ANHANG

Siliciumorganische Verbindungen

Von der gezielten Synthese stereochemisch reiner Systeme zur selektiven Spaltung der Si–O–Si-Einheit in Disiloxanen

Dissertation

zur Erlangung des naturwissenschaftlichen Doktorgrades
der Technischen Universität Dortmund

vorgelegt von
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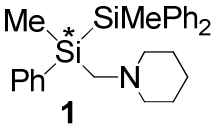
aus Gunzenhausen

Dortmund 2009

8 Anhang

8.1 Übersicht zentraler Verbindungen

Anmerkung: Systeme, die sowohl enantiomerenrein als auch racemisch vorkommen, wurden hier nur mit der jeweiligen Nummer und ohne Stereodeskriptoren versehen (das stereogene Zentrum wurde durch einen Stern gekennzeichnet).



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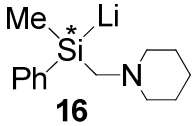

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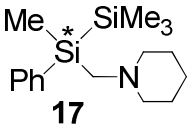

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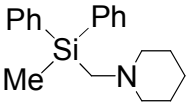

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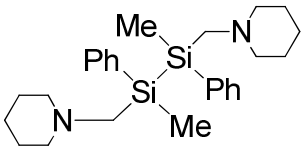

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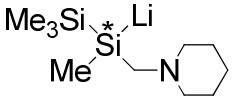

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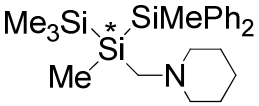

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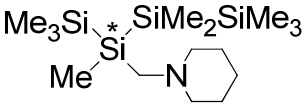

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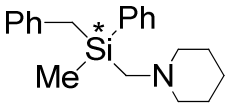

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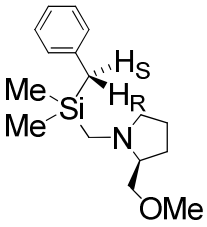

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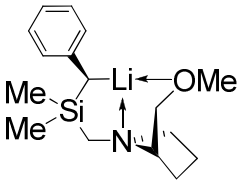

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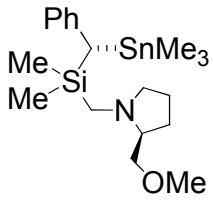

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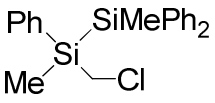

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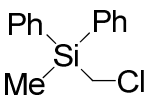

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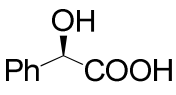

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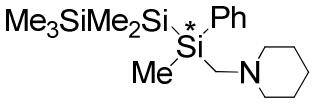

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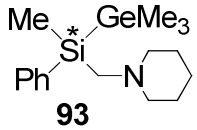
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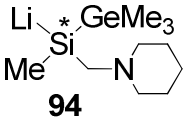
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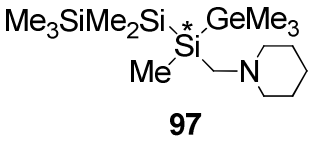
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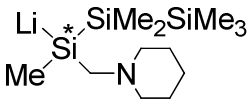
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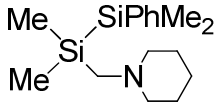
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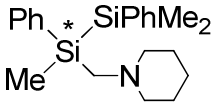
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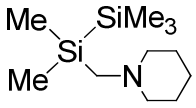
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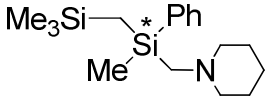
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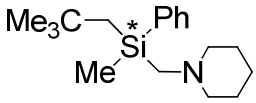
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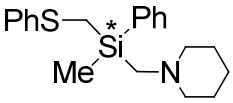
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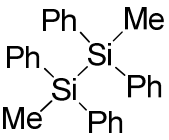
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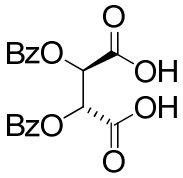
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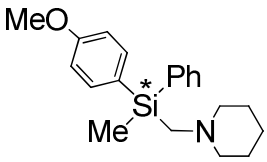
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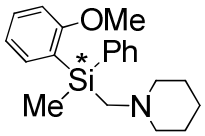
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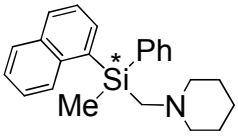
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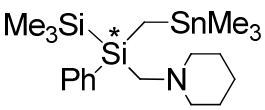
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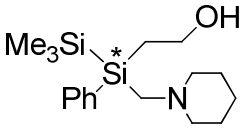
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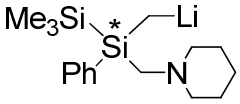
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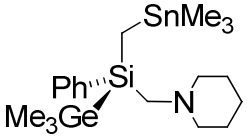
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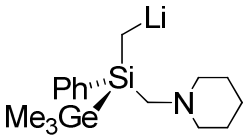
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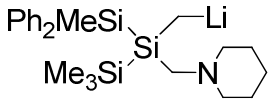

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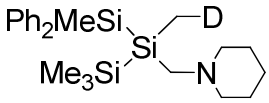

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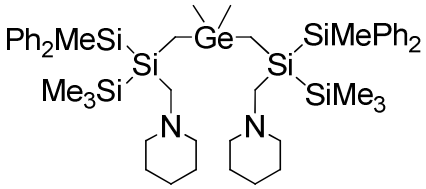

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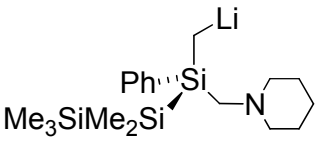

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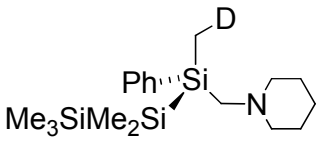

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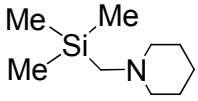

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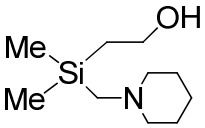

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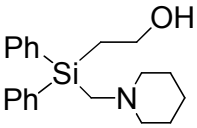

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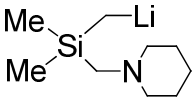

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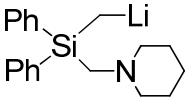

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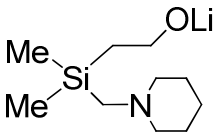

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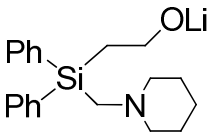

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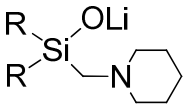

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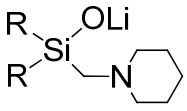

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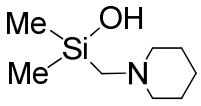

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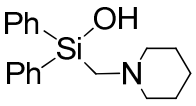

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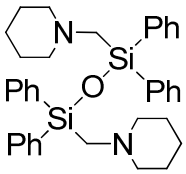

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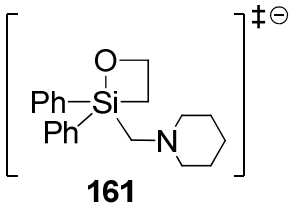

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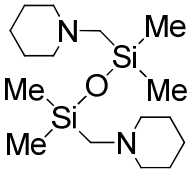

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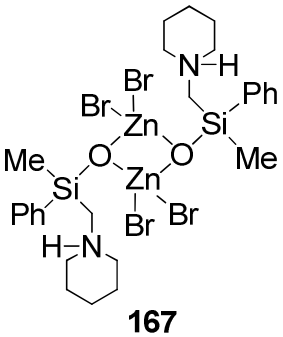

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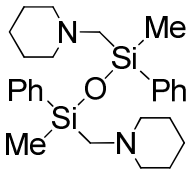

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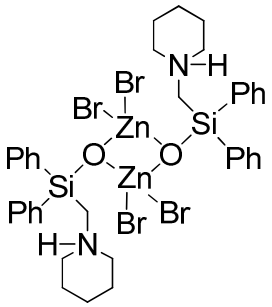

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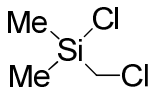
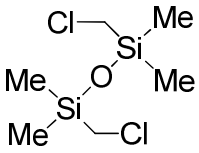


170



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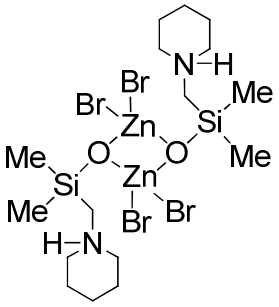

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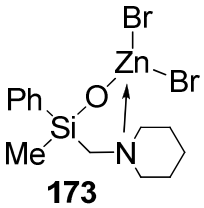

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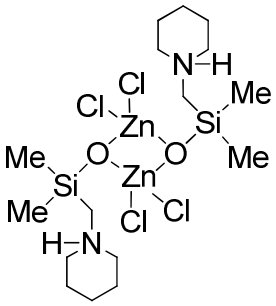

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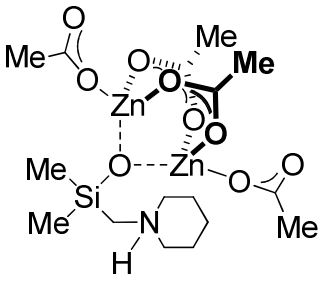
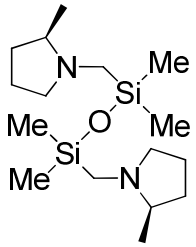
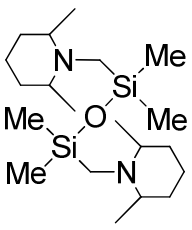


175



(*R*,*R*)-**176**



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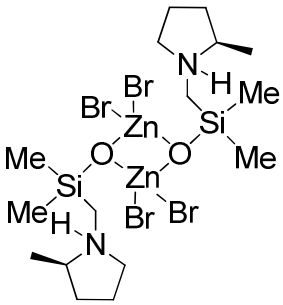
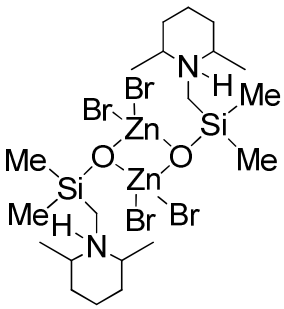
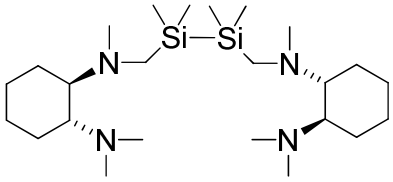


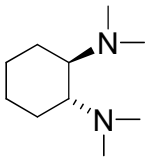
(*R*,*R*)-**178**



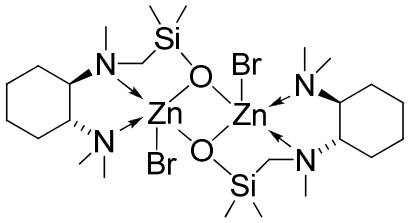
179



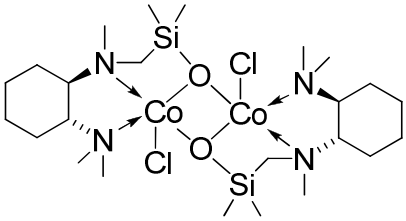
(*R*,*R*,*R*,*R*)-**180**



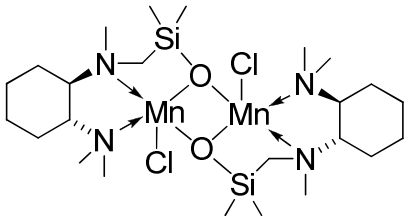
(*R*,*R*)-**181**



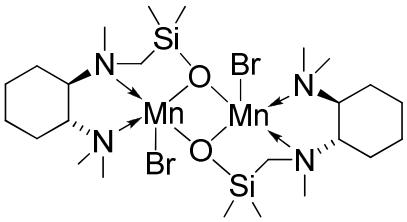
(*R*,*R*,*R*,*R*)-**182**



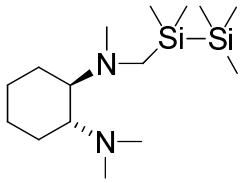
(*R*,*R*,*R*,*R*)-**183**



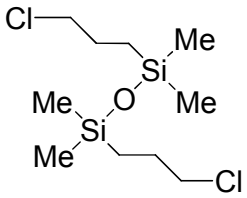
(*R*,*R*,*R*,*R*)-**184**



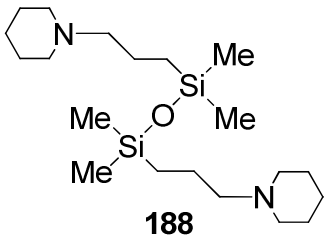
(*R*,*R*,*R*,*R*)-**185**



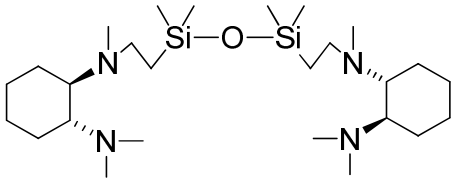
(*R*,*R*)-**186**



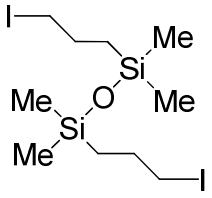
187



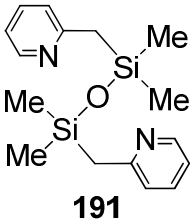
188



(*R*,*R*,*R*,*R*)-**189**



190



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8.2 Daten der Einkristallröntgenstrukturanalysen

(*S*)-1·HCl

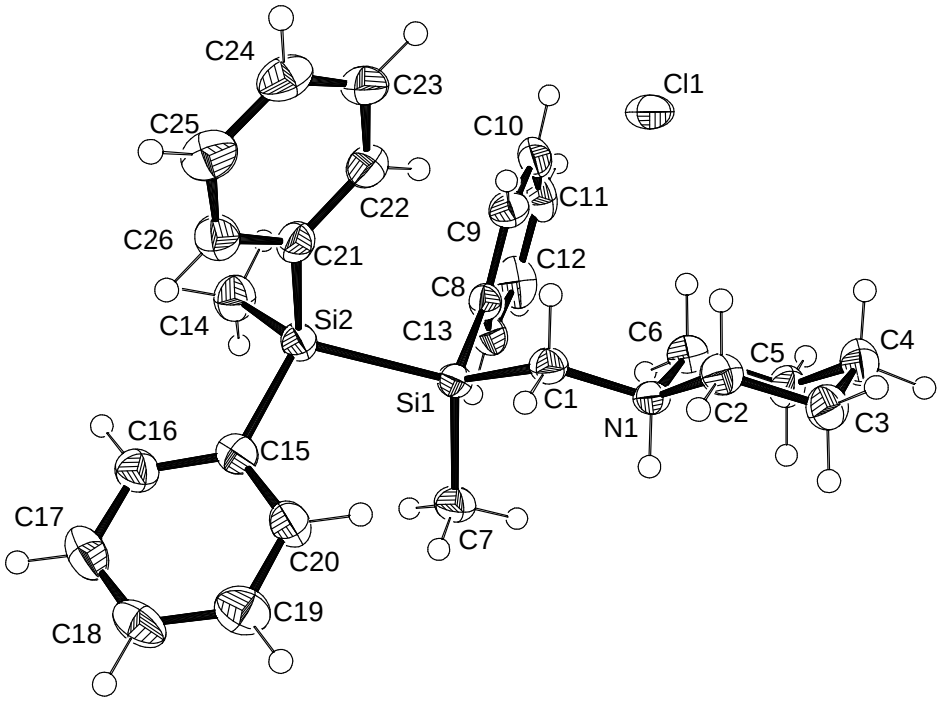

Abb. A.1 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von (*S*)-**1**·HCl im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.1 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*S*)-**1**·HCl.

Atom	x	y	z	U(eq)
Cl(1)	961(1)	5415(1)	2476(1)	37(1)
Si(1)	2862(1)	2109(1)	2080(1)	26(1)
Si(2)	4062(1)	2397(1)	1007(1)	29(1)
N(1)	149(2)	2535(2)	2569(1)	25(1)
C(3)	–2128(3)	2952(3)	2977(2)	36(1)
C(17)	4390(4)	301(3)	–646(2)	44(1)
C(8)	3754(3)	2682(2)	2864(2)	28(1)
C(2)	–1097(3)	3127(2)	2409(2)	32(1)
C(16)	4679(4)	1011(3)	–121(2)	38(1)
C(6)	655(3)	2779(3)	3299(2)	30(1)
C(1)	1158(3)	2715(2)	1993(2)	28(1)
C(11)	4931(4)	3529(3)	4090(2)	46(1)
C(18)	3132(4)	–79(3)	–695(2)	44(1)
C(19)	2153(4)	245(3)	–239(2)	47(1)
C(10)	4387(4)	4142(3)	3574(2)	39(1)
C(21)	3634(3)	3622(3)	555(2)	31(1)
C(24)	3083(4)	5454(3)	–126(2)	42(1)

C(26)	3721(4)	3724(3)	–188(2)	37(1)
C(23)	2974(4)	5371(3)	614(2)	42(1)
C(9)	3795(3)	3723(2)	2974(2)	32(1)
C(14)	5853(3)	2419(3)	1259(2)	41(1)
C(7)	2687(4)	726(2)	2229(2)	36(1)
C(4)	–1611(4)	3194(3)	3724(2)	40(1)
C(22)	3248(4)	4466(3)	944(2)	37(1)
C(12)	4925(4)	2504(3)	3994(2)	44(1)
C(5)	–374(3)	2591(3)	3866(2)	34(1)
C(20)	2446(4)	968(3)	280(2)	38(1)
C(15)	3721(3)	1364(2)	347(2)	32(1)
C(13)	4354(3)	2085(3)	3384(2)	35(1)
C(25)	3455(4)	4635(3)	–531(2)	44(1)

Tab. A.2 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*S*)-**1**·HCl.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	45(1)	24(1)	42(1)	1(1)	–1(1)	6(1)
Si(1)	28(1)	24(1)	26(1)	–1(1)	0(1)	–1(1)
Si(2)	29(1)	30(1)	28(1)	–3(1)	1(1)	1(1)
N(1)	24(1)	22(1)	31(1)	0(1)	–2(1)	–1(1)
C(3)	29(2)	36(2)	44(2)	2(2)	–1(2)	6(2)
C(17)	57(3)	42(2)	33(2)	–1(2)	4(2)	18(2)
C(8)	24(2)	33(2)	26(1)	–3(1)	1(1)	0(1)
C(2)	28(2)	29(2)	39(2)	3(1)	–5(2)	5(1)
C(16)	44(2)	33(2)	38(2)	1(2)	3(2)	3(2)
C(6)	31(2)	31(2)	30(2)	1(1)	–4(1)	–1(1)
C(1)	32(2)	26(2)	27(2)	1(1)	0(1)	–1(1)
C(11)	35(2)	67(3)	35(2)	–20(2)	–1(2)	4(2)
C(18)	66(3)	37(2)	29(2)	–9(2)	–9(2)	6(2)
C(19)	46(2)	47(2)	47(2)	–7(2)	–12(2)	–1(2)
C(10)	31(2)	40(2)	45(2)	–13(2)	8(2)	–1(2)
C(21)	26(2)	34(2)	31(2)	0(1)	2(1)	–3(1)
C(24)	36(2)	38(2)	53(2)	14(2)	–6(2)	–3(2)
C(26)	35(2)	40(2)	36(2)	–4(2)	–2(2)	–1(2)
C(23)	43(2)	27(2)	58(2)	1(2)	8(2)	–2(2)
C(9)	31(2)	32(2)	34(2)	2(1)	–3(2)	–2(1)
C(14)	35(2)	47(2)	40(2)	–1(2)	–1(2)	1(2)
C(7)	45(2)	26(2)	38(2)	0(1)	5(2)	–1(2)
C(4)	37(2)	44(2)	39(2)	–5(2)	7(2)	2(2)
C(22)	38(2)	37(2)	36(2)	2(2)	6(2)	–5(2)
C(12)	37(2)	62(2)	34(2)	5(2)	–7(2)	15(2)
C(5)	34(2)	39(2)	30(2)	–1(2)	4(1)	–1(2)
C(20)	36(2)	40(2)	36(2)	–8(2)	2(2)	4(2)
C(15)	38(2)	30(2)	28(2)	1(1)	–2(1)	2(2)
C(13)	35(2)	37(2)	34(2)	–1(2)	1(1)	6(2)

C(25)	50(2)	46(2)	37(2)	9(2)	–9(2)	–6(2)

(*R*)-1·HBr

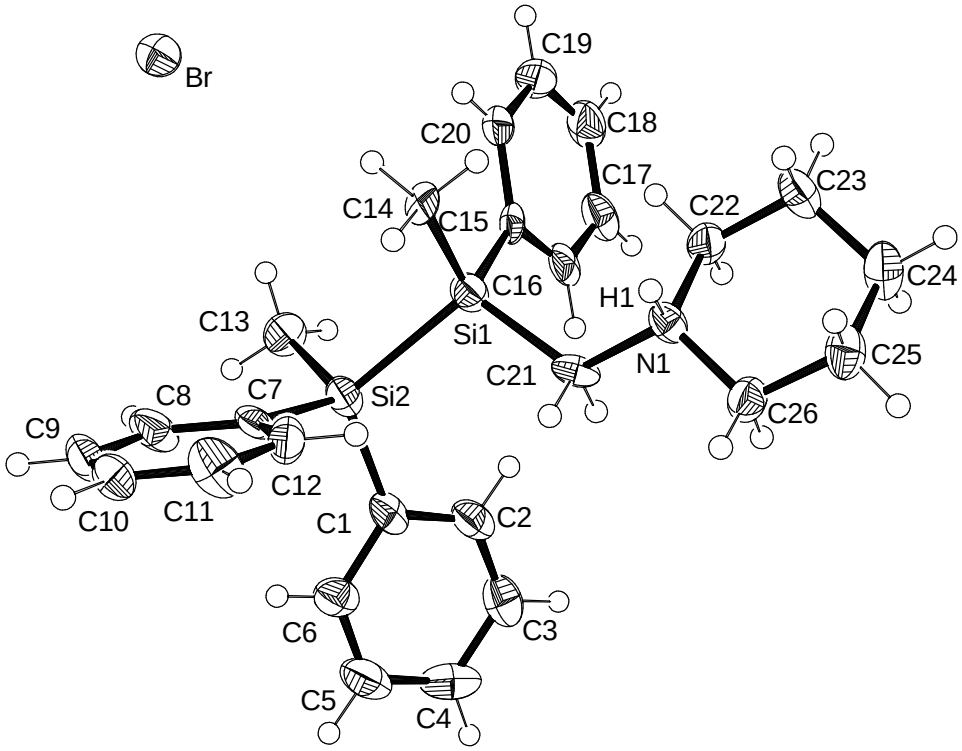

Abb. A.2 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von (*R*)-**1**·HBr im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber – mit Ausnahme des Wasserstoffatoms am Stickstoff – weggelassen.

