (N_{Si}) und **66·Me$_3$Al** (ÜZ) [B3LYP/6−31+G(d)].

66·Me$_3$Al				**ÜZ**			
Si	−0.14731400	0.47732100	1.32599200	Si	0.56761300	−1.06572700	1.23582700
N	−1.64537400	0.63956100	0.24188700	N	1.44891800	−0.25521400	−0.11337900
C	0.80528700	2.08649600	1.62877400	C	0.32141400	−2.95222400	1.13528900
C	−0.82756000	0.00190600	3.02103800	C	1.57579600	−0.83798300	2.82629200
C	0.99348500	−0.84513900	0.52859800	C	−1.14219300	−0.25588300	1.58720400
C	−1.66082600	1.63245800	−0.92809700	C	1.74635600	−0.96957200	−1.42301500
C	−0.49562700	1.31494400	−1.87513700	C	0.44258500	−1.37437500	−2.13471400
C	−2.99870600	1.51728800	−1.68186000	C	2.53271300	−0.06163400	−2.39658500
N	2.26324700	−0.33564000	−0.01866200	N	−2.04534500	0.03955600	0.46772000
C	3.30936500	−0.27895000	1.00818900	C	−2.70230900	−1.16652300	−0.04362700
C	4.59527300	0.35996800	0.47486200	C	−3.56573100	−0.87067200	−1.27454400
C	5.10504600	−0.38987000	−0.76373700	C	−4.60713600	0.21420800	−0.96994600
C	3.98046800	−0.52817600	−1.79898500	C	−3.92225900	1.44301400	−0.35751800
C	2.72019800	−1.13038500	−1.16938600	C	−3.05013600	1.04724900	0.83827800
H	−2.39865100	0.95119000	0.86454500	H	2.58455800	0.36153500	0.27939700
H	1.52639500	1.89167900	2.43324800	H	−0.38388700	−3.21168700	1.93718700
H	1.37242900	2.44117100	0.76332200	H	−0.09581000	−3.34248600	0.20287000
H	0.15118300	2.89012500	1.98376600	H	1.25123100	−3.49381000	1.34382800
H	0.01205800	−0.20108000	3.69921700	H	1.02169500	−1.23896000	3.68560300
H	−1.46898500	−0.88091800	3.01449000	H	1.81994300	0.20495800	3.04806100
H	−1.39230700	0.83827200	3.45483800	H	2.52045100	−1.39299400	2.75836600
H	0.42170200	−1.28981700	−0.29214900	H	−0.92627000	0.69095600	2.09214100
H	1.16889100	−1.67745900	1.23763000	H	−1.64978400	−0.88240200	2.35544500
C	−1.55663600	3.08693500	−0.42258500	C	2.63502600	−2.20708800	−1.16856600
H	−0.49560500	2.02887600	−2.70693500	H	0.66345400	−1.79623600	−3.12353800
H	0.47731200	1.38853600	−1.37587500	H	−0.11470900	−2.12965000	−1.57497000
H	−0.59340300	0.30994700	−2.29345900	H	−0.20740000	−0.50343500	−2.26812500
H	−3.00891400	2.23876500	−2.50708000	H	2.80748800	−0.64982800	−3.27962500
H	−3.84672200	1.74812000	−1.02717900	H	3.46134200	0.31795000	−1.95892800
H	−3.15352200	0.52418600	−2.10460700	H	1.93784200	0.78470700	−2.74234800
H	2.93499400	0.29246100	1.86343800	H	−1.93627900	−1.90455400	−0.29631600
H	3.53330700	−1.30123300	1.38393200	H	−3.33540400	−1.62438400	0.74875800
H	5.35441100	0.36171000	1.26798900	H	−4.05439800	−1.79736700	−1.60364600
H	4.39127200	1.40823300	0.21680200	H	−2.91388700	−0.53862000	−2.09400100
H	5.97124400	0.12466500	−1.19911100	H	−5.15793100	0.48878500	−1.87883600
H	5.44893500	−1.39165100	−0.46507000	H	−5.34754400	−0.18204000	−0.25845400
H	4.30107700	−1.15929700	−2.63810400	H	−4.66671700	2.18180200	−0.03277200
H	3.73308000	0.45956400	−2.21177400	H	−3.28920600	1.92965500	−1.11196000
H	1.91148100	−1.16046000	−1.90773200	H	−2.52613200	1.92728300	1.22652900
H	2.92205800	−2.17948700	−0.86518600	H	−3.69765700	0.66767200	1.65884800

Al	−2.58078200	−1.34834500	−0.16528000	**Al**	1.42233600	1.74857300	−0.02282100
C	−2.03067400	−1.97007200	−1.98966500	**C**	1.18051100	2.87364000	−1.63851500
H	−1.75348100	3.77525700	−1.25251300	**H**	2.90150200	−2.68271500	−2.12040600
H	−0.57075500	3.32921200	−0.02623400	**H**	2.14152700	−2.96141500	−0.55503800
H	−2.30561100	3.29059800	0.35406100	**H**	3.56610700	−1.91408100	−0.66854900
C	−1.96192100	−2.67596500	1.20471500	**C**	0.74298500	2.65251500	1.60594200
C	−4.50747200	−0.90266200	0.15349400	**C**	3.54637600	1.40644800	0.56135100
H	−0.94702700	−2.12922500	−2.09511300	**H**	0.39926000	2.49518200	−2.31242900
H	−2.35426900	−1.37055400	−2.85066600	**H**	2.08886100	3.00756000	−2.24016100
H	−2.48648600	−2.59400400	2.16707900	**H**	0.84664400	2.13957700	2.56801200
H	−0.88955700	−2.76447900	1.41869800	**H**	−0.30913200	2.94964000	1.49585300
H	−5.03593300	−0.45701900	−0.69959100	**H**	4.37566600	0.80194600	0.17015600
H	−4.67415600	−0.23821100	1.01710200	**H**	3.65545300	1.46763000	1.64998000
H	−2.26260300	−3.64960800	0.78249300	**H**	1.31588300	3.59011800	1.68692800
H	−2.48875100	−2.96418200	−2.11937000	**H**	0.85829600	3.87413800	−1.31512300
H	−5.03584800	−1.83798300	0.39596600	**H**	3.72898500	2.41718700	0.15801400

Tabelle 8.116 Standardorientierung von **66·Et_3Al** (N) und **66·Me_3Al** (N) [B3LYP/6−31+G(d)].

66·Et_3Al				**66·Me_3Al**			
Si	1.85168300	−0.10949400	1.04992800	**Si**	1.45477100	−1.12756000	0.77780900
C	2.11334600	−1.59092800	2.21115100	**N**	1.97081700	0.30972600	−0.05030800
C	2.52730400	1.40072900	1.97406700	**C**	1.81655500	−2.68725800	−0.23844600
N	2.56702800	−0.30256500	−0.53619800	**C**	2.22715800	−1.40457800	2.49011400
C	3.94350400	−0.64183600	−0.96499100	**C**	−0.42436700	−1.04612700	1.22160100
C	4.14353600	−2.17364200	−0.99703900	**C**	3.23611600	0.64450000	−0.74984900
C	4.15372600	−0.07073100	−2.38148400	**C**	3.21468100	0.08997700	−2.19093300
C	−0.06219400	−0.18935500	0.79341300	**C**	3.35192200	2.17885800	−0.80231400
N	−1.03295300	0.71634900	0.07417200	**N**	−1.51765200	−0.56075000	0.30557600
C	−0.54402700	1.24367200	−1.24094300	**C**	−1.26762000	−1.08593700	−1.07604200
C	0.42964000	2.42544200	−1.15375600	**C**	−2.42923500	−0.84731800	−2.04076100
C	−0.15126400	3.56497700	−0.30557200	**C**	−3.71954500	−1.48653400	−1.51726300
C	−0.58711400	3.03415300	1.06722700	**C**	−4.01122200	−0.95681100	−0.10863900
C	−1.54132700	1.84600600	0.91739400	**C**	−2.80943000	−1.14076800	0.82195600
Al	−2.76073400	−0.52792400	−0.34361900	**H**	1.40527900	1.13230700	0.12702900
C	−5.31152600	0.04280900	−1.75619700	**H**	1.41473400	−3.57266700	0.27203700
C	−3.68832500	−0.80984900	1.42182900	**H**	1.38718000	−2.65428800	−1.24553700
C	−3.87901700	0.60194500	−1.58893400	**H**	2.89664800	−2.84588500	−0.34562200
H	−1.05051300	−1.88276500	−1.80604200	**H**	1.77116700	−2.26188200	3.00453900
H	−2.69937300	−2.32487700	−2.12229700	**H**	2.09945200	−0.52353500	3.13089100
C	−1.80712600	−3.45566200	−0.51373900	**H**	3.30244800	−1.60587300	2.41397700
H	1.70699600	−2.51862400	1.78994700	**H**	−0.52001700	−0.49889000	2.16358300
H	1.63165500	−1.42656900	3.18447400	**H**	−0.64173900	−2.10106600	1.46635300
H	3.18031300	−1.75895400	2.40446000	**C**	4.45842700	0.07988000	0.00224100
H	2.56281400	2.30887500	1.36365300	**H**	4.13172500	0.35860100	−2.73126500
H	1.91721300	1.60874600	2.86256700	**H**	3.13261300	−1.00241500	−2.19276000
H	3.54550100	1.20141100	2.32846100	**H**	2.35952900	0.49600800	−2.74285900
C	4.96982900	−0.00979400	−0.01199100	**H**	4.26315300	2.48039200	−1.33154200
H	5.14807000	−2.43721700	−1.35246700	**H**	3.38935000	2.60214700	0.20880600
H	4.00850700	−2.60621800	0.00048600	**H**	2.49602100	2.61863100	−1.32851400
H	3.41534600	−2.64480000	−1.66921500	**H**	−0.35255000	−0.61651900	−1.44197800
H	5.15385000	−0.31368200	−2.76050600	**H**	−1.08503900	−2.17012700	−0.99696800
H	4.03598700	1.01854300	−2.37974400	**H**	−2.15053600	−1.26536600	−3.01663600
H	3.42196300	−0.49050100	−3.08441900	**H**	−2.57428700	0.22920100	−2.18808800
H	−0.47055900	−0.31768300	1.80221400	**H**	−4.55975800	−1.27012700	−2.18819300
H	−0.18273700	−1.17675800	0.32728900	**H**	−3.60509600	−2.58090900	−1.49231000
H	−0.10546200	0.40670000	−1.79225400	**H**	−4.86182800	−1.48524200	0.34153200
H	−1.43466000	1.55781400	−1.79526200	**H**	−4.28604400	0.09918100	−0.16170300
H	0.62970800	2.76952500	−2.17736100	**H**	−3.00065700	−0.69286800	1.80229400
H	1.39174100	2.09588800	−0.74907100	**H**	−2.64686900	−2.21925500	0.97977100

H	0.58326200	4.37209100	−0.19158400	Al	−1.57379900	1.65684500	0.42999300
H	−1.02097400	4.00083300	−0.81960100	C	−0.85665000	2.31145800	−1.32250100
H	−1.10405100	3.81569600	1.63963300	H	5.38686600	0.35012300	−0.51552300
H	0.29019200	2.74520600	1.65462600	H	4.42805200	−1.01464900	0.06224100
H	−1.82101800	1.43140800	1.88938400	H	4.50570400	0.47776000	1.02210500
H	−2.46480800	2.19253000	0.43858200	C	−3.44969400	2.26300900	0.78272900
H	−4.14548400	0.14438800	1.73483300	C	−0.46371400	2.09319700	2.04524700
H	−4.55462400	−1.43644400	1.14274600	H	−0.05722900	1.71974600	−1.78754500
C	−3.00835000	−1.46180000	2.64294600	H	−0.44418500	3.32115900	−1.16614300
H	−3.95686100	1.65192500	−1.25956800	H	−3.99057900	1.72344300	1.57344000
H	−3.40966400	0.64605600	−2.58618600	H	−4.10258900	2.30027000	−0.10059400
H	−5.91408700	0.62269100	−2.47154800	H	0.59338400	1.79703500	2.06906100
C	−1.99525400	−2.13692900	−1.29347200	H	−0.91848200	1.72660400	2.97853500
H	−5.30178900	−0.99464300	−2.11939700	H	−3.36039600	3.30269800	1.13779600
H	−5.85784600	0.04150100	−0.80373300	H	−1.65169000	2.42441600	−2.07394500
H	−3.71099500	−1.64493500	3.46990600	H	−0.47358800	3.19257200	2.12478000
H	−2.55290000	−2.42775800	2.39008200				
H	−2.20724400	−0.83095100	3.05459700				
H	−1.46725800	−4.28464500	−1.15298900				
H	−2.74503000	−3.77865000	−0.04329200				
H	−1.07129200	−3.35741000	0.29681300				
H	1.90311000	−0.63329900	−1.23198900				
H	5.98570900	−0.21481500	−0.36787400				
H	4.89192700	−0.42190500	1.00106000				
H	4.84065100	1.07646200	0.04338200				

8.3.3 Angaben zu den quantenchemischen Rechnungen aus Kapitel 4.3

8.117 Berechnete Energien der optimierten Verbindungen [B3LYP/6−31+G(d)].

Verbindung	SCF [Hartree]	ZPE [Hartree]
[LiN(^{t}Bu)SiMe$_2$(CH$_2$NC$_5$H$_{10}$)]$_2$−*C*$_2$	−1760.38655716	−1759.62148000
[LiN(^{t}Bu)SiMe$_2$(CH$_2$NC$_5$H$_{10}$)]$_2$−*C*$_i$	−1760.36947880	−1759.60377100
[LiN(Me)SiMe$_2$(CH$_2$NC$_5$H$_{10}$)]$_2$−*C*$_2$	−1524.50543994	−1523.91170200
[LiN(Me)SiMe$_2$(CH$_2$NC$_5$H$_{10}$)]$_2$−*C*$_i$	−1524.50476013	−1523.90953500
LiN(Me)SiMe$_2$(CH$_2$NC$_5$H$_{10}$)	−762.221480747	−761.925052
[LiN(Me)SiMe$_2$(CH$_2$NC$_5$H$_{10}$)]$_2$ (nur eine koordinierende Piperidingruppe)	−1524.46700212	−1523.873815
[LiN(Me)SiMe$_2$(CH$_2$NC$_5$H$_{10}$)]$_2$−*C*$_2$ (CPCM, Benzol)	−1524.50760731	−1523.913965
LiN(Me)SiMe$_2$(CH$_2$NC$_5$H$_{10}$) (CPCM, Benzol)	−762.233849606	−761.938283
[LiN(Me)SiMe$_2$(CH$_2$NC$_5$H$_{10}$)]$_2$ (nur eine koordinierende Piperidingruppe) (CPCM, Benzol)	−1524.48456357	−1523.891649
102	−1071.11809926	−1070.67919100

Tabelle 8.118 Standardorientierung von [LiN(**^{t}Bu**)SiMe$_2$(CH$_2$NC$_5$H$_{10}$)]$_2$ mit C_2− und C_i−Symmetrie [Minima, B3LYP/6−31+G(d)].

C_2				C_i			
C	2.77900200	0.11258500	−2.44685200	C	0.93797800	−2.44586900	−2.39433000
C	−2.77900200	−0.11258500	−2.44685200	C	−2.04138500	−1.99832700	−1.78449500
C	0.95496000	−2.14838800	−1.70545900	C	−3.94954200	−0.46936400	−1.71601000
C	−0.95496000	2.14838800	−1.70545900	C	−0.60606900	−4.51871700	−0.88289600
C	−0.97243000	−3.61331600	−1.46002700	C	−4.84449500	0.43255500	−0.85891400
C	0.97243000	3.61331600	−1.46002700	C	−3.50344800	−1.92336400	0.15012300
C	3.91620900	−2.08513100	−0.77871200	C	−5.46303500	−0.34016500	0.31316600
C	−3.91620900	2.08513100	−0.77871200	C	−4.36365000	−1.07506600	1.09049700
C	−1.85111300	−4.44790000	−0.52386000	C	1.72170400	−3.04595100	1.60283800
C	1.85111300	4.44790000	−0.52386000	C	0.37425700	−2.28499000	1.69482800
C	−0.97243000	3.94745100	−0.05521000	C	0.53457600	−1.17996000	2.75443500
C	0.97243000	−3.94745100	−0.05521000	C	−0.68591700	−3.25865500	2.27272800
C	1.01759800	5.48513800	0.23885900	N	−2.87808900	−1.11559400	−0.92144600
C	−1.01759800	−5.48513800	0.23885900	N	0.00249400	−1.66289400	0.39229900
C	−0.16581000	4.79783100	0.93084200	Si	−0.35985400	−2.62412100	−1.00278900
C	0.16581000	−4.79783100	0.93084200	Li	−1.20396000	−0.04201100	−0.03547600
C	3.79268100	0.82818200	1.24001600	C	−0.93797800	2.44586900	2.39433000
C	−3.79268100	−0.82818200	1.24001600	C	2.04138500	1.99832700	1.78449500
C	2.44114700	0.16507600	1.60574800	C	3.94954200	0.46936400	1.71601000
C	−2.44114700	−0.16507600	1.60574800	C	0.60606900	4.51871700	0.88289600
C	1.64633400	1.21816500	2.41755100	C	4.84449500	−0.43255500	0.85891400
C	−1.64633400	−1.21816500	2.41755100	C	3.50344800	1.92336400	−0.15012300
C	2.71833800	−1.02923800	2.55250500	C	5.46303500	0.34016500	−0.31316600
C	−2.71833800	1.02923800	2.55250500	C	4.36365000	1.07506600	−1.09049700
H	3.15456100	−0.48073200	−3.29296100	C	−1.72170400	3.04595100	−1.60283800
H	−3.15456100	0.48073200	−3.29296100	C	−0.37425700	2.28499000	−1.69482800
H	−1.91703000	−0.68702200	−2.80878600	C	−0.53457600	1.17996000	−2.75443500
H	1.91703000	0.68702200	−2.80878600	C	0.68591700	3.25865500	−2.27272800
H	1.41133700	−2.81972600	−2.46011900	N	2.87808900	1.11559400	0.92144600
H	−1.41133700	2.81972600	−2.46011900	N	−0.00249400	1.66289400	−0.39229900
H	−0.55654000	−4.26468600	−2.25379100	Si	0.35985400	2.62412100	1.00278900
H	0.55654000	4.26468600	−2.25379100	Li	1.20396000	0.04201100	0.03547600
H	3.56610400	0.83061400	−2.18029900	H	0.57924100	−2.87169700	−3.34246100
H	−3.56610400	−0.83061400	−2.18029900	H	1.21377000	−1.40275700	−2.59292300
H	0.25741800	−1.51300500	−2.26975700	H	1.85750200	−2.98315100	−2.12383300
H	−0.25741800	1.51300500	−2.26975700	H	−2.63986700	−2.87487600	−2.10150000
H	−1.57104100	−2.84321300	−1.95541000	H	−1.82167200	−1.45060100	−2.70755200
H	1.57104100	2.84321300	−1.95541000	H	−4.56667900	−1.24968400	−2.20180500
H	−3.99988900	2.73931300	−1.65805900	H	−3.48280400	0.11293200	−2.51700400
H	3.99988900	−2.73931300	−1.65805900	H	−0.70025700	−4.90471300	−1.90812100
H	2.63654300	4.93594400	−1.11538700	H	0.23476500	−5.04678300	−0.41827100
H	−2.63654300	−4.93594400	−1.11538700	H	−1.51948800	−4.80494300	−0.34840600
H	4.82392500	−1.46921100	−0.75897100	H	−5.62546100	0.86727600	−1.49620400
H	−1.45099900	4.60847300	−0.80465400	H	−4.24925100	1.27005700	−0.47119100
H	1.45099900	−4.60847300	−0.80465400	H	−4.13115000	−2.71279300	−0.30897100
H	0.63903800	6.23949000	−0.46727800	H	−2.70684600	−2.42228100	0.70207000
H	−4.82392500	1.46921100	−0.75897100	H	−6.18606900	−1.07452600	−0.07219800
H	−0.63903800	−6.23949000	−0.46727800	H	−6.02039900	0.33770300	0.97187800
H	−2.35694900	−3.78126900	0.18713500	H	−4.79774900	−1.72540100	1.86095400
H	−3.93646600	2.72738500	0.10824100	H	−3.72685500	−0.34695700	1.61432400
H	2.35694900	3.78126900	0.18713500	H	2.51463000	−2.37626100	1.25183800
H	3.93646600	−2.72738500	0.10824100	H	1.65962200	−3.88245400	0.89866100
H	1.77305000	−3.42328700	0.47155700	H	2.02836200	−3.45409500	2.57624800
H	−1.77305000	3.42328700	0.47155700	H	1.30914500	−0.46803100	2.46409200
H	1.63721500	6.01952600	0.97018600	H	−0.40404200	−0.63025500	2.88686500
H	3.63330300	1.67157900	0.55725300	H	0.82019700	−1.59630800	3.72931200
H	−1.63721500	−6.01952600	0.97018600	H	−0.88672100	−4.10066100	1.60762400

H	−3.63330300	−1.67157900	0.55725300	H	−1.62927300	−2.73389300	2.46329400
H	4.47139600	0.12158800	0.75252600	H	−0.34457700	−3.67317700	3.23102500
H	−4.47139600	−0.12158800	0.75252600	H	−0.57924100	2.87169700	3.34246100
H	−0.83527300	5.53905300	1.38627600	H	−1.21377000	1.40275700	2.59292300
H	0.83527300	−5.53905300	1.38627600	H	−1.85750200	2.98315100	2.12383300
H	0.20059200	4.15991700	1.74689500	H	2.63986700	2.87487600	2.10150000
H	−0.20059200	−4.15991700	1.74689500	H	1.82167200	1.45060100	2.70755200
H	4.30604300	1.20865500	2.13378100	H	4.56667900	1.24968400	2.20180500
H	1.52773000	2.15192100	1.84915200	H	3.48280400	−0.11293200	2.51700400
H	−1.52773000	−2.15192100	1.84915200	H	0.70025700	4.90471300	1.90812100
H	−4.30604300	−1.20865500	2.13378100	H	−0.23476500	5.04678300	0.41827100
H	3.31438400	−1.79696000	2.04898900	H	1.51948800	4.80494300	0.34840600
H	−3.31438400	1.79696000	2.04898900	H	5.62546100	−0.86727600	1.49620400
H	−0.65300200	−0.84729400	2.69777200	H	4.24925100	−1.27005700	0.47119100
H	0.65300200	0.84729400	2.69777200	H	4.13115000	2.71279300	0.30897100
H	−1.77600000	1.49074200	2.87206800	H	2.70684600	2.42228100	−0.70207000
H	1.77600000	−1.49074200	2.87206800	H	6.18606900	1.07452600	0.07219800
H	2.16471000	1.48551800	3.34646100	H	6.02039900	−0.33770300	−0.97187800
H	−2.16471000	−1.48551800	3.34646100	H	4.79774900	1.72540100	−1.86095400
H	3.26626100	−0.71756500	3.45316000	H	3.72685500	0.34695700	−1.61432400
H	−3.26626100	0.71756500	3.45316000	H	−2.51463000	2.37626100	−1.25183800
N	0.13811300	−2.94057900	−0.74705100	H	−1.65962200	3.88245400	−0.89866100
N	−0.13811300	2.94057900	−0.74705100	H	−2.02836200	3.45409500	−2.57624800
N	1.64623300	−0.25199100	0.42255200	H	−1.30914500	0.46803100	−2.46409200
N	−1.64623300	0.25199100	0.42255200	H	0.40404200	0.63025500	−2.88686500
Si	2.33950600	−1.00868200	−0.96180600	H	−0.82019700	1.59630800	−3.72931200
Si	−2.33950600	1.00868200	−0.96180600	H	0.88672100	4.10066100	−1.60762400
Li	−0.18648400	−1.17516800	0.36279600	H	1.62927300	2.73389300	−2.46329400
Li	0.18648400	1.17516800	0.36279600	H	0.34457700	3.67317700	−3.23102500

Tabelle 8.119 Standardorientierung von [LiN(**Me**)$SiMe_2(CH_2NC_5H_{10})]_2$ mit C_2− und C_i−Symmetrie [Minima, B3LYP/6−31+G(d)].

C_i				C_2			
C	0.94613300	−2.76576700	−2.56164900	C	−3.35641100	0.25291200	−1.71312600
C	−1.83942700	−1.82405500	−1.86968200	C	3.35641100	−0.25291200	−1.71312600
C	−3.73352800	−0.29278500	−1.65353700	C	−1.22897200	2.35530700	−1.27207900
C	−0.60589600	−4.42163100	−0.55031700	C	1.22897200	−2.35530700	−1.27207900
C	−4.61993300	0.51527000	−0.70063000	C	0.96818100	3.43209300	−1.32633800
C	−3.40808000	−2.03215700	−0.00532700	C	−0.96818100	−3.43209300	−1.32633800
C	−5.31842800	−0.39966700	0.31510500	C	−3.88407900	2.28014500	0.46625000
C	−4.28729800	−1.29704400	1.01217300	C	3.88407900	−2.28014500	0.46625000
C	0.81961900	−2.15682100	1.39754800	C	2.16421000	3.93142700	−0.50991100
N	−2.72795900	−1.09536100	−0.92408300	C	−2.16421000	−3.93142700	−0.50991100
N	0.22933900	−1.57365000	0.18610100	C	0.56799400	−3.92717100	0.47790700
Si	−0.25337700	−2.62417100	−1.08298200	C	−0.56799400	3.92717100	0.47790700
Li	−1.16838100	−0.15360700	0.09509700	C	−1.73157600	−4.98544400	0.51919600
C	−0.94613300	2.76576700	2.56164900	C	1.73157600	4.98544400	0.51919600
C	1.83942700	1.82405500	1.86968200	C	−0.56799400	−4.45037600	1.36355300
C	3.73352800	0.29278500	1.65353700	C	0.56799400	4.45037600	1.36355300
C	0.60589600	4.42163100	0.55031700	C	−2.18608200	−0.17263700	2.01589600
C	4.61993300	−0.51527000	0.70063000	C	2.18608200	0.17263700	2.01589600
C	3.40808000	2.03215700	0.00532700	H	−3.89544600	0.91356100	−2.40730000
C	5.31842800	0.39966700	−0.31510500	H	3.89544600	−0.91356100	−2.40730000
C	4.28729800	1.29704400	−1.01217300	H	2.63978500	0.33335900	−2.30375800
C	−0.81961900	2.15682100	−1.39754800	H	−2.63978500	−0.33335900	−2.30375800
N	2.72795900	1.09536100	0.92408300	H	−1.74572700	3.18223200	−1.79802300
N	−0.22933900	1.57365000	−0.18610100	H	1.74572700	−3.18223200	−1.79802300
Si	0.25337700	2.62417100	1.08298200	H	0.56300300	4.25797100	−1.94340900
Li	1.16838100	0.15360700	−0.09509700	H	−0.56300300	−4.25797100	−1.94340900

H	0.52966900	−3.37497200	−3.37676200	H	−4.09171900	−0.45045700	−1.29921100
H	1.19006300	−1.77954100	−2.98008100	H	4.09171900	0.45045700	−1.29921100
H	1.89111500	−3.23448300	−2.25512700	H	−0.78748200	1.73323500	−2.06392300
H	−2.42074500	−2.57588100	−2.43958700	H	0.78748200	−1.73323500	−2.06392300
H	−1.49860400	−1.09053300	−2.61458000	H	1.28483100	2.63992700	−2.01362800
H	−4.36171500	−0.96043800	−2.27541100	H	−1.28483100	−2.63992700	−2.01362800
H	−3.20076800	0.37797400	−2.33544000	H	4.28888200	−3.00507300	−0.25297600
H	−1.06072300	−4.98746800	−1.37457700	H	−4.28888200	3.00507300	−0.25297600
H	0.32725200	−4.93546200	−0.28303700	H	−2.91910900	−4.34062000	−1.19359300
H	−1.27658100	−4.49873900	0.31408700	H	2.91910900	4.34062000	−1.19359300
H	−5.35612400	1.08005900	−1.28711000	H	−4.71790500	1.63682100	0.77790100
H	−3.99900500	1.25282100	−0.17284700	H	1.01612100	−4.76630900	−0.09007800
H	−4.02726900	−2.74192400	−0.58880100	H	−1.01612100	4.76630900	−0.09007800
H	−2.64496200	−2.61896400	0.51302900	H	−1.40993900	−5.89761800	−0.00538200
H	−6.05318400	−1.02998100	−0.20791900	H	4.71790500	−1.63682100	0.77790100
H	−5.87680500	0.19258600	1.05100500	H	1.40993900	5.89761800	−0.00538200
H	−4.78381800	−2.03554400	1.65476800	H	2.62829700	3.07743700	0.00309700
H	−3.64965900	−0.68630500	1.66842700	H	3.55790600	−2.83764600	1.35290900
H	−0.52966900	3.37497200	3.37676200	H	−2.62829700	−3.07743700	0.00309700
H	−1.19006300	1.77954100	2.98008100	H	−3.55790600	2.83764600	1.35290900
H	−1.89111500	3.23448300	2.25512700	H	−1.36077300	3.49768000	1.09631900
H	2.42074500	2.57588100	2.43958700	H	1.36077300	−3.49768000	1.09631900
H	1.49860400	1.09053300	2.61458000	H	−2.57570900	−5.27011700	1.15985100
H	4.36171500	0.96043800	2.27541100	H	2.57570900	5.27011700	1.15985100
H	3.20076800	−0.37797400	2.33544000	H	−0.17383200	−5.23205600	2.02558800
H	1.06072300	4.98746800	1.37457700	H	0.17383200	5.23205600	2.02558800
H	−0.32725200	4.93546200	0.28303700	H	−0.92584800	−3.63786400	2.01286700
H	1.27658100	4.49873900	−0.31408700	H	0.92584800	3.63786400	2.01286700
H	5.35612400	−1.08005900	1.28711000	N	−0.10006200	2.88610600	−0.46122400
H	3.99900500	−1.25282100	0.17284700	N	0.10006200	−2.88610600	−0.46122400
H	4.02726900	2.74192400	0.58880100	N	−1.55206800	0.34217500	0.79753600
H	2.64496200	2.61896400	−0.51302900	N	1.55206800	−0.34217500	0.79753600
H	6.05318400	1.02998100	0.20791900	Si	−2.49371000	1.23500900	−0.32032000
H	5.87680500	−0.19258600	−1.05100500	Si	2.49371000	−1.23500900	−0.32032000
H	4.78381800	2.03554400	−1.65476800	Li	0.25613000	1.13230600	0.59658600
H	3.64965900	0.68630500	−1.66842700	Li	−0.25613000	−1.13230600	0.59658600
H	0.22408700	−2.98048600	1.83030600	H	2.62451700	−0.61411300	2.65652000
H	1.83989600	−2.56253300	1.25579600	H	2.99556500	0.90743300	1.83763500
H	0.90261000	−1.40311500	2.19848800	H	1.44953700	0.68863000	2.66104400
H	−1.83989600	2.56253300	−1.25579600	H	−2.62451700	0.61411300	2.65652000
H	−0.90261000	1.40311500	−2.19848800	H	−2.99556500	−0.90743300	1.83763500
H	−0.22408700	2.98048600	−1.83030600	H	−1.44953700	−0.68863000	2.66104400

Tabelle 8.120 Standardorientierung von [LiN(**Me**)$SiMe_2(CH_2NC_5H_{10})]_2$ mit nur einer koordinierenden Piperidingruppe in der Gasphase und in Benzol [Minima, B3LYP/6−31+G(d)].

Gasphase				**Benzol**			
C	−0.79737900	−3.35733100	−0.74409300	C	−1.06481900	−3.60036700	0.28115400
C	0.93201500	3.57597800	−1.31786800	C	1.10685100	3.81989500	−0.70797600
C	−2.58039300	−1.07782200	−1.37993300	C	−2.08517700	−0.99675700	−0.87464200
C	2.40554100	0.92735900	−1.33184300	C	2.10572000	1.05100300	−1.35922100
C	−3.45619600	1.25187100	−1.76319100	C	−2.90123900	1.23606900	−0.25357500
C	2.85683300	−1.45525900	−1.63171800	C	2.18823900	−1.29145500	−2.03730800
C	−3.06546700	−2.89930100	1.18380900	C	−3.13253500	−2.14935300	1.93283100
C	3.43018000	3.39308500	0.37702300	C	3.87224300	3.10105400	0.28127500
C	−3.08823300	2.18120200	−0.58882600	C	−3.86099400	2.36457200	−0.65251300
C	3.16788300	−2.79715800	−0.96149200	C	2.55089500	−2.72849700	−1.65242000
C	3.98462800	−0.23146500	0.12798500	C	3.92066300	−0.39624900	−0.59964800
C	−4.72134400	−0.22550000	−0.33455900	C	−4.49645100	−0.46337100	−0.92388600
C	4.43846100	−2.70976500	−0.10604500	C	4.02635900	−2.83942300	−1.24811100

C	−4.14697600	2.08627400	0.52280300	C	−5.32149500	1.89751100	−0.57296900
C	4.33635400	−1.52737700	0.86535200	C	4.34702500	−1.80218500	−0.16482400
C	−4.40496400	0.62162200	0.91655500	C	−5.50958500	0.59792400	−1.36881500
C	−0.37512600	−1.50926800	2.42265200	C	0.19817700	−1.60119200	2.80869800
C	1.03062600	2.32948600	2.43106300	C	1.90008100	2.10841000	2.75285400
H	−1.46741800	−4.07048300	−1.24320700	H	−0.62815900	−4.16132900	1.11850500
H	1.54686700	3.93625600	−2.15487500	H	0.08103600	3.51048300	−0.94856800
H	0.04281200	3.09222100	−1.74254400	H	1.03944200	4.66088200	−0.00425500
H	−0.11140400	−2.96067800	−1.50459200	H	−1.91727700	−4.18534000	−0.09134700
H	−2.85863900	−1.93519100	−2.02175200	H	−2.33880700	−1.81599500	−1.56413800
H	3.23640000	1.22276300	−2.00228000	H	2.72994300	1.38161500	−2.21291000
H	−4.37303000	1.65223600	−2.22900900	H	−3.01964000	1.02687800	0.83324100
H	3.65213300	−1.20832400	−2.36143200	H	2.74287900	−0.99865200	−2.94972700
H	−0.19518500	−3.92863800	−0.02449700	H	−0.31343500	−3.56965900	−0.51861700
H	0.58897400	4.46026400	−0.76373800	H	1.56470700	4.20288300	−1.63113500
H	−1.75045100	−0.60028700	−1.92176400	H	−1.14576100	−0.57588600	−1.26984000
H	1.55150900	0.72745000	−1.99549600	H	1.07866100	1.00027600	−1.75023500
H	−2.67872100	1.27359000	−2.53508300	H	−1.86327700	1.55944200	−0.41016600
H	1.91629400	−1.51860900	−2.19051100	H	1.12040800	−1.21767200	−2.27217300
H	4.05957700	3.64760100	−0.48643000	H	4.32708500	3.34460100	−0.68844500
H	−3.77477400	−3.44090700	0.54405500	H	−3.90977200	−2.73505000	1.42476900
H	3.27175800	−3.56666600	−1.73713700	H	2.32481400	−3.39180800	−2.49750100
H	−2.98850300	3.21666400	−0.94280100	H	−3.62955700	2.67792600	−1.67995300
H	−2.57164400	−3.64992900	1.81636700	H	−2.82894100	−2.71874600	2.82298000
H	4.81435100	0.04633300	−0.55092300	H	4.52881800	−0.07713200	−1.46849700
H	−5.67938900	0.12516000	−0.75466000	H	−3.69451900	3.23323200	−0.00103200
H	5.31184300	−2.56779500	−0.76001900	H	4.66289700	−2.65732100	−2.12715500
H	3.12353600	4.34021900	0.84082700	H	3.83052700	4.03328300	0.86110400
H	−5.08370100	2.52771100	0.14886200	H	−4.59144300	−1.36203100	−1.54626200
H	−2.09337700	1.89969500	−0.20596100	H	−4.72617800	−0.76393000	0.11684600
H	4.06142000	2.86721400	1.10345300	H	4.55404500	2.42283400	0.80839200
H	2.31616800	−3.09410000	−0.33526900	H	1.91598900	−3.04834300	−0.81539700
H	−3.64462200	−2.24933300	1.85087700	H	−3.59119500	−1.21645400	2.28364900
H	−4.86331500	−1.27651700	−0.06808400	H	−5.99651600	2.68050000	−0.94293900
H	3.86287900	0.58653400	0.84255100	H	4.10903900	0.31839400	0.20540100
H	4.60168900	−3.64721100	0.44021000	H	4.25517800	−3.85274800	−0.89422200
H	−3.85450100	2.68376600	1.39718600	H	−5.58965900	1.71974300	0.48006500
H	5.28010300	−1.38292300	1.40675400	H	5.42087500	−1.79153100	0.06290500
H	−5.23721800	0.55830200	1.63199600	H	−6.52766200	0.20750800	−1.23645500
H	3.56736600	−1.73521000	1.62425700	H	3.82847300	−2.06956800	0.76781100
H	−3.51958200	0.20773900	1.41930500	H	−5.37162100	0.79713500	−2.44080500
N	−3.71462400	−0.13054400	−1.38531300	N	−3.12590100	0.03687100	−1.05684100
N	2.73093800	−0.35502500	−0.64825600	N	2.48413500	−0.32910600	−0.95079100
N	−0.74364700	−0.95195200	1.10502900	N	−0.35965200	−0.95538700	1.60218800
N	1.01099900	1.68113300	1.11121700	N	1.46313900	1.61866300	1.43633300
Si	−1.76439600	−1.96384200	0.14296100	Si	−1.61540300	−1.84448100	0.81357000
Si	1.89977600	2.39802700	−0.17313200	Si	2.11689400	2.38638300	0.04136700
Li	−0.75106600	0.95237300	1.19958900	Li	−0.29525700	0.96452200	1.95789800
Li	1.10743200	−0.29141600	0.65334000	Li	1.31814700	−0.28962300	0.77730900
H	2.02362700	2.31815100	2.91455800	H	2.98137900	1.97836200	2.93875200
H	0.70017400	3.38468700	2.42835600	H	1.68116700	3.17687500	2.93741600
H	0.36214300	1.80919800	3.14425600	H	1.40124700	1.55708100	3.57285500
H	−1.22415300	−1.59483300	3.12389400	H	−0.51919300	−1.69099900	3.64627500
H	0.08340700	−2.51612900	2.37846700	H	0.58823100	−2.62101300	2.63274400
H	0.36586500	−0.86652000	2.93466600	H	1.05042900	−1.02286600	3.21167500

Tabelle 8.121 Standardorientierung von LiN(**Me**)$SiMe_2(CH_2NC_5H_{10})$ in der Gasphase und in Benzol [Minima, B3LYP/6−31+G(d)].

Gasphase				Benzol			
C	3.18142000	−1.56909300	−0.45705200	C	3.16958400	−1.62699200	−0.32796100
C	0.18692400	−1.23336000	−0.06118600	C	0.17605200	−1.21872000	−0.06067700
C	−2.15695300	−1.14835000	−0.79135400	C	−2.16041600	−1.14783000	−0.77702400
C	2.27887300	−0.04246100	1.99341300	C	2.23469200	0.05750300	1.98482600
C	−3.39417900	−0.27221600	−1.01359000	C	−3.41487000	−0.29484100	−0.98742600
C	−1.42245700	0.22899200	1.06224500	C	−1.40838000	0.27775200	1.03181300
C	−3.82445900	0.41995600	0.28700600	C	−3.83121800	0.40755100	0.31167200
C	−2.63343100	1.15569700	0.91474400	C	−2.63981800	1.17774400	0.89487300
C	2.78242700	2.04721400	−1.00023000	C	2.84871600	1.98343100	−1.01969600
H	3.15362800	−2.49782200	0.13058900	H	3.10056900	−2.51340400	0.31891500
H	3.02746600	−1.83049800	−1.51214900	H	3.04956700	−1.95771400	−1.36832800
H	0.01502600	−1.95945100	0.75572200	H	−0.00649100	−1.92892500	0.76909100
H	−2.40729600	−1.98448500	−0.11103000	H	−2.38613200	−1.97474600	−0.07636900
H	4.19755200	−1.16172900	−0.36685600	H	4.18939600	−1.23105800	−0.22589700
H	0.28131800	−1.82991800	−0.97903200	H	0.27285800	−1.83452500	−0.96626000
H	−1.82758500	−1.59311400	−1.73738000	H	−1.84460400	−1.60477200	−1.72227700
H	2.28486600	−0.99021600	2.55004700	H	2.20724400	−0.86077800	2.58846500
H	−4.20710700	−0.89111800	−1.41413100	H	−4.22400400	−0.93390200	−1.36425100
H	3.27663700	0.40371200	2.10725500	H	3.24155800	0.48444800	2.09463700
H	−1.65580800	−0.57512000	1.78594100	H	−1.60970800	−0.51189600	1.78122200
H	−4.19578000	−0.33690200	0.99357000	H	−4.17029500	−0.34483800	1.03939900
H	−3.16901900	0.48598900	−1.77928400	H	−3.21550200	0.45736100	−1.76582400
H	1.56872900	0.63395700	2.48593800	H	1.53135600	0.77362400	2.42848600
H	−0.56373700	0.78001000	1.45596200	H	−0.55334800	0.85608000	1.39300500
H	−4.65497300	1.11237500	0.10106000	H	−4.67911400	1.08128300	0.13354000
H	−2.89825800	1.55765500	1.90076700	H	−2.88684100	1.59290900	1.88057100
H	−2.35979500	2.02042900	0.28995500	H	−2.39808200	2.03262900	0.24465200
N	−1.02657300	−0.37368000	−0.23230600	N	−1.02571600	−0.35232600	−0.25377300
N	1.68740600	1.10877400	−0.79797500	N	1.73120400	1.05780800	−0.88199700
Si	1.88545600	−0.29927200	0.13882700	Si	1.87149300	−0.30011100	0.13750900
Li	−0.05585700	1.06319400	−1.26331200	Li	−0.04033800	1.06393300	−1.41742400
H	3.16028200	2.49950300	−0.06288600	H	3.17048400	2.44503700	−0.06472900
H	3.66117800	1.60149200	−1.50418500	H	3.75771400	1.52637000	−1.45863500
H	2.46903600	2.89154700	−1.63552000	H	2.58902300	2.82460200	−1.68427400

Tabelle 8.122 Standardorientierung von $[LiN(\mathbf{Me})SiMe_2(CH_2NC_5H_{10})]_2$ mit C_2−Symmetrie in Benzol [Minima, B3LYP/6−31+G(d)].

C_2							
C	3.51854100	−0.18166900	−1.55788000	H	2.76584500	4.28774500	−1.40386600
C	−3.51854100	0.18166900	−1.55788000	H	−2.76584500	−4.28774500	−1.40386600
C	1.37595100	−2.29611300	−1.24755400	H	4.71201900	−1.53201600	1.04149300
C	−1.37595100	2.29611300	−1.24755400	H	−1.12198100	4.74310800	−0.15877700
C	−0.81410400	−3.37194200	−1.42533100	H	1.12198100	−4.74310800	−0.15877700
C	0.81410400	3.37194200	−1.42533100	H	1.29887300	5.88174600	−0.21426400
C	3.92358100	−2.19480600	0.65860500	H	−4.71201900	1.53201600	1.04149300
C	−3.92358100	2.19480600	0.65860500	H	−1.29887300	−5.88174600	−0.21426400
C	−2.04043800	−3.90143100	−0.67592400	H	−2.52694900	−3.06677800	−0.15192300
C	2.04043800	3.90143100	−0.67592400	H	−3.54110500	2.76867300	1.51192100
C	−0.64982100	3.92622200	0.42186500	H	2.52694900	3.06677800	−0.15192300
C	0.64982100	−3.92622200	0.42186500	H	3.54110500	−2.76867300	1.51192100
C	1.64534700	4.99074400	0.33087000	H	1.41596600	−3.51840800	1.08696900
C	−1.64534700	−4.99074400	0.33087000	H	−1.41596600	3.51840800	1.08696900
C	0.51861300	4.48521700	1.24095200	H	2.51360800	5.30086200	0.92638200
C	−0.51861300	−4.48521700	1.24095200	H	−2.51360800	−5.30086200	0.92638200
C	2.13693400	0.29034800	2.05269900	H	0.14685500	5.29154900	1.88665000

C	−2.13693400	−0.29034800	2.05269900	H	−0.14685500	−5.29154900	1.88665000
H	4.11355500	−0.83806000	−2.20935400	H	0.90505700	3.70033600	1.90809400
H	−4.11355500	0.83806000	−2.20935400	H	−0.90505700	−3.70033600	1.90809400
H	−2.83467000	−0.39187300	−2.19776300	N	0.21618800	−2.85251300	−0.49843800
H	2.83467000	0.39187300	−2.19776300	N	−0.21618800	2.85251300	−0.49843800
H	1.92536100	−3.10899200	−1.76249100	N	1.55985800	−0.28343700	0.83331300
H	−1.92536100	3.10899200	−1.76249100	N	−1.55985800	0.28343700	0.83331300
H	−0.38040200	−4.17573400	−2.05194900	Si	2.57360100	−1.17145600	−0.22387700
H	0.38040200	4.17573400	−2.05194900	Si	−2.57360100	1.17145600	−0.22387700
H	4.21301900	0.53379900	−1.09648600	Li	−0.21618800	−1.14344700	0.59994000
H	−4.21301900	−0.53379900	−1.09648600	Li	0.21618800	1.14344700	0.59994000
H	0.96480500	−1.66466400	−2.04872100	H	−2.55805800	0.46279100	2.74384300
H	−0.96480500	1.66466400	−2.04872100	H	−2.94343500	−1.02845600	1.87459200
H	−1.10362400	−2.55707500	−2.09819700	H	−1.36845700	−0.82268600	2.64619000
H	1.10362400	2.55707500	−2.09819700	H	2.55805800	−0.46279100	2.74384300
H	−4.40367600	2.90172600	−0.03182000	H	2.94343500	1.02845600	1.87459200
H	4.40367600	−2.90172600	−0.03182000	H	1.36845700	0.82268600	2.64619000

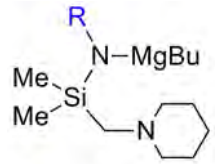
Tabelle 8.123 Standardorientierung von **102** [Minimum, B3LYP/6−31+G(d)].

102							
C	2.16502400	0.04336300	−2.24521700	H	−2.20444000	2.13446900	−1.75631200
C	1.66134500	2.36892300	−2.25358300	H	2.43143200	−2.69596200	0.90375700
C	2.45878400	−1.11433900	−1.29501000	H	−0.68612400	2.98792200	0.11283600
C	−2.75814900	−1.88269100	−1.49452600	H	3.61758700	−0.54493100	1.33363100
C	0.18650900	−1.98819600	−0.82729600	H	−1.89829900	−3.41760200	1.19300600
C	1.82802600	−1.77139000	0.98956100	H	−3.51232100	0.99721900	−1.39698500
C	−2.93291600	1.83514700	−0.99223800	H	0.93204800	−2.02391900	1.56293700
C	2.62673800	−0.73287000	1.77608900	H	−3.62315200	2.67504300	−0.82220900
C	−1.98048200	−2.33783000	1.38731700	H	−3.01733300	−2.14176200	1.69084000
C	−1.43902200	2.65359400	0.84207200	H	3.48126300	1.77244900	2.17906300
C	−2.19318900	1.41175300	0.30474500	H	−0.92773700	2.40743600	1.78253100
C	2.49136400	1.50711700	2.57884800	H	−2.11215200	3.50098500	1.03197500
C	−3.25729200	1.02460100	1.36339100	H	−1.34673400	−2.09988100	2.25215300
H	3.01633000	0.20035900	−2.92552700	H	2.78432700	−1.09504700	2.80350200
H	1.27042900	−0.15335000	−2.85371600	H	1.83405200	2.37832900	2.53442300
H	0.74395300	2.22004700	−2.83907100	H	−3.87389500	0.18789100	1.01081500
H	2.49819000	2.59185300	−2.93088400	H	2.59670200	1.18678800	3.62503300
H	2.61853700	−2.03614500	−1.88333000	H	−2.77089200	0.71457500	2.29611000
H	−2.58183700	−1.37763800	−2.45347400	H	−3.93514100	1.86061500	1.58848600
H	0.15209200	−1.82990000	−1.91223100	N	1.38219800	−1.26708700	−0.31113500
H	−2.69056700	−2.96720500	−1.66644000	N	−1.22353900	0.35515400	0.04509400
H	3.39686900	−0.89381700	−0.77449900	O	1.94940200	1.22094700	−1.46023500
H	1.51953300	3.20660800	−1.56714100	O	1.88470600	0.48604000	1.79852400
H	0.30880200	−3.07952700	−0.68913300	Si	−1.50902800	−1.30205900	−0.16122100
H	−3.79406100	−1.66998800	−1.19799700	Li	0.65834500	0.61915100	0.12533200

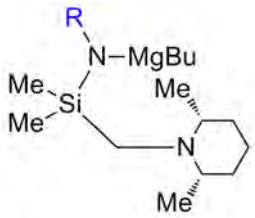
8.3.4 Angaben zu den quantenchemischen Rechnungen aus Kapitel 4.4.3 – Dimere

8.124 Berechnete Energien der optimierten Verbindungen [B3LYP/6−31+G(d)].

Verbindung	SCF [Hartree]	ZPE [Hartree]
110M	−1230.58099359	−1230.078642
110C	−2461.17887956	−2460.17176
110N	−2461.15088594	−2460.141302
111M	−1191.26899472	−1190.795046
111C	−2382.55354912	−2381.602446
111N	−2382.5615695	−2381.607668
112M	−1112.63474844	−1112.216885
112C	−2225.29038633	−2224.453292
112N	−2225.31597626	−2224.476613
113M	−1191.25987804	−1190.786581
113C	−2382.51981291	−2381.570918
113N	−2382.52806558	−2381.575459
114M	−1269.89112544	−1269.360961
114C	−2539.78134664	−2538.717617
114N	−2539.75781898	−2538.693155
115M	−1309.20559936	−1308.647553
115C	−2618.40312344	−2617.282408
115N	−2618.36132581	−2617.239893



R = ^{t}Bu (**110**)
R = ^{i}Pr (**111**)
R = Me (**112**)



R = Me (**113**)
R = ^{i}Pr (**114**)
R = ^{t}Bu (**115**)

Tabelle 8.125 Standardorientierung von **110C** und **110N** [B3LYP/6−31+G(d)].

110C				110N			
C	0.61110300	4.05105400	−3.78532700	C	−0.89971800	−0.84540700	−3.73434700
C	0.36410800	2.56200800	−3.51047500	C	1.55442000	−1.33883500	−3.41052400
C	−3.24074500	−1.91322000	−3.12523900	C	0.32169100	−0.62537400	−2.80751400
C	0.38189500	2.19832500	−2.01540600	C	−0.84692800	−3.86773200	−2.47098600
C	3.32405700	−3.60242800	−1.72499800	C	5.07469500	1.53464000	−1.38561300
C	−1.33008100	−2.92417600	−1.86464400	C	3.81642700	2.37550900	−1.59943500
C	4.89369400	2.21791500	−1.52313200	C	−5.55018100	2.06574800	−1.28442900
C	−2.79463200	−2.45647800	−1.74453500	C	−6.60890700	2.79182800	−0.44396800
C	−3.64691900	−3.70371500	−1.41040000	C	−3.23009600	0.89310400	−1.29592300
C	0.12741300	0.70159500	−1.71028900	C	5.80044800	1.96836900	−0.10656300
C	2.30505300	−2.50746300	−1.37519100	C	−4.31414100	1.62100500	−0.47939800
C	3.83849300	−0.57088000	−1.13784400	C	1.72148900	3.21734100	−0.72774800
C	−5.90590700	−0.65967000	−0.85917900	C	−4.85531700	−2.25601200	−0.23981300
C	3.89173000	−4.24991900	−0.45246800	C	−3.44639500	−2.82865800	−0.42651400
C	−3.36921200	2.09459100	−0.76904600	C	1.47669100	−3.74959600	−0.66585000

C	−4.42960900	3.17389500	−0.50406400	C	4.82812200	1.93193200	1.07833400
C	4.42960900	−3.17389500	0.50406400	C	−1.22347600	3.81559400	−0.65424200
C	−3.89173000	4.24991900	0.45246800	C	3.53459000	2.69439000	0.78323800
C	5.90590700	0.65967000	0.85917900	C	6.16471500	−3.29014100	1.27081400
C	3.36921200	−2.09459100	0.76904600	C	4.15005500	−1.75822200	0.79202000
C	−3.83849300	0.57088000	1.13784400	C	−1.19129200	−3.09028200	0.47177200
C	3.64691900	3.70371500	1.41040000	C	−5.43099300	−2.57345800	1.14446200
C	−4.89369400	−2.21791500	1.52313200	C	2.85935000	−1.09301400	1.31085400
C	−2.30505300	2.50746300	1.37519100	C	4.87639100	−2.65606300	1.81199200
C	−3.32405700	3.60242800	1.72499800	C	−4.42689100	−2.14492500	2.22003500
C	2.79463200	2.45647800	1.74453500	C	−3.06027300	−2.77700600	1.95372300
C	−0.12741300	−0.70159500	1.71028900	C	0.44207200	4.45587900	1.71644800
C	1.33008100	2.92417600	1.86464400	C	−0.41144600	1.14437700	2.36329400
C	−0.38189500	−2.19832500	2.01540600	C	−1.76395500	1.80419100	2.71961800
C	3.24074500	1.91322000	3.12523900	C	0.67002100	1.60155400	3.36994100
C	−0.36410800	−2.56200800	3.51047500	H	−0.71075900	−0.39220800	−4.71648000
C	−0.61110300	−4.05105400	3.78532700	H	1.76736500	−0.95888300	−4.41817400
H	0.59101000	4.27143800	−4.85988900	H	−1.11571300	−1.89943200	−3.90454300
H	−0.60321200	2.26290000	−3.94170400	H	1.40592700	−2.41866900	−3.49851000
H	1.12459900	1.96107900	−4.03120400	H	−1.79534400	−0.37356600	−3.31746200
H	−3.15204500	−2.67633600	−3.91146500	H	5.72524500	1.64704000	−2.26265900
H	−0.15347200	4.67566100	−3.30423900	H	−0.18270500	−3.96223000	−3.33785200
H	1.58753800	4.37007200	−3.39841700	H	−6.00073400	1.18305600	−1.76285400
H	−2.62386800	−1.05369700	−3.41485400	H	−1.83543600	−3.57830400	−2.83678000
H	−4.28417900	−1.58065500	−3.09362300	H	3.30539700	2.07622600	−2.51965700
H	−1.21500600	−3.69845300	−2.63471900	H	−5.22042800	2.71895200	−2.10603900
H	4.13962500	−3.18060400	−2.32716800	H	−7.47382100	3.09105200	−1.04982600
H	2.82844400	−4.35279500	−2.35446600	H	4.10207300	3.43686500	−1.72425700
H	5.65862100	1.74862700	−2.15899900	H	2.44464700	−1.17482700	−2.79062800
H	−3.52364700	−4.48223400	−2.17481600	H	−0.94433300	−4.87503600	−2.04221900
H	4.05698200	2.51200200	−2.16978000	H	−3.69940900	0.03554500	−1.81001100
H	1.93328100	−2.01894100	−2.28140700	H	−2.92355200	1.55970100	−2.12308700
H	0.88469900	0.11787900	−2.26999800	H	4.80274400	0.47306900	−1.32188300
H	−0.78985800	0.41732700	−2.26603400	H	6.18986600	2.98900800	−0.23986000
H	3.38859100	−0.25031400	−2.08785800	H	1.40308800	3.09078600	−1.76606700
H	−0.67482100	−2.08967700	−2.14385600	H	6.66488600	1.32194800	0.08838700
H	−5.75659800	0.08428200	−1.65123900	H	−3.05183400	−2.50425900	−1.39185300
H	−4.71558400	−3.46142700	−1.36636100	H	−5.49837900	−2.66040900	−1.03257900
H	−0.36545400	2.82159500	−1.49984800	H	−6.97854400	2.15172700	0.36861300
H	4.74292000	−1.13146500	−1.41663700	H	2.22300700	−3.68030600	−1.46603000
H	−4.71944900	3.61902100	−1.46483100	H	2.09540800	4.25759800	−0.66870500
H	1.34743800	2.50645600	−1.58941000	H	−6.19586900	3.69979700	0.01579000
H	−6.28865400	−1.57069700	−1.33722400	H	−4.82205200	−1.17134400	−0.37886300
H	5.33264600	3.13620600	−1.11461300	H	−1.53873900	3.17726300	−1.48442900
H	−3.75776600	1.30633100	−1.41775400	H	−4.66153100	0.98258400	0.35038800
H	−2.51853100	2.55304900	−1.28852600	H	1.22368000	−4.81291200	−0.55257900
H	4.67832800	−4.97230500	−0.70409600	H	−3.49953400	−3.93553600	−0.45096600
H	−0.98293800	−3.33745900	−0.91032400	H	−3.88875400	2.51299000	0.00613700
H	1.44249200	−2.96601800	−0.87651300	H	5.95937400	−3.91516700	0.39145000
H	−3.35250600	−4.12616200	−0.44273900	H	3.93648800	−2.36370100	−0.10155200
H	−6.70275100	−0.28964100	−0.19839000	H	3.75845100	3.77485700	0.70732500
H	5.33826300	−2.72024800	0.08736200	H	−0.88648100	4.77273400	−1.07744700
H	3.09395700	−4.81590000	0.05193400	H	6.88784100	−2.52137200	0.96605900
H	6.70275100	0.28964100	0.19839000	H	4.86634900	−0.99421100	0.45208100
H	−3.09395700	4.81590000	−0.05193400	H	1.95456600	−3.42079100	0.25938200
H	−5.33826300	2.72024800	−0.08736200	H	4.58954700	0.89626200	1.32953100
H	3.35250600	4.12616200	0.44273900	H	−6.39535700	−2.06911000	1.28458500
H	−4.67832800	4.97230500	0.70409600	H	5.28710200	2.37900400	1.97000700
H	6.28865400	1.57069700	1.33722400	H	−1.33231000	−4.19036300	0.52108300
H	−5.33264600	−3.13620600	1.11461300	H	−2.11549000	4.02447800	−0.05166900
H	0.98293800	3.33745900	0.91032400	H	−5.62019100	−3.65391400	1.23427500

H	−1.44249200	2.96601800	0.87651300	H	6.65237000	−3.92431800	2.02220400
H	4.71944900	−3.61902100	1.46483100	H	2.83254800	2.56925700	1.61131200
H	4.71558400	3.46142700	1.36636100	H	−0.58321700	−2.84539800	1.35110200
H	2.51853100	−2.55304900	1.28852600	H	−4.33040500	−1.05046300	2.22672300
H	3.75776600	−1.30633100	1.41775400	H	0.45885400	5.40071200	1.15467700
H	5.75659800	−0.08428200	1.65123900	H	4.18814300	−3.44844600	2.14238900
H	−4.74292000	1.13146500	1.41663700	H	2.21459700	−1.89550000	1.71459200
H	−1.34743800	−2.50645600	1.58941000	H	3.11731000	−0.49792900	2.20711400
H	0.36545400	−2.82159500	1.49984800	H	−3.15233600	−3.88018100	2.01289800
H	3.52364700	4.48223400	2.17481600	H	5.10571900	−2.06225900	2.70973500
H	−5.65862100	−1.74862700	2.15899900	H	−2.56650100	1.42993200	2.07255700
H	−4.05698200	−2.51200200	2.16978000	H	1.39389400	4.38826200	2.25279000
H	−3.38859100	0.25031400	2.08785800	H	−2.34348600	−2.48317400	2.72603600
H	−2.82844400	4.35279500	2.35446600	H	−4.76772600	−2.44471900	3.21976700
H	0.67482100	2.08967700	2.14385600	H	−0.35735400	4.54651500	2.45880600
H	−4.13962500	3.18060400	2.32716800	H	−1.73582900	2.89216600	2.61017300
H	−1.93328100	2.01894100	2.28140700	H	1.63162100	1.12913100	3.14160900
H	0.78985800	−0.41732700	2.26603400	H	0.80655300	2.68288200	3.38457000
H	−0.88469900	−0.11787900	2.26999800	H	−2.04243200	1.58640800	3.75896600
H	1.21500600	3.69845300	2.63471900	H	0.38812600	1.29752700	4.38632000
H	4.28417900	1.58065500	3.09362300	N	0.08073000	−1.03204800	−1.36476800
H	−1.58753800	−4.37007200	3.39841700	N	2.84735200	2.27476800	−0.47253700
H	0.15347200	−4.67566100	3.30423900	N	−2.49772300	−2.41054100	0.63080000
H	2.62386800	1.05369700	3.41485400	N	−0.03882900	1.39610300	0.91247600
H	3.15204500	2.67633600	3.91146500	Mg	−1.43095400	0.15899400	−0.37656600
H	−1.12459900	−1.96107900	4.03120400	Mg	1.55030700	0.12787500	0.09361800
H	0.60321200	−2.26290000	3.94170400	Si	−0.10321400	−2.77898600	−1.08150400
H	−0.59101000	−4.27143800	4.85988900	Si	0.16943700	3.08647800	0.40903200
N	−2.88857400	−1.40357700	−0.71209600	C	0.61764700	0.87659500	−2.84381300
N	2.82781200	−1.44813200	−0.46450300	H	−0.21993300	1.46701700	−2.45520400
N	−2.82781200	1.44813200	0.46450300	H	1.51310700	1.09910100	−2.25908700
N	2.88857400	1.40357700	0.71209600	H	0.80975300	1.22383500	−3.86627100
Mg	−1.37979200	−0.15474400	−0.15815800	C	−0.57421300	−0.36622100	2.57519300
Mg	1.37979200	0.15474400	0.15815800	H	−1.34986900	−0.77636900	1.92012700
Si	4.32206700	1.02254300	−0.14974300	H	0.36376500	−0.90141500	2.39626600
Si	−4.32206700	−1.02254300	0.14974300	H	−0.88472900	−0.58232200	3.60464700

Tabelle 8.126 Standardorientierung von **111C** und **111N** [B3LYP/6−31+G(d)].