Tab. A.3 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*)-**1**·HBr.

Atom	x	y	z	U(eq)
Br(1)	8875(1)	4533(1)	7510(1)	41(1)
C(1)	3683(6)	1416(7)	5587(3)	32(3)
C(2)	3349(6)	596(9)	5978(3)	40(3)
C(3)	3061(7)	–282(8)	5665(3)	46(3)
C(4)	3118(6)	–386(8)	4921(3)	46(3)
C(5)	3431(7)	448(10)	4517(3)	51(3)
C(6)	3708(6)	1303(7)	4844(3)	39(3)
C(7)	3753(7)	3606(6)	5366(3)	31(2)
C(8)	4710(6)	3993(7)	4910(3)	45(3)
C(9)	4423(7)	4655(8)	4403(3)	39(3)
C(10)	3140(8)	5009(7)	4330(3)	48(3)
C(11)	2182(7)	4677(8)	4770(3)	49(3)
C(12)	2461(7)	3990(7)	5280(3)	37(3)
C(13)	5919(5)	2603(7)	6276(3)	40(3)
C(14)	2726(6)	4232(6)	7229(3)	32(3)

C(15)	3833(6)	2338(7)	7879(3)	26(2)
C(16)	3864(6)	1344(7)	7998(3)	36(3)
C(17)	4423(6)	928(7)	8608(3)	42(3)
C(18)	4938(7)	1555(9)	9120(4)	51(3)
C(19)	4938(7)	2548(8)	9020(3)	43(3)
C(20)	4367(6)	2954(7)	8404(3)	39(3)
C(21)	1206(5)	2271(6)	7003(2)	27(2)
C(22)	719(6)	2185(6)	8310(3)	34(3)
C(23)	–361(6)	2360(7)	8868(3)	42(3)
C(24)	–1576(6)	1710(7)	8726(3)	45(3)
C(25)	–2100(6)	1940(7)	7977(3)	39(3)
C(26)	–1050(5)	1822(6)	7412(3)	35(2)
N(1)	184(5)	2391(5)	7576(3)	28(2)
Si(1)	2912(2)	2889(2)	7091(1)	31(1)
Si(2)	4112(2)	2611(2)	6026(1)	31(1)

Tab. A.4 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*)-**1**·HBr.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	47(1)	36(1)	41(1)	0(1)	–1(1)	7(1)
C(1)	15(4)	55(9)	27(4)	–1(4)	6(3)	10(4)
C(2)	40(5)	53(11)	27(4)	–5(5)	5(4)	5(5)
C(3)	40(5)	56(11)	42(5)	8(5)	12(4)	7(6)
C(4)	37(5)	50(10)	52(5)	–25(5)	–17(4)	21(6)
C(5)	47(6)	76(12)	28(4)	–7(5)	–3(4)	4(6)
C(6)	26(5)	56(10)	34(4)	–7(4)	–3(4)	2(5)
C(7)	29(4)	48(8)	18(3)	–9(3)	5(4)	–2(5)
C(8)	27(5)	83(11)	24(4)	–5(4)	–2(4)	–3(5)
C(9)	40(5)	51(10)	26(4)	5(4)	7(4)	–3(5)
C(10)	66(6)	55(11)	23(4)	17(4)	–13(4)	–18(6)
C(11)	44(5)	61(10)	42(4)	13(5)	–4(4)	18(6)
C(12)	34(5)	44(10)	34(4)	9(4)	0(4)	–11(4)
C(13)	25(4)	53(9)	42(4)	0(4)	–4(4)	–3(5)
C(14)	52(4)	6(9)	37(4)	4(3)	11(3)	–5(4)
C(15)	20(4)	25(8)	33(3)	4(4)	12(3)	–1(5)
C(16)	17(4)	64(10)	27(4)	–1(4)	9(4)	–3(5)
C(17)	28(5)	67(11)	31(4)	8(4)	6(4)	6(5)
C(18)	46(6)	78(12)	28(4)	14(5)	–6(4)	–16(6)
C(19)	48(5)	55(11)	28(4)	3(4)	–9(4)	–15(6)
C(20)	32(5)	53(10)	31(4)	–4(4)	9(3)	–16(5)
C(21)	31(4)	25(7)	24(3)	–10(3)	–3(3)	17(5)
C(22)	28(4)	47(9)	28(3)	5(4)	–5(3)	–8(4)
C(23)	44(5)	57(10)	26(3)	5(4)	9(4)	3(5)
C(24)	33(5)	59(11)	45(4)	16(4)	5(4)	–3(5)
C(25)	24(4)	42(9)	50(4)	3(4)	9(4)	4(5)
C(26)	28(4)	40(7)	37(4)	3(4)	0(4)	–5(4)

N(1)	24(3)	36(7)	24(3)	0(4)	3(3)	6(3)
Si(1)	29(1)	39(2)	25(1)	1(1)	0(1)	–1(1)
Si(2)	26(1)	44(2)	24(1)	3(1)	1(1)	1(1)

(*R*)-17·HI

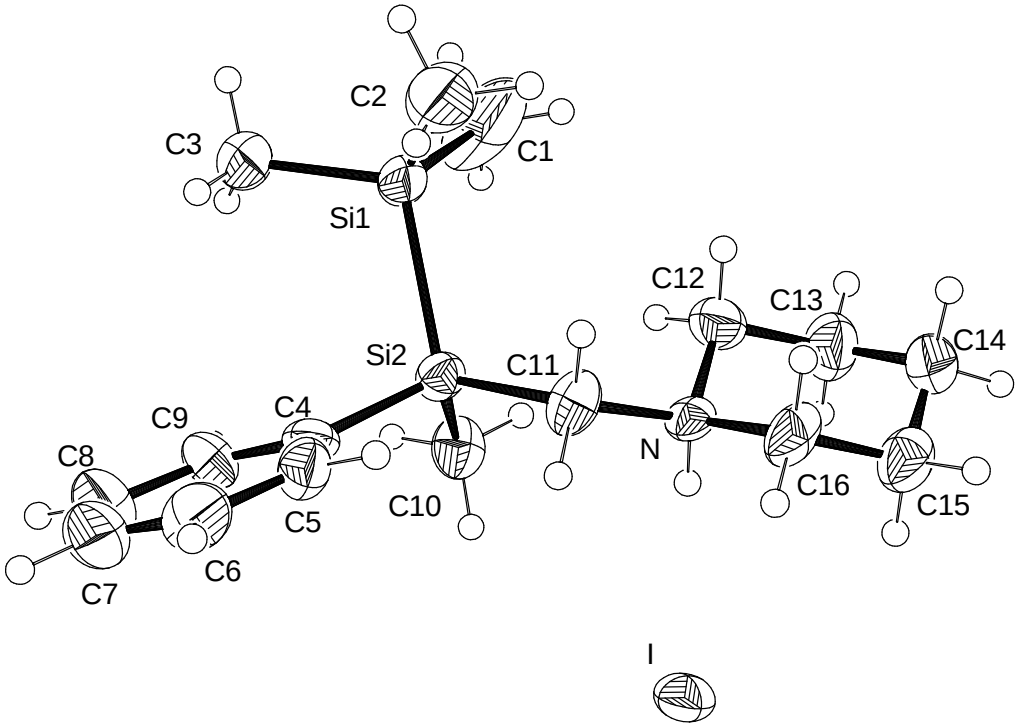

Abb. A.3 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von (*R*)-**17**·HI im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.5 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*)-**17**·HI.

Atom	x	y	z	U(eq)
C(2)	1172(12)	6381(10)	5089(4)	58(3)
C(3)	–752(13)	5202(14)	6049(5)	96(5)
C(4)	4900(11)	6997(9)	6372(4)	49(2)
C(5)	4196(9)	4413(9)	5809(3)	40(2)
C(6)	4000(11)	3095(8)	5899(4)	44(2)
C(7)	4602(13)	2202(10)	5529(4)	59(3)
C(8)	5399(15)	2586(13)	5061(5)	70(3)
C(9)	5601(13)	3862(10)	4946(4)	63(3)
C(10)	4996(11)	4750(8)	5328(4)	46(2)
C(11)	2907(13)	4806(7)	6961(3)	44(2)
C(12)	2010(12)	6747(9)	7501(4)	50(2)
C(13)	2206(15)	7461(9)	8052(3)	60(2)
C(14)	1803(12)	6616(12)	8541(4)	70(3)
C(15)	2810(13)	5408(9)	8519(3)	55(2)

C(16)	2564(12)	4705(8)	7980(3)	48(2)
C(1A)	320(20)	8012(13)	6106(6)	142(7)
I(1)	7224(1)	5723(1)	7772(1)	51(1)
N(1)	3017(8)	5551(7)	7493(3)	34(2)
Si(1)	916(3)	6389(3)	5866(1)	48(1)
Si(2)	3347(2)	5675(2)	6279(1)	36(1)

Tab. A.6 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*)-**17**·HI.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(2)	58(6)	73(7)	42(5)	5(5)	–4(5)	15(5)
C(3)	54(7)	172(15)	62(7)	17(8)	0(6)	–23(8)
C(4)	55(6)	45(5)	46(5)	3(4)	6(4)	–11(4)
C(5)	32(4)	41(5)	46(5)	–8(4)	–7(3)	12(4)
C(6)	52(5)	42(5)	37(5)	–6(4)	–5(4)	2(4)
C(7)	77(7)	39(5)	61(7)	–14(5)	–19(6)	15(5)
C(8)	69(7)	71(7)	71(7)	–27(6)	–6(6)	26(6)
C(9)	68(7)	57(7)	64(7)	–4(5)	16(5)	9(5)
C(10)	48(5)	36(5)	54(6)	–8(4)	6(4)	10(4)
C(11)	57(5)	37(4)	39(4)	–2(3)	–7(4)	–10(4)
C(12)	41(5)	59(6)	51(5)	14(4)	4(4)	10(5)
C(13)	74(6)	61(6)	45(5)	–8(4)	0(5)	10(6)
C(14)	45(6)	125(10)	42(6)	1(6)	4(4)	0(6)
C(15)	47(5)	78(7)	39(4)	14(4)	–1(4)	–19(5)
C(16)	51(6)	56(5)	38(4)	24(3)	–4(4)	–11(4)
C(1A)	209(17)	111(11)	107(11)	–52(9)	–88(11)	120(11)
I(1)	32(1)	63(1)	58(1)	–7(1)	–3(1)	3(1)
N(1)	26(3)	41(4)	36(3)	2(3)	–6(3)	–8(3)
Si(1)	49(2)	60(2)	35(1)	–5(1)	–6(1)	22(1)
Si(2)	38(1)	36(1)	34(1)	2(1)	–3(1)	2(1)

(*R*)-93·MeI

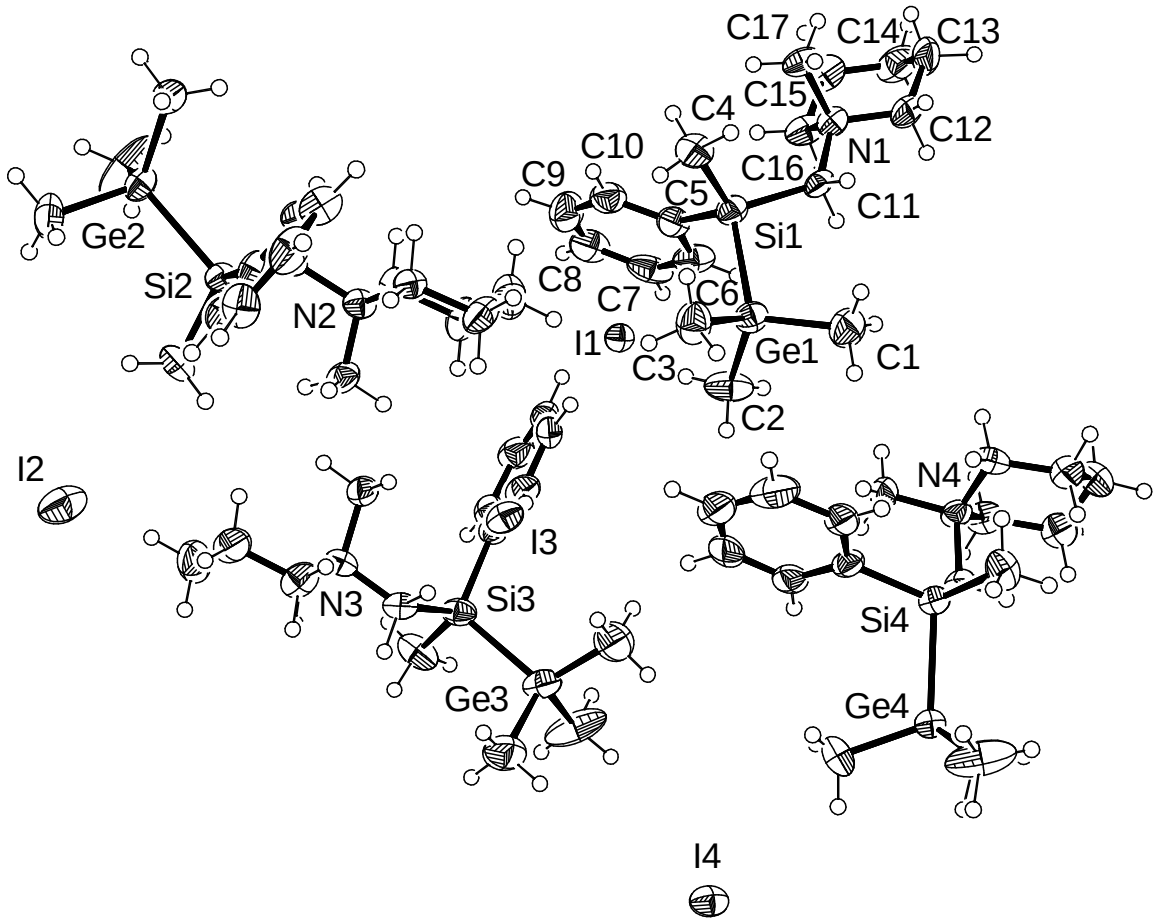

Abb. A.4 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von (*R*)-**93**·MeI im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome sowie dem Großteil der Kohlenstoffatome wurde der Übersicht halber weggelassen.

Tab. A.7 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*)-**93**·MeI.

Atom	x	y	z	U(eq)
C(1)	9239(15)	1853(7)	1469(7)	51(3)
C(2)	9644(16)	1157(6)	1095(9)	59(4)
C(3)	8910(20)	1139(7)	149(9)	73(4)
C(4)	9318(17)	1732(7)	–258(7)	58(3)
C(5)	8910(15)	2445(7)	116(8)	52(3)
C(6)	9398(14)	3161(6)	1405(7)	48(3)
C(7)	12502(18)	2970(20)	2776(13)	189(16)
C(9)	9830(40)	3490(20)	4515(12)	190(15)
C(11)	9870(20)	1476(10)	3798(7)	92(6)
C(13)	11410(50)	4937(19)	3627(17)	240(20)
C(14)	12850(30)	4768(19)	2200(40)	360(40)
C(15)	9284(9)	4558(4)	2647(4)	12(2)
C(16)	5736(14)	5040(6)	8385(8)	49(3)

C(17)	5304(17)	5675(7)	8792(9)	64(4)
C(18)	6076(17)	5641(8)	9746(9)	70(4)
C(19)	5667(16)	4889(8)	10115(8)	62(4)
C(20)	6121(13)	4296(7)	9634(7)	52(3)
C(21)	5512(14)	3722(7)	8209(9)	59(4)
C(22)	2486(18)	3948(12)	6826(11)	99(6)
C(23)	7540(20)	2326(16)	7062(17)	148(10)
C(24)	4240(60)	2410(30)	5550(30)	430(60)
C(25)	3800(40)	810(20)	6620(20)	205(16)
C(26)	1640(30)	2024(13)	7140(18)	150(10)
C(27)	4940(30)	1509(14)	8284(12)	150(10)
C(28)	5510(50)	5350(30)	6010(30)	250(20)
Ge(1)	10981(3)	4596(1)	2527(2)	119(1)
Ge(2)	6108(4)	4405(2)	6197(2)	147(1)
N(1)	9698(11)	2483(5)	1010(6)	42(2)
N(2)	5260(13)	4359(5)	8721(6)	45(3)
O(1)	6386(12)	7720(6)	10301(7)	86(3)
O(2)	6144(14)	8503(5)	9134(7)	72(3)
O(3)	7147(9)	7319(5)	9082(6)	65(3)
O(4)	4398(9)	7519(6)	9033(8)	91(4)
O(5)	2095(8)	4511(4)	8794(5)	56(2)
O(6)	1058(11)	3333(5)	8820(6)	70(3)
O(7)	–667(11)	4274(6)	8738(6)	86(3)
O(8)	1256(11)	4088(5)	10016(5)	67(2)
S(1)	5999(3)	7724(2)	9390(2)	51(1)
S(2)	934(3)	4073(2)	9069(2)	51(1)
Si(1)	10403(4)	3361(2)	2526(2)	55(1)
Si(2)	8888(6)	3006(4)	3476(3)	101(2)
Si(3)	8439(10)	1881(4)	3776(4)	118(2)
Si(4)	4658(6)	3679(3)	7055(3)	91(2)
Si(5)	5152(9)	2490(5)	6703(8)	192(5)
Si(6)	3699(10)	1682(4)	7168(5)	138(3)
C(8)	6890(30)	3450(30)	3100(20)	260(30)
C(12)	8030(60)	1932(18)	4756(18)	270(30)
C(30)	8100(40)	4295(18)	6180(30)	230(20)
C(29)	5610(70)	4530(40)	5210(20)	420(50)
C(10)	7010(80)	1840(80)	2971(18)	820(150)
C(1)	9239(15)	1853(7)	1469(7)	51(3)
C(2)	9644(16)	1157(6)	1095(9)	59(4)
C(3)	8910(20)	1139(7)	149(9)	73(4)
C(4)	9318(17)	1732(7)	–258(7)	58(3)
C(5)	8910(15)	2445(7)	116(8)	52(3)
C(6)	9398(14)	3161(6)	1405(7)	48(3)
C(7)	12502(18)	2970(20)	2776(13)	189(16)
C(9)	9830(40)	3490(20)	4515(12)	190(15)
C(11)	9870(20)	1476(10)	3798(7)	92(6)

C(13)	11410(50)	4937(19)	3627(17)	240(20)
C(14)	12850(30)	4768(19)	2200(40)	360(40)
C(15)	9284(9)	4558(4)	2647(4)	12(2)
C(16)	5736(14)	5040(6)	8385(8)	49(3)
C(17)	5304(17)	5675(7)	8792(9)	64(4)
C(18)	6076(17)	5641(8)	9746(9)	70(4)
C(19)	5667(16)	4889(8)	10115(8)	62(4)
C(20)	6121(13)	4296(7)	9634(7)	52(3)
C(21)	5512(14)	3722(7)	8209(9)	59(4)
C(22)	2486(18)	3948(12)	6826(11)	99(6)
C(23)	7540(20)	2326(16)	7062(17)	148(10)
C(24)	4240(60)	2410(30)	5550(30)	430(60)
C(25)	3800(40)	810(20)	6620(20)	205(16)
C(26)	1640(30)	2024(13)	7140(18)	150(10)
C(27)	4940(30)	1509(14)	8284(12)	150(10)
C(28)	5510(50)	5350(30)	6010(30)	250(20)
Ge(1)	10981(3)	4596(1)	2527(2)	119(1)
Ge(2)	6108(4)	4405(2)	6197(2)	147(1)
N(1)	9698(11)	2483(5)	1010(6)	42(2)
N(2)	5260(13)	4359(5)	8721(6)	45(3)
O(1)	6386(12)	7720(6)	10301(7)	86(3)
O(2)	6144(14)	8503(5)	9134(7)	72(3)
O(3)	7147(9)	7319(5)	9082(6)	65(3)
O(4)	4398(9)	7519(6)	9033(8)	91(4)
O(5)	2095(8)	4511(4)	8794(5)	56(2)

Tab. A.8 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*)-**93**·MeI.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	48(7)	66(8)	41(7)	–1(6)	18(5)	–12(6)
C(2)	58(8)	35(7)	79(9)	8(6)	1(7)	–4(6)
C(3)	101(12)	53(9)	65(9)	–21(7)	18(8)	–17(8)
C(4)	78(9)	64(9)	37(6)	–7(6)	20(6)	–17(7)
C(5)	49(7)	52(7)	59(8)	–12(6)	21(6)	–5(6)
C(6)	46(7)	49(7)	47(7)	–7(5)	5(5)	0(5)
C(7)	28(9)	430(50)	98(14)	–70(20)	–17(9)	–21(16)
C(9)	210(30)	290(40)	52(12)	16(17)	–4(14)	–90(30)
C(11)	135(15)	117(14)	13(6)	11(7)	–12(7)	–12(13)
C(13)	370(50)	220(40)	120(20)	–70(20)	70(30)	–210(40)
C(14)	77(17)	150(30)	760(100)	–130(50)	–120(30)	–19(18)
C(15)	35(5)	0(3)	0(3)	–15(3)	–1(3)	15(3)
C(16)	32(6)	50(7)	60(8)	10(6)	–4(5)	11(5)
C(17)	59(9)	53(9)	82(10)	–12(7)	21(7)	–5(7)
C(18)	59(9)	67(10)	88(10)	4(8)	27(8)	–7(7)
C(19)	54(8)	83(10)	54(8)	1(7)	19(6)	–25(7)
C(20)	37(7)	75(9)	41(6)	1(6)	3(5)	–14(6)

C(21)	32(7)	53(8)	94(10)	–24(7)	19(6)	7(6)
C(22)	52(9)	149(17)	97(11)	–8(12)	14(8)	3(10)
C(23)	81(13)	190(30)	190(20)	–48(19)	80(15)	11(14)
C(24)	300(50)	550(100)	340(60)	–390(70)	–160(50)	240(60)
C(25)	170(30)	200(30)	230(40)	–40(30)	0(30)	–50(30)
C(26)	190(30)	94(15)	190(30)	–14(16)	100(20)	–19(16)
C(27)	210(20)	170(20)	96(14)	84(15)	80(15)	68(19)
C(28)	220(40)	330(70)	250(40)	0(40)	150(30)	120(40)
Ge(1)	128(2)	95(2)	127(2)	–22(1)	9(1)	–7(1)
Ge(2)	138(2)	185(3)	132(2)	10(2)	56(2)	39(2)
N(1)	23(5)	43(6)	66(7)	6(5)	20(5)	1(4)
N(2)	20(5)	44(6)	70(7)	3(5)	3(5)	0(4)
O(1)	81(7)	77(7)	110(9)	–4(6)	41(6)	–27(6)
O(2)	105(9)	52(6)	57(7)	–4(5)	11(6)	8(5)
O(3)	31(4)	58(5)	115(8)	–29(5)	37(5)	1(4)
O(4)	13(4)	104(8)	161(11)	–24(7)	30(5)	–8(4)
O(5)	31(4)	47(5)	97(6)	1(5)	26(4)	–10(4)
O(6)	74(6)	67(7)	68(6)	6(5)	15(5)	–31(5)
O(7)	40(5)	125(10)	87(7)	13(6)	0(5)	1(5)
O(8)	75(6)	71(6)	55(5)	10(5)	18(4)	–8(5)
S(1)	31(2)	50(2)	76(2)	–11(2)	22(1)	1(1)
S(2)	30(2)	51(2)	75(2)	9(2)	15(1)	–3(1)
Si(1)	53(2)	55(2)	54(2)	–7(2)	0(2)	2(2)
Si(2)	60(3)	179(6)	67(3)	–11(3)	16(2)	–16(3)
Si(3)	158(6)	104(4)	97(4)	–3(3)	41(4)	–30(4)
Si(4)	66(3)	92(3)	106(4)	–30(3)	1(2)	15(2)
Si(5)	103(5)	170(8)	304(12)	–165(9)	48(6)	–7(5)
Si(6)	151(6)	116(5)	151(6)	–18(4)	42(5)	–12(4)
C(8)	110(20)	360(60)	290(50)	–170(40)	–40(20)	100(30)
C(12)	570(80)	150(30)	90(19)	–17(18)	80(30)	–60(40)
C(30)	200(30)	170(30)	400(50)	–130(30)	210(40)	–50(20)
C(29)	480(90)	660(130)	110(20)	200(50)	70(40)	190(90)
C(10)	420(80)	2000(400)	42(17)	–30(60)	30(30)	–690(160)
C(1)	48(7)	66(8)	41(7)	–1(6)	18(5)	–12(6)
C(2)	58(8)	35(7)	79(9)	8(6)	1(7)	–4(6)
C(3)	101(12)	53(9)	65(9)	–21(7)	18(8)	–17(8)
C(4)	78(9)	64(9)	37(6)	–7(6)	20(6)	–17(7)
C(5)	49(7)	52(7)	59(8)	–12(6)	21(6)	–5(6)
C(6)	46(7)	49(7)	47(7)	–7(5)	5(5)	0(5)
C(7)	28(9)	430(50)	98(14)	–70(20)	–17(9)	–21(16)
C(9)	210(30)	290(40)	52(12)	16(17)	–4(14)	–90(30)
C(11)	135(15)	117(14)	13(6)	11(7)	–12(7)	–12(13)
C(13)	370(50)	220(40)	120(20)	–70(20)	70(30)	–210(40)
C(14)	77(17)	150(30)	760(100)	–130(50)	–120(30)	–19(18)
C(15)	35(5)	0(3)	0(3)	–15(3)	–1(3)	15(3)
C(16)	32(6)	50(7)	60(8)	10(6)	–4(5)	11(5)

C(17)	59(9)	53(9)	82(10)	–12(7)	21(7)	–5(7)
C(18)	59(9)	67(10)	88(10)	4(8)	27(8)	–7(7)
C(19)	54(8)	83(10)	54(8)	1(7)	19(6)	–25(7)
C(20)	37(7)	75(9)	41(6)	1(6)	3(5)	–14(6)
C(21)	32(7)	53(8)	94(10)	–24(7)	19(6)	7(6)
C(22)	52(9)	149(17)	97(11)	–8(12)	14(8)	3(10)
C(23)	81(13)	190(30)	190(20)	–48(19)	80(15)	11(14)
C(24)	300(50)	550(100)	340(60)	–390(70)	–160(50)	240(60)
C(25)	170(30)	200(30)	230(40)	–40(30)	0(30)	–50(30)
C(26)	190(30)	94(15)	190(30)	–14(16)	100(20)	–19(16)
C(27)	210(20)	170(20)	96(14)	84(15)	80(15)	68(19)
C(28)	220(40)	330(70)	250(40)	0(40)	150(30)	120(40)
Ge(1)	128(2)	95(2)	127(2)	–22(1)	9(1)	–7(1)
Ge(2)	138(2)	185(3)	132(2)	10(2)	56(2)	39(2)
N(1)	23(5)	43(6)	66(7)	6(5)	20(5)	1(4)
N(2)	20(5)	44(6)	70(7)	3(5)	3(5)	0(4)
O(1)	81(7)	77(7)	110(9)	–4(6)	41(6)	–27(6)
O(2)	105(9)	52(6)	57(7)	–4(5)	11(6)	8(5)
O(3)	31(4)	58(5)	115(8)	–29(5)	37(5)	1(4)
O(4)	13(4)	104(8)	161(11)	–24(7)	30(5)	–8(4)
O(5)	31(4)	47(5)	97(6)	1(5)	26(4)	–10(4)

rac-92·MeI

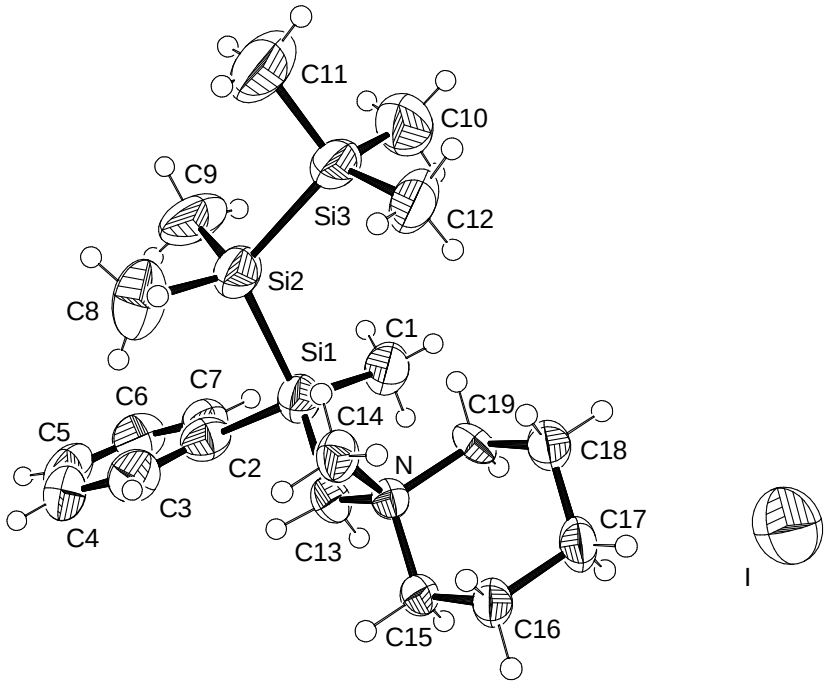

Abb. A.5 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von *rac*-**92**·MeI im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.9 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von *rac*-**92**·MeI.

Atom	x	y	z	U(eq)
I	6027(1)	997(1)	2628(1)	54(1)
N	4267(4)	8949(3)	1743(6)	37(1)
C(1)	3231(7)	10784(6)	3472(10)	66(2)
Si(1)	2876(2)	10218(1)	1922(2)	54(1)
C(2)	2518(6)	10934(4)	526(10)	57(2)
Si(2)	1511(2)	9545(2)	2191(3)	68(1)
C(3)	2328(7)	10693(5)	–764(11)	67(3)
Si(3)	1402(2)	8807(2)	4147(3)	75(1)
C(4)	1952(7)	11187(6)	–1728(12)	76(3)
C(5)	1727(7)	11950(6)	–1361(13)	78(3)
C(6)	1945(7)	12220(5)	–79(12)	70(3)
C(7)	2329(6)	11696(5)	846(10)	60(2)
C(8)	1138(11)	8965(7)	630(16)	107(5)
C(9)	702(8)	10399(7)	2384(16)	104(5)
C(10)	1488(10)	9490(10)	5614(14)	114(5)
C(11)	252(9)	8359(9)	4020(20)	129(6)
C(12)	2251(7)	7995(6)	4411(13)	82(3)
C(13)	3890(6)	9715(4)	1223(8)	44(2)
C(14)	3613(6)	8302(4)	1358(9)	48(2)
C(15)	5162(5)	8798(4)	1173(7)	39(2)
C(16)	5640(6)	8079(4)	1755(8)	47(2)
C(17)	5780(6)	8150(5)	3267(8)	56(2)
C(18)	4889(6)	8281(4)	3869(8)	51(2)
C(19)	4411(6)	9008(4)	3263(7)	42(2)

Tab. A.10 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von *rac*-**92**·MeI.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I	62(1)	52(1)	46(1)	–8(1)	–3(1)	–1(1)
N	37(4)	41(3)	33(3)	–1(2)	0(3)	1(2)
C(1)	59(7)	77(5)	62(6)	–13(5)	–6(5)	11(4)
Si(1)	53(2)	57(1)	53(1)	–4(1)	–3(1)	7(1)
C(2)	49(6)	52(4)	71(6)	3(4)	11(4)	6(4)
Si(2)	52(2)	76(2)	74(2)	11(1)	–4(1)	5(1)
C(3)	64(7)	58(5)	79(7)	–3(5)	3(5)	12(4)
Si(3)	46(2)	95(2)	83(2)	31(2)	2(1)	4(1)
C(4)	60(7)	99(7)	67(7)	5(5)	–13(5)	7(5)
C(5)	48(6)	82(6)	104(9)	38(6)	–8(6)	9(5)
C(6)	65(7)	57(5)	87(8)	19(5)	10(6)	7(4)
C(7)	53(6)	65(5)	63(6)	–4(4)	4(4)	4(4)
C(8)	97(11)	110(9)	109(11)	–20(7)	–34(9)	–2(7)
C(9)	49(7)	112(9)	154(13)	46(8)	24(7)	26(6)

C(10)	93(11)	175(13)	75(9)	4(9)	10(7)	34(9)
C(11)	64(10)	140(12)	177(18)	60(11)	–21(9)	–9(7)
C(12)	53(7)	90(7)	100(9)	24(6)	–22(6)	–9(5)
C(13)	56(5)	37(3)	38(4)	7(3)	0(3)	4(3)
C(14)	49(5)	43(4)	52(5)	9(3)	–8(4)	0(3)
C(15)	38(5)	45(3)	33(4)	–5(3)	0(3)	0(3)
C(16)	46(5)	55(4)	39(4)	0(3)	–5(3)	10(3)
C(17)	57(6)	72(5)	37(4)	–4(4)	–13(4)	14(4)
C(18)	52(6)	56(4)	45(5)	2(3)	–3(4)	5(3)
C(19)	58(5)	44(3)	23(3)	–2(3)	8(3)	–3(3)

(*R*)-97·H_2SO_4

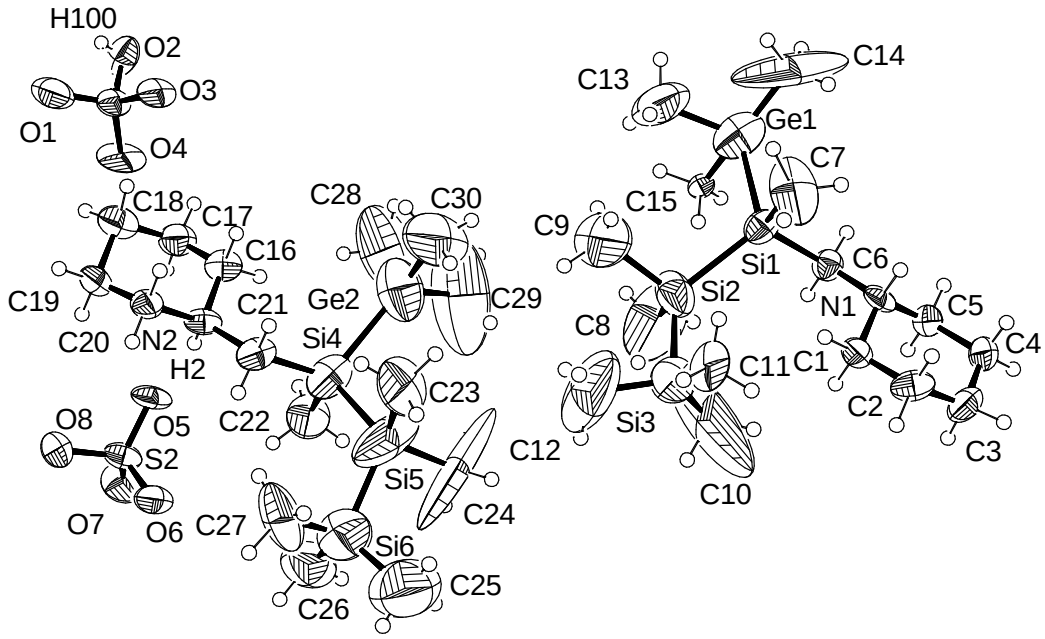

Abb. A.6 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von (*R*)-**97**·H_2SO_4 im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.11 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*)-**97**·H_2SO_4.

Atom	x	y	z	U(eq)
C(1)	9235(15)	1853(7)	1468(7)	51(3)
C(2)	9641(16)	1157(6)	1095(9)	59(4)
C(3)	8910(20)	1139(7)	147(9)	72(4)
C(4)	9306(17)	1732(7)	–258(7)	59(3)
C(5)	8911(15)	2445(7)	117(8)	52(3)
C(6)	9394(14)	3162(6)	1401(7)	48(3)
C(7)	12511(18)	2970(20)	2786(13)	193(16)
C(9)	9780(40)	3500(20)	4523(12)	189(16)
C(11)	9880(20)	1473(11)	3800(7)	92(6)

C(13)	11420(50)	4933(19)	3618(17)	230(20)
C(14)	12840(30)	4780(20)	2190(40)	310(30)
C(15)	9283(9)	4558(4)	2649(4)	12(2)
C(16)	5736(14)	5040(6)	8388(8)	49(3)
C(17)	5298(17)	5676(7)	8793(9)	64(4)
C(18)	6065(17)	5641(8)	9742(9)	70(4)
C(19)	5664(16)	4888(8)	10112(8)	62(4)
C(20)	6122(13)	4296(7)	9632(7)	52(3)
C(21)	5513(14)	3721(7)	8202(9)	60(4)
C(22)	2489(18)	3948(12)	6827(11)	100(6)
C(23)	7530(20)	2324(16)	7056(17)	147(10)
C(24)	4220(60)	2400(30)	5550(30)	410(50)
C(25)	3800(40)	820(20)	6620(20)	213(15)
C(26)	1660(30)	2026(13)	7146(18)	150(10)
C(27)	4940(30)	1513(15)	8288(13)	149(11)
C(28)	5530(40)	5340(30)	6040(30)	240(20)
Ge(1)	10981(3)	4596(1)	2528(2)	120(1)
Ge(2)	6106(4)	4405(2)	6196(2)	148(1)
N(1)	9693(11)	2483(5)	1008(6)	42(2)
N(2)	5254(12)	4361(5)	8721(6)	44(3)
O(1)	6378(12)	7721(6)	10296(7)	87(3)
O(2)	6147(14)	8503(5)	9135(7)	71(3)
O(3)	7146(9)	7320(5)	9082(6)	64(3)
O(4)	4401(9)	7519(6)	9034(8)	92(4)
O(5)	2098(8)	4510(4)	8796(5)	57(2)
O(6)	1054(11)	3333(5)	8819(6)	70(3)
O(7)	–671(11)	4274(6)	8738(6)	86(3)
O(8)	1276(11)	4086(5)	10020(5)	66(2)
S(1)	5997(3)	7724(2)	9388(2)	51(1)
S(2)	935(3)	4073(2)	9069(2)	52(1)
Si(1)	10404(4)	3360(2)	2526(2)	55(1)
Si(2)	8888(6)	3005(4)	3476(3)	102(2)
Si(3)	8442(10)	1880(4)	3777(4)	119(2)
Si(4)	4657(5)	3678(3)	7055(3)	91(2)
Si(5)	5157(9)	2487(5)	6706(8)	195(5)
Si(6)	3702(10)	1681(4)	7167(5)	138(2)
C(8)	6880(30)	3430(30)	3110(20)	270(30)
C(12)	8040(60)	1936(19)	4766(18)	270(20)
C(30)	8100(40)	4303(18)	6170(30)	230(20)
C(29)	5640(80)	4530(40)	5200(20)	420(40)
C(10)	7160(80)	1700(70)	2975(17)	750(140)

Tab. A.12 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*)-**97**·H_2SO_4.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	48(7)	65(9)	41(7)	0(6)	16(5)	–12(6)
C(2)	59(9)	34(7)	78(9)	7(6)	1(7)	–5(6)
C(3)	101(12)	52(9)	66(9)	–20(7)	20(8)	–19(8)
C(4)	79(9)	63(9)	37(7)	–8(6)	22(6)	–17(7)
C(5)	49(7)	52(8)	60(8)	–12(6)	22(6)	–4(6)
C(6)	45(7)	50(7)	47(7)	–6(5)	4(5)	–1(5)
C(7)	28(9)	440(50)	99(15)	–80(20)	–19(9)	–22(16)
C(9)	210(30)	290(40)	54(11)	12(17)	–6(14)	–100(30)
C(11)	129(15)	122(15)	13(6)	11(7)	–13(7)	–8(13)
C(13)	350(50)	220(40)	130(20)	–60(20)	70(30)	–200(40)
C(14)	91(18)	170(30)	600(90)	–50(40)	–100(30)	–60(20)
C(15)	34(5)	0(3)	0(3)	–15(3)	–1(3)	15(3)
C(16)	31(6)	49(7)	59(8)	9(6)	–4(5)	12(5)
C(17)	59(9)	54(9)	81(10)	–10(7)	21(7)	–6(7)
C(18)	61(9)	67(10)	87(10)	3(8)	27(8)	–6(7)
C(19)	56(8)	80(10)	55(8)	–1(7)	22(6)	–27(7)
C(20)	37(7)	75(9)	42(7)	3(6)	3(5)	–15(6)
C(21)	33(7)	53(8)	97(10)	–25(7)	18(6)	7(6)
C(22)	51(9)	148(17)	98(12)	–10(12)	12(8)	2(10)
C(23)	81(13)	200(30)	190(20)	–46(19)	77(15)	13(14)
C(24)	320(50)	510(90)	320(60)	–360(70)	–140(40)	210(60)
C(25)	200(30)	200(30)	230(40)	–30(30)	0(30)	–50(30)
C(26)	190(30)	97(15)	190(30)	–11(16)	100(20)	–17(16)
C(27)	200(30)	170(20)	97(14)	85(15)	81(16)	70(20)
C(28)	200(30)	300(50)	260(40)	0(40)	140(30)	100(30)
Ge(1)	129(2)	95(2)	128(2)	–22(1)	9(1)	–7(1)
Ge(2)	138(2)	185(3)	132(2)	11(2)	56(2)	40(2)
N(1)	22(5)	44(6)	66(7)	4(5)	20(4)	0(4)
N(2)	22(5)	41(6)	67(7)	2(5)	4(5)	0(4)
O(1)	84(7)	77(7)	111(9)	–5(6)	44(6)	–28(6)
O(2)	102(9)	52(6)	57(7)	–4(5)	12(6)	7(5)
O(3)	31(4)	59(5)	113(7)	–29(5)	38(5)	1(4)
O(4)	14(4)	106(8)	161(11)	–26(7)	31(5)	–8(5)
O(5)	32(4)	47(5)	98(6)	–1(5)	28(4)	–12(4)
O(6)	73(6)	67(7)	69(6)	5(5)	15(5)	–31(5)
O(7)	39(5)	125(10)	87(7)	15(6)	0(5)	2(5)
O(8)	81(7)	70(6)	50(5)	9(5)	20(4)	–11(5)
S(1)	31(2)	50(2)	76(2)	–11(2)	21(1)	1(1)
S(2)	30(2)	51(2)	76(2)	9(2)	15(1)	–3(1)
Si(1)	53(2)	55(2)	54(2)	–7(2)	0(2)	2(2)
Si(2)	61(3)	180(6)	67(3)	–10(3)	16(2)	–17(3)
Si(3)	162(6)	104(4)	96(4)	–4(3)	42(4)	–31(4)
Si(4)	65(3)	93(3)	106(4)	–30(3)	0(2)	15(2)

Si(5)	100(5)	175(8)	312(12)	–171(9)	48(6)	–6(5)
Si(6)	149(6)	116(5)	152(6)	–16(4)	41(5)	–11(4)
C(8)	120(20)	390(60)	270(40)	–180(50)	–40(20)	110(30)
C(12)	550(80)	160(30)	90(19)	–15(19)	60(30)	–50(40)
C(30)	210(30)	170(30)	380(50)	–130(30)	210(40)	–50(20)
C(29)	550(100)	610(120)	90(20)	160(40)	80(40)	200(90)
C(10)	420(80)	1800(400)	37(16)	–80(60)	50(30)	–600(150)

(*S*,*R*,*S*)-85·MeI

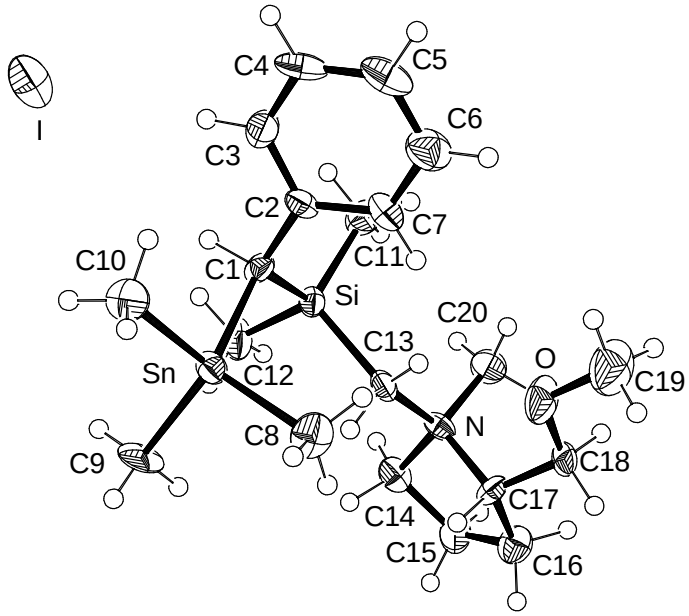

Abb. A.7 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von (*S*,*R*,*S*)-**85**·MeI im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.13 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*S*,*R*,*S*)-**85**·MeI.