111C				111N			
C	0.71665000	4.01054300	−3.78746100	C	−0.59741700	−0.52368600	−3.67691400
C	0.45480200	2.52280400	−3.51921200	C	1.79497800	−1.14284700	−3.20352300
C	−3.12718700	−2.02267600	−3.06988800	C	0.52935100	−0.47981800	−2.62604600
C	0.38883700	2.16817800	−2.02330000	C	−0.92080800	−3.68775100	−2.42516300
C	3.23011000	−3.62433400	−1.86981000	C	4.58602100	1.24877300	−1.92950500
C	4.90269000	2.18164800	−1.47417200	C	3.25848200	2.00717100	−1.96613000
C	−2.60258000	−2.38319800	−1.66383400	C	−5.29356700	2.35576600	−1.70672600
C	−3.14228300	−3.76349100	−1.24126900	C	−6.44522100	3.08941300	−1.00638800
C	0.11703700	0.67355000	−1.72302200	C	−3.08674300	1.00879500	−1.40727200
C	2.24835600	−2.51215300	−1.47415900	C	5.52299100	1.84801900	−0.87487600
C	3.84121900	−0.62140300	−1.15554000	C	−4.25800900	1.75438900	−0.73666400
C	−5.84481300	−0.61991200	−0.93421300	C	1.32456400	2.85488400	−0.76861200
C	3.78029700	−4.33745300	−0.62544100	C	−4.75969300	−2.00788100	−0.15645900
C	−3.33763800	2.21397800	−0.68114300	C	−3.35323700	−2.59947800	−0.27532300
C	−4.36022900	3.31714100	−0.36629300	C	1.44006400	−3.79092800	−0.62599800
C	4.36022900	−3.31714100	0.36629300	C	4.80591200	1.88677500	0.47895600
C	−3.78029700	4.33745300	0.62544100	C	−1.35612000	3.86945900	0.07296900
C	5.84481300	0.61991200	0.93421300	C	3.43726700	2.56372500	0.38574500
C	3.33763800	−2.21397800	0.68114300	C	6.16721700	−3.35873100	1.39869800
C	−3.84121900	0.62140300	1.15554000	C	4.14147600	−1.84655300	0.89720800
C	3.14228300	3.76349100	1.24126900	C	−1.09701200	−2.80981800	0.59988600

C	−4.90269000	−2.18164800	1.47417200	C	−5.30027200	−2.09258900	1.27423800
C	−2.24835600	2.51215300	1.47415900	C	2.90382000	−1.09581000	1.43005900
C	−3.23011000	3.62433400	1.86981000	C	4.94289100	−2.62327900	1.96008800
C	2.60258000	2.38319800	1.66383400	C	−4.27677500	−1.48098400	2.23642400
C	−0.11703700	−0.67355000	1.72302200	C	−2.90862700	−2.14163700	2.05917400
C	−0.38883700	−2.16817800	2.02330000	C	0.78172300	3.96768200	2.12506200
C	3.12718700	2.02267600	3.06988800	C	−0.55963300	0.72791300	2.44696200
C	−0.45480200	−2.52280400	3.51921200	C	−1.86190800	1.40610400	2.91349400
C	−0.71665000	−4.01054300	3.78746100	C	0.51521400	0.85515000	3.54347200
H	0.76031500	4.22524100	−4.86245100	H	−0.29238600	0.03228200	−4.57383100
H	−0.48629400	2.22037500	−4.00276700	H	2.11466100	−0.63790500	−4.12448100
H	1.24424200	1.91991300	−3.99262100	H	−0.82201500	−1.54794400	−3.98851600
H	−2.85619500	−2.79056500	−3.80838800	H	1.60946900	−2.19332500	−3.45885100
H	−0.07558800	4.63694500	−3.35596100	H	−1.51631100	−0.06820900	−3.29759000
H	1.66811700	4.33225500	−3.34463100	H	5.03891200	1.28988700	−2.92855100
H	−2.70967600	−1.06540800	−3.40333500	H	−0.20884400	−3.89850800	−3.23369900
H	−4.22033900	−1.92799300	−3.06629400	H	−5.69870200	1.55183000	−2.33963000
H	4.05663300	−3.20263000	−2.45707200	H	−1.79587200	−3.21050900	−2.87448900
H	2.71071400	−4.33383200	−2.52686100	H	2.59253000	1.59051700	−2.72625200
H	5.70438200	1.73632900	−2.08119900	H	−4.77820500	3.04713400	−2.39020900
H	−2.84573100	−4.54136600	−1.95794900	H	−7.16135100	3.50488200	−1.72703400
H	4.08793700	2.46594600	−2.15222100	H	3.44917200	3.05944600	−2.24687400
H	1.89013300	−1.97706700	−2.35937000	H	2.62966700	−1.11747600	−2.49424600
H	0.89323800	0.08710700	−2.25308100	H	0.76263000	0.58868400	−2.50746700
H	−0.78185300	0.38085400	−2.30274600	H	−1.23999300	−4.66110500	−2.02706800
H	3.41693400	−0.27931900	−2.10969000	H	−3.51370700	0.23363000	−2.07238400
H	−5.65991700	0.10532600	−1.73608200	H	−2.60185600	1.71334700	−2.11019300
H	−4.23982500	−3.76057500	−1.19570600	H	4.40476800	0.18995300	−1.70454300
H	−0.38587900	2.79614700	−1.55605200	H	5.81055900	2.86626300	−1.17761700
H	4.74663900	−1.18577700	−1.42268500	H	0.75530000	2.51722600	−1.64549400
H	−4.64176200	3.80754200	−1.30719500	H	6.44892200	1.26461900	−0.80185400
H	1.32981500	2.47698300	−1.54588900	H	−2.98139500	−2.44861100	−1.28962700
H	−6.19915300	−1.54473800	−1.40916500	H	−5.41229900	−2.54940700	−0.85377200
H	5.30377700	3.10491200	−1.03785400	H	−6.99912500	2.41403400	−0.34022500
H	−3.75860100	1.46172000	−1.35254800	H	2.20920700	−3.72728500	−1.40483100
H	−2.47818100	2.66358400	−1.19381600	H	1.62853400	3.89320400	−0.99851500
H	4.54012200	−5.07673200	−0.90798900	H	−6.07080400	3.92051200	−0.39358800
H	1.37112200	−2.96213700	−0.98829000	H	−4.74193600	−0.96481900	−0.48387800
H	−2.76431500	−4.04422700	−0.25180000	H	−1.81592600	3.43963400	−0.82163700
H	−6.67332800	−0.24069800	−0.31930500	H	−4.79699500	1.08519500	−0.04520500
H	5.28055400	−2.87855700	−0.04080800	H	1.12683400	−4.84278500	−0.56600700
H	2.96552700	−4.89357300	−0.13756400	H	−3.39842900	−3.69074200	−0.10269300
H	6.67332800	0.24069800	0.31930500	H	−3.87870500	2.56942800	−0.10246700
H	−2.96552700	4.89357300	0.13756400	H	5.87314200	−4.08908100	0.63289700
H	−5.28055400	2.87855700	0.04080800	H	3.85510200	−2.55592500	0.10730700
H	2.76431500	4.04422700	0.25180000	H	3.57123500	3.63973700	0.17164800
H	−4.54012200	5.07673200	0.90798900	H	−1.01056800	4.88256900	−0.17759000
H	6.19915300	1.54473800	1.40916500	H	6.87157500	−2.65768900	0.93036500
H	−5.30377700	−3.10491200	1.03785400	H	4.83423400	−1.14414600	0.40564300
H	−1.37112200	2.96213700	0.98829000	H	1.90961200	−3.52615500	0.32531600
H	4.64176200	−3.80754200	1.30719500	H	4.67935700	0.86992000	0.85943800
H	4.23982500	3.76057500	1.19570600	H	−6.26491100	−1.57622600	1.35192700
H	2.47818100	−2.66358400	1.19381600	H	5.40208900	2.43369500	1.22108700
H	3.75860100	−1.46172000	1.35254800	H	−1.30980800	−3.87130500	0.82951000
H	5.65991700	−0.10532600	1.73608200	H	−2.14174100	3.97539000	0.83048300
H	−4.74663900	1.18577700	1.42268500	H	−5.47774500	−3.14380700	1.54725100
H	−1.32981500	−2.47698300	1.54588900	H	6.71144400	−3.90073900	2.18279200
H	0.38587900	−2.79614700	1.55605200	H	2.92815000	2.48732500	1.34785000
H	2.84573100	4.54136600	1.95794900	H	−0.44092600	−2.46271400	1.41092700
H	−5.70438200	−1.73632900	2.08119900	H	−4.19719100	−0.40204500	2.05595000
H	−4.08793700	−2.46594600	2.15222100	H	1.05890600	4.93795700	1.68927300

H	−3.41693400	0.27931900	2.10969000	H	4.27298900	−3.34586200	2.44988900
H	−2.71071400	4.33383200	2.52686100	H	2.28535500	−1.82384600	1.99180800
H	−4.05663300	3.20263000	2.45707200	H	3.25321200	−0.39729600	2.21444600
H	−1.89013300	1.97706700	2.35937000	H	−2.99428000	−3.21686100	2.30266800
H	0.78185300	−0.38085400	2.30274600	H	5.26100700	−1.92479900	2.74874800
H	−0.89323800	−0.08710700	2.25308100	H	−2.65323300	1.32648300	2.15980500
H	4.22033900	1.92799300	3.06629400	H	−0.77113900	−0.34948400	2.38318200
H	−1.66811700	−4.33225500	3.34463100	H	1.65442400	3.58694400	2.66273800
H	0.07558800	−4.63694500	3.35596100	H	−2.17909900	−1.71746900	2.75429700
H	2.70967600	1.06540800	3.40333500	H	−4.59078600	−1.60772100	3.28064800
H	2.85619500	2.79056500	3.80838800	H	0.00011000	4.17096900	2.86797600
H	−1.24424200	−1.91991300	3.99262100	H	−1.70176400	2.47309400	3.11082800
H	0.48629400	−2.22037500	4.00276700	H	1.44993300	0.37515600	3.24065300
H	−0.76031500	−4.22524100	4.86245100	H	0.72392600	1.90062700	3.78907300
N	−2.83793700	−1.32122600	−0.68043200	H	−2.22984600	0.95476600	3.84408800
N	2.80730700	−1.50638400	−0.52347000	H	0.17042800	0.36483200	4.46396500
N	−2.80730700	1.50638400	0.52347000	N	0.15893400	−0.98729600	−1.26682300
N	2.83793700	1.32122600	0.68043200	N	2.53774900	1.99198000	−0.66058600
Mg	−1.36933000	−0.06497900	−0.12997900	N	−2.36064300	−2.01866100	0.67725600
Mg	1.36933000	0.06497900	0.12997900	N	−0.13123500	1.15285700	1.07719500
Si	4.29895400	0.96689000	−0.13280700	Mg	−1.49680000	0.05841400	−0.28811500
Si	−4.29895400	−0.96689000	0.13280700	Mg	1.51588400	0.01564400	0.18762600
H	−1.50895300	−2.50769600	−1.77120100	Si	−0.06985600	−2.71137800	−1.02144300
H	1.50895300	2.50769600	1.77120100	Si	0.10983300	2.85660900	0.72429700

Tabelle 8.127 Standardorientierung von **112C** und **112N** [B3LYP/6−31+G(d)].

112C				112N			
C	0.76499400	4.01389000	−3.76403600	C	0.25807200	−0.50243500	−2.55654300
C	0.48088600	2.52797800	−3.50827800	C	−0.92185500	−3.49952300	−2.59731300
C	0.39105500	2.16626100	−2.01530500	C	3.53769400	1.74044400	−2.51883700
C	3.22873100	−3.62527200	−1.89486500	C	2.27381000	2.41864100	−1.98769100
C	4.92535400	2.21986900	−1.42856800	C	−4.65490800	2.65209000	−2.19458700
C	−2.70229500	−2.47099400	−1.51516500	C	−5.88929200	3.47987000	−1.81232300
C	0.10049300	0.67329200	−1.72481000	C	−2.71357800	1.14435400	−1.34544600
C	2.25812800	−2.50103600	−1.50538800	C	4.77351900	2.21463200	−1.74478500
C	3.87672000	−0.63551800	−1.17137600	C	−3.95931900	1.97930900	−0.99541600
C	−5.80849800	−0.63969500	−0.99608900	C	0.82519100	2.90287500	−0.09734900
C	3.75949100	−4.34765200	−0.64733600	C	−4.74410100	−1.73999300	−0.13245400
C	−3.33179200	2.22160100	−0.65968800	C	−3.44318000	−2.53301000	−0.27663900
C	−4.34332400	3.33703200	−0.35200500	C	1.41665700	−3.82257200	−0.72705200
C	4.34332400	−3.33703200	0.35200500	C	4.54468800	2.02011300	−0.24170600
C	−3.75949100	4.34765200	0.64733600	C	−1.50023100	3.41051900	1.81199500
C	5.80849800	0.63969500	0.99608900	C	3.22602700	2.64249600	0.22182100
C	3.33179200	−2.22160100	0.65968800	C	6.48063100	−3.12490400	0.95412400
C	−3.87672000	0.63551800	1.17137600	C	4.31391400	−1.76890500	0.62541500
C	−4.92535400	−2.21986900	1.42856800	C	−1.18955100	−2.99054000	0.52672800
C	−2.25812800	2.50103600	1.50538800	C	−5.27522100	−1.76773000	1.30543500
C	−3.22873100	3.62527200	1.89486500	C	3.10897200	−1.05107000	1.26288500
C	2.70229500	2.47099400	1.51516500	C	5.28908900	−2.42544300	1.62190500
C	−0.10049300	−0.67329200	1.72481000	C	−4.16326700	−1.34912700	2.27506200
C	−0.39105500	−2.16626100	2.01530500	C	−2.90980100	−2.19960400	2.06091600
C	−0.48088600	−2.52797800	3.50827800	C	1.18455400	2.90623600	3.07596100
C	−0.76499400	−4.01389000	3.76403600	C	−0.10888300	−0.03719900	2.77227200
H	0.82768700	4.23444700	−4.83694200	H	3.63309500	1.96346900	−3.58929500
H	−0.45728400	2.23991100	−4.00605800	H	−0.17799200	−3.62249300	−3.39549100
H	1.26926400	1.91813300	−3.97465000	H	−4.94185500	1.87596700	−2.92017200
H	−0.02590300	4.64754600	−3.34068800	H	−1.74862900	−2.91272200	−3.01350800
H	1.71342200	4.32086000	−3.30443100	H	1.39238000	2.08743200	−2.54087500
H	4.06526600	−3.21339700	−2.47491500	H	−3.92652200	3.29424500	−2.71236200
H	2.70546400	−4.32697200	−2.55720800	H	−6.35796800	3.94094100	−2.69129600

H	5.81935600	1.86677600	−1.96168600	H	2.35533600	3.51151100	−2.13281900
H	4.15276700	2.44216700	−2.17569300	H	−0.02465500	0.55525800	−2.61037900
H	1.91440000	−1.95994500	−2.39270800	H	−1.30775900	−4.50111200	−2.36484100
H	0.87386800	0.08082900	−2.25273800	H	−3.00094900	0.42645800	−2.14027800
H	−0.80000200	0.39070900	−2.30723700	H	−2.00279300	1.81984200	−1.86211000
H	3.47000200	−0.29255400	−2.13272400	H	3.43755400	0.64969600	−2.43010600
H	−5.60645500	0.10849900	−1.77238200	H	4.95098300	3.27885000	−1.96106700
H	−0.38386500	2.79969800	−1.55579000	H	0.03362900	2.70610400	−0.83355400
H	4.77799500	−1.21376600	−1.42152300	H	5.66863500	1.67067400	−2.07044500
H	−4.60936700	3.83317100	−1.29441100	H	−3.05863300	−2.43332300	−1.29377600
H	1.32866200	2.46373400	−1.52367900	H	−5.48124000	−2.16015600	−0.82885700
H	−6.09337600	−1.56802300	−1.50988400	H	−6.64829200	2.85628900	−1.32063700
H	5.19416600	3.16845700	−0.94447000	H	2.15523300	−3.71390500	−1.53160300
H	−3.75454000	1.47681500	−1.33832600	H	1.02131600	3.98921900	−0.15331800
H	−2.46178600	2.66240300	−1.16202100	H	−5.62590700	4.28661400	−1.11511900
H	4.51238100	−5.09584200	−0.92500900	H	−4.56742100	−0.70517300	−0.44185500
H	1.37092500	−2.94024400	−1.02776900	H	−2.19167100	3.27782900	0.97461600
H	−6.68826400	−0.30781500	−0.42734300	H	−4.71128800	1.36149500	−0.47668200
H	5.27322900	−2.90974900	−0.04521600	H	1.13423000	−4.88403700	−0.68701600
H	2.93353400	−4.89442500	−0.16780600	H	−3.63796900	−3.60753100	−0.10537200
H	6.68826400	0.30781500	0.42734300	H	−3.69873700	2.76789000	−0.27311400
H	−2.93353400	4.89442500	0.16780600	H	6.14342100	−3.91716000	0.27206900
H	−5.27322900	2.90974900	0.04521600	H	3.96847700	−2.54755800	−0.07173700
H	−4.51238100	5.09584200	0.92500900	H	3.27332500	3.74180400	0.11291700
H	6.09337600	1.56802300	1.50988400	H	−1.27540600	4.48231900	1.90117400
H	−5.19416600	−3.16845700	0.94447000	H	7.07688700	−2.41571700	0.36395900
H	−1.37092500	2.94024400	1.02776900	H	4.89537100	−1.06915300	0.00210200
H	4.60936700	−3.83317100	1.29441100	H	1.91714800	−3.56982400	0.21338400
H	2.46178600	−2.66240300	1.16202100	H	4.53805500	0.95239500	−0.00211500
H	3.75454000	−1.47681500	1.33832600	H	−6.14591100	−1.10820500	1.40503700
H	5.60645500	−0.10849900	1.77238200	H	5.35969700	2.47167900	0.33872200
H	−4.77799500	1.21376600	1.42152300	H	−1.50475300	−4.04525600	0.62851100
H	−1.32866200	−2.46373400	1.52367900	H	−2.02845700	3.11497100	2.72848700
H	0.38386500	−2.79969800	1.55579000	H	−5.61419500	−2.78340200	1.55909400
H	−5.81935600	−1.86677600	1.96168600	H	7.14912000	−3.58538500	1.69305200
H	−4.15276700	−2.44216700	2.17569300	H	3.06920600	2.42935900	1.28048900
H	−3.47000200	0.29255400	2.13272400	H	−0.53030700	−2.79860900	1.38365300
H	−2.70546400	4.32697200	2.55720800	H	−3.91897600	−0.28768200	2.12758300
H	−4.06526600	3.21339700	2.47491500	H	1.53788900	3.93846000	2.95043500
H	−1.91440000	1.95994500	2.39270800	H	4.73370900	−3.15072700	2.23567400
H	0.80000200	−0.39070900	2.30723700	H	2.58543600	−1.78629000	1.90627700
H	−0.87386800	−0.08082900	2.25273800	H	3.49667400	−0.30731000	1.98693900
H	−1.71342200	−4.32086000	3.30443100	H	−3.14310600	−3.25973800	2.26888800
H	0.02590300	−4.64754600	3.34068800	H	5.65589700	−1.65787100	2.32002900
H	−1.26926400	−1.91813300	3.97465000	H	−0.01733500	−1.12270900	2.64111400
H	0.45728400	−2.23991100	4.00605800	H	2.06267900	2.26794200	3.22719700
H	−0.82768700	−4.23444700	4.83694200	H	−2.11710800	−1.90216200	2.75058500
N	−2.83982700	−1.30722300	−0.64373400	H	−4.48851400	−1.45806800	3.31763500
N	2.82165300	−1.50367500	−0.54813300	H	0.60191700	2.88045600	4.00636000
N	−2.82165300	1.50367500	0.54813300	N	0.11622500	−1.01490600	−1.16986500
N	2.83982700	1.30722300	0.64373400	N	2.04054300	2.14978200	−0.53967300
Mg	−1.36813500	−0.06256800	−0.12127200	N	−2.37822300	−2.09457200	0.67212500
Mg	1.36813500	0.06256800	0.12127200	N	−0.09342900	0.66522900	1.46524500
Si	4.31154300	0.95199700	−0.14486200	Mg	−1.48033600	−0.06549000	−0.03581600
Si	−4.31154300	−0.95199700	0.14486200	Mg	1.51284000	−0.06425200	0.19293900
H	−1.73390600	−2.46437700	−2.04029600	Si	−0.10878000	−2.74547900	−1.04891600
H	1.73390600	2.46437700	2.04029600	Si	0.08766800	2.39909000	1.60342700
H	−2.75080000	−3.43378800	−0.97341500	H	−0.39221300	−1.01851000	−3.27595700
H	−3.47187300	−2.51637500	−2.30658300	H	−1.03327700	0.13974600	3.34745300
H	3.47187300	2.51637500	2.30658300	H	0.72973900	0.25205600	3.42140400
H	2.75080000	3.43378800	0.97341500	H	1.28666000	−0.58810400	−2.94492300

Tabelle 8.128 Standardorientierung von **110M** und **111M** [B3LYP/6−31+G(d)].

110M				111M			
C	−6.03113200	−1.89880400	−0.17640200	C	−6.03139600	−1.38794700	−0.24651600
C	−4.63754300	−2.52221600	−0.02321500	C	−4.71671400	−2.14361700	−0.01232900
C	2.58177600	−2.15531700	1.84914500	C	−3.46293700	−1.25519000	−0.11737600
C	−3.48529600	−1.50885900	−0.15573700	C	1.84745300	−3.09141700	1.60363900
C	1.64261400	−3.36535100	−0.13619400	C	2.42865900	−2.40081300	0.35752700
C	2.42108200	−2.10808500	0.30982100	C	2.42571600	−3.37032800	−0.83982900
C	3.82548900	−2.17708900	−0.33127800	C	−2.12787300	−1.98958500	0.11150700
C	−2.07446300	−2.11055100	−0.01130900	C	3.55920000	0.99837700	1.17964800
C	3.27942100	1.50033100	1.01658200	C	−0.24732500	1.76486900	1.22597600
C	−0.55059900	1.73443300	1.23514600	C	−0.29177500	3.29557500	1.35543400
C	−0.72239700	3.24659500	1.44885700	C	−1.43913200	3.88818800	0.52213700
C	−1.95309500	3.77473600	0.69458200	C	1.15857000	1.52179600	−0.81565700
C	0.77961300	1.71376100	−0.87085800	C	3.76346800	0.25610700	−1.75055200
C	3.44859400	0.86628600	−1.93956100	C	−1.30883900	1.84904500	−0.96274000
C	−1.71032700	1.83067700	−0.90164900	C	−1.37106500	3.38180600	−0.92733300
C	−1.90648900	3.34799400	−0.78115000	H	−6.90155400	−2.05103000	−0.16048400
H	−6.82483000	−2.65010000	−0.07694900	H	−4.73418200	−2.61605100	0.98097800
H	−4.56118100	−3.01996300	0.95485900	H	−4.62900700	−2.96582500	−0.73774800
H	−4.50188300	−3.31212400	−0.77669500	H	−6.15893200	−0.57746700	0.48396100
H	3.11419600	−3.05986900	2.17443600	H	−6.05683500	−0.93609100	−1.24738300
H	−6.20744400	−1.12779600	0.58589300	H	2.39717800	−4.00926500	1.85192800
H	−6.14692200	−1.42260200	−1.15945300	H	2.98723500	−4.28897200	−0.61956200
H	1.59884300	−2.14766400	2.33732000	H	−2.06445200	−2.83209200	−0.60042300
H	3.14113600	−1.28434100	2.20950600	H	−2.15906100	−2.47416300	1.10405700
H	2.16592900	−4.28536500	0.15432700	H	1.88660100	−2.42131600	2.47038800
H	4.33994200	−3.10520700	−0.05076200	H	2.95252500	1.13846400	2.08298800
H	−1.95556900	−2.91176900	−0.76232600	H	2.87117400	−2.89795400	−1.72258200
H	−2.01566100	−2.63730800	0.95880700	H	−3.57226000	−0.42969600	0.60655000
H	0.64476200	−3.40331300	0.32216300	H	−0.40942400	3.55165300	2.41627400
H	2.72707500	1.49231300	1.96448900	H	−3.46874500	−0.77674100	−1.11104400
H	4.45855300	−1.34372000	−0.00214900	H	4.37440500	0.31141500	1.44461800
H	−3.64216100	−0.71781100	0.59749500	H	0.60409800	1.35166500	1.77497300
H	−0.81501800	3.43791100	2.52568400	H	−1.16163700	1.34406200	1.66943000
H	−3.58540400	−1.00722700	−1.13268300	H	0.79683500	−3.37104800	1.43672200
H	4.24072400	1.00281600	1.20046100	H	1.39588700	−3.65533700	−1.09593900
H	0.35647000	1.37087000	1.72684000	H	4.02165900	1.96295200	0.92834000
H	−1.40483300	1.21170800	1.68973900	H	−2.40120000	3.58755400	0.96392100
H	1.51737500	−3.37211300	−1.22596200	H	0.66537600	3.72898100	1.03734200
H	3.75572200	−2.14269000	−1.42447800	H	−1.40881800	4.98441400	0.55132700
H	3.50548700	2.54688500	0.76742200	H	4.60704800	−0.41820600	−1.55179900
H	−2.86485400	3.36945400	1.15890000	H	−2.23567400	1.43577400	−0.54476500
H	0.17849800	3.77842900	1.11658200	H	1.46651000	2.57098800	−0.69916700
H	−2.01647100	4.86666500	0.77956600	H	4.18864500	1.24890300	−1.95504600
H	4.46115200	0.47933300	−1.77522800	H	3.27115500	−0.09623100	−2.66593900
H	−2.57656300	1.31301400	−0.47035900	H	1.02241900	1.37082000	−1.89514000
H	0.98834200	2.78673000	−0.74753300	H	−2.25021700	3.71274500	−1.49502500
H	3.54886400	1.93007900	−2.20000600	H	−0.49325600	3.80546600	−1.43344000
H	3.03296100	0.34590200	−2.81191100	H	−1.22717200	1.48373500	−1.99249800
H	0.61979200	1.56630600	−1.94792900	N	1.70690800	−1.15700800	0.05068300
H	−2.83605900	3.62585800	−1.29438400	N	−0.17711200	1.26650700	−0.18133800
H	−1.09331300	3.87412800	−1.29899100	Mg	−0.27155200	−0.94723900	−0.01079300
H	−1.64217800	1.52609800	−1.95198600	Si	2.55493400	0.29373800	−0.28004400
N	1.66893900	−0.90146300	−0.09637800	H	3.48858600	−2.18526400	0.58768600
N	−0.49803500	1.31727300	−0.19801000				
Mg	−0.33400700	−0.88294600	−0.14176300				
Si	2.33305600	0.64999400	−0.40810800				

Tabelle 8.129 Standardorientierung von **112M** und **113M** [B3LYP/6−31+G(d)].

112M				**113M**			
C	6.02447400	−0.48375600	0.09964000	C	−0.63627900	3.41885400	−0.14319600
C	4.90173700	−1.51224400	−0.09068800	C	2.69530200	2.82558800	−1.41320100
C	3.48729500	−0.91938400	0.04994700	C	0.95178600	−1.80807900	−1.19375800
C	−1.99665000	−3.22042700	−0.53770300	C	2.10268900	−2.82672900	−1.12846500
C	2.33920800	−1.93025200	−0.13827900	C	2.07011900	−3.61689500	0.18686600
C	−3.77986100	−0.10291300	−1.31909800	C	2.14476900	0.11167900	−0.05987800
C	−0.22670100	1.41381900	−1.17867300	C	2.47704200	2.73131800	1.60889600
C	−0.49937800	2.92325900	−1.27090900	C	0.87473300	−1.63623100	1.24651200
C	0.47085300	3.71585000	−0.38137900	C	2.00748600	−2.66904300	1.39247800
C	−1.61950900	0.82130900	0.80005900	C	−2.73343100	−0.69316200	−0.27926100
C	−3.94258600	−1.00644400	1.57309000	C	−4.01504900	0.10992800	0.02515200
C	0.71923200	1.64911100	1.05135200	C	−5.32318700	−0.69679200	−0.07006500
C	0.46312500	3.16255300	1.05204000	C	−6.58087500	0.12541500	0.24081800
H	7.01625900	−0.94146100	−0.00581400	H	2.37711100	2.44050200	−2.39074000
H	4.99331300	−1.97944500	−1.08239200	H	2.02259000	−3.50892500	−1.98481000
H	5.01844500	−2.32610200	0.64002300	H	2.53789700	3.91225400	−1.42455500
H	5.95195900	0.32422900	−0.64097300	H	3.77800700	2.65982700	−1.32041300
H	5.97609900	−0.02323300	1.09568700	H	1.18462300	−4.26987300	0.19268400
H	2.46600400	−2.74732900	0.59360300	H	3.06446800	−2.30549300	−1.23366200
H	2.46027900	−2.42105000	−1.12059300	H	2.94454300	−4.27525100	0.26216000
H	−3.17803100	0.19490400	−2.18678700	H	2.32039000	3.81731400	1.65428200
H	3.39293100	−0.09433000	−0.67679500	H	−0.06864500	−2.19367900	1.15306300
H	−0.40344400	3.23024000	−2.32035500	H	2.70959800	−0.06165000	−0.98117700
H	3.41580300	−0.44499800	1.04294600	H	−3.95583900	0.54775900	1.03525600
H	−4.42473100	−0.93020100	−1.64542000	H	−4.09286200	0.96985000	−0.66007100
H	−0.95356900	0.84943700	−1.77007400	H	3.56191100	2.56221100	1.66111500
H	0.76968400	1.20670300	−1.59563300	H	2.02374800	2.30077600	2.51058300
H	−4.44081200	0.73661800	−1.06236800	H	2.84432300	−0.14397300	0.74474400
H	1.48814200	3.63673600	−0.79380700	H	1.84278400	−3.23854300	2.31634100
H	−1.53550800	3.13743300	−0.97975100	H	2.96995600	−2.15383900	1.51559700
H	0.21246300	4.78202400	−0.38568600	H	−2.82888800	−1.13944700	−1.28594300
H	−4.63470200	−1.81239400	1.29534300	H	−2.69164500	−1.56130800	0.40401200
H	1.72580500	1.44954600	0.66126500	H	−6.54422300	0.53663900	1.25855200
H	−2.13153100	1.78971700	0.70435300	H	−6.68225600	0.97162600	−0.45185000
H	−4.55552000	−0.12728300	1.81622300	H	−5.26308300	−1.55319600	0.61839400
H	−3.42343000	−1.32089900	2.48752400	H	−5.40312400	−1.12491400	−1.08058000
H	−1.49159200	0.65798400	1.87873900	H	−7.49236700	−0.48062000	0.16025000
H	1.23577300	3.65067800	1.65990200	N	0.02427200	2.11216400	−0.11349000
H	−0.49910900	3.38039000	1.53464400	N	0.96757200	−0.84174600	−0.03340000
H	0.68011300	1.24472800	2.06900700	Mg	−0.88333300	0.36217000	−0.17108100
N	−1.56607600	−1.87288300	−0.15958300	Si	1.72798700	2.00939300	0.01135500
N	−0.23889400	0.86787000	0.21312900	C	0.75861700	−0.73880200	2.48183200
Mg	0.31468300	−1.27249100	−0.01894500	H	−0.04448200	0.00263700	2.38661600
Si	−2.71350100	−0.64494700	0.16598500	H	0.53248700	−1.35722700	3.35759400
H	−2.58492300	−3.24031000	−1.47211000	H	1.68594600	−0.19555400	2.68826900
H	−1.13359800	−3.88130000	−0.70534900	C	0.88214300	−1.09676200	−2.54899900
H	−2.61240800	−3.70966600	0.23696700	H	0.07674500	−0.35216000	−2.58725600
				H	1.81654200	−0.58874600	−2.80855200
				H	0.67847700	−1.83458800	−3.33294400
				H	0.01028800	−2.36326900	−1.07083700
				H	−1.72524400	3.31146900	−0.25299100
				H	−0.30386700	4.05237600	−0.98415200
				H	−0.47582000	4.00483300	0.77886600

Tabelle 8.130 Standardorientierung von **114M** und **115M** [B3LYP/6−31+G(d)].

114M				**115M**			
C	−0.85780400	3.58549500	−1.65057000	C	0.00649700	3.58343700	−1.64856700
C	−1.01362500	2.91730500	−0.26984800	C	−0.20633200	3.08042100	−0.19974200
C	−0.90964500	3.97241600	0.84694500	C	0.40472200	4.11192500	0.77642200
C	2.69207900	2.83473200	−0.87020600	C	3.29435000	2.08917200	−0.97400600
C	1.31713100	−1.94167100	−1.29768900	C	0.80823300	−2.22973700	−1.28461300
C	2.56583300	−2.83680800	−1.21836900	C	1.82035600	−3.38802000	−1.27756500
C	2.52101900	−3.74614600	0.01684600	C	1.65137400	−4.26396000	−0.02911300
C	2.18251600	−0.01659400	0.09784500	C	2.18656600	−0.55839400	0.02043200
C	2.03097500	2.38327300	2.04674100	C	2.71567200	1.78092900	1.97982100
C	1.03078200	−2.01302900	1.13199700	C	0.68131400	−2.23385000	1.15880400
C	2.25989800	−2.92755200	1.28850800	C	1.67433400	−3.40823200	1.24434900
C	−2.55285200	−1.27905000	−0.50567500	C	−2.64105800	−0.87442700	−0.48128300
C	−3.87101400	−0.73103600	0.08041600	C	−3.90882400	−0.29339800	0.17491200
C	−5.09524400	−1.64436500	−0.11551800	C	−5.20712400	−1.06215000	−0.13315600
C	−6.39250300	−1.07419900	0.47328900	C	−6.45510400	−0.45663300	0.52283300
H	−1.60589500	4.37700500	−1.79686900	H	−0.44254600	4.57439100	−1.80323500
H	−0.98000100	2.84584000	−2.45073300	H	−0.44961000	2.88704600	−2.36313500
H	0.13689100	4.03501700	−1.75958700	H	1.07330600	3.65493400	−1.88564000
H	−1.68527700	4.74158200	0.73474100	H	−0.07519900	5.09267700	0.66278100
H	2.53733600	2.57516400	−1.92525900	H	3.03172300	1.86154900	−2.01520600
H	0.06362300	4.48082500	0.82446800	H	1.47702800	4.25254100	0.59379200
H	2.62867100	−3.43963800	−2.13365400	H	1.67845600	−3.98733900	−2.18620300
H	2.51224600	3.91273100	−0.76749300	H	3.37995500	3.17979700	−0.88700600
H	−1.02589300	3.50758700	1.83251100	H	0.27525700	3.78641800	1.81513000
H	3.75225700	2.66384000	−0.63290600	H	4.29450300	1.67443700	−0.78143400
H	1.71731600	−4.48698500	−0.10927300	H	0.69086200	−4.79690600	−0.09040500
H	3.46844500	−2.21044800	−1.19471400	H	2.84274700	−2.98741300	−1.32470900
H	3.45583800	−4.31260200	0.11134200	H	2.43369000	−5.03206800	0.01187000
H	1.87004000	3.46019800	2.17991500	H	2.89240700	2.85710600	2.09610800
H	0.16775700	−2.65668400	0.90759100	H	−0.31993100	−2.66019300	1.00294900
H	2.83905600	−0.04054900	−0.77761600	H	2.74238300	−0.70950900	−0.91009900
H	−3.75667000	−0.54124600	1.16065300	H	−3.78504300	−0.25519000	1.27008000
H	−4.10114100	0.25083200	−0.36419000	H	−4.05068700	0.75358500	−0.13701000
H	3.09333600	2.18733000	2.25299500	H	3.67906400	1.27710500	2.14540800
H	1.43860800	1.86989900	2.81435400	H	2.03302100	1.47575400	2.78231900
H	2.83891100	−0.26352800	0.94055400	H	2.83977400	−0.96520400	0.80187300
H	2.09273500	−3.59448000	2.14416700	H	1.41648100	−4.01963700	2.11889400
H	3.14455300	−2.32458400	1.53490600	H	2.68938400	−3.02765200	1.42254600
H	−2.70281500	−1.47294800	−1.58315500	H	−2.81112400	−0.93372500	−1.57264400
H	−2.36327300	−2.27740100	−0.07014400	H	−2.53933800	−1.92936600	−0.16482600
H	−6.29674200	−0.90568400	1.55436600	H	−6.35815400	−0.43655900	1.61670900
H	−6.64703600	−0.11075800	0.01184100	H	−6.61625200	0.57691200	0.18836900
H	−4.88352800	−2.62391800	0.33903300	H	−5.08915400	−2.10654400	0.19310100
H	−5.22965500	−1.83170300	−1.19141800	H	−5.34607400	−1.09945900	−1.22413700
H	−7.24154100	−1.75189300	0.31696700	H	−7.35960200	−1.02905400	0.28023300
N	−0.11014200	1.76977200	−0.09408700	N	0.36334100	1.72650800	−0.02826400
N	1.13215700	−1.09520900	−0.06098600	N	0.90925500	−1.36314200	−0.05186500
Mg	−0.80826200	−0.07759000	−0.25851200	Mg	−0.75245900	0.08037800	−0.17887700
Si	1.56004600	1.82143400	0.28343800	Si	2.01950800	1.36853700	0.24988600
C	0.71513400	−1.25542300	2.42471100	C	0.64030600	−1.42474400	2.45746200
H	−0.14670600	−0.58435000	2.31679700	H	−0.06101100	−0.58264200	2.40036500
H	0.47109500	−1.97464200	3.21441700	H	0.30759800	−2.07157800	3.27687700
H	1.56139200	−0.65486600	2.77193000	H	1.62136900	−1.02243400	2.72809000
C	1.27763800	−1.11614400	−2.58793900	C	−1.72528600	3.02771700	0.06909700
H	0.40868000	−0.44725600	−2.62952500	H	−2.22923200	2.34452700	−0.62858000
H	2.17316800	−0.50126800	−2.72331800	H	−1.92727200	2.68374300	1.09154300
H	1.20892400	−1.79354100	−3.44632900	H	−2.19094100	4.01381100	−0.05376100
H	0.43693100	−2.60118200	−1.30666600	C	0.87043200	−1.41887200	−2.58340100

H	−2.04914700	2.53614600	−0.23008000	H	0.17243900	−0.57188100	−2.58292800
				H	1.87080300	−1.02402300	−2.78791600
				H	0.59317800	−2.06583800	−3.42307600
				H	−0.19859900	−2.66682000	−1.22418200

Tabelle 8.131 Standardorientierung von **113C** und **113N** [B3LYP/6−31+G(d)].

113C				**113N**			
C	0.25429400	3.37253600	−4.42632900	C	0.10995000	−0.12338200	−2.82200800
C	−0.09266000	1.98252800	−3.87693300	C	−0.93951800	−3.01423500	−3.29803800
C	0.17409500	1.83324000	−2.36873600	C	5.02964300	0.80124300	−1.10058500
C	3.63394800	−2.96305900	−2.77708500	C	3.89276500	1.74701400	−1.52023100
C	5.36640200	2.04847400	−1.33112600	C	−5.32684900	2.77510300	−1.24659000
C	−2.42193100	−2.82190900	−0.63661900	C	−6.11313800	3.76369400	−0.37520700
C	−0.15891500	0.44029100	−1.77976800	C	−3.39225200	1.03644400	−1.34826200
C	2.80944400	−1.77994300	−2.23361600	C	5.78131500	1.29348000	0.13059200
C	4.41174400	−0.81785800	−0.56027200	C	−4.19749100	2.04113300	−0.49818000
C	−5.47742400	−1.14107900	−1.55902900	C	1.90187900	3.02328400	−0.82388000
C	3.43541700	−4.23166400	−1.94619700	C	−4.75689800	−1.72604100	0.55602200
C	−2.89623600	2.73618000	−0.04058700	C	−3.63483800	−2.62285800	0.00870400
C	−3.72847300	3.92419800	0.47687500	C	1.36859700	−3.57646200	−1.51953200
C	3.72847300	−3.92419800	−0.47687500	C	4.77745100	1.53604800	1.25154800
C	−3.43541700	4.23166400	1.94619700	C	−0.89605300	3.46570100	−1.73997600
C	5.47742400	1.14107900	1.55902900	C	3.61771700	2.44402600	0.82171500
C	2.89623600	−2.73618000	0.04058700	C	5.29957000	−3.89865200	1.83711300
C	−4.41174400	0.81785800	0.56027200	C	3.62489400	−2.07101200	1.13046100
C	−5.36640200	−2.04847400	1.33112600	C	−1.20284700	−3.06810100	−0.05066900
C	−2.80944400	1.77994300	2.23361600	C	−4.79467500	−1.70224500	2.08291000
C	−3.63394800	2.96305900	2.77708500	C	2.28150900	−1.35841700	1.39076000
C	2.42193100	2.82190900	0.63661900	C	3.94663000	−3.22450300	2.10118000
C	0.15891500	−0.44029100	1.77976800	C	−3.39872000	−1.40803900	2.62879400
C	−0.17409500	−1.83324000	2.36873600	C	−2.34424900	−2.35888200	2.03730300
C	0.09266000	−1.98252800	3.87693300	C	−0.27126000	4.49126600	0.97410400
C	−0.25429400	−3.37253600	4.42632900	C	−0.73094800	1.57007000	1.99082300
H	0.05603600	3.44312900	−5.50313800	H	5.71198900	0.69585400	−1.95347900
H	−1.15036000	1.75866000	−4.08038800	H	−0.15817300	−2.92272800	−4.06451400
H	0.48517000	1.21912300	−4.41840200	H	−6.01476200	2.02754500	−1.66925000
H	−0.33437300	4.15490200	−3.92865900	H	−1.79612000	−2.42126700	−3.63157800
H	1.31429900	3.60898900	−4.26588800	H	−4.89358100	3.30618100	−2.10744200
H	4.69979800	−2.69504900	−2.79564100	H	−6.90418800	4.26805800	−0.94506000
H	3.33928900	−3.13016100	−3.82144300	H	−1.24448900	−4.06915500	−3.28574300
H	6.39328400	1.67734800	−1.45852200	H	−4.10223700	0.30275000	−1.76487100
H	4.87387100	2.02144000	−2.31139700	H	−3.01417200	1.57424700	−2.23652200
H	0.39128000	−0.31650200	−2.36863300	H	4.61046600	−0.19464200	−0.90526800
H	−1.19208500	0.18742500	−2.08497300	H	6.31326800	2.22713200	−0.10627200
H	5.02447200	−0.94194000	−1.46030500	H	1.79579800	2.96683200	−1.90866200
H	−5.05056200	−0.53355700	−2.36796600	H	6.54049800	0.56399300	0.43926600
H	−0.39437400	2.61057400	−1.83783600	H	−5.71155800	−2.09394500	0.15835800
H	4.94927100	−1.37291800	0.21331600	H	−6.58923800	3.25388700	0.47334600
H	−3.51299800	4.79585400	−0.15504400	H	2.09588400	−3.25962500	−2.27922200
H	1.22685200	2.08441800	−2.17313200	H	2.35193300	4.01498000	−0.63814100
H	−5.54829400	−2.17278600	−1.92899900	H	−5.45453200	4.54054700	0.03644500
H	5.44263700	3.10329900	−1.03431300	H	−4.62109700	−0.71234900	0.16660100
H	4.08193100	−5.03974500	−2.31098800	H	−0.84927900	2.72038900	−2.54006600
H	1.75268100	−2.08169900	−2.27586400	H	−4.64606400	1.53202200	0.37219500
H	−6.50498100	−0.79298300	−1.38154600	H	1.13279400	−4.63069500	−1.72310200
H	4.79773200	−3.70257400	−0.34866800	H	−3.79816700	−3.64583400	0.39943900
H	2.39866400	−4.58538800	−2.05074900	H	−3.52689100	2.80252400	−0.06513800
H	6.50498100	0.79298300	1.38154600	H	5.34187900	−4.31945000	0.82353900
H	−2.39866400	4.58538800	2.05074900	H	3.65884100	−2.47279400	0.10502200
H	−4.79773200	3.70257400	0.34866800	H	4.04770600	3.42335000	0.53826600

H	−4.08193100	5.03974500	2.31098800	H	−0.47188100	4.39963400	−2.13814700
H	5.54829400	2.17278600	1.92899900	H	6.12541400	−3.18025800	1.92958600
H	−5.44263700	−3.10329900	1.03431300	H	4.46036500	−1.35791200	1.18213100
H	−1.75268100	2.08169900	2.27586400	H	1.86437100	−3.52595900	−0.54619300
H	3.51299800	−4.79585400	0.15504400	H	4.37117600	0.58445000	1.60839000
H	5.05056200	0.53355700	2.36796600	H	−5.51844000	−0.95886700	2.44050800
H	−4.94927100	1.37291800	−0.21331600	H	5.26691800	2.01399200	2.11000800
H	−1.22685200	−2.08441800	2.17313200	H	−1.57485900	−4.10226300	−0.16215700
H	0.39437400	−2.61057400	1.83783600	H	−1.95380900	3.65097000	−1.52927800
H	−6.39328400	−1.67734800	1.45852200	H	−5.13080300	−2.67906000	2.46204500
H	−4.87387100	−2.02144000	2.31139700	H	5.49120400	−4.71598900	2.54417700
H	−5.02447200	0.94194000	1.46030500	H	−0.40569500	−3.13696200	0.69202400
H	−3.33928900	3.13016100	3.82144300	H	−3.11566300	−0.36897900	2.40885700
H	−4.69979800	2.69504900	2.79564100	H	0.11952000	5.40575200	0.50777300
H	1.19208500	−0.18742500	2.08497300	H	3.14453600	−3.97560400	2.04041300
H	−0.39128000	0.31650200	2.36863300	H	1.51819300	−2.15144900	1.46784800
H	−1.31429900	−3.60898900	4.26588800	H	2.31817400	−0.93263200	2.41216100
H	0.33437300	−4.15490200	3.92865900	H	3.92089000	−2.83841100	3.13135600
H	−0.48517000	−1.21912300	4.41840200	H	0.14588300	4.42820300	1.98375100
H	1.15036000	−1.75866000	4.08038800	H	−3.38866300	−1.51142900	3.72097500
H	−0.05603600	−3.44312900	5.50313800	H	−1.35564900	4.62593000	1.08006000
N	−2.77280400	−1.47641000	−0.18701600	N	0.01735000	−0.77982300	−1.48933900
N	3.05874500	−1.46923200	−0.77289600	N	2.87837800	1.95064500	−0.40926500
N	−3.05874500	1.46923200	0.77289600	N	−2.27954400	−2.19003400	0.52926100
N	2.77280400	1.47641000	0.18701600	N	−0.27483400	1.44872900	0.57909700
Mg	−1.40763400	−0.06542700	0.13286500	Mg	−1.64421700	0.11429200	−0.46453600
Mg	1.40763400	0.06542700	−0.13286500	Mg	1.35738300	0.09626200	0.06052400
Si	4.41017400	1.04507800	−0.02000400	Si	−0.20524700	−2.51631600	−1.61159300
Si	−4.41017400	−1.04507800	0.02000400	Si	0.06763200	3.00531200	−0.16873700
C	−2.99894500	0.55331500	3.13458400	C	−3.72506300	−2.70905000	−1.51461300
H	−2.57343900	−0.35868800	2.70965900	H	−3.09449900	−3.49754000	−1.92564600
H	−2.50961000	0.73586400	4.09759200	H	−4.75954900	−2.94507900	−1.78976200
H	−4.05793600	0.36161800	3.33576100	H	−3.46803900	−1.76069500	−1.99369300
C	2.99894500	−0.55331500	−3.13458400	C	2.70341600	2.66116800	2.02681700
H	2.50961000	−0.73586400	−4.09759200	H	3.30550100	3.03958600	2.86098200
H	2.57343900	0.35868800	−2.70965900	H	1.91849800	3.39198700	1.84154800
H	4.05793600	−0.36161800	−3.33576100	H	2.24589300	1.72070700	2.35002900
C	3.16858300	−2.51997400	1.53457500	H	−2.68914200	−3.39256200	2.22665600
H	4.24037600	−2.52280000	1.75851200	H	4.32957600	2.73911100	−1.73767000
H	2.75218300	−1.58238400	1.91002600	C	3.28349900	1.19254400	−2.81252500
H	2.71748100	−3.33844500	2.10506500	H	2.87199300	0.19024400	−2.65085600
C	−3.16858300	2.51997400	−1.53457500	H	2.50282400	1.81718000	−3.25131800
H	−2.75218300	1.58238400	−1.91002600	H	4.07733400	1.10237000	−3.56257900
H	−4.24037600	2.52280000	−1.75851200	C	−1.00346200	−2.19678900	2.76441900
H	−2.71748100	3.33844500	−2.10506500	H	−0.36129700	−3.07683900	2.68160200
H	−1.83523200	3.00344600	0.07849400	H	−0.42972800	−1.33866300	2.40813800
H	1.83523200	−3.00344600	−0.07849400	H	−1.19486100	−2.04559600	3.83264300
H	2.86591800	3.08746900	1.61315100	H	0.34462600	0.94197400	−2.71939100
H	2.72314600	3.61375000	−0.07342200	H	−0.82791300	−0.17897100	−3.39446400
H	1.33246000	2.93132800	0.76215200	H	0.89631400	−0.54835400	−3.46435300
H	−1.33246000	−2.93132800	−0.76215200	H	−0.86851100	0.58264800	2.44139600
H	−2.72314600	−3.61375000	0.07342200	H	−0.01994500	2.09906200	2.64144600
H	−2.86591800	−3.08746900	−1.61315100	H	−1.69423800	2.09585200	2.08247600

Tabelle 8.132 Standardorientierung von **114C** und **114N** [B3LYP/6−31+G(d)].

114C				**114N**			
C	0.77273600	−3.76517800	4.04364700	C	1.57743300	−1.77696400	−2.68202600
C	0.43774000	−2.31527800	3.66968400	C	0.17346300	−1.24841800	−2.33728300
C	−1.74242900	2.87083300	2.89044600	C	−0.40613800	−4.31900300	−1.62749000
C	0.46284100	−2.04988500	2.15395300	C	5.60275800	1.58785800	−1.59643000

C	4.33180900	2.41985000	2.24806400	C	4.28926300	2.37896000	−1.72865600
C	5.28008300	−2.47295500	0.38310900	C	−5.28995700	2.73367900	−0.97112700
C	−1.85939700	2.86419700	1.35086600	C	−6.21429300	3.52401600	−0.03533600
C	−2.45888100	4.19997700	0.86957400	C	−3.16337300	1.25037300	−1.15980500
C	0.14060100	−0.59341700	1.73808100	C	6.43402700	2.02788000	−0.39740400
C	3.31100300	1.36273900	1.78197800	C	−4.11023300	2.05411700	−0.24997600
C	4.44840400	0.45199900	−0.26232600	C	2.24183200	3.13123900	−0.64260400
C	−5.15961500	1.51312300	2.46579800	C	−5.56487000	−1.95200000	−0.85213200
C	4.10072100	3.77819800	1.58505300	C	−4.25367800	−2.73959500	−0.69604000
C	−3.04286100	−2.53999400	0.37023800	C	0.60182700	−3.62264200	1.06920100
C	−4.07431800	−3.59633700	−0.06613800	C	5.56487000	1.95200000	0.85213200
C	4.07562000	3.59605000	0.06750500	C	−0.60182700	3.62264200	−1.06920100
C	−4.09824700	−3.77985400	−1.58354600	C	4.25367800	2.73959500	0.69604000
C	5.15644600	−1.51235400	−2.46945500	C	6.21429300	−3.52401600	0.03533600
C	3.04346900	2.54047500	−0.36909700	C	4.11023300	−2.05411700	0.24997600
C	−4.44843500	−0.45212700	0.26049600	C	−2.24183200	−3.13123900	0.64260400
C	2.45783000	−4.20011300	−0.86811600	C	−6.43402700	−2.02788000	0.39740400
C	−5.27865600	2.47267100	−0.38737700	C	3.16337300	−1.25037300	1.15980500
C	−3.30919900	−1.36430600	−1.78212900	C	5.28995700	−2.73367900	0.97112700
C	−4.32929000	−2.42220000	−2.24799100	C	−5.60275800	−1.58785800	1.59643000
C	1.85800900	−2.86445900	−1.34933100	C	−4.28926300	−2.37896000	1.72865600
C	−0.14028100	0.59434600	−1.73757800	C	0.40613800	4.31900300	1.62749000
C	−0.46319600	2.05089700	−2.15264400	C	−0.17346300	1.24841800	2.33728300
C	1.73930600	−2.87178900	−2.88877800	C	−1.57743300	1.77696400	2.68202600
C	−0.43784500	2.31732100	−3.66819300	H	1.75093600	−1.75113300	−3.76607700
C	−0.77358800	3.76728400	−4.04124000	H	1.72187300	−2.80589100	−2.34415100
H	0.74866200	−3.91824100	5.12979100	H	6.17108300	1.71270300	−2.52697900
H	−0.55380800	−2.05200300	4.06672400	H	0.62298200	−4.69633900	−1.66699400
H	1.14841400	−1.63563200	4.16254600	H	−5.87240300	1.96636600	−1.50272800
H	−1.14546600	3.72492300	3.24182100	H	−0.69212600	−4.04441100	−2.64689800
H	0.05809400	−4.46746500	3.59385400	H	−4.89262700	3.40316900	−1.74848800
H	1.77343000	−4.04499300	3.68951000	H	−7.04052700	3.99526100	−0.58285400
H	−1.26778600	1.95024000	3.24830000	H	2.35963000	−1.16821700	−2.20873700
H	−2.73320600	2.93789100	3.35609600	H	−1.03997800	−5.16377500	−1.32590000
H	5.35174100	2.07202300	2.03239200	H	−3.75491700	0.48231900	−1.68315600
H	4.25783800	2.50033100	3.34046700	H	−2.80919900	1.92194500	−1.96146600
H	6.29345000	−2.05811900	0.48814800	H	5.36242300	0.51925800	−1.50864400
H	−1.83614500	5.04792800	1.18564000	H	6.78505600	3.06010900	−0.54686500
H	4.84295400	−2.54765200	1.38596300	H	1.91355700	3.01757400	−1.67698400
H	0.83239500	0.07530100	2.28232300	H	7.32828600	1.40018200	−0.29183200
H	−0.80677700	−0.31385000	2.23668000	H	−6.10137500	−2.35525000	−1.72064500
H	5.28699300	0.54304800	0.43969700	H	−6.65346900	2.87221300	0.73199900
H	−4.67142800	0.90949500	3.24189300	H	1.63383100	−3.73584500	0.72206900
H	−3.46212300	4.35631000	1.28748800	H	2.51180200	4.20757600	−0.56114700
H	−0.23948400	−2.74246000	1.66849000	H	−5.66495500	4.31976100	0.48577500
H	4.78503400	0.97435700	−1.16136600	H	−5.32805900	−0.90516600	−1.07886400
H	−3.83361100	−4.54110700	0.43881800	H	−0.62611700	3.01784800	−1.98231700
H	1.44781900	−2.34484800	1.76456700	H	−4.52282600	1.40219600	0.53711100
H	−5.20682900	2.54620600	2.83427400	H	0.24149200	−4.62143700	1.35648500
H	5.39201600	−3.49504500	0.00008700	H	−4.52549700	−3.80474000	−0.52963800
H	4.88056300	4.49168000	1.87973600	H	−3.54990500	2.83496400	0.29008400
H	2.31561200	1.73464800	2.06456600	H	5.66495500	−4.31976100	−0.48577500
H	−2.53987200	4.22103800	−0.22260600	H	3.54990500	−2.83496400	−0.29008400
H	−6.19718700	1.16150600	2.36758400	H	4.52549700	3.80474000	0.52963800
H	5.07179800	3.29638600	−0.28858400	H	−0.24149200	4.62143700	−1.35648500
H	3.14236000	4.19961100	1.92373400	H	6.65346900	−2.87221300	−0.73199900
H	6.19408600	−1.16051900	−2.37274600	H	4.52282600	−1.40219600	−0.53711100
H	−3.13949800	−4.20125800	−1.92113700	H	0.62611700	−3.01784800	1.98231700
H	−5.07086500	−3.29674300	0.28897500	H	5.32805900	0.90516600	1.07886400
H	2.54018300	−4.22062800	0.22397000	H	−7.32828600	−1.40018200	0.29183200
H	−4.87763400	−4.49386300	−1.87815400	H	6.10137500	2.35525000	1.72064500

H	5.20334200	−2.54531700	−2.83830900	H	−2.51180200	−4.20757600	0.56114700
H	−5.39098800	3.49495500	−0.00499300	H	−1.63383100	3.73584500	−0.72206900
H	−2.31345500	−1.73608700	−2.06364900	H	−6.78505600	−3.06010900	0.54686500
H	3.83491200	4.54135600	−0.43644500	H	7.04052700	−3.99526100	0.58285400
H	3.46052200	−4.35684200	−1.28719600	H	−1.91355700	−3.01757400	1.67698400
H	4.66691200	−0.90861000	−3.24461200	H	−5.36242300	−0.51925800	1.50864400
H	−4.78611900	−0.97423800	1.15928400	H	1.03997800	5.16377500	1.32590000
H	−1.44843900	2.34506300	−1.76331700	H	4.89262700	−3.40316900	1.74848800
H	0.23861500	2.74353700	−1.66651300	H	2.80919900	−1.92194500	1.96146600
H	1.83453800	−5.04810200	−1.18298200	H	3.75491700	−0.48231900	1.68315600
H	−6.29193600	2.05799600	−0.49388500	H	5.87240300	−1.96636600	1.50272800
H	−4.83987700	2.54682200	−1.38954900	H	−2.35963000	1.16821700	2.20873700
H	−5.28620100	−0.54339400	−0.44247000	H	0.69212600	4.04441100	2.64689800
H	−4.25449300	−2.50367900	−3.34026400	H	−6.17108300	−1.71270300	2.52697900
H	−5.34949500	−2.07450400	−2.03339100	H	−0.62298200	4.69633900	1.66699400
H	0.80740300	0.31560900	−2.23605800	H	−1.72187300	2.80589100	2.34415100
H	−0.83151100	−0.07447100	−2.28238500	H	−1.75093600	1.75113300	3.76607700
H	2.72955300	−2.93922900	−3.35549300	N	−0.12953500	−1.31820300	−0.86201600
H	−1.77453100	4.04626600	−3.68715900	N	3.45401200	2.29103800	−0.48277900
H	−0.05946800	4.46967700	−3.59078300	N	−3.45401200	−2.29103800	0.48277900
H	1.26441800	−1.95129100	−3.24655100	N	0.12953500	1.31820300	0.86201600
H	1.14182700	−3.72595800	−3.23908200	Mg	−1.42892800	0.31648100	−0.31296400
H	−1.14800300	1.63760600	−4.16170100	Mg	1.42892800	−0.31648100	0.31296400
H	0.55395100	2.05488800	−4.06516700	Si	−0.54731100	−2.95676800	−0.29350900
H	−0.74933100	3.92110600	−5.12727100	Si	0.54731100	2.95676800	0.29350900
N	−2.54308200	1.67292400	0.83304500	C	0.02289200	0.17866200	−2.88539400
N	3.23884500	1.18360100	0.27952500	H	−1.00261900	0.55536100	−2.78519600
N	−3.23822100	−1.18380700	−0.27979200	H	0.70499200	0.87936100	−2.38531800
N	2.54244900	−1.67309100	−0.83276700	H	0.26855200	0.20982400	−3.95361200
Mg	−1.40218600	0.17568400	0.14334000	C	−0.02289200	−0.17866200	2.88539400
Mg	1.40229200	−0.17533800	−0.14306000	H	−0.70499200	−0.87936100	2.38531800
Si	4.22916700	−1.40312100	−0.80255300	H	1.00261900	−0.55536100	2.78519600
Si	−4.22979900	1.40313800	0.80037600	H	−0.26855200	−0.20982400	3.95361200
C	−3.56176600	−0.04498400	−2.51966300	C	−3.47319900	−2.66004400	−2.01072000
H	−2.96971000	0.78462700	−2.12733400	H	−2.66236900	−3.38505700	−2.06319600
H	−3.30395900	−0.16937000	−3.57719700	H	−4.14949800	−2.87869500	−2.84537800
H	−4.61529300	0.24695300	−2.46904600	H	−3.06772500	−1.65476900	−2.16444800
C	3.56362300	0.04266700	2.51813800	C	3.47319900	2.66004400	2.01072000
H	3.30667100	0.16619600	3.57598000	H	4.14949800	2.87869500	2.84537800
H	2.97099200	−0.78639300	2.12549300	H	2.66236900	3.38505700	2.06319600
H	4.61701200	−0.24957600	2.46644500	H	3.06772500	1.65476900	2.16444800
C	2.99397000	2.47216900	−1.90072300	H	−4.55278100	−3.44561600	1.88912500
H	3.99631800	2.44041200	−2.34057700	H	4.55278100	3.44561600	−1.88912500
H	2.43885200	1.60770200	−2.27108900	C	3.56860700	1.87555400	−2.98888100
H	2.50354700	3.37293000	−2.28402500	H	3.19837900	0.85557500	−2.84073200
C	−2.99447400	−2.47017200	1.90183500	H	2.73470400	2.50347200	−3.31396800
H	−2.43970000	−1.60528400	2.27175500	H	4.28298700	1.85051400	−3.81964800
H	−3.99713900	−2.43805000	2.34093500	C	−3.56860700	−1.87555400	2.98888100
H	−2.50425700	−3.37051600	2.28637800	H	−2.73470400	−2.50347200	3.31396800
H	−2.05738300	−2.87371800	0.01155400	H	−3.19837900	−0.85557500	2.84073200
H	2.05836000	2.87419200	−0.00938400	H	−4.28298700	−1.85051400	3.81964800
H	−0.82102000	2.85052500	0.96743300	H	−0.55111500	−1.85923000	−2.89329100
H	0.82006600	−2.85043600	−0.96472400	H	0.55111500	1.85923000	2.89329100

Tabelle 8.133 Standardorientierung von **115C** und **115N** [B3LYP/6−31+G(d)].