Atom	x	y	z	U(eq)
C(1)	8512(5)	8840(3)	4473(2)	30(1)
C(2)	9570(5)	8166(3)	4146(2)	29(1)
C(3)	9530(6)	7264(3)	4343(3)	38(1)
C(4)	10463(7)	6640(4)	4042(3)	47(1)
C(5)	11501(7)	6899(4)	3536(3)	52(2)
C(6)	11595(6)	7782(4)	3341(3)	47(1)
C(7)	10644(6)	8405(4)	3638(3)	39(1)
C(8)	7269(7)	9515(4)	2724(3)	49(1)
C(9)	4914(6)	9831(4)	4153(3)	46(1)
C(10)	5776(6)	7646(3)	3634(5)	43(1)
C(11)	11155(6)	9659(4)	5293(3)	48(2)
C(12)	8036(6)	10356(4)	5540(3)	45(2)
C(13)	9482(6)	10672(3)	4046(3)	33(1)

C(14)	9244(6)	12229(3)	4500(2)	35(1)
C(15)	9695(7)	13150(4)	4238(3)	49(2)
C(16)	10273(6)	13021(3)	3474(3)	41(1)
C(17)	10174(5)	12015(3)	3314(2)	31(1)
C(18)	11410(6)	11699(3)	2817(3)	38(1)
C(19)	12481(8)	10451(5)	2255(4)	69(2)
C(20)	11727(6)	11543(4)	4366(3)	38(1)
I	5625(1)	2615(1)	3479(1)	46(1)
N	10181(4)	11589(3)	4078(2)	26(1)
O	11360(5)	10762(2)	2730(2)	50(1)
Si	9332(2)	9893(1)	4855(1)	28(1)
Sn	6613(1)	8978(1)	3734(1)	31(1)

Tab. A.14 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*S*,*R*,*S*)-**85**·MeI.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	27(2)	32(3)	29(2)	0(2)	3(2)	–2(2)
C(2)	23(2)	37(3)	28(2)	–3(3)	–7(2)	9(2)
C(3)	38(3)	42(3)	34(3)	4(3)	–6(2)	1(3)
C(4)	56(4)	39(3)	47(3)	–1(4)	–10(3)	14(3)
C(5)	52(3)	52(3)	52(3)	–11(4)	–5(3)	24(3)
C(6)	32(3)	68(4)	41(3)	–3(3)	2(3)	12(3)
C(7)	31(2)	48(3)	38(3)	–3(2)	5(3)	9(2)
C(8)	54(3)	55(4)	37(3)	–2(3)	–3(3)	–4(3)
C(9)	37(3)	50(4)	50(3)	–5(3)	7(3)	13(3)
C(10)	38(3)	39(3)	51(3)	–3(3)	–11(2)	–6(2)
C(11)	42(3)	55(4)	45(3)	18(3)	–15(3)	–9(3)
C(12)	46(4)	48(3)	42(3)	–10(3)	15(3)	–11(3)
C(13)	32(3)	31(3)	35(3)	0(2)	0(2)	–1(2)
C(14)	34(3)	41(3)	29(2)	–3(2)	7(2)	1(2)
C(15)	59(4)	38(3)	49(3)	–6(3)	10(3)	0(3)
C(16)	47(3)	38(3)	38(3)	6(2)	1(3)	–4(2)
C(17)	33(3)	32(3)	26(2)	6(2)	2(2)	–6(2)
C(18)	42(3)	44(3)	29(3)	0(2)	4(2)	–9(3)
C(19)	82(5)	62(4)	61(4)	–9(4)	38(4)	–6(4)
C(20)	31(3)	48(3)	36(3)	4(2)	–9(2)	–5(3)
I	33(1)	73(1)	33(1)	–1(1)	0(1)	3(1)
N	25(2)	29(2)	25(2)	–4(2)	–1(2)	–1(2)
O	62(3)	46(2)	42(2)	–5(2)	23(3)	1(3)
Si	28(1)	31(1)	26(1)	0(1)	2(1)	–2(1)
Sn	26(1)	33(1)	33(1)	–3(1)	1(1)	2(1)

(*R*,*S*)-78·Quinuklidin

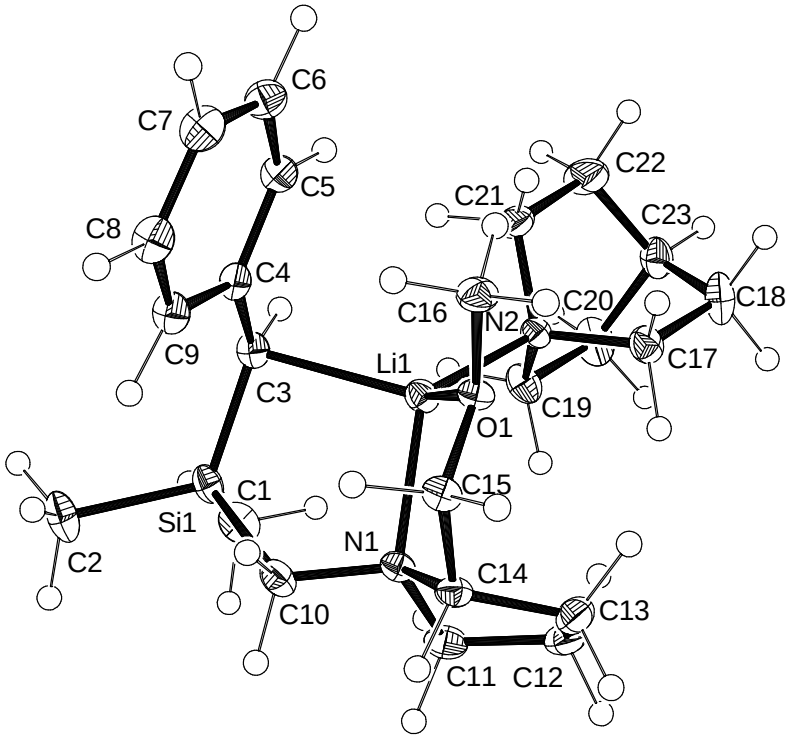

Abb. A.8 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von (*R*,*S*)-**78**·Quinuklidin im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Messung der Hochaufgelösten Daten

Alle Details zur Messung der Hochaufgelösten Daten finden sich in der in Zusammenarbeit mit der Arbeitsgruppe um *D. Stalke* entandenen Publikation sowie der Dissertation von *H. Ott*. Im Rahmen dieser Dissertation sind nur die wichtigsten Werte und Ergebnisse dieser Messungen aufgeführt (Tab. A.15 bis Tab. A.19).

Lokales Koordinatensystemen.

Tab. A.15 Definition des lokalen Koordinatensystems.

Atom	Atom 1	Axe 1	Atom 2	Axe 2	R/L
Si(1)	C(3)	X	C(10)	Y	R
O(1)	Li(1)	X	C(15)	Y	R
N(1)	Li(1)	X	C(10)	Y	R
N(2)	Li(1)	Z	C(17)	X	R
C(1)	Si(1)	Z	C(2)	X	R
C(2)	Si(1)	Z	C(1)	X	L
C(3)	Li(1)	Z	C(4)	X	R
C(4)	C(5)	X	C(9)	Y	R
C(5)	C(4)	X	C(6)	Y	R
C(6)	C(5)	X	C(7)	Y	R

C(7)	C(6)	X	C(8)	Y	R
C(8)	C(7)	Y	C(9)	X	L
C(9)	C(8)	Y	C(4)	X	L
C(10)	Si(1)	X	N(1)	Y	R
C(11)	C(12)	X	N(1)	Y	R
C(12)	C(11)	Y	C(13)	X	R
C(13)	C(12)	X	C(14)	Y	L
C(14)	C(13)	X	N(1)	Y	L
C(15)	C(14)	X	O(1)	Y	R
C(16)	O(1)	Z	H(16A)	X	R
C(17)	C(18)	Y	N(2)	X	R
C(18)	C(17)	Y	C(23)	X	L
C(19)	C(20)	Y	N(2)	X	R
C(20)	C(19)	Y	C(23)	X	L
C(21)	C(22)	Y	N(2)	X	R
C(22)	C(21)	Y	C(23)	X	L
C(23)	N(2)	Z	C(18)	X	R
Li(1)	C(3)	Z	N(1)	X	R
H(1A)	C(1)	Z	H(1B)	Y	R
H(1B)	C(1)	Z	H(1C)	Y	R
H(1C)	C(1)	Z	H(1A)	Y	R
H(2A)	C(2)	Z	H(2B)	Y	R
H(2B)	C(2)	Z	H(2C)	Y	R
H(2C)	C(2)	Z	H(2A)	Y	R
H(3A)	C(3)	Z	C(4)	Y	R
H(5A)	C(5)	Z	C(6)	Y	R
H(6A)	C(6)	Z	C(5)	Y	R
H(7A)	C(7)	Z	C(8)	Y	R
H(8A)	C(8)	Z	C(9)	Y	R
H(9A)	C(9)	Z	C(8)	Y	R
H(10A)	C(10)	Z	H(10B)	Y	R
H(10B)	C(10)	Z	H(10A)	Y	R
H(11A)	C(11)	Z	H(11B)	Y	R
H(11B)	C(11)	Z	H(11A)	Y	R
H(12A)	C(12)	Z	H(12B)	Y	R
H(12B)	C(12)	Z	H(12A)	Y	R
H(13A)	C(13)	Z	H(13B)	Y	R
H(13B)	C(13)	Z	H(13A)	Y	R
H(14A)	C(14)	Z	N(1)	Y	R
H(15A)	C(15)	Z	H(15B)	Y	R
H(15B)	C(15)	Z	H(15A)	Y	R
H(16A)	C(16)	Z	H(16B)	Y	R
H(16B)	C(16)	Z	H(16C)	Y	R
H(16C)	C(16)	Z	H(16A)	Y	R
H(17A)	C(17)	Z	H(17B)	Y	R
H(17B)	C(17)	Z	H(17A)	Y	R

H(18A)	C(18)	Z	H(18B)	Y	R
H(18B)	C(18)	Z	H(18A)	Y	R
H(19A)	C(19)	Z	H(19B)	Y	R
H(19B)	C(19)	Z	H(19A)	Y	R
H(20A)	C(20)	Z	H(20B)	Y	R
H(20B)	C(20)	Z	H(20A)	Y	R
H(21A)	C(21)	Z	H(21B)	Y	R
H(21B)	C(21)	Z	H(21A)	Y	R
H(22A)	C(22)	Z	H(22B)	Y	R
H(22B)	C(22)	Z	H(22A)	Y	R
H(23A)	C(23)	Z	C(22)	Y	R

R-Werte der Multipol-Verfeinerung

R-Werte nach dem finalen Verfeinerungsschritt (alle Parameter ausser κ')

R{ *F* } = 0.0203 R_{all}{ *F* } = 0.0295 *R*w{ *F* } = 0.0160
R{*F*2} = 0.0244 R_{all}{*F*2} = 0.0252 *R*w{*F*2} = 0.0312
GOFw = 2.5948
*N*ref/*N*v = 34.1347

Hirshfeld-Test nach dem finalen Verfeinerungsschritt

Tab. A.16 Abweichungen der Mean-Square Displacement Amplitudes (DMSDA) ($1 \cdot 10^{-4}$ Å^2) entlang der interatomaren Vektoren.

Atom → Atom		d [Å]	DMSDA	Atom	d [Å]	DMSDA	Atom	d [Å]	DMSDA
Si(1)	C(1)	1.8817	11	C(2)	1.8860	13	C(3)	1.8131	5
	C(10)	1.9070	6						
O(1)	C(15)	1.4202	10	C(16)	1.4208	9			
N(1)	C(10)	1.4811	6	C(11)	1.4695	10	C(14)	1.4762	3
N(2)	C(17)	1.4772	6	C(19)	1.4754	6	C(21)	1.4776	–2
C(3)	C(4)	1.4343	5						
C(4)	C(5)	1.4272	2	C(9)	1.4266	2			
C(5)	C(6)	1.3859	4						
C(6)	C(7)	1.3947	0						
C(7)	C(8)	1.3992	4						
C(8)	C(9)	1.3902	–4						
C(11)	C(12)	1.5226	0						
C(12)	C(13)	1.5382	–3						
C(13)	C(14)	1.5399	3						
C(14)	C(15)	1.5143	1						
C(17)	C(18)	1.5403	1						
C(18)	C(23)	1.5235	2						
C(19)	C(20)	1.5435	7						
C(20)	C(23)	1.5278	–3						
C(21)	C(22)	1.5367	2						
C(22)	C(23)	1.5251	3						

Populations- sowie Kontraktions-/Expansions-Parameter

Tab. A.17 Monopole Populationen, radiale Parameter und Nettoatomladungen.

Atom	Pval	Kappa	Kappa’	Nettoladung
Si(1)	2.951(53)	1.205(8)	0.930(6)	+1.049(53)
O(1)	6.503(24)	0.969(2)	0.928(13)	–0.502(24)
N(1)	5.358(26)	0.975(2)	0.924(11)	–0.358(26)
N(2)	5.287(28)	0.975(2)	0.906(11)	–0.286(28)
Li(1)	0.000	–	–	+1.000
C(1)	4.540(33)	0.961(2)	0.942(12)	–0.540(33)
C(2)	4.540	0.961(2)	0.942(12)	–0.540
C(3)	4.683(37)	0.961(2)	0.954(13)	–0.683(37)
C(4)	3.908(23)	1.009(1)	0.939(12)	+0.092(23)
C(5)	4.119(22)	1.009(1)	0.945(9)	–0.119(22)
C(6)	4.139(22)	1.009(1)	0.948(9)	–0.139(22)
C(7)	4.167(22)	1.009(1)	1.005(12)	–0.166(22)
C(8)	3.988(23)	1.009(1)	0.948(9)	+0.011(23)
C(9)	4.182(22)	1.009(1)	0.945(9)	–0.181(22)
C(10)	4.546(35)	0.961(2)	0.945(12)	–0.546(35)
C(11)	4.335(25)	0.990(1)	0.923(8)	–0.335(25)
C(12)	4.212(17)	0.990(1)	0.916(9)	–0.211(17)
C(13)	4.212	0.990(1)	0.916(9)	–0.211(21)
C(14)	4.107(21)	0.990(1)	0.923(8)	–0.106(23)
C(15)	4.326(23)	0.990(1)	0.922(10)	–0.325(26)
C(16)	4.247(26)	0.990(1)	0.898(9)	–0.246(18)
C(17)	4.212(18)	0.990(1)	0.906(7)	–0.211(22)
C(18)	4.142(22)	0.990(1)	0.914(8)	–0.142
C(19)	4.212	0.990(1)	0.906(7)	–0.211
C(20)	4.142	0.990(1)	0.914(8)	–0.142
C(21)	4.212	0.990(1)	0.906(7)	–0.211
C(22)	4.142	0.990(1)	0.914(8)	–0.142
C(23)	4.338(77)	0.964(6)	0.906(10)	–0.338(77)
H(1A)	0.887(8)	1.100	1.180	+0.112(8)
H(1B)	0.887	1.100	1.180	+0.112
H(1C)	0.887	1.100	1.180	+0.112
H(2A)	0.887	1.100	1.180	+0.112
H(2B)	0.887	1.100	1.180	+0.112
H(2C)	0.887	1.100	1.180	+0.112
H(3A)	0.846(15)	1.100	1.180	+0.154(15)
H(5A)	0.909(7)	1.100	1.180	+0.090(7)
H(6A)	0.909	1.100	1.180	+0.090
H(7A)	0.909	1.100	1.180	+0.090
H(8A)	0.909	1.100	1.180	+0.090
H(9A)	0.909	1.100	1.180	+0.090
H(10A)	0.852(11)	1.100	1.180	+0.148(11)

H(10B)	0.852	1.100	1.180	+0.148
H(11A)	0.892(10)	1.100	1.180	+0.108(10)
H(11B)	0.892	1.100	1.180	+0.108
H(12A)	0.932(7)	1.100	1.180	+0.068(7)
H(12B)	0.932	1.100	1.180	+0.068
H(13A)	0.932	1.100	1.180	+0.068
H(13B)	0.932	1.100	1.180	+0.068
H(14A)	0.890(13)	1.100	1.180	+0.109(13)
H(15A)	0.852(10)	1.100	1.180	+0.148(10)
H(15B)	0.852	1.100	1.180	+0.148
H(16A)	0.891(9)	1.100	1.180	+0.108(9)
H(16B)	0.891	1.100	1.180	+0.108
H(16C)	0.891	1.100	1.180	+0.108
H(17A)	0.848(6)	1.100	1.180	+0.151(6)
H(17B)	0.848	1.100	1.180	+0.151
H(18A)	0.848	1.100	1.180	+0.151
H(18B)	0.848	1.100	1.180	+0.151
H(19A)	0.848	1.100	1.180	+0.151
H(19B)	0.848	1.100	1.180	+0.151
H(20A)	0.848	1.100	1.180	+0.151
H(20B)	0.848	1.100	1.180	+0.151
H(21A)	0.848	1.100	1.180	+0.151
H(21B)	0.848	1.100	1.180	+0.151
H(22A)	0.848	1.100	1.180	+0.151
H(22B)	0.848	1.100	1.180	+0.151
H(23A)	0.868(21)	1.100	1.180	+0.132(21)

Bindungskritische Punkte

Tab. A.18 Liste der BCP's über einem Schwellenwert von $\rho(r_{BCP}) = 0.045$ eÅ^{-3}.