115C				**115N**			
C	0.29149300	3.34657900	−4.51123600	C	−0.86288300	−1.32004100	−3.38640500
C	−0.01870500	1.96474100	−3.92098900	C	1.48035000	−1.98561700	−2.72610600
C	−2.87807100	−2.60236200	−2.72453300	C	0.26270500	−1.11076600	−2.34952600
C	0.25099800	1.86613200	−2.40890600	C	−0.61119800	−4.39193700	−1.62614500

C	3.68721700	−2.91196200	−2.70775800	C	5.77281200	1.76231000	−1.70272300
C	5.15589500	2.05077100	−1.54056900	C	4.44162400	2.53340000	−1.79361800
C	−2.55035600	−2.76987900	−1.21909900	C	−5.31705600	2.65222000	−1.01358700
C	−3.32023000	−4.00067900	−0.68273300	C	−6.24594600	3.45433500	−0.09246100
C	−0.05533200	0.48470700	−1.78124200	C	−3.14518800	1.23515100	−1.18595400
C	2.85074900	−1.72556800	−2.18778400	C	6.62887400	2.19502500	−0.51899600
C	4.40107500	−0.77215100	−0.47018300	C	−4.09617900	2.05146200	−0.29150800
C	−5.84755400	−1.19944200	−1.26324700	C	2.35591400	3.12217700	−0.64776800
C	3.46295400	−4.18037500	−1.88428100	C	−5.78426600	−2.11507700	−0.74670000
C	−2.86861900	2.68406800	−0.08628100	C	−4.46114600	−2.88713500	−0.60907100
C	−3.71695600	3.87032000	0.40907400	C	0.49599800	−3.65295200	0.96573600
C	3.71695600	−3.87032000	−0.40907400	C	5.78426600	2.11507700	0.74670000
C	−3.46295400	4.18037500	1.88428100	C	−0.49599800	3.65295200	−0.96573600
C	5.84755400	1.19944200	1.26324700	C	4.46114600	2.88713500	0.60907100
C	2.86861900	−2.68406800	0.08628100	C	6.24594600	−3.45433500	0.09246100
C	−4.40107500	0.77215100	0.47018300	C	4.09617900	−2.05146200	0.29150800
C	3.32023000	4.00067900	0.68273300	C	−2.35591400	−3.12217700	0.64776800
C	−5.15589500	−2.05077100	1.54056900	C	−6.62887400	−2.19502500	0.51899600
C	−2.85074900	1.72556800	2.18778400	C	3.14518800	−1.23515100	1.18595400
C	−3.68721700	2.91196200	2.70775800	C	5.31705600	−2.65222000	1.01358700
C	2.55035600	2.76987900	1.21909900	C	−5.77281200	−1.76231000	1.70272300
C	0.05533200	−0.48470700	1.78124200	C	−4.44162400	−2.53340000	1.79361800
C	−0.25099800	−1.86613200	2.40890600	C	0.61119800	4.39193700	1.62614500
C	2.87807100	2.60236200	2.72453300	C	−0.26270500	1.11076600	2.34952600
C	0.01870500	−1.96474100	3.92098900	C	−1.48035000	1.98561700	2.72610600
C	−0.29149300	−3.34657900	4.51123600	C	0.86288300	1.32004100	3.38640500
H	0.08801300	3.38047900	−5.58877400	H	−0.48973800	−1.10738400	−4.39661100
H	−1.07059000	1.70809900	−4.11531300	H	1.84351400	−1.72543600	−3.72863500
H	0.57757900	1.20084000	−4.44104100	H	−1.24395000	−2.34102200	−3.38609500
H	−2.61056000	−3.50108000	−3.29839600	H	1.23621800	−3.04913700	−2.73523500
H	−0.31548600	4.12771700	−4.03422800	H	−1.70423700	−0.64517100	−3.19443200
H	1.34571100	3.61445900	−4.36269600	H	6.31819400	1.90469200	−2.64457800
H	−2.32518800	−1.75241900	−3.14124600	H	0.41169500	−4.78472700	−1.67387100
H	−3.94544800	−2.41363800	−2.87617800	H	−5.88392500	1.83938700	−1.49147700
H	4.75427400	−2.64905800	−2.69872200	H	−0.93818200	−4.20405200	−2.65092500
H	3.41922400	−3.07673900	−3.75963000	H	−4.96330700	3.29652700	−1.83214400
H	6.04215900	1.53399300	−1.93716700	H	−7.10196400	3.86872600	−0.64009000
H	−3.02604700	−4.91304900	−1.21851500	H	2.30878500	−1.83851600	−2.02318400
H	4.43130200	2.14784800	−2.35754400	H	−1.23673300	−5.20240600	−1.22817400
H	0.49494700	−0.27359300	−2.36419100	H	−3.71992100	0.41044300	−1.63832100
H	−1.08892300	0.22711400	−2.08346200	H	−2.83998300	1.86873800	−2.03834200
H	5.08220700	−0.98193300	−1.30441400	H	5.54512200	0.68979800	−1.62258900
H	−5.59665700	−0.64644300	−2.17760200	H	6.97656400	3.22806800	−0.66961800
H	−4.40304500	−3.88732900	−0.80993400	H	1.98700700	2.94117700	−1.65781000
H	−0.33408900	2.64611700	−1.90235600	H	7.52548500	1.56706500	−0.43577200
H	4.86049200	−1.26780900	0.38866900	H	−6.33413100	−2.52497500	−1.60367300
H	−3.48753200	4.74134100	−0.21887100	H	−6.64209800	2.82557200	0.71635200
H	1.29895500	2.14666700	−2.22372200	H	1.51702600	−3.75523300	0.58167700
H	−6.09303000	−2.22805700	−1.55537500	H	2.54407400	4.21945900	−0.62227200
H	5.47325000	3.06391200	−1.26455300	H	−5.71333000	4.29342400	0.37514200
H	4.11794500	−4.98955800	−2.23127100	H	−5.55605400	−1.06673800	−0.98195100
H	1.79661800	−2.02341000	−2.26426600	H	−0.55514000	3.08262200	−1.89874300
H	−3.11691100	−4.14907000	0.38410100	H	−4.46499700	1.42264700	0.53564100
H	−6.76704500	−0.75955200	−0.84959700	H	0.14892200	−4.66127000	1.23370200
H	4.78181700	−3.64488000	−0.25333600	H	−4.71298700	−3.95073400	−0.40258100
H	2.42873300	−4.53142400	−2.01623200	H	−3.55172300	2.87903500	0.19222100
H	6.76704500	0.75955200	0.84959700	H	5.71333000	−4.29342400	−0.37514200
H	−2.42873300	4.53142400	2.01623200	H	3.55172300	−2.87903500	−0.19222100
H	−4.78181700	3.64488000	0.25333600	H	4.71298700	3.95073400	0.40258100
H	3.11691100	4.14907000	−0.38410100	H	−0.14892200	4.66127000	−1.23370200
H	−4.11794500	4.98955800	2.23127100	H	6.64209800	−2.82557200	−0.71635200

H	6.09303000	2.22805700	1.55537500	H	4.46499700	−1.42264700	−0.53564100
H	−5.47325000	−3.06391200	1.26455300	H	0.55514000	−3.08262200	1.89874300
H	−1.79661800	2.02341000	2.26426600	H	5.55605400	1.06673800	0.98195100
H	3.48753200	−4.74134100	0.21887100	H	−7.52548500	−1.56706500	0.43577200
H	4.40304500	3.88732900	0.80993400	H	6.33413100	2.52497500	1.60367300
H	5.59665700	0.64644300	2.17760200	H	−2.54407400	−4.21945900	0.62227200
H	−4.86049200	1.26780900	−0.38866900	H	−1.51702600	3.75523300	−0.58167700
H	−1.29895500	−2.14666700	2.22372200	H	−6.97656400	−3.22806800	0.66961800
H	0.33408900	−2.64611700	1.90235600	H	7.10196400	−3.86872600	0.64009000
H	3.02604700	4.91304900	1.21851500	H	−1.98700700	−2.94117700	1.65781000
H	−6.04215900	−1.53399300	1.93716700	H	−5.54512200	−0.68979800	1.62258900
H	−4.43130200	−2.14784800	2.35754400	H	1.23673300	5.20240600	1.22817400
H	−5.08220700	0.98193300	1.30441400	H	4.96330700	−3.29652700	1.83214400
H	−3.41922400	3.07673900	3.75963000	H	2.83998300	−1.86873800	2.03834200
H	−4.75427400	2.64905800	2.69872200	H	3.71992100	−0.41044300	1.63832100
H	1.08892300	−0.22711400	2.08346200	H	5.88392500	−1.83938700	1.49147700
H	−0.49494700	0.27359300	2.36419100	H	−2.30878500	1.83851600	2.02318400
H	3.94544800	2.41363800	2.87617800	H	0.93818200	4.20405200	2.65092500
H	−1.34571100	−3.61445900	4.36269600	H	−6.31819400	−1.90469200	2.64457800
H	0.31548600	−4.12771700	4.03422800	H	−0.41169500	4.78472700	1.67387100
H	2.32518800	1.75241900	3.14124600	H	−1.23621800	3.04913700	2.73523500
H	2.61056000	3.50108000	3.29839600	H	1.70423700	0.64517100	3.19443200
H	−0.57757900	−1.20084000	4.44104100	H	1.24395000	2.34102200	3.38609500
H	1.07059000	−1.70809900	4.11531300	H	−1.84351400	1.72543600	3.72863500
H	−0.08801300	−3.38047900	5.58877400	H	0.48973800	1.10738400	4.39661100
N	−2.85403600	−1.52891100	−0.46907200	N	−0.18468200	−1.32334900	−0.91107100
N	3.05574000	−1.41279500	−0.72042700	N	3.63855100	2.38655300	−0.53090800
N	−3.05574000	1.41279500	0.72042700	N	−3.63855100	−2.38655300	0.53090800
N	2.85403600	1.52891100	0.46907200	N	0.18468200	1.32334900	0.91107100
Mg	−1.43792200	−0.17292800	0.05605900	Mg	−1.37355700	0.38696900	−0.34749600
Mg	1.43792200	0.17292800	−0.05605900	Mg	1.37355700	−0.38696900	0.34749600
Si	4.44417500	1.11311000	−0.03212700	Si	−0.68396500	−2.95225400	−0.36319300
Si	−4.44417500	−1.11311000	0.03212700	Si	0.68396500	2.95225400	0.36319300
C	−3.07824300	0.50532100	3.08622300	C	0.70545200	0.35604700	−2.50403300
H	−2.61836500	−0.40545400	2.69707600	H	−0.11919500	1.05806900	−2.32886900
H	−2.64283200	0.70082600	4.07246500	H	1.54109600	0.62324300	−1.84285700
H	−4.14395000	0.30377700	3.23103300	H	1.05780200	0.55038000	−3.52231100
C	3.07824300	−0.50532100	−3.08622300	C	−0.70545200	−0.35604700	2.50403300
H	2.64283200	−0.70082600	−4.07246500	H	−1.54109600	−0.62324300	1.84285700
H	2.61836500	0.40545400	−2.69707600	H	0.11919500	−1.05806900	2.32886900
H	4.14395000	−0.30377700	−3.23103300	H	−1.05780200	−0.55038000	3.52231100
C	−1.04666600	−3.09463700	−1.10127500	C	−3.73418700	−2.83347900	−1.94947900
H	−0.43920600	−2.27649900	−1.50791200	H	−2.88056300	−3.50722900	−1.99335200
H	−0.76667500	−3.25636800	−0.05482400	H	−4.42314000	−3.13782400	−2.74625900
H	−0.78971000	−4.00044600	−1.66597700	H	−3.40021100	−1.81595600	−2.16608300
C	1.04666600	3.09463700	1.10127500	C	3.73418700	2.83347900	1.94947900
H	0.76667500	3.25636800	0.05482400	H	4.42314000	3.13782400	2.74625900
H	0.43920600	2.27649900	1.50791200	H	2.88056300	3.50722900	1.99335200
H	0.78971000	4.00044600	1.66597700	H	3.40021100	1.81595600	2.16608300
C	3.10309700	−2.48110700	1.58914400	H	−4.67816900	−3.61118500	1.92263000
H	4.16777900	−2.51049200	1.84398600	H	4.67816900	3.61118500	−1.92263000
H	2.69869300	−1.53755700	1.96203000	C	3.73812800	2.05907300	−3.07334000
H	2.61947400	−3.29444000	2.13994100	H	3.50132500	0.99154800	−3.01491100
C	−3.10309700	2.48110700	−1.58914400	H	2.82610100	2.60806600	−3.32130600
H	−2.69869300	1.53755700	−1.96203000	H	4.42553600	2.19836100	−3.91559700
H	−4.16777900	2.51049200	−1.84398600	C	−3.73812800	−2.05907300	3.07334000
H	−2.61947400	3.29444000	−2.13994100	H	−2.82610100	−2.60806600	3.32130600
H	−1.81271100	2.94852400	0.06448000	H	−3.50132500	−0.99154800	3.01491100
H	1.81271100	−2.94852400	−0.06448000	H	−4.42553600	−2.19836100	3.91559700

8.3.5 Angaben zu den quantenchemischen Rechnungen aus Kapitel 4.4.3 – Reaktionsbarrieren

Tabelle 8.134 Berechnete Energien der optimierten Verbindungen [B3LYP/6−31+G(d)].

Verbindung	SCF [Hartree]	ZPE [Hartree]
BuH	−158.463204695	−158.330834
65 (R = ^{i}Pr, R' = H)	−833.897173228	−833.534456
66 (R = ^{t}Bu, R' = H)	−873.210621215	−872.819872
(S)−69 (R = CH(Me)(Ph), R' = H)	−1025.63836924	−1025.22293
90 (R = ^{i}Pr, R' = Me)	−912.516763359	−912.097284
116 (R = ^{t}Bu, R' = Me)	−951.833068753	−951.386245
R = Me, R' = Me	−833.884550196	−833.522164
R = Ph, R' = H	−947.019810019	−946.660295
R = Me, R' = H	−755.261889451	−754.955961
$[Bu_2Mg]_2$	−1031.56747258	−1031.082647
65·$MgBu_2$ (R = ^{i}Pr, R' = H)	−1349.69858646	−1349.091104
65·$MgBu_2$ (ÜZ, R = ^{i}Pr, R' = H)	−1349.67679299	−1349.073737
66·$MgBu_2$ (R = ^{t}Bu, R' = H)	−1389.01230263	−1388.376562
66·$MgBu_2$ (ÜZ, R = ^{t}Bu, R' = H)	−1388.98659758	−1388.35493
[(S)−69]·$MgBu_2$ [R = CH(Me)(Ph), R' = H]	−1541.44325287	−1540.783084
[(S)−69]·$MgBu_2$ [ÜZ, R = CH(Me)(Ph), R' = H]	−1541.41755072	−1540.761724
90·$MgBu_2$ (R = ^{i}Pr, R' = Me)	−1428.31029184	−1427.646176
90·$MgBu_2$ (ÜZ, R = ^{i}Pr, R' = Me)	−1428.29115724	−1427.631894
116·$MgBu_2$ (R = ^{t}Bu, R' = Me)	−1467.62172231	−1466.929718
116·$MgBu_2$ (ÜZ, R = ^{t}Bu, R' = Me)	−1467.60025228	−1466.912284
$MgBu_2$−Addukt mit R = Me, R' = Me	−1349.68312545	−1349.075668
$MgBu_2$−Addukt mit R = Me, R' = Me (ÜZ)	−1349.66093903	−1349.058503
$MgBu_2$−Addukt mit R = Ph, R' = H	−1462.81685908	−1462.213504
$MgBu_2$−Addukt mit R = Ph, R' = H (ÜZ)	−1462.79790034	−1462.199248
$MgBu_2$−Addukt mit R = Me, R' = H	−1271.06987007	−1270.519086
$MgBu_2$−Addukt mit R = Me, R' = H (ÜZ)	−1271.04562927	−1270.499858
$[Me_3SiN(^{t}Bu)H]·MgBu_2$	−1138.2986105	−1137.804622
$[Me_3SiN(^{t}Bu)H]·MgBu_2$ (ÜZ)	−1138.26431043	−1137.774892
66·$Mg(CH_2SiMe_3)_2$	−1970.50265236	−1969.834075

66·Mg(CH$_2$SiMe$_3$)$_2$ (ÜZ)	−1970.46914115	−1969.80462

Tabelle 8.135 Standardorientierung von **66·Mg(CH$_2$SiMe$_3$)$_2$** und **66·Mg(CH$_2$SiMe$_3$)$_2$ (ÜZ)** [B3LYP/6−31+G(d)].

66·Mg(CH$_2$SiMe$_3$)$_2$				**ÜZ**			
C	0.35374800	1.88347700	−1.29367700	**C**	−0.72625800	1.82188300	−1.27786200
C	−0.13809100	−1.45195100	−2.87967500	**C**	−0.00742300	−1.91075600	−2.57076600
C	1.20025200	−2.17992200	−2.75860500	**C**	1.43034500	−2.41293200	−2.43828900
C	−4.69877900	0.76707000	−1.17450100	**C**	−4.64991600	0.10392800	−0.93024200
C	−2.20022800	−0.74086100	−1.84938000	**C**	−2.12876500	−1.38862700	−1.51499000
C	−3.82097600	2.00784600	2.08728000	**C**	−3.77121700	1.63111700	2.07960400
N	−2.18560100	0.77025400	0.62102700	**N**	−2.03405900	0.40581200	0.72416400
N	−0.88605100	−1.38904700	−1.58902700	**N**	−0.69965500	−1.75157200	−1.25656200
C	−1.34702700	2.27738500	2.37242700	**C**	−1.38235800	2.33439700	2.13793500
Si	−3.29667400	−0.22289600	−0.37211100	**Si**	−3.15998800	−0.68423500	−0.05147200
C	−2.46351900	1.27855600	2.01587800	**C**	−2.31766900	1.11345600	2.01102900
C	1.00029600	−3.60466200	−2.23046100	**C**	1.48228000	−3.74226300	−1.67581500
C	−1.09371000	−2.76901000	−1.06962500	**C**	−0.65267200	−3.04504500	−0.51107400
C	0.20924000	−3.55799900	−0.91913800	**C**	0.76624000	−3.58849400	−0.32960500
C	−4.05950800	−1.67375700	0.56393200	**C**	−3.85832200	−2.08116500	1.03295800
C	1.00117000	−0.90145800	1.64265600	**C**	1.52475700	−0.38168400	1.57429900
C	−2.44637200	0.11405100	3.01840200	**C**	−2.06433300	0.17484100	3.21088700
H	0.16001100	1.58079000	−2.33902500	**H**	−1.00309400	1.29321100	−2.20675300
H	−1.95723600	1.59193200	0.05211300	**H**	−1.46663100	1.19406500	−0.21677100
H	−0.45675200	2.60265200	−1.06132100	**H**	−1.48296400	2.62357000	−1.20042500
H	0.01031600	−0.42531100	−3.22457600	**H**	−0.03507700	−0.94026700	−3.07737200
H	−0.77041500	−1.96541800	−3.62742200	**H**	−0.59081400	−2.61724900	−3.18751400
H	1.68156300	−2.18839700	−3.74471700	**H**	1.85465300	−2.51901500	−3.44479300
H	1.86657900	−1.62327100	−2.08724300	**H**	2.03933200	−1.66496800	−1.91661200
H	−4.32385100	1.66247200	−1.68629100	**H**	−4.34553700	0.96673000	−1.53575700
H	−5.21926400	0.15554100	−1.92404700	**H**	−5.12932100	−0.62181700	−1.60239600
H	−5.44666000	1.09251700	−0.44272200	**H**	−5.41604200	0.44706300	−0.22561200
H	−1.99644200	0.18942600	−2.39686800	**H**	−2.12828800	−0.60375500	−2.28013300
H	−2.79702400	−1.36813700	−2.53907500	**H**	−2.64609200	−2.25188100	−1.97060600
H	−3.86831600	2.83062300	1.36325800	**H**	−3.99680500	2.28184100	1.22692600
H	−4.65747200	1.32804000	1.88720200	**H**	−4.49569900	0.80793300	2.08410300
H	−3.97600100	2.43143200	3.08691900	**H**	−3.93259300	2.20791500	2.99894600
H	−1.32563700	3.11956800	1.66938900	**H**	−1.56588500	3.06299900	1.34114500
H	−1.51028700	2.68640300	3.37587100	**H**	−1.54470600	2.83818300	3.09827000
H	−0.36294900	1.79909000	2.36026800	**H**	−0.32742000	2.04279600	2.09542400
H	0.45161700	−4.19910600	−2.97662000	**H**	0.99204800	−4.52788200	−2.27020700
H	1.96673600	−4.09910200	−2.07677800	**H**	2.52120500	−4.05819100	−1.52512400
H	−1.77602500	−3.30700800	−1.75432100	**H**	−1.26394700	−3.78415700	−1.05895800
H	−1.59465600	−2.69649700	−0.10116300	**H**	−1.12964900	−2.89285800	0.46162800
H	0.82030800	−3.09576300	−0.13729000	**H**	1.33812500	−2.91290100	0.31599100
H	−0.04088600	−4.57011600	−0.57559400	**H**	0.70024600	−4.55156900	0.19257500
H	−4.88044000	−1.33905600	1.20911900	**H**	−4.59529900	−1.69386300	1.74755500
H	−4.48861400	−2.37322400	−0.16584300	**H**	−4.37952600	−2.81603700	0.40385300
H	−3.35169300	−2.23218100	1.18346500	**H**	−3.09450200	−2.61555700	1.60860700
H	0.70207100	−0.28023600	2.50689500	**H**	1.23406500	0.34747600	2.35292500
H	0.42920200	−1.83959500	1.76799100	**H**	1.20503800	−1.35523400	1.99371200
H	−3.29242200	−0.56368700	2.87200400	**H**	−2.72472600	−0.69819400	3.17835000
H	−1.51992200	−0.46106000	2.93741200	**H**	−1.02869000	−0.18178900	3.21418300
H	−2.51690100	0.50700100	4.03930800	**H**	−2.24627700	0.69646600	4.15992300
Mg	0.09140900	0.11333500	−0.04055700	**Mg**	−0.01464700	−0.05828700	0.12000100
Si	1.93364700	2.87857000	−1.30410300	**Si**	0.83969900	2.80787100	−1.66162300
Si	2.80733600	−1.27921200	1.94353700	**Si**	3.39640800	−0.37531700	1.59476800
C	2.24413100	3.68212100	0.39471400	**C**	1.40055000	3.82962100	−0.16505000

H	3.16844800	4.27520900	0.39333500	H	2.29110600	4.42431700	−0.40719900
H	1.42244800	4.36144500	0.66108200	H	0.61383100	4.52966100	0.14572400
H	2.33071900	2.93886500	1.19645500	H	1.64756600	3.20470000	0.70041000
C	3.42891000	1.78825900	−1.75955400	C	2.25253900	1.66897000	−2.23467200
H	3.57655100	0.96711600	−1.04713600	H	2.54781100	0.93931800	−1.47140800
H	3.30018400	1.34179600	−2.75556500	H	1.96975200	1.11439100	−3.13990800
H	4.35823900	2.37305600	−1.78399200	H	3.14798600	2.25423200	−2.48216600
C	1.90795500	4.30432700	−2.57590200	C	0.50783600	4.02619200	−3.08712500
H	1.08713100	5.00506800	−2.37060200	H	−0.28436600	4.73978500	−2.82413300
H	2.84430700	4.87958900	−2.56656900	H	1.40551400	4.60768000	−3.33798600
H	1.76374800	3.92381900	−3.59641700	H	0.18759100	3.50214500	−3.99743800
C	3.77754500	0.31207900	2.32827100	C	4.09079700	1.39178200	1.47603200
H	3.79492000	1.00350400	1.47759400	H	3.85153400	1.87141700	0.51992400
H	3.33952000	0.84936200	3.18042200	H	3.69249300	2.03142800	2.27484800
H	4.82016900	0.08348800	2.58727900	H	5.18436200	1.38441900	1.57756700
C	3.67686800	−2.13013300	0.47283200	C	4.19527000	−1.39532800	0.19496900
H	3.22279900	−3.10003900	0.22975100	H	3.85022000	−2.43780900	0.19658600
H	3.65284100	−1.51311400	−0.43467200	H	3.98788900	−0.97592000	−0.79750400
H	4.73266300	−2.31959300	0.70963900	H	5.28671400	−1.41685600	0.31675200
C	3.05353600	−2.44619400	3.43657000	C	4.06565700	−1.11790000	3.22115400
H	4.11554100	−2.65569700	3.62633000	H	5.16380700	−1.10196100	3.25665100
H	2.63287500	−2.00883800	4.35220600	H	3.69694600	−0.56080400	4.09285000
H	2.55001300	−3.40962700	3.27607800	H	3.74618100	−2.16187600	3.34443900

Tabelle 8.136 Standardorientierung von **[Me$_3$SiN(^{t}Bu)H]·MgBu$_2$** und **[Me$_3$SiN(^{t}Bu)H]·MgBu$_2$ (ÜZ)** [B3LYP/6−31+G(d)].

[Me$_3$SiN(^{t}Bu)H]·MgBu$_2$				ÜZ			
C	−3.14004100	−1.97873200	−0.03574800	C	0.84567400	2.79323900	−0.23179700
C	−1.79607700	−1.62159500	−0.70452900	C	0.34756500	1.54276100	−0.98127800
C	4.17353800	−0.74180700	−1.39636400	C	−3.76186500	−0.64449700	−1.83984800
C	1.42542200	−0.72154500	−2.75391100	C	−0.84709700	−1.51656400	−2.28588900
C	2.97171100	−2.14674700	1.64536300	C	−3.04244200	1.60043600	0.99064100
N	1.46171000	−0.80464200	0.15520300	N	−1.49729200	−0.20023600	0.21758800
C	0.79731200	−1.23893800	2.49493200	C	−1.14034900	0.82136200	2.43352400
Si	2.39151000	−0.12063100	−1.24649700	Si	−2.20649500	−1.29772500	−0.97115400
C	1.99313900	−0.95862700	1.56198300	C	−2.20289900	0.37170200	1.40484800
C	2.39323300	1.76320000	−1.17696100	C	−2.59023300	−3.03464500	−0.30695800
C	−0.92696400	2.01122000	0.91776900	C	2.29869000	−1.40914500	1.02154900
C	−1.69361000	3.00195800	0.01656500	C	3.54735000	−1.41002500	0.11546000
C	2.68704600	0.33645700	2.00781700	C	−3.11868700	−0.65933800	2.09005000
H	−3.79000600	−1.08880700	−0.00181400	H	1.56964400	2.51241700	0.55299000
H	−2.97649700	−2.25804300	1.01925200	H	0.00331900	3.25914700	0.30380200
H	−1.99293700	−1.38784900	−1.76750100	H	1.19800600	1.09809300	−1.54045600
H	1.12666800	−1.72832000	−0.13583500	H	−0.77690000	0.72956700	−0.37974100
H	−1.17113300	−2.53554300	−0.74004200	H	−0.33531300	1.85758300	−1.78694000
H	4.22888800	−1.83536900	−1.45742600	H	−3.59414200	0.34319600	−2.28694000
H	4.60794000	−0.34124900	−2.32262800	H	−4.05651100	−1.32908400	−2.64676200
H	4.81727800	−0.41439000	−0.57208000	H	−4.61829900	−0.56131500	−1.15929400
H	1.43576600	−1.81589800	−2.83637000	H	−0.55838200	−0.57344900	−2.76396600
H	1.88338900	−0.32186300	−3.66792500	H	−1.21782700	−2.18175000	−3.07686900
H	2.48262600	−3.07978100	1.33632700	H	−2.40953800	2.36890900	0.53232600
H	3.84809600	−1.99463600	1.00934000	H	−3.81199700	1.32133000	0.26364200
H	3.32273000	−2.28309500	2.67524000	H	−3.54310800	2.04654100	1.85963700
H	0.22030000	−2.10830100	2.15493100	H	−0.45447000	1.56425700	2.00539300
H	1.14325100	−1.45016900	3.51327700	H	−1.60558100	1.28985600	3.30921300
H	0.12806800	−0.37057200	2.56142000	H	−0.55937200	−0.03737500	2.79988300
H	3.03818800	2.15671300	−0.38358900	H	−3.47310800	−3.06305100	0.34081400
H	2.77143600	2.15639200	−2.13008300	H	−2.78204300	−3.71389000	−1.14913200
H	1.39014000	2.17596300	−1.02065000	H	−1.74721200	−3.44763000	0.26153700
H	−1.46262000	1.94147600	1.88304200	H	2.57407400	−0.99644500	2.00773900

H	0.05269000	2.45296500	1.17496500	H	2.00266800	−2.45235800	1.22686600
H	−2.68295700	2.58867200	−0.24019100	H	3.86624300	−0.37560800	−0.09178900
H	−1.17107300	3.12154600	−0.94850800	H	3.30302500	−1.84330700	−0.86834900
H	3.59550600	0.53416000	1.42814600	H	−3.95192100	−0.95328700	1.44194000
H	2.01818600	1.19777900	1.91333000	H	−2.56220300	−1.56267100	2.36379600
H	2.98464000	0.25200700	3.05900300	H	−3.55178800	−0.23594400	3.00521800
C	−3.92604700	−3.11777200	−0.71184300	C	1.50405500	3.86324700	−1.12051800
H	−3.29284500	−4.01756200	−0.74190700	H	0.78607200	4.16968800	−1.89541000
H	−4.11309000	−2.84376900	−1.76092800	H	2.35269400	3.41056400	−1.65368500
C	−5.25594300	−3.44838600	−0.02162100	C	1.98306200	5.09644800	−0.34418800
H	−5.92136800	−2.57490700	−0.00586100	H	2.72767800	4.82273700	0.41499000
H	−5.78774900	−4.26181900	−0.53185400	H	2.44448600	5.83676000	−1.00929600
H	−5.09635200	−3.75832300	1.02005600	H	1.14913500	5.58882700	0.17346400
C	−1.90377000	4.40443200	0.61738800	C	4.75296900	−2.17713600	0.68862400
H	−0.92149500	4.83798500	0.85881100	H	4.45122700	−3.21637300	0.88689800
H	−2.43397100	4.30224600	1.57604500	H	5.01632000	−1.74528100	1.66554200
C	−2.67764100	5.36159700	−0.29893700	C	5.98276400	−2.16442800	−0.22865500
H	−2.80481400	6.35024900	0.16053700	H	6.82104000	−2.71989200	0.21052100
H	−2.15595600	5.50464600	−1.25496300	H	5.75627800	−2.61991400	−1.20194800
H	−3.67812400	4.96989400	−0.52622800	H	6.32640200	−1.13860200	−0.41722200
Mg	−0.70489500	0.01897500	0.15385800	Mg	0.60136400	−0.36063000	0.32001800
H	0.37499000	−0.40708800	−2.75050700	H	0.06567500	−1.99538500	−1.89897700

Tabelle 8.137 Standardorientierung von **$MgBu_2$−Addukt mit R = Me, R′ = Me** und **$MgBu_2$−Addukt mit R = Me, R′ = Me (ÜZ)** [B3LYP/6−31+G(d)].

$MgBu_2$−Addukt mit R = Me, R′ = Me				**ÜZ**			
C	−0.59167200	3.36630400	0.51048900	C	−0.66691300	3.49876800	0.32618500
C	−0.26185900	2.03891600	1.22615400	C	−0.22233300	2.13013500	0.87747900
C	0.65380500	−1.86859700	2.14579600	C	0.52881400	−1.82523700	2.09572300
C	−0.80299800	−2.30561900	2.37151200	C	−0.89487000	−2.40296700	2.16311700
C	3.68753700	1.54292800	0.37787100	C	4.09126000	1.42627000	0.53554700
C	2.37210400	−1.25409600	0.47922600	C	2.40268000	−1.10856800	0.64479200
N	1.41875800	0.91123200	−1.43557000	N	1.50112900	1.11462300	−1.04741200
N	0.91127500	−1.57520300	0.67804600	N	0.94726900	−1.53913400	0.66280600
Si	2.87856600	0.20433600	−0.67577000	Si	2.96586400	0.32810800	−0.52662500
C	1.20487200	0.82357200	−2.90051400	C	1.49442600	1.94925200	−2.26064500
C	−1.17543500	−3.54166300	1.55721300	C	−1.05452100	−3.67847400	1.34044200
C	0.58710900	−2.81720400	−0.12485700	C	0.81835700	−2.81817900	−0.14553500
C	−0.86022800	−3.28475900	0.08620600	C	−0.59889500	−3.40732400	−0.09069600
C	4.10531500	−0.40607900	−1.97702800	C	4.01972800	−0.26809400	−1.98685800
C	−2.08747900	−0.10127700	−1.38036200	C	−2.07585400	−0.26825500	−1.49691500
C	−3.44657900	−0.21123500	−0.65952000	C	−3.39508400	−0.48808100	−0.73055100
H	−1.56394700	3.28495100	−0.00288700	H	−1.37444600	3.35218800	−0.50546800
H	0.14014500	3.56444200	−0.29738300	H	0.20090200	4.01718400	−0.11370600
H	−1.00208900	1.90667100	2.03774600	H	−1.12138900	1.64093900	1.30831700
H	1.32926000	1.88792400	−1.14913100	H	0.83270400	1.66379000	−0.12899400
H	0.70284200	2.16329900	1.75337900	H	0.44091300	2.28752800	1.74467800
H	1.31145500	−2.71487800	2.42061900	H	1.22891400	−2.58851000	2.48093400
H	−0.93856400	−2.49377000	3.44377700	H	−1.13330000	−2.58975400	3.21759200
H	−1.47188500	−1.47106000	2.11529400	H	−1.61113500	−1.64499900	1.81329200
H	2.97807000	1.97300800	1.09472900	H	3.55936200	1.81919700	1.41124200
H	4.53204200	1.13484200	0.94881900	H	4.97510900	0.88131500	0.89556300
H	4.07694000	2.36029200	−0.24231000	H	4.45381200	2.28749200	−0.04054900
H	2.80217400	−0.99591300	1.44922400	H	2.65869900	−0.76042500	1.64670800
H	2.90694400	−2.16711000	0.17371200	H	3.03466300	−1.99729500	0.49049600
H	−0.60261500	−4.40858300	1.91944300	H	−0.44713100	−4.48283800	1.78163200
H	−2.23699400	−3.78558000	1.68776600	H	−2.09638000	−4.02107300	1.35705700
H	−1.54157500	−2.52713200	−0.31804900	H	−1.29774600	−2.72175900	−0.58493400
H	−1.00874900	−4.19661400	−0.50658400	H	−0.59691500	−4.33496300	−0.67722500
H	4.46550100	0.42293100	−2.59870900	H	4.52795900	0.59043900	−2.44520100

H	4.98165400	−0.84630500	−1.48302500	H	4.80306900	−0.96399500	−1.65729900
H	3.69044800	−1.16841300	−2.64585200	H	3.43963100	−0.76100600	−2.77451100
H	−2.14305900	0.77523400	−2.05704300	H	−2.20012500	0.62532700	−2.13727200
H	−1.98321300	−0.96317500	−2.06497400	H	−1.94123900	−1.09851600	−2.21397100
H	−3.58494400	0.65396500	0.01025100	H	−3.56716200	0.34630800	−0.03030300
H	−3.45608000	−1.09335000	0.00540100	H	−3.32407300	−1.38892900	−0.09611000
C	−0.62957400	4.61944100	1.40686300	C	−1.31667100	4.43941300	1.35621100
H	0.33982600	4.71995500	1.91822600	H	−0.61358500	4.59521800	2.18825200
H	−1.37490500	4.45950300	2.19987800	H	−2.19559900	3.94014900	1.79068200
C	−0.95066700	5.91626800	0.65159300	C	−1.73304200	5.79697200	0.77508900
H	−1.92826900	5.85366900	0.15517800	H	−2.45986500	5.67357400	−0.03870400
H	−0.97430700	6.78387500	1.32370200	H	−2.19301600	6.43932500	1.53675500
H	−0.20054500	6.11919400	−0.12514800	H	−0.86786800	6.33506800	0.36515000
C	−4.68122600	−0.30421400	−1.57672600	C	−4.64911100	−0.63411500	−1.61315200
H	−4.56628600	−1.17480100	−2.24045900	H	−4.49492000	−1.46931900	−2.31301800
H	−4.69895000	0.57758600	−2.23456300	H	−4.75007100	0.26745700	−2.23529900
C	−6.01233100	−0.40714700	−0.81963000	C	−5.94345800	−0.85926600	−0.82038600
H	−6.86744900	−0.47350400	−1.50493800	H	−6.81369600	−0.95682900	−1.48211000
H	−6.03404200	−1.29647700	−0.17488800	H	−5.88381300	−1.77354000	−0.21417600
H	−6.17011800	0.46846500	−0.17560200	H	−6.13944900	−0.02329300	−0.13552000
Mg	−0.37375600	0.32571000	−0.12129800	Mg	−0.27881200	0.11831500	−0.40145300
C	0.96149000	−0.69178500	3.08119400	C	0.59562500	−0.59790300	3.01483900
H	0.75484100	−1.00911500	4.10984900	H	0.31551600	−0.91062000	4.02711600
H	2.00407400	−0.36256100	3.05843900	H	1.58576700	−0.14151100	3.08659200
H	0.33101700	0.17168700	2.85600400	H	−0.10747100	0.17865900	2.70111500
H	0.21014900	1.20450100	−3.14972400	H	0.50505000	2.40536400	−2.39209900
C	0.84559900	−2.64096100	−1.62417100	C	1.24673000	−2.63632100	−1.60475900
H	0.16824000	−1.89606500	−2.05246400	H	0.63636300	−1.88400100	−2.11804300
H	1.87769700	−2.36320300	−1.85292700	H	2.29745600	−2.36235100	−1.70763800
H	0.65160600	−3.59356200	−2.13013900	H	1.10496200	−3.58520000	−2.13415900
H	1.26035600	−3.61244500	0.24883500	H	1.50522200	−3.54710000	0.32286000
H	1.24729100	−0.21922900	−3.22102500	H	1.70168800	1.36035100	−3.16481000
H	1.95423800	1.38866500	−3.47127800	H	2.22629300	2.77110000	−2.22206200

Tabelle 8.138 Standardorientierung von **90·MgBu$_2$** und **90·MgBu$_2$ (ÜZ)** [B3LYP/6−31+G(d)].

90·MgBu$_2$				ÜZ			
C	−1.40966300	2.92703100	1.21433300	C	0.67253200	3.29879100	0.81680400
C	−0.82968500	1.58573100	1.71383400	C	0.38924700	1.83938600	1.22164900
C	0.39851800	−2.24904200	2.20578100	C	−0.91594300	−2.04518600	2.08774900
C	−1.07606700	−2.68674700	2.19737000	C	−2.43780900	−1.94264200	1.89087500
C	4.14435200	0.99891600	0.88687600	C	3.90299800	−0.62474800	1.35632900
C	2.25310000	−1.34565500	0.84398200	C	1.30628200	−2.12881400	0.99308600
C	2.39101800	3.18600500	−1.80352900	C	3.62429900	1.69100500	−1.56638000
N	1.50007400	1.15885200	−0.58301900	N	1.75365500	0.26894100	−0.63388100
N	0.81139000	−1.76892800	0.82228100	N	−0.17545800	−1.90548400	0.76498700
Si	2.90942100	0.10921800	−0.24176100	Si	2.63152200	−1.08901200	0.02368100
C	1.32170800	2.08503000	−1.75147200	C	2.19531900	1.15068800	−1.74231000
C	−1.34294700	−3.81036000	1.19781400	C	−2.98016200	−2.98646800	0.91912100
C	0.63870900	−2.93052800	−0.13165600	C	−0.68873500	−2.97851100	−0.17961500
C	−0.81974500	−3.40960200	−0.17961500	C	−2.20719400	−2.89525700	−0.39340300
C	3.87537500	−0.42657700	−1.77413600	C	3.57843500	−2.16646500	−1.22300400
C	−1.87185700	−0.16174200	−1.54025000	C	−1.99686300	0.67341800	−1.55373300
C	−3.33626200	−0.43014300	−1.13758100	C	−3.33294300	1.08589300	−0.90360200
C	1.20820100	1.33701200	−3.08147300	C	2.01693200	0.50375300	−3.12500900
H	−2.30805300	2.74198700	0.60292800	H	0.09135200	3.55370400	−0.08351900
H	−0.69588200	3.42308200	0.53089100	H	1.73002200	3.40290900	0.52452600
H	−1.55762900	1.15333700	2.42625100	H	−0.68515900	1.77989000	1.49541800
H	1.34921600	1.72835300	0.25617000	H	1.27091500	0.99623000	0.27551300
H	0.05641000	1.81234600	2.34116400	H	0.91949200	1.61648200	2.16300400
H	1.01716500	−3.13779300	2.43200900	H	−0.68446700	−3.05578200	2.46995900

H	−1.34336400	−3.00821500	3.21151300	H	−2.91361100	−2.04712400	2.87382900
H	−1.70832400	−1.81539400	1.97266200	H	−2.68795300	−0.93425100	1.53079300
H	3.65663800	1.42270200	1.77420900	H	3.46078800	0.01974500	2.12653700
H	4.92064000	0.30638300	1.24048400	H	4.30097000	−1.51903200	1.85679200
H	4.65095400	1.81796500	0.36232700	H	4.75630800	−0.08576200	0.92662500
H	2.46962200	−0.98612400	1.85092400	H	1.51455200	−1.90160000	2.03908900
H	2.90544600	−2.22807800	0.71563800	H	1.52388000	−3.20472000	0.89295800
H	2.44812700	3.73092500	−0.85353600	H	3.74315200	2.17292800	−0.58970500
H	3.38369400	2.77203100	−2.02070800	H	4.36840600	0.88756700	−1.64461300
H	2.15403800	3.91179800	−2.59108800	H	3.85779300	2.43191600	−2.34167700
H	−0.83504200	−4.72596500	1.53642100	H	−2.86557600	−3.99101800	1.35313700
H	−2.41437600	−4.04136900	1.15157400	H	−4.05299900	−2.83469400	0.74853700
H	−1.44172200	−2.61505900	−0.60772500	H	−2.45110500	−1.95911800	−0.91034500
H	−0.87264100	−4.26113500	−0.87018900	H	−2.49367800	−3.71279200	−1.06711500
H	4.41971600	0.42713700	−2.19579800	H	4.49312600	−1.65364400	−1.54619200
H	4.62928900	−1.16514200	−1.46839900	H	3.89324700	−3.10305600	−0.74167900
H	3.27804100	−0.87248600	−2.57225700	H	3.01290600	−2.42456300	−2.12314600
H	−1.85458000	0.79382600	−2.10049400	H	−1.62458800	1.53373100	−2.14107600
H	−1.56906100	−0.92003600	−2.28583100	H	−2.19842500	−0.10564400	−2.31100500
H	−3.67390000	0.34047400	−0.42475200	H	−3.15981700	1.89052800	−0.16931700
H	−3.41483500	−1.38451400	−0.58706300	H	−3.75087500	0.24584800	−0.32190900
H	2.16096700	0.89517200	−3.38911700	H	2.68626400	−0.35414200	−3.25630100
H	0.44928100	0.55132000	−3.02803900	H	0.98570900	0.16025300	−3.26544300
H	0.90547000	2.03990000	−3.86621300	H	2.24162200	1.22647900	−3.92013600
C	−1.78125500	3.94140900	2.31311000	C	0.37110900	4.34790200	1.90183700
H	−0.88958400	4.14485900	2.92563600	H	0.95138000	4.10331300	2.80428000
H	−2.51248900	3.47420600	2.98942000	H	−0.68756200	4.26837800	2.19048900
C	−2.34885600	5.26208800	1.77546900	C	0.67832700	5.78733100	1.46856200
H	−3.25862000	5.09045000	1.18467500	H	0.08745300	6.07025600	0.58733500
H	−2.60569900	5.95562200	2.58674100	H	0.45193100	6.50704100	2.26543300
H	−1.62476900	5.76889600	1.12283700	H	1.73821300	5.90499000	1.20593600
C	−4.34619500	−0.47916100	−2.30057500	C	−4.42178600	1.56302500	−1.88329700
H	−4.02875000	−1.25548700	−3.01344200	H	−4.60931500	0.76732800	−2.62013500
H	−4.29927900	0.47334800	−2.84939900	H	−4.03322300	2.41914200	−2.45433800
C	−5.79129300	−0.74694300	−1.85864900	C	−5.73993400	1.95482300	−1.20240900
H	−6.48031500	−0.77595000	−2.71286900	H	−6.49118200	2.28541200	−1.93111200
H	−5.87366300	−1.70829800	−1.33324900	H	−6.16669900	1.10824800	−0.64728400
H	−6.14615800	0.03327400	−1.17193800	H	−5.58883900	2.77407800	−0.48671500
Mg	−0.48352200	0.15169300	0.09816200	Mg	−0.36794200	0.14556000	−0.26806100
C	0.61182700	−1.22058700	3.32611900	C	−0.49786600	−1.01946600	3.14986600
H	0.14268700	−1.60474300	4.23885100	H	−1.08654200	−1.20294500	4.05572900
H	1.66381000	−1.04718700	3.57152600	H	0.55366300	−1.07500700	3.44083800
H	0.14473200	−0.26269200	3.08566400	H	−0.70030900	0.00356700	2.82210600
H	0.35415900	2.57228900	−1.57492800	H	1.52285000	2.02172700	−1.71358300
C	1.13381600	−2.62430500	−1.54622000	C	0.01977700	−2.96680000	−1.53632000
H	0.65547600	−1.72755000	−1.95300100	H	−0.12389400	−2.01745100	−2.06504300
H	2.21774800	−2.50918700	−1.59267200	H	1.08891800	−3.16244000	−1.45630000
H	0.87232700	−3.46177400	−2.20270200	H	−0.40987100	−3.75594100	−2.16364000
H	1.25641400	−3.75731900	0.26958500	H	−0.46874400	−3.94565500	0.30914200

Tabelle 8.139 Standardorientierung von **116·MgBu$_2$** und **116·MgBu$_2$ (ÜZ)** [B3LYP/6−31+G(d)].

116·MgBu$_2$				**ÜZ**			
C	−0.68885700	3.20160100	1.26130000	C	1.59079300	3.00548900	0.91215600
C	−0.50872000	1.72027900	1.65339100	C	0.82708200	1.68763200	1.13225800
C	−0.58144300	−2.27286900	2.20570400	C	−1.56584700	−1.55181700	2.18724800
C	−2.09249900	−2.37279800	1.93928700	C	−3.03596000	−1.19450900	1.91241500
C	3.87432600	0.18699500	1.54980800	C	3.44075100	−1.14347000	1.63984300
C	1.61865500	−1.77788500	1.20726900	C	0.62215000	−2.19993400	1.24523800
C	3.62290700	1.75771700	−1.97970100	C	3.94218900	0.39399200	−1.67182200
N	1.81580200	0.66495700	−0.58173800	N	1.70586100	−0.23862200	−0.71072100

N	0.15168500	−1.89779700	0.92423600	**N**	−0.75805800	−1.67676600	0.90202200
C	1.28299100	2.62421100	−1.98104100	**C**	1.85821200	1.54981000	−2.42323500
Si	2.79902100	−0.61662500	0.21387700	**Si**	2.19887700	−1.60542200	0.27797000
C	2.13802000	1.34681100	−1.89703700	**C**	2.43408000	0.20146000	−1.94445000
C	−2.41767700	−3.43693400	0.89316700	**C**	−3.72814400	−2.19391300	0.99140100
C	−0.09470200	−3.01328200	−0.06759700	**C**	−1.44324100	−2.68823100	−0.00131900
C	−1.59232100	−3.18681300	−0.36676100	**C**	−2.90904200	−2.33144800	−0.28769500
C	3.97168100	−1.59522300	−0.90780900	**C**	2.97747900	−3.11305900	−0.58210400
C	−1.84218900	0.23820700	−1.65354000	**C**	−1.89715800	1.09999300	−1.56380500
C	−3.33289600	0.28560200	−1.25705800	**C**	−3.22295400	1.62287700	−0.97682600
C	1.77217100	0.42350000	−3.06866000	**C**	2.24493800	−0.81602400	−3.08933500
H	−1.51091800	3.30137900	0.53299600	**H**	1.18171100	3.52937700	0.03466500
H	0.20732500	3.57006500	0.73368900	**H**	2.64394200	2.79050300	0.66532500
H	−1.38903300	1.43946400	2.26324900	**H**	−0.22849000	1.96649200	1.33515400
H	1.73852700	1.41108900	0.11736600	**H**	1.45055000	0.70896300	0.10600400
H	0.34107500	1.65468700	2.36151600	**H**	1.17239900	1.23478300	2.07638700
H	−0.22116500	−3.28021100	2.48763000	**H**	−1.53578300	−2.54735900	2.66562900
H	−2.59456400	−2.60497700	2.88644500	**H**	−3.55210700	−1.13562600	2.87884900
H	−2.47000700	−1.39174700	1.61771600	**H**	−3.08516600	−0.19002500	1.47022500
H	3.27555700	0.79778700	2.23772900	**H**	3.10155200	−0.27786100	2.22096100
H	4.39127400	−0.57308300	2.15147500	**H**	3.59071500	−1.97951600	2.33748500
H	4.64260500	0.83411500	1.10927700	**H**	4.42137300	−0.89217000	1.21735400
H	1.71420900	−1.37051100	2.21420400	**H**	0.82750100	−1.92979300	2.28186000
H	2.07374000	−2.78467500	1.26097500	**H**	0.59002200	−3.30183700	1.24360300
H	3.90586200	2.37892100	−1.12093000	**H**	4.10034000	1.11707200	−0.86350100
H	4.29092700	0.89176700	−2.01531800	**H**	4.42680700	−0.54698500	−1.38571800
H	3.80318800	2.34553200	−2.88789100	**H**	4.45635900	0.76686400	−2.56674100
H	1.53774200	3.32631900	−1.17808400	**H**	1.98084600	2.33172300	−1.66909400
H	1.46284100	3.13228100	−2.93536600	**H**	2.37717800	1.87698900	−3.33220600
H	0.21483500	2.39948700	−1.91471400	**H**	0.79249100	1.46662000	−2.66442300
H	−2.18341500	−4.43134400	1.30222800	**H**	−3.80970700	−3.17011100	1.49235800
H	−3.48910000	−3.43607100	0.65740700	**H**	−4.75023400	−1.86630100	0.76482400
H	−1.95540200	−2.29190900	−0.88319000	**H**	−2.94995000	−1.39815300	−0.86250100
H	−1.70040800	−4.02551800	−1.06661200	**H**	−3.32298800	−3.11899000	−0.93028600
H	4.91097800	−1.04840400	−1.04703300	**H**	3.96391100	−2.86843700	−0.99388200
H	4.22412300	−2.53581900	−0.39925200	**H**	3.13546100	−3.89356700	0.17565800
H	3.58379700	−1.85203200	−1.89645600	**H**	2.38369200	−3.55280200	−1.38934700
H	−1.63363300	1.15020100	−2.24479600	**H**	−1.38223600	1.95955800	−2.03107600
H	−1.69858700	−0.58781900	−2.37459200	**H**	−2.13056300	0.43063900	−2.41277300
H	−3.50758200	1.12480200	−0.56317800	**H**	−3.02165200	2.30201500	−0.13105700
H	−3.60738300	−0.61967200	−0.68707200	**H**	−3.80935000	0.79187300	−0.54978200
H	2.34525100	−0.50834900	−3.05296800	**H**	2.68229200	−1.78996200	−2.85236900
H	0.70579500	0.17888700	−3.05236000	**H**	1.17990600	−0.96126700	−3.30288000
H	1.99082300	0.92609300	−4.01814600	**H**	2.72470200	−0.45266200	−4.00729300
C	−0.96766600	4.16689600	2.42965900	**C**	1.56878100	3.97777400	2.10482600
H	−0.14743600	4.08762100	3.15957900	**H**	1.98855700	3.47095000	2.98666700
H	−1.87412200	3.83236900	2.95589700	**H**	0.52319800	4.20960300	2.35657500
C	−1.13419000	5.63107700	2.00083400	**C**	2.33582500	5.28167800	1.84812000
H	−1.96954800	5.74525600	1.29710400	**H**	1.91410100	5.82714500	0.99354800
H	−1.33097800	6.28688900	2.85892200	**H**	2.30155100	5.94957000	2.71815600
H	−0.23003000	6.00328500	1.49973300	**H**	3.39219400	5.08289600	1.62319300
C	−4.32736300	0.42097600	−2.42620800	**C**	−4.13123700	2.36728000	−1.97435800
H	−4.17592000	−0.41925200	−3.12098800	**H**	−4.34829000	1.70022900	−2.82221400
H	−4.08236300	1.33091400	−2.99425300	**H**	−3.57426100	3.21824800	−2.39344600
C	−5.79783600	0.46906800	−1.98954200	**C**	−5.44635900	2.86602900	−1.36106900
H	−6.47473700	0.56961200	−2.84796800	**H**	−6.06410000	3.39471600	−2.09829200
H	−6.08157200	−0.44415200	−1.44876500	**H**	−6.04240200	2.03176400	−0.96657800
H	−5.98364000	1.31853900	−1.31857700	**H**	−5.25801800	3.55753500	−0.52874000
Mg	−0.45342600	0.27077800	0.01592100	**Mg**	−0.38677000	0.24159400	−0.30587600
C	−0.32927600	−1.33748800	3.39697100	**C**	−1.00680600	−0.52203600	3.17799300
H	−1.02637600	−1.61008900	4.19729300	**H**	−1.60098800	−0.57442300	4.09739300

H	0.67511900	−1.42902000	3.82110500	H	0.03512400	−0.68396100	3.46254400
H	−0.50581500	−0.29129300	3.14027600	H	−1.09174300	0.49651000	2.78837800
H	0.26921600	−3.94232200	0.41194500	H	−1.43011200	−3.64641400	0.55004000
C	0.67071800	−2.83411100	−1.37842400	C	−0.70781700	−2.89494300	−1.32749100
H	0.43328000	−1.87732300	−1.85216200	H	−0.70140800	−1.98276600	−1.93456400
H	1.75069600	−2.91425400	−1.24812700	H	0.32066500	−3.23008600	−1.19861600
H	0.37434500	−3.62744300	−2.07384700	H	−1.23355100	−3.66483900	−1.90356600

Tabelle 8.140 Standardorientierung von **[(S)−69]·$MgBu_2$** und **[(S)−69]·$MgBu_2$ (ÜZ)** [B3LYP/6−31+G(d)].