Bindung A–B	d [Å]	Pfadlänge	$\rho(r_{BCP})$ [eÅ^{-3}]	$\nabla 2\rho(rBCP)$ [eÅ^{-5}]	d1 A–BCP	d2 B–BCP	λ1/λ2/λ3	ε
Si1–C1	1.8817(3)	1.88198	0.816(4)	3.313(7)	0.7721	1.1099	–3.78 –3.49 10.58	0.09
Si1–C2	1.8860(3)	1.88670	0.809(4)	3.247(6)	0.7737	1.1129	–3.73 –3.43 10.41	0.09
Si1–C3	1.8131(4)	1.81405	0.903(7)	4.168(12)	0.7612	1.0523	–4.21 –3.89 12.27	0.08
Si1–C10	1.9070(4)	1.90725	0.814(6)	2.502(10)	0.7819	1.1251	–3.64 –3.47 9.61	0.05
O1–Li1	1.9820(6)	1.98252	0.150(1)	4.804(1)	1.2327	0.7495	–1.05 –1.00	0.05

							6.85	
O1–C15	1.4202(4)	1.42028	1.862(16)	–12.155(74)	0.8628	0.5575	–14.19 –13.50 15.54	0.05
O1–C16	1.4208(4)	1.42078	1.896(15)	–15.932(67)	0.8480	0.5728	–15.76 –14.92 14.76	0.06
N1–Li1	2.1618(5)	2.16385	0.113(1)	3.225(1)	1.3754	0.7870	–0.71 –0.67 4.61	0.06
N1–C10	1.4811(4)	1.48221	1.762(17)	–13.947(73)	0.8789	0.6029	–12.60 –12.39 11.05	0.02
N1–C11	1.4695(4)	1.46961	1.880(13)	–13.075(43)	0.8569	0.6127	–13.81 –13.05 13.78	0.06
N1–C14	1.4762(4)	1.47762	1.833(12)	–12.774(37)	0.8509	0.6262	–13.57 –12.71 13.51	0.07
N2–Li1	2.1180(5)	2.11804	0.131(1)	3.700(1)	1.3480	0.7701	–0.86 –0.85 5.41	0.01
N2–C17	1.4772(4)	1.47795	1.866(8)	–13.787(28)	0.8468	0.6305	–14.18 –13.30 13.69	0.07
N2–C19	1.4754(4)	1.47589	1.877(7)	–14.066(16)	0.8479	0.6278	–14.26 –13.43 13.62	0.06
N2–C21	1.4776(4)	1.47826	1.870(7)	–13.869(16)	0.8483	0.6296	–14.22 –13.31 13.66	0.07
C3–Li1	2.2725(6)	2.27892	0.086(2)	2.166(1)	1.4465	0.8261	–0.46 –0.41 3.03	0.13
C3–C4	1.4343(4)	1.43688	2.022(13)	–16.760(41)	0.7132	0.7211	–14.84 –12.48 10.57	0.19
C4–C5	1.4272(5)	1.42822	2.115(12)	–17.886(30)	0.7030	0.7245	–16.23 –13.71 12.05	0.18
C5–C6	1.3859(5)	1.38726	2.250(12)	–20.388(33)	0.6665	0.7194	–17.60 –14.44 11.65	0.22
C6–C7	1.3947(6)	1.39781	2.198(15)	–19.125(37)	0.6912	0.7036	–17.42 –14.07 12.37	0.24
C7–C8	1.3992(6)	1.40054	2.177(15)	–18.176(42)	0.7493	0.6505	–16.82 –13.56 12.20	0.24
C8–C9	1.3902(5)	1.39206	2.221(12)	–19.851(32)	0.6780	0.7130	–17.51	0.25

							–14.04 11.70	
C9–C4	1.4266(4)	1.42682	2.048(11)	–17.477(29)	0.7386	0.6880	–15.94 –13.02 11.49	0.22
C11–C12	1.5226(5)	1.52617	1.726(9)	–12.034(19)	0.7661	0.7571	–11.65 –11.01 10.62	0.06
C12–C13	1.5382(5)	1.54075	1.623(5)	–10.565(10)	0.7691	0.7695	–10.79 –10.05 10.28	0.07
C13–C14	1.5399(4)	1.54067	1.697(10)	–11.669(19)	0.7700	0.7700	–11.37 –10.64 10.34	0.07
C14–C15	1.5143(4)	1.51488	1.832(10)	–15.148(27)	0.7341	0.7803	–12.69 –12.64 10.18	0.00
C17–C18	1.5403(5)	1.54052	1.747(7)	–14.751(19)	0.7705	0.7698	–12.68 –11.72 9.66	0.08
C18–C23	1.5235(5)	1.52400	1.828(9)	–16.346(24)	0.7365	0.7872	–13.12 –12.25 9.03	0.07
C19–C20	1.5435(5)	1.54372	1.739(0)	–14.611(0)	0.7729	0.7706	–12.61 –11.66 9.66	0.08
C20–C23	1.5278(6)	1.52820	1.797(14)	–16.303(37)	0.7463	0.7817	–12.82 –12.36 8.88	0.04
C21–C22	1.5367(4)	1.53696	1.754(0)	–14.926(0)	0.7695	0.7672	–12.77 –11.81 9.65	0.08
C22–C23	1.5251(5)	1.52592	1.819(13)	–16.679(36)	0.7411	0.7843	–13.28 –12.28 8.88	0.08
C1–H1A	1.0850(3)	1.08520	1.747(9)	–17.593(30)	0.7059	0.3792	–15.47 –14.60 12.47	0.06
C1–H1B	1.0850(3)	1.08697	1.733(7)	–17.157(25)	0.7064	0.3795	–15.17 –14.53 12.54	0.04
C1–H1C	1.0850(3)	1.08564	1.756(8)	–17.494(25)	0.7062	0.3791	–15.34 –14.61 12.45	0.05
C2–H2A	1.0850(3)	1.08634	1.741(1)	–17.187(0)	0.7074	0.3783	–15.31 –14.44 12.57	0.06
C2–H2B	1.0850(3)	1.08673	1.738(1)	–17.150(0)	0.7069	0.3789	–15.25 –14.46 12.55	0.05

C2–H2C	1.0850(3)	1.08686	1.738(1)	–16.988(0)	0.7071	0.3788	–15.17 –14.40 12.58	0.05
C3–H3A	1.0760(3)	1.08281	1.677(20)	–15.991(75)	0.7476	0.3304	–16.25 –14.56 14.82	0.12
C5–H5A	1.0760(3)	1.07614	1.810(11)	–18.473(35)	0.7315	0.3446	–17.61 –16.43 15.57	0.07
C6–H6A	1.0760(4)	1.08041	1.761(11)	–17.610(23)	0.7270	0.3506	–16.87 –16.09 15.35	0.05
C7–H7A	1.0760(4)	1.07605	1.771(13)	–18.424(29)	0.7263	0.3497	–17.30 –16.31 15.18	0.06
C8–H8A	1.0760(4)	1.07637	1.724(11)	–16.706(25)	0.7168	0.3593	–16.05 –15.43 14.77	0.04
C9–H9A	1.0760(4)	1.07722	1.782(11)	–18.152(23)	0.7236	0.3528	–17.10 –15.94 14.89	0.07
C10–H10A	1.0850(3)	1.08879	1.731(14)	–17.349(47)	0.7316	0.3548	–16.07 –14.61 13.32	0.10
C10–H10B	1.0850(3)	1.08540	1.747(11)	–18.038(34)	0.7315	0.3536	–16.32 –15.02 13.30	0.09
C11–H11A	1.0850(4)	1.08908	1.680(15)	–15.120(46)	0.7308	0.3552	–15.12 –14.60 14.60	0.04
C11–H11B	1.0850(4)	1.08721	1.790(11)	–17.468(22)	0.7493	0.3361	–16.87 –16.22 15.63	0.04
C12–H12A	1.0850(3)	1.08763	1.725(10)	–15.687(26)	0.7027	0.3833	–15.22 –14.04 13.57	0.08
C12–H12B	1.0850(3)	1.08628	1.724(8)	–15.304(17)	0.7043	0.3810	–14.92 –14.23 13.85	0.05
C13–H13A	1.0850(3)	1.08772	1.724(0)	–15.779(0)	0.7020	0.3839	–15.19 –14.11 13.52	0.08
C13–H13B	1.0850(3)	1.08831	1.710(0)	–15.028(0)	0.7038	0.3823	–14.76 –14.12 13.86	0.04
C14–H14A	1.0850(3)	1.08528	1.725(15)	–16.584(50)	0.7237	0.3614	–15.52 –15.02 13.96	0.03
C15–H15A	1.0850(3)	1.08553	1.812(13)	–20.375(46)	0.7354	0.3497	–17.33 –16.62	0.04

							13.58	
C15–H15B	1.0850(3)	1.08568	1.812(10)	–20.366(30)	0.7353	0.3498	–17.34 –16.60 13.57	0.04
C16–H16A	1.0850(3)	1.08682	1.852(12)	–20.590(39)	0.7205	0.3654	–17.66 –16.15 13.22	0.09
C16–H16B	1.0850(3)	1.08753	1.849(7)	–20.616(23)	0.7207	0.3655	–17.63 –16.22 13.23	0.09
C16–H16C	1.0850(3)	1.08662	1.853(7)	–20.703(24)	0.7203	0.3655	–17.68 –16.23 13.20	0.09
C17–H17A	1.0850(3)	1.08981	1.709(6)	–17.155(21)	0.7236	0.3628	–15.65 –14.85 13.34	0.05
C17–H17B	1.0850(3)	1.08975	1.710(6)	–17.153(16)	0.7238	0.3626	–15.65 –14.85 13.35	0.05
C18–H18A	1.0850(3)	1.09491	1.634(6)	–14.599(18)	0.7198	0.3676	–14.60 –13.62 13.62	0.07
C18–H18B	1.0850(4)	1.09535	1.629(7)	–14.370(18)	0.7200	0.3676	–14.49 –13.53 13.65	0.07
C19–H19A	1.0850(3)	1.08999	1.706(0)	–17.108(0)	0.7234	0.3631	–15.61 –14.83 13.34	0.05
C19–H19B	1.0850(3)	1.09055	1.703(0)	–17.004(0)	0.7233	0.3633	–15.56 –14.78 13.34	0.05

Integration der atomaren Basins.

Die Ladungen für alle Atome wurden durch die Integration der zero-flux Oberflächen bestimmt.

Tab. A.19 Integrierte Bader-Ladungen [e], Qualitätfaktor L und atomares Volumen (zero-flux Oberfläche).

Atom	Ladung [e]	L (Lagrangian)	Volumen V(001) (Å^3)	Volumen V(tot) (Å^3)
Si(1)	2.1454	–3.36E–04	6.298	6.357
O(1)	–1.3213	5.70E–04	13.143	14.485
N(1)	–1.2197	4.03E–04	10.424	10.525
N(2)	–1.1247	–7.13E–04	10.792	10.792
Li(1)	0.9359	–1.21E–05	3.669	3.669
C(1)	–0.7699	4.09E–04	13.713	94.881
C(2)	–0.7936	8.19E–04	13.950	142.386
C(3)	–0.9692	1.38E–04	15.313	28.398
C(4)	0.0731	5.24E–04	9.412	18.181

C(5)	–0.1915	1.73E–04	12.010	80.230
C(6)	–0.2243	4.20E–04	12.317	91.622
C(7)	–0.3297	6.28E–04	13.086	100.651
C(8)	0.0022	5.87E–04	11.940	69.648
C(9)	–0.2948	1.19E–03	12.341	30.061
C(10)	–0.5233	–9.54E–04	10.866	25.221
C(11)	–0.0046	1.43E–03	8.947	36.574
C(12)	–0.2333	2.64E–03	10.061	43.887
C(13)	–0.2403	5.87E–03	9.613	61.713
C(14)	0.1734	4.66E–03	6.637	6.776
C(15)	0.1020	3.86E–03	7.964	25.950
C(16)	0.2385	–8.20E–05	9.566	48.219
C(17)	0.0464	4.10E–03	8.888	18.954
C(18)	–0.3056	3.56E–03	10.343	119.279
C(19)	0.0418	2.37E–03	9.203	12.784
C(20)	–0.3143	4.99E–03	10.3628	112.150
C(21)	0.0471	4.09E–03	8.612	10.892
C(22)	–0.3125	3.80E–03	10.257	107.327
C(23)	–0.0482	2.09E–03	7.441	12.510
H(1A)	0.1049	5.50E–04	6.599	33.749
H(1B)	0.1076	2.44E–04	6.697	297.440
H(1C)	0.0858	4.12E–04	6.669	236.817
H(2A)	0.1203	–4.68E–04	6.059	138.970
H(2B)	0.1159	2.71E–05	6.321	259.469
H(2C)	0.1073	1.26E–05	6.488	279.832
H(3A)	0.1912	7.03E–04	6.079	37.402
H(5A)	0.1738	8.97E–04	5.706	28.400
H(6A)	0.1808	1.89E–05	6.185	287.062
H(7A)	0.1780	–3.20E–06	6.175	390.435
H(8A)	0.1684	–6.07E–06	6.266	334.025
H(9A)	0.1688	3.99E–04	5.803	18.244
H(10A)	0.1687	5.96E–04	5.376	26.062
H(10B)	0.1480	–4.17E–04	6.064	109.981
H(11A)	0.0992	3.97E–06	6.686	179.016
H(11B)	0.1140	2.73E–04	6.666	38.593
H(12A)	0.0755	2.12E–04	6.589	341.308
H(12B)	0.0880	2.71E–04	6.061	17.201
H(13A)	0.0716	–3.13E–04	6.611	332.114
H(13B)	0.0908	8.42E–04	6.097	59.059
H(14A)	0.1078	1.82E–04	6.533	135.698
H(15A)	0.1436	2.45E–04	6.044	38.418
H(15B)	0.1425	2.85E–05	6.354	179.425
H(16A)	0.0755	–3.48E–04	6.285	23.252
H(16B)	0.0855	–1.21E–04	6.741	43.168
H(16C)	0.0831	–1.83E–04	6.606	300.782
H(17A)	0.1669	–1.95E–04	6.128	39.510

H(17B)	0.1663	–1.05E–04	5.743	16.556
H(18A)	0.2013	4.73E–05	5.789	219.379
H(18B)	0.2066	6.13E–05	5.753	182.583
H(19A)	0.1663	2.94E–04	5.965	15.936
H(19B)	0.1697	–3.71E–04	6.100	14.701
H(20A)	0.2054	2.56E–05	5.762	181.438
H(20B)	0.2046	3.75E–06	5.800	195.933
H(21A)	0.1689	–1.42E–04	5.717	19.735
H(21B)	0.1674	8.19E–05	6.159	17.907
H(22A)	0.2034	7.45E–05	5.730	209.788
H(22B)	0.2020	1.66E–06	5.843	232.551
H(23A)	0.0541	–4.11E–07	7.342	315.737

[*rac*-**134**]$_4$

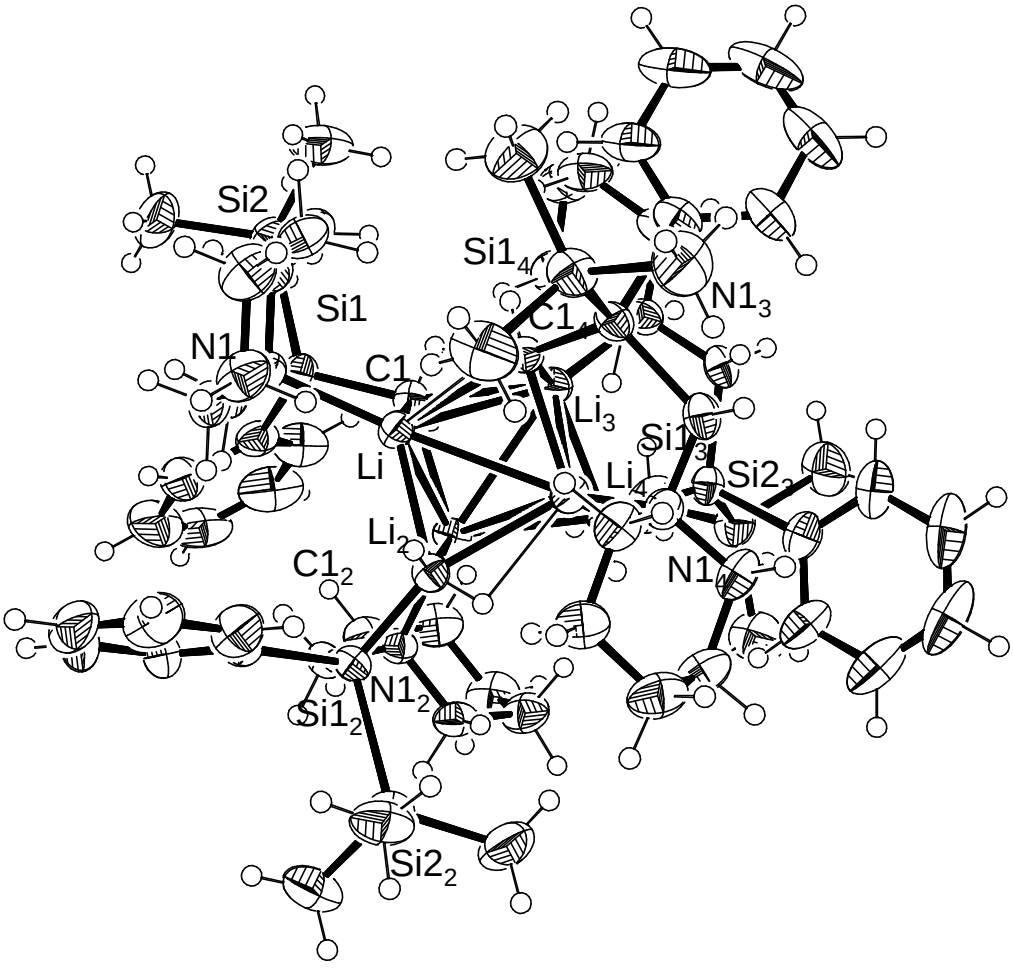

Abb. A.9 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von [*rac*-**134**]$_4$ im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome sowie dem Großteil der Kohlenstoffatome wurde der Übersicht halber weggelassen.

Tab. A.20 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von [*rac*-**134**]$_4$.

Atom	x	y	z	U(eq)
C(1)	5706(2)	5984(2)	9376(2)	34(1)
C(2)	6439(2)	6240(2)	7882(2)	44(1)
C(3)	6244(3)	6040(2)	7196(2)	58(1)
C(4)	6876(4)	5806(3)	6725(2)	83(2)
C(5)	7693(4)	5778(3)	6914(3)	83(2)
C(6)	7911(3)	5980(3)	7589(3)	76(1)
C(7)	7294(2)	6213(2)	8068(2)	60(1)
C(8)	7010(2)	8281(2)	8703(2)	68(1)
C(9)	5515(3)	8535(3)	7727(2)	75(1)
C(10)	5295(3)	8663(2)	9295(3)	76(1)
C(11)	4555(2)	6316(2)	8134(2)	39(1)
C(12)	3671(2)	7154(2)	8899(2)	44(1)
C(13)	2895(2)	7209(2)	9359(2)	53(1)
C(14)	2114(2)	6853(3)	9006(2)	66(1)
C(15)	2297(2)	5980(2)	8725(2)	59(1)
C(16)	3075(2)	5998(2)	8248(2)	49(1)
C(17)	4583(9)	8856(14)	5719(9)	330(14)
C(18)	4570(20)	7920(40)	5286(14)	740(60)
C(19)	4432(8)	7728(16)	5882(6)	246(9)
C(20)	4473(15)	6929(13)	5504(12)	311(12)
C(21)	4336(7)	6115(8)	5871(5)	179(4)
Li	4377(3)	5471(3)	9410(2)	34(1)
N(1)	3832(1)	6293(1)	8626(1)	36(1)
Si(1)	5619(1)	6585(1)	8551(1)	35(1)
Si(2)	5853(1)	8066(1)	8578(1)	48(1)

Tab. A.21 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von [*rac*-**134**]$_4$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	32(2)	37(2)	34(2)	1(1)	1(1)	1(1)
C(2)	53(2)	33(2)	47(2)	4(1)	13(2)	–1(1)
C(3)	76(3)	55(2)	43(2)	2(2)	19(2)	5(2)
C(4)	125(5)	70(3)	55(2)	–6(2)	41(3)	–1(3)
C(5)	98(4)	49(2)	100(4)	–6(2)	66(3)	–3(2)
C(6)	57(2)	58(2)	113(4)	–2(2)	38(3)	–9(2)
C(7)	47(2)	55(2)	79(3)	–6(2)	21(2)	–9(2)
C(8)	73(2)	48(2)	85(3)	15(2)	–6(2)	–17(2)
C(9)	89(3)	66(3)	69(3)	28(2)	–6(2)	–4(2)
C(10)	88(3)	43(2)	96(3)	–15(2)	23(3)	–9(2)
C(11)	50(2)	38(2)	30(2)	6(1)	–2(1)	1(1)
C(12)	47(2)	33(2)	51(2)	5(1)	–7(2)	3(1)
C(13)	46(2)	46(2)	66(2)	2(2)	1(2)	14(1)

C(14)	40(2)	74(3)	85(3)	5(2)	–4(2)	15(2)
C(15)	41(2)	56(2)	79(3)	5(2)	–13(2)	3(2)
C(16)	48(2)	48(2)	52(2)	2(2)	–20(2)	1(2)
C(17)	169(10)	550(30)	272(17)	330(20)	–32(10)	–47(15)
C(18)	360(40)	1600(160)	260(30)	270(50)	–170(30)	–520(70)
C(19)	145(8)	460(30)	132(9)	–90(14)	6(7)	–9(12)
C(20)	410(30)	258(19)	270(20)	34(17)	160(20)	33(18)
C(21)	165(8)	214(11)	158(8)	–14(8)	–28(7)	26(8)
Li	35(2)	32(2)	36(2)	5(2)	–3(2)	–1(2)
N(1)	36(1)	35(1)	36(1)	4(1)	–4(1)	3(1)
Si(1)	40(1)	33(1)	32(1)	4(1)	4(1)	–2(1)
Si(2)	57(1)	36(1)	51(1)	7(1)	4(1)	–6(1)

[*t*-BuLi·(*R*)-134]$_2$

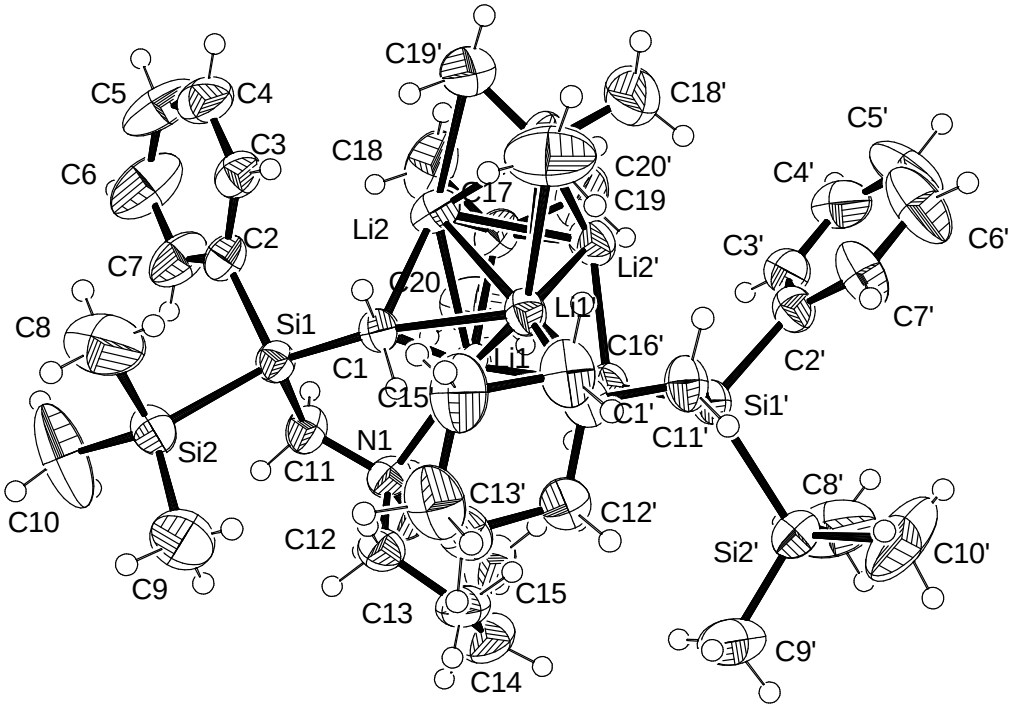

Abb. A.10 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von [*t*-BuLi·(*R*)-**134**]$_2$ im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.22 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter (Å$^2 \cdot 10^3$) von [*t*-BuLi·(*R*)-**134**]$_2$.