[(S)−69]·$MgBu_2$				ÜZ			
C	1.11121000	3.35595900	−1.13581300	C	0.17661800	2.86473400	1.28952000
C	1.39270000	1.89893200	−1.55351600	C	−0.04727300	1.36565200	1.55295000
C	2.43019800	−1.32846500	−2.50952100	C	−2.47851300	−1.73752600	2.07743900
C	3.86363100	−1.11734700	−2.01900800	C	−3.89356000	−1.44268600	1.57579600
C	−2.88559700	−2.01282800	−1.90934100	C	2.85590700	−2.06095400	1.62953500
C	0.13016600	−1.86722000	−1.96869800	C	−0.14856800	−2.19675100	1.55015400
N	−1.21580000	−0.01632800	−0.20945800	N	1.07714900	−0.39175500	−0.31458300
N	1.47881800	−1.61099300	−1.39636600	N	−1.48063700	−1.84044900	0.97230000
Si	−1.38103800	−1.69751800	−0.81153900	Si	1.39543800	−1.94880800	0.42918800
C	−1.98222300	0.45435000	0.98644900	C	1.92196500	0.05971700	−1.44679800
C	4.36015700	−2.32661900	−1.21842600	C	−4.35318500	−2.49856100	0.56155600
C	1.94293000	−2.80122700	−0.63459700	C	−1.91525600	−2.89856400	0.01596800
C	3.36640700	−2.64131000	−0.09419100	C	−3.31197500	−2.64060300	−0.55561400
C	−1.40911500	−2.85191900	0.67767500	C	1.62472100	−3.31991800	−0.86254600
C	1.65848200	−0.06629100	1.99238800	C	−2.37322400	0.95982400	−1.57783500
C	2.98209100	0.53413700	2.50866300	C	−3.83853300	1.30937100	−1.25510100
H	1.69997700	3.60794300	−0.23793200	H	−0.44709900	3.19526900	0.44351400
H	0.05741100	3.46725800	−0.82817300	H	1.21656500	3.02817400	0.96337000
H	2.44080500	1.85147800	−1.90711400	H	−1.08728300	1.24239000	1.93154500
H	−1.32166400	0.66521600	−0.96485900	H	0.72249000	0.48580400	0.55259900
H	0.79560100	1.68449800	−2.46461600	H	0.56647000	1.05060400	2.41457700
H	2.07271700	−0.43555300	−3.02948500	H	−2.13759100	−0.95183600	2.75980400
H	2.40179700	−2.17225100	−3.22418400	H	−2.47311300	−2.68684500	2.64246400
H	4.50473300	−0.93045300	−2.88985000	H	−4.56864000	−1.41106700	2.44048900
H	3.90587800	−0.21307300	−1.39750800	H	−3.92468900	−0.44748500	1.11450500
H	−2.92226900	−1.32062400	−2.75992700	H	2.81031300	−1.28029800	2.39866000
H	−2.85472300	−3.03271100	−2.31621200	H	2.86477000	−3.03466700	2.13929700
H	−3.82216900	−1.90324100	−1.35233000	H	3.81330200	−1.95130000	1.10801800
H	−0.03539400	−1.11713100	−2.75566700	H	0.01204500	−1.53564500	2.41169500
H	0.11410100	−2.84410300	−2.48779900	H	−0.18617200	−3.22249100	1.95915900
H	4.45405000	−3.19674100	−1.88578900	H	−4.48080700	−3.46528100	1.07166500
H	5.35798600	−2.13363900	−0.80580200	H	−5.33030400	−2.22899800	0.14330300
H	1.89486600	−3.68719500	−1.29623200	H	−1.89733000	−3.87250900	0.53778700
H	1.24868100	−2.97207900	0.19130300	H	−1.17783600	−2.95431000	−0.78984600
H	3.37874100	−1.83788600	0.65122400	H	−3.29344700	−1.72910900	−1.16577800
H	3.64380200	−3.56648800	0.42732700	H	−3.57011800	−3.47024500	−1.22601900
H	−2.39342800	−2.82873400	1.16027600	H	2.63101100	−3.26376100	−1.29684900
H	−1.22607000	−3.88702600	0.36302000	H	1.52926100	−4.31174000	−0.40083300
H	−0.65837100	−2.58969400	1.43146000	H	0.90733000	−3.26391600	−1.68980500
H	0.84400400	0.32278900	2.63316400	H	−1.86308900	1.89708700	−1.86703200
H	1.66577300	−1.15405000	2.20265400	H	−2.35575900	0.34850800	−2.50012400
H	2.98299300	1.62547400	2.35075100	H	−3.88852800	1.92963900	−0.34442200
H	3.83076700	0.15924500	1.90987200	H	−4.40846100	0.39572100	−1.01728700
C	1.40142700	4.42320600	−2.20869400	C	−0.10032300	3.79250900	2.48563700
H	0.81304800	4.19052700	−3.10971300	H	0.52471600	3.47618500	3.33418800
H	2.45708200	4.34437300	−2.50878600	H	−1.14312800	3.65571100	2.80908200
C	1.10210300	5.85884400	−1.75625800	C	0.15180700	5.27567800	2.18494700
H	1.69962000	6.12898600	−0.87521600	H	−0.48319600	5.62611300	1.36056700
H	1.32432500	6.58961100	−2.54479100	H	−0.05820500	5.90657700	3.05780000
H	0.04444200	5.97680400	−1.48335200	H	1.19599100	5.44941600	1.89273900

C	3.29847800	0.26652700	3.99254100	C	−4.59208900	2.05001000	−2.37625000
H	3.31514700	−0.82123300	4.16102300	H	−4.55605100	1.43899300	−3.29073400
H	2.47087500	0.65436600	4.60560300	H	−4.05261000	2.97923800	−2.61161000
C	4.62164100	0.88085300	4.46927500	C	−6.05147500	2.37583100	−2.03227300
H	4.81152400	0.66736300	5.52928600	H	−6.55328800	2.90550600	−2.85213200
H	5.47127300	0.48819300	3.89422700	H	−6.62533900	1.46154200	−1.82827300
H	4.61884500	1.97216200	4.34566100	H	−6.11613600	3.01081400	−1.13843400
Mg	1.13265700	0.32037700	−0.07864800	Mg	−1.04545800	0.08431800	−0.14280500
H	−1.65249600	−0.17522200	1.81926500	H	1.87913500	−0.70639400	−2.23660500
C	−3.49768100	0.30483600	0.85530100	C	3.39968600	0.23330200	−1.08869600
C	−4.20516700	0.92189000	−0.18831500	C	3.80012300	1.01700700	0.00435300
C	−4.22176100	−0.42444100	1.80778200	C	4.39347900	−0.36179900	−1.87742400
C	−5.59269100	0.80390100	−0.28319700	C	5.15233200	1.20125200	0.29746600
H	−3.67071100	1.50203000	−0.93810600	H	3.04580200	1.47900500	0.63606700
C	−5.61274500	−0.54587500	1.71919400	C	5.75076300	−0.18399500	−1.58720100
H	−3.69308600	−0.89989300	2.63196000	H	4.10311700	−0.97230900	−2.73115400
C	−6.30253300	0.06638900	0.67077100	C	6.13484300	0.59947700	−0.49695400
H	−6.12125900	1.28954200	−1.09983200	H	5.44113100	1.81301000	1.14902400
H	−6.15386700	−1.11765700	2.46905500	H	6.50411800	−0.65884400	−2.21143900
H	−7.38308700	−0.02549900	0.59767200	H	7.18786800	0.74027400	−0.26631300
C	−1.60964700	1.90713800	1.31860500	C	1.37826000	1.35968600	−2.07017400
H	−2.15278400	2.23841500	2.21019900	H	2.00590000	1.66575400	−2.91481900
H	−0.53756200	2.00457000	1.51312200	H	0.35620800	1.22011900	−2.43973200
H	−1.87515300	2.58279300	0.49681900	H	1.37529400	2.17835500	−1.34239100

Tabelle 8.141 Standardorientierung von **$MgBu_2$−Addukt mit R = Ph, R′ = H** und **$MgBu_2$−Addukt mit R = Ph, R′ = H (ÜZ)** [B3LYP/6−31+G(d)].

$MgBu_2$−Addukt mit R = Ph, R' = H				**ÜZ**			
C	0.65632500	2.46151400	2.35298600	**C**	0.79942400	2.41941300	1.98619700
C	−0.21469000	1.18981300	2.28414900	**C**	0.29376900	0.96437100	1.98505600
C	−2.36340500	−1.62499400	1.99178900	**C**	−2.21261700	−1.94515100	1.83492600
C	−3.66152700	−0.93151300	1.57333000	**C**	−3.56810100	−1.41313200	1.36616900
C	2.78836400	−3.11709200	1.28174500	**C**	3.10882000	−2.64209000	1.45646600
C	−0.19822200	−2.49537600	1.33281700	**C**	0.07308500	−2.56183100	1.27360900
N	1.58131300	−0.58246500	0.09182700	**N**	1.50924300	−0.49755100	−0.06190100
N	−1.40739000	−1.77164700	0.85611600	**N**	−1.19490700	−1.96956900	0.74266800
Si	1.38322200	−2.36343500	0.27050700	**Si**	1.68433300	−2.20834800	0.28868500
C	−4.34666000	−1.68447700	0.42691200	**C**	−4.10671700	−2.23692300	0.18940200
C	−2.05700400	−2.53091500	−0.24487800	**C**	−1.70552700	−2.79892900	−0.38726100
C	−3.35667000	−1.88112900	−0.72734800	**C**	−3.05314400	−2.30667800	−0.92306000
C	1.32599200	−3.18687200	−1.42043300	**C**	1.89249100	−3.23893600	−1.28361400
C	−1.27335500	1.13502500	−1.60216100	**C**	−1.66692800	1.21067100	−1.46100900
C	−2.53060200	2.02784400	−1.58319000	**C**	−3.03750100	1.83840900	−1.14201300
H	0.22536200	3.24356600	1.70660800	**H**	0.35080400	2.97119800	1.14471000
H	1.65767100	2.26400400	1.92868100	**H**	1.88302200	2.42894900	1.79204800
H	−1.18951100	1.42280100	2.75367300	**H**	−0.79188500	0.98252400	2.23109300
H	1.78055700	−0.17692100	1.01034500	**H**	1.12297600	0.15847400	0.92078000
H	0.23118800	0.43254900	2.96349800	**H**	0.73320500	0.42243200	2.84052200
H	−1.85868800	−1.05122700	2.77401500	**H**	−1.81315500	−1.32665600	2.64515400
H	−2.59091600	−2.62801600	2.39870200	**H**	−2.33006200	−2.96996700	2.23035000
H	−4.31866000	−0.86519400	2.44963300	**H**	−4.26404000	−1.43718300	2.21419100
H	−3.44316000	0.10016700	1.26552800	**H**	−3.47170000	−0.36052900	1.06724900
H	2.87429300	−2.65476500	2.27301300	**H**	3.04966800	−2.07706700	2.39488200
H	2.63532200	−4.19396200	1.43199500	**H**	3.10904000	−3.71153400	1.70736200
H	3.75041900	−2.99110100	0.76991100	**H**	4.07729500	−2.41646100	0.99297100
H	0.07700500	−2.05982300	2.30336700	**H**	0.24443900	−2.11359400	2.26083600
H	−0.44233800	−3.55427300	1.54123900	**H**	−0.07000400	−3.64217100	1.45247000
H	−4.69527700	−2.66373500	0.78877900	**H**	−4.34943900	−3.25309900	0.53491600
H	−5.23338500	−1.13892500	0.08224700	**H**	−5.03747800	−1.80052000	−0.19213000
H	−2.26347900	−3.56002700	0.10606900	**H**	−1.80028600	−3.84375500	−0.04026600

H	−1.34974300	−2.60740900	−1.07444800	H	−0.95365600	−2.79201600	−1.18182300
H	−3.12386000	−0.91465800	−1.18795800	H	−2.92672000	−1.31618300	−1.37632000
H	−3.79019900	−2.51641400	−1.51049500	H	−3.37481700	−2.98600300	−1.72272800
H	2.31443000	−3.15463900	−1.89388900	H	2.87911700	−3.04940300	−1.72494500
H	1.05022800	−4.24302900	−1.30303400	H	1.83467600	−4.31282100	−1.06128200
H	0.61441000	−2.72945500	−2.11442700	H	1.14664400	−3.01145900	−2.05338200
H	−0.43857400	1.73723400	−2.00614400	H	−0.97601300	2.02426000	−1.74791800
H	−1.42057900	0.33422200	−2.35283200	H	−1.76395600	0.60179100	−2.37944400
H	−2.39192400	2.85052600	−0.86213300	H	−2.95962700	2.47806900	−0.24719400
H	−3.40064100	1.46090800	−1.20699100	H	−3.76788600	1.05457500	−0.87671800
C	0.85322500	3.05942000	3.75931300	C	0.52849000	3.20513400	3.28110300
H	1.29342900	2.29132000	4.41392400	H	0.98438300	2.66764700	4.12634600
H	−0.13464000	3.28928100	4.18579000	H	−0.55484500	3.21207600	3.47458200
C	1.72952000	4.31903800	3.78343800	C	1.05216500	4.64685800	3.24665000
H	1.29564100	5.11488100	3.16349900	H	0.58822000	5.21734100	2.43126900
H	1.84484600	4.71570600	4.80052400	H	0.84217100	5.17648000	4.18457300
H	2.73467400	4.11043900	3.39223000	H	2.13837900	4.67008200	3.08731900
C	−2.92621900	2.64573600	−2.93816300	C	−3.64831600	2.68029900	−2.27818100
H	−3.08585400	1.83487800	−3.66532500	H	−3.74588600	2.04860600	−3.17408200
H	−2.07708900	3.23193000	−3.31998000	H	−2.94084900	3.47867000	−2.54635600
C	−4.17645300	3.53357600	−2.87507200	C	−5.01073000	3.29503100	−1.93133700
H	−4.42599200	3.95695000	−3.85673500	H	−5.41342600	3.88591800	−2.76396000
H	−5.04996000	2.96525700	−2.52723300	H	−5.74804700	2.51716100	−1.68993800
H	−4.03196500	4.37095800	−2.17920000	H	−4.93557400	3.95850800	−1.05935100
Mg	−0.58267400	0.37712600	0.29758500	Mg	−0.58991400	0.10487700	0.01297700
C	2.51016700	−0.04092700	−0.86937400	C	2.47394300	0.17510000	−0.87483000
C	2.17018900	0.00594000	−2.22790800	C	3.68160800	0.64617400	−0.32600100
C	3.75183100	0.46601400	−0.45804600	C	2.23017200	0.40966600	−2.23988900
C	3.06973100	0.52912600	−3.15908900	C	4.61145400	1.32611700	−1.11565600
H	1.19009600	−0.33332200	−2.54667300	H	3.87952500	0.48151900	0.73034200
C	4.64058200	1.00506000	−1.39106600	C	3.16389700	1.08471400	−3.02967600
H	4.01985300	0.44298700	0.59641100	H	1.29483300	0.06624700	−2.67498100
C	4.30787200	1.03085900	−2.74796000	C	4.36025100	1.54654800	−2.47328300
H	2.78811700	0.56401800	−4.20835200	H	5.53464500	1.68546900	−0.66675100
H	5.59487900	1.40150100	−1.05368100	H	2.95034300	1.25571500	−4.08220700
H	4.99958400	1.44816100	−3.47462700	H	5.08400100	2.07587900	−3.08747000

Tabelle 8.142 Standardorientierung von **$MgBu_2$−Addukt mit R = Me, R′ = H** und **$MgBu_2$−Addukt mit R = Me, R′ = H (ÜZ)** [B3LYP/6−31+G(d)].

$MgBu_2$−Addukt mit R = Me, R’ = H				**ÜZ**			
C	0.98770500	3.34238300	0.50889000	C	0.42718000	3.40496400	0.43632200
C	0.69751900	1.99566500	1.20439600	C	0.51115900	1.93684300	0.89302700
C	0.10375200	−1.23980200	2.60111400	C	−0.03201500	−1.59031400	2.29093100
C	−1.36639700	−1.00082500	2.95081900	C	−1.53374200	−1.88366500	2.30350700
C	4.23316800	−1.74610500	−0.86935900	C	4.58922900	−0.09363400	−0.04590000
C	1.74178900	−1.78728000	0.89379700	C	2.02137400	−1.36954900	0.99991200
N	1.79309000	0.05721100	−1.32433600	N	1.76943300	0.48825100	−1.12092200
N	0.29966500	−1.52529500	1.15095400	N	0.54297300	−1.59714800	0.91329600
Si	2.35017700	−1.58557900	−0.90712500	Si	2.89121300	−0.73354800	−0.59388600
C	1.68565000	0.47590400	−2.74151700	C	1.97182900	1.23790100	−2.36960000
C	−2.23529200	−2.19722000	2.54486700	C	−1.83986400	−3.22582300	1.62708100
C	−0.51108200	−2.70983100	0.76284200	C	0.27480500	−2.91608800	0.27202400
C	−2.00079000	−2.53099000	1.06658000	C	−1.21730200	−3.25913500	0.22543700
C	1.63392700	−2.78312200	−2.17435100	C	3.18958600	−2.07518900	−1.90204200
C	−1.79731600	0.26090300	−1.44768600	C	−2.04209700	0.07749600	−1.51370300
C	−3.17118100	0.79339300	−0.99261300	C	−3.40080400	0.17230100	−0.79262600
H	0.06514300	3.72803300	0.04412500	H	−0.35286500	3.50880000	−0.33482900
H	1.69158400	3.19810500	−0.33270200	H	1.37004100	3.68621100	−0.06070100
H	0.01208000	2.19358800	2.04986400	H	−0.45268900	1.68212300	1.38656600
H	2.30909300	0.76874000	−0.80272300	H	1.32761300	1.22501900	−0.18317900

H	1.63476600	1.65491800	1.69254000	H	1.25075200	1.85098700	1.70852500
H	0.69975600	−0.35615700	2.84588900	H	0.17486800	−0.60897500	2.73008500
H	0.49597400	−2.08971500	3.19021300	H	0.50000400	−2.34326700	2.89965500
H	−1.44167400	−0.80658000	4.02820300	H	−1.88055200	−1.88083500	3.34456700
H	−1.71733500	−0.09214200	2.44282700	H	−2.07564000	−1.07834400	1.78940100
H	4.68940900	−1.04151800	−0.16277000	H	4.49961900	0.68198400	0.72458400
H	4.53998400	−2.75741600	−0.57142300	H	5.21591700	−0.90036800	0.35787900
H	4.66725700	−1.55262900	−1.85840500	H	5.13388300	0.34441700	−0.89234900
H	2.31222200	−1.03993900	1.46347600	H	2.17606900	−0.57165100	1.73755900
H	2.03578700	−2.76726900	1.31395000	H	2.50930800	−2.26787900	1.41689400
H	−1.97511700	−3.06653300	3.16773600	H	−1.42585800	−4.04438200	2.23487800
H	−3.29567900	−1.98317100	2.72562200	H	−2.92260200	−3.38928900	1.56923600
H	−0.12508600	−3.59649900	1.30124500	H	0.81895300	−3.69670600	0.83386800
H	−0.36748300	−2.89019900	−0.30548600	H	0.69551300	−2.89595500	−0.73790200
H	−2.40104200	−1.73102300	0.43355500	H	−1.73595400	−2.54740700	−0.42846200
H	−2.52431200	−3.45432400	0.78685600	H	−1.32997300	−4.25187600	−0.22861400
H	2.17478500	−2.70250400	−3.12583200	H	3.85366900	−1.69624500	−2.69005900
H	1.73786800	−3.81971100	−1.83004000	H	3.67847800	−2.95701000	−1.46671500
H	0.57357400	−2.60089700	−2.38030900	H	2.26580700	−2.40738400	−2.38990300
H	−1.51195300	0.81356700	−2.36381700	H	−1.95970500	0.93920100	−2.20216700
H	−1.92494600	−0.78417500	−1.79284600	H	−2.06031700	−0.80180100	−2.18408600
H	−3.08031000	1.85107200	−0.69417900	H	−3.41947500	1.05781500	−0.13574100
H	−3.50474400	0.26724800	−0.08061600	H	−3.53748700	−0.69160300	−0.11950300
C	1.56549700	4.45120900	1.40976300	C	0.14728900	4.42689400	1.55191600
H	2.49620000	4.08588700	1.87036600	H	0.92735300	4.33443200	2.32257700
H	0.86615700	4.62778700	2.24039500	H	−0.80046300	4.16566700	2.04611100
C	1.83758100	5.77150200	0.67622800	C	0.08456200	5.87773300	1.05696900
H	0.91598000	6.17831900	0.23887200	H	−0.70958800	6.00775800	0.30991300
H	2.25088800	6.53437300	1.34871900	H	−0.11467100	6.57724100	1.87865500
H	2.55455600	5.62925000	−0.14413200	H	1.03084900	6.17770100	0.58730400
C	−4.30280100	0.68714400	−2.03295000	C	−4.62863400	0.24119100	−1.72021300
H	−4.40993400	−0.36629400	−2.33411900	H	−4.62769300	−0.64285600	−2.37551400
H	−4.00117900	1.23163100	−2.94035800	H	−4.52153500	1.11094700	−2.38519700
C	−5.65458000	1.21997200	−1.53852300	C	−5.96628600	0.32721200	−0.97333900
H	−6.43487500	1.12763500	−2.30524900	H	−6.81591500	0.37847500	−1.66626400
H	−5.99541100	0.67089100	−0.65013700	H	−6.11783600	−0.54843400	−0.32746100
H	−5.58482400	2.28051000	−1.26157300	H	−6.00598200	1.21863400	−0.33296800
Mg	−0.13177700	0.44561100	−0.07844900	Mg	−0.21716000	0.10169500	−0.40584800
H	1.27363900	1.48817700	−2.79549200	H	1.18459700	1.99497800	−2.48367500
H	2.65190200	0.46624100	−3.26559500	H	2.93587900	1.76907400	−2.39866800
H	0.99395900	−0.18731800	−3.26561900	H	1.92212800	0.58758600	−3.25456500

Tabelle 8.143 Standardorientierung von **65·MgBu₂** und **65·MgBu₂ (ÜZ)** [B3LYP/6−31+G(d)].

65·MgBu₂				**ÜZ**			
C	0.02683200	3.29382800	−1.08282500	C	−0.67344700	3.17779000	−0.94665500
C	0.10321400	1.83690200	−1.58615100	C	−0.52579300	1.68619900	−1.29844700
C	0.54492100	−1.57037700	−2.61839000	C	0.86124900	−1.77101100	−2.34491800
C	2.07237200	−1.64649100	−2.56590400	C	2.37646700	−1.80711300	−2.13585100
C	−4.36958600	−0.99568300	−0.49040600	C	−4.21168000	−0.95993200	−0.82888300
C	−1.55804000	−1.62584700	−1.41229600	C	−1.36431100	−1.80099100	−1.35524400
C	−3.46992000	1.55032600	2.15410100	C	−3.57060900	1.43631100	1.82175500
N	−1.83217300	0.29757000	0.69517300	N	−1.73524000	0.13490100	0.68143100
N	−0.07729200	−1.65732600	−1.26600200	N	0.10302600	−1.77713800	−1.05936700
Si	−2.59955000	−1.21940500	0.14087300	Si	−2.56215800	−1.26838000	0.05760400
C	−2.04092600	1.01073700	1.99673700	C	−2.11150100	0.95259100	1.85612400
C	2.53906900	−2.92951400	−1.86733900	C	2.79066100	−3.02694100	−1.30304500
C	0.34732200	−2.91737200	−0.60085100	C	0.47942500	−2.98363100	−0.26945700
C	1.86937500	−3.04323000	−0.49320500	C	1.98459800	−3.06714100	0.00190700
C	−2.59524800	−2.57298200	1.45605400	C	−2.86476900	−2.66029400	1.31324100
C	1.78471900	0.09594000	1.57445000	C	2.01529600	0.49097700	1.49166000

C	3.26439600	0.41229300	1.27575800	C	3.42701100	0.73946000	0.92608000
C	−1.62515200	0.16055100	3.19917500	C	−1.79736300	0.25481800	3.18964200
H	0.91719200	3.52304400	−0.47443300	H	0.01596600	3.43681100	−0.12737200
H	−0.82896800	3.41899200	−0.39342500	H	−1.68467200	3.35956200	−0.54772200
H	0.94985100	1.77130400	−2.29636100	H	0.49779000	1.53769500	−1.70946600
H	−1.97002900	0.99246500	−0.04627400	H	−1.32461300	0.88871800	−0.25840500
H	−0.78875800	1.64830000	−2.21979800	H	−1.18128800	1.44855400	−2.15444200
H	0.22586700	−0.62465400	−3.06567900	H	0.56827700	−0.87199500	−2.89709600
H	0.15204600	−2.39223300	−3.24551400	H	0.54588400	−2.64340400	−2.94484500
H	2.45871000	−1.59296500	−3.59160500	H	2.86366400	−1.81999900	−3.11905700
H	2.46521500	−0.76814200	−2.03579300	H	2.70453700	−0.88658600	−1.63441700
H	−4.43628400	−0.20281600	−1.24588700	H	−4.13302100	−0.13314600	−1.54548500
H	−4.73963100	−1.92182600	−0.95057200	H	−4.53476600	−1.85315800	−1.38166600
H	−5.05848500	−0.73694700	0.32234800	H	−5.01134000	−0.70903200	−0.12165900
H	−1.79224800	−0.82708800	−2.12957100	H	−1.53646300	−1.07710600	−2.16180300
H	−1.91439700	−2.56165100	−1.88314500	H	−1.63996900	−2.78699700	−1.76977800
H	−3.76375100	2.16381600	1.29372500	H	−3.79608800	1.93658600	0.87341800
H	−4.19568700	0.73344700	2.25464300	H	−4.27013600	0.59808700	1.94015700
H	−3.54575600	2.17612000	3.05181400	H	−3.76461300	2.14518200	2.63682800
H	2.27160500	−3.80083900	−2.48445500	H	2.60402300	−3.94457300	−1.88095200
H	3.63089800	−2.93692700	−1.76354300	H	3.86566300	−2.99971600	−1.08855800
H	−0.05990100	−3.77539500	−1.16909200	H	0.14827200	−3.88217400	−0.82083700
H	−0.09976700	−2.94710100	0.39622400	H	−0.07801000	−2.96191300	0.67182000
H	2.24521600	−2.25745900	0.17187100	H	2.28579300	−2.23493000	0.64995000
H	2.10525400	−4.00583000	−0.02137100	H	2.18512000	−3.99288300	0.55616700
H	−3.41760500	−2.43240400	2.16777000	H	−3.71020700	−2.41490400	1.96876300
H	−2.75109800	−3.54605600	0.97182100	H	−3.12131200	−3.59452800	0.79500700
H	−1.66404700	−2.62798200	2.02778300	H	−2.00042500	−2.85801900	1.95688100
H	1.44571300	0.80236100	2.35687600	H	1.71197100	1.39043400	2.05941300
H	1.72955000	−0.89626600	2.06284300	H	2.07904900	−0.30339200	2.25862200
H	3.34696900	1.40824500	0.80971200	H	3.39666800	1.54344700	0.17186200
H	3.66133600	−0.29082900	0.52210000	H	3.78385700	−0.15372400	0.38509300
H	−2.32763100	−0.65952100	3.38147900	H	−2.42906600	−0.62965600	3.33563100
H	−0.62160500	−0.25288700	3.06413600	H	−0.74910300	−0.06260400	3.22742900
H	−1.61335700	0.78671900	4.09859400	H	−1.97533100	0.93431800	4.03316900
C	−0.09577000	4.37199800	−2.17649100	C	−0.43184800	4.15430700	−2.11103200
H	−0.99097800	4.16244300	−2.78204500	H	−1.12404000	3.90943800	−2.93071400
H	0.76037900	4.27779800	−2.86118400	H	0.58073000	3.99060800	−2.50939300
C	−0.16545400	5.80646400	−1.63557600	C	−0.59681600	5.62929000	−1.72250400
H	0.72967200	6.05232100	−1.04870200	H	0.10531000	5.90987100	−0.92625500
H	−0.24408200	6.54338800	−2.44547400	H	−0.41504100	6.29508300	−2.57561700
H	−1.03575200	5.94185400	−0.97883400	H	−1.61119400	5.83148700	−1.35355000
C	4.20841500	0.37629500	2.49298800	C	4.49521400	1.10979100	1.97225900
H	4.15162700	−0.62023500	2.95695500	H	4.54389300	0.31091800	2.72747000
H	3.83592300	1.08370400	3.24906500	H	4.16812300	2.01331600	2.50778800

Tabelle 8.144 Standardorientierung von **66·MgBu$_2$** und **66·MgBu$_2$ (ÜZ)** [B3LYP/6−31+G(d)].

66·MgBu$_2$				**ÜZ**			
C	0.41221500	3.29567300	−1.14903800	C	−0.47696600	3.10770700	−1.09603800
C	0.31780700	1.81605600	−1.57279700	C	−0.52567200	1.59364300	−1.36119100
C	0.82381600	−1.54382500	−2.60259900	C	1.16779600	−1.82471200	−2.26061000
C	2.32591700	−1.70823200	−2.36872200	C	2.65639300	−1.89824400	−1.91488300
C	−4.25943400	−0.71651200	−1.12161600	C	−4.03877600	−1.02701500	−1.22489500
C	−1.40600000	−1.50321700	−1.66501100	C	−1.13907500	−1.79098900	−1.50096200
C	−3.82635800	0.97196700	2.04905700	C	−3.62968000	1.56229800	1.28235800
N	−1.89447700	0.27297800	0.58494200	N	−1.76651600	0.02794500	0.62075300
N	0.03811400	−1.63228700	−1.33789900	N	0.28811800	−1.78433200	−1.05573900
C	−1.63285100	2.18170600	2.11396400	C	−1.36498100	1.76930300	2.33443100
Si	−2.63372500	−1.13569700	−0.24671100	Si	−2.47972100	−1.35392800	−0.19118900
C	−2.29722400	0.80360400	1.94214700	C	−2.39104700	0.77125600	1.75924200

C	2.63133000	−3.04388700	−1.68081900	C	2.95651000	−3.10054200	−1.00968200
C	0.30541200	−2.93669800	−0.67722700	C	0.56211700	−2.97679600	−0.20444000
C	1.79385800	−3.17143700	−0.40215100	C	2.03159000	−3.07672200	0.21337400
C	−2.93373900	−2.61043400	0.89396500	C	−2.86739800	−2.87634000	0.88248200
C	1.73944200	−0.02699400	1.66553400	C	2.04364500	0.59710400	1.46965000
C	3.24789800	0.17334300	1.41355000	C	3.49537300	0.64789000	0.95765800
C	−1.79211500	−0.13893400	3.04631000	C	−2.80850400	−0.17982700	2.89808000
H	1.28807000	3.44192400	−0.49512200	H	0.29292200	3.33415700	−0.34103900
H	−0.45769800	3.57175000	−0.52839600	H	−1.43048100	3.43129800	−0.64830700
H	1.17165900	1.61564000	−2.24998300	H	0.43315900	1.30468300	−1.84687500
H	−1.95670700	1.06019400	−0.06997700	H	−1.32816200	0.82916600	−0.28856700
H	−0.56967200	1.70559300	−2.23055500	H	−1.27224300	1.39253700	−2.14904100
H	0.61005300	−0.57223600	−3.05584600	H	0.95268300	−0.93201300	−2.85699100
H	0.46732100	−2.32687600	−3.29771000	H	0.88324500	−2.70157500	−2.86946900
H	2.83943700	−1.63725400	−3.33590400	H	3.22620500	−1.96126200	−2.85075900
H	2.69484300	−0.87648800	−1.75344300	H	2.96871100	−0.97222800	−1.41636700
H	−4.15867400	0.17074500	−1.75945800	H	−3.93290200	−0.13021500	−1.84724000
H	−4.57752900	−1.54805500	−1.76484700	H	−4.24450700	−1.87623000	−1.89159000
H	−5.07029500	−0.52387700	−0.41004000	H	−4.92665000	−0.89113300	−0.59532000
H	−1.50340300	−0.65503800	−2.35581000	H	−1.22835600	−1.03985400	−2.29516000
H	−1.74970900	−2.39028200	−2.23101600	H	−1.37116900	−2.76269100	−1.97398700
H	−4.20910000	1.62943200	1.25890600	H	−3.36046900	2.25468800	0.47669500
H	−4.34695800	0.00989100	1.97543400	H	−4.41197000	0.89396000	0.90588200
H	−4.09638100	1.41635100	3.01468400	H	−4.05970300	2.14876100	2.10445400
H	−1.96137000	2.88279000	1.33646100	H	−1.01382800	2.47183000	1.57168900
H	−1.90201700	2.61172200	3.08521900	H	−1.81748300	2.35780700	3.14179100
H	−0.54162300	2.10735500	2.06918100	H	−0.49547400	1.24781300	2.75055700
H	2.39196900	−3.87118400	−2.36619900	H	2.79825600	−4.03282600	−1.57258700
H	3.69980600	−3.12389800	−1.44682300	H	4.00748700	−3.09279300	−0.69680900
H	−0.08726500	−3.74820100	−1.31919100	H	0.26798700	−3.88432400	−0.76210400
H	−0.25415500	−2.96579000	0.26126900	H	−0.08077300	−2.92139500	0.67875400
H	2.13982500	−2.44622200	0.34239600	H	2.28669600	−2.22461900	0.85562200
H	1.90866900	−4.16870000	0.04215800	H	2.15914300	−3.98406200	0.81739500
H	−3.79601300	−2.43994800	1.54932000	H	−3.86101600	−2.79830700	1.33987400
H	−3.16905300	−3.48642100	0.27464100	H	−2.87532100	−3.77651100	0.25230700
H	−2.07953600	−2.87140700	1.52546300	H	−2.14722100	−3.03981800	1.69148000
H	1.43730200	0.69438600	2.44872800	H	1.78479500	1.60420200	1.84469300
H	1.59088300	−1.01676800	2.13873100	H	2.01400400	−0.04207600	2.37243900
H	3.42370200	1.17508800	0.98756600	H	3.55816600	1.28153300	0.05688500
H	3.60695300	−0.53205200	0.64352200	H	3.82355200	−0.35371100	0.63346000
H	−2.28755900	−1.11346300	3.01237400	H	−3.61863200	−0.85183300	2.59558400
H	−0.71185600	−0.29108800	2.96679000	H	−1.96077400	−0.79165700	3.22756200
H	−2.00334200	0.29974300	4.02859900	H	−3.16651700	0.39553700	3.76129500
C	0.50740900	4.31130600	−2.30393300	C	−0.20856900	3.98279600	−2.33340300
H	−0.36875600	4.18826200	−2.95913200	H	−0.97693800	3.77200600	−3.09226100
H	1.38336900	4.06136500	−2.92114000	H	0.75095000	3.68336000	−2.78090200
C	0.60452900	5.77215900	−1.84400000	C	−0.18508600	5.48634100	−2.02885200
H	1.48929700	5.93001800	−1.21271000	H	0.59786500	5.73040000	−1.29868600
H	0.67573300	6.46310800	−2.69413300	H	0.00607400	6.07948400	−2.93199800
H	−0.27542900	6.06223200	−1.25370100	H	−1.14296600	5.82029800	−1.60819900
C	4.15330500	0.01531500	2.65018100	C	4.52754600	1.16823900	1.97608900
H	3.99994500	−0.98777400	3.07690100	H	4.48418500	0.53862400	2.87754400
H	3.82286100	0.72583600	3.42257800	H	4.23098300	2.17763600	2.29714700
C	5.64555900	0.22775800	2.36128400	C	5.96477300	1.20095100	1.43953800
H	6.25680800	0.10623400	3.26504800	H	6.67049700	1.57790600	2.19081500
H	6.01140500	−0.49034500	1.61463600	H	6.30099500	0.19805800	1.14285400
H	5.83309300	1.23529300	1.96642500	H	6.04343400	1.84867300	0.55595900
Mg	0.42442800	0.27675200	−0.02997700	Mg	0.38554100	0.09319800	0.21045000

Tabelle 8.145 Standardorientierung von **90 (R = ^{i}Pr, R′ = Me)** und **Ligand mit R = Me, R′ = Me** [B3LYP/6−31+G(d)].

90 (R = ^{i}Pr, R′ = Me)				Ligand: R = Me, R′ = Me			
C	2.15142000	−0.90600300	0.91473600	C	1.67795400	1.24330000	−0.46338800
C	3.18106000	−1.46983300	−0.07748700	C	2.91152700	1.23678800	0.45239100
C	−2.38882700	−0.42593300	2.15305300	C	−2.99872100	1.56986400	−0.76987500
C	0.37383800	0.75567300	1.29095300	C	−0.30574300	0.00468200	−1.22866300
C	−2.63262700	−2.28575400	−1.29971800	N	−1.64307600	−0.14811400	1.33995700
N	−1.44348200	−0.15475200	−0.75423600	N	0.87501500	0.00453200	−0.31446300
N	1.34627400	0.18613000	0.31194000	Si	−2.01983400	−0.00372100	−0.34706100
Si	−1.49022000	0.58584600	0.81648100	C	−2.54206100	0.00030700	2.47359600
C	−2.45929900	−0.78451800	−1.60017200	C	3.77130900	−0.01054300	0.26352000
C	4.07200400	−0.38371100	−0.67466200	C	1.66531100	−1.24435400	−0.45604800
C	2.16157900	1.25668300	−0.31600000	C	2.89683200	−1.24620600	0.46198200
C	3.18646500	0.68646200	−1.30793300	C	−3.07711500	−1.46135400	−0.94216000
C	−2.30229300	2.30124800	0.82036000	H	−0.65657600	−0.01724000	1.54652400
C	−3.80133900	−0.04803500	−1.51387400	H	2.03711400	1.32051300	−1.51292000
H	−0.49079300	−0.43355600	−0.98555200	H	3.49295200	2.14628200	0.25276100
H	2.70964400	−0.50628000	1.78908500	H	2.57446600	1.29553300	1.49785400
H	3.78236800	−2.22598300	0.44385200	H	−2.46691400	2.47926500	−0.46491200
H	2.64438100	−1.98928500	−0.88513200	H	−3.19715300	1.64069200	−1.84829400
H	−1.97807900	−1.43879100	2.24399500	H	−3.97322400	1.57483500	−0.26322000
H	−2.30311600	0.06138500	3.13459300	H	−0.25676300	0.87413400	−1.89823600
H	−3.46069000	−0.52299300	1.93644100	H	−0.24873600	−0.85619800	−1.90892900
H	0.51998800	0.28464200	2.27162300	H	4.20159500	−0.01711200	−0.74926100
H	0.60421800	1.81582600	1.46899500	H	4.61474500	−0.01233700	0.96637100
H	−1.67384700	−2.81142000	−1.38501600	H	2.55774500	−1.29362300	1.50729900
H	−3.00889800	−2.43708700	−0.28033900	H	3.46795300	−2.16370500	0.26964300
H	−3.33805700	−2.75279000	−2.00051700	H	−4.03522900	−1.49834800	−0.40656500
H	4.69262000	0.06600800	0.11491600	H	−3.30990700	−1.37981400	−2.01265200
H	4.76097700	−0.80947400	−1.41590400	H	−2.57190300	−2.42029400	−0.77530700
H	2.64809100	0.25907700	−2.16664300	C	0.84697700	2.49702100	−0.14942400
H	3.79220300	1.51731700	−1.69237600	H	0.01034700	2.64576100	−0.83684900
H	−3.38050100	2.24159200	0.62728000	H	0.44440900	2.44309500	0.86933800
H	−2.17500800	2.78849200	1.79724400	H	1.48542200	3.38581600	−0.21890900
H	−1.86532200	2.95650300	0.05724000	C	0.82087100	−2.48946900	−0.14354000
H	−4.22674900	−0.10842600	−0.50345600	H	0.40397400	−2.42675200	0.86793300
H	−3.68678000	1.00933000	−1.77571100	H	−0.00964300	−2.63459400	−0.83953800
H	−4.52831700	−0.49626700	−2.20125400	H	1.45396400	−3.38282800	−0.20389600
C	1.26343100	−2.06201100	1.40072700	H	2.02704500	−1.32597300	−1.50443600
H	0.58130000	−1.77837100	2.20664600	H	−2.20338700	−0.60480700	3.32554900
H	0.66326600	−2.45682200	0.57244900	H	−2.64638600	1.04189800	2.82146400
H	1.89551500	−2.87249600	1.78276700	H	−3.54467100	−0.35724000	2.20923600
C	1.28460200	2.28067000	−1.05244000				
H	0.66986100	1.78350500	−1.81130000				
H	0.61581700	2.83383500	−0.38787500				
H	1.92632200	3.01596200	−1.55249700				
H	2.72540200	1.79250500	0.47855000				
H	−2.11236400	−0.69706300	−2.64202200				

Tabelle 8.146 Standardorientierung von **(*S*)−69 [R = CH(Me)(Ph), R′ = H]** und **116 (R = ^{t}Bu, R′ = Me)** [B3LYP/6−31+G(d)].

(*S*)−69 [R = CH(Me)(Ph), R′ = H]				116 (R = ^{t}Bu, R′ = Me)			
C	−3.44361200	−0.69536000	−1.49875400	C	−2.29853900	−0.15876600	1.28184000
C	−4.10778300	−1.93258400	−0.88629800	C	−3.25145300	1.03685300	1.12409500
C	1.00069800	2.27908800	−1.59588500	C	2.07820800	−1.82977900	1.75904600
C	−1.79719800	1.06418400	−1.18338700	C	−0.61923100	−1.59389900	0.20441000
N	0.34425700	0.22827000	0.55296200	C	2.69862800	1.98359700	1.24281400
N	−2.51468200	−0.05610500	−0.55765400	N	1.39658000	0.43356300	−0.20066600

Si	−0.20983100	1.65119600	−0.28109600	**N**	−1.49817200	−0.39644500	0.05414800
C	1.57565600	0.02102200	1.30391500	**Si**	1.28267900	−1.26896900	0.12500100
C	−4.82809300	−1.57972200	0.42191600	**C**	2.50102200	1.40409100	−0.17786200
C	−3.21031700	0.35082100	0.66833400	**C**	−4.14311800	0.91381100	−0.10832400
C	−3.87177600	−0.84166600	1.36817600	**C**	−2.31146500	−0.48390500	−1.18575000
C	−0.50914700	3.09356200	0.91436300	**C**	−3.25802100	0.71685500	−1.33621700
H	−0.24806500	−0.59127700	0.45649300	**C**	2.04489400	−2.35296900	−1.23340500
H	−2.87890100	−0.97696800	−2.39529600	**C**	3.80537400	0.73173000	−0.64055900
H	−4.22737600	0.02392100	−1.82158900	**H**	0.47542500	0.86813300	−0.15029400
H	−4.80918800	−2.36355200	−1.61284700	**H**	−2.91845200	−1.05802100	1.48924500
H	−3.33579000	−2.68981100	−0.69145800	**H**	−3.85443000	1.11794900	2.03784800
H	1.23576200	1.49665700	−2.32725100	**H**	−2.65388700	1.95767700	1.05272300
H	0.58599600	3.13976700	−2.13860500	**H**	1.67472000	−1.28218500	2.61941000
H	1.94953000	2.60361300	−1.14951100	**H**	1.89934800	−2.90101600	1.92846400
H	−1.46133400	0.72653100	−2.17360100	**H**	3.16608400	−1.68396800	1.75623800
H	−2.47620800	1.92342100	−1.37615200	**H**	−0.84088100	−2.09586500	1.15622100
H	−5.69088700	−0.93349600	0.19950400	**H**	−0.88254700	−2.34234700	−0.55593100
H	−5.22617900	−2.48362900	0.90089300	**H**	1.77809500	2.46894400	1.59015600
H	−3.98045200	1.11934500	0.43872500	**H**	2.94850700	1.18841600	1.95453600
H	−2.48164100	0.81592900	1.33981500	**H**	3.50425500	2.72981000	1.26520700
H	−3.08764800	−1.52992400	1.71274900	**H**	−4.82115500	0.05455900	0.00441800
H	−4.40466600	−0.48617500	2.25983100	**H**	−4.77518200	1.80435700	−0.22147700
H	0.42744600	3.39625700	1.40178400	**H**	−2.65727400	1.62250700	−1.50631100
H	−0.89111100	3.97411600	0.38041100	**H**	−3.86689500	0.56398100	−2.23668000
H	−1.22562000	2.84160200	1.70487700	**H**	3.13992300	−2.28902500	−1.24291300
H	1.85510900	0.97949100	1.76605700	**H**	1.78350100	−3.40924900	−1.07875900
C	2.77464300	−0.42569200	0.45638400	**H**	1.68717700	−2.05878800	−2.22734900
C	2.61813300	−1.26436100	−0.65459700	**H**	4.10136000	−0.08183000	0.03295400
C	4.07150600	−0.03280100	0.81597200	**H**	3.69551200	0.32054300	−1.65012100
C	3.72698000	−1.70355000	−1.38319600	**H**	4.62558500	1.45912200	−0.65325100
H	1.61809600	−1.56022800	−0.96128200	**C**	−1.40080700	0.09478400	2.50228500
C	5.18471100	−0.46554900	0.08975700	**H**	−0.75441500	−0.75152400	2.74913800
H	4.21300900	0.62543800	1.67251300	**H**	−0.76226200	0.96962600	2.33209800
C	5.01567900	−1.30633600	−1.01379100	**H**	−2.02610200	0.29302000	3.38104400
H	3.58403000	−2.35249600	−2.24427800	**C**	2.15796200	2.55199300	−1.14850800
H	6.18090800	−0.14164800	0.38204700	**H**	1.22000300	3.04187900	−0.85540000
H	5.87802300	−1.64264600	−1.58405700	**H**	2.94570700	3.31547200	−1.15232200
C	1.33494700	−0.98180100	2.44940200	**H**	2.03684500	2.16998800	−2.16845400
H	2.24443300	−1.13446500	3.04072300	**C**	−1.42733700	−0.56987900	−2.43909800
H	0.53856400	−0.62018500	3.10991100	**H**	−0.76248100	0.29906300	−2.49864600
H	1.03461500	−1.95702700	2.04390400	**H**	−0.80767800	−1.47004100	−2.47126900
				H	−2.06317000	−0.58132700	−3.33244600
				H	−2.93831200	−1.40121400	−1.14106000

Tabelle 8.147 Standardorientierung von **$[Bu_2Mg]_2$** und **66 (R = ^{t}Bu, R′ = H)** [B3LYP/6−31+G(d)].

$[Bu_2Mg]_2$				**66 (R = ^{t}Bu, R′ = H)**			
C	4.33551100	0.33186200	0.12044900	**C**	2.89728600	−0.53904100	−1.17980100
C	3.35211800	−0.84607700	−0.02567700	**C**	3.79426600	0.69987300	−1.09695400
C	−0.57397000	−1.71242400	−0.13795800	**C**	−2.12153700	−2.35055600	−1.02006600
C	0.25529600	−3.02522800	−0.21059700	**C**	0.78867700	−1.54283100	−0.50353800
H	4.12866900	0.88633000	1.05041700	**C**	−3.01274100	1.38140300	−1.55858300
H	4.18012100	1.06006400	−0.69223400	**N**	−1.23660200	0.44545200	−0.09272000
H	3.54141900	−1.57360400	0.78296100	**N**	1.69885700	−0.39974000	−0.34173400
H	3.58924100	−1.39789500	−0.95228100	**C**	−1.98625300	2.73653600	0.29746500
H	−1.26383100	−1.83164400	0.72111300	**Si**	−1.01810500	−1.27179400	0.08883300
H	−1.24704300	−1.72595800	−1.01841600	**C**	−2.41869600	1.32054400	−0.13176600
H	0.91651900	−3.10908400	0.66674400	**C**	4.18900400	0.99576900	0.35581800
H	0.93068700	−3.00366500	−1.08095400	**C**	2.06319000	−0.18046500	1.06258200
C	5.82093400	−0.07308200	0.12448300	**C**	2.93514700	1.06827200	1.23628200
H	6.04438000	−0.61261300	−0.80791100	**C**	−1.29107100	−1.88444000	1.86436400

H	5.99015600	−0.79283000	0.93921500	C	−3.48811100	0.80427400	0.84682200
C	6.78336300	1.11181200	0.27692800	H	−0.40251200	0.88856200	−0.47402000
H	6.60409500	1.65021300	1.21719300	H	2.57120100	−0.69839200	−2.21434100
H	7.83081500	0.78475500	0.27646800	H	3.48011000	−1.43761000	−0.88167900
H	6.66012900	1.83192500	−0.54307200	H	4.68538800	0.54321900	−1.71902300
C	−0.59527600	−4.30473100	−0.29451100	H	3.25233300	1.55922600	−1.51554900
H	−1.24797200	−4.23958100	−1.17698500	H	−2.03679400	−2.06348800	−2.07548300
H	−1.26413400	−4.34351900	0.57732000	H	−1.83489700	−3.40832100	−0.93696900
C	0.24104200	−5.58841100	−0.36312600	H	−3.18064300	−2.28417700	−0.74016900
H	−0.39770500	−6.47762900	−0.42612800	H	0.71622400	−1.75220000	−1.57999700
H	0.89878700	−5.58826300	−1.24195200	H	1.21166000	−2.46428700	−0.04786000
H	0.87646500	−5.69750800	0.52526400	H	−2.26003300	1.73989700	−2.27156600
Mg	1.28070400	−0.41198900	−0.03764900	H	−3.33790100	0.38706600	−1.88491300
C	−4.31496600	−0.35747800	−0.02771800	H	−3.87712800	2.05721200	−1.60763000
C	−3.37431100	0.86362900	0.00885600	H	−1.20931100	3.12582800	−0.37392500
C	0.56127700	1.77344600	0.06486200	H	−2.83169100	3.43487200	0.26816400
C	−0.26985100	3.08657600	0.10469300	H	−1.57996600	2.72342500	1.31523400
H	−4.11987600	−0.95971600	−0.92998000	H	4.84706400	0.19416900	0.72434200
H	−4.09964800	−1.02797400	0.82026300	H	4.76223900	1.92972400	0.41974000
H	−3.61540200	1.52810700	−0.83895800	H	2.60204300	−1.06640500	1.46426300
H	−3.60264700	1.46571800	0.90554300	H	1.14312200	−0.07194600	1.64517500
H	1.25733300	1.87706400	−0.79161000	H	2.34367500	1.95410800	0.96668500
H	1.22730900	1.80386600	0.94994900	H	3.20823300	1.17189100	2.29469900
H	−0.92491800	3.15213700	−0.77903100	H	−2.34839800	−1.82149500	2.15080700
H	−0.95135500	3.08166100	0.97046000	H	−0.99116200	−2.93712200	1.95922200
C	−5.81554100	−0.01384700	0.00353300	H	−0.71639800	−1.30458000	2.59599800
H	−6.02657900	0.57516400	0.90841100	H	−3.83207500	−0.20093200	0.57414000
H	−6.04782200	0.64326900	−0.84764600	H	−3.09679500	0.76845200	1.86963100
C	−6.72884800	−1.24623800	−0.03307700	H	−4.36486400	1.46239900	0.83679100
H	−6.56206300	−1.83618600	−0.94417100				
H	−7.78928900	−0.96523200	−0.00888700				
H	−6.53994600	−1.90508300	0.82494200				
C	0.57849800	4.36872200	0.16891200				
H	1.22573900	4.32136900	1.05649400				
H	1.25266600	4.39153300	−0.69939600				
C	−0.26006700	5.65218600	0.20744100				
H	0.37700400	6.54348800	0.25609400				
H	−0.92245100	5.66842700	1.08260000				
H	−0.89088000	5.74247300	−0.68632800				
Mg	−1.29388500	0.47169200	−0.01535000				

Tabelle 8.148 Standardorientierung von **65 (R = ^{i}Pr, R' = H)** und **Ligand mit R = Ph, R' = H** [B3LYP/6−31+G(d)].

65 (R = ^{i}Pr, R' = H)				**Ligand: R = Ph, R' = H**			
C	2.65909700	−0.55931700	−1.21143000	C	−3.38264800	0.01151400	−1.12469400
C	3.58536700	0.65949900	−1.15494800	C	−3.93148900	−1.41401900	−1.00981300
C	−2.40332100	−2.32380000	−0.84643700	C	1.05324400	2.97525400	−1.15089600
C	0.54513000	−1.51132600	−0.47617900	C	−1.58595800	1.53037200	−0.50570300
C	−2.52807800	2.38143400	0.98271100	N	0.84616900	0.06972500	−0.27525100
N	−1.50942500	0.49487900	−0.27592300	N	−2.16993100	0.19387700	−0.31331000
N	1.48853200	−0.39140500	−0.34001600	Si	0.25581300	1.70104000	−0.00254000
Si	−1.24457100	−1.17354300	0.11828200	C	−4.20645700	−1.78141500	0.45429900
C	−2.71118500	1.30927500	−0.10598900	C	−2.43946600	−0.09084600	1.10182700
C	4.02802300	0.94760400	0.28565500	C	−2.95776900	−1.51842600	1.30584800
C	1.89970500	−0.18417400	1.05221300	C	0.49994500	2.28367100	1.78248600
C	2.80222300	1.04532800	1.20312300	H	0.09576600	−0.57305200	−0.52293300
C	−1.52980500	−1.56865400	1.95516000	H	−3.12948300	0.23356400	−2.16792400
C	−3.14708000	1.94342600	−1.43774500	H	−4.16681700	0.73682200	−0.81908600
H	−0.67978700	1.01801300	−0.54537700	H	−4.84604600	−1.49792400	−1.61125300
H	2.30067500	−0.71080800	−2.23628300	H	−3.19775800	−2.11222600	−1.43571200

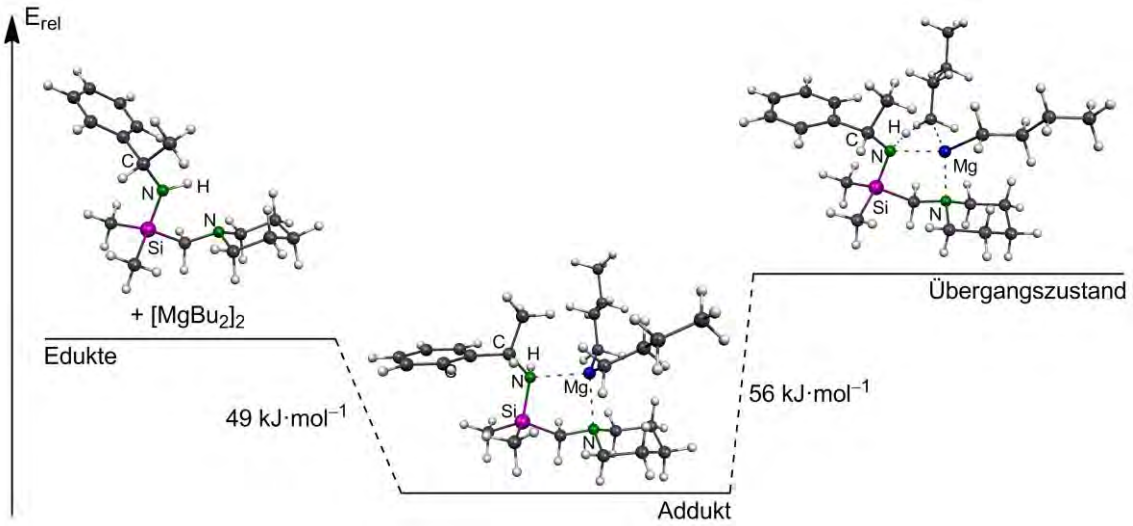
H	3.22953400	−1.47096400	−0.92893200	H	0.99405400	2.65354300	−2.19767100
H	4.45506900	0.48331300	−1.80160000	H	0.54330200	3.94471100	−1.06635700
H	3.05045000	1.52991500	−1.55936000	H	2.11085000	3.14412300	−0.91569900
H	−2.28843800	−2.18997300	−1.92904600	H	−1.61706600	1.74972000	−1.58187000
H	−2.20877600	−3.37916000	−0.61175000	H	−2.20263000	2.31754400	−0.02235500
H	−3.45535300	−2.12898200	−0.59889200	H	−5.04059700	−1.17107100	0.83226100
H	0.45152300	−1.73104500	−1.54873000	H	−4.51867800	−2.83016900	0.53887000
H	0.94705600	−2.43941400	−0.01507200	H	−3.17886000	0.63346100	1.50658600
H	−2.25910400	1.92129500	1.93992100	H	−1.51272700	0.05006400	1.66718100
H	−1.72302400	3.07486900	0.70362400	H	−2.16500000	−2.22723700	1.02971700
H	−3.44367400	2.97027300	1.12455100	H	−3.17255400	−1.67390900	2.37109000
H	4.67997300	0.13264600	0.63527000	H	1.56240300	2.41952000	2.01953100
H	4.62193400	1.86957000	0.33234800	H	0.00501500	3.25160200	1.93948400
H	2.43170300	−1.08242700	1.43599700	H	0.09011800	1.57518700	2.51136700
H	1.00177100	−0.06061600	1.66547000	C	2.10355700	−0.52297900	−0.17293100
H	2.22244700	1.94436000	0.95223500	C	3.25199900	0.21411300	0.17917500
H	3.10867500	1.14051200	2.25317400	C	2.25973700	−1.90187000	−0.42790600
H	−2.58161200	−1.40200000	2.22486400	C	4.49908200	−0.40588800	0.27068000
H	−1.30539400	−2.62163900	2.17356400	H	3.17154000	1.27876800	0.38015000
H	−0.91912700	−0.94979100	2.62261000	C	3.50883900	−2.51261400	−0.33403600
H	−2.36496300	2.61642000	−1.81491000	H	1.38726900	−2.49160000	−0.70377100
H	−3.31884900	1.17071200	−2.19485400	C	4.64330000	−1.77257100	0.01642300
H	−4.06744500	2.53027900	−1.32067700	H	5.36633600	0.19090600	0.54434500
H	−3.51549200	0.63414600	0.22067200	H	3.59473300	−3.57764300	−0.53774900
				H	5.61631000	−2.25024300	0.08875700

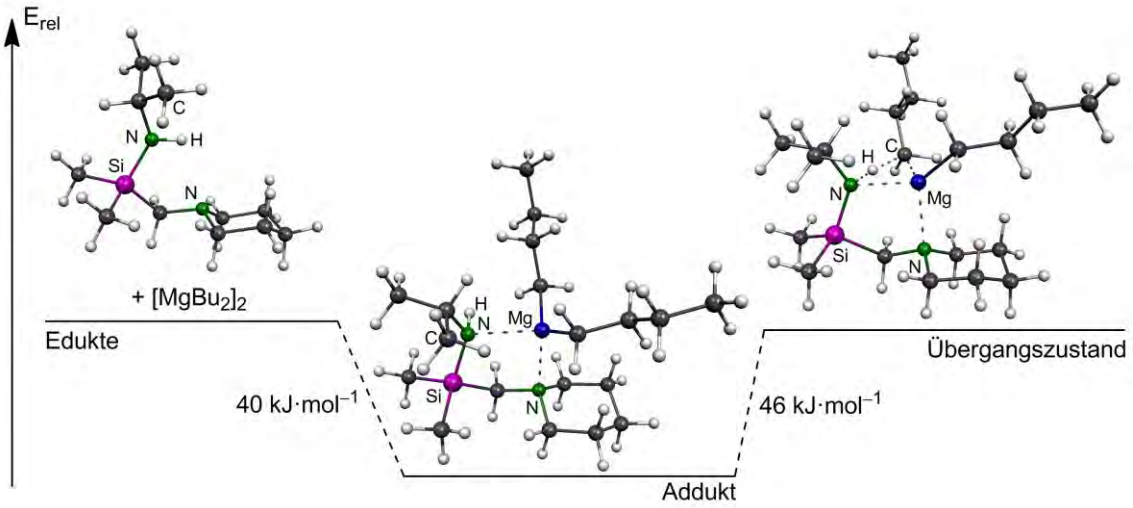
Tabelle 8.149 Standardorientierung von **BuH** und **Ligand mit R = Me, R′ = Me** [B3LYP/6−31+G(d)].

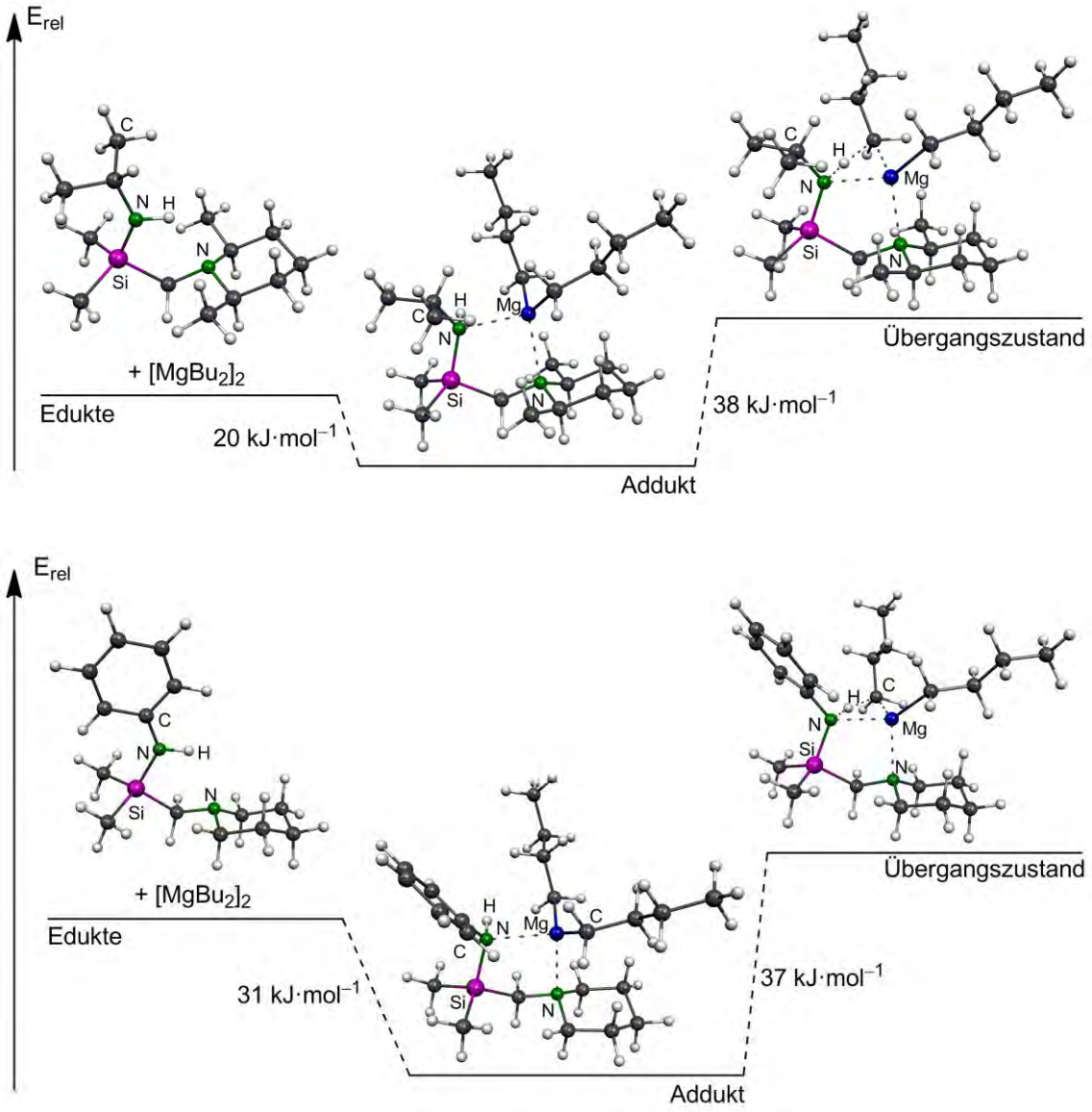
BuH				**Ligand: R = Me, R' = Me**			
C	1.96457700	−0.12112700	−0.00000200	C	2.17218300	−1.24595500	−0.63333000
H	2.11257800	−0.75302100	−0.88553900	C	3.37972300	−0.36911500	−0.98030500
H	2.11263900	−0.75287900	0.88562300	C	−3.18059800	−1.47374300	−0.55695600
H	2.75310800	0.64151600	−0.00009300	C	−0.16267400	−1.27708700	0.03154400
C	0.56913100	0.51456800	0.00000300	N	−1.60051200	1.11441700	−0.74886900
H	0.46482300	1.16804900	0.87896800	N	1.02504300	−0.44117500	−0.19404600
H	0.46481700	1.16803900	−0.87896800	Si	−1.83346000	−0.34610400	0.16257600
C	−0.56913100	−0.51456700	0.00000400	C	−2.61511200	2.07324300	−1.16138500
H	−0.46482200	−1.16804100	0.87897400	C	3.77269100	0.51988400	0.20711700
H	−0.46481900	−1.16804700	−0.87896200	C	1.36967600	0.36045500	0.98511200
C	−1.96457700	0.12112700	−0.00000300	C	2.54928800	1.29900100	0.70749800
H	−2.11260100	0.75296400	−0.88557500	C	−2.34533500	0.03432200	1.94831000
H	−2.75310800	−0.64151700	−0.00002300	H	−0.72281000	1.17896000	−1.25424600
H	−2.11261700	0.75293600	0.88558600	H	1.86472900	−1.82665300	−1.51108600
				H	2.45968100	−1.97638900	0.15403500
				H	4.21846900	−1.01067600	−1.28131400
				H	3.12443300	0.25970200	−1.84445400
				H	−2.96298400	−1.74153600	−1.59864400
				H	−3.27708400	−2.40534600	0.01734700
				H	−4.16253100	−0.98235500	−0.54013500
				H	−0.26220200	−1.94411000	−0.83628000
				H	−0.02632900	−1.94788700	0.90812700
				H	4.16136900	−0.11073100	1.02126900
				H	4.58162500	1.20669900	−0.07384000
				H	1.61737300	−0.30113500	1.84405300
				H	0.49188400	0.94792300	1.27093900
				H	2.24455100	2.03479900	−0.04946100
				H	2.78977500	1.85616300	1.62254500
				H	−3.29195800	0.59077800	1.97316400
				H	−2.49988900	−0.88961500	2.52154600
				H	−1.59666500	0.63751700	2.47483200
				H	−2.20087300	3.08929400	−1.21031700

	H	−3.42943700	2.09742000	−0.42716100
	H	−3.06346700	1.84390900	−2.14222300

8.3.5.1 Weitere Molekelbilder berechneter Strukturen







8.3.6 Angaben zu den quantenchemischen Rechnungen aus Kapitel 4.5.2

8.150 Berechnete Energien der optimierten Verbindungen [B3LYP/6−31+G(d)].

Verbindung	SCF [Hartree]	ZPE [Hartree]
122	−2963.2576404	−2962.710638
122−Diastereomer 1	−2963.25323792	−2962.706043
122−Diastereomer 2	−2963.25128248	−2962.703642
122−Diastereomer 3	−2963.25166656	−2962.70486

Tabelle 8.151 Standardorientierung von **122** und **122−Diastereomer 1** [B3LYP/6−31+G(d)].

122				D1			
C	2.62834200	2.59709100	−2.37422700	C	−1.73566500	−3.48510700	−1.53141800
C	1.35789400	1.88592600	−1.86821100	C	−0.67872700	−2.47630100	−1.03729600
C	3.15461900	−1.25447500	−1.42828700	C	−2.80984800	0.29408100	−1.93724400
C	4.47155200	−0.65963200	−0.92590100	C	−4.13322400	−0.30327500	−1.45519300
C	−2.02676200	−2.65013100	−1.06566300	C	2.08539900	2.40250900	−1.52963400
C	0.86492200	−1.85742200	−0.94528900	C	−0.72889000	1.37540600	−1.38914800
C	−3.57107000	0.48015800	0.21074800	C	3.50442000	−0.05420800	0.37655200
N	−1.10054700	0.19438500	−0.27457900	N	1.20656000	0.82830100	0.84789100
N	2.08866400	−1.23050600	−0.39851000	N	−1.96597400	0.78939300	−0.82172300
C	−1.99492700	2.44534900	0.24053800	C	2.57471300	−0.02519800	2.71162800
Si	−0.82388300	−1.54742800	−0.10349200	Si	0.69558100	2.05703300	−0.30122000
Zn	1.36682800	1.18321400	0.02066600	Zn	−1.22820400	−1.24744200	0.44624900
C	−2.13508200	0.93356900	0.48502500	C	2.58880400	0.69038200	1.34851800
C	4.96040900	−1.38476300	0.33336700	C	−4.92779300	0.71725000	−0.63255400
C	2.53976100	−1.95081700	0.81293900	C	−2.71236200	1.79180600	−0.02983700
C	3.84576500	−1.39265300	1.38568600	C	−4.04822600	1.26068800	0.49914100
C	−0.94446000	−1.97563000	1.73028200	C	0.24910800	3.69696400	0.54704200
C	1.45172700	1.43125300	2.01353500	C	−1.55689400	−0.81693100	2.37955300
C	2.53537200	2.40372500	2.52124700	C	−2.65040400	−1.67274400	3.05391600
H	2.51546000	3.00201700	−3.39277200	H	−1.34082900	−4.16154400	−2.30568300
H	3.49456200	1.92210600	−2.39754900	H	−2.61243800	−2.98662000	−1.96621400
H	2.90340200	3.43949700	−1.72543400	H	−2.10523500	−4.11914100	−0.71436400
H	1.09540600	1.07689800	−2.57124900	H	−0.29933700	−1.89525200	−1.89152500
H	0.51689900	2.59687700	−1.92236600	H	0.18996800	−3.03835500	−0.66098700
H	−1.04582200	0.53428900	−1.23395000	H	0.53347400	0.61790000	1.58012200
H	2.79226300	−0.69228300	−2.29424000	H	−2.22853300	−0.45206200	−2.48703300
H	3.32326000	−2.29928200	−1.75722100	H	−3.01736500	1.12939200	−2.63442900
H	5.21583000	−0.72183800	−1.73026300	H	−4.70754900	−0.63904500	−2.32805000
H	4.32679900	0.40676000	−0.70790100	H	−3.93198300	−1.19653300	−0.84758000
H	−1.99366500	−2.44874900	−2.14420100	H	2.40235700	1.49798600	−2.05942000
H	−1.78265500	−3.71149500	−0.92144200	H	1.75277700	3.13627700	−2.27574100
H	−3.06001200	−2.49733200	−0.73458100	H	2.97015400	2.82117900	−1.03545800
H	0.72997800	−1.47278600	−1.96692300	H	−0.25628300	0.59533000	−2.00015700
H	1.01644700	−2.94906800	−1.06778300	H	−0.99850900	2.18753100	−2.09652700
H	−1.92947500	0.74853800	1.54585000	H	3.04046600	1.68265900	1.51619100
H	−7.27167700	−0.59232900	−0.44752700	H	5.94239400	−2.03249500	−1.94673200
H	−6.37684200	−0.53839100	1.87708700	H	6.77597100	−0.10102300	−0.61067800
H	−2.15661200	2.68875900	−0.81721100	H	2.14425300	−1.02868800	2.61476600
H	−2.73938200	2.99684200	0.82507200	H	3.59238100	−0.12956500	3.10158200
H	−0.99739900	2.79303700	0.52507300	H	1.98266200	0.54072600	3.44215300
H	5.23617000	−2.41913300	0.07761700	H	−5.24535100	1.54503000	−1.28445200
H	5.86325600	−0.90495800	0.73150800	H	−5.84122000	0.26426500	−0.22742700
H	2.67738600	−3.02355200	0.56739700	H	−2.89318600	2.69033300	−0.65232100
H	1.74799300	−1.89126800	1.56330900	H	−2.08331700	2.10277000	0.80823100
H	3.67358500	−0.37324000	1.74972100	H	−3.85461200	0.46676400	1.23014800
H	4.13237100	−1.99938000	2.25462000	H	−4.55751200	2.07168700	1.03571400
H	−1.99106500	−1.94657000	2.05851100	H	1.15913400	4.17009900	0.93948200
H	−0.57866400	−2.99393800	1.91293700	H	−0.21092800	4.40461600	−0.15538100
H	−0.37334500	−1.28996400	2.36573000	H	−0.43902900	3.57103900	1.39100400
H	0.46617700	1.80442700	2.33512700	H	−0.61042000	−0.98456800	2.91749000
H	1.56834000	0.46026400	2.51880700	H	−1.79410200	0.24905900	2.51998200
H	2.41952400	3.40303400	2.08027400	H	−2.42150300	−2.74453700	2.98643900
H	3.54751500	2.06300700	2.26144900	H	−3.63467300	−1.53040000	2.58650800
H	2.51574200	2.53288400	3.61540400	H	−2.77087700	−1.43779200	4.12294500
C	−4.41545600	0.12259300	1.26999700	C	4.85566100	0.30586800	0.28128600
C	−5.74085300	−0.26216800	1.03950600	C	5.73236700	−0.40017600	−0.54730400
C	−6.24321200	−0.29276500	−0.26295200	C	5.26518000	−1.48272100	−1.29779300
C	−5.41181700	0.06589200	−1.32987800	C	3.91822000	−1.84831700	−1.21171600
C	−4.09080500	0.44860700	−1.09243400	C	3.04574500	−1.13906500	−0.38185200
H	−4.03342700	0.14603300	2.28927500	H	5.22672600	1.15228000	0.85805000

H	−3.45701600	0.72085200	−1.93407100	H	1.99771100	−1.41730400	−0.33009700
H	−5.79411100	0.04762100	−2.34770300	H	3.54273300	−2.68653900	−1.79398800

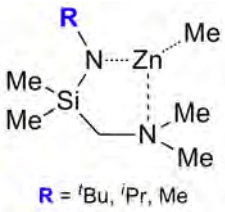
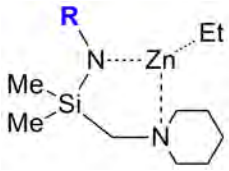
Tabelle 8.152 Standardorientierung von **122−Diastereomer 2** und **122−Diastereomer 3** [B3LYP/6−31+G(d)].

D2				D3			
C	3.41207500	2.83784100	−1.44292900	C	−1.43819900	−3.39677200	−2.10005500
C	2.01657500	2.18333500	−1.50362000	C	−0.60100900	−2.12953400	−1.83058800
C	3.31269800	−1.29896300	−0.96863200	C	−3.50359000	−0.11751800	−0.99129900
C	4.32526800	−1.16365200	0.17095200	C	−4.29027200	−1.12676200	−0.15196000
C	−1.48082000	−0.43944100	−3.09038000	C	0.48237700	3.25666100	−2.16632800
C	0.99682100	−1.39629200	−1.64322500	C	−1.69749800	1.46622500	−1.13008700
C	−3.34858900	0.59924700	0.47086100	C	3.30783200	0.35461900	−0.03965700
N	−0.93278300	0.25598100	−0.15850300	N	1.06783400	1.39882500	0.05685100
N	1.91148400	−1.23519500	−0.49314100	N	−2.37266800	0.48804900	−0.24897200
C	−2.11545600	2.27758400	−1.04371300	C	2.98644300	2.64620900	1.08889300
Si	−0.86669000	−1.01640100	−1.40110600	Si	−0.16565200	2.47400500	−0.57077200
Zn	1.43066400	1.26240200	0.18228400	Zn	−0.66226100	−1.43083400	0.03994000
C	−2.01721100	1.25345400	0.09019700	C	2.51996200	1.66871500	−0.00376000
C	4.09641200	−2.24256000	1.23583100	C	−4.81385600	−0.47715000	1.13412000
C	1.66778400	−2.28030900	0.52162200	C	−2.85999800	1.13213500	0.98902200
C	2.63742800	−2.20175500	1.70525100	C	−3.65149000	0.17783900	1.88887000
C	−1.83084300	−2.57333900	−0.91693500	C	−0.65594000	3.88798000	0.60160000
C	1.16953400	1.27699000	2.18099500	C	−0.30890300	−1.44483500	2.00924300
C	2.39006000	1.70166100	3.02130300	C	0.97452300	−2.18788300	2.43082800
H	3.67525800	3.36735700	−2.37274500	H	−1.32272500	−3.76587600	−3.13133000
H	4.20549700	2.09847700	−1.26476900	H	−2.51213800	−3.22390100	−1.94494200
H	3.47922000	3.57209200	−0.62887400	H	−1.15157500	−4.22154400	−1.43373800
H	1.97396800	1.50040900	−2.36557500	H	−0.88165900	−1.34485300	−2.54888400
H	1.27100500	2.96479600	−1.72163200	H	0.45607200	−2.35141900	−2.03998000
H	−0.68655800	−0.15052900	0.74444500	H	0.83119900	0.84397200	0.87688000
H	3.45059600	−0.49663300	−1.70018000	H	−3.09386900	−0.59853800	−1.88451400
H	3.47973300	−2.25911300	−1.49709300	H	−4.18720100	0.68475700	−1.33373600
H	5.33819800	−1.23143800	−0.24622100	H	−5.11567500	−1.52138600	−0.75826900
H	4.23178900	−0.16787800	0.62489900	H	−3.64457300	−1.98047000	0.09690900
H	−1.00077200	0.49098600	−3.41282300	H	0.82510200	2.50268700	−2.88526000
H	−1.23609600	−1.21164600	−3.83271200	H	−0.31356500	3.83833300	−2.64965500
H	−2.56721900	−0.29964100	−3.12136400	H	1.31365500	3.94762600	−1.98049000
H	1.33126200	−0.69573400	−2.41837800	H	−1.36786200	0.92108700	−2.02429500
H	1.10754300	−2.40926800	−2.08300100	H	−2.43756400	2.21247400	−1.49022100
H	−1.68327700	1.80656600	0.97707700	H	2.69605200	2.15750600	−0.97065900
H	−6.65465800	−1.18079700	1.57038500	H	5.28378300	−3.01183700	−0.28473300
H	−6.37745200	−0.38088900	−0.77095300	H	5.62938100	−1.49065800	1.65613600
H	−2.42885300	1.83631300	−1.99320500	H	2.78403900	2.25262300	2.09250900
H	−2.84021000	3.05615300	−0.78067300	H	4.05969500	2.85900000	1.01102600
H	−1.14078400	2.74854000	−1.20135400	H	2.44773200	3.59453300	0.99362200
H	4.32140900	−3.23171800	0.80879400	H	−5.56620300	0.28402200	0.87765200
H	4.77688100	−2.10130800	2.08478400	H	−5.31591000	−1.21837000	1.76841300
H	1.74589900	−3.28007600	0.04838100	H	−3.49435000	2.00280100	0.72809400
H	0.63738700	−2.18208600	0.88163300	H	−1.99517300	1.51719600	1.53703900
H	2.45586700	−1.27430500	2.25976800	H	−2.97650500	−0.59622200	2.27109700
H	2.42312500	−3.03424600	2.38811800	H	−4.01720100	0.74150500	2.75692400
H	−2.90697300	−2.36783500	−0.87081400	H	0.15511100	4.62456800	0.66721700
H	−1.67338500	−3.37004800	−1.65675500	H	−1.54839900	4.41616200	0.23994500
H	−1.53224700	−2.97020200	0.06074300	H	−0.86420900	3.54325100	1.62103400
H	0.34451600	1.97850300	2.38818300	H	−0.29993900	−0.42275600	2.42161500
H	0.80996100	0.29653500	2.53542300	H	−1.17386400	−1.93220200	2.48580700
H	2.73968100	2.70414500	2.74103400	H	1.87500600	−1.73513600	1.99811400
H	3.24209700	1.02216000	2.88047200	H	0.95825500	−3.23447400	2.09886300

H	2.17943400	1.72681500	4.10251500	H	1.11196600	−2.20142900	3.52371900
C	−4.39643700	0.39945700	−0.43944600	C	4.22203700	−0.01640800	0.95449600
C	−5.57756700	−0.23972000	−0.04788500	C	4.92831500	−1.22279300	0.86926100
C	−5.73521400	−0.68746400	1.26574500	C	4.73484700	−2.07596400	−0.21689400
C	−4.70475200	−0.48290300	2.18848200	C	3.82610200	−1.71599900	−1.21886000
C	−3.52888500	0.15644400	1.79141500	C	3.12221200	−0.51591100	−1.12664300
H	−4.30489000	0.75027400	−1.46366300	H	4.39610100	0.63110300	1.80816500
H	−2.73748700	0.32248400	2.52113200	H	2.40895800	−0.24883000	−1.90250300
H	−4.81990000	−0.81285900	3.21812100	H	3.66547400	−2.37158500	−2.07131000

8.3.7 Angaben zu den quantenchemischen Rechnungen aus Kapitel 4.5.4

Tabelle 8.153 Berechnete Energien der optimierten Verbindungen [B3LYP/6−31+G(d)].

Verbindung		SCF [Hartree]	ZPE [Hartree]
$Me_2(CH_2NMe_2)SiN(^tBu)ZnMe$		−2574.97499034	−2574.624306
$[Me_2(CH_2NMe_2)SiN(^tBu)ZnMe]_2$		−5149.91306301	−5149.207325
$Me_2(CH_2NMe_2)SiN(^iPr)ZnMe$		−2535.66079139	−2535.337895
$[Me_2(CH_2NMe_2)SiN(^iPr)ZnMe]_2$		−5071.32032401	−5070.669884
$Me_2(CH_2NMe_2)SiN(Me)ZnMe$		−2457.02930383	−2456.763439
$[Me_2(CH_2NMe_2)SiN(Me)ZnMe]_2$		−4914.07156925	−4913.536209
$Me_2(CH_2NC_5H_{10})SiN(^tBu)ZnEt$ (127)		−2731.02457288	−2730.578719
$Me_2(CH_2NC_5H_{10})SiN(^iPr)ZnEt$		−2691.7130233	−2691.295527
$Me_2(CH_2NC_5H_{10})SiN(Me)ZnEt$		−2613.07851025	−2612.717449
$Me_2(CH_2NC_5H_{10})SiN(Cy)ZnEt$ (126		−2808.45310576	−2807.968997
$[Me_2(CH_2NC_5H_{10})SiN(^tBu)]_2Zn$		−3524.40828594	−3523.644653
$[Me_2(CH_2NC_5H_{10})SiN(^iPr)]_2Zn$		−3445.79407725	−3445.086362
$[Me_2(CH_2NC_5H_{10})SiN(Me)]_2Zn$		−3288.53300565	−3287.940843
$Me_2(CH_2NC_5H_{10})SiN(^tBu)ZnEt$ in THF		−2731.02729452	−2730.582343
$Me_2(CH_2NC_5H_{10})SiN(^iPr)ZnEt$ in THF		−2691.71582144	−2691.2992
$[Me_2(CH_2NC_5H_{10})SiN(^tBu)]_2Zn$ in THF		−3524.41093921	−3523.648361
$[Me_2(CH_2NC_5H_{10})SiN(^iPr)]_2Zn$ in THF		−3445.79722423	−3445.090626
$[Me_2(CH_2NC_5H_{10})SiN(C_2H_4OMe)ZnEt]_2$ (128)		−5533.83950521	−5532.991945
$ZnEt_2$		−1937.61384161	−1937.484949
$ZnEt_2$ in THF		−1937.61611569	−1937.48784
EtH		−79.833585	−79.758649
Ligand mit R = ^{i}Pr, R' = Me		−912.517197435	−912.097627

Ligand mit R = ^{t}Bu, R’ = Me	−951.833442136	−951.386419
67 (R = C_2H_4OMe, R’ = H)	−909.100392899	−908.732359
64 (R = Cy, R’ = H)	−950.636101191	−950.207042
65·$ZnEt_2$ (R = ^{i}Pr, R’ = H)	−2771.51552348	−2771.02147
65·$ZnEt_2$ (ÜZ, R = ^{i}Pr, R’ = H)	−2771.4718633	−2770.982751
66·$ZnEt_2$ (R = ^{t}Bu, R’ = H)	−2810.82637397	−2810.303943
66·$ZnEt_2$ (ÜZ, R = ^{t}Bu, R’ = H)	−2810.78027076	−2810.262282
[(S)−69]·$ZnEt_2$ [R = CH(Me)(Ph), R’ = H]	−2963.2576404	−2962.710638
[(S)−69]·$ZnEt_2$ [ÜZ, R = CH(Me)(Ph), R’ = H]	−2963.21189845	−2962.669267
67·$ZnEt_2$ (R = C_2H_4OMe, R’ = H)	−2846.72099923	−2846.221978
67·$ZnEt_2$ (ÜZ, R = C_2H_4OMe, R’ = H)	−2846.67418006	−2846.179735
64·$ZnEt_2$ (R = Cy, R’ = H)	−2888.2546382	−2887.694327
64·$ZnEt_2$ (ÜZ, R = Cy, R’ = H)	−2888.20836024	−2887.652698
$ZnEt_2$−Addukt mit R = Me, R’ = H	−2692.88358725	−2692.446168
$ZnEt_2$−Addukt mit R = Me, R’ = H (ÜZ)	−2692.84051209	−2692.408219
$ZnEt_2$−Addukt mit R = Ph, R’ = H	−2884.63354989	−2884.143219
$ZnEt_2$−Addukt mit R = Ph, R’ = H (ÜZ)	−2884.59364375	−2884.108217
$ZnEt_2$−Addukt mit R = ^{t}Bu, R’ = Me	−2889.4442696	−2888.866041
$ZnEt_2$−Addukt mit R = ^{t}Bu, R’ = Me (ÜZ)	−2889.39990638	−2888.825527
$ZnEt_2$−Addukt mit R = ^{i}Pr, R’ = Me	−2850.13192055	−2849.581801
$ZnEt_2$−Addukt mit R = ^{i}Pr, R’ = Me (ÜZ)	−2850.09039766	−2849.544524
[$Me_3SiN(^tBu)H$]·$ZnEt_2$	−2560.12499226	−2559.744606
[$Me_3SiN(^tBu)H$]·$ZnEt_2$ (ÜZ)	−2560.06822029	−2559.692718

Tabelle 8.154 Standardorientierung von $Me_2(CH_2NMe_2)SiN(^tBu)ZnMe$ und $Me_2(CH_2NMe_2)SiN(^iPr)ZnMe$ [B3LYP/6−31+G(d)].

$Me_2(CH_2NMe_2)SiN(^tBu)ZnMe$				$Me_2(CH_2NMe_2)SiN(^iPr)ZnMe$			
C	−2.24780200	−1.27452100	1.59233800	C	3.02613700	0.99254900	1.19350100
C	−2.02393400	−2.28117100	−0.69810500	H	1.45951100	2.35676900	0.73901100
C	−2.07248900	−0.95355300	0.08871700	C	1.89715700	1.46589400	0.26162700
C	−3.31463200	−0.17425200	−0.39532800	C	2.47410000	1.93081100	−1.08936500
C	2.00426700	−2.74541200	−0.15778300	C	−2.33648000	2.54319500	0.10085500
C	−1.15457300	2.42764600	1.46243500	C	1.56856800	−2.23777000	1.37415200
C	2.34354200	0.94956100	1.48964700	C	−2.10915900	−1.38589900	1.32095100
N	−0.81701800	−0.19426800	−0.13381900	N	0.81888500	0.47224300	0.09769000
Zn	0.83774700	−1.15567600	−0.12106700	Zn	−0.96640600	1.13016900	0.04067400
Si	−0.65931300	1.52624100	−0.14412800	Si	1.01210800	−1.22458600	−0.14264500

N	2.10024500	0.73105300	0.05414200	**N**	−1.85023600	−0.96513600	−0.06674500
C	1.21664000	1.78539000	−0.50874300	**C**	−0.75957300	−1.77299900	−0.67802100
C	3.38635800	0.65611400	−0.65937700	**C**	−3.09483100	−1.05087100	−0.84997000
C	−1.51012600	2.48222600	−1.55369000	**C**	2.15170900	−1.77222900	−1.56470700
H	−3.15971900	−1.85838700	1.77829900	**H**	3.75125600	1.79823000	1.36637200
H	−1.39275200	−1.85480200	1.96145800	**H**	2.62529200	0.67706900	2.16314300
H	−2.30727600	−0.35217900	2.18200000	**H**	3.57535800	0.14664300	0.75890300
H	−2.95002600	−2.85436400	−0.56273600	**H**	3.21149200	2.73384000	−0.95219700
H	−1.19354200	−2.91457900	−0.36168800	**H**	2.96783700	1.10178800	−1.61110000
H	−1.89081300	−2.08675000	−1.76889200	**H**	1.67485800	2.30699600	−1.73872400
H	−4.22344800	−0.77138200	−0.25058300	**H**	−2.96251300	2.52578300	−0.80089600
H	−3.45064100	0.76031400	0.16221300	**H**	−1.88815100	3.54121000	0.17353100
H	−3.23412800	0.06817800	−1.46071100	**H**	−2.99963300	2.41444100	0.96656300
H	1.43819400	−3.67382400	−0.01609000	**H**	1.01622900	−1.97454600	2.28458800
H	2.76952400	−2.70077200	0.62877000	**H**	2.63367000	−2.08297500	1.58647700
H	2.52728700	−2.82343200	−1.12046000	**H**	1.42727000	−3.31309500	1.19528100
H	−0.69334900	1.98786700	2.35516000	**H**	−1.19957500	−1.28529800	1.91730200
H	−2.24148000	2.39887800	1.61396400	**H**	−2.88717000	−0.75231200	1.75865800
H	−0.86469800	3.48696300	1.42122600	**H**	−2.44334400	−2.43642800	1.36441300
H	1.39514700	0.97265300	2.03098600	**H**	−0.94693800	−2.85026700	−0.51619100
H	2.95483400	0.13366500	1.88828600	**H**	−0.81094100	−1.61174700	−1.76279600
H	2.86948500	1.90354000	1.66499900	**H**	−3.86338200	−0.41983100	−0.39244100
H	1.57420500	2.78785800	−0.20949600	**H**	−3.46735600	−2.08777400	−0.90158200
H	1.31676600	1.73908200	−1.60109800	**H**	−2.91437000	−0.69345500	−1.86787500
H	3.99109300	−0.15596300	−0.24404800	**H**	3.20626800	−1.56109800	−1.34641400
H	3.94848900	1.60140400	−0.57526400	**H**	2.07035200	−2.85548100	−1.73348900
H	3.20819500	0.44794700	−1.71828500	**H**	1.90032000	−1.26514000	−2.50447300
H	−2.58955100	2.59275200	−1.39942000				
H	−1.08918900	3.49514900	−1.63210600				
H	−1.36071300	1.98340000	−2.51961700				

Tabelle 8.155 Standardorientierung von $[Me_2(CH_2NMe_2)SiN(^tBu)ZnMe]_2$ und $[Me_2(CH_2NMe_2)SiN(^iPr)ZnMe]_2$ [B3LYP/6−31+G(d)].

$[Me_2(CH_2NMe_2)SiN(^tBu)ZnMe]_2$				**$[Me_2(CH_2NMe_2)SiN(^iPr)ZnMe]_2$**			
C	−0.52823600	2.84794400	−1.79605400	**C**	0.68740800	−188.276.300	2.74170400
Zn	−0.50199400	1.09495100	−0.84871100	**Zn**	0.53222500	−101.428.800	0.93557700
N	−1.44700700	0.14698700	0.71991100	**N**	1.24213700	0.89605300	0.32570600
N	−2.76959300	0.14109800	−2.42437000	**N**	2.26948600	−208.196.400	−0.40755700
C	−3.10846000	−1.01825300	−1.58190800	**C**	2.66890100	−100.580.300	−1.34976700
Si	−2.88171800	−0.83909000	0.32249900	**Si**	2.73496200	0.76283600	−0.60222100
C	0.52823600	−2.84794400	1.79605400	**C**	−0.53753100	164.195.700	−2.85223400
Zn	0.50199400	−1.09495100	0.84871100	**Zn**	−0.50765200	0.96559100	−0.95804000
N	1.44700700	−0.14698700	−0.71991100	**N**	−1.27566500	−0.89160300	−0.25806400
N	2.76959300	−0.14109800	2.42437000	**N**	−2.27115400	211.628.800	0.17913900
C	3.10846000	1.01825300	1.58190800	**C**	−2.68622100	116.939.200	1.24607400
Si	2.88171800	0.83909000	−0.32249900	**Si**	−2.72449400	−0.68061900	0.72323800

C	−1.54188700	1.06289300	1.92549200	C	1.13210800	192.072.200	1.40920100
C	−2.78148200	−0.21345400	−3.84690100	C	2.04642200	−334.859.200	−1.13021100
C	−3.68809800	1.25846300	−2.19905200	C	3.32157800	−232.765.800	0.59535200
C	−4.59968600	−0.25836400	0.93418200	C	4.37567200	100.702.600	0.34431500
C	−2.79865600	−2.63600300	0.92799800	C	2.94323800	191.886.400	−2.09377300
C	1.54188700	−1.06289300	−1.92549200	C	−1.23063700	−194.791.000	−1.31561800
C	2.78148200	0.21345400	3.84690100	C	−2.07190900	346.902.500	0.73123600
C	3.68809800	−1.25846300	2.19905200	C	−3.29830600	220.809.800	−0.87505300
C	4.59968600	0.25836400	−0.93418200	C	−4.41155000	−106.021.000	−0.08739900
C	2.79865600	2.63600300	−0.92799800	C	−2.82068500	−164.829.600	2.35316800
C	−2.54146400	2.22510000	1.71873200	C	1.95441000	162.061.200	2.67767800
C	−0.16978200	1.70563900	2.16998800	H	0.08393000	191.063.400	1.73368800
C	−1.90161000	0.27509500	3.20583400	C	1.43580300	334.932.200	0.92027900
C	1.90161000	−0.27509500	−3.20583400	C	−1.45932500	−336.501.900	−0.75870400
C	0.16978200	−1.70563900	−2.16998800	H	−0.21200700	−192.283.200	−1.72068400
C	2.54146400	−2.22510000	−1.71873200	C	−2.15032400	−170.426.600	−2.52769900
H	−0.21837200	3.66979700	−1.13757200	H	0.19644400	−128.359.800	3.52057600
H	−1.53390600	3.08469100	−2.15918100	H	1.73316200	−200.542.100	3.05248800
H	0.14962400	2.84910000	−2.65783000	H	0.21955000	−287.651.800	2.76191900
H	−4.16121600	−1.33004400	−1.75367000	H	3.63211600	−125.797.600	−1.83441700
H	−2.50119500	−1.86626600	−1.91680800	H	1.92264900	−0.98356400	−2.15531000
H	0.21837200	−3.66979700	1.13757200	H	0.06461000	100.701.200	−3.51719800
H	1.53390600	−3.08469100	2.15918100	H	−1.55351000	165.857.600	−3.26844400
H	−0.14962400	−2.84910000	2.65783000	H	−0.13602200	266.126.100	−2.93359500
H	4.16121600	1.33004400	1.75367000	H	−3.66274200	147.475.400	1.66887100
H	2.50119500	1.86626600	1.91680800	H	−1.96187200	126.203.800	2.06586600
H	−2.08367800	−1.03420300	−4.03695100	H	1.31395700	−321.000.700	−1.92684500
H	−2.47108200	0.64992700	−4.44548100	H	1.67316200	−410.906.100	−0.43744000
H	−3.78588700	−0.53262300	−4.18550700	H	2.98414500	−371.392.400	−1.58394400
H	−3.43694400	2.08210900	−2.87303000	H	3.02059500	−315.695.700	1.24033800
H	−3.60342100	1.62519800	−1.17383300	H	3.46865000	−144.920.300	1.22211500
H	−4.74043300	0.96764300	−2.38162700	H	4.27937900	−258.225.100	0.10926900
H	−5.30626800	−1.03718200	0.61413000	H	5.19800100	0.69517600	−0.31528000
H	−4.94292300	0.68166900	0.49115000	H	4.47526400	0.44942500	1.28014200
H	−4.69583900	−0.17396600	2.02134700	H	4.54255500	206.703.900	0.57287800
H	−3.70797700	−3.16343400	0.60746200	H	3.86912900	166.132.500	−2.62742600
H	−2.75065800	−2.69928800	2.02160600	H	3.03445500	296.544.700	−1.77784200
H	−1.93898500	−3.18679100	0.53526100	H	2.11525600	185.919.500	−2.80492100
H	2.47108200	−0.64992700	4.44548100	H	−1.70026900	413.731.400	−0.05177000
H	2.08367800	1.03420300	4.03695100	H	−1.34504200	344.341.900	1.54405100
H	3.78588700	0.53262300	4.18550700	H	−3.01862100	387.807.000	1.12443100
H	3.60342100	−1.62519800	1.17383300	H	−3.41264500	124.927.100	−1.38023300
H	3.43694400	−2.08210900	2.87303000	H	−2.98976900	294.759.600	−1.61804600
H	4.74043300	−0.96764300	2.38162700	H	−4.27280500	250.811.400	−0.45291500
H	5.30626800	1.03718200	−0.61413000	H	−5.19494700	−0.72609400	0.60765600
H	4.69583900	0.17396600	−2.02134700	H	−4.55378000	−213.921.200	−0.22514100

H	4.94292300	−0.68166900	−0.49115000	H	−4.59790800	−0.57510200	−1.04958400
H	3.70797700	3.16343400	−0.60746200	H	−3.74797600	−138.149.700	2.87970600
H	1.93898500	3.18679100	−0.53526100	H	−1.98106500	−145.088.000	3.02497800
H	2.75065800	2.69928800	−2.02160600	H	−2.84870100	−273.041.600	2.17430800
H	−3.57364300	1.88438300	1.63456700	H	3.02839300	174.033.900	2.50821600
H	−2.29091700	2.79102000	0.81387700	H	1.77201400	0.60378700	3.03657900
H	−2.49586100	2.91905100	2.56830500	H	1.66918300	231.751.000	3.47743800
H	0.14866500	2.31714000	1.31624900	H	0.86441200	359.701.900	0.01961100
H	0.58463900	0.93744300	2.35815700	H	2.50057300	346.944.900	0.68614700
H	−0.19864700	2.36521600	3.04609600	H	1.19195800	408.739.700	1.69581300
H	−1.16326500	−0.51222900	3.39393300	H	−2.49413300	−349.230.400	−0.41750300
H	−2.88559900	−0.19707000	3.14353300	H	−0.79910900	−357.278.300	0.09015000
H	−1.91652300	0.94317800	4.07646900	H	−1.27647800	−412.413.600	−1.53065700
H	2.88559900	0.19707000	−3.14353300	H	−2.02515800	−0.69034900	−2.91870600
H	1.16326500	0.51222900	−3.39393300	H	−3.20508200	−185.795.500	−2.28357000
H	1.91652300	−0.94317800	−4.07646900	H	−1.89558400	−240.767.700	−3.33196200
H	−0.58463900	−0.93744300	−2.35815700				
H	−0.14866500	−2.31714000	−1.31624900				
H	0.19864700	−2.36521600	−3.04609600				
H	2.29091700	−2.79102000	−0.81387700				
H	3.57364300	−1.88438300	−1.63456700				
H	2.49586100	−2.91905100	−2.56830500				

Tabelle 8.156 Standardorientierung von $Me_2(CH_2NMe_2)SiN(Me)ZnMe$, $[Me_2(CH_2NMe_2)SiN(Me)ZnMe]_2$ und EtH [B3LYP/6−31+G(d)].

$Me_2(CH_2NMe_2)SiN(Me)ZnMe$				$[Me_2(CH_2NMe_2)SiN(Me)ZnMe]_2$			
C	3.11213900	−1.30618200	−0.07171700	C	−0.77665600	−2.43168900	−2.15093000
Zn	1.20061500	−0.84712400	−0.02239700	Zn	−0.64885700	−1.18331000	−0.58322700
N	−0.65951500	−1.17035400	0.06647700	N	−0.98026900	0.91876400	−0.73629200
N	0.85761700	1.43493200	−0.03639600	N	−2.61337000	−1.43958700	0.70833200
C	−0.51433800	1.60195000	−0.59141300	C	−2.90856700	−0.06818400	1.20427400
Si	−1.71564200	0.17912900	−0.09448900	Si	−2.54181900	1.33748400	−0.05743000
C	−1.19172300	−2.51838200	0.28730900	C	0.77347500	2.42672100	2.15463000
C	1.85477800	2.18054800	−0.82237900	Zn	0.64821100	1.18174100	0.58398600
C	0.91455800	1.86588900	1.37059600	N	0.98164500	−0.92036900	0.73485000
C	−2.70970000	0.60511800	1.47182100	N	2.61253200	1.44246800	−0.70418500
C	−2.98726700	0.02515000	−1.49778300	C	2.90915800	0.07270500	−1.20380200
H	−1.88770200	−2.83329500	−0.50835600	Si	2.54281400	−1.33687300	0.05381300
H	−0.38751900	−3.26502800	0.31072300	C	−0.74911700	1.39381600	−2.11821800
H	−1.73196800	−2.61042900	1.24511500	C	−2.61371500	−2.41452400	1.81486900

H	3.27346700	−2.38601900	0.02920600
H	3.66020200	−0.81164200	0.74108300
H	3.56786500	−0.98998200	−1.01916100
H	−0.90053300	2.61065500	−0.35721400
H	−0.42653200	1.55346400	−1.68465500
H	1.84708000	1.82675500	−1.85743100
H	2.85311500	2.01163700	−0.40644100
H	1.64491500	3.26370200	−0.81857800
H	1.92122000	1.69814000	1.76656000
H	0.20432700	1.28945100	1.96798300
H	0.66967800	2.93720500	1.47175400
H	−3.30191200	1.52052600	1.33593200
H	−2.07184900	0.74443500	2.35321100
H	−3.41579300	−0.20212900	1.70881700
H	−3.56106100	0.95336000	−1.62623500
H	−3.71183900	−0.77377400	−1.29272300
H	−2.50202900	−0.20773000	−2.45401700

EtH			
C	0.00000000	0.00000000	0.76628800
H	−0.51042700	0.88512500	1.16529700
H	1.02175400	−0.00052000	1.16529700
H	−0.51132800	−0.88460500	1.16529700
C	0.00000000	0.00000000	−0.76628800
H	0.51132800	−0.88460500	−1.16529700
H	−1.02175400	−0.00052000	−1.16529700
H	0.51042700	0.88512500	−1.16529700

C	−3.62209600	−1.87346400	−0.27632700
C	−3.89939900	1.48108700	−1.38579100
C	−2.63854700	2.96114400	0.91556200
C	0.75178500	−1.39746500	2.11630100
C	2.61279400	2.42069000	−1.80783600
C	3.62009500	1.87428300	0.28260100
C	3.90143600	−1.48440500	1.38067700
C	2.63947300	−2.95706100	−0.92492500
H	−0.57483000	2.48062400	−2.17383100
H	0.12736200	0.90222100	−2.55639300
H	−1.58970200	1.16613400	−2.78910300
H	1.59438900	−1.17386300	2.78601300
H	−0.12220300	−0.90386900	2.55719600
H	0.57418700	−2.48382200	2.17005700
H	−0.00565200	−2.21457100	−2.90346800
H	−1.74584600	−2.35166900	−2.66159500
H	−0.64715400	−3.48223300	−1.85560400
H	−3.94452600	−0.01397100	1.58976700
H	−2.25533600	0.11267300	2.06835100
H	−0.00419100	2.21444700	2.90162800
H	1.73860300	2.33873100	2.67170600
H	0.65395700	3.47868200	1.86003400
H	3.94542200	0.02039800	−1.58872400
H	2.25669400	−0.10619000	−2.06886100
H	−1.90032800	−2.11495000	2.58307000
H	−2.32810800	−3.40107800	1.43504500
H	−3.61333200	−2.49069800	2.27653100
H	−3.38661400	−2.88533700	−0.61597900
H	−3.61773400	−1.21591000	−1.14499300
H	−4.63262300	−1.86931800	0.16742400
H	−4.89103300	1.43921500	−0.91544300
H	−3.86604700	0.70547100	−2.15900100
H	−3.82912700	2.45078700	−1.89591200
H	−3.66169100	3.13428800	1.27738500
H	−2.37468000	3.81164700	0.27292700
H	−1.96361400	2.98041100	1.77683400
H	2.32625700	3.40589200	−1.42521700
H	1.90003600	2.12289400	−2.57731900
H	3.61261300	2.49896900	−2.26869300
H	3.61577500	1.21388200	1.14911500
H	3.38323100	2.88477900	0.62537700
H	4.63093700	1.87264200	−0.16042200
H	4.89259300	−1.44131800	0.90943600
H	3.83156600	−2.45551800	1.88815300
H	3.86901500	−0.71094800	2.15608800
H	3.66220100	−3.12796500	−1.28899200

				H	1.96318700	−2.97380100	−1.78518200
				H	2.37732800	−3.81010700	−0.28497800

Tabelle 8.157 Standardorientierung von $ZnEt_2$ in der Gasphase und in THF [B3LYP/6−31+G(d)].

$ZnEt_2$				$ZnEt_2$ in THF			
Zn	−0.00000100	0.37855400	0.00000000	Zn	0.00000000	−0.42800400	−0.00010200
C	−1.97153200	0.39483200	0.00001700	C	1.97650700	−0.37121300	−0.00237300
C	1.97153100	0.39483100	−0.00001600	C	−1.97650500	−0.37120900	0.00255100
H	−2.30083400	0.97278000	0.87617000	H	2.33181900	−0.93593400	0.87260600
C	−2.65369600	−0.98816600	−0.00001200	C	2.59194600	1.04278500	0.00243100
H	−2.30084800	0.97282200	−0.87610400	H	2.32956200	−0.92893000	−0.88274100
H	−3.75040800	−0.90293700	−0.00000200	H	3.69243900	1.01353000	0.00060100
H	−2.37932600	−1.58051000	0.88244800	H	2.28900300	1.61738600	0.88764300
H	−2.37933900	−1.58046800	−0.88250400	H	2.28626400	1.62456400	−0.87713400
C	2.65369900	−0.98816400	0.00001200	C	−2.59194800	1.04278300	−0.00228900
H	2.30084600	0.97282300	0.87610300	H	−2.32928300	−0.92879700	0.88311700
H	2.30083100	0.97278000	−0.87617000	H	−2.33208700	−0.93606200	−0.87223100
H	3.75041000	−0.90293100	0.00000100	H	−3.69244000	1.01352100	−0.00082000
H	2.37933100	−1.58050900	−0.88244800	H	−2.28871400	1.61748800	−0.88733400
H	2.37934500	−1.58046600	0.88250500	H	−2.28655500	1.62445900	0.87744400

Tabelle 8.158 Standardorientierung von $Me_2(CH_2NC_5H_{10})SiN(^tBu)ZnEt$ in der Gasphase und in THF [B3LYP/6−31+G(d)].

$Me_2(CH_2NC_5H_{10})SiN(^tBu)ZnEt$				$Me_2(CH_2NC_5H_{10})SiN(^tBu)ZnEt$ in THF			
H	−2.86779000	−1.00225100	2.76360200	H	−2.87687300	−0.99603500	2.76038500
H	1.54761800	1.84878700	2.23575900	H	1.54435800	1.85455000	2.22825900
H	1.40434100	−2.38744800	2.15261100	H	1.40649700	−2.37782800	2.16102700
H	3.23388100	−0.06856800	2.16227100	H	3.24000500	−0.05358500	2.15718500
H	3.01512000	−2.63442800	1.46934300	H	3.02113400	−2.62190800	1.48047600
C	−2.71978500	−0.65928600	1.73166800	C	−2.72449300	−0.65231400	1.72905000
H	−2.41905500	0.39616300	1.78892900	H	−2.42277900	0.40325300	1.78841500
H	−0.66126700	−1.33919500	1.65887100	H	−0.66711200	−1.33674000	1.66674300
H	2.81384200	2.92310100	1.59717800	H	2.80670500	2.93193200	1.58476700
C	1.94351600	−2.65936900	1.23715100	C	1.94929900	−2.65281700	1.24842700
H	4.43613600	1.05464400	1.49631000	H	4.43608800	1.07269500	1.48302600
H	−4.79616300	−0.13592500	1.33445300	H	−4.79838600	−0.12608500	1.32295100
C	2.00184300	2.23946500	1.31730600	C	1.99589200	2.24505900	1.30823500
H	1.69002200	−3.70131600	0.99569400	H	1.69823700	−3.69610600	1.00956400
H	−1.84496100	−2.55402800	1.14329400	H	−1.85147800	−2.54753800	1.14152300
C	3.63133200	0.35676700	1.23370300	C	3.63357700	0.36972600	1.22584500
H	−4.39092700	−1.81836000	0.99354800	H	−4.39236400	−1.81023700	0.98350000
C	−1.59082500	−1.47825900	1.10124300	C	−1.59417800	−1.47310200	1.10398000
C	−4.01554100	−0.78646200	0.92104900	C	−4.01684300	−0.77821600	0.91266700
H	−1.42439800	3.67799900	0.87922000	H	−1.38326500	3.66666400	0.89521600
H	1.24488500	2.83052400	0.78539900	H	1.23494900	2.83040700	0.77601500

H	4.08380200	−0.45392100	0.64996500	H	4.08679300	−0.44214300	0.64428800
H	−2.83826500	2.64977800	0.64772900	H	−2.82566000	2.68472200	0.63993400
C	2.52228800	1.08068900	0.43899500	C	2.51802900	1.08520800	0.43178700
C	−2.11263700	3.28368600	0.11997500	C	−2.07720700	3.30268800	0.12568300
N	1.40090400	0.17134900	0.10502400	N	1.40160400	0.17161100	0.10236600
H	−2.67309900	4.14252300	−0.28011300	H	−2.60868700	4.18375500	−0.26753800
Si	1.51876300	−1.51681100	−0.22911600	Si	1.51934500	−1.51841400	−0.22364200
N	−1.33567500	−1.09952100	−0.31077300	N	−1.33053800	−1.09345200	−0.30867500
H	−0.49181500	−3.01107900	−0.75220100	H	−0.49363700	−3.01178200	−0.73646300
Zn	−0.28013500	0.95186500	−0.39842600	Zn	−0.29808500	0.92709000	−0.39777500
C	−3.74809400	−0.43815400	−0.54885500	C	−3.74334300	−0.43113600	−0.55650400
H	3.95986100	2.37448000	−0.61630800	H	3.94845800	2.38425500	−0.62883100
H	−3.52365700	0.63084600	−0.64121700	H	−3.51827000	0.63824500	−0.64871300
C	−0.24804600	−1.94006000	−0.88077900	C	−0.24516200	−1.94345200	−0.87390000
C	3.14370800	1.67612000	−0.84716100	C	3.13506400	1.68129200	−0.85687800
H	−2.85005800	−2.32126200	−1.14837200	H	−2.84397900	−2.31511200	−1.14780300
H	−4.63630700	−0.63349800	−1.16344800	H	−4.62904400	−0.62702600	−1.17501100
C	−1.36461200	2.51254000	−0.98526900	C	−1.34451900	2.51934100	−0.98157700
C	−2.57793300	−1.24987500	−1.11067800	C	−2.57235400	−1.24418200	−1.11421200
H	3.74102400	−1.89269700	−1.37891500	H	3.74672400	−1.89420100	−1.36600300
H	−0.68047200	3.20109400	−1.50231700	H	−0.64435400	3.19485000	−1.49587100
H	2.38407600	2.21951200	−1.42240100	H	2.37051600	2.21871400	−1.43147500
C	2.68566900	−2.04007000	−1.64064700	C	2.69223400	−2.04587600	−1.63013700
H	3.54551200	0.88262300	−1.48751900	H	3.53894300	0.88721100	−1.49549900
H	2.55961700	−3.10599600	−1.87838100	H	2.56688900	−3.11343400	−1.86168800
H	−2.08021000	2.18145400	−1.75223500	H	−2.06823100	2.20389600	−1.74796500
H	−0.23805100	−1.76045700	−1.96480600	H	−0.23533100	−1.77035500	−1.95931800
H	−2.35312800	−0.93650400	−2.13618000	H	−2.34282700	−0.93327000	−2.13972600
H	2.48934700	−1.46637900	−2.55533300	H	2.49424600	−1.47709400	−2.54777900

Tabelle 8.159 Standardorientierung von $Me_2(CH_2NC_5H_{10})SiN(^iPr)ZnEt$ in der Gasphase und in THF [B3LYP/6−31+G(d)].

$Me_2(CH_2NC_5H_{10})SiN(^iPr)ZnEt$				$Me_2(CH_2NC_5H_{10})SiN(^iPr)ZnEt$ in THF			
H	−2.78342600	−1.02941100	2.67858700	H	−2.79124300	−1.02574400	2.67274000
H	2.31871500	2.74286400	−0.84813700	H	2.28244800	2.75422100	−0.86602500
H	1.56043900	−2.27346000	2.25462200	H	1.57039700	−2.24831400	2.26857400
H	1.47308100	2.58098100	1.62003600	H	1.44929000	2.58825000	1.60466700
H	3.24777800	−2.13649100	1.74949400	H	3.26024700	−2.10619700	1.76528200
C	−2.60088700	−0.70479000	1.64622700	C	−2.60270100	−0.70144700	1.64105700
H	−2.34289300	0.36222400	1.69114900	H	−2.34447600	0.36600900	1.68718900
H	−0.51821800	−1.30855300	1.68430300	H	−0.52129300	−1.30941600	1.69477000
H	3.99331700	2.65010500	−0.26373800	H	3.96118000	2.68776600	−0.28616500
C	2.24431200	−2.42941800	1.41193200	C	2.25844200	−2.40839500	1.42977800
H	3.16091500	2.50207300	2.16492400	H	3.14125800	2.53397400	2.14411200
H	−4.67433700	−0.26918800	1.14271100	H	−4.67274100	−0.26506100	1.12405200
C	3.12641500	2.05075000	−0.57381800	C	3.10164800	2.07525100	−0.59240500
H	2.28012500	−3.50713000	1.20090200	H	2.29882500	−3.48759300	1.22604000

H	−1.63287400	−2.57847500	1.14851800	H	−1.63478100	−2.57547900	1.14685400
C	2.31191600	1.89840600	1.81708200	C	2.29846600	1.91829800	1.80099400
H	−4.19328100	−1.94312900	0.86415900	H	−4.18918300	−1.94077100	0.85072400
C	−1.41510200	−1.49538100	1.08805000	C	−1.41420800	−1.49349900	1.09140600
C	−3.85254500	−0.90001500	0.78185800	C	−3.84899000	−0.89738400	0.76891400
H	−1.44450100	3.64275400	0.92928900	H	−1.41512700	3.62860800	0.94989100
H	3.40056800	1.48268900	−1.46976300	H	3.38125700	1.50790900	−1.48744400
H	2.01246500	1.22092300	2.62469300	H	2.01029700	1.23869800	2.61113600
H	−2.79711300	2.54524000	0.65411000	H	−2.78929300	2.56261100	0.65790000
C	2.66396500	1.10370800	0.54793900	C	2.65566700	1.12343500	0.53269600
C	−2.09588400	3.22438900	0.15082500	C	−2.07318900	3.23329800	0.16455000
N	1.54432200	0.24905600	0.12334700	N	1.54652400	0.25540100	0.11399300
H	−2.69270500	4.05840300	−0.24908100	H	−2.65225000	4.08504200	−0.22602100
Si	1.74729800	−1.43836400	−0.13580900	Si	1.75588600	−1.43388100	−0.12771900
N	−1.10819400	−1.14404900	−0.32068800	N	−1.09615400	−1.14110900	−0.31718700
H	−0.18569700	−3.04364700	−0.64524900	H	−0.17533600	−3.04537200	−0.62090300
Zn	−0.13491600	0.99735100	−0.37621000	Zn	−0.15895600	0.96487500	−0.37673700
C	−3.53050400	−0.57770700	−0.68305000	C	−3.51872400	−0.57834800	−0.69504200
H	−3.34087400	0.49638600	−0.79252400	H	−3.33043000	0.49626000	−0.80644400
C	0.02650400	−1.97199500	−0.81592600	C	0.03906000	−1.97686200	−0.80443600
H	3.53015400	0.46848400	0.80450300	H	3.53297500	0.50199900	0.78770700
H	−2.54041500	−2.44072100	−1.19205500	H	−2.52343700	−2.44081400	−1.19184500
H	−4.38172700	−0.82083900	−1.33200800	H	−4.36561300	−0.82500500	−1.34880200
C	−1.28706000	2.51072700	−0.94946200	C	−1.27622500	2.51317800	−0.94065100
C	−2.30726500	−1.35949800	−1.17001600	C	−2.29245800	−1.35980800	−1.17451000
H	4.03090800	−1.61324100	−1.18033000	H	4.04499900	−1.60794800	−1.16325100
H	−0.62540600	3.24049800	−1.43844600	H	−0.59701800	3.23366100	−1.42091300
C	3.01540600	−1.91253000	−1.47200200	C	3.03159300	−1.91440900	−1.45604300
H	3.03742000	−2.99806200	−1.64265300	H	3.05597400	−3.00178100	−1.61565200
H	−1.96748400	2.15996800	−1.73928300	H	−1.96372100	2.18204900	−1.73323600
H	0.06847300	−1.84154200	−1.90599400	H	0.08109200	−1.85679000	−1.89602900
H	−2.04779000	−1.06372300	−2.19267400	H	−2.02652100	−1.06666400	−2.19657200
H	2.79116800	−1.42433700	−2.42889500	H	2.80560600	−1.43590100	−2.41765600

Tabelle 8.160 Standardorientierung von $Me_2(CH_2NC_5H_{10})SiN(Me)ZnEt$ und $[Me_2(CH_2NC_5H_{10})SiN(Me)Zn]_2$ [B3LYP/6−31+G(d)].

$Me_2(CH_2NC_5H_{10})SiN(Me)ZnEt$				$[Me_2(CH_2NC_5H_{10})SiN(Me)Zn]_2$			
H	−2.17779000	−1.85014400	2.49645000	H	4.51739100	0.50365200	−2.61716900
H	2.34284400	−1.54370100	2.25436600	H	−4.51616300	−0.50516100	−2.61753900
H	3.90369600	−0.81162400	1.86815100	H	3.57226300	1.91775500	−2.14154200
C	−2.07496600	−1.37966900	1.51027100	H	−3.56906300	−1.91824500	−2.14285900
H	−2.17599900	−0.29661300	1.66429100	C	4.14345400	1.06684500	−1.75131500
H	0.08780800	−1.28473900	1.62976100	C	−4.14167600	−1.06855800	−1.75204700
C	3.06844400	−1.38753700	1.44716100	N	−1.63442400	0.60890700	−1.28697100
H	−4.15985200	−1.57160500	0.91168900	H	5.02272000	1.46374800	−1.22532100
H	3.46881100	−2.36943600	1.15948800	N	1.63340600	−0.60654500	−1.28897900

H	−0.53361700	−2.78481600	0.91785800
H	−3.15930300	−2.97097500	0.52258300
C	−0.67892800	−1.68900600	0.96378400
C	−3.16748400	−1.87096300	0.55234500
H	−2.33465800	3.12263500	1.35425900
H	−3.30312000	1.73885100	0.84624200
C	−2.81518300	2.65439000	0.48546000
N	1.56258600	1.01878200	0.31127800
H	−3.61784100	3.33293700	0.15811100
Si	2.32680000	−0.47729900	−0.05109500
N	−0.45676500	−1.11808600	−0.38800700
H	1.05035500	−2.57399600	−0.80356300
Zn	−0.25669600	1.20857500	−0.19359400
C	−2.91485500	−1.31642100	−0.85582600
H	−3.06958300	−0.23096100	−0.85923700
C	0.90375400	−1.48057500	−0.87601300
H	−1.36361100	−2.71485200	−1.44764200
H	−3.62295300	−1.74478600	−1.57680200
C	−1.80413300	2.36912100	−0.64190100
C	−1.49079100	−1.62266500	−1.32663000
H	4.58112300	0.19913000	−0.93907000
H	−1.38360700	3.32183300	−0.99531500
C	3.72671300	−0.36708800	−1.33266100
H	4.10180100	−1.36162300	−1.61130100
H	−2.32835000	1.94277300	−1.50978500
H	0.93580800	−1.24106900	−1.94765800
H	−1.30475900	−1.16523600	−2.30483500
H	3.39164300	0.13673700	−2.24817400
C	2.32362600	2.15603900	0.83478600
H	3.14951700	2.46226100	0.16982000
H	1.68321500	3.03872500	0.96244500
H	2.76618100	1.94661100	1.82347200

H	0.20525400	4.47757400	−0.52294300
H	1.64396300	2.48386400	−0.90570800
H	−5.02051200	−1.46730500	−1.22672500
H	−4.68963400	2.00126300	−0.90662500
H	−1.64276700	−2.48381800	−0.90598800
H	−0.73411100	2.97877000	−0.47399200
H	−0.20315300	−4.47685200	−0.52364700
H	4.68716400	−2.00368300	−0.90754400
H	0.73547500	−2.97762200	−0.47402900
Si	−3.11019000	0.06402800	−0.61833700
Si	3.10969300	−0.06488900	−0.61890300
Zn	−0.00026800	0.00036700	−0.45321200
C	0.02714500	3.56228700	0.05621600
C	1.33058600	2.76066700	0.10433700
C	−0.02558100	−3.56169200	0.05587300
C	−4.31978600	1.42188900	−0.04982500
C	−1.32940300	−2.76070000	0.10403500
C	4.31695500	−1.42491600	−0.05048800
H	2.13534500	3.38265200	0.53979600
H	−3.84412800	2.12873500	0.64191400
H	−2.13392600	−3.38320100	0.53918800
H	−5.20014600	0.99853600	0.45411400
H	5.19719900	−1.00327900	0.45510500
H	3.83958100	−2.13205200	0.63977100
H	−1.44517400	4.40318000	1.42079200
N	1.21402500	1.50967800	0.90384300
C	−0.47283400	3.89718100	1.46632000
N	−1.21353800	−1.50987900	0.90388700
H	1.44683600	−4.40245200	1.42043100
C	2.54546100	0.84041900	0.98474300
C	−2.54534000	−0.84136300	0.98499400
C	0.47430000	−3.89683000	1.46594700
H	0.22581400	4.59263400	1.95598400
H	3.30149100	1.56294400	1.34384500
H	−3.30092000	−1.56434900	1.34411000
H	−0.22416700	−4.59268800	1.95529100
H	−1.37000300	1.97524500	1.88348300
H	1.37067500	−1.97468200	1.88379800
H	2.47081400	0.07275800	1.76630500
H	−2.47101100	−0.07371800	1.76660900
C	−0.57392500	2.60948700	2.29257300
C	0.57476100	−2.60933100	2.29256700
C	0.75062500	1.84421000	2.27571500
C	−0.75006300	−1.84453400	2.27571400
H	1.52949200	2.45014200	2.77594800
H	−1.52873900	−2.45087000	2.77575100

H	0.66712700	0.90793500	2.83735200
H	−0.83901000	2.82967800	3.33506800
H	−0.66697900	−0.90834800	2.83756200
H	0.83977200	−2.82968400	3.33504700
C	1.58023000	−1.30084100	−2.57563400
H	2.08082300	−0.74388300	−3.38714000
H	2.04818900	−2.30151200	−2.54401500
H	0.54287200	−1.45275200	−2.90305800
C	−1.58216800	1.30427900	−2.57310500
H	−2.07113300	0.74171000	−3.38787400
H	−2.06240100	2.29916400	−2.54368300
H	−0.54484800	1.46914700	−2.89431100

Tabelle 8.161 Standardorientierung von $[Me_2(CH_2NC_5H_{10})SiN(^tBu)Zn]_2$ in der Gasphase und in THF [B3LYP/6−31+G(d)].