Atom	x	y	z	U(eq)
C(1)	10477(2)	4439(2)	3337(3)	42(1)
C(2)	10154(2)	2923(2)	4452(3)	45(1)
C(3)	10701(2)	3333(2)	5356(4)	51(1)
C(4)	10722(3)	2990(3)	6444(5)	71(1)
C(5)	10209(3)	2236(4)	6662(5)	97(2)

C(6)	9680(3)	1816(3)	5785(6)	101(2)
C(7)	9638(2)	2150(2)	4701(5)	72(1)
C(8)	11715(3)	3376(5)	2135(6)	110(2)
C(9)	10836(5)	3513(5)	–17(5)	113(2)
C(10)	10198(4)	1998(3)	1327(9)	141(4)
C(11)	9017(2)	2934(2)	2608(4)	48(1)
C(12)	9101(2)	3730(2)	884(3)	51(1)
C(13)	8866(2)	4256(2)	273(4)	62(1)
C(14)	7999(3)	3884(3)	214(5)	78(1)
C(15)	7654(2)	3592(3)	1480(6)	76(1)
C(16)	7926(2)	3059(2)	2001(4)	61(1)
C(17)	8992(3)	4181(3)	5848(5)	78(1)
C(18)	9132(3)	3668(3)	6766(6)	95(2)
C(19)	8738(4)	4640(4)	6697(5)	94(2)
C(20)	8219(3)	3590(4)	5153(6)	115(2)
C(21)	10000	10000	6110(90)	220(30)
C(22)	10000	10000	7710(80)	210(30)
Li(1)	9288(3)	4334(3)	3609(5)	44(1)
Li(2)	10236(4)	4549(4)	5304(6)	55(1)
N(1)	8772(2)	3468(2)	2122(3)	44(1)
Si(1)	10099(1)	3414(1)	2989(1)	39(1)
Si(2)	10732(1)	3069(1)	1527(1)	52(1)

Tab. A.23 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von [*t*-BuLi·(*R*)-**134**]$_2$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	46(2)	36(2)	44(2)	–2(1)	–2(2)	20(2)
C(2)	39(2)	48(2)	54(2)	9(2)	4(1)	24(2)
C(3)	44(2)	61(2)	53(2)	6(2)	3(2)	31(2)
C(4)	64(2)	113(4)	54(2)	3(3)	–2(2)	59(3)
C(5)	66(3)	139(5)	86(4)	67(4)	10(3)	51(3)
C(6)	64(3)	83(3)	133(5)	56(4)	–2(3)	19(3)
C(7)	57(2)	54(2)	92(3)	28(2)	–7(2)	18(2)
C(8)	63(3)	187(7)	86(4)	–26(4)	–8(3)	67(4)
C(9)	171(6)	166(6)	55(3)	8(3)	24(4)	124(5)
C(10)	124(5)	63(3)	211(9)	–42(4)	65(6)	27(3)
C(11)	40(2)	35(2)	66(2)	1(2)	–5(2)	16(1)
C(12)	49(2)	46(2)	50(2)	–7(2)	–11(2)	19(2)
C(13)	66(3)	60(2)	51(2)	–2(2)	–18(2)	26(2)
C(14)	74(3)	70(3)	85(3)	–7(2)	–35(3)	32(2)
C(15)	47(2)	73(3)	110(4)	–5(3)	–24(2)	32(2)
C(16)	39(2)	49(2)	86(3)	–1(2)	–13(2)	15(2)
C(17)	90(3)	87(3)	84(3)	–16(2)	–29(3)	65(3)
C(18)	96(4)	103(4)	109(4)	39(3)	35(3)	68(3)
C(19)	124(5)	120(4)	77(3)	30(3)	37(3)	89(4)
C(20)	76(4)	152(6)	92(4)	4(4)	18(3)	37(4)

C(21)	130(20)	180(20)	370(100)	0	0	87(19)
C(22)	110(30)	180(40)	390(70)	0	0	120(30)
Li(1)	41(3)	38(3)	52(3)	5(2)	2(2)	19(2)
Li(2)	56(3)	62(4)	51(3)	8(3)	–4(3)	33(3)
N(1)	35(1)	38(1)	52(2)	0(1)	–9(1)	13(1)
Si(1)	37(1)	33(1)	44(1)	0(1)	–2(1)	16(1)
Si(2)	51(1)	51(1)	55(1)	–10(1)	0(1)	26(1)

[*t*-BuLi·(*R*)-138]$_2$

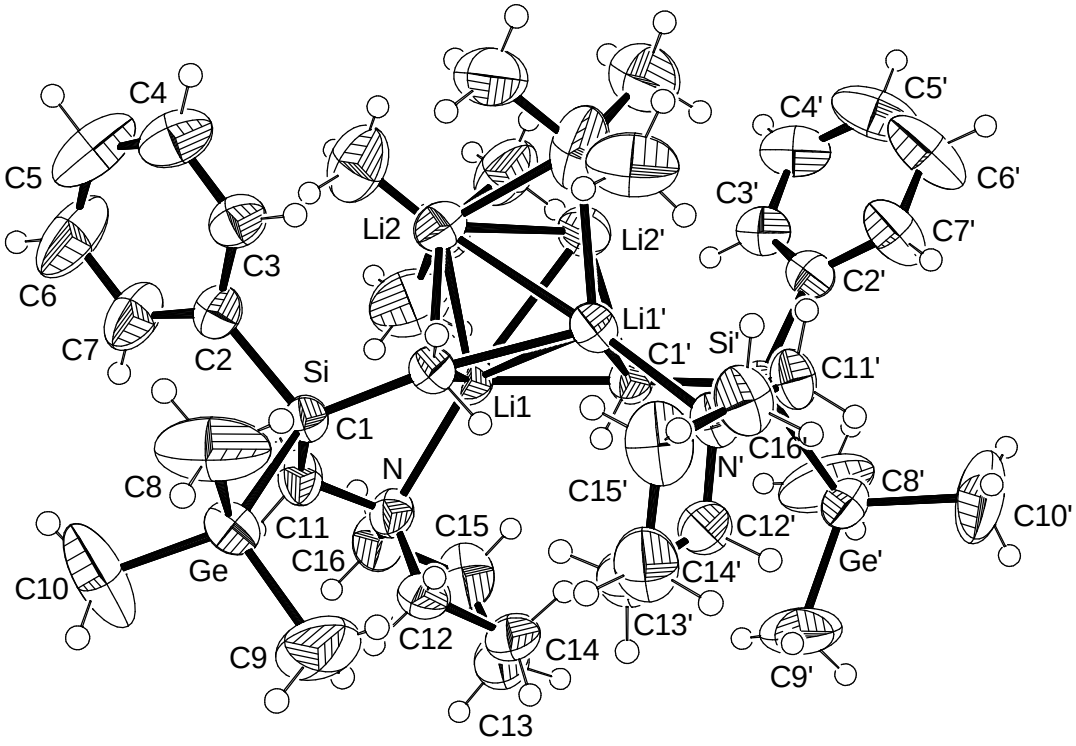

Abb. A.11 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von [*t*-BuLi·(*R*)-**138**]$_2$ im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.24 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter (Å$^2 \cdot 10^3$) von [*t*-BuLi·(*R*)-**138**]$_2$.

Atom	x	y	z	U(eq)
C(1)	10476(3)	4440(3)	3362(5)	46(1)
C(2)	10149(3)	2923(3)	4469(5)	46(1)
C(3)	10709(3)	3338(4)	5354(5)	54(1)
C(4)	10734(4)	2993(4)	6469(9)	73(2)
C(5)	10212(4)	2236(5)	6645(8)	93(3)
C(6)	9688(4)	1828(5)	5802(9)	103(3)
C(7)	9641(3)	2153(4)	4720(8)	77(2)
C(8)	11744(4)	3357(6)	2151(8)	115(4)
C(9)	10869(7)	3560(7)	–72(7)	120(3)

C(10)	10166(6)	1944(4)	1282(13)	136(5)
C(11)	9014(3)	2938(3)	2648(6)	52(1)
C(12)	9110(3)	3738(3)	907(5)	57(1)
C(13)	8871(4)	4254(4)	306(6)	64(2)
C(14)	8010(4)	3894(4)	221(7)	81(2)
C(15)	7655(3)	3598(4)	1505(8)	77(2)
C(16)	7918(3)	3065(3)	2032(7)	63(2)
C(17)	9003(5)	4185(5)	5850(9)	92(3)
C(18)	9132(5)	3677(5)	6786(9)	99(3)
C(19)	8737(5)	4642(5)	6712(7)	95(2)
C(20)	8237(6)	3633(7)	5194(9)	117(3)
Li(1)	9291(5)	4338(5)	3626(8)	47(2)
Li(2)	10236(6)	4557(5)	5323(9)	57(2)
N	8778(2)	3480(2)	2141(4)	47(1)
Si	10090(1)	3414(1)	3023(1)	42(1)
Ge	10719(1)	3062(1)	1524(1)	54(1)

Tab. A.25 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von [*t*-BuLi·(*R*)-**138**]$_2$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	50(3)	41(2)	45(3)	–2(2)	–3(2)	22(2)
C(2)	41(2)	49(3)	52(3)	7(2)	6(2)	26(2)
C(3)	47(3)	65(3)	53(3)	4(3)	0(2)	31(3)
C(4)	57(3)	120(5)	60(3)	11(4)	2(3)	58(4)
C(5)	72(4)	128(7)	86(5)	57(5)	18(4)	54(5)
C(6)	68(4)	91(5)	129(7)	60(5)	–7(5)	24(4)
C(7)	61(3)	60(3)	96(5)	26(4)	–10(4)	20(3)
C(8)	81(5)	213(11)	72(5)	–24(6)	–3(4)	89(6)
C(9)	179(9)	179(9)	55(4)	23(5)	40(5)	130(8)
C(10)	121(7)	63(4)	206(12)	–39(6)	58(8)	31(4)
C(11)	42(3)	38(2)	70(3)	2(2)	–5(2)	15(2)
C(12)	61(3)	53(3)	48(3)	–6(2)	–13(2)	20(3)
C(13)	75(4)	64(3)	53(3)	–2(3)	–22(3)	36(3)
C(14)	89(5)	71(4)	84(5)	–8(4)	–38(4)	42(4)
C(15)	51(3)	74(4)	108(5)	–3(4)	–19(4)	34(3)
C(16)	40(3)	54(3)	85(4)	0(3)	–12(3)	16(2)
C(17)	114(6)	91(5)	103(6)	–35(4)	–56(5)	75(5)
C(18)	103(6)	112(6)	114(7)	29(5)	30(5)	78(5)
C(19)	121(6)	119(6)	76(5)	29(4)	28(4)	83(6)
C(20)	100(6)	151(9)	87(7)	19(6)	23(5)	53(6)
Li(1)	48(4)	39(4)	47(4)	4(3)	0(3)	19(4)
Li(2)	64(5)	59(5)	51(5)	4(4)	–5(4)	33(4)
N	44(2)	42(2)	54(2)	2(2)	–9(2)	21(2)
Si	44(1)	37(1)	44(1)	–1(1)	–2(1)	20(1)
Ge	55(1)	53(1)	53(1)	–10(1)	0(1)	28(1)

(*Rac*-**139**)$_2$

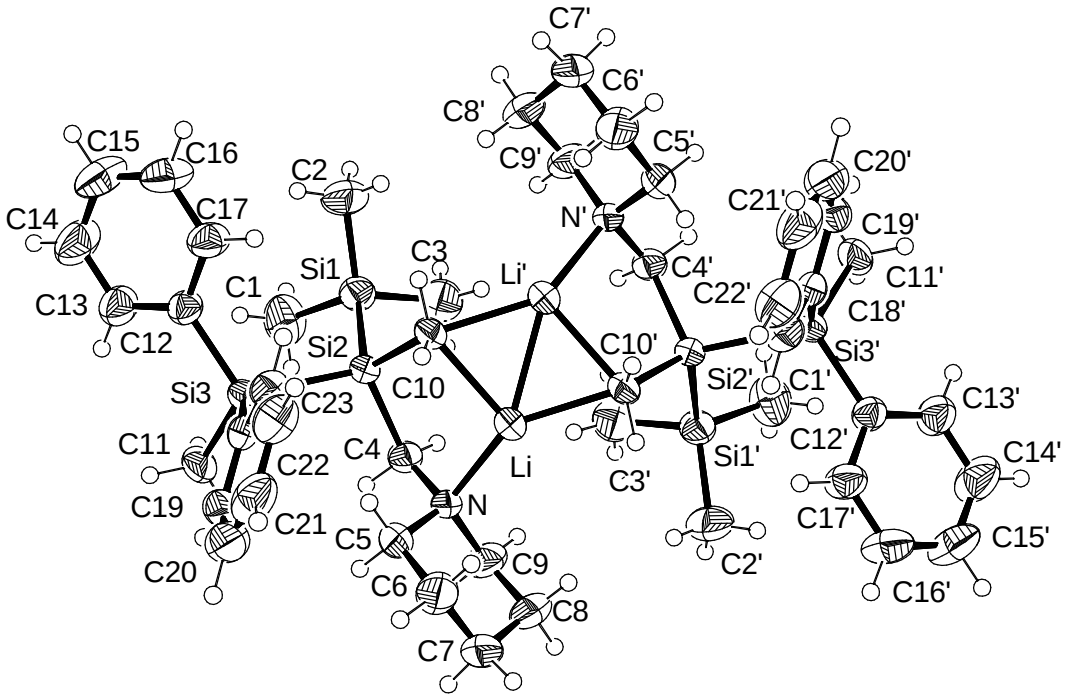

Abb. A.12 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von (*rac*-**139**)$_2$ im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.26 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter (Å$^2 \cdot 10^3$) von (*rac*-**139**)$_2$.

Atom	x	y	z	U(eq)
C(1)	2403(2)	24(1)	3321(3)	77(1)
C(2)	2473(2)	705(1)	5361(2)	73(1)
C(3)	1102(2)	42(1)	3594(3)	65(1)
C(4)	543(1)	932(1)	927(2)	41(1)
C(5)	169(1)	1746(1)	–384(2)	50(1)
C(6)	–440(1)	2153(1)	–1200(3)	67(1)
C(7)	–1117(2)	1856(1)	–2205(2)	71(1)
C(8)	–1339(1)	1410(1)	–1653(2)	67(1)
C(9)	–703(1)	1017(1)	–845(2)	60(1)
C(10)	952(1)	1754(1)	2993(2)	39(1)
C(11)	2260(1)	1193(1)	905(2)	54(1)
C(12)	3154(1)	1628(1)	3523(2)	42(1)
C(13)	3760(1)	1396(1)	3589(2)	57(1)
C(14)	4443(2)	1391(1)	4663(3)	77(1)
C(15)	4544(2)	1619(1)	5704(3)	75(1)
C(16)	3960(2)	1853(1)	5677(2)	65(1)
C(17)	3274(1)	1858(1)	4601(2)	54(1)
C(18)	1957(1)	2366(1)	1476(2)	42(1)
C(19)	1738(1)	2503(1)	294(2)	56(1)

C(20)	1487(1)	3034(1)	–180(3)	70(1)
C(21)	1462(1)	3445(1)	525(3)	70(1)
C(22)	1683(1)	3327(1)	1711(3)	64(1)
C(23)	1927(1)	2793(1)	2174(2)	48(1)
C(24)	4353(4)	10145(3)	8124(9)	253(6)
C(25)	4405(7)	9853(5)	6919(13)	371(10)
C(26)	5000	9724(17)	7500	630(40)
Li	–186(2)	1668(2)	1470(3)	48(1)
N	–66(1)	1326(1)	148(1)	37(1)
Si(1)	1863(1)	477(1)	3728(1)	48(1)
Si(2)	1343(1)	1254(1)	2426(1)	34(1)
Si(3)	2214(1)	1622(1)	2062(1)	39(1)

Tab. A.27 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*rac*-**139**)$_2$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	80(2)	66(2)	100(2)	6(2)	59(2)	21(2)
C(2)	66(2)	92(2)	42(1)	15(1)	18(1)	5(2)
C(3)	70(2)	58(2)	68(2)	16(1)	39(2)	3(1)
C(4)	41(1)	43(1)	36(1)	–5(1)	20(1)	–4(1)
C(5)	43(1)	68(2)	43(1)	10(1)	26(1)	–1(1)
C(6)	56(2)	80(2)	63(2)	29(1)	30(1)	8(1)
C(7)	55(2)	113(2)	39(1)	21(1)	23(1)	22(2)
C(8)	41(1)	96(2)	43(1)	1(1)	9(1)	–7(1)
C(9)	47(1)	70(2)	41(1)	–9(1)	11(1)	–15(1)
C(10)	41(1)	48(1)	34(1)	–6(1)	24(1)	–3(1)
C(11)	54(1)	72(2)	47(1)	–22(1)	35(1)	–15(1)
C(12)	38(1)	45(1)	41(1)	–7(1)	20(1)	–2(1)
C(13)	45(1)	67(2)	56(2)	–11(1)	25(1)	3(1)
C(14)	44(1)	94(2)	74(2)	–11(2)	19(1)	17(1)
C(15)	49(2)	79(2)	58(2)	–8(1)	4(1)	9(1)
C(16)	68(2)	62(2)	40(1)	–9(1)	14(1)	10(1)
C(17)	49(1)	61(1)	42(1)	–9(1)	19(1)	8(1)
C(18)	32(1)	57(1)	38(1)	–4(1)	19(1)	–11(1)
C(19)	51(1)	73(2)	44(1)	0(1)	27(1)	–17(1)
C(20)	56(2)	92(2)	53(2)	18(2)	23(1)	–19(2)
C(21)	47(1)	66(2)	77(2)	20(2)	22(1)	–9(1)
C(22)	51(1)	57(2)	71(2)	–4(1)	26(1)	–5(1)
C(23)	39(1)	55(1)	41(1)	–2(1)	16(1)	–6(1)
C(24)	167(7)	139(5)	242(9)	–13(6)	–24(6)	–11(5)
C(25)	220(11)	296(13)	285(14)	–59(11)	–62(10)	78(10)
C(26)	110(11)	980(90)	500(40)	0	–20(20)	0
Li	40(2)	72(2)	37(2)	–2(2)	24(2)	0(2)
N	32(1)	49(1)	27(1)	–2(1)	15(1)	–5(1)
Si(1)	48(1)	51(1)	44(1)	9(1)	25(1)	10(1)
Si(2)	33(1)	41(1)	29(1)	–2(1)	17(1)	–1(1)

Si(3)	36(1)	51(1)	32(1)	–10(1)	21(1)	–6(1)

147·HBr

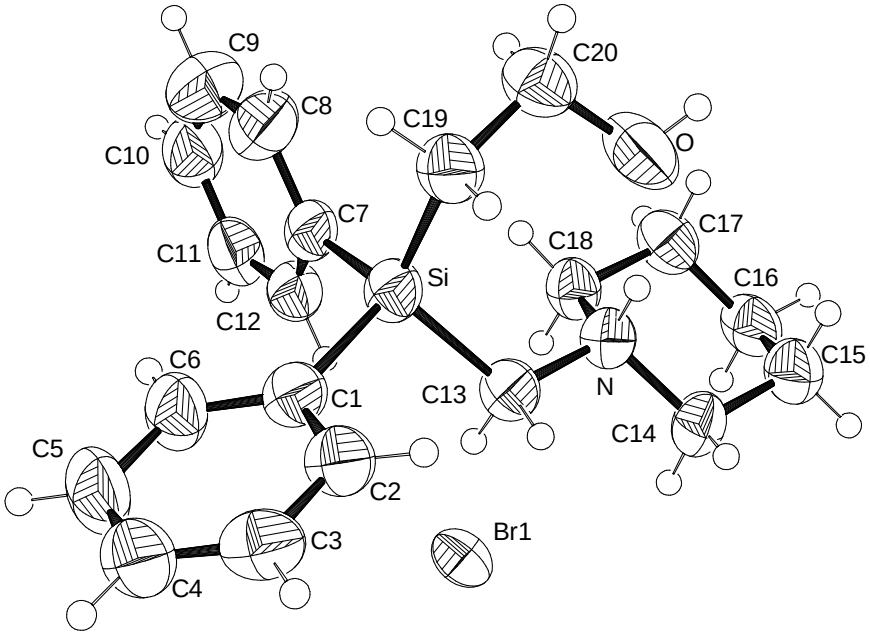

Abb. A.13 Thermische Auslenkungsellipsoide (50 % Aufenthaltswahrscheinlichkeit) der Molekülstruktur von **147**·HBr im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.28 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) von **147**·HBr.