$[Me_2(CH_2NC_5H_{10})SiN(^tBu)Zn]_2$				$[Me_2(CH_2NC_5H_{10})SiN(^tBu)Zn]_2$ in THF			
C	1.85031900	−1.66007600	3.27473600	C	1.85272400	−1.65966700	3.27597500
C	−3.50834500	−0.21487100	2.66230200	C	−3.49710100	−0.23253900	2.67227900
C	3.40120600	0.21280800	2.69783800	C	3.39318300	0.22221700	2.70338400
C	0.99615600	0.69851600	3.08092800	C	0.98441100	0.69346800	3.08004500
C	1.97099900	−0.33486800	2.48234200	C	1.96645900	−0.33384600	2.48212600
C	−3.86570900	−1.64133600	0.63337000	C	−3.86292000	−1.64867400	0.63819300
C	−1.88996000	−2.00987100	2.11743700	C	−1.87892300	−2.02254800	2.10966600
C	−2.79071600	−0.92864300	1.49093700	C	−2.78360900	−0.93874200	1.49330800
C	−2.69588600	2.88244000	1.59524300	C	−2.70482200	2.87349200	1.60380600
C	3.56262600	−2.86993400	0.25961700	C	3.56844200	−2.86715500	0.26070800
N	1.67501200	−0.54388800	1.03990300	N	1.67530000	−0.54467600	1.04103200
N	−1.98070900	0.01602400	0.66486900	N	−1.97903400	0.01052600	0.66926300
Si	2.82217600	−1.14774000	−0.10242100	Si	2.82438200	−1.14551400	−0.10114000
Si	−2.58781900	1.57588900	0.20139000	Si	−2.58922800	1.56744200	0.20712500
Zn	−0.11529200	−0.36782400	0.33315800	Zn	−0.11273400	−0.37443400	0.31192200
C	1.85006900	3.46113500	0.09285300	C	1.84412500	3.46254400	0.09929600
C	0.33381600	3.30132900	−0.04058500	C	0.32802000	3.29901100	−0.03207500
C	−1.05250700	−3.64683300	−1.51807800	C	−1.05299400	−3.63558100	−1.52861300
C	4.33927000	−0.06843200	−0.51948200	C	4.34445300	−0.06500700	−0.50943800
C	0.36036900	−3.05988500	−1.47471500	C	0.35995400	−3.05005500	−1.47599700
C	−4.32023000	1.60376100	−0.60076200	C	−4.32554600	1.59484700	−0.58998000
N	−0.04316800	2.34855100	−1.10086900	N	−0.04914200	2.34764200	−1.09398100
C	2.48152200	3.90513400	−1.23176500	C	2.47220900	3.91113100	−1.22549900
N	0.40626300	−1.58271400	−1.64088100	N	0.40919900	−1.57015100	−1.63828200
C	−1.50880600	2.25903500	−1.23119100	C	−1.51498600	2.25901500	−1.22338000
C	1.82636900	−1.15087100	−1.74276000	C	1.83255300	−1.14483300	−1.74164000
C	−1.80893700	−3.21914900	−2.78084600	C	−1.80188000	−3.20477200	−2.79484800
C	2.05273100	2.95043300	−2.35264900	C	2.04399900	2.95757900	−2.34771400
C	−1.75896500	−1.69302300	−2.91736800	C	−1.75129600	−1.67820400	−2.92721000
C	0.53028900	2.79143600	−2.38825900	C	0.52193600	2.79583500	−2.38192500

C	−0.31426900	−1.19432700	−2.88193300	C	−0.30687200	−1.17991000	−2.88412000
H	2.04826300	−1.50572200	4.34445300	H	2.04934800	−1.50293400	4.34589300
H	2.56829400	−2.39959100	2.90361700	H	2.57516100	−2.39476000	2.90438600
H	0.84921600	−2.08982500	3.17406700	H	0.85405400	−2.09488400	3.17393800
H	−4.03714400	−0.94213900	3.29192300	H	−4.02270100	−0.96455700	3.29943500
H	−4.25418600	0.50390100	2.30619500	H	−4.24439200	0.48834300	2.32317800
H	−2.78989900	0.32330900	3.29001900	H	−2.77569500	0.30239000	3.29985900
H	3.57473500	0.42422700	3.76049300	H	3.56033600	0.43654700	3.76677300
H	4.16451500	−0.50956800	2.38548200	H	4.16170700	−0.49624800	2.39461200
H	3.55611100	1.13986500	2.13546900	H	3.54418600	1.14887100	2.13913200
H	−0.04738800	0.38816500	2.96171100	H	−0.05689000	0.37863200	2.95428600
H	1.11657600	1.66876000	2.58590500	H	1.10230500	1.66510800	2.58710800
H	1.18306700	0.83799200	4.15320400	H	1.16723000	0.83073300	4.15359600
H	−4.44119800	−2.35633600	1.23710200	H	−4.42751600	−2.37402200	1.24015600
H	−4.57052000	−0.92496400	0.20307200	H	−4.57599500	−0.93085900	0.22361600
H	−3.40372900	−2.19063600	−0.19251000	H	−3.40527900	−2.18458100	−0.19861600
H	−1.30043600	−2.53751600	1.35705100	H	−1.29726800	−2.54928200	1.34290800
H	−2.48931200	−2.76299400	2.64398500	H	−2.47481100	−2.77521700	2.64104500
H	−1.19814900	−1.57125200	2.84211800	H	−1.17967200	−1.58448200	2.82743600
H	−3.63655200	2.79126700	2.15198300	H	−3.64327300	2.77272100	2.16311800
H	−1.87925600	2.79835200	2.32161400	H	−1.88380700	2.79515900	2.32604100
H	−2.66705900	3.89727400	1.17521200	H	−2.68511700	3.88787000	1.18158400
H	4.31491500	−2.81168000	1.05719500	H	4.31276700	−2.80905600	1.06603600
H	2.81503400	−3.60845100	0.57136200	H	2.81867600	−3.60891700	0.55973800
H	4.07421300	−3.26328900	−0.63032700	H	4.08815900	−3.25206600	−0.62844200
H	2.06087700	4.18935900	0.88722100	H	2.05374200	4.18975000	0.89549600
H	2.27874200	2.50218200	0.40849900	H	2.27562100	2.50352900	0.41133400
H	−0.08644700	2.95150800	0.90491900	H	−0.08922500	2.94527100	0.91350300
H	−0.12371700	4.29158200	−0.24920800	H	−0.13199300	4.28876600	−0.23768300
H	−0.97025100	−4.74011800	−1.46162800	H	−0.97022400	−4.72918200	−1.47397300
H	−1.61220700	−3.32805000	−0.63287400	H	−1.61777400	−3.31839900	−0.64578600
H	5.14425500	−0.17876700	0.21630100	H	5.14265600	−0.17124400	0.23460100
H	4.08825400	0.99671100	−0.57856200	H	4.09020000	0.99901600	−0.57630800
H	4.75266600	−0.36732100	−1.49398500	H	4.76430900	−0.36947700	−1.47963400
H	0.84498500	−3.30766100	−0.52674400	H	0.83848900	−3.30079400	−0.52553700
H	0.96640400	−3.51899100	−2.27820200	H	0.96909200	−3.50631400	−2.27779000
H	−5.11889300	1.35315800	0.10782200	H	−5.12085500	1.34373400	0.12251000
H	−4.53185500	2.61717400	−0.97066400	H	−4.53654500	2.60860800	−0.96004100
H	−4.40087100	0.91640500	−1.45201400	H	−4.40624700	0.90605500	−1.44020200
H	3.57552100	3.93933400	−1.14982400	H	3.56670100	3.94803100	−1.14489700
H	2.14952100	4.92616200	−1.47342600	H	2.13613100	4.93172400	−1.46452300
H	−1.92768100	3.25494000	−1.49531800	H	−1.93437400	3.25661700	−1.48106100
H	−1.72430000	1.61656400	−2.09651600	H	−1.73105700	1.62065300	−2.09157200
H	2.34009600	−1.73352000	−2.53026300	H	2.34279100	−1.73091800	−2.52821900
H	1.81788600	−0.11088100	−2.08924200	H	1.82823500	−0.10502200	−2.08884400
H	−2.84694300	−3.57262200	−2.74425800	H	−2.84039000	−3.55891900	−2.76526000

H	−1.34588400	−3.68316000	−3.66473000	H	−1.33191200	−3.66553100	−3.67684500
H	2.52044600	1.97062400	−2.19715800	H	2.51301800	1.97791800	−2.19420600
H	2.39338700	3.31581800	−3.33054900	H	2.38222100	3.32518100	−3.32590200
H	−2.32097400	−1.22448800	−2.10073900	H	−2.31780700	−1.21151300	−2.11226200
H	−2.21920100	−1.36919600	−3.86000300	H	−2.20542800	−1.35124600	−3.87204100
H	0.07219300	3.75978400	−2.68039400	H	0.06250200	3.76526800	−2.66813300
H	0.24270500	2.06612500	−3.15848300	H	0.23429600	2.07333300	−3.15459300
H	0.23823500	−1.59661500	−3.75206000	H	0.24969000	−1.58294500	−3.75038700
H	−0.27953600	−0.10381400	−2.95301800	H	−0.27090300	−0.08945700	−2.95431100

Tabelle 8.162 Standardorientierung von $[Me_2(CH_2NC_5H_{10})SiN(^iPr)Zn]_2$ in der Gasphase und in THF [B3LYP/6−31+G(d)].

$[Me_2(CH_2NC_5H_{10})SiN(^iPr)Zn]_2$				$[Me_2(CH_2NC_5H_{10})SiN(^iPr)Zn]_2$ in THF			
H	1.91026100	0.13891800	4.37232200	H	−1.89966400	−0.14513500	4.37676600
H	−1.91061000	−0.14830300	4.37153400	H	1.90042300	0.14595600	4.37641400
H	3.34278400	1.97337500	3.35279700	H	−3.32551500	−1.98126100	3.35658100
H	2.69441600	−1.08447500	3.35210600	H	−2.69207800	1.07772000	3.36034100
C	1.87364500	−0.35818300	3.39285400	C	−1.86728000	0.35552100	3.39845300
H	−2.69505200	1.07728000	3.35418700	H	2.69221600	−1.07743900	3.36015400
C	−1.87418600	0.35100400	3.39318200	C	1.86770800	−0.35491000	3.39822000
H	−0.93208900	0.90532400	3.33052800	H	0.92829000	−0.91348000	3.33297000
H	0.93147700	−0.91226900	3.32913400	H	−0.92809500	0.91445300	3.33295400
H	−3.34371000	−1.98033100	3.34767300	H	3.32688400	1.98116300	3.35574500
C	3.30560600	1.45166400	2.38752100	C	−3.29320600	−1.45727600	2.39191000
H	4.17551500	0.78302700	2.34546300	H	−4.16576200	−0.79170200	2.35239300
H	1.17804100	1.39627700	2.39359500	H	−1.16555900	−1.39292500	2.39254800
C	1.98830900	0.66484000	2.24401800	C	−1.97910300	−0.66446000	2.24562600
H	−4.17609500	−0.78745100	2.34303400	H	4.16649400	0.79123300	2.35145600
C	−3.30633600	−1.45636100	2.38362900	C	3.29418600	1.45712500	2.39111700
H	−1.17878700	−1.40138100	2.39022000	H	1.16649900	1.39354600	2.39200200
C	−1.98888800	−0.66946800	2.24207900	C	1.97977200	0.66476700	2.24514700
H	3.41429400	2.19623400	1.59122200	H	−3.40006900	−2.20034600	1.59396200
H	−4.54454300	1.89357900	1.71533600	H	4.53734800	−1.89882600	1.72423200
H	4.54526900	−1.89575500	1.71179400	H	−4.53719900	1.89876100	1.72444900
H	−3.14013600	2.93491400	1.45665300	H	3.13456400	−2.94276600	1.45418200
H	−3.41504400	−2.19902000	1.58555200	H	3.40114300	2.20010100	1.59309700
H	3.14173000	−2.93753800	1.45031600	H	−3.13498700	2.94322900	1.45346500
C	−3.84689800	2.26546000	0.95322000	C	3.84398100	−2.27060500	0.95769100
C	3.84805900	−2.26631100	0.94864700	C	−3.84419200	2.27043200	0.95753200
N	1.80508400	0.06136500	0.91217300	N	−1.80097800	−0.05670400	0.91773000
H	−4.43722600	2.86764400	0.24782700	H	4.43730400	−2.86847700	0.25081000
N	−1.80533700	−0.06315500	0.91155700	N	1.80130700	0.05675900	0.91741200
H	0.85313700	4.46919800	0.34341400	H	−0.86632000	−4.45979000	0.33706100
H	−1.01794000	2.84335400	0.51228800	H	1.00508400	−2.83693900	0.51461500
H	4.43897000	−2.86632800	0.24189500	H	−4.43798700	2.86763500	0.25047400
H	5.20392900	0.43950700	0.07613500	H	−5.20544100	−0.42766400	0.09398400

H	1.01932600	−2.84456500	0.50759000	H	−1.00545100	2.83643700	0.51476400
H	1.44378100	2.80224700	0.33445000	H	−1.45558500	−2.79113300	0.32778500
H	−0.85126300	−4.47075400	0.33619200	H	0.86572600	4.45956500	0.33753900
H	−5.20328700	−0.43980600	0.07575600	H	5.20570700	0.42722600	0.09306200
H	−1.44251200	−2.80402600	0.33121400	H	1.45524200	2.79099500	0.32769000
Si	3.00447200	−0.81098800	0.04466700	Si	−3.00038200	0.81471300	0.05120300
Si	−3.00431800	0.81162100	0.04589700	Si	3.00045800	−0.81499600	0.05087400
Zn	−0.00004400	−0.00075500	0.18042000	Zn	0.00010700	0.00003600	0.15544900
C	0.88594600	3.54456400	−0.24732500	C	−0.89698900	−3.53401700	−0.25276900
C	−0.54654200	3.04798500	−0.45187500	C	0.53678400	−3.03946900	−0.45172000
C	−0.88471600	−3.54484500	−0.25250500	C	0.89646900	3.53397000	−0.25256400
C	4.46774700	0.16961700	−0.69082100	C	−4.46955500	−0.16549800	−0.67641300
C	0.54747300	−3.04732300	−0.45674000	C	−0.53722800	3.03925400	−0.45154200
C	−4.46833200	−0.16667400	−0.69121700	C	4.46976800	0.16472200	−0.67716500
H	−1.14490500	3.83396600	−0.95060900	H	1.13460900	−3.82512000	−0.95072300
H	4.14811600	1.09766600	−1.17950100	H	−4.15109700	−1.09696800	−1.15947300
H	1.14583900	−3.83195300	−0.95755300	H	−1.13521000	3.82487000	−0.95040500
H	4.99393300	−0.43794000	−1.44152400	H	−4.99248400	0.44061000	−1.43084500
H	−4.99584200	0.44350000	−1.43884800	H	4.99259200	−0.44183600	−1.43130700
H	−4.14908200	−1.09276100	−1.18387600	H	4.15139300	1.09597000	−1.16071400
H	2.63801900	4.05948200	−1.43297600	H	−2.64620600	−4.04496900	−1.44484500
N	−0.61940400	1.80592100	−1.26687500	N	0.61551900	−1.79499700	−1.26515900
C	1.58953700	3.77668000	−1.58924600	C	−1.59627600	−3.76351600	−1.59747700
N	0.61948300	−1.80341500	−1.26904600	N	−0.61569500	1.79488600	−1.26515500
H	−2.63718800	−4.05792200	−1.43839000	H	2.64541500	4.04565300	−1.44471000
C	−2.04489300	1.44650200	−1.49817600	C	2.04505400	−1.44604100	−1.49521400
C	2.04480100	−1.44321300	−1.50042200	C	−2.04513900	1.44554100	−1.49508900
C	−1.58893400	−3.77423700	−1.59455300	C	1.59552700	3.76400600	−1.59728600
H	1.10988100	4.61240900	−2.12108400	H	−1.11492000	−4.59900300	−2.12839900
H	−2.57237300	2.29759600	−1.96944800	H	2.56691600	−2.30270400	−1.96206200
H	2.57215800	−2.29323300	−1.97370800	H	−2.56715300	2.30185200	−1.96240600
H	−1.10912500	−4.60850300	−2.12855500	H	1.11394000	4.59958900	−2.12784800
H	2.09494200	1.71297800	−1.97621800	H	−2.09761300	−1.69825600	−1.98579900
H	−2.09546400	−1.70987500	−1.97639800	H	2.09744200	1.69903700	−1.98665700
H	−2.05719200	0.63830900	−2.24160300	H	2.06432200	−0.64059500	−2.24140900
H	2.05643300	−0.63350500	−2.24219100	H	−2.06417300	0.63970100	−2.24084600
C	1.49672700	2.50456300	−2.44038500	C	−1.49839100	−2.49087200	−2.44749600
C	−1.49720800	−2.50010400	−2.44281000	C	1.49781400	2.49165100	−2.44783600
C	0.04734200	2.03529000	−2.57467600	C	−0.04803700	−2.02390200	−2.57710100
C	−0.04810200	−2.02990900	−2.57694700	C	0.04760000	2.02416200	−2.57721900
H	−0.53175100	2.79033900	−3.13937100	H	0.53163200	−2.78149500	−3.13679500
H	0.53091900	−2.78333200	−3.14385300	H	−0.53243400	2.78163500	−3.13669600
H	−0.00561100	1.10211200	−3.14527700	H	0.00901100	−1.09199300	−3.14899000
H	1.90512100	2.67274800	−3.44565000	H	−1.90217100	−2.65774400	−3.45505400
H	0.00412000	−1.09530900	−3.14526900	H	−0.00922700	1.09231600	−3.14923100
H	−1.90614100	−2.66611800	−3.44821700	H	1.90123800	2.65908900	−3.45544100

Tabelle 8.163 Standardorientierung des Liganden $Me_2(CH_2NC_7H_{104})SiN(^tBu)H$ und $Me_2(CH_2NC_7H_{104})SiN(^iPr)H$ [B3LYP/6−31+G(d)].

Ligand mit R = ^{t}Bu, R' = Me				Ligand mit R = ^{i}Pr, R' = Me			
C	−2.73758900	−0.19907400	1.07595300	**C**	2.56956400	−0.55612500	0.95514400
C	−3.46377300	1.14142800	0.84829300	**C**	3.41137800	−1.31517500	−0.08987600
C	2.23507400	−2.34858300	1.11860000	**C**	−2.57499300	0.63135400	2.14953700
C	−0.59460800	−1.36183500	0.58726400	**C**	0.34130000	0.49967900	1.27321300
C	3.38914200	1.34988100	1.51455800	**C**	−3.33474300	−2.38776600	−0.36732500
N	1.55980800	0.46529700	0.08342400	**N**	−1.63328400	−0.56678700	−0.51654700
N	−1.47695400	−0.22149500	0.29496200	**N**	1.31701000	−0.06672000	0.32905500
Si	1.21476100	−1.23781300	−0.03796500	**Si**	−1.44792000	0.73719600	0.62297200
C	2.80177800	1.25480700	0.08698800	**C**	−2.79593300	−1.18297600	−1.16149200
C	−3.69354300	1.45960900	−0.63173400	**C**	3.67685600	−0.49968200	−1.35790900
C	−1.68437600	−0.01084200	−1.16032300	**C**	1.55231900	0.80458800	−0.85042500
C	−2.37198800	1.34458200	−1.39826600	**C**	2.35407600	0.03436500	−1.91453100
C	1.45976400	−1.94314500	−1.78384800	**C**	−1.75726500	2.45209100	−0.13115000
C	3.83705400	0.61120700	−0.85165600	**C**	−3.90395000	−0.15716400	−1.42571200
H	0.76305700	0.98459900	0.44773800	**H**	−0.79485400	−1.14029200	−0.57695700
H	−3.40893600	−1.01776600	0.74521700	**H**	3.17084900	0.29775100	1.32812600
H	−4.42065700	1.11908700	1.38663400	**H**	4.35893500	−1.61747500	0.37547300
H	−2.85632100	1.93748500	1.30391600	**H**	2.87399500	−2.23803600	−0.35437600
H	2.17427200	−2.01128500	2.16070800	**H**	−2.48332500	−0.33900300	2.65315100
H	1.86887000	−3.38420900	1.08062200	**H**	−2.31750600	1.41281800	2.87830300
H	3.29560200	−2.37455500	0.83792300	**H**	−3.63183600	0.77257400	1.88967900
H	−0.47367300	−1.42066900	1.67363400	**H**	0.21190400	−0.21697300	2.09032500
H	−1.03409800	−2.33654300	0.29106900	**H**	0.69808100	1.43171700	1.75772400
H	2.65863900	1.79759700	2.19973400	**H**	−2.53995200	−3.12277400	−0.19113300
H	3.64130000	0.35412700	1.89642400	**H**	−3.71820500	−2.06741500	0.60949300
H	4.29824700	1.96571800	1.53709200	**H**	−4.14744500	−2.89081700	−0.90898600
H	−4.43767800	0.76700400	−1.04964600	**H**	4.35679600	0.33310500	−1.12936600
H	−4.11413400	2.46772600	−0.74332500	**H**	4.18722900	−1.11778400	−2.10830400
H	−0.67955600	0.06575000	−1.59019300	**H**	0.56062000	0.99323100	−1.27652100
H	−1.69131900	2.13957200	−1.06479900	**H**	1.74226500	−0.80926600	−2.26224000
H	−2.53094400	1.48758700	−2.47541300	**H**	2.52762900	0.68562500	−2.78138400
H	2.52569800	−2.03140600	−2.02844000	**H**	−2.82435400	2.60559500	−0.33603800
H	1.02756000	−2.95082000	−1.85344800	**H**	−1.44601900	3.24130900	0.56699500
H	0.99299400	−1.32373200	−2.55801000	**H**	−1.21523900	2.60272000	−1.07162200
H	4.10539900	−0.40046600	−0.52368800	**H**	−4.30689200	0.24762200	−0.48811000
H	3.45124600	0.55101700	−1.87533100	**H**	−3.53173700	0.67736500	−2.02956100
H	4.75895900	1.20428600	−0.86658300	**H**	−4.73674700	−0.62517000	−1.96325400
C	−2.40796400	−1.15957800	−1.89970500	**H**	−2.46439600	−1.55727700	−2.14298300
H	−2.42311300	−0.95168800	−2.97679800	**C**	2.18166100	2.18247000	−0.54037200
H	−1.89594000	−2.11751400	−1.76059000	**H**	2.26204500	2.76683600	−1.46542900
H	−3.44592900	−1.28655400	−1.57440600	**H**	1.56622800	2.76080000	0.15667600
C	−2.50158500	−0.38514400	2.58185700	**H**	3.18648900	2.10510200	−0.11135500

H	−2.20420300	−1.40420400	2.84707100	C	2.30821500	−1.48553400	2.14926300
H	−1.73078800	0.30808400	2.94208100	H	1.92897300	−0.95820100	3.02974500
H	−3.43058300	−0.16980100	3.12269700	H	1.59276900	−2.27249700	1.87887100
C	2.47580000	2.67297000	−0.42207000	H	3.24758300	−1.96814300	2.44369800
H	1.72901800	3.15581900	0.22222600				
H	3.37043100	3.30776800	−0.42716800				
H	2.07083000	2.63306300	−1.43961500				

Tabelle 8.164 Standardorientierung von **65**·$ZnEt_2$ (R = ^{i}Pr, R′ = H) und **65**·$ZnEt_2$ (ÜZ, R = ^{i}Pr, R′ = H) [B3LYP/6−31+G(d)].

65·$ZnEt_2$ (R = ^{i}Pr, R' = H)				**ÜZ**			
C	1.67014300	2.73874100	−2.30857900	C	1.06444600	2.81770000	2.28139000
C	0.47092700	1.84613400	−1.93096300	C	0.32883300	1.48446200	2.05170300
C	2.30892200	−1.25501500	−1.35754600	C	−2.27288200	−1.14766000	1.45998300
C	3.58811300	−0.59940300	−0.83384800	C	−3.55445500	−0.47668500	0.96377400
C	−2.83587500	−2.75491200	−1.14554000	C	2.96590200	−2.24032000	1.35316800
C	0.01935300	−1.89638400	−0.93034400	C	−0.00644200	−1.88813400	0.97761200
C	−4.50601400	0.34863800	0.10063700	C	2.52495100	0.94044400	−2.25501100
N	−2.02876200	0.11634400	−0.34672200	N	1.62822500	0.18099400	−0.03458800
N	1.20978300	−1.22745900	−0.36420900	N	−1.19243200	−1.16012800	0.43280300
C	−2.97788700	2.35414100	0.10764500	C	4.03781900	0.87426600	−0.22498600
Si	−1.69967200	−1.60970200	−0.14427300	Si	1.68648300	−1.54984400	0.13095100
Zn	0.39805300	1.18948100	−0.02844600	Zn	−0.42468100	0.89636900	−0.08730000
C	−3.08143800	0.85143900	0.39637500	C	2.59443800	1.05893400	−0.72337600
C	4.05777600	−1.26779800	0.46357900	C	−4.06999200	−1.14951500	−0.31478800
C	1.64027400	−1.89800600	0.88180700	C	−1.68250000	−1.83925700	−0.79869700
C	2.90906900	−1.28174500	1.47885100	C	−2.95326600	−1.20015600	−1.36505300
C	−1.87068200	−2.02594500	1.68878700	C	1.90206600	−2.52771600	−1.48477100
C	0.42050900	1.47463500	1.96189700	C	−1.21464000	2.21844300	−1.36845700
C	1.45882200	2.48947700	2.48165400	C	−2.46758500	2.99467800	−0.92422000
H	1.62470900	3.10039100	−3.34850500	H	0.86903700	3.25631900	3.27201400
H	2.62612100	2.20828400	−2.20054200	H	0.77385700	3.56846700	1.53473800
H	1.72908200	3.62663100	−1.66486100	H	2.15274600	2.69177500	2.19846300
H	0.41862300	0.99583800	−2.63107900	H	−0.75576100	1.66036200	2.18230400
H	−0.45641500	2.41737700	−2.10207500	H	0.57960300	0.77386800	2.85710000
H	−2.00811500	0.42556600	−1.31885700	H	1.11768100	0.75756900	1.00810600
H	1.95991300	−0.73735700	−2.25577700	H	−1.88217700	−0.63125000	2.34179600
H	2.52092400	−2.30545700	−1.64097700	H	−2.48815600	−2.19054500	1.75488600
H	4.36085200	−0.66175300	−1.61087800	H	−4.30553900	−0.52441100	1.76245200
H	3.39887200	0.46763300	−0.65642900	H	−3.36031400	0.58665800	0.77279300
H	−2.80690700	−2.51689600	−2.21687300	H	2.93799200	−1.70358900	2.30954600
H	−2.53287600	−3.80494400	−1.03496300	H	2.78016800	−3.30370600	1.55990500
H	−3.88010900	−2.67883400	−0.82106900	H	3.98648400	−2.15999800	0.95967700
H	−0.09683700	−1.53431600	−1.96258900	H	0.12368200	−1.54968500	2.01315400
H	0.20009800	−2.98650800	−1.02612100	H	−0.23216200	−2.96779400	1.03648800
H	−4.74562300	0.46665300	−0.96440200	H	2.85488500	−0.04852000	−2.59545600

H	−4.62667600	−0.70945500	0.35744000	H	1.50041700	1.09944700	−2.60957200
H	−5.24618700	0.91704000	0.67811800	H	3.17009000	1.68996500	−2.73187900
H	−3.15155700	2.55832500	−0.95778700	H	4.43376800	−0.10987600	−0.50894700
H	−3.73135500	2.90831200	0.67941000	H	4.70058700	1.63415400	−0.65889700
H	−1.99100700	2.74418300	0.37221700	H	4.08885300	0.95866700	0.86638400
H	−2.87345600	0.69461700	1.46217500	H	2.29958000	2.08995900	−0.47198700
H	4.37627300	−2.29939000	0.24967600	H	−4.40370100	−2.17167100	−0.08085000
H	4.93007400	−0.74540800	0.87592200	H	−4.94232800	−0.61350400	−0.70804400
H	1.81714900	−2.97316800	0.67442000	H	−1.87680700	−2.90060100	−0.55911800
H	0.82327700	−1.83894500	1.60473000	H	−0.87877100	−1.81774200	−1.53968800
H	2.69126300	−0.25823600	1.80457100	H	−2.72685600	−0.18621100	−1.71466800
H	3.18562200	−1.85242100	2.37499800	H	−3.26914300	−1.77885500	−2.24249500
H	−2.92592300	−2.01676500	1.99033100	H	2.94428500	−2.48446800	−1.82654700
H	−1.48682400	−3.03319700	1.89382100	H	1.66008300	−3.58809800	−1.32801800
H	−1.33527400	−1.32015100	2.33294600	H	1.27551200	−2.15597300	−2.30327100
H	−0.58463000	1.82064400	2.25067400	H	−0.40645900	2.93574300	−1.57702600
H	0.55461600	0.51659400	2.48713700	H	−1.41137200	1.72017200	−2.32978200
H	1.32462200	3.47688800	2.01964000	H	−2.30277700	3.52647000	0.02217900
H	2.48817000	2.17665600	2.25646100	H	−3.33115900	2.33266000	−0.77175700
H	1.40411300	2.63680900	3.57234800	H	−2.77687500	3.74802400	−1.66546600

Tabelle 8.165 Standardorientierung von **66**·$ZnEt_2$ (R = ^{t}Bu, R′ = H) und **66**·$ZnEt_2$ (ÜZ, R = ^{t}Bu, R′ = H) [B3LYP/6−31+G(d)].

66·$ZnEt_2$ (R = ^{t}Bu, R' = H)				**ÜZ**			
C	1.81756600	−2.38279500	2.64901800	C	0.86732800	2.76689200	2.30259900
C	0.56931300	−1.67961900	2.07689900	C	0.30357700	1.36092100	2.03752100
C	2.44404500	1.31313000	1.23503100	C	−2.50116800	−1.00795700	1.44443200
C	3.71887200	0.71612800	0.63622700	C	−3.74182200	−0.28701900	0.91610700
C	−2.71704900	2.66064700	1.44178600	C	2.64350100	−2.56402500	1.36444100
C	0.11275100	1.86186100	0.95682700	C	−0.27474700	−1.87629100	1.03119700
C	−4.45707800	−0.34544700	0.21257700	C	3.90761900	0.74754500	0.42731400
N	−1.95626600	−0.09311300	0.28171300	N	1.58397600	−0.00779300	−0.05634100
N	1.28405000	1.22396200	0.31501700	N	−1.40152400	−1.09479400	0.44133000
C	−2.92798500	−2.33439400	0.14549700	C	2.42050100	2.10192800	−1.06847700
Si	−1.64979800	1.64620100	0.24036600	Si	1.42974700	−1.73493600	0.15935700
Zn	0.64900100	−1.21391600	0.11713300	C	2.78449500	0.66874800	−0.63307700
C	−3.09575000	−0.86827900	−0.29553400	C	−4.26219300	−0.94852700	−0.36655400
C	4.07212700	1.39886300	−0.69055100	C	−1.90480200	−1.76970500	−0.78697200
C	1.60011700	1.89297900	−0.96615900	C	−3.12632000	−1.07172100	−1.38988700
C	2.86476600	1.34448200	−1.63388300	C	1.45084200	−2.80076200	−1.42044200
C	−1.88690200	2.38658300	−1.48263100	C	3.32604500	−0.07022000	−1.87398300
C	0.81702300	−1.77334000	−1.80344800	H	0.62236000	3.14578100	3.30650700
C	2.08685400	−2.57555400	−2.15409400	H	0.48071600	3.49973600	1.58188400
H	1.70373600	−2.65898200	3.70949400	H	1.96203900	2.78523700	2.21773100
H	2.71318100	−1.74955500	2.58177100	H	−0.79017400	1.39318800	2.20133400
H	2.04498700	−3.30771100	2.10215800	H	0.65794600	0.66613200	2.81743700

H	0.34973300	−0.78834200	2.68774900	H	1.08525300	0.63824600	0.98171600
H	−0.29723100	−2.34673400	2.21412300	H	−2.10415200	−0.49720500	2.32670000
H	−1.75750100	−0.45415500	1.21534600	H	−2.77067000	−2.03452300	1.75204500
H	2.17534800	0.79107900	2.15848400	H	−4.50966400	−0.29684700	1.70022800
H	2.62313800	2.37503000	1.49594100	H	−3.49964500	0.76480600	0.72191700
H	4.53371500	0.82404400	1.36372700	H	2.72889100	−2.00683900	2.30528300
H	3.57799900	−0.36164100	0.47563900	H	2.31311600	−3.58410800	1.60620300
H	−2.64197300	2.28251500	2.46954800	H	3.64991600	−2.64718100	0.93559000
H	−2.40389300	3.71357600	1.45469700	H	−0.12271000	−1.49657400	2.04859800
H	−3.77659500	2.63822800	1.16091300	H	−0.57833900	−2.93312300	1.14192500
H	0.04946800	1.46636300	1.97996500	H	3.56619000	1.29349200	1.31378500
H	0.29748400	2.94907100	1.07859800	H	4.22248800	−0.25110300	0.74865000
H	−4.50150400	−0.36927500	1.30827100	H	4.78919300	1.26597800	0.02796500
H	−4.63322200	0.68683100	−0.11186300	H	2.00471200	2.68192700	−0.23893300
H	−5.28129400	−0.95831900	−0.17400100	H	3.31315600	2.62857700	−1.42849400
H	−2.94650300	−2.42372400	1.23964300	H	1.68607900	2.08852200	−1.88076700
H	−3.74275700	−2.95034900	−0.25208800	H	−4.65398800	−1.94912300	−0.12925200
H	−1.97917900	−2.74581800	−0.21404200	H	−5.09654500	−0.37308300	−0.78584600
H	4.34804700	2.44710700	−0.49946600	H	−2.16172100	−2.81436100	−0.53279800
H	4.94432600	0.92084700	−1.15374300	H	−1.08907500	−1.80544700	−1.51307100
H	1.72124500	2.98068200	−0.78809900	H	−2.83691700	−0.07647800	−1.74674900
H	0.74593500	1.76770000	−1.63536900	H	−3.45287800	−1.64438200	−2.26738800
H	2.68598400	0.30963600	−1.94469600	H	2.47384700	−3.07721600	−1.70209400
H	3.05548100	1.92522100	−2.54583900	H	0.90061200	−3.73595000	−1.24697300
H	−2.95204900	2.50645300	−1.71538500	H	0.99936600	−2.30104700	−2.28472700
H	−1.43863900	3.38855800	−1.50906500	H	3.71316900	−1.06409000	−1.62142300
H	−1.43361400	1.79343500	−2.28256800	H	2.54497200	−0.18830300	−2.63362300
H	−0.06048200	−2.40043200	−2.02559300	H	4.15246000	0.49499500	−2.32363900
H	0.72903600	−0.90527100	−2.47430500	Zn	−0.45110400	0.88715300	−0.11859300
H	2.16730800	−3.48679500	−1.54627300	C	−1.22752200	2.26274400	−1.35701300
H	3.00541500	−1.99871000	−1.97602200	C	−2.56983500	2.92612700	−1.00229200
H	2.11241100	−2.89196400	−3.20913100	H	−0.45734800	3.04361300	−1.42295000
C	−3.05822700	−0.80386600	−1.83225600	H	−1.28685700	1.82908300	−2.36716100
H	−3.26888200	0.20328700	−2.20384900	H	−2.55225300	3.37516600	−0.00028100
H	−2.07931300	−1.11330700	−2.21040700	H	−3.40458400	2.21322000	−1.01929500
H	−3.81936600	−1.47211100	−2.25233500	H	−2.83244500	3.72982600	−1.70764700

Tabelle 8.166 Standardorientierung von [(*S*)−**69**]·$ZnEt_2$ (R = CH(Me)(Ph), R′ = H) und [(*S*)−**69**]·$ZnEt_2$ (ÜZ, R = CH(Me)(Ph), R′ = H) [B3LYP/6−31+G(d)].

[(S)−69]·$ZnEt_2$ [R = CH(Me)(Ph), R′ = H]				ÜZ			
C	2.62834200	2.59709100	−2.37422700	C	0.23199300	2.94228900	1.97309800
C	1.35789400	1.88592600	−1.86821100	C	−0.28191700	1.49531800	1.88618900
C	3.15461900	−1.25447500	−1.42828700	C	−3.16441300	−0.99980200	1.54285300
C	4.47155200	−0.65963200	−0.92590100	C	−4.43352800	−0.30729300	1.04459000
C	−2.02676200	−2.65013100	−1.06566300	C	1.98999600	−2.45246200	1.31139200
C	0.86492200	−1.85742200	−0.94528900	C	−0.94763000	−1.85825400	1.05687900

C	−3.57107000	0.48015800	0.21074800	**C**	3.28921200	0.30998900	−0.55364400
N	−1.10054700	0.19438500	−0.27457900	**N**	0.81546800	0.00624200	−0.20572900
N	2.08866400	−1.23050600	−0.39851000	**N**	−2.10772100	−1.10635400	0.49658900
C	−1.99492700	2.44534900	0.24053800	**C**	1.66580500	1.98590600	−1.48430900
Si	−0.82388300	−1.54742800	−0.10349200	**Si**	0.71844600	−1.71209100	0.11686000
Zn	1.36682800	1.18321400	0.02066600	**Zn**	−1.21354100	0.87052800	−0.15954600
C	−2.13508200	0.93356900	0.48502500	**C**	1.87604800	0.50688700	−1.10972700
C	4.96040900	−1.38476300	0.33336700	**C**	−4.99815200	−1.01125500	−0.19625800
C	2.53976100	−1.95081700	0.81293900	**C**	−2.65366300	−1.82390400	−0.68868100
C	3.84576500	−1.39265300	1.38568600	**C**	−3.90447300	−1.15422700	−1.26213200
C	−0.94446000	−1.97563000	1.73028200	**C**	0.78771800	−2.74323700	−1.47769200
C	1.45172700	1.43125300	2.01353500	**C**	−2.06228000	2.22837700	−1.37245200
C	2.53537200	2.40372500	2.52124700	**C**	−3.43485000	2.82331200	−1.01178500
H	2.51546000	3.00201700	−3.39277200	**H**	0.07113600	3.40055900	2.96079000
H	3.49456200	1.92210600	−2.39754900	**H**	−0.26065900	3.58899700	1.23504300
H	2.90340200	3.43949700	−1.72543400	**H**	1.31025400	3.00052900	1.77096800
H	1.09540600	1.07689800	−2.57124900	**H**	−1.35356600	1.49131200	2.16249600
H	0.51689900	2.59687700	−1.92236600	**H**	0.18585800	0.88235300	2.67528300
H	−1.04582200	0.53428900	−1.23395000	**H**	0.43360100	0.73661400	0.80921600
H	2.79226300	−0.69228300	−2.29424000	**H**	−2.73571100	−0.45784200	2.39152800
H	3.32326000	−2.29928200	−1.75722100	**H**	−3.40958300	−2.01846900	1.89376200
H	5.21583000	−0.72183800	−1.73026300	**H**	−5.16894100	−0.30176500	1.85920300
H	4.32679900	0.40676000	−0.70790100	**H**	−4.21085600	0.74048900	0.81018700
H	−1.99366500	−2.44874900	−2.14420100	**H**	2.00983700	−1.91511600	2.26735700
H	−1.78265500	−3.71149500	−0.92144200	**H**	1.75592500	−3.50545000	1.52272500
H	−3.06001200	−2.49733200	−0.73458100	**H**	3.00269200	−2.41546600	0.89443800
H	0.72997800	−1.47278600	−1.96692300	**H**	−0.74835600	−1.43815100	2.05081100
H	1.01644700	−2.94906800	−1.06778300	**H**	−1.23469400	−2.91214100	1.22385200
H	−1.92947500	0.74853800	1.54585000	**H**	1.83223200	−0.05933600	−2.05399300
H	−7.27167700	−0.59232900	−0.44752700	**H**	6.93280900	−0.12000500	0.79873700
H	−6.37684200	−0.53839100	1.87708700	**H**	6.34292400	−0.91224200	−1.48913500
H	−2.15661200	2.68875900	−0.81721100	**H**	1.67375000	2.62765300	−0.59665800
H	−2.73938200	2.99684200	0.82507200	**H**	2.46883000	2.32368700	−2.14957000
H	−0.99739900	2.79303700	0.52507300	**H**	0.71125500	2.12240700	−2.00249800
H	5.23617000	−2.41913300	0.07761700	**H**	−5.36913200	−2.00823000	0.08543200
H	5.86325600	−0.90495800	0.73150800	**H**	−5.85513300	−0.45626900	−0.59698400
H	2.67738600	−3.02355200	0.56739700	**H**	−2.89130600	−2.86161700	−0.39122400
H	1.74799300	−1.89126800	1.56330900	**H**	−1.86670500	−1.87768000	−1.44513800
H	3.67358500	−0.37324000	1.74972100	**H**	−3.63872800	−0.16767300	−1.65966400
H	4.13237100	−1.99938000	2.25462000	**H**	−4.26159700	−1.75521800	−2.10818600
H	−1.99106500	−1.94657000	2.05851100	**H**	1.82502400	−2.84598300	−1.82135800
H	−0.57866400	−2.99393800	1.91293700	**H**	0.40609300	−3.75840900	−1.30490900
H	−0.37334500	−1.28996400	2.36573000	**H**	0.21248900	−2.30279900	−2.30084000
H	0.46617700	1.80442700	2.33512700	**H**	−1.33034000	3.04719200	−1.42034100
H	1.56834000	0.46026400	2.51880700	**H**	−2.09908000	1.81322800	−2.39138800
H	2.41952400	3.40303400	2.08027400	**H**	−3.44180500	3.25491900	−0.00191700

H	3.54751500	2.06300700	2.26144900	H	−4.23605900	2.07337900	−1.04587000
H	2.51574200	2.53288400	3.61540400	H	−3.73108300	3.62697700	−1.70366200
C	−4.41545600	0.12259300	1.26999700	C	4.28376500	−0.28610500	−1.34064700
C	−5.74085300	−0.26216800	1.03950600	C	5.58913900	−0.44259600	−0.86136800
C	−6.24321200	−0.29276500	−0.26295200	C	5.92064100	0.00074900	0.42073700
C	−5.41181700	0.06589200	−1.32987800	C	4.93741900	0.60071900	1.21559500
C	−4.09080500	0.44860700	−1.09243400	C	3.63659900	0.75089700	0.73224000
H	−4.03342700	0.14603300	2.28927500	H	4.03510600	−0.63375100	−2.34230200
H	−3.45701600	0.72085200	−1.93407100	H	2.87795400	1.20637000	1.36314900
H	−5.79411100	0.04762100	−2.34770300	H	5.18472700	0.94933000	2.21570500

Tabelle 8.167 Standardorientierung von **67**·$ZnEt_2$ (R = C_2H_4OMe, R′ = H) und **67**·$ZnEt_2$ (ÜZ, R = C_2H_4OMe, R′ = H) [B3LYP/6−31+G(d)].

67·$ZnEt_2$ [R = C_2H_4OMe, R′ = H]				**ÜZ**			
C	−3.07990100	−1.48292300	1.50946400	C	0.57331600	1.42060500	3.59893400
C	−4.24788900	−1.53968900	0.51751300	C	−0.16627000	0.40668700	2.70591700
C	−1.77559000	−1.96682400	0.86849900	C	−2.67902600	−1.41273200	0.60148900
C	−2.13834400	2.40457800	2.45098700	C	−3.75495400	−0.44685900	0.10310000
C	−3.86648300	−0.79757700	−0.76891900	C	2.40970000	−3.08737000	1.24297900
C	1.76364000	−1.85029200	1.59588000	C	−0.41227900	−2.26199200	0.40714600
C	−0.94722200	1.55899500	1.95715500	N	1.53184400	−0.22917700	0.59929400
C	−2.54888200	−1.32672200	−1.33869000	N	−1.37020300	−1.22781100	−0.08679800
C	−0.20174300	−1.78509200	−0.97219000	Si	1.44956600	−1.89888100	0.11807800
C	2.73086800	−2.28331000	−1.30612700	Zn	−0.38689400	0.79624100	0.39774700
C	2.43211000	1.27619200	0.50544700	C	2.74141800	0.59583000	0.58347600
C	3.90329800	1.35637400	0.10783400	C	−3.95228400	−0.57433800	−1.41254700
C	−2.19634400	2.59471600	−2.40266300	C	−1.55376500	−1.37239800	−1.55654100
C	5.90873700	0.10344800	0.02011300	C	−2.60423100	−0.41524600	−2.12672100
C	−0.90671500	1.89835200	−1.92532900	C	1.99643500	−2.27175300	−1.66378000
H	−3.28586300	−2.10277700	2.39192000	C	−0.91153800	2.58610300	−0.32137900
H	−5.15237800	−1.10592600	0.96221000	C	−2.05583600	3.33258600	0.38704600
H	−4.48229100	−2.58845200	0.27936700	H	0.16445500	1.48183000	4.61959700
H	−2.94560200	−0.45476800	1.86382700	H	0.53034200	2.43315100	3.17594000
H	−1.86047400	−3.04771400	0.63521400	H	1.63707400	1.16298100	3.69908400
H	−2.11347900	2.58504700	3.53793500	H	−1.23494200	0.68934500	2.67222600
H	−0.94990400	−1.85411900	1.57493300	H	−0.16872800	−0.58367700	3.19238700
H	−3.10395800	1.92645200	2.23322400	H	0.82244200	0.00097600	1.63447200
H	1.51171900	−2.90755800	1.74788200	H	−2.50814200	−1.28089200	1.67434900
H	−0.92029200	0.60612900	2.50838700	H	−3.01437900	−2.45441700	0.44507600
H	1.16400000	−1.25717200	2.29535700	H	−4.68879400	−0.65819500	0.63963600
H	−4.64939700	−0.90301200	−1.53107200	H	−3.46845600	0.58177000	0.35527200
H	2.81922800	−1.71894900	1.86238700	H	2.10929000	−2.97919400	2.29243600
H	−3.76521200	0.27642700	−0.56246900	H	2.25372300	−4.13534800	0.95268000
H	−2.16137000	3.38947500	1.96515500	H	3.48967500	−2.89635700	1.18938900
H	−2.67739000	−2.38335700	−1.64753300	H	−0.52877300	−2.30872500	1.49694600
H	−0.01480200	2.07669100	2.23362200	H	−0.71072800	−3.25511200	0.02544500

H	−0.29462200	−2.88365600	−1.09146900	H	−4.37952900	−1.56164500	−1.64476100
H	2.36451400	0.94339200	1.54579700	H	−4.66851700	0.17413800	−1.77300700
H	−2.26460200	−0.75713200	−2.22887700	H	−1.84999600	−2.41588500	−1.77197800
H	2.58392500	−3.37008100	−1.24231700	H	−0.58637500	−1.20523300	−2.03735100
H	−0.13747900	−1.39108000	−1.99713600	H	−2.25109300	0.61723600	−2.02400900
H	3.75823900	−2.06017100	−1.00015100	H	−2.70545700	−0.61515100	−3.20128300
H	−3.05785100	1.91279200	−2.38938700	H	3.09051600	−2.32708400	−1.73307800
H	2.02513700	2.29645300	0.47681700	H	1.60549400	−3.24559400	−1.98955700
H	−2.45769700	3.44413900	−1.75739200	H	1.65809600	−1.51510700	−2.38060600
H	6.29790500	−0.88710300	0.26940200	H	0.00867600	3.18327700	−0.26059400
H	4.39267500	2.15954600	0.68634200	H	−1.12918600	2.50266400	−1.39614900
H	6.47347700	0.86404300	0.58193900	H	−1.85697400	3.45775600	1.45970200
H	2.62404600	−2.00009800	−2.36165800	H	−3.01468300	2.80238300	0.30256500
H	1.52156400	0.76350600	−1.27162300	H	−2.21750900	4.34018800	−0.02798900
H	−0.66036500	1.08089900	−2.62417800	H	2.53777200	1.51765700	1.14627500
H	−2.11853900	2.98572700	−3.43008400	H	3.58167100	0.09839700	1.09885000
H	−0.07172300	2.61486200	−2.01670100	C	3.25470100	1.00351600	−0.79753200
H	4.00011000	1.60796700	−0.96311100	H	4.16675700	1.61420800	−0.66911800
H	6.04549600	0.28576000	−1.05755300	H	3.53117500	0.11897600	−1.39533400
O	4.53768500	0.11552100	0.37413900	O	2.26386000	1.75289500	−1.47838600
Si	1.49979100	−1.35804800	−0.20452600	C	2.69399400	2.23488000	−2.73505100
Zn	−0.85948400	1.22507700	−0.02370100	H	1.86189200	2.79905000	−3.16438800
N	−1.43359600	−1.23036400	−0.36771900	H	3.56661100	2.90076200	−2.63370000
N	1.58673500	0.40588600	−0.31964800	H	2.96083400	1.40864300	−3.41453200

Tabelle 8.168 Standardorientierung von **64**·$ZnEt_2$ (R = Cy, R′ = H) und **64**·$ZnEt_2$ (ÜZ, R = Cy, R′ = H) [B3LYP/6−31+G(d)].

64·$ZnEt_2$ [R = Cy, R' = H]				**ÜZ**			
C	−1.69366600	−2.76217400	−2.49640000	C	−0.98533700	−1.91710500	2.77405300
C	−0.68375900	−1.68184600	−2.06152900	C	−0.05460200	−0.77638300	2.33022600
C	−3.23735200	0.74994800	−1.18251200	C	3.26015800	0.68432900	1.11425600
C	−4.26166200	−0.23724200	−0.61906300	C	4.20073500	−0.42891200	0.65237400
C	1.33453700	3.57178700	−1.13972700	C	−1.31644700	3.47802000	1.13337600
C	−1.17322200	1.96611400	−0.84757400	C	1.29622300	2.04591700	0.68614600
N	1.36238500	0.54566900	−0.50998800	N	−1.07335300	0.55611500	0.09724400
N	−2.10638500	0.98432400	−0.25381000	N	2.10858800	0.89632900	0.19148600
Si	0.61041000	2.10914000	−0.17032200	Si	−0.48915000	2.19581600	0.00152700
Zn	−0.67381700	−1.13634800	−0.12176100	Zn	0.63960300	−0.83267700	0.10641700
C	−4.80252600	0.24007700	0.73370900	C	4.71496400	−0.16848000	−0.76965300
C	−2.61464400	1.47543900	1.04545300	C	2.61644700	1.18652200	−1.17723000
C	−3.63255900	0.52528800	1.68261600	C	3.53479100	0.08713500	−1.71644100
C	0.78632400	2.44893800	1.67868400	C	−0.57308700	2.90145900	−1.76190400
C	−0.49808600	−1.52063500	1.84362500	C	0.90477500	−2.56331700	−0.87463100
C	−1.22292100	−2.78575900	2.34550400	C	2.04689800	−3.50433400	−0.45190500
H	−1.59875100	−3.03312800	−3.56035600	H	−0.83243200	−2.22133300	3.82060000
H	−2.73255100	−2.43870300	−2.34503200	H	−0.84361600	−2.81321900	2.15524300

H	−1.56575800	−3.68820600	−1.91986000	H	−2.04151700	−1.63021600	2.67831100
H	−0.81288500	−0.79140700	−2.69986700	H	0.99271000	−1.10093900	2.47925400
H	0.33280000	−2.04731000	−2.28131700	H	−0.15931400	0.08333700	3.01319200
H	1.35032200	0.29066800	−1.49787400	H	−0.70377200	−0.04580900	1.20647500
H	−2.82332600	0.37051200	−2.12156400	H	2.85178900	0.45921600	2.10422700
H	−3.73594500	1.71448300	−1.40505200	H	3.81925200	1.63404400	1.19655900
H	−5.07375600	−0.35766100	−1.34768500	H	5.03497400	−0.49547300	1.36254200
H	−3.78814700	−1.22128500	−0.50375200	H	3.67596200	−1.39109100	0.68934000
H	1.29160900	3.40026100	−2.22317900	H	−1.37125800	3.12739300	2.17138700
H	0.77744900	4.49544600	−0.93160000	H	−0.75839500	4.42500000	1.12808700
H	2.38321400	3.75421100	−0.87793800	H	−2.33895700	3.70588800	0.80725600
H	−1.03574300	1.68764600	−1.90282100	H	1.17406100	1.90566600	1.76774600
H	−1.63896800	2.97237900	−0.87320200	H	1.86751200	2.98367500	0.56298200
H	−5.39482900	1.15644800	0.58918900	H	5.37862400	0.70937600	−0.76372700
H	−5.47741400	−0.50846300	1.16748100	H	5.31479000	−1.01599500	−1.12318600
H	−3.08334300	2.47016100	0.89961000	H	3.16284700	2.14711900	−1.15234100
H	−1.76549400	1.61482400	1.71823200	H	1.75517900	1.32243100	−1.83632700
H	−3.13193800	−0.41346700	1.94595600	H	2.95809400	−0.83537700	−1.85131000
H	−3.98929900	0.97308700	2.61939200	H	3.89114600	0.39053500	−2.70921900
H	1.82303200	2.70938200	1.92751300	H	−1.59929200	3.20283400	−2.00884800
H	0.16065400	3.29858900	1.97954900	H	0.05329200	3.79864100	−1.85775700
H	0.50479000	1.58528300	2.29088800	H	−0.25356800	2.18302600	−2.52595700
H	0.57696500	−1.62060500	2.06211600	H	−0.04960100	−3.09633300	−0.76095100
H	−0.83078800	−0.65238500	2.43262000	H	0.98632100	−2.34771600	−1.95115300
H	−0.87838000	−3.68479400	1.81675500	H	1.99662600	−3.75412200	0.61643300
H	−2.30911800	−2.72772600	2.18724500	H	3.03691900	−3.06447800	−0.63155000
H	−1.06931200	−2.96920600	3.42123300	H	2.02443900	−4.45714600	−1.00350600
C	2.61649600	0.07526800	0.12285600	C	−2.40213300	0.22457800	−0.46777800
C	2.88174700	−1.39587800	−0.24234200	C	−2.48577700	−1.23183600	−0.95962500
C	3.85180600	0.93352200	−0.22606000	C	−3.54715600	0.50379400	0.53189000
H	2.45746800	0.12830600	1.20898000	H	−2.58235900	0.86042400	−1.35348600
C	4.16412000	−1.93602600	0.41144200	C	−3.86531300	−1.56662500	−1.55192300
H	2.97004500	−1.47606000	−1.33790300	H	−2.27908400	−1.90667700	−0.11609800
H	2.02089900	−2.00703300	0.04938800	H	−1.70268300	−1.40989800	−1.70645700
C	5.13669300	0.39966000	0.43067800	C	−4.93107900	0.17149300	−0.05207700
H	3.97288300	0.94346300	−1.32071000	H	−3.37326200	−0.10062100	1.43408900
H	3.68488900	1.97442400	0.07912100	H	−3.51546300	1.55305200	0.85099300
C	5.38672900	−1.07182500	0.06992300	C	−4.99789900	−1.27798000	−0.55546200
H	4.32906200	−2.97472300	0.09703900	H	−3.88975800	−2.61910000	−1.86450800
H	4.03012400	−1.96004000	1.50356400	H	−4.02454700	−0.96856500	−2.46280800
H	5.99266300	1.01956000	0.13283100	H	−5.70847700	0.35117000	0.70282100
H	5.05011800	0.49436200	1.52412400	H	−5.14729700	0.85428400	−0.88863600
H	6.27677600	−1.44618100	0.59258600	H	−5.97392700	−1.47755600	−1.01803600
H	5.59844100	−1.15050900	−1.00746900	H	−4.90953900	−1.96332800	0.30115800

Tabelle 8.169 Standardorientierung des $ZnEt_2$–Addukt mit R = Me, R′ = H und ÜZ [B3LYP/6–31+G(d)].

$ZnEt_2$–Addukt mit R = Me, R’ = H				ÜZ			
C	2.10512700	2.37790300	−2.27013500	C	0.95322100	3.37443900	1.65606300
C	0.68837300	1.91674300	−1.87606300	C	0.45722500	1.91629600	1.66200600
C	1.45709900	−1.68800500	−1.42058400	C	−1.53913400	−1.26223200	1.67998600
C	2.88275100	−1.46531000	−0.91050400	C	−2.97625800	−0.92931300	1.27546000
C	−3.93473000	−1.33267200	−1.07830000	C	3.80387400	−1.25417000	0.96570800
C	−0.91408300	−1.61449200	−0.94817400	C	0.77315300	−1.60333100	0.99920800
N	−2.06814800	0.97155300	−0.31677700	N	1.79901900	0.62761700	−0.39296200
N	0.43474000	−1.35656500	−0.40292300	N	−0.58927100	−1.20029300	0.53283300
Si	−2.40433600	−0.75689900	−0.11944300	Si	2.24526800	−1.02301500	−0.08958100
Zn	0.41294300	1.28339400	0.01623400	Zn	−0.33878400	0.89630700	−0.30389500
C	−2.82767100	1.99923600	0.41516900	C	2.54892400	1.49135400	−1.31127300
C	3.14459900	−2.27204600	0.36654900	C	−3.46538800	−1.85952900	0.15779100
C	0.65846500	−2.15154200	0.82176300	C	−1.04586400	−2.12656000	−0.53988400
C	2.06127400	−1.95792600	1.40463400	C	−2.47342400	−1.83737800	−1.01225100
C	−2.67367600	−1.08937300	1.71772600	C	2.48877700	−2.03320500	−1.67876400
C	0.57749200	1.48061100	2.00876000	C	−1.52488700	1.85595500	−1.60097200
C	1.90411600	2.07843800	2.51820900	C	−2.77499800	2.54955900	−1.02943100
H	2.16346500	2.74810400	−3.30645900	H	0.76135100	3.90426900	2.60178500
H	2.83829500	1.56449500	−2.18295800	H	0.47161200	3.95638300	0.85894200
H	2.45831000	3.19032300	−1.62110100	H	2.03614700	3.42570200	1.47635400
H	0.35167200	1.13933100	−2.58248800	H	−0.62814500	1.92030000	1.87591300
H	−0.00666300	2.76118100	−2.02613200	H	0.89571100	1.37297500	2.51604400
H	−1.96150200	1.24542400	−1.29271900	H	1.28781800	1.23892300	0.62105800
H	1.26929100	−1.06159700	−2.29833100	H	−1.18063100	−0.56485800	2.44315300
H	1.33808700	−2.74468700	−1.73555500	H	−1.50007300	−2.27757000	2.11425400
H	3.58908400	−1.74352500	−1.70337700	H	−3.61700300	−1.01172400	2.16258800
H	3.03036100	−0.39560400	−0.71176700	H	−3.02955400	0.11489000	0.94109600
H	−3.82263600	−1.17736600	−2.15906500	H	3.72715500	−0.71289300	1.91684100
H	−4.13237700	−2.40093300	−0.91758400	H	3.99092200	−2.31254200	1.19313400
H	−4.82947100	−0.78380200	−0.75759000	H	4.69106400	−0.87448500	0.44222700
H	−0.92867400	−1.23314800	−1.98020500	H	0.93502100	−1.11247200	1.96730100
H	−1.09719600	−2.70461300	−1.04112700	H	0.78914900	−2.68888100	1.20103100
H	−2.78849900	1.78845800	1.48718500	H	2.48948200	1.14305100	−2.35325100
H	3.13116300	−3.34710300	0.13071800	H	−3.55332700	−2.88470100	0.54811300
H	4.14074200	−2.04817700	0.76843500	H	−4.46528700	−1.56268000	−0.18139800
H	0.50032900	−3.22649700	0.59584800	H	−0.98676800	−3.16140500	−0.15585700
H	−0.09314600	−1.86461900	1.56132200	H	−0.34361500	−2.05201500	−1.37461300
H	2.16633900	−0.92257700	1.74896200	H	−2.50435000	−0.85935900	−1.50613800
H	2.16583700	−2.60319000	2.28660300	H	−2.74516100	−2.58614600	−1.76734600
H	−3.64968300	−0.70339200	2.03883000	H	3.44385300	−1.76883300	−2.15157500
H	−2.67160600	−2.16745100	1.92142000	H	2.52176900	−3.11056900	−1.46803300
H	−1.90665000	−0.62275000	2.34524500	H	1.70070300	−1.85802300	−2.42056700
H	−0.24974700	2.13295200	2.33257800	H	−0.88174900	2.61251900	−2.07547000
H	0.39612600	0.51642000	2.50849800	H	−1.81843400	1.17682000	−2.41509300

H	2.09149600	3.07036200	2.08542700	H	−2.51640800	3.26197600	−0.23502800
H	2.76683100	1.45263400	2.24984600	H	−3.48335500	1.83114100	−0.59415800
H	1.92732600	2.19790500	3.61349300	H	−3.32919900	3.11228400	−1.79693400
H	−3.88433100	2.06096200	0.11237400	H	2.13651500	2.50861100	−1.28882800
H	−2.37112500	2.98293800	0.25843900	H	3.61498600	1.56976300	−1.04554200

Tabelle 8.170 Standardorientierung des $ZnEt_2$–Addukt mit R = Ph, R′ = H und ÜZ [B3LYP/6−31+G(d)].

$ZnEt_2$–Addukt mit R = Ph, R' = H				**ÜZ**			
C	−1.49650100	−2.93009400	−2.37947600	C	−0.88017500	−2.02417900	2.84728400
C	−0.50555400	−1.83621700	−1.93432200	C	0.04195200	−0.88383500	2.37877100
C	−3.05518700	0.73629200	−1.29586400	C	3.11626500	0.82526800	1.05830000
C	−4.11374400	−0.20592900	−0.71865300	C	4.09249500	−0.24358000	0.56546000
C	1.64622300	3.43177400	−1.22965600	C	−1.67555500	3.28640300	1.23743500
C	−0.98227100	1.93245000	−0.95564900	C	1.06207900	2.07494300	0.69012800
C	3.60755700	−0.55848800	−1.18921300	C	−3.59248800	0.00271300	0.63955400
N	1.48017200	0.47537800	−0.55653800	N	−1.19318500	0.41465200	0.25590600
N	−1.94994800	0.99553600	−0.34425600	N	1.92767900	0.97370100	0.16986200
C	3.25169200	0.08180000	1.11188800	C	−2.59970800	−0.67758400	−1.45140700
Si	0.77999100	2.07902500	−0.22989800	Si	−0.75896600	2.09649100	0.08340700
Zn	−0.58121900	−1.26253700	−0.01230000	Zn	0.61743400	−0.86980300	0.15223600
C	2.77687300	0.01535600	−0.20942900	C	−2.45430300	−0.07578000	−0.18721700
C	−4.68746200	0.34602700	0.59152000	C	4.56022600	0.05251100	−0.86537100
C	−2.48709000	1.55641500	0.91372900	C	2.38065800	1.29583400	−1.21220000
C	−3.54271300	0.65639200	1.56272600	C	3.34672900	0.25392700	−1.78227700
C	0.88733500	2.53470800	1.59674600	C	−0.98908500	2.73490200	−1.68486300
C	−0.43732800	−1.46760200	1.96933500	C	0.83938800	−2.50643900	−0.97580500
C	−1.17959700	−2.67448600	2.57742500	C	1.92040300	−3.52368800	−0.56769100
H	−1.35851100	−3.22583700	−3.43149500	H	−0.66669200	−2.35446700	3.87525900
H	−2.54052200	−2.60488400	−2.27604800	H	−0.78764600	−2.90495100	2.19895100
H	−1.38759400	−3.84065100	−1.77564200	H	−1.93453800	−1.72196600	2.81684500
H	−0.61488200	−0.96221000	−2.59838200	H	1.09238300	−1.21685800	2.48022300
H	0.51970900	−2.20534500	−2.10208400	H	−0.02586300	−0.03031400	3.07381400
H	1.23987300	0.15651400	−1.49379100	H	−0.70861000	−0.13749800	1.30813900
H	−2.62050300	0.30601000	−2.20372900	H	2.75076300	0.58390500	2.06092600
H	−3.53103600	1.69633600	−1.58057800	H	3.63115700	1.80090100	1.12092900
H	−4.90473000	−0.34933600	−1.46598800	H	4.94495700	−0.28245800	1.25551500
H	−3.66129900	−1.19077400	−0.54014500	H	3.60860700	−1.22823500	0.60422300
H	1.56018500	3.26145000	−2.31024400	H	−1.57466300	2.99100900	2.28910800
H	1.22613800	4.42315300	−1.01413300	H	−1.29855600	4.31353800	1.13827200
H	2.71552200	3.46674800	−0.98593700	H	−2.74700200	3.30900700	1.00162400
H	−0.82487300	1.60894900	−1.99518700	H	0.99450000	1.93735700	1.77685900
H	−1.42568200	2.94625500	−1.03640900	H	1.56572300	3.04568600	0.53576300
H	5.49374900	−1.48363400	−1.63700500	H	−5.68667100	−0.42941700	0.87792600
C	4.87415000	−1.04209400	−0.86016200	C	−4.82540700	−0.49904600	0.21710400
H	2.61270800	0.47343200	1.89539600	H	−1.72866300	−0.75982100	−2.09653200
C	4.52673700	−0.38977900	1.43100000	C	−3.83456800	−1.17447100	−1.87446400

H	3.25464700	−0.62338700	−2.21678700	H	−3.49595900	0.45632200	1.62310000
H	−5.25726500	1.26448000	0.38405400	H	5.17843600	0.96287400	−0.86571200
H	−5.38985900	−0.36845700	1.03868700	H	5.19354600	−0.76064800	−1.24017000
H	−2.93121100	2.55255200	0.70992800	H	2.87008700	2.28668100	−1.19742700
H	−1.65616500	1.70968700	1.60581900	H	1.49561000	1.38361700	−1.84757900
H	−3.06927200	−0.27742500	1.88758400	H	2.81967800	−0.69783800	−1.91535100
H	−3.91980700	1.15555700	2.46480400	H	3.66295800	0.58660400	−2.77921100
H	1.91727600	2.79488600	1.86900900	H	−2.05746900	2.86584900	−1.89873800
H	0.26951100	3.42129800	1.79085600	H	−0.50677800	3.71260100	−1.81766800
H	0.55124800	1.73517000	2.26502700	H	−0.59059800	2.05324400	−2.44472500
H	0.63695300	−1.56233900	2.18956900	H	−0.14322100	−2.99920700	−0.95532600
H	−0.76095000	−0.54536000	2.47466500	H	0.99213300	−2.20697900	−2.02383800
H	−0.84216300	−3.62079800	2.13405000	H	1.78019200	−3.87515700	0.46306600
H	−2.26465400	−2.61863000	2.41163300	H	2.93237200	−3.09947700	−0.62533300
H	−1.02889700	−2.76010400	3.66527200	H	1.91685400	−4.41609200	−1.21267400
H	6.33683200	−1.32595700	0.70748100	H	−5.91545800	−1.48050400	−1.37201900
H	4.87020700	−0.32938800	2.46097100	H	−3.91767000	−1.63588600	−2.85598300
C	5.34862100	−0.95395600	0.45170300	C	−4.95604800	−1.08901100	−1.04397400

Tabelle 8.171 Standardorientierung des $ZnEt_2$–Addukt mit R = ^{t}Bu, R′ = Me und ÜZ [B3LYP/6−31+G(d)].

$ZnEt_2$–Addukt mit R = ^{t}Bu, R’ = Me				ÜZ			
C	1.23085200	3.24864600	−2.17793600	C	1.86903300	2.70862900	2.26840300
C	0.01007800	2.41623200	−1.73826400	C	0.85793700	1.57566700	2.01872100
C	2.64685100	−1.17561600	−1.35285700	C	−2.69437900	−0.66219700	1.15311700
C	3.76757900	−0.19098800	−0.97019200	C	−3.71034700	0.15489100	0.33743700
C	−2.22498200	−3.35921800	−0.57300200	C	2.45314300	−2.17687100	1.99416600
C	0.37220700	−1.91186800	−0.76837400	C	−0.38751100	−1.56870200	1.20210300
C	−4.26323300	−0.41283900	−1.46281600	C	4.12845000	−0.33659500	−0.63104700
N	−2.02512600	−0.28229900	−0.36231300	N	1.68771000	−0.05711000	−0.09809800
N	1.52213600	−1.07813400	−0.38014100	N	−1.38704000	−0.79134100	0.40880900
C	−3.49437400	1.69290000	−0.33617900	C	2.98636400	1.84225000	−1.02820000
Si	−1.32389300	−1.83516000	0.12445200	Si	1.39762800	−1.68301700	0.49426800
Zn	−0.01989700	1.89303900	0.17990200	Zn	−0.17447100	1.11912100	−0.04943700
C	−3.44730200	0.15378700	−0.27919000	C	2.78697600	0.31356000	−1.03820700
C	4.25349300	−0.36470000	0.47004800	C	−3.93308500	−0.38960900	−1.07609500
C	1.96100700	−1.32666000	1.02152800	C	−1.60647500	−1.41959700	−0.95051900
C	3.05414100	−0.31937800	1.41952800	C	−2.58561400	−0.57103700	−1.78068000
C	−1.31459800	−2.02908800	2.00843100	C	1.58140500	−3.11760400	−0.74267100
C	−0.00223900	1.92048200	2.16619700	C	−0.70258000	2.68592900	−1.19516600
C	0.83538600	3.05317100	2.79333500	C	−2.08088100	3.34856000	−1.02931300
H	1.18322200	3.53300200	−3.24047900	H	1.74116100	3.18861500	3.25062400
H	2.17212900	2.70176100	−2.03658000	H	1.78333700	3.49955200	1.51167500
H	1.31422000	4.17994700	−1.60226300	H	2.90343900	2.34001000	2.23010400
H	−0.06654600	1.51655400	−2.36687700	H	−0.15174400	1.99857700	2.17182300
H	−0.90613000	2.99431500	−1.93327400	H	0.95012500	0.81823500	2.81429000
H	−1.63860800	0.02939400	−1.25268300	H	1.45119100	0.72937300	0.90429300

C	2.21020000	−0.89316400	−2.79802500	C	−2.54204100	−0.03939300	2.54553100
H	0.09251300	−1.63867300	−1.79305100	H	−0.25578200	−1.04611100	2.15244000
H	3.06690300	−2.20137300	−1.33081200	H	−3.09461600	−1.68071200	1.28972800
H	4.60032800	−0.32040000	−1.67381300	H	−4.65729300	0.17048400	0.89202500
H	3.38737900	0.83119800	−1.10853800	H	−3.36031700	1.19349500	0.28425900
H	−2.23946400	−3.36437800	−1.67038400	H	2.45873000	−1.38883100	2.75700400
H	−1.72508400	−4.28101300	−0.24492400	H	2.07285900	−3.09506400	2.46374000
H	−3.26477400	−3.41842600	−0.22878000	H	3.49469300	−2.36591100	1.70745100
H	3.10097100	−0.79993000	−3.43010100	H	−3.54028000	0.10693000	2.97344700
H	0.64531900	−2.98516400	−0.83544200	H	−0.77892700	−2.56665500	1.45996300
H	−3.83715500	−0.08313500	−2.41916000	H	4.40322600	−0.05234800	0.39133700
H	−4.26674000	−1.50766300	−1.45404600	H	4.08483500	−1.43083100	−0.68195700
H	−5.30466200	−0.06808700	−1.42579500	H	4.93517100	−0.01279800	−1.30096300
H	−3.03035200	2.06742000	−1.25613400	H	3.27698900	2.19897600	−0.03593300
H	−4.53107000	2.05072100	−0.31461600	H	3.77755300	2.12305300	−1.73400900
H	−2.96427000	2.12973200	0.51746500	H	2.07312600	2.36633700	−1.32725100
H	4.78823300	−1.31942500	0.57172000	H	−4.47270400	−1.34541300	−1.02711600
H	4.97458600	0.42200700	0.72741100	H	−4.57044700	0.29541000	−1.64914300
H	1.08845000	−1.10845700	1.64309400	H	−0.62997100	−1.37010200	−1.44278800
H	2.61969000	0.68795000	1.40120400	H	−2.13830500	0.41220100	−1.96496900
H	3.36283400	−0.51432300	2.45495700	H	−2.71688500	−1.04797500	−2.76036400
H	−2.30278000	−2.33507800	2.37147300	H	2.63210300	−3.26559400	−1.02039700
H	−0.60599100	−2.81011900	2.31134200	H	1.24894500	−4.04771400	−0.26078200
H	−1.04264700	−1.10323000	2.52552600	H	1.00914100	−3.00129800	−1.66853200
H	−1.04772600	2.01491300	2.49762700	H	0.07163500	3.43720600	−0.97998700
H	0.34230400	0.95087800	2.55075600	H	−0.55437300	2.41169800	−2.25072500
H	0.49525800	4.04366600	2.46273400	H	−2.27656100	3.63465500	0.01293900
H	1.89690300	2.97514900	2.52268000	H	−2.89944800	2.68669000	−1.34072200
H	0.78584500	3.04922800	3.89315100	H	−2.17381600	4.26432100	−1.63351200
C	−4.06980000	−0.31084800	1.04645800	C	2.42798400	−0.11212800	−2.47816100
H	−4.13576500	−1.40303700	1.10739100	H	2.30667100	−1.19690300	−2.56052500
H	−3.48923400	0.05005300	1.90184500	H	1.49154600	0.36310600	−2.79313200
H	−5.08907500	0.08169400	1.13614100	H	3.21373300	0.19019200	−3.18292100
H	1.65390400	0.04912000	−2.85847400	H	−2.05330100	0.93919600	2.49769400
H	1.59735400	−1.69154300	−3.22716000	H	−1.98250400	−0.66907900	3.24211000
C	2.38832500	−2.77855800	1.33955000	C	−2.03117300	−2.90198700	−0.92902100
H	2.62015300	−2.86310800	2.40829300	H	−2.10855900	−3.25645500	−1.96359300
H	1.59224600	−3.49849100	1.12230100	H	−1.30047600	−3.53907300	−0.42530400
H	3.27813200	−3.09332600	0.78463100	H	−3.00447700	−3.06428200	−0.45632700

Tabelle 8.172 Standardorientierung des $ZnEt_2$–Addukt mit R = ^{i}Pr, R′ = Me und ÜZ [B3LYP/6−31+G(d)].

$ZnEt_2$–Addukt mit R = ^{i}Pr, R’ = Me				ÜZ			
C	−0.05573500	3.59772000	2.24432300	C	2.03013500	2.89776900	1.86812700
C	0.54535400	2.22488000	1.88512700	C	0.92239300	1.82684200	1.84844100
C	−2.82414700	−1.04143800	1.21125500	C	−2.48629100	−0.69199100	1.27343800
C	−3.70268600	0.21208000	1.03409100	C	−3.58258000	0.07142000	0.51135000

C	1.87544700	−3.59445600	0.34130300	**C**	2.72451600	−2.13589400	1.79175900
C	−0.68900700	−2.06446400	0.50265600	**C**	−0.16350400	−1.55478500	1.17143300
C	3.92988200	−0.79142500	1.72712600	**C**	4.22046500	0.24011100	−0.59904200
N	1.77947900	−0.50956100	0.45601000	**N**	1.75228800	0.06171700	−0.13132300
N	−1.65544700	−0.97749300	0.29364100	**N**	−1.23550800	−0.81488400	0.43638800
Si	1.06816200	−1.97881400	−0.25021700	**Si**	1.58524300	−1.59842300	0.37004100
Zn	0.65310100	1.80873700	−0.06211600	**Zn**	−0.15091500	1.12658000	−0.13890000
C	3.21819600	−0.14691700	0.52633100	**C**	2.79185100	0.63729800	−1.00827300
C	−4.12658400	0.44925600	−0.41671400	**C**	−3.90274900	−0.54061800	−0.85436000
C	−2.04488800	−0.82485500	−1.13362600	**C**	−1.53274900	−1.47909800	−0.89244200
C	−2.88875100	0.44934700	−1.31602300	**C**	−2.61107300	−0.69430100	−1.66069400
C	1.18294900	−1.95968600	−2.13819800	**C**	1.80161400	−2.91388700	−0.98492400
C	0.71853300	2.00569700	−2.04158900	**C**	−0.70915300	2.55458100	−1.43219800
C	0.43079700	3.42649000	−2.56617000	**C**	−1.86251700	3.48924700	−1.02548200
H	−0.08578300	3.77323000	3.33107900	**H**	2.03730000	3.49581900	2.79230000
H	−1.08559200	3.69862100	1.87671700	**H**	1.91858400	3.60087700	1.03201800
H	0.52079800	4.42182900	1.80373600	**H**	3.02754200	2.44627600	1.77424000
H	−0.04441100	1.43115200	2.36897100	**H**	−0.04642000	2.34310500	1.97129000
H	1.55815000	2.14985800	2.31278800	**H**	1.00421900	1.18306000	2.73956500
H	1.35497100	−0.32633800	1.36521300	**H**	1.45362200	0.84556500	0.84573500
C	−2.41194700	−1.14780200	2.68726100	**C**	−2.23867800	−0.01479800	2.62677300
H	−0.46757700	−2.11714500	1.57506800	**H**	0.01580800	−1.01204100	2.10372300
H	−3.44121800	−1.93215800	0.97558200	**H**	−2.85064000	−1.71333200	1.47563500
H	−4.58533700	0.11251700	1.67940600	**H**	−4.48148600	0.09411900	1.14046200
H	−3.13551000	1.08141800	1.39697500	**H**	−3.26140100	1.11436400	0.38430600
H	1.83544600	−3.69994600	1.43274600	**H**	2.71634700	−1.40469200	2.60950400
H	1.36175600	−4.46245800	−0.09439700	**H**	2.41659600	−3.10619700	2.20615500
H	2.92837600	−3.66006000	0.04089800	**H**	3.76292900	−2.24169100	1.45450900
H	−3.29296000	−0.98766000	3.31950800	**H**	−3.20330100	0.13893900	3.12361600
H	−1.11046000	−3.06250500	0.26010000	**H**	−0.51103200	−2.55663200	1.47021800
H	3.41480600	−0.54921400	2.66508600	**H**	4.40166000	0.46403000	0.45810400
H	3.96453900	−1.88286300	1.62987800	**H**	4.39698800	−0.83246200	−0.75630000
H	4.96053100	−0.42301500	1.80930100	**H**	4.96248400	0.78628400	−1.19563200
H	−4.82956200	−0.33378100	−0.73377800	**H**	−4.39328900	−1.51468800	−0.72077900
H	−4.66433300	1.40212100	−0.50594700	**H**	−4.61472800	0.09333000	−1.39739500
H	−1.10885900	−0.66671600	−1.67813500	**H**	−0.60038700	−1.39690100	−1.46077300
H	−2.26413100	1.31771200	−1.06915800	**H**	−2.22195300	0.29947000	−1.90707900
H	−3.16881000	0.54832200	−2.37290100	**H**	−2.80035500	−1.20572600	−2.61300500
H	2.17205000	−2.29393900	−2.47331400	**H**	2.85505600	−2.96795000	−1.28850800
H	0.44643000	−2.64936900	−2.57034700	**H**	1.53210700	−3.90619900	−0.59796500
H	1.00585900	−0.96627900	−2.56172800	**H**	1.21001400	−2.73308500	−1.88829900
H	1.71751300	1.68681300	−2.37653300	**H**	0.19966600	3.15717100	−1.58318900
H	0.01447000	1.29721400	−2.50158700	**H**	−0.92507600	2.10789900	−2.41392900
H	1.13843200	4.16212200	−2.16108700	**H**	−1.66839400	3.98005900	−0.06241100
H	−0.57518100	3.76750000	−2.28740400	**H**	−2.81398300	2.94977400	−0.92275700
H	0.49696800	3.49006500	−3.66350700	**H**	−2.03257400	4.28907100	−1.76307900

C	3.95002100	−0.44765000	−0.78416900	C	2.54465200	0.33465300	−2.49575700
H	4.03103100	−1.52652200	−0.96560400	H	2.63808300	−0.73785800	−2.70562700
H	3.44341000	0.01050000	−1.63911000	H	1.54063900	0.65636200	−2.79479700
H	4.96921200	−0.04762100	−0.73831400	H	3.27128200	0.86333100	−3.12669700
H	−1.67237100	−0.37773000	2.93916400	H	−1.76496700	0.96471500	2.50444800
H	−2.00364000	−2.12752000	2.95349900	H	−1.62118000	−0.61301000	3.30177600
C	−2.73277000	−2.05490000	−1.77100500	C	−1.88431300	−2.97795300	−0.80789100
H	−2.93504700	−1.85213300	−2.82974800	H	−2.06446100	−3.35309100	−1.82202100
H	−2.09960100	−2.94729200	−1.72705600	H	−1.07142500	−3.57312600	−0.38483700
H	−3.68697400	−2.30277300	−1.29456500	H	−2.78800400	−3.17328500	−0.22245300
H	3.25909200	0.94342800	0.67561000	H	2.71858100	1.72944400	−0.89065100

Tabelle 8.173 Standardorientierung von [$Me_3SiN(^tBu)H{\cdot}ZnEt_2$ und ÜZ [B3LYP/6−31+G(d)].

[$Me_3SiN(^tBu)H{\cdot}ZnEt_2$				ÜZ			
Si	−1.10006300	0.00026700	0.12248600	Si	1.64202500	−1.20204600	0.34160500
C	0.56555000	0.88449100	−0.03320100	C	0.53950200	−2.25459900	1.47491200
C	−2.49786600	1.26676400	−0.00480000	C	1.98775100	−2.24793900	−1.20606200
N	−1.12949100	−1.14766700	−1.23156700	N	0.71850600	0.27345600	0.00811500
C	−2.04496500	−2.30111600	−1.44448500	C	1.26051700	1.48711200	−0.68056600
C	−1.18785400	−0.79507800	1.84558100	C	3.28951500	−0.91778200	1.23959800
C	−1.97932600	−2.70567200	−2.93038000	C	0.08510100	2.33862100	−1.20856500
C	−3.48728600	−1.89701800	−1.10085300	C	2.15448000	1.12288800	−1.88185500
C	−1.62251400	−3.51167500	−0.58176900	C	2.07006500	2.34112800	0.32033400
Zn	−0.57741800	0.42877300	−3.78138000	Zn	−1.30747700	−0.13934300	−0.25873300
C	1.22291100	−0.39892400	−3.84144300	C	−1.29233000	0.69359300	1.90365600
C	2.18733600	0.19386200	−4.88859400	C	−1.95035200	2.08148800	1.99536300
C	−2.26925400	1.42926700	−4.01255600	C	−2.82179500	−0.78401400	−1.35607000
C	−2.60972200	1.82687800	−5.46281600	C	−4.04994400	−1.27484300	−0.56840500
H	1.41059000	0.18624900	0.02291600	H	0.31524500	−1.75804000	2.42548700
H	0.68442900	1.60441800	0.78688000	H	1.06141600	−3.19259300	1.70679900
H	0.65654300	1.44141400	−0.97344800	H	−0.41669900	−2.53816900	1.01303300
H	−3.48320100	0.83364700	0.20145800	H	2.74898700	−1.80625200	−1.85868000
H	−2.53705800	1.72525300	−0.99922100	H	1.07992600	−2.39208200	−1.80593200
H	−2.33567800	2.06842000	0.72850400	H	2.34676800	−3.24325400	−0.91002800
H	−2.13342100	−1.32375600	2.01832800	H	4.02811400	−0.39893300	0.61663400
H	−1.10581000	−0.01971700	2.61976600	H	3.72701100	−1.88541000	1.52102200
H	−0.37147900	−1.51015600	2.00720100	H	3.15767700	−0.33488900	2.15946400
H	−2.60997200	−3.58154700	−3.12575900	H	0.45083500	3.26473700	−1.66845300
H	−0.95344100	−2.96197000	−3.22339400	H	−0.60015300	2.62485100	−0.40246700
H	−2.32623800	−1.88778000	−3.57214000	H	−0.47966600	1.79546300	−1.97857300
H	−4.17247600	−2.71961400	−1.33543100	H	2.47089700	2.03079300	−2.41090500
H	−3.79680400	−1.01877600	−1.67725600	H	1.61655300	0.48579600	−2.59303100
H	−3.60448600	−1.67033900	−0.03476300	H	3.06254500	0.59612600	−1.56801400
H	−2.27605000	−4.37463800	−0.76350900	H	2.44869100	3.25279200	−0.15962900
H	−1.66565800	−3.27198900	0.48552700	H	2.92795100	1.78639500	0.71225300
H	−0.59483000	−3.81564600	−0.81929700	H	1.44407300	2.63895700	1.16946500

H	1.09599600	−1.47611000	−4.02921700	H	−0.59667200	0.56079000	2.74822500
H	1.67671100	−0.32136100	−2.84205000	H	−2.05285000	−0.08810300	2.08026600
H	3.16886000	−0.30388600	−4.87811900	H	−2.45970000	2.24938300	2.95587500
H	2.36971200	1.26266900	−4.71590100	H	−2.70167600	2.23664100	1.20839500
H	1.79148100	0.09789300	−5.90808000	H	−1.20860700	2.88455600	1.88723500
H	−2.21248100	2.33454200	−3.38934800	H	−2.44763900	−1.58309000	−2.01073300
H	−3.08558400	0.82865000	−3.58725500	H	−3.10944200	0.03961300	−2.02496500
H	−3.55397100	2.38872100	−5.52676900	H	−4.85672700	−1.60814300	−1.23816700
H	−2.71644700	0.94921900	−6.11404300	H	−4.46709600	−0.48672500	0.07094200
H	−1.83084400	2.46088500	−5.90643800	H	−3.80488400	−2.12197700	0.08487600
H	−0.18242900	−1.42604600	−1.48716600	H	−0.11352200	0.57160900	0.99828500

Tabelle 8.174 Standardorientierung von $[Me_2(CH_2NC_5H_{10})SiN(C_2H_4OMe)ZnEt]_2$ (**128**) und **67** (R = C_2H_4OMe, R′ = H) [B3LYP/6−31+G(d)].

$[Me_2(CH_2NC_5H_{10})SiN(C_2H_4OMe)ZnEt]_2$ (128)				67 (R = C_2H_4OMe, R' = H)			
C	2.30551100	0.47418700	2.26399400	C	2.92979000	−0.23489300	−1.08711100
C	6.99164500	0.21964400	0.98635600	C	3.48559000	1.19156900	−1.02306900
C	2.25070400	2.85769200	2.05906600	C	−1.52928400	−3.18723800	−1.09893100
C	1.49120800	−0.76005800	1.89443500	C	1.09010200	−1.70011500	−0.48440500
C	6.14730700	−1.04717500	0.81265700	N	−1.43653100	−0.29437300	−0.16662100
C	−1.39503700	−3.63839000	1.93394900	N	1.67881700	−0.36406000	−0.32984400
C	−1.96947100	1.68202900	2.32442200	Si	−0.74646600	−1.87805400	0.03213100
C	−1.97167400	−2.25018000	1.60304800	C	−2.85051500	0.04488800	−0.19501300
C	4.05483500	−1.99334200	0.06600900	C	3.69063600	1.63658800	0.43095100
C	−5.88926100	−1.13564500	1.07385500	C	1.87748600	−0.00557300	1.07778300
C	7.22895400	0.90909400	−0.36340000	C	2.39817200	1.42766800	1.23082600
C	−5.08010900	0.16186900	1.16655400	C	−0.97491200	−2.49690200	1.81011500
C	1.72197000	−3.78457900	−0.14310300	H	−0.85133500	0.39578000	−0.62955000
C	−7.22891500	−0.90919000	0.36326100	H	2.72732200	−0.51198000	−2.12850000
C	5.88928600	1.13555900	−1.07396600	H	3.69323300	−0.94759800	−0.70480000
C	5.08010600	−0.16194100	−1.16661400	H	4.42995200	1.23733500	−1.58145500
C	−1.72200700	3.78460100	0.14310400	H	2.77881200	1.86931600	−1.52113800
C	−4.05485500	1.99333500	−0.06600000	H	−1.45806600	−2.89651900	−2.15463600
C	−6.99158400	−0.21970700	−0.98647300	H	−1.03655100	−4.16260600	−0.98478000
C	1.97168400	2.25021200	−1.60299100	H	−2.59251500	−3.33547000	−0.86771400
C	−6.14728200	1.04712800	−0.81272300	H	1.11858700	−1.94798500	−1.55479800
C	1.96945400	−1.68199100	−2.32440300	H	1.70798300	−2.47779700	0.01682300
C	1.39509100	3.63845200	−1.93384600	H	4.49930900	1.04217600	0.88301200
C	−2.25071600	−2.85767600	−2.05902100	H	4.00817400	2.68658300	0.47409600
C	−1.49121600	0.76007300	−1.89441100	H	2.58920000	−0.71107100	1.56095500
C	−2.30551800	−0.47417400	−2.26396500	H	0.91990800	−0.10577300	1.59793100
H	2.44608000	0.53610300	3.35440300	H	1.62593700	2.12320400	0.87507100
H	2.41637600	3.00297400	3.13547500	H	2.56110700	1.63974700	2.29588000
H	5.93567700	−1.49504300	1.79141800	H	−2.04104400	−2.56574400	2.06597200
H	7.94434600	−0.04450000	1.46418500	H	−0.54765100	−3.50055900	1.93758500
H	−2.02444400	−4.19499200	2.64650100	H	−0.50332900	−1.83338600	2.54435700

H	2.04037100	−1.63809500	2.26931300
H	−0.39383400	−3.56970400	2.37861900
H	6.46837700	0.90729700	1.66563600
H	0.55631700	−0.73144300	2.47425900
H	3.28333200	0.45746400	1.76393700
H	−2.61141300	2.36893900	2.89184800
H	−2.11407400	−1.69557900	2.54322700
H	−0.93041200	1.88455500	2.61010400
H	−2.20947600	0.66354500	2.64597700
H	4.05201500	−2.44934400	1.06751400
H	3.21507900	2.87355900	1.53462200
H	−6.04489700	−1.53372100	2.08487900
H	6.72743700	−1.79975500	0.23499000
H	1.74049300	−4.03807600	0.92406100
H	1.61595900	3.65969200	1.67687900
H	−1.29741600	−4.26805800	1.03959900
H	−4.10665200	−0.04709500	1.61680600
H	−5.60518900	0.87488300	1.83989500
H	7.76221300	1.85881000	−0.22628800
H	−2.98335000	−2.37090900	1.18878700
H	4.55272600	−2.74960500	−0.58377600
H	−7.87210100	−0.27211000	0.98914700
H	7.87211100	0.27198800	−0.98928800
H	−5.30094200	−1.88225000	0.52341400
H	2.41104000	−4.46928600	−0.65620900
H	−7.76215200	−1.85891400	0.22611600
H	0.71092100	−4.00193900	−0.50811100
H	5.30099500	1.88218800	−0.52352600
H	−0.71097500	4.00198500	0.50814600
H	−2.41110700	4.46930500	0.65617300
H	−4.55277500	2.74956700	0.58379800
H	5.60515600	−0.87498300	−1.83994900
H	2.98336900	2.37089400	−1.18873800
H	4.10664200	0.04703000	−1.61684900
H	−6.72744500	1.79968100	−0.23505500
H	1.29749200	4.26809500	−1.03947500
H	6.04490500	1.53360900	−2.08500200
H	−1.74049600	4.03808100	−0.92406400
H	−1.61598400	−3.65967300	−1.67680800
H	−7.94427700	0.04442400	−1.46432400
H	−6.46828100	−0.90733400	−1.66575200
H	−4.05204100	2.44936000	−1.06749400
H	−3.21510500	−2.87353300	−1.53460200
H	2.61141700	−2.36887600	−2.89183600
H	2.20943700	−0.66349600	−2.64594200
H	2.11405400	1.69563500	−2.54318900
H	−3.40452300	−0.64765500	0.45293300
H	−3.28470100	−0.04569900	−1.20571300
C	−3.11555500	1.45888700	0.30672300
H	−4.20175000	1.65648800	0.32772600
H	−2.71756600	1.57914900	1.32783100
O	−2.47487700	2.37232000	−0.57329300
C	−2.59972500	3.72101100	−0.16792400
H	−2.14908400	3.88527500	0.82395700
H	−2.07244900	4.32956500	−0.90727900
H	−3.65612300	4.03310600	−0.13167200

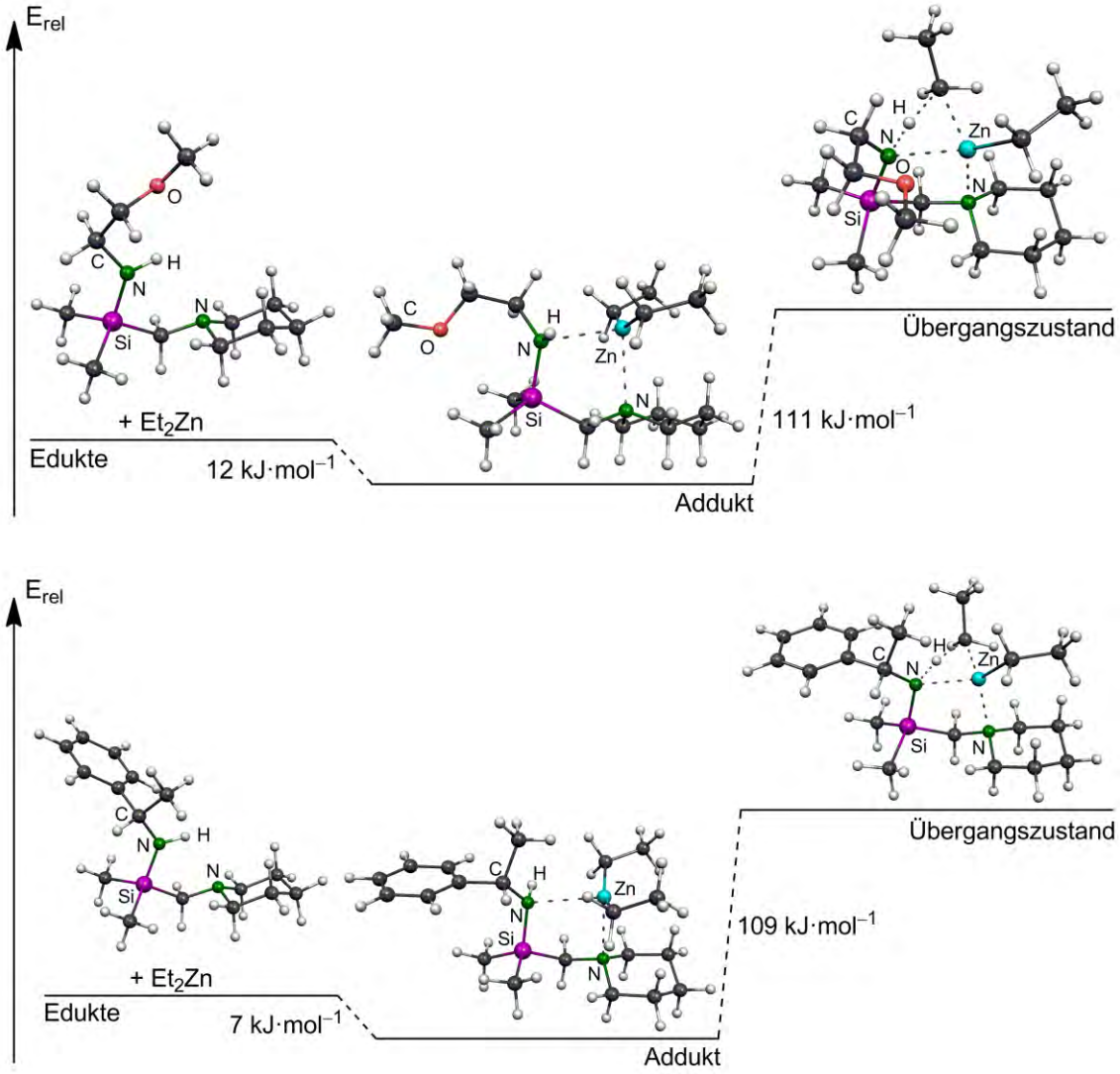
H	0.93040100	−1.88453900	−2.61009300
H	2.02451600	4.19505700	−2.64638000
H	−3.28334300	−0.45744700	−1.76391500
H	−5.93563500	1.49502200	−1.79146900
H	0.39388600	3.56981200	−2.37851700
H	−0.55632400	0.73146000	−2.47423400
H	−2.04038300	1.63810800	−2.26929200
H	−2.41636200	−3.00297200	−3.13543300
H	−2.44607700	−0.53609900	−3.35437500
N	4.86419400	−0.77164900	0.15028800
N	1.19970400	−0.84498200	0.43952500
N	−4.86417800	0.77161800	−0.15032800
N	−1.19971800	0.84500200	−0.43950100
O	1.56542000	1.63025100	1.82627400
O	−1.56543400	−1.63023500	−1.82622800
Si	2.20168000	−1.97260900	−0.46913500
Si	−2.20170100	1.97263100	0.46915000
Zn	−0.93400900	−1.06627300	0.34986300
Zn	0.93399400	1.06630500	−0.34982800

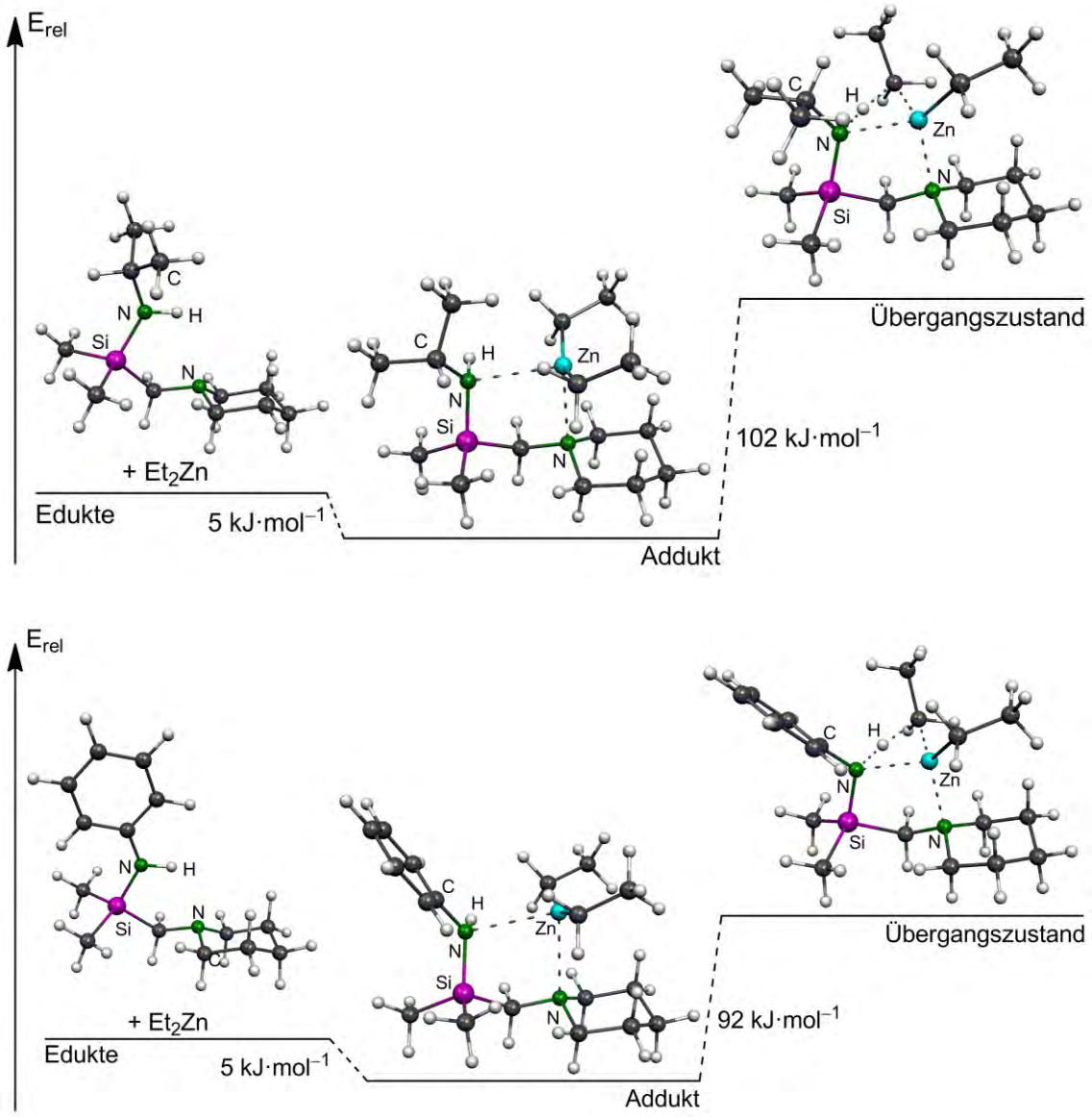
Tabelle 8.175 Standardorientierung von $Me_2(CH_2NC_5H_{10})SiN(Cy)ZnEt$ (**126**) und **64** (R = Cy, R′ = H) [B3LYP/6−31+G(d)].

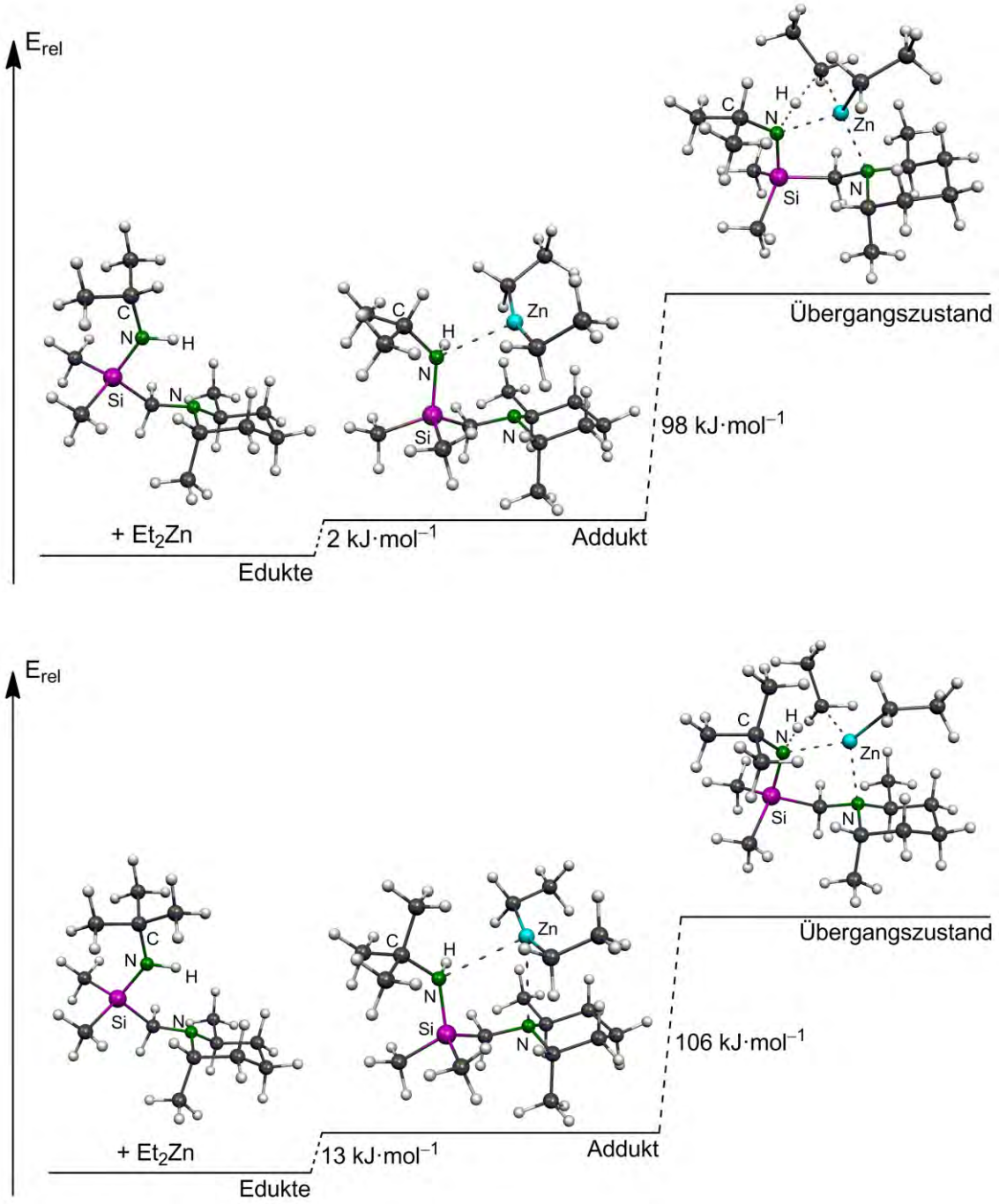
$Me_2(CH_2NC_5H_{10})SiN(Cy)ZnEt$ (126)				**64 (R = Cy, R' = H)**			
C	0.85276200	3.18650700	−1.79175800	**C**	−3.54880100	−0.07916800	−1.17142700
C	3.01203700	−0.23005800	−0.95090400	**C**	−3.97552700	−1.54985100	−1.22209300
C	−3.46438700	0.12792500	−0.90701600	**C**	0.58008200	3.32650700	−0.74001700
C	4.50358100	−0.41665900	−0.62417200	**C**	−1.87284600	1.50140400	−0.40202300
C	0.44343500	−3.68094700	−1.02688000	**N**	0.77036100	0.35260100	−0.24130400
C	−1.69194200	1.80062100	−0.81132300	**N**	−2.33948300	0.10807700	−0.35932200
C	−0.76374200	−2.76444900	−0.75264000	**Si**	−0.07416900	1.80585500	0.18586700
C	−4.09681000	−1.12760500	−0.30002300	**C**	−4.18736700	−2.11071300	0.19042600
C	2.23571200	0.44856900	0.19792700	**C**	−2.55650700	−0.36002500	1.01337000
C	4.70182100	−1.18885000	0.68976300	**C**	−2.94823500	−1.84130400	1.05410600
C	−4.36687200	−0.94900200	1.19992700	**C**	0.05884100	2.22173300	2.03469500
C	−2.50920100	0.76373700	1.23500000	**H**	0.19498200	−0.40323100	−0.60420800
C	0.26020500	3.33979800	1.17339200	**H**	−3.33944500	0.28602600	−2.18372700
C	2.45118400	−0.33557800	1.50918300	**H**	−4.38483500	0.53532200	−0.77172300
C	3.93935400	−0.52476500	1.84710300	**H**	−4.89308400	−1.64002300	−1.81837700
C	−3.08911900	−0.48210000	1.90878700	**H**	−3.19535300	−2.12766200	−1.73667700
H	0.79821200	2.62276000	−2.73156700	**H**	0.53669000	3.17948600	−1.82617500
H	−3.20913900	−0.04399200	−1.95860900	**H**	−0.00106700	4.22629100	−0.49565500
H	2.88716100	0.36010500	−1.86806900	**H**	1.62497700	3.53751400	−0.47611000
H	−1.70721200	1.66249600	−1.90113400	**H**	−1.89345500	1.82051900	−1.45341500
H	0.31800500	4.13604700	−1.93462700	**H**	−2.57515800	2.18032900	0.12935300
H	5.00860500	−0.93492400	−1.45059400	**H**	−5.06289900	−1.62519200	0.64777500

H	1.02083400	−3.34486900	−1.89790500	**H**	−4.40683700	−3.18559800	0.15201800
H	−1.45101900	−2.79988000	−1.61138000	**H**	−3.34700900	0.24543200	1.50888200
H	1.90816600	3.43590400	−1.61898400	**H**	−1.63357700	−0.20733300	1.58116400
H	−5.02788400	−1.34431100	−0.83959900	**H**	−2.10403100	−2.44094700	0.68654900
H	4.98341400	0.57089900	−0.53857900	**H**	−3.12729100	−2.13845000	2.09584800
H	0.13886200	−4.72016000	−1.22515500	**H**	1.10414800	2.41043800	2.31505400
H	2.55445000	−1.21270500	−1.14562800	**H**	−0.50707300	3.13196000	2.27532900
H	−4.19125800	0.96144800	−0.87928900	**H**	−0.31206500	1.41557500	2.67821800
H	−3.43006700	−1.98339900	−0.45684400	**C**	2.17508800	0.00919000	−0.04594200
H	−2.37652900	2.64359100	−0.60214300	**C**	2.35691700	−1.16422800	0.93949800
H	2.70411600	1.43931200	0.34843100	**C**	2.88603800	−0.29871300	−1.38014700
H	1.13658600	−3.70764300	−0.17600900	**H**	2.66812300	0.89026700	0.39484200
H	−1.33653300	−3.15984100	0.09936500	**C**	3.83402200	−1.54300000	1.13865100
H	5.77089800	−1.26315300	0.93099100	**H**	1.80548400	−2.03366700	0.54684500
H	4.33704400	−2.21948400	0.56139200	**H**	1.89025800	−0.90595800	1.89870200
H	−5.15907600	−0.19919300	1.34581400	**C**	4.36422200	−0.67467100	−1.18384300
H	−4.73294500	−1.88557400	1.63856500	**H**	2.35696800	−1.13202500	−1.86962800
H	−0.25651800	4.29309100	0.99615600	**H**	2.78923300	0.56700000	−2.04741700
H	−3.21917100	1.60595400	1.34141100	**C**	4.52646300	−1.84363700	−0.19977900
H	1.31171500	3.58005100	1.38166900	**H**	3.91343600	−2.40619700	1.81307400
H	4.39006000	0.45695400	2.06057500	**H**	4.35714500	−0.71172600	1.63657600
H	1.97111100	−1.32256400	1.40407000	**H**	4.82048700	−0.92381700	−2.15128600
H	−2.34190100	−1.28743100	1.89564800	**H**	4.91274800	0.19923500	−0.79891800
H	−1.57683700	1.06120000	1.72148200	**H**	5.59090800	−2.06012900	−0.03758100
H	1.92961600	0.18031800	2.32596500	**H**	4.08547100	−2.75130900	−0.63996300
H	−0.15635900	2.89419800	2.08456500				
H	4.04536800	−1.11936300	2.76469900				
H	−3.28834500	−0.25078000	2.96296400				
N	−2.22523400	0.54981900	−0.20514400				
N	0.81069000	0.62691400	−0.10889700				
Si	0.13354500	2.19083100	−0.33949600				
Zn	−0.34097800	−0.86055600	−0.38848700				

8.3.7.1 *Weitere Molekelbilder berechneter Strukturen*




E_rel
C
H
Zn
N
N
Si
Übergangszustand
C
N
H
Si
N
+ Et2Zn
C
H
Zn
N
Si
N
102 kJ·mol−1
Edukte
5 kJ·mol−1
Addukt
E_rel
C
H
Zn
N
Si
N
Übergangszustand
N
H
Si
N
C
+ Et2Zn
C
H
Zn
N
Si
N
92 kJ·mol−1
Edukte
5 kJ·mol−1
Addukt



8.3.8 Angaben zu den quantenchemischen Rechnungen aus Kapitel 4.5.5

8.176 Berechnete Energien der optimierten Verbindungen [B3LYP/6−31+G(d)].

Verbindung	SCF [Hartree]	ZPE [Hartree]
$^{t}BuNH_2{\cdot}ZnEt_2$	−2151.4374414	−2151.158291
$^{t}BuNH_2{\cdot}ZnEt_2$ (ÜZ)	−2151.37876066	−2151.105474

$(^t\text{BuNH}_2)_2\cdot\text{ZnEt}_2$	−2365.25651959	−2364.827054
$(^t\text{BuNH}_2)_2\cdot\text{ZnEt}_2$ (ÜZ)	−2365.20933546	−2364.785084

Tabelle 8.177 Standardorientierung von $^t\text{BuNH}_2\cdot\text{ZnEt}_2$ und $^t\text{BuNH}_2\cdot\text{ZnEt}_2$ (ÜZ) [B3LYP/6−31+G(d)].

$^t\text{BuNH}_2\cdot\text{ZnEt}_2$				ÜZ			
C	2.51570500	−0.12074500	0.02787300	C	−2.28645800	−0.30301800	0.03138500
N	1.23778800	−0.76471700	−0.39817800	N	−1.05151600	0.29953900	−0.51920300
C	2.67404200	1.18008000	−0.77256000	C	−2.62911000	−1.60121100	−0.72525600
C	3.71417400	−1.05424700	−0.23524700	C	−3.45218900	0.69786200	−0.09935800
C	2.40237000	0.18188500	1.52970000	C	−2.03771900	−0.61711700	1.51707000
H	1.27814700	−0.96598000	−1.39976800	H	−1.20512900	0.59061800	−1.48827200
Zn	−1.07337600	−0.01535500	−0.07362700	Zn	0.86433600	−0.29171400	−0.15847500
C	−1.74893600	−1.89299500	0.00227500	C	0.82343800	1.94372400	0.61826600
H	3.31882900	0.65743600	1.89711600	H	−2.92945500	−1.05875800	1.97657500
H	2.24978800	−0.73846800	2.10857200	H	−1.78256400	0.29105400	2.07537700
H	1.56216500	0.85525900	1.72872100	H	−1.21557900	−1.33623700	1.63588500
H	3.59662600	1.69702800	−0.48504500	H	−3.53855500	−2.06802400	−0.32512000
H	1.83023700	1.85369600	−0.59687100	H	−1.80965000	−2.32548300	−0.64463200
H	2.73147500	0.97495900	−1.84992000	H	−2.79700700	−1.39883900	−1.79092100
H	4.65632000	−0.58516700	0.07400200	H	−4.38136300	0.28307600	0.31128800
H	3.79617900	−1.29813700	−1.30232500	H	−3.63508900	0.94681700	−1.15291700
H	3.61099800	−1.99503200	0.32098800	H	−3.22470900	1.62827300	0.43337300
C	−1.05606100	1.97643800	−0.08363700	C	2.35307400	−1.59412500	−0.18282400
C	−3.27722300	−2.07819300	0.06517800	C	1.15621700	3.04868300	−0.40246400
H	−1.28835000	−2.37895200	0.87893800	H	1.75557800	1.61386600	1.11170200
H	−1.35252200	−2.43668600	−0.87158600	H	0.22923300	2.36062400	1.44843500
H	−3.57422800	−3.13774900	0.11244800	H	1.64120400	3.92664300	0.04980200
H	−3.77398600	−1.64622300	−0.81368300	H	0.24897200	3.41039700	−0.90701500
H	−3.70858500	−1.58554600	0.94650200	H	1.83157400	2.68502900	−1.18972300
C	−2.42324200	2.65526800	0.13068600	C	3.71621700	−1.05889900	0.29028300
H	−0.62885300	2.30969500	−1.04259800	H	2.43332700	−1.98214400	−1.20809300
H	−0.35054200	2.32505200	0.68670300	H	2.04864700	−2.45107700	0.43510500
H	−2.35531500	3.75436400	0.11219600	H	4.49314100	−1.83734000	0.25723900
H	−2.86714100	2.37882400	1.09627700	H	3.67442200	−0.68968000	1.32278600
H	−3.14595100	2.36701500	−0.64414600	H	4.06749200	−0.22725400	−0.33342800

Tabelle 8.178 Standardorientierung von $(^t\text{BuNH}_2)_2\cdot\text{ZnEt}_2$ und $(^t\text{BuNH}_2)_2\cdot\text{ZnEt}_2$ (ÜZ) [B3LYP/6−31+G(d)].

$(^t\text{BuNH}_2)_2\cdot\text{ZnEt}_2$				ÜZ			
C	−2.97853400	−1.00269800	−0.08775200	C	2.77476900	−0.75610600	−0.57600000
N	−1.63423300	−0.71704200	−0.66955300	N	1.47251100	−0.67410900	0.12081200
C	−2.76640800	−1.63325600	1.29633000	C	2.57562600	−1.31257300	−2.00018800
C	−3.77403900	−1.96621500	−0.99156500	C	3.73069100	−1.67872400	0.20867600
C	−3.72204600	0.33552500	0.03927400	C	3.37711200	0.65749800	−0.65603200
H	−1.10077900	−1.58557800	−0.73342900	H	1.11439400	−1.61737000	0.28589200
Zn	−0.09461200	1.03905200	0.05116900	Zn	0.00471600	0.77984800	−0.08754800
C	−0.16157000	2.02477600	−1.71422200	C	0.81888900	0.98779700	2.22034300
H	−4.72344100	0.18138400	0.45742800	H	4.34909900	0.63196500	−1.16307200
H	−3.83816900	0.81680400	−0.94019000	H	3.52550700	1.08018200	0.34406600
H	−3.17603300	1.02296200	0.69325800	H	2.72209600	1.33389600	−1.21781300
H	−3.73096800	−1.84269200	1.77300700	H	3.52808000	−1.38006200	−2.54271000
H	−2.19425200	−0.96564000	1.94707500	H	1.90055900	−0.66612000	−2.57347200
H	−2.22338100	−2.58470100	1.21637700	H	2.13720800	−2.31892000	−1.96761700
H	−4.76379800	−2.17968500	−0.56903900	H	4.70659500	−1.75947200	−0.28725700
H	−3.24658500	−2.92197800	−1.10834500	H	3.31450000	−2.69192000	0.29194200
H	−3.92307600	−1.53582100	−1.99045200	H	3.89107300	−1.29515300	1.22300300

C	−0.06884100	1.01827300	2.06198000	C	−0.40510800	2.37694400	−1.22065900
C	0.86404800	3.15692700	−1.92152700	C	0.66546000	0.05295700	3.43642300
H	−1.17511200	2.44500900	−1.82408700	H	−0.01573900	1.71458300	2.23091500
H	−0.06344900	1.29936600	−2.54311500	H	1.71748300	1.61314900	2.34653100
H	0.76832300	3.65873900	−2.89840600	H	0.62745600	0.57855900	4.40369600
H	1.90025500	2.79109800	−1.85985700	H	1.49825100	−0.66279700	3.49668200
H	0.76363600	3.93458800	−1.15261100	H	−0.25556900	−0.55052400	3.38067900
C	0.89673600	2.01952100	2.72686500	C	−1.46199900	3.34188100	−0.65054300
H	0.16164700	−0.00024200	2.41413300	H	−0.71506500	2.04182700	−2.22237400
H	−1.09038700	1.22404500	2.42069600	H	0.53587100	2.92443800	−1.37602900
H	0.86965200	1.97813900	3.82820400	H	−1.63638100	4.21142100	−1.30376300
H	0.66266000	3.05423600	2.44182400	H	−1.16407100	3.73510700	0.33059700
H	1.93992500	1.84072900	2.42998900	H	−2.43665500	2.85107800	−0.51620100
H	−1.74385500	−0.38170400	−1.62843400	H	1.31993400	0.03021200	1.16637800
C	2.71148400	−1.42441400	−0.17675200	C	−2.69068800	−1.19514100	−0.18176200
N	1.91602100	−0.29570300	−0.73429000	N	−1.77309500	−0.36886600	0.66778500
C	1.75531400	−2.61026900	0.02486000	C	−1.84744300	−2.28468900	−0.85922400
C	3.85561700	−1.82602100	−1.12981900	C	−3.78755700	−1.83610100	0.68955700
C	3.28439900	−0.96797300	1.17294300	C	−3.31991600	−0.26962200	−1.23245700
H	1.60747100	−0.52300200	−1.68114300	H	−1.39000400	−0.94783800	1.41818600
H	2.48313800	−0.66418700	1.85293600	H	−2.55167100	0.20862200	−1.84798200
H	3.96214700	−0.11396400	1.04312700	H	−3.91461100	0.52133900	−0.75833300
H	3.85608700	−1.77651500	1.64286400	H	−3.98709200	−0.83844600	−1.88950100
H	0.95112100	−2.34269400	0.71841500	H	−1.06099300	−1.84459700	−1.48060600
H	2.28914800	−3.47607300	0.43311900	H	−2.47855700	−2.91419100	−1.49625400
H	1.30677900	−2.92062600	−0.92923500	H	−1.37094800	−2.93744000	−0.11609400
H	3.46257900	−2.14418800	−2.10447900	H	−3.35229300	−2.49131700	1.45504700
H	4.44391900	−2.65604700	−0.71889300	H	−4.46886400	−2.44107800	0.07952200
H	4.53726600	−0.98287400	−1.29931500	H	−4.38603300	−1.06964100	1.19841200
H	2.51642700	0.52369600	−0.84329200	H	−2.31997400	0.35116500	1.14497800

8.3.9 Angaben zu den quantenchemischen Rechnungen aus Kapitel 4.6.3

8.179 Berechnete Energien der optimierten Verbindungen [B3LYP/6−31+G(d)].

Verbindung	SCF [Hartree]	ZPE [Hartree]
$(AlMe_3)_2$	−724.408239356	−724.191125
132	−1419.84054206	−1419.400731
133	−2119.701389	−2118.970238
134	−1395.26022101	−1394.751192
$Me_3Si(CH_2NC_5H_{10})$	−699.891823905	−699.6032
$(Me_2SiO)_3$	−1334.03145343	−1333.792417
$[(Me_2SiO)_3]\cdot AlMe_3$	−1696.23753265	−1695.889067

134·$AlMe_3$ (Koordination an N)	−1757.47955593	−1756.859608
134·$AlMe_3$ (Koordination an O)	−1757.45742373	−1756.837657
$Me_3SiOSiMe_2(CH_2NC_5H_{10})$	−1144.56806362	−1144.199902
$[Me_3SiOSiMe_2(CH_2NC_5H_{10})]\cdot AlMe_3$ (Koordination an N)	−1506.78886551	−1506.309204
$[Me_3SiOSiMe_2(CH_2NC_5H_{10})]\cdot AlMe_3$ (Koordination an O)	−1506.76559654	−1506.286537
$[Me_3SiOSiMe_2(CH_2NC_5H_{10})]\cdot 2AlMe_3$ (Koordination an N und O)	−1868.98179093	−1868.390926
$Me_2(CH_2NC_5H_{10})SiOAlMe_2$	−1057.61303794	−1057.282479
$[Me_2(CH_2NC_5H_{10})SiOAlMe_2]_2$	−2115.24083885	−2114.579765
$[H_3SiOSiMe_2(CH_2NMe_2)]\cdot AlMe_3$ (Gasphase)	−1272.05936565	−1271.732341
$[H_3SiOSiMe_2(CH_2NMe_2)]\cdot AlMe_3$ (Gasphase, ÜZ)	−1271.95967941	−1271.634042
$[H_3SiOSiMe_2(CH_2NMe_2)]\cdot AlMe_3$ (H_2O)	−1272.06560268	−1271.739942
$[H_3SiOSiMe_2(CH_2NMe_2)]\cdot AlMe_3$ (H_2O, ÜZ)	−1271.99157675	−1271.666515

Tabelle 8.180 Standardorientierung von **132** und **$Me_3SiOSiMe_2(CH_2NC_5H_{10})$** [B3LYP/6−31+G(d)].