Atom	x	y	z	U(eq)
Br(1)	3396(1)	2717(1)	5965(1)	70(1)
C(1)	6941(9)	–1071(7)	7932(6)	64(2)
C(2)	6698(9)	–2363(7)	7163(6)	67(2)
C(3)	5786(10)	–3525(8)	7209(7)	74(2)
C(4)	5083(11)	–3394(9)	8022(8)	83(2)
C(5)	5270(13)	–2124(10)	8775(8)	96(3)
C(6)	6206(11)	–987(9)	8734(7)	83(2)
C(7)	8312(9)	2032(7)	8994(6)	64(2)
C(8)	9611(12)	2421(10)	9967(7)	85(2)
C(9)	9637(14)	3541(12)	10825(8)	105(3)
C(10)	8358(13)	4337(12)	10728(8)	99(3)
C(11)	7031(11)	3997(10)	9763(7)	82(2)
C(12)	7029(10)	2848(8)	8910(6)	70(2)
C(13)	7154(9)	690(7)	6468(6)	62(2)
C(14)	7102(9)	1473(8)	4818(6)	66(2)
C(15)	7978(10)	2428(9)	4365(7)	76(2)
C(16)	8039(10)	3944(9)	4979(7)	76(2)

C(17)	8960(10)	4171(8)	6186(7)	73(2)
C(18)	8115(9)	3200(7)	6654(6)	64(2)
C(19)	10373(9)	–53(8)	8004(7)	71(2)
C(20)	11652(10)	896(9)	7866(7)	78(2)
N	7981(7)	1694(6)	6026(5)	58(1)
O	11048(7)	1030(8)	6773(6)	100(2)
Si	8261(2)	461(2)	7869(2)	61(1)

Tab. A.29 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) von **147**·HBr.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	63(1)	62(1)	92(1)	25(1)	32(1)	4(1)
C(1)	72(4)	56(4)	64(4)	24(3)	16(4)	2(3)
C(2)	71(4)	58(4)	74(5)	27(4)	18(4)	6(3)
C(3)	74(5)	55(4)	84(5)	25(4)	9(4)	3(3)
C(4)	89(6)	74(5)	93(6)	42(5)	24(5)	–1(4)
C(5)	119(8)	88(6)	93(6)	33(5)	48(6)	–13(5)
C(6)	107(7)	71(5)	74(5)	18(4)	39(5)	–13(4)
C(7)	74(5)	59(4)	60(4)	25(3)	19(3)	–7(3)
C(8)	96(6)	83(6)	72(5)	25(5)	18(5)	4(5)
C(9)	104(8)	114(8)	80(6)	15(6)	18(6)	2(6)
C(10)	105(7)	105(7)	77(6)	2(5)	40(6)	–23(6)
C(11)	84(6)	87(6)	88(6)	23(5)	48(5)	9(4)
C(12)	73(5)	73(5)	68(4)	22(4)	26(4)	–1(4)
C(13)	69(4)	51(4)	69(4)	24(3)	24(3)	1(3)
C(14)	78(5)	69(4)	57(4)	23(3)	25(4)	11(4)
C(15)	80(5)	86(6)	72(5)	35(4)	31(4)	10(4)
C(16)	67(4)	90(6)	88(5)	55(5)	27(4)	5(4)
C(17)	74(5)	67(5)	89(5)	34(4)	32(4)	6(4)
C(18)	72(4)	55(4)	69(4)	18(3)	30(4)	4(3)
C(19)	68(4)	74(5)	77(5)	35(4)	23(4)	1(4)
C(20)	66(5)	79(5)	96(6)	35(5)	29(4)	14(4)
N	63(3)	54(3)	61(3)	18(3)	24(3)	10(3)
O	66(3)	136(5)	130(5)	77(5)	45(4)	19(3)
Si	68(1)	57(1)	63(1)	25(1)	22(1)	3(1)

$(146)_2 \cdot H_2CoCl_4$

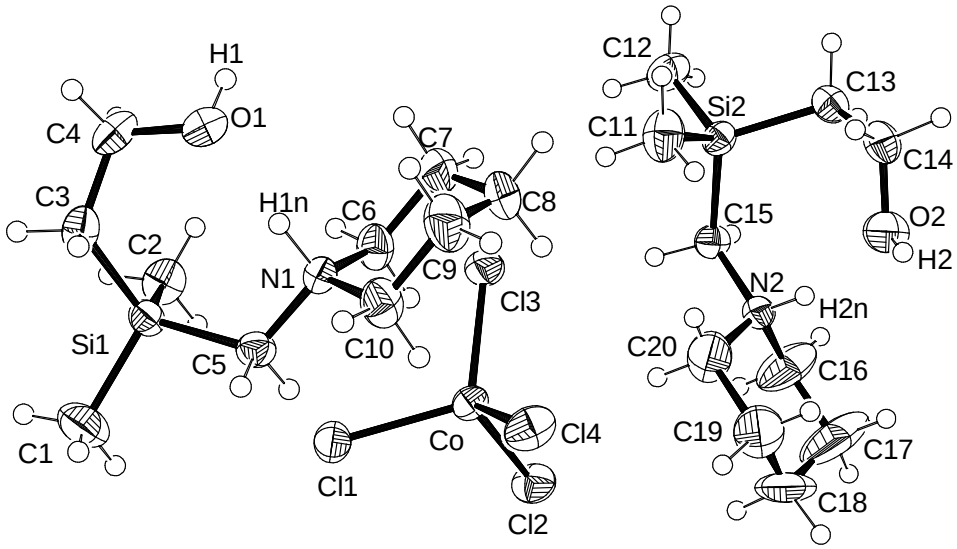

Abb. A.14 Thermische Auslenkungsellipsoide (50 % Aufenthaltswahrscheinlichkeit) der Molekülstruktur von $(\mathbf{146})_2 \cdot H_2CoCl_4$ im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.30 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) von $(\mathbf{146})_2 \cdot H_2CoCl_4$.

Atom	x	y	z	U(eq)
C(1)	833(4)	7054(5)	2424(1)	63(1)
C(2)	1520(3)	7570(3)	1458(1)	45(1)
C(3)	1774(3)	9759(3)	2140(1)	41(1)
C(4)	2426(3)	10660(3)	1806(1)	47(1)
C(5)	3618(3)	7357(3)	2221(1)	34(1)
C(6)	5166(3)	7588(3)	1593(1)	41(1)
C(7)	6350(3)	8307(4)	1413(1)	51(1)
C(8)	7499(3)	8180(4)	1730(1)	56(1)
C(9)	7111(3)	8663(4)	2191(1)	58(1)
C(10)	5936(3)	7918(4)	2362(1)	45(1)
C(11)	8940(4)	6726(4)	534(1)	53(1)
C(12)	8446(4)	6306(3)	−468(1)	48(1)
C(13)	11107(3)	5687(3)	−74(1)	37(1)
C(14)	11981(3)	5463(3)	327(1)	42(1)
C(15)	8655(3)	3984(3)	97(1)	34(1)
C(16)	9260(5)	1731(4)	293(2)	80(2)
C(17)	9906(6)	872(4)	640(2)	112(2)
C(18)	9284(5)	1021(6)	1092(3)	128(3)
C(19)	9332(5)	2418(7)	1233(2)	103(2)
C(20)	8682(5)	3291(6)	887(1)	80(2)
Cl(1)	2989(1)	4190(1)	1479(1)	44(1)
Cl(2)	5236(1)	1792(1)	1000(1)	48(1)

Cl(3)	5475(1)	5274(1)	634(1)	44(1)
Cl(4)	6517(1)	4295(1)	1772(1)	51(1)
Co	5064(1)	3918(1)	1216(1)	32(1)
N(1)	4803(2)	8054(2)	2049(1)	29(1)
N(2)	9277(2)	3107(2)	438(1)	32(1)
O(1)	3797(3)	10442(2)	1820(1)	50(1)
O(2)	11715(2)	4199(3)	508(1)	52(1)
Si(1)	1945(1)	7967(1)	2044(1)	32(1)
Si(2)	9310(1)	5700(1)	39(1)	31(1)

Tab. A.31 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) von (**146**)$_2$·H_2CoCl_4.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	42(2)	86(3)	60(2)	28(2)	4(2)	−10(2)
C(2)	47(2)	50(2)	38(2)	−6(2)	−11(2)	2(2)
C(3)	38(2)	46(2)	40(2)	−6(1)	−1(1)	10(2)
C(4)	51(2)	34(2)	55(2)	3(2)	−10(2)	13(2)
C(5)	35(2)	35(2)	31(2)	5(1)	−1(1)	−1(1)
C(6)	38(2)	50(2)	34(2)	−6(1)	3(1)	7(2)
C(7)	46(2)	58(2)	50(2)	8(2)	17(2)	12(2)
C(8)	29(2)	59(2)	79(3)	11(2)	12(2)	2(2)
C(9)	35(2)	66(3)	71(3)	−9(2)	−5(2)	−7(2)
C(10)	34(2)	61(2)	41(2)	0(2)	−7(1)	0(2)
C(11)	49(2)	54(2)	57(2)	−20(2)	−2(2)	5(2)
C(12)	52(2)	45(2)	47(2)	9(2)	−14(2)	5(2)
C(13)	36(2)	40(2)	37(2)	−2(1)	5(1)	−3(1)
C(14)	30(2)	47(2)	48(2)	−4(2)	−3(1)	−8(1)
C(15)	34(2)	35(2)	32(1)	2(1)	−6(1)	−3(1)
C(16)	102(4)	30(2)	108(4)	−1(2)	−48(3)	−1(2)
C(17)	125(5)	35(2)	175(6)	24(3)	−79(5)	−1(3)
C(18)	61(3)	136(6)	187(7)	135(6)	−35(4)	−34(3)
C(19)	76(3)	170(6)	62(3)	70(4)	13(3)	36(4)
C(20)	74(3)	122(4)	44(2)	35(2)	22(2)	39(3)
Cl(1)	41(1)	49(1)	42(1)	2(1)	2(1)	7(1)
Cl(2)	64(1)	33(1)	47(1)	−7(1)	5(1)	2(1)
Cl(3)	41(1)	48(1)	43(1)	13(1)	−2(1)	1(1)
Cl(4)	59(1)	52(1)	42(1)	2(1)	−22(1)	−1(1)
Co	36(1)	31(1)	30(1)	−1(1)	−4(1)	2(1)
N(1)	28(1)	29(1)	29(1)	−1(1)	–2(1)	4(1)
N(2)	28(1)	33(1)	35(1)	4(1)	−1(1)	−2(1)
O(1)	53(2)	39(1)	59(2)	14(1)	4(1)	8(1)
O(2)	44(1)	57(2)	54(2)	12(1)	−18(1)	−13(1)
Si(1)	28(1)	39(1)	29(1)	3(1)	0(1)	−1(1)
Si(2)	32(1)	30(1)	33(1)	−1(1)	−5(1)	1(1)

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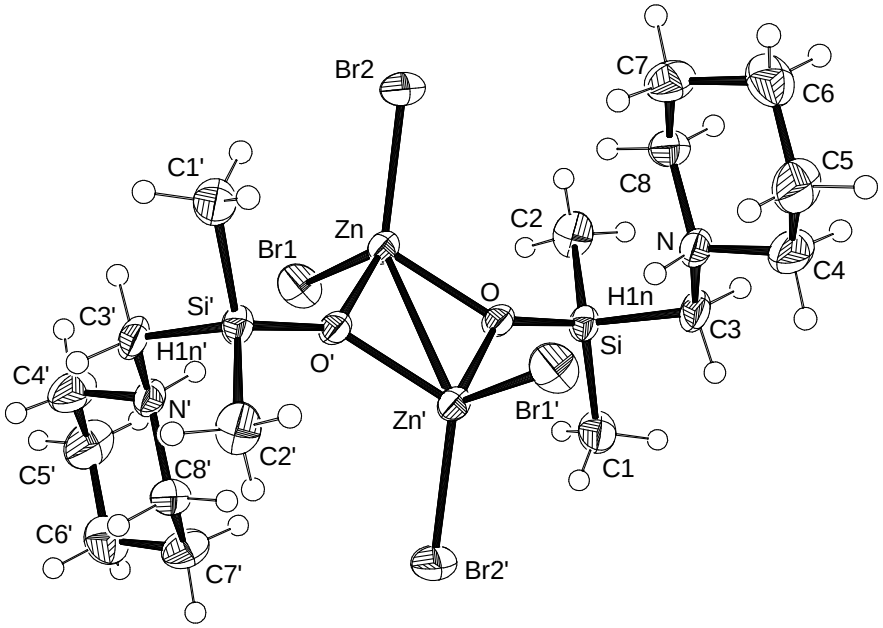

Abb. A.15 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von **172** im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber – mit Ausnahme der Wasserstoffatome an den Stickstoffen – weggelassen.

Tab. A.32 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) von **172**.

Atom	x	y	z	U(eq)
Br(1)	11776(1)	1157(1)	2930(1)	37(1)
Br(2)	12450(1)	1289(1)	6816(1)	45(1)
C(1)	8683(3)	2535(2)	5027(3)	37(1)
C(2)	6394(3)	1333(2)	3579(3)	38(1)
C(3)	6637(2)	1306(2)	6433(2)	30(1)
C(4)	6341(3)	815(2)	8663(3)	47(1)
C(5)	7085(3)	458(2)	9919(2)	48(1)
C(6)	8302(3)	1069(2)	10451(3)	44(1)
C(7)	9377(3)	1207(2)	9446(3)	38(1)
C(8)	8633(3)	1566(2)	8192(2)	31(1)
N	7407(2)	968(1)	7678(2)	24(1)
O	8979(2)	645(1)	5083(2)	23(1)
Si	7770(1)	1433(1)	5002(1)	22(1)
Zn	11135(1)	669(1)	4999(1)	23(1)

Tab. A.33 Anisotrope Auslenkungsparameter (Å^2 x 10^3) von **172**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	52(1)	26(1)	35(1)	3(1)	11(1)	–7(1)
Br(2)	33(1)	54(1)	46(1)	–24(1)	–11(1)	0(1)
C(1)	42(1)	26(1)	43(2)	6(1)	2(1)	3(1)
C(2)	34(1)	50(2)	29(1)	2(1)	–6(1)	8(1)
C(3)	24(1)	42(1)	25(1)	1(1)	–1(1)	7(1)
C(4)	30(1)	84(2)	27(1)	3(1)	9(1)	–7(1)
C(5)	46(2)	75(2)	25(1)	7(1)	8(1)	–11(1)
C(6)	52(2)	56(2)	25(1)	–2(1)	0(1)	6(1)
C(7)	38(1)	43(1)	30(1)	2(1)	–6(1)	–3(1)
C(8)	32(1)	27(1)	32(1)	1(1)	–3(1)	–3(1)
N	24(1)	27(1)	22(1)	–1(1)	4(1)	2(1)
O	19(1)	19(1)	30(1)	0(1)	1(1)	2(1)
Si	21(1)	23(1)	21(1)	2(1)	0(1)	4(1)
Zn	19(1)	22(1)	27(1)	–3(1)	1(1)	–1(1)

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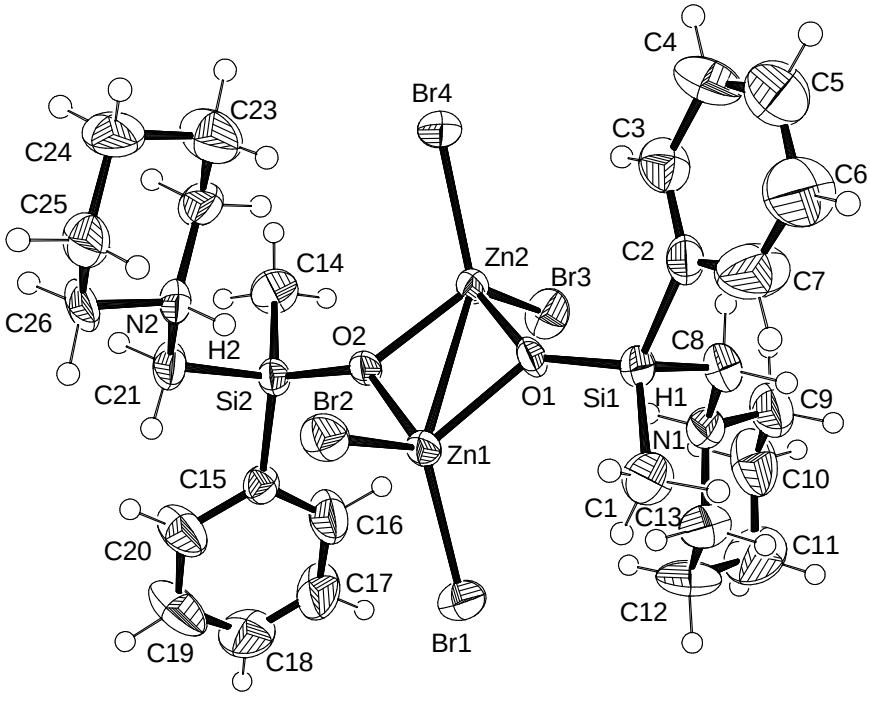

Abb. A.16 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von **167** im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber – mit Ausnahme der Wasserstoffatome an den Stickstoffen – weggelassen.

Tab. A.34 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter ($Å^2$ x 10^3) von **167**.

Atom	x	y	z	U(eq)
Br(1)	9159(1)	3767(1)	9631(1)	52(1)
Br(2)	10828(1)	4290(1)	7915(1)	43(1)
Br(3)	5107(1)	5710(1)	9232(1)	52(1)
Br(4)	6446(1)	6300(1)	7492(1)	51(1)
C(1)	7195(8)	2838(3)	8208(4)	60(2)
C(2)	5540(7)	3675(4)	7208(3)	42(2)
C(3)	5068(8)	4312(4)	6892(3)	52(2)
C(4)	4473(9)	4263(5)	6267(4)	69(2)
C(5)	4361(10)	3557(5)	5976(4)	82(3)
C(6)	4840(13)	2919(5)	6290(5)	112(4)
C(7)	5383(10)	3002(5)	6895(4)	86(3)
C(8)	4509(7)	3748(4)	8540(4)	54(2)
C(9)	3068(8)	3950(5)	9512(4)	66(2)
C(10)	3039(9)	4110(5)	10211(4)	79(3)
C(11)	3774(11)	3527(5)	10582(4)	88(3)
C(12)	5269(10)	3447(5)	10317(4)	82(3)
C(13)	5289(8)	3295(4)	9617(4)	60(2)
C(14)	8601(7)	7110(3)	9091(4)	52(2)
C(15)	10148(6)	6024(3)	9931(3)	34(1)
C(16)	9190(8)	5805(5)	10391(4)	65(2)
C(17)	9562(10)	5689(5)	11040(4)	82(3)
C(18)	10821(10)	5795(5)	11239(4)	70(2)
C(19)	11816(9)	6010(5)	10814(4)	78(3)
C(20)	11480(7)	6153(5)	10154(4)	65(2)
C(21)	11269(6)	6325(4)	8604(3)	45(2)
C(22)	10220(7)	6653(4)	7543(3)	47(2)
C(23)	10157(8)	6457(5)	6821(4)	70(2)
C(24)	11607(8)	6523(5)	6522(4)	69(2)
C(25)	12617(7)	6029(4)	6888(3)	54(2)
C(26)	12638(6)	6221(4)	7601(3)	49(2)
N(1)	4516(6)	3881(3)	9250(3)	45(1)
N(2)	11220(5)	6170(3)	7887(2)	33(1)
O(1)	7100(4)	4444(2)	8258(2)	30(1)
O(2)	8696(4)	5563(2)	8758(2)	30(1)
Si(1)	6192(2)	3716(1)	8062(1)	37(1)
Si(2)	9605(2)	6221(1)	9087(1)	30(1)
Zn(1)	8983(1)	4460(1)	8665(1)	32(1)
Zn(2)	6790(1)	5531(1)	8408(1)	31(1)

Tab. A.35 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) von **167**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	60(1)	45(1)	50(1)	14(1)	−10(1)	−5(1)
Br(2)	40(1)	41(1)	50(1)	−2(1)	0(1)	7(1)
Br(3)	43(1)	46(1)	66(1)	−2(1)	14(1)	5(1)
Br(4)	44(1)	49(1)	59(1)	23(1)	−12(1)	−2(1)
C(1)	73(6)	30(3)	78(6)	−6(3)	−23(4)	−4(3)
C(2)	36(4)	46(4)	44(4)	0(3)	−1(3)	−14(3)
C(3)	59(5)	56(4)	42(4)	−12(3)	−2(4)	−6(4)
C(4)	72(6)	93(7)	42(5)	1(5)	−19(4)	12(5)
C(5)	94(7)	90(7)	63(6)	−7(5)	−15(5)	−12(5)
C(6)	178(12)	72(6)	85(8)	−12(5)	−60(8)	−34(7)
C(7)	140(9)	59(5)	61(6)	−2(4)	−30(6)	0(5)
C(8)	46(5)	55(4)	59(5)	3(4)	−16(4)	−16(3)
C(9)	48(5)	88(6)	61(6)	6(5)	−3(4)	−18(4)
C(10)	56(6)	115(7)	67(6)	−18(6)	16(5)	−24(5)
C(11)	123(9)	100(7)	40(5)	11(5)	12(5)	−17(6)
C(12)	97(7)	93(6)	55(6)	34(5)	−26(5)	8(5)
C(13)	64(5)	55(5)	61(5)	15(4)	−4(4)	1(4)
C(14)	57(5)	29(3)	69(5)	−1(3)	−4(4)	7(3)
C(15)	38(4)	33(3)	32(3)	−2(3)	−2(3)	−6(3)
C(16)	43(5)	99(6)	54(5)	7(4)	1(4)	−23(4)
C(17)	76(6)	128(8)	42(5)	27(5)	0(5)	−47(6)
C(18)	90(7)	83(6)	37(4)	7(4)	−6(5)	−6(5)
C(19)	49(5)	132(8)	52(5)	−13(5)	−18(4)	15(5)
C(20)	37(4)	113(7)	44(4)	2(4)	0(4)	5(4)
C(21)	35(4)	62(4)	38(4)	5(3)	3(3)	−20(3)
C(22)	39(4)	50(4)	53(5)	16(3)	9(4)	3(3)
C(23)	49(5)	110(7)	52(5)	8(5)	5(4)	16(5)
C(24)	56(5)	112(7)	40(5)	28(5)	4(4)	10(5)
C(25)	35(4)	79(5)	48(5)	8(4)	10(3)	−3(4)
C(26)	16(3)	82(5)	48(4)	6(4)	3(3)	−8(3)
N(1)	44(4)	52(3)	40(4)	11(3)	−6(3)	−14(3)
N(2)	25(3)	37(3)	38(3)	0(2)	4(3)	−8(2)
O(1)	21(2)	30(2)	40(3)	−4(2)	−9(2)	−4(2)
O(2)	23(2)	21(2)	45(2)	3(2)	−7(2)	2(2)
Si(1)	39(1)	34(1)	38(1)	2(1)	−10(1)	−11(1)
Si(2)	25(1)	26(1)	40(1)	−1(1)	−2(1)	−2(1)
Zn(1)	26(1)	25(1)	44(1)	3(1)	−7(1)	0(1)
Zn(2)	23(1)	27(1)	45(1)	6(1)	−5(1)	0(1)

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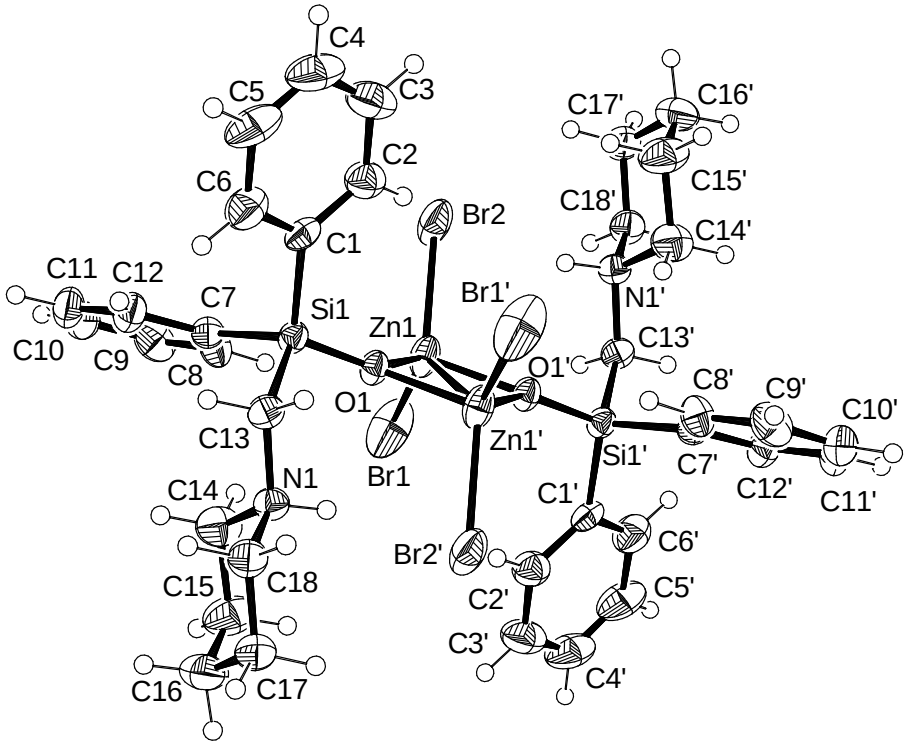

Abb. A.17 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von **169** im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber – mit Ausnahme der Wasserstoffatome an den Stickstoffen – weggelassen.