132				$Me_3SiOSiMe_2(CH_2NC_5H_{10})$			
H	−1.17321300	−1.54631700	−2.89758900	H	2.32563000	−2.57130300	−1.42042700
H	0.28190200	0.95674900	−3.10340200	H	3.72239100	−3.09488600	−0.46402300
H	−0.90371000	2.20377300	−2.73484000	C	2.81023600	−2.48386400	−0.43969900
H	−0.66765000	−3.16944600	−2.38634000	H	2.13542200	−2.92422600	0.30526500
H	0.81181400	2.59326700	−2.69071800	H	3.89071000	0.00733800	−2.33433800
C	0.08014300	1.81111100	−2.44140500	Si	0.40696400	1.09232400	0.03130700
C	−1.22162600	−2.27231600	−2.07733600	C	4.34971700	0.04701300	−1.33837400
H	−2.27012900	−2.55659600	−1.94202400	C	0.50861200	2.30682800	1.47037500
H	1.48596100	−1.01790600	−1.91010600	H	5.29992800	−0.50114800	−1.38790300
H	2.77157100	0.85074000	−1.89229400	Si	3.20206700	−0.68294600	−0.02840400
H	−4.15028600	−1.13674800	−1.22871400	O	1.78938600	0.17764200	−0.01670900
H	4.21450400	−0.98823200	−1.01360900	C	0.27203200	2.03925500	−1.59710300
H	5.08708500	0.53791900	−0.99580300	H	4.94990200	−1.12394100	1.71310300
H	−3.28636200	2.12589000	−1.34881300	C	−1.03269800	−0.12121900	0.33577900
C	1.35624200	−1.14418200	−0.82892100	C	4.00428700	−0.56671700	1.67721500
C	2.95987200	0.77029600	−0.81843300	N	−2.35087300	0.54772900	0.33997600
C	4.25224500	−0.00203500	−0.53172300	C	−3.29007200	0.05233200	1.35630500
H	2.03594700	−1.94922900	−0.52607400	H	3.34730900	−0.97773800	2.45430500
Si	−0.49738600	−1.56231400	−0.49740200	C	−3.91944300	−1.31417000	1.02590600
H	3.04354800	1.79051900	−0.42211200	C	−4.60693200	−1.26435700	−0.34847200
Al	0.06379900	1.38977100	−0.50819800	C	−3.63266500	−0.74479000	−1.41836800
C	−4.06712100	−1.12871600	−0.13181200	H	4.22239100	0.47523500	1.94364800
H	−4.41084000	2.34744300	−0.01686200	C	−2.99857200	0.59112500	−0.97884500
N	1.73916400	0.16325400	−0.18873500	H	−0.43683900	2.85162300	1.58285600
C	−3.35792300	2.12150300	−0.25050400	H	1.30737300	3.04312100	1.31515900
H	−3.80671300	−2.14903000	0.18689200	H	0.71191200	1.78796000	2.41575600
O	−1.08197400	−0.01948500	−0.12743700	H	0.20936900	1.36327800	−2.45909000

H	−5.08683400	−0.95193300	0.24704200	H	1.15980100	2.66988400	−1.73656100
H	−0.18810100	−3.70741600	0.71023700	H	−0.60595500	2.69648700	−1.61453900
H	−2.77773300	2.97719300	0.12159500	H	−0.85355300	−0.53729500	1.33741900
H	−0.49117200	3.65981700	0.56320600	H	−0.98262900	−0.98855100	−0.34714500
Al	−2.91276800	0.35294100	0.57287800	H	−4.09299700	0.79986800	1.45080700
C	−0.69919800	−2.76179900	0.93681300	H	−2.77203100	0.02280600	2.32200200
H	5.36475400	−0.77801100	1.17282200	H	−4.63773900	−1.59016500	1.81039700
C	4.47972800	−0.16015500	0.97920600	H	−3.13951000	−2.08974400	1.02319800
H	−1.75661900	−2.99030000	1.10774400	H	−5.47509400	−0.58887700	−0.29165700
C	0.18040000	2.83455600	0.83338200	H	−4.99673500	−2.25245400	−0.62607300
H	1.19252900	3.26542100	0.88208000	H	−4.14788100	−0.60448800	−2.37865100
H	3.13430000	−1.82338900	1.35846200	H	−2.84640500	−1.49330200	−1.59201500
H	4.68135400	0.82720500	1.42033200	H	−2.26575600	0.92759200	−1.71905700
C	1.97405700	0.01936700	1.29047700	H	−3.78462300	1.36059400	−0.93592000
C	3.23915700	−0.76988700	1.64912700	H	4.58318300	1.09719400	−1.12162100
H	−0.29175800	−2.37336100	1.87683100				
H	1.08267200	−0.43253300	1.73225200				
H	−0.09184900	2.52527100	1.85047900				
H	2.05041500	1.03516300	1.69134200				
H	3.34469800	−0.76255900	2.74115600				
C	−2.65721100	0.32977900	2.55666400				
H	−2.30419700	−0.64223600	2.93480100				
H	−1.94730300	1.09224100	2.91084600				
H	−3.60953300	0.53173900	3.07140100				

Tabelle 8.181 Standardorientierung von **133** und **$[Me_2(CH_2NC_5H_{10})SiOAlMe_2]_2$** [B3LYP/6−31+G(d)].

133				**$[Me_2(CH_2NC_5H_{10})SiOAlMe_2]_2$**			
C	−5.31182200	−2.55262600	−0.88946800	H	1.76110700	−3.45318800	−1.58546800
C	−3.79034000	−2.35784000	−0.96644800	Al	−0.92583600	−1.09388300	−0.09119400
C	0.38454800	−1.70165700	−1.97577200	C	−1.29955400	−1.80922100	−1.89954600
C	−5.91122500	−1.64684800	0.19642900	H	2.66954600	−4.24443700	−0.28633300
C	−3.42348200	−0.87731100	−1.13435600	O	−0.97378900	0.78207000	0.00963400
C	5.29289400	−1.02677000	−1.79496200	C	−1.43353700	−2.04922800	1.56826300
C	5.92438000	−1.96206700	−0.75544300	C	1.85894500	−3.53355600	−0.49651300
C	3.81612600	−0.78742500	−1.47993900	H	0.93226800	−3.97501300	−0.11085200
C	1.16693800	−3.13051400	0.65065300	H	3.51996800	−1.20204600	−1.64146200
C	−5.47693500	−0.18846600	−0.00260900	H	4.16659900	0.83264900	−2.26347700
C	5.68747700	−1.41624800	0.65925200	Si	−2.23721700	1.86755500	0.30335100
C	−5.07471600	2.27115500	−2.21156500	H	6.29658800	−0.41858600	−1.84497900
C	−3.37973000	−0.23024000	1.27603700	H	6.64408900	1.24477800	−2.31206700
C	4.20636900	−1.12152400	0.91397000	C	3.76792900	−1.15115700	−0.57182000
C	2.11956500	−0.08527800	0.14779900	C	−2.42502400	2.10485500	2.16606400
C	−1.41805500	−1.13918000	3.31641500	C	4.72548800	0.99391400	−1.33612200
C	−1.86115600	2.11060500	−1.47909000	C	6.20928900	0.62671200	−1.51480600
C	3.56102700	2.63245500	−1.65993300	H	4.64306600	−1.81605800	−0.44517200
C	6.28633500	2.00685100	0.15706300	Si	2.23719700	−1.86752500	0.30340200
C	−0.91863200	1.62836400	2.10238500	H	4.64659700	2.06559700	−1.10151300
C	−4.16954400	3.12720900	0.88608600	N	4.04470900	0.26225200	−0.25021500
C	3.43297600	2.45134900	1.75233000	Al	0.92583100	1.09392800	−0.09137200
H	−5.55931700	−3.60379500	−0.69621700	O	0.97379100	−0.78201800	0.00973400
H	−5.75785800	−2.29588200	−1.86173700	C	−1.85906600	3.53356900	−0.49664500
H	−3.37382800	−2.91073700	−1.81858700	H	3.33555600	−2.66983000	2.40580800
H	1.19939900	−2.18059200	−2.53123800	C	−3.76798200	1.15109400	−0.57172500
H	−0.49982700	−2.34346800	−2.07797700	C	2.42507600	−2.10477000	2.16612100
H	−3.31145300	−2.77055100	−0.06845800	C	1.43377100	2.04956300	1.56783800
H	5.36251400	−1.45805100	−2.80173300	H	8.01617900	0.48800500	−0.29641700
H	0.16119300	−0.74536800	−2.46370100	N	−4.04468100	−0.26229400	−0.24988800
H	−7.00789000	−1.67847300	0.16494600	C	6.97515800	0.82176000	−0.19642600
H	5.47837700	−2.96442900	−0.84726100	C	−4.72518900	−0.99420300	−1.33581700
H	−5.62391100	−2.01086900	1.19149400	H	1.57078800	−2.66815000	2.56127800

H	−3.81785400	−0.51252000	−2.09024900	C	−6.20893200	−0.62705200	−1.51497100
H	3.28357200	−1.74867400	−1.54869800	H	6.38132200	−1.00992800	0.80175300
H	1.98933100	−3.66341000	0.15747400	C	−6.97516000	−0.82185100	−0.19676300
H	6.99879500	−2.07677400	−0.94268100	C	1.29946300	1.80899200	−1.89983000
H	0.27707600	−3.77026400	0.58227900	H	7.01101900	1.89605100	0.04295200
H	−2.34349900	−0.73750200	−1.14738200	C	4.77923600	0.45306400	1.01389400
H	3.36195700	−0.10088800	−2.19921900	H	2.50761800	2.27081300	1.60739800
H	−5.88903700	0.18250400	−0.94561600	C	−6.27270000	−0.07388300	0.94776900
H	5.82860200	−0.07214200	−1.81859200	C	6.27238100	0.07403100	0.94806900
H	−5.07621700	1.47438300	−2.97168700	H	2.46465800	−1.15250600	2.70660700
H	−3.67505000	−1.23067600	1.61997000	H	4.27662300	−0.10991100	1.80530300
H	−1.64968200	−2.19598400	3.13340700	H	−2.14952200	−2.50414800	−1.90725000
H	3.64543400	−2.06684100	0.92858300	H	4.69586400	1.51628500	1.28014000
H	1.41906200	−3.02993800	1.71314500	H	6.74447000	0.30586600	1.91243500
H	−5.86000000	0.45407100	0.79567500	C	−4.77955900	−0.45282100	1.01407400
H	6.02162700	−2.13912500	1.41472000	H	−0.43656000	−2.35504400	−2.30583700
H	4.09144400	2.28504900	−2.55956500	H	−1.52903900	−1.00980000	−2.61849100
H	−6.11127500	2.39215100	−1.86437400	H	1.18345400	1.48038000	2.47462800
H	1.76556300	0.77450700	−0.43515600	H	0.91572800	3.01704500	1.65027500
H	−1.85339000	1.76450700	−2.52403900	H	2.14941400	2.50393100	−1.90770200
H	−4.82571100	3.19701100	−2.75476700	H	−0.91592000	−3.01695800	1.65047500
H	6.27501100	−0.50596600	0.80576100	H	−2.50747400	−2.26994500	1.60833000
H	−1.09185700	1.53539400	−0.94913300	H	−1.18252000	−1.48014100	2.47492000
H	−3.86821200	0.47069900	1.96600800	H	−3.33529300	2.67025700	2.40574700
H	−0.41377000	−1.08943500	3.75618800	H	−1.57053200	2.66793700	2.56120200
H	6.86947200	1.53296000	−0.64458100	H	−2.46494600	1.15261800	2.70656600
H	2.48614700	2.48819700	−1.84100200	H	−1.76073500	3.45310600	−1.58554600
H	−2.12091800	−0.76991300	4.07504900	H	0.43642600	2.35477700	−2.30610000
H	2.01242100	0.21584000	1.19523700	H	−0.93269600	3.97536800	−0.11063600
H	4.07067300	−0.64152300	1.88848500	H	−2.66999100	4.24421200	−0.28689900
H	3.71426100	3.72287200	−1.62573200	H	−3.52012500	1.20187100	−1.64139500
H	−1.50654700	3.15291900	−1.50120400	H	−4.64313700	1.81595900	−0.44506600
H	6.70749200	1.67052200	1.11569100	H	−4.64635000	−2.06582700	−1.10092800
H	−5.18106400	2.92180000	1.26984100	H	−4.16604500	−0.83315300	−2.26305100
H	6.51033700	3.08485200	0.09495700	H	−6.64351400	−1.24526500	−2.31223400
H	−0.96848600	2.29417500	1.23689700	H	−6.29613700	0.41818600	−1.84535600
H	0.12126700	1.60545700	2.45209600	H	−7.01108500	−1.89609400	0.04281200
H	−3.47595800	3.03033700	1.73180500	H	−8.01615300	−0.48810900	−0.29709300
H	−1.52095700	2.07544400	2.90334800	H	−6.74501400	−0.30556900	1.91206200
H	2.35873900	2.66900000	1.67397800	H	−6.38168500	1.01004300	0.80123600
H	−4.16751200	4.19375300	0.61097900	H	−4.27719100	0.11040000	1.80546400
H	3.56422800	1.74898000	2.59071200	H	−4.69620000	−1.51596700	1.28063800
H	3.91579600	3.38783700	2.07251600	H	1.52883300	1.00953800	−2.61876000
O	−0.55547800	−0.82422900	0.57097800				
Al	−3.72573500	2.05602100	−0.74546000				
Al	4.29044800	1.86739100	0.03926000				
Si	0.79956300	−1.46202600	−0.15368400				
Si	−1.51105700	−0.11453000	1.73003700				
N	−3.98538900	0.02399300	−0.07408100				
N	3.59492600	−0.22029900	−0.11446500				

Tabelle 8.182 Standardorientierung von **134** und **[$Me_3SiOSiMe_2(CH_2NC_5H_{10})$]·2$AlMe_3$** [B3LYP/6−31+G(d)].

134				**[$Me_3SiOSiMe_2(CH_2NC_5H_{10})$]·2$AlMe_3$**			
H	−0.84411200	2.08604600	−2.91913200	H	2.89618300	0.47261000	−2.64813400
H	−2.05431800	3.26116700	−2.37334400	Al	3.24176600	1.31038600	0.58029800
C	−1.15112600	2.71365000	−2.07294300	C	2.09178100	2.83818600	0.00108300
H	−0.35624600	3.45085800	−1.90405300	H	2.89564300	−1.08048700	−3.49630100
H	−2.23517700	−0.24847500	−1.75190900	C	3.71593500	1.06338200	2.50149500
H	−2.67374400	−2.28370600	−1.00704500	C	4.87409000	1.17241600	−0.56570600
Si	1.01427200	−0.04831500	0.72916700	C	2.39859800	−0.49840500	−2.70886500

H	−4.84403900	−1.47165700	−1.96087100
H	−5.04076000	−3.09004800	−1.28684800
C	−2.73936500	0.34864000	−0.97833400
C	0.89571600	0.32870400	2.57270600
C	−3.46845600	−1.92789300	−0.34131000
C	−4.84613300	−2.04192800	−1.02060800
H	−3.60597600	0.80794200	−1.49319900
Si	−1.44888900	1.67963900	−0.52106000
H	−3.45574200	−2.57990800	0.54608600
N	−3.12269200	−0.57057600	0.11010700
O	−0.02334700	0.93266300	−0.12830600
C	0.53631000	−1.84692600	0.41348500
H	−2.92395100	3.30521000	0.70464300
C	2.74310100	0.44254000	0.08731000
C	−1.96294700	2.81235300	0.90191100
H	−6.92099500	−1.51257000	−0.59032200
N	3.86304500	−0.28119600	0.71802200
C	−5.94433200	−1.50401400	−0.08888200
C	5.10928800	0.49474200	0.81284900
H	−1.21116100	3.60022000	1.04140500
C	5.86597600	0.64652500	−0.52060800
H	−5.66064900	0.61478800	−0.44933700
C	6.15093600	−0.73544600	−1.13165400
H	−6.03329000	−2.17074300	0.78337600
C	−4.17411300	−0.05068200	0.99741200
C	4.85686400	−1.55891100	−1.22943200
C	−5.59331800	−0.08719500	0.39387200
H	−2.04852400	2.26891200	1.85010100
H	−3.91352100	0.96866300	1.29686800
H	−4.16422200	−0.66351500	1.91194800
H	−6.31644400	0.25806800	1.14557900
C	4.13404800	−1.60283900	0.13227300
H	1.66814100	−0.22023300	3.12547300
H	−0.08239900	0.03934600	2.97712200
H	1.04047100	1.39802400	2.77217300
H	0.68937500	−2.13414000	−0.63452600
H	−0.52840100	−1.97775700	0.64401400
H	1.10570600	−2.54216100	1.04279900
H	2.83870200	1.50423900	0.35626100
H	2.76612200	0.42488600	−1.01869800
H	5.76151200	−0.02092100	1.53495200
H	4.87392200	1.47531700	1.24302300
H	6.80152300	1.19836900	−0.35395000
H	5.26512500	1.24556000	−1.22010000
H	6.87039300	−1.26970600	−0.49109800
H	6.62370700	−0.63608800	−2.11765000
H	5.07286500	−2.58438300	−1.55987800
H	4.19656400	−1.11824400	−1.98964900
H	3.19226700	−2.15230100	0.04574800
H	4.76151400	−2.15641000	0.84779400

H	1.36386200	−0.32976200	−3.03309100
H	4.92569800	−1.43379400	−0.66375500
Si	0.37638300	−0.45181100	1.02631800
C	4.11192700	−2.15854000	−0.61253300
C	0.20360000	−2.18505400	1.73780400
H	4.35275700	−2.98866800	−1.29011300
Si	2.43459200	−1.46062800	−1.09029800
O	1.90117400	−0.37536600	0.17487200
C	0.37497600	0.73156700	2.48069100
H	1.67130800	−3.46862900	−2.21444200
C	−0.81162800	0.05116000	−0.41062100
C	1.30376200	−2.95741200	−1.31286500
N	−2.26562800	0.41639800	−0.29057400
C	−2.78780000	0.78212900	−1.66126300
H	0.24457700	−2.74385100	−1.48533500
C	−2.25009200	2.10375800	−2.22503800
C	−2.51355900	3.26371200	−1.25375100
C	−1.97463800	2.91866900	0.14215400
H	1.37998600	−3.67377300	−0.48882800
H	1.58168400	2.65673100	−0.95699600
C	−2.52242200	1.57333700	0.63257600
H	2.75348900	3.70130500	−0.17177000
H	1.33400900	3.17575100	0.71984200
H	3.63311100	0.02361600	2.85125900
H	3.13949800	1.68801900	3.19626300
H	4.77308500	1.34215100	2.62848900
H	5.65180500	0.53327000	−0.12659800
H	5.28438600	2.19658200	−0.55096300
H	4.78138600	0.90479900	−1.62441800
H	−0.48586300	−2.16445300	2.58809100
H	1.17956900	−2.51676400	2.11561500
H	−0.16698100	−2.93515900	1.03758800
H	0.48552600	1.78504500	2.21578300
H	1.17277800	0.47236900	3.18307600
H	−0.57457100	0.60788300	3.01608200
H	−0.77902600	−0.77954200	−1.12414900
H	−0.26890600	0.87594000	−0.88995500
H	−3.87539500	0.84763200	−1.56889000
H	−2.56741000	−0.05649800	−2.32855000
H	−2.74635900	2.28304300	−3.18750900
H	−1.17684500	2.03314100	−2.44314200
H	−3.59667500	3.44659100	−1.19196000
H	−2.05640500	4.18873200	−1.62487100
H	−2.26453500	3.68751500	0.86995300
H	−0.87872000	2.90724700	0.12581000
H	−2.12585100	1.31575000	1.61447400
H	−3.61161300	1.64163800	0.73590100
Al	−3.51853700	−1.20579800	0.37949800
C	−5.37429900	−0.65262700	−0.13421000
C	−3.30778000	−1.22834000	2.37324300
C	−2.86153400	−2.77187900	−0.67966400
H	−6.07319600	−1.32101800	0.39410000
H	−5.60202700	−0.76012500	−1.20469700
H	−5.66234700	0.36820300	0.16033200
H	−3.53559800	−2.23818800	2.74868500
H	−4.04328000	−0.55504200	2.83832500
H	−2.33096000	−0.96279800	2.79627300
H	−3.59861400	−3.58350200	−0.57434400
H	−1.89907700	−3.19624800	−0.36568600
H	−2.79301800	−2.57454200	−1.76091300
H	4.08182100	−2.56640600	0.40568200

Tabelle 8.183 Standardorientierung von **$Me_3Si(CH_2NC_5H_{10})$** und **$(AlMe_3)_2$** [B3LYP/6−31+G(d)].

$Me_3Si(CH_2NC_5H_{10})$				$(AlMe_3)_2$			
H	−2.97355400	−1.34196400	1.98998100	Al	1.31567400	−0.00006300	0.00012000
H	−2.73818000	0.34584500	2.47144900	C	−0.00002100	−0.22475700	−1.70452200
C	−2.61301000	−1.13092000	−1.31661200	C	2.26186800	1.72969600	−0.10816700
C	−3.05471700	−0.30307700	1.64442400	C	2.26364400	−1.72888400	0.10792800
H	−4.11768600	−0.10174200	1.45817200	Al	−1.31551600	−0.00004600	−0.00008500
H	−0.27403100	−1.53812000	0.79754600	C	−2.26392600	−1.72862500	0.10804100
H	1.40872500	−2.33261600	−0.39907200	C	−2.26179800	1.72970100	−0.10815800
H	2.47973900	−1.14710200	1.53220100	C	−0.00000300	0.22301600	1.70484200
H	3.71611000	−1.81138600	0.46313900	H	−0.00005100	−1.27913300	−2.00151700
C	−0.21470900	−0.47342400	0.52798200	H	0.84966700	0.25486000	−2.21622500
C	1.84684400	−1.33715000	−0.53761500	H	2.82277900	1.94279000	0.81299700
C	2.92146200	−1.05534200	0.52932700	H	1.58081800	2.57625300	−0.27143100
H	0.10686400	0.03616300	1.45691000	H	2.99344600	1.74024700	−0.92902100
Si	−2.01805300	−0.00237100	0.08179200	H	2.99544500	−1.73881400	0.92859200
H	2.32297200	−1.33541400	−1.53051800	H	2.82454200	−1.94124000	−0.81341500
N	0.75635100	−0.35086300	−0.57519700	H	1.58351800	−2.57618400	0.27122900
H	−1.82113600	2.50557300	0.29851100	H	−0.00053600	1.27710300	2.00285500
C	−2.23373500	1.80925600	−0.44283700	H	0.84983100	−0.25668000	2.21624500
H	4.21205300	0.59658600	1.14167300	H	−2.99472700	−1.73871400	0.92959400
C	3.49810000	0.35753200	0.34255600	H	−1.58392800	−2.57627500	0.27006400
H	−3.30148700	2.04242500	−0.55191000	H	−2.82603300	−1.94030000	−0.81272500
H	1.90634000	1.48660100	1.28778800	H	−2.82323200	1.94225600	0.81281600
H	4.06219200	0.39272600	−0.60285900	H	−2.99294200	1.74058800	−0.92939500
C	1.30265100	1.00290300	−0.74931700	H	−1.58077600	2.57643800	−0.27062100
C	2.36856000	1.39924000	0.29415200	H	−0.84930900	0.25511600	−2.21663300
H	−1.75479200	2.01958100	−1.40659300	H	−0.84914600	−0.25776400	2.21633700
H	0.47714800	1.72078800	−0.74225400				
H	1.75577900	1.04759400	−1.75162500				
H	2.76664500	2.39312000	0.04715000				
H	−2.60331200	−2.18553900	−1.01207300				
H	−1.96339000	−1.03440000	−2.19483100				
H	−3.63738400	−0.88358000	−1.62384400				

Tabelle 8.184 Standardorientierung von **$134{\cdot}AlMe_3$ (Koordination an N)** und **$134{\cdot}AlMe_3$ (Koordination an O)** [B3LYP/6−31+G(d)].

$134{\cdot}AlMe_3$ (Koordination an N)				$134{\cdot}AlMe_3$ (Koordination an O)			
H	−0.55203400	−0.84255500	−2.93614000	H	−0.61999200	1.52487500	3.11519600
Al	2.00901500	2.09829200	0.87663600	Al	−0.75447000	2.80723800	0.12960000
C	3.54747500	3.26953400	1.41180700	C	0.92275500	3.61320100	0.85602000
H	0.61675900	−2.13803300	−3.25470600	H	−0.92408600	−0.07377300	3.81258000
C	1.17876200	1.20623300	2.45775700	C	−1.32517200	3.24222200	−1.73637800
C	0.78516100	2.92670400	−0.47181300	C	−2.33771200	3.02345300	1.33884000
C	−0.12386600	−1.76882500	−2.53353100	C	−0.38560400	0.46232200	3.01892600
H	−0.93124700	−2.50989700	−2.48453300	H	0.68671600	0.33556800	3.21501700
H	1.43401500	0.63730800	−1.69523600	H	−3.19441500	0.53493300	1.04994400
H	3.55625900	1.77407400	−1.79190000	H	−3.28746000	0.61776100	−1.28480800
Si	−1.90531300	−1.36523800	1.12208700	Si	1.09814700	0.25985100	−0.97135500
H	4.55663800	−0.42301500	−2.48463100	H	−5.39961500	0.28209400	0.01427200
H	5.81418400	0.76119400	−2.17361400	H	−5.74555100	0.25631800	−1.71391300
C	1.97015400	−0.17973000	−1.19881500	C	−2.71262300	−0.44772500	1.04871100
C	−2.86288600	−2.72979900	0.22278200	C	0.56615700	−1.32275100	−1.84923400
C	4.03316500	1.13494800	−1.04258700	C	−3.73193300	−0.38018000	−1.21193100
C	5.03186800	0.16409800	−1.68771200	C	−5.23970900	−0.29378600	−0.90883800
H	2.53956000	−0.67954300	−1.99734700	H	−3.15705900	−0.98383000	1.90291700
Si	0.62571500	−1.49884000	−0.81908700	Si	−0.84306600	−0.27722300	1.34368200
H	4.57127100	1.78809700	−0.35102700	H	−3.59182700	−0.86152000	−2.19199700

N	2.93073700	0.47758200	−0.24854800	**N**	−2.96774300	−1.16175300	−0.22775600
O	−0.54602200	−0.96615500	0.21783600	**O**	−0.19922900	0.76137000	0.09220200
C	−1.34205800	−2.03395100	2.79700200	**C**	1.43629300	1.56154500	−2.28264600
H	2.07255200	−3.55484500	−0.88864400	**H**	−0.30484700	−2.48654700	2.23171900
C	−2.89775500	0.24751400	1.45353200	**C**	2.64983900	0.09755900	0.15070600
C	1.31639200	−3.14886200	−0.20517400	**C**	−0.07189100	−1.99616400	1.27574600
H	6.29847000	−1.51255600	−1.11148000	**H**	−6.89630800	−1.64424200	−0.46530800
N	−3.84910800	0.82539300	0.49479100	**N**	3.33235100	−1.20523200	0.12056700
C	5.63760600	−0.77675800	−0.63682800	**C**	−5.83791700	−1.70133100	−0.75058600
C	−3.26839200	1.13420100	−0.80951200	**C**	4.23963500	−1.42476300	1.26080300
H	0.49987600	−3.88135400	−0.15812700	**H**	1.01832100	−2.00388800	1.16273700
C	−4.22518800	1.98990700	−1.64755500	**C**	5.56151700	−0.63822600	1.18218200
H	3.98564200	−2.17413200	−0.51353000	**H**	−5.19285800	−2.08336700	1.28446600
C	−5.59432500	1.30899300	−1.78456700	**C**	6.28765300	−0.94382200	−0.13788400
H	6.25942100	−0.19427200	0.05894300	**H**	−5.80154800	−2.21960300	−1.72170400
C	3.54315400	−0.45921200	0.74645000	**C**	−3.53950200	−2.50526300	−0.06556500
C	−6.14359600	0.93145500	−0.40139800	**C**	5.34964600	−0.72111900	−1.33565000
C	4.51929200	−1.47868200	0.14581100	**C**	−5.04056800	−2.51313300	0.28340900
H	1.76012200	−3.09164200	0.79487000	**H**	−0.50021600	−2.60706300	0.47647500
H	2.73061400	−0.94570900	1.28973100	**H**	−2.96082500	−3.04333300	0.69428000
H	3.96750200	3.88400900	0.60208800	**H**	1.13853500	3.27679300	1.88116500
H	4.07870000	0.16619300	1.47128200	**H**	−3.39202100	−3.04304400	−1.01464300
H	4.93455500	−2.08183000	0.96355900	**H**	−5.40160400	−3.54990500	0.32836000
C	−5.11768100	0.10867100	0.38781500	**C**	4.03062800	−1.49563000	−1.14164700
H	4.38728100	2.74696500	1.89593300	**H**	0.79977000	4.70638900	0.91162200
H	3.16637500	3.97736900	2.16566900	**H**	1.83292000	3.43779600	0.26524400
H	0.55552000	0.34124800	2.20570400	**H**	−1.70463400	2.37881700	−2.30306000
H	0.52395600	1.92742800	2.97233200	**H**	−0.55256300	3.71885200	−2.35344200
H	1.91854600	0.87921300	3.20387500	**H**	−2.16209100	3.95474000	−1.67102300
H	1.28181800	3.22162600	−1.40909200	**H**	−3.28531000	2.77918500	0.83751600
H	0.36988600	3.85468100	−0.04839000	**H**	−2.37880400	4.10849100	1.53514100
H	−0.07565400	2.29884700	−0.74080900	**H**	−2.35229300	2.54168200	2.32336100
H	−3.77321800	−2.99580400	0.77510300	**H**	0.90359300	−1.29591700	−2.89294200
H	−2.25590700	−3.64183500	0.13996100	**H**	−0.52744800	−1.40561100	−1.85129500
H	−3.16554300	−2.43360000	−0.78793300	**H**	0.97757200	−2.22211200	−1.38267600
H	−0.81034200	−1.27321400	3.38032800	**H**	1.68509500	2.54835900	−1.88393300
H	−0.66891600	−2.89268800	2.67636700	**H**	0.60699900	1.67419500	−2.98652100
H	−2.20203800	−2.37123500	3.39096200	**H**	2.30833600	1.20294500	−2.84910500
H	−2.13709500	1.01230500	1.67262300	**H**	2.31102500	0.26598700	1.18075100
H	−3.43764400	0.10101100	2.40113900	**H**	3.31800800	0.95204500	−0.06842200
H	−3.02038900	0.20953300	−1.37507600	**H**	4.46615600	−2.50159200	1.29136400
H	−2.32606500	1.66860400	−0.64704300	**H**	3.69788400	−1.18673400	2.18402000
H	−3.78128700	2.17147900	−2.63545700	**H**	6.19401700	−0.89729600	2.04206700
H	−4.34414900	2.96620900	−1.15878700	**H**	5.35821200	0.43946300	1.25432300
H	−5.48816700	0.39805000	−2.39418800	**H**	6.61997300	−1.99373500	−0.13104800
H	−6.29991300	1.96161500	−2.31510000	**H**	7.19216600	−0.32979100	−0.23507800
H	−7.07489800	0.35719500	−0.49731900	**H**	5.82752400	−1.04718100	−2.26944200
H	−6.37659100	1.84337900	0.16467500	**H**	5.14364400	0.35267200	−1.44833600
H	−5.49004700	−0.08116400	1.40248700	**H**	3.34785900	−1.30700500	−1.97788700
H	−4.99810700	−0.87963100	−0.10295100	**H**	4.24863600	−2.57427900	−1.15253400

Tabelle 8.185 Standardorientierung von **[$Me_3SiOSiMe_2(CH_2NC_5H_{10})$]·$AlMe_3$ (Koordination an O)** und **[$Me_3SiOSiMe_2(CH_2NC_5H_{10})$]·$AlMe_3$ (Koordination an N)** [B3LYP/6−31+G(d)].

[$Me_3SiOSiMe_2(CH_2NC_5H_{10})$]·$AlMe_3$ (Koordination an O)				[$Me_3SiOSiMe_2(CH_2NC_5H_{10})$]·$AlMe_3$ (Koordination an N)			
H	−2.16219800	1.32045700	−2.55125800	**H**	3.39708400	2.62923100	−0.51749900
Al	−2.87992700	−1.22170600	−0.46911200	**H**	4.81655400	2.18772800	−1.47959200
C	−1.86720300	−2.19814400	−1.89677900	**C**	3.81365500	1.85794600	−1.17774900
H	−1.72015600	3.02114600	−2.32883600	**H**	3.19251900	1.81937700	−2.08160600
C	−3.43543100	−2.15689300	1.20640100	**H**	4.51733600	1.02128800	1.95303800
C	−4.41226500	−0.18416700	−1.22724700	**Si**	0.87771200	−0.91075900	0.54194000

C	−1.47843500	1.99350600	−2.02656600	C	4.92851000	0.28861800	1.24717900
H	−0.46072100	1.77698100	−2.37514200	C	0.86560400	−2.69558900	−0.05295200
H	−4.09073400	2.09223200	0.05989900	H	5.95771200	0.59260400	1.01465500
Si	0.06089500	−0.55232400	0.94584100	Si	3.87814500	0.17902700	−0.31696800
C	−3.20268700	2.44215500	0.58913100	O	2.33076100	−0.24189800	0.10888700
C	0.29872700	0.18348200	2.66647100	C	0.73884500	−0.81957900	2.41961700
H	−3.20622600	3.54045800	0.57212800	H	5.60392900	−0.87921700	−1.78788200
Si	−1.59015600	1.82980100	−0.15549500	C	−0.32710000	0.21531000	−0.46348200
O	−1.38135900	0.14496900	0.23526200	C	4.57728600	−1.12629700	−1.48665400
C	−0.09683800	−2.40757100	1.16419600	N	−1.77214000	0.48370200	−0.14921400
H	−0.33570200	3.90035200	0.15262300	C	−2.32554900	1.46022600	−1.15894800
C	1.49428100	−0.25489200	−0.27918600	H	3.97497600	−1.20841700	−2.40026800
C	−0.23012300	2.90377400	0.60417700	C	−1.76611900	2.88534400	−1.05002400
N	2.75366700	−0.74187100	0.32060000	C	−1.95158200	3.44561100	0.36813700
C	3.52736600	0.29784700	1.01566100	C	−1.38564000	2.46733100	1.40797500
H	0.79314100	2.57180900	0.40600200	H	4.60001700	−2.11612600	−1.01373600
C	4.30619800	1.23967500	0.07519300	C	−1.97155400	1.06184600	1.22107400
C	5.19922400	0.43475700	−0.88312500	H	−0.09870300	−3.18773500	0.10402300
C	4.37917600	−0.64412300	−1.60934100	H	1.63055500	−3.27168900	0.48394000
H	−0.35110200	3.02981100	1.68547500	H	1.09939900	−2.74963900	−1.12313100
H	−0.88665900	−1.76626200	−2.14597500	H	0.78334300	0.21189200	2.78941900
C	3.61647300	−1.51005800	−0.59075100	H	1.58812300	−1.35976600	2.85849300
H	−2.45163600	−2.18336800	−2.82906100	H	−0.17711600	−1.28588600	2.79918900
H	−1.69562300	−3.25699000	−1.65423700	H	−0.30946100	−0.19211000	−1.48188400
H	−3.19126600	−1.60139200	2.12435300	H	0.21609400	1.16673100	−0.51612000
H	−3.01581500	−3.16542200	1.31742200	H	−3.40826400	1.48747400	−1.00504200
H	−4.53046900	−2.26700900	1.19906500	H	−2.14658300	1.03818900	−2.15218400
H	−5.09314500	0.21829300	−0.46523500	H	−2.29247900	3.50911000	−1.78393800
H	−4.99075200	−0.94996000	−1.77221600	H	−0.70545700	2.91323600	−1.33015600
H	−4.21538600	0.61213800	−1.95588700	H	−3.02422500	3.59547200	0.56127700
H	1.08928600	−0.37729500	3.18058900	H	−1.47384200	4.42877100	0.46046000
H	−0.62211700	0.05662400	3.25034400	H	−1.62348100	2.80361500	2.42542800
H	0.57038600	1.24185300	2.68921900	H	−0.29002000	2.43783400	1.34111500
H	−0.40933900	−2.93757200	0.26136900	H	−1.55923500	0.36018900	1.94568300
H	−0.77637900	−2.67766700	1.97721600	H	−3.05471400	1.09621700	1.38627800
H	0.90894400	−2.75868000	1.43049200	Al	−3.01267600	−1.26674600	−0.32034200
H	1.56662500	0.77309400	−0.66997200	C	−4.88044200	−0.53787000	−0.38208900
H	1.25788200	−0.87739400	−1.15253600	C	−2.72475700	−2.31639500	1.36228900
H	4.24107200	−0.21232900	1.67976700	C	−2.40808900	−2.07906500	−2.04547200
H	2.85081000	0.86980300	1.65972600	H	−5.57168800	−1.38122000	−0.22413700
H	4.90691900	1.93731900	0.67453400	H	−5.16264800	−0.09116700	−1.34682200
H	3.60375800	1.85367100	−0.50679700	H	−5.12685400	0.19645700	0.40031200
H	6.00160400	−0.05071000	−0.30597000	H	−3.37032100	−3.20702500	1.29284500
H	5.69132800	1.10059700	−1.60371400	H	−3.05981400	−1.77655700	2.26091000
H	5.03124600	−1.28150200	−2.22186400	H	−1.71539700	−2.69417500	1.56775900
H	3.66550700	−0.16779400	−2.29730400	H	−3.05860600	−2.93798600	−2.27415000
H	3.00325600	−2.26541300	−1.09487100	H	−1.37982400	−2.46531700	−2.05123700
H	4.34315800	−2.05487000	0.03097900	H	−2.50345800	−1.39600300	−2.90345000
H	−3.28636300	2.12972900	1.63758100	H	4.97785000	−0.67879000	1.76284600

Tabelle 8.186 Standardorientierung von **$Me_2(CH_2NC_5H_{10})SiOAlMe_2$** [B3LYP/6−31+G(d)].

$Me_2(CH_2NC_5H_{10})SiOAlMe_2$			
H	−3.11619700	−0.36258200	−2.13589000
H	−0.97928000	2.10768100	−2.26098300
H	−1.59735600	3.43156500	−1.28224900
H	−3.08934500	−2.11881600	−1.86812400
H	0.12659200	3.33808000	−1.62806000
C	−0.75564600	2.72938400	−1.38114700
C	−3.18873700	−1.14465200	−1.37020300
H	−4.19889000	−1.09473100	−0.94392100

H	−0.27198300	−0.57260500	−1.89145300
H	1.43461000	0.91883400	−1.99114800
H	2.50404500	−1.33708200	−1.93315800
H	3.73212600	−0.07750400	−1.95373900
C	−0.13946800	−0.91999400	−0.85916600
C	1.87814500	0.54833400	−1.06321300
C	2.93984700	−0.52297100	−1.33853400
H	0.34171300	−1.90333600	−0.92209800
Si	−1.89026500	−0.90757100	−0.02073000
H	2.34357700	1.40638700	−0.55974800
Al	−0.55661200	1.70115600	0.30890700
N	0.75912700	0.08583900	−0.18054300
O	−1.90454400	0.58603300	0.65554900
H	−1.99629500	−3.28146700	0.79048600
H	−0.38558800	3.53576200	2.10112400
C	−2.09547100	−2.28985800	1.25234400
H	4.22002700	−1.89587600	−0.23138700
C	3.51684700	−1.07890200	−0.02799700
H	−3.09593300	−2.23567600	1.70106100
C	0.20601600	2.63358300	1.88493400
H	1.24014900	2.97811300	1.73238900
H	1.92232100	−2.46166200	0.48229800
H	4.08951700	−0.28822400	0.47961100
C	1.33578600	−0.45521700	1.09522700
C	2.38538300	−1.55593100	0.89496500
H	−1.36996000	−2.22464000	2.07191700
H	0.50777800	−0.80624800	1.71607700
H	0.19236200	2.02479700	2.79952600
H	1.79143800	0.39283900	1.61770700
H	2.78048800	−1.83444300	1.88032700

Tabelle 8.187 Standardorientierung von **[$H_3SiOSiMe_2(CH_2NMe_2)$]·$AlMe_3$ (H_2O)** und **[$H_3SiOSiMe_2(CH_2NMe_2)$]·$AlMe_3$ (H_2O, ÜZ)** [B3LYP/6−31+G(d)].

[$H_3SiOSiMe_2(CH_2NMe_2)$]·$AlMe_3$ (H_2O)				ÜZ			
H	−5.35089200	−0.94781600	−0.34130600	H	−4.80895600	−2.02962200	−0.32865100
H	−4.65171400	0.07204700	1.74506300	H	−4.72251200	−0.44990100	1.44565400
H	−3.85642400	−2.13555900	1.15131200	H	−3.02530400	−2.10030100	1.24523500
H	0.60484800	−1.67545500	−2.40897800	H	0.88270000	−1.27119200	−2.78350600
H	0.96096500	−3.16588000	−0.49082900	H	0.80933200	−3.08204200	−1.18710600
H	−0.45482200	1.95428200	−2.17230600	H	−1.51196400	3.08535000	−1.42673300
Si	−1.44531100	0.59674800	−0.30236200	Si	−0.71668000	1.11177200	−0.15142800
H	−2.21835200	2.08083100	−2.10471300	H	−0.48583000	2.08076800	−2.45975000
C	−1.37563900	1.38364500	−2.00746100	C	−1.26956800	2.04745600	−1.69188800
H	−1.46801400	0.63704700	−2.80536100	H	−2.16352100	1.57935200	−2.10991500
Si	−4.22602100	−0.79801700	0.61619100	Si	−3.84569000	−1.13349300	0.41898000
O	−2.94820600	−0.12625200	−0.18538000	O	−2.99437200	−0.15060900	−0.52387300
C	−1.32308300	1.88067500	1.06640800	C	−1.58685700	1.54859100	1.46926100
H	−1.50998800	1.42400300	2.04648700	H	−1.52397900	0.72438000	2.19036900
C	−0.29561800	−0.92170000	−0.01602600	C	−0.27384000	−0.74430100	−0.41745600
H	−2.07956000	2.66075700	0.90993900	H	−2.64639500	1.74397500	1.28660300
N	1.14135400	−1.03771100	−0.44337000	N	1.18787300	−1.04289900	−0.69258100
C	1.25424200	−0.93406100	−1.92337800	C	1.51856700	−0.68957500	−2.10604300
H	−0.34196800	2.36379600	1.10478200	H	−1.13498200	2.43430200	1.93426500
C	1.60893000	−2.39965100	−0.04439200	C	1.44708000	−2.50733600	−0.50568300
Al	2.47989000	0.34305600	0.46040000	Al	2.30116200	−0.04107100	0.63011700
C	1.97210500	0.30093300	2.39763200	C	1.84645800	−0.55105400	2.46624900
C	4.29348100	−0.43471500	0.09850900	C	4.09399500	0.38648500	−0.03096800
C	2.25193100	2.08348500	−0.51012800	C	1.04245200	1.97731200	0.15418600
H	−0.84007200	−1.76133900	−0.48045900	H	−0.87193200	−1.16250000	−1.23244700
H	−0.32083200	−1.10873900	1.06506700	H	−0.55242200	−1.29462400	0.48593600

H	2.28983800	−1.12077100	−2.21847300	H	2.56778100	−0.91711800	−2.30831500
H	0.97332800	0.06536400	−2.25246800	H	1.34039600	0.37260000	−2.28016200
H	2.66338600	0.94923600	2.96025100	H	2.24255000	0.19181900	3.17248000
H	2.06608900	−0.70271800	2.84003200	H	2.31360500	−1.51254900	2.72324200
H	0.95824600	0.65970000	2.62205300	H	0.77143400	−0.64650100	2.66119900
H	5.05160800	0.30885700	0.39426000	H	4.57748000	1.11102500	0.63863600
H	4.48669600	−0.66211100	−0.96104400	H	4.11679100	0.80841100	−1.04326200
H	4.51280800	−1.34640400	0.67344500	H	4.72555900	−0.51361700	−0.03533500
H	2.55657300	2.01736000	−1.56569400	H	1.79363300	1.97338800	−0.64923600
H	2.93851100	2.80703200	−0.03992000	H	1.53672500	1.89882800	1.14413500
H	1.25872300	2.54975300	−0.48886700	H	0.74280000	3.03549000	0.19283500
H	1.57449000	−2.49233800	1.04385500	H	1.21828800	−2.79313600	0.52379600
H	2.63468100	−2.55058000	−0.38527300	H	2.49694200	−2.72887100	−0.72410200

Tabelle 8.188 Standardorientierung von **[$H_3SiOSiMe_2(CH_2NMe_2)$]·$AlMe_3$ (Gasphase)** und **[$H_3SiOSiMe_2(CH_2NMe_2)$]·$AlMe_3$ (Gasphase, ÜZ)** [B3LYP/6−31+G(d)].

[$H_3SiOSiMe_2(CH_2NMe_2)$]·$AlMe_3$ (Gasphase)				ÜZ			
H	5.30226400	−0.59036300	0.61979500	H	4.61862500	−2.17381900	−0.46158500
H	4.91968100	−0.05941200	−1.71164400	H	4.78780300	−0.68745100	1.39514600
H	4.18544400	−2.18471700	−0.81711900	H	4.86293400	0.17182700	−0.82517900
H	−0.48682900	−1.98602700	2.11936100	H	0.74412400	−2.14800000	0.70524700
H	−0.94647500	−3.20851100	0.03311500	H	−0.39499300	−2.95331900	−1.40784500
H	0.56018000	1.62690600	2.36282400	H	1.46137500	2.28500700	1.97133900
Si	1.42586200	0.59188300	0.23770600	Si	0.54006200	1.27422800	−0.07525700
H	2.31469800	1.77572400	2.20581700	H	1.81101300	0.54173300	1.91681900
C	1.46669900	1.09582200	2.05111000	C	1.03979800	1.29556400	1.74527900
H	1.61070300	0.23588600	2.71613600	H	0.19667700	1.14648300	2.43314700
Si	4.35423800	−0.73767100	−0.51587800	Si	4.13270500	−0.83393600	0.03981200
O	2.90398600	−0.07809300	−0.12358200	O	2.53285300	−0.66008200	0.04247900
C	1.20434400	2.07445900	−0.89333500	C	1.65598100	2.24944200	−1.23328200
H	1.32945300	1.78396500	−1.94337000	H	2.62334400	1.74561200	−1.31575700
C	0.27318300	−0.89204900	−0.20020200	C	0.01576000	−0.33699700	−0.98447000
H	1.96901200	2.82783200	−0.66381800	H	1.82083900	3.26474200	−0.85037900
N	−1.13031300	−1.09517900	0.28874400	N	−0.94112400	−1.25906100	−0.25106900
C	−1.16123900	−1.19070700	1.76937800	C	−0.26731200	−1.82331500	0.97116400
H	0.22282300	2.54706400	−0.79088400	H	1.22120300	2.33921000	−2.23715300
C	−1.61476800	−2.38966800	−0.26929400	C	−1.30311000	−2.39716900	−1.15143900
Al	−2.54568700	0.39459700	−0.35506300	Al	−2.51522500	−0.12773400	0.15412200
C	−2.10371300	0.61424700	−2.29274100	C	−3.62126900	0.20457500	−1.42588500
C	−4.30911200	−0.48792200	−0.00547900	C	−3.07134000	−0.16599300	2.02992900
C	−2.25195800	1.95853700	0.86118200	C	−1.14310100	2.27861800	−0.05718300
H	0.85762400	−1.78055900	0.09471800	H	0.94674700	−0.88066500	−1.18382200
H	0.23112200	−0.91125900	−1.29606400	H	−0.47652700	−0.05763500	−1.92606900
H	−2.17929300	−1.41979500	2.09330000	H	−0.87595700	−2.64332200	1.36185000
H	−0.86147400	−0.24137500	2.21035000	H	−0.17263300	−1.05161100	1.73331600
H	−2.85920600	1.27098600	−2.75198100	H	−4.27931600	1.06740700	−1.26078600
H	−2.14343200	−0.32747200	−2.86152800	H	−4.27427400	−0.65513900	−1.63398700
H	−1.13005900	1.07777500	−2.50090700	H	−3.04533100	0.40317200	−2.33777600
H	−5.09959700	0.27271300	−0.10463200	H	−3.93290700	0.49350300	2.19530700
H	−4.42506800	−0.90485900	1.00692100	H	−2.28334100	0.13895200	2.72846000
H	−4.56418300	−1.28606700	−0.71779800	H	−3.38180100	−1.17966900	2.32185400
H	−2.56306400	1.74568400	1.89511200	H	−1.96188000	1.95567100	0.62118900
H	−2.90879400	2.77243400	0.51413500	H	−1.57504800	2.45555200	−1.04941500
H	−1.24349600	2.38940000	0.90898800	H	−0.90393500	3.26591900	0.36425600
H	−1.63555500	−2.32952900	−1.35977400	H	−1.75900400	−2.01404600	−2.06684300
H	−2.62424600	−2.59048000	0.09290000	H	−2.00594000	−3.06793400	−0.64570300

Tabelle 8.189 Standardorientierung von **$(Me_2SiO)_3$** und **$[(Me_2SiO)_3]\cdot AlMe_3$** [B3LYP/6−31+G(d)].

$(Me_2SiO)_3$				$[(Me_2SiO)_3]\cdot AlMe_3$			
O	−1.10462500	1.08747300	0.00721800	O	1.73297400	−1.28645400	0.34821100
O	1.49515100	0.41262400	0.01620000	O	−0.65064200	−0.00325700	−0.06310000
O	−0.38951000	−1.49762100	−0.03649500	O	1.76104500	1.25267300	−0.30218100
Si	0.44486500	1.71161400	0.00767000	Si	0.15663200	−1.54655300	−0.10642500
Si	1.26069300	−1.24070100	−0.00400100	Si	0.12628300	1.54218100	−0.25441900
Si	−1.70581600	−0.47028500	−0.00599000	Si	2.76654400	0.01276700	0.18168400
C	0.70980000	2.71392800	−1.55306500	C	0.10778000	−2.16529900	−1.87118100
H	0.57300700	2.09229400	−2.44624300	H	0.56146800	−1.43958000	−2.55760900
H	−0.00143000	3.54729800	−1.61155700	H	0.67332900	−3.10175100	−1.95637500
H	1.72352800	3.13216600	−1.58704700	H	−0.91705300	−2.35350400	−2.20639200
C	0.70556500	2.73218600	1.55724400	C	−0.55815700	−2.71275300	1.16094900
H	0.00756000	3.57795500	1.59402700	H	0.06471100	−3.61701900	1.16770500
H	0.54845600	2.12747300	2.45855300	H	−0.51708100	−2.27313600	2.16311000
H	1.72540000	3.13492500	1.59653800	H	−1.58930600	−3.01001500	0.95663800
C	2.03103100	−1.95991800	−1.55317300	C	−0.31587300	2.30455500	−1.90023400
H	3.11315300	−1.77992500	−1.57450200	H	−1.34077900	2.68090400	−1.93763400
H	1.86803700	−3.04346800	−1.60884900	H	0.36758500	3.14215100	−2.08985000
H	1.59797400	−1.50854100	−2.45396000	H	−0.18475600	1.58091000	−2.71367000
C	1.97877100	−1.98997500	1.55648900	C	−0.25570700	2.58021000	1.25271700
H	1.81603300	−3.07472200	1.58348000	H	0.25730400	3.54670800	1.16697300
H	3.05908700	−1.80923800	1.61981200	H	−1.32456200	2.77268100	1.38037300
H	1.51342000	−1.55852200	2.45097500	H	0.11061800	2.08795700	2.16147800
C	−2.69333000	−0.76975400	1.55836900	C	3.55431200	0.38851400	1.83689900
H	−3.55163300	−0.08911400	1.61988100	H	4.18312400	−0.44747400	2.16780700
H	−3.07467900	−1.79797800	1.59258800	H	4.18774900	1.28238000	1.77982500
H	−2.07521100	−0.61165900	2.45044900	H	2.79511500	0.56086600	2.60890300
C	−2.73230300	−0.72928400	−1.55188600	C	4.03382600	−0.30346900	−1.15792600
H	−3.12551200	−1.75255900	−1.59716600	H	4.68216900	0.57092700	−1.29539300
H	−3.58460400	−0.03883800	−1.57842800	H	4.67326100	−1.15781200	−0.90351600
H	−2.13430900	−0.55924300	−2.45530500	H	3.55147600	−0.51717100	−2.11900900
				Al	−2.76606600	−0.02800800	0.20183700
				C	−3.45187300	1.69950000	−0.52979100
				C	−3.37160500	−1.53921100	−0.95524300
				C	−2.92926600	−0.20328900	2.18015900
				H	−4.52262700	1.70563500	−0.26567400
				H	−3.41279400	1.75635000	−1.62629400
				H	−3.04360200	2.63694500	−0.13114300
				H	−4.46998200	−1.57146200	−0.86881900
				H	−3.02175400	−2.55088200	−0.71346100
				H	−3.16092000	−1.36184200	−2.02010800
				H	−2.80116600	−1.22636700	2.55801200
				H	−3.93765800	0.11759800	2.48473000
				H	−2.22508100	0.43632700	2.73220900

8.4 Angaben zu sonstigen Kooperationsprojekten

Tabelle 8.190 Lumineszenzmessungen, E_{max} = Wellenlänge der maximalen Emission, I_{max} = maximale Intensität der Emission, λ_{ex} bzw $\lambda_{excitation}$ = Wellenlänge der Anregung.

	RT								77K	
X = I	$\lambda_{excitation}$ = 440 nm		$\lambda_{xcitation}$ = 440 nm		$\lambda_{excitation}$ = 315 nm		$\lambda_{excitation}$ = 370 nm		$\lambda_{excitation}$ = 440 nm	
	E_{max}/λ	I_{max}	E_2/λ	I_2	E_{max}/λ	I_{max}	E_{max}/λ	I_{max}	E_{max}/λ	I_{max}
$NR_2 = NC_5H_{10}$	713	2281377	487	842093	536	415520	–	–	–	–
$NR_2 = NC_4H_8O$	692	256598	500	231785	538	1539891	–	–	–	–
R = Bu	682	3686204	496	486946	–	–	–	–	–	–
R = ^{i}Pr	697	496754	506	102344	546	528271	–	–	713	2281377
$R = C_2H_4OMe$	474	3437091	686	696983	–	–	–	67825944	–	–
X =Br	$\lambda_{excitation}$ = 440 nm		$\lambda_{excitation}$ = 440 nm		$\lambda_{excitation}$ = 315 nm		$\lambda_{excitation}$ = 370 nm			
	E_{max}/λ	I_{max}	E_2/λ	I_2	E_{max}/λ	I_{max}	E_{max}/λ	I_{max}		
$NR_2 = NC_5H_{10}$	479	646785	672 (small)	131218	–	–	414	9442489	–	–
$NR_2 = NC_4H_8O$	485	342612	–	–	–	–	415	3233970	–	–
R = Bu	624	593557	478	566962	–	–	413	8395066	–	–
R = ^{i}Pr	467	538764	–	–	–	–	438	4776992	–	–
$R = C_2H_4OMe$	493	454135	–	–	–	–	436	3059458	–	–

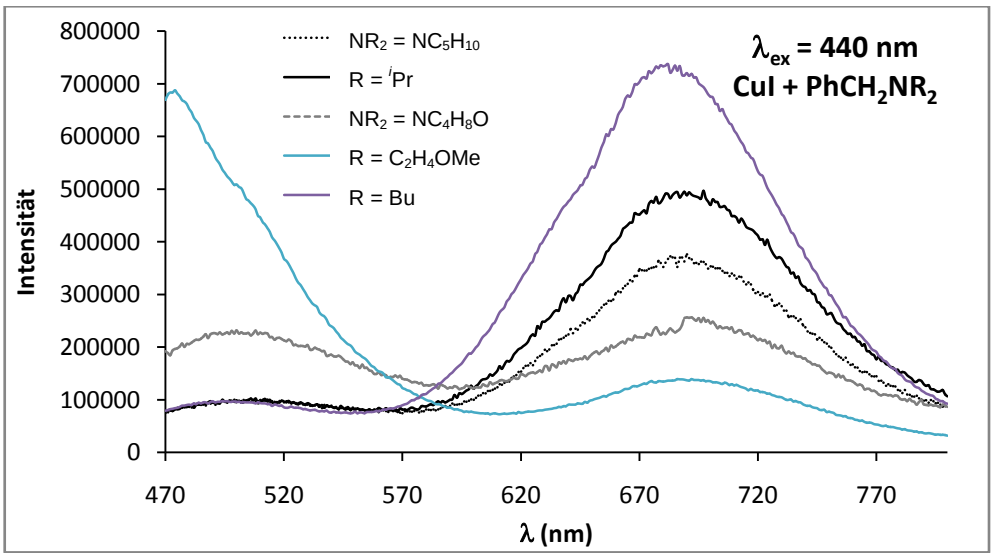


Abb. 8.35 Emmissionsspektrum (Intensität von $R = C_2H_4OMe$, Bu auf 1/5 herabgesetzt)

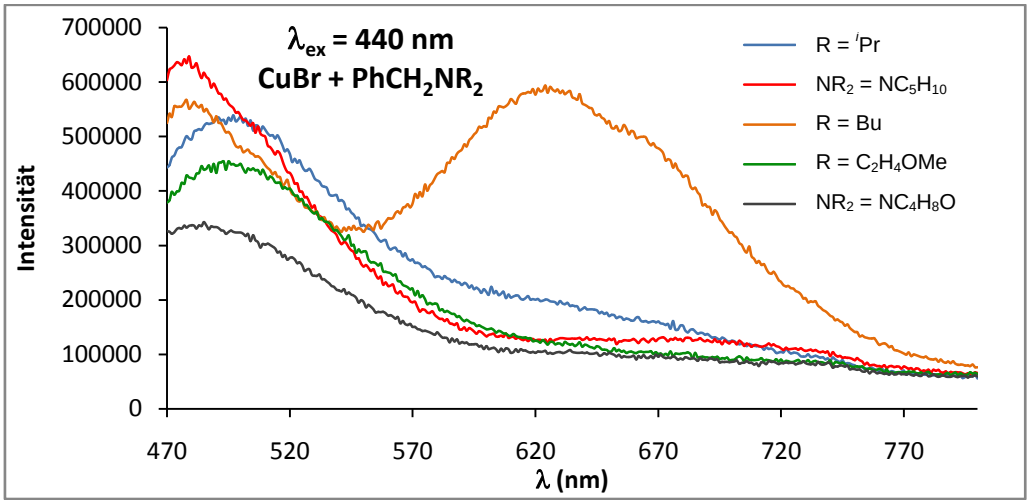


Abb. 8.36 Emmissionsspektrum

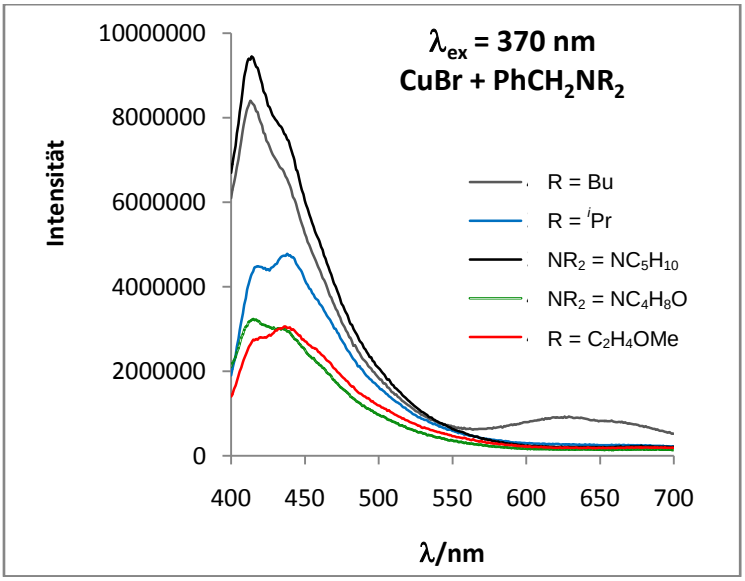


Abb. 8.37 Emmissionsspektrum