Tab. A.36 Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter (Å^2 x 10^3) von **169**.

Atom	x	y	z	U(eq)
Br(1)	2474(1)	6623(1)	74(1)	88(1)
Br(2)	6345(1)	7008(1)	834(1)	63(1)
C(1)	7053(6)	4259(4)	2377(4)	37(2)
C(2)	8006(7)	4824(5)	2024(4)	46(2)
C(3)	9365(7)	4817(5)	2400(6)	60(2)
C(4)	9801(8)	4241(6)	3116(6)	65(2)
C(5)	8901(8)	3668(6)	3455(5)	67(2)
C(6)	7513(7)	3676(5)	3088(5)	53(2)
C(7)	4229(6)	4929(4)	2696(4)	33(1)
C(8)	3442(6)	5688(4)	2470(4)	42(2)
C(9)	2741(7)	6173(5)	3094(5)	51(2)
C(10)	2859(7)	5860(5)	3974(5)	53(2)
C(11)	3593(6)	5076(5)	4212(4)	52(2)
C(12)	4284(7)	4621(5)	3596(4)	42(2)
C(13)	4721(6)	2999(4)	1870(4)	34(2)
C(14)	2188(6)	3239(5)	1657(5)	55(2)
C(15)	896(7)	2956(5)	1078(5)	64(2)

C(16)	660(7)	1898(6)	1145(5)	64(2)
C(17)	1858(7)	1371(5)	851(5)	54(2)
C(18)	3187(7)	1678(4)	1410(4)	43(2)
N(1)	3382(5)	2722(3)	1356(4)	34(1)
O(1)	4933(4)	4695(3)	882(2)	32(1)
Si(1)	5213(2)	4283(1)	1893(1)	32(1)
Zn(1)	4591(1)	5919(1)	268(1)	41(1)

Tab. A. 37 Anisotrope Auslenkungsparameter ($Å^2$ x 10^3) von **169**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	88(1)	113(1)	59(1)	–5(1)	–5(1)	62(1)
Br(2)	107(1)	45(1)	38(1)	–6(1)	13(1)	–24(1)
C(1)	40(4)	38(4)	31(4)	–6(3)	–1(3)	1(3)
C(2)	43(4)	46(4)	50(4)	–6(3)	2(3)	2(3)
C(3)	36(4)	62(5)	82(6)	–22(5)	6(4)	–3(4)
C(4)	41(4)	78(6)	73(6)	–21(5)	–9(4)	12(5)
C(5)	63(6)	74(6)	56(5)	–5(4)	–25(4)	19(5)
C(6)	49(5)	58(5)	50(5)	–7(4)	–2(4)	3(4)
C(7)	34(3)	29(3)	37(4)	0(3)	2(3)	–4(3)
C(8)	40(4)	45(4)	42(4)	6(3)	6(3)	0(3)
C(9)	42(4)	43(4)	71(5)	–4(4)	14(4)	2(3)
C(10)	45(4)	70(5)	47(5)	–14(4)	15(3)	–2(4)
C(11)	47(4)	77(5)	32(4)	6(4)	7(3)	–1(4)
C(12)	49(4)	44(4)	35(4)	–1(3)	5(3)	0(3)
C(13)	31(3)	38(4)	34(4)	–1(3)	2(3)	2(3)
C(14)	40(4)	57(5)	69(5)	–18(4)	7(4)	7(4)
C(15)	43(4)	69(6)	76(6)	–19(4)	–14(4)	6(4)
C(16)	39(4)	83(6)	71(5)	–20(5)	6(4)	–17(4)
C(17)	53(5)	56(5)	51(5)	–8(4)	4(4)	–18(4)
C(18)	50(4)	31(4)	48(4)	0(3)	8(3)	–5(3)
N(1)	37(3)	34(3)	32(3)	0(2)	2(2)	–3(2)
O(1)	40(2)	29(2)	27(2)	2(2)	3(2)	0(2)
Si(1)	35(1)	30(1)	29(1)	1(1)	2(1)	–1(1)
Zn(1)	58(1)	33(1)	33(1)	3(1)	7(1)	9(1)

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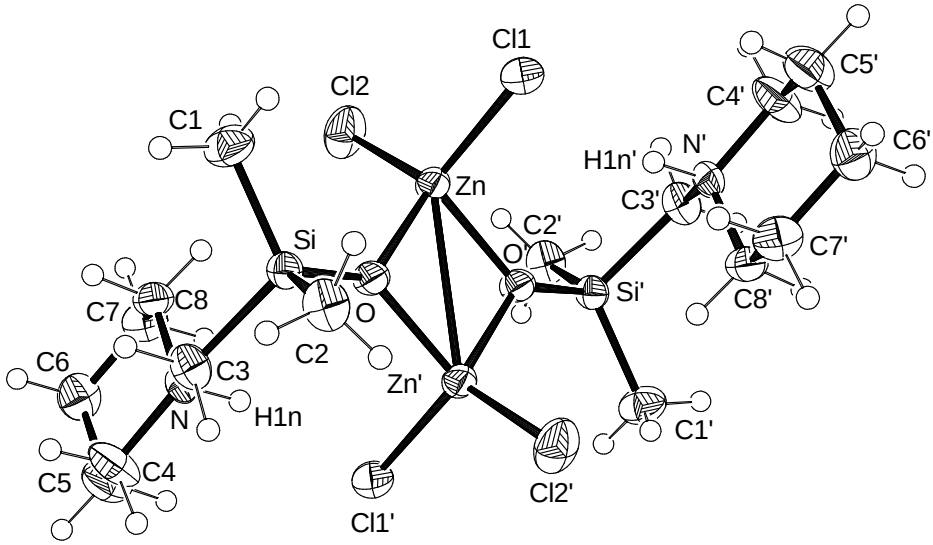

Abb. A.18 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von **174** im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber – mit Ausnahme der Wasserstoffatome an den Stickstoffen – weggelassen.

Tab. A.38 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von **174**.

Atom	x	y	z	U(eq)
C(1)	8577(4)	7401(2)	–28(4)	42(1)
C(2)	6321(4)	8682(3)	–1533(3)	41(1)
C(3)	6562(4)	8696(3)	1356(3)	34(1)
C(4)	6310(4)	9193(3)	3611(4)	49(1)
C(5)	7089(4)	9543(3)	4876(4)	49(1)
C(6)	8319(4)	8898(3)	5417(4)	44(1)
C(7)	9390(4)	8757(3)	4398(3)	40(1)
C(8)	8610(4)	8403(2)	3126(3)	33(1)
Cl(1)	11751(1)	8888(1)	–2010(1)	41(1)
Cl(2)	12404(1)	8662(1)	1680(1)	51(1)
N	7364(3)	9032(2)	2613(3)	28(1)
O	8960(2)	9337(1)	37(2)	28(1)
Si	7698(1)	8546(1)	–72(1)	26(1)
Zn	11138(1)	9303(1)	–26(1)	28(1)

Tab. A.39 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von **174**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	40(2)	29(2)	58(3)	–7(2)	3(2)	–1(2)
C(2)	37(2)	48(3)	37(2)	1(2)	1(2)	–5(2)
C(3)	24(2)	44(2)	32(2)	0(2)	0(2)	–6(2)
C(4)	30(2)	82(3)	37(2)	1(2)	12(2)	11(2)

C(5)	48(2)	65(3)	37(2)	–4(2)	12(2)	9(2)
C(6)	46(2)	53(3)	33(2)	3(2)	0(2)	–1(2)
C(7)	36(2)	41(2)	40(2)	–3(2)	–3(2)	3(2)
C(8)	32(2)	28(2)	39(2)	–3(2)	6(2)	4(2)
Cl(1)	51(1)	30(1)	45(1)	–2(1)	16(1)	5(1)
Cl(2)	38(1)	55(1)	58(1)	24(1)	–7(1)	2(1)
N	23(2)	31(2)	31(2)	4(1)	10(1)	–2(1)
O	20(1)	24(1)	42(1)	1(1)	5(1)	–1(1)
Si	23(1)	26(1)	30(1)	–1(1)	3(1)	–3(1)
Zn	21(1)	25(1)	37(1)	4(1)	5(1)	1(1)

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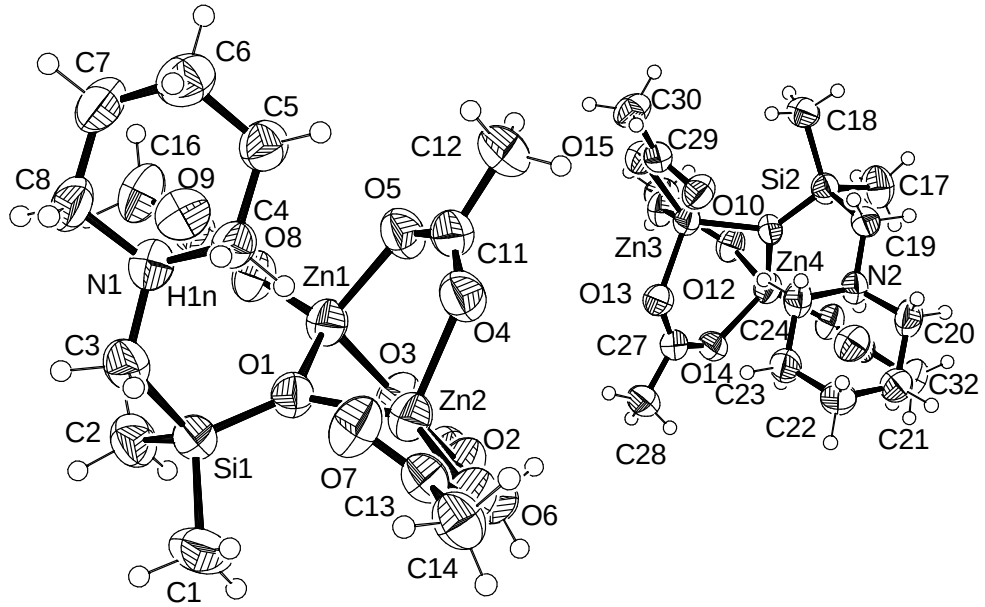

Abb. A.19 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von **175** im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber – mit Ausnahme der Wasserstoffatome an den Stickstoffen – weggelassen.

Tab. A.40 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von **175**.

Atom	x	y	z	U(eq)
C(1)	6931(5)	2408(1)	5585(3)	45(1)
C(2)	8946(6)	3054(2)	4893(3)	61(1)
C(3)	7610(5)	3195(1)	6461(2)	36(1)
C(4)	9455(4)	3269(1)	7682(2)	33(1)
C(5)	9742(5)	3171(1)	8560(2)	38(1)
C(6)	8542(5)	3374(1)	9025(3)	46(1)
C(7)	6939(5)	3245(2)	8686(3)	53(1)
C(8)	6641(5)	3323(1)	7794(3)	45(1)
C(9)	7400(4)	1961(1)	7576(3)	35(1)

C(10)	6049(5)	1715(1)	7799(3)	59(1)
C(11)	12627(5)	2450(1)	8017(3)	39(1)
C(12)	13484(5)	2472(2)	8841(3)	55(1)
C(13)	12339(5)	1837(1)	5872(3)	36(1)
C(14)	13054(6)	1520(1)	5379(3)	51(1)
C(15)	13070(5)	3427(1)	6001(2)	33(1)
C(16)	13943(5)	3801(1)	5808(3)	41(1)
C(17)	1056(5)	–305(1)	6143(3)	53(1)
C(18)	3051(5)	290(1)	5297(2)	44(1)
C(19)	1162(4)	582(1)	6609(2)	36(1)
C(20)	2713(4)	921(1)	7742(3)	39(1)
C(21)	2888(5)	992(2)	8639(3)	49(1)
C(22)	1450(5)	1196(1)	8908(3)	46(1)
C(23)	27(5)	940(1)	8645(3)	43(1)
C(24)	–129(4)	861(1)	7752(3)	38(1)
C(25)	1215(5)	–429(1)	8394(3)	36(1)
C(26)	–213(5)	–581(1)	8735(3)	49(1)
C(27)	6147(5)	156(1)	8755(3)	36(1)
C(28)	6807(6)	294(2)	9573(3)	60(2)
C(29)	6372(4)	–716(1)	7039(2)	33(1)
C(30)	7270(5)	–1074(1)	6777(3)	51(1)
C(31)	6591(4)	804(1)	6192(2)	31(1)
C(32)	7238(5)	1103(1)	5635(3)	45(1)
N(1)	7861(3)	3127(1)	7352(2)	29(1)
N(2)	1313(3)	668(1)	7499(2)	27(1)
O(1)	9999(3)	2594(1)	6309(2)	30(1)
O(2)	11861(4)	3446(1)	6330(2)	53(1)
O(3)	13637(3)	3084(1)	5822(2)	42(1)
O(4)	13028(3)	2687(1)	7491(2)	43(1)
O(5)	11538(3)	2195(1)	7911(2)	45(1)
O(6)	12878(3)	2188(1)	5859(2)	47(1)
O(7)	11264(3)	1721(1)	6272(2)	43(1)
O(8)	8394(3)	1772(1)	7195(2)	39(1)
O(9)	7511(4)	2326(1)	7746(2)	46(1)
O(10)	3794(3)	49(1)	6954(2)	29(1)
O(11)	5477(3)	894(1)	6561(2)	44(1)
O(12)	7222(3)	454(1)	6254(2)	34(1)
O(13)	6564(3)	338(1)	8153(2)	40(1)
O(14)	5214(3)	–139(1)	8728(2)	41(1)
O(15)	6961(3)	–372(1)	6965(2)	40(1)
O(16)	5114(3)	–786(1)	7325(2)	39(1)
O(17)	2172(3)	–687(1)	8169(2)	42(1)
O(18)	1431(4)	–58(1)	8335(2)	50(1)
Si(1)	8470(1)	2796(1)	5817(1)	32(1)
Si(2)	2370(1)	144(1)	6270(1)	30(1)
Zn(1)	12247(1)	2712(1)	6333(1)	33(1)

Zn(2)	10134(1)	2092(1)	6936(1)	31(1)
Zn(3)	6016(1)	181(1)	7021(1)	29(1)
Zn(4)	3875(1)	–362(1)	7808(1)	31(1)

Tab. A.41 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von **175**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	38(2)	51(3)	44(3)	–13(2)	–9(2)	2(2)
C(2)	65(3)	76(4)	42(3)	22(3)	–1(3)	4(3)
C(3)	36(2)	35(2)	35(2)	3(2)	–3(2)	4(2)
C(4)	25(2)	38(2)	37(2)	–5(2)	5(2)	–4(2)
C(5)	37(2)	35(2)	41(3)	–7(2)	0(2)	–4(2)
C(6)	55(3)	44(3)	41(3)	–10(2)	19(2)	–7(2)
C(7)	45(3)	65(3)	52(3)	–13(3)	25(2)	–2(2)
C(8)	31(2)	47(3)	62(3)	–12(2)	16(2)	7(2)
C(9)	31(2)	29(2)	44(3)	1(2)	3(2)	–1(2)
C(10)	46(3)	49(3)	88(4)	–19(3)	32(3)	–11(2)
C(11)	35(2)	39(3)	42(3)	–3(2)	5(2)	8(2)
C(12)	51(3)	67(4)	44(3)	2(3)	–9(2)	–2(2)
C(13)	38(2)	34(3)	37(2)	2(2)	3(2)	11(2)
C(14)	66(3)	35(3)	55(3)	0(2)	19(3)	17(2)
C(15)	29(2)	35(2)	36(2)	2(2)	1(2)	–2(2)
C(16)	41(2)	33(3)	48(3)	5(2)	6(2)	–5(2)
C(17)	45(3)	45(3)	66(3)	–12(2)	–9(2)	–12(2)
C(18)	44(3)	50(3)	37(2)	–5(2)	–1(2)	4(2)
C(19)	32(2)	41(3)	35(2)	0(2)	1(2)	7(2)
C(20)	27(2)	39(3)	50(3)	–10(2)	12(2)	–9(2)
C(21)	37(2)	57(3)	52(3)	–16(2)	3(2)	–5(2)
C(22)	51(3)	44(3)	44(3)	–15(2)	6(2)	3(2)
C(23)	36(2)	50(3)	47(3)	–8(2)	21(2)	4(2)
C(24)	24(2)	43(3)	48(3)	–7(2)	10(2)	5(2)
C(25)	33(2)	36(3)	40(2)	4(2)	6(2)	–4(2)
C(26)	37(2)	49(3)	63(3)	–1(2)	16(2)	–8(2)
C(27)	29(2)	46(3)	33(2)	–1(2)	6(2)	–2(2)
C(28)	63(3)	84(4)	33(3)	–5(3)	2(2)	–29(3)
C(29)	32(2)	32(2)	34(2)	1(2)	1(2)	6(2)
C(30)	54(3)	40(3)	61(3)	–4(2)	21(3)	12(2)
C(31)	30(2)	35(2)	28(2)	–2(2)	1(2)	–8(2)
C(32)	47(3)	47(3)	43(3)	13(2)	16(2)	–1(2)
N(1)	27(2)	21(2)	40(2)	–3(2)	6(2)	1(1)
N(2)	24(2)	24(2)	34(2)	–2(2)	5(1)	2(1)
O(1)	23(1)	30(2)	36(2)	2(1)	3(1)	–2(1)
O(2)	45(2)	44(2)	74(2)	2(2)	25(2)	1(1)
O(3)	43(2)	26(2)	59(2)	–1(1)	17(2)	1(1)
O(4)	35(2)	48(2)	46(2)	8(2)	–3(1)	–11(1)
O(5)	42(2)	48(2)	45(2)	11(2)	–5(2)	–11(1)

O(6)	45(2)	33(2)	65(2)	–2(2)	22(2)	0(1)
O(7)	45(2)	27(2)	59(2)	–2(1)	18(2)	2(1)
O(8)	31(2)	29(2)	58(2)	–3(1)	14(1)	–5(1)
O(9)	61(2)	24(2)	54(2)	–3(1)	9(2)	–2(1)
O(10)	22(1)	26(2)	37(2)	4(1)	3(1)	–1(1)
O(11)	45(2)	43(2)	48(2)	4(2)	21(2)	1(1)
O(12)	34(2)	29(2)	40(2)	4(1)	8(1)	0(1)
O(13)	38(2)	51(2)	31(2)	2(1)	4(1)	–14(1)
O(14)	41(2)	47(2)	35(2)	5(1)	5(1)	–10(1)
O(15)	32(2)	33(2)	56(2)	7(2)	10(1)	4(1)
O(16)	35(2)	29(2)	56(2)	3(1)	15(1)	1(1)
O(17)	36(2)	34(2)	60(2)	4(2)	19(2)	–2(1)
O(18)	59(2)	28(2)	63(2)	11(2)	10(2)	–4(1)
Si(1)	31(1)	34(1)	30(1)	0(1)	–1(1)	3(1)
Si(2)	24(1)	29(1)	35(1)	–7(1)	0(1)	0(1)
Zn(1)	27(1)	32(1)	41(1)	2(1)	7(1)	–2(1)
Zn(2)	28(1)	26(1)	41(1)	1(1)	5(1)	0(1)
Zn(3)	23(1)	31(1)	32(1)	3(1)	4(1)	–3(1)
Zn(4)	27(1)	25(1)	41(1)	3(1)	8(1)	–2(1)

(*R*,*R*)-176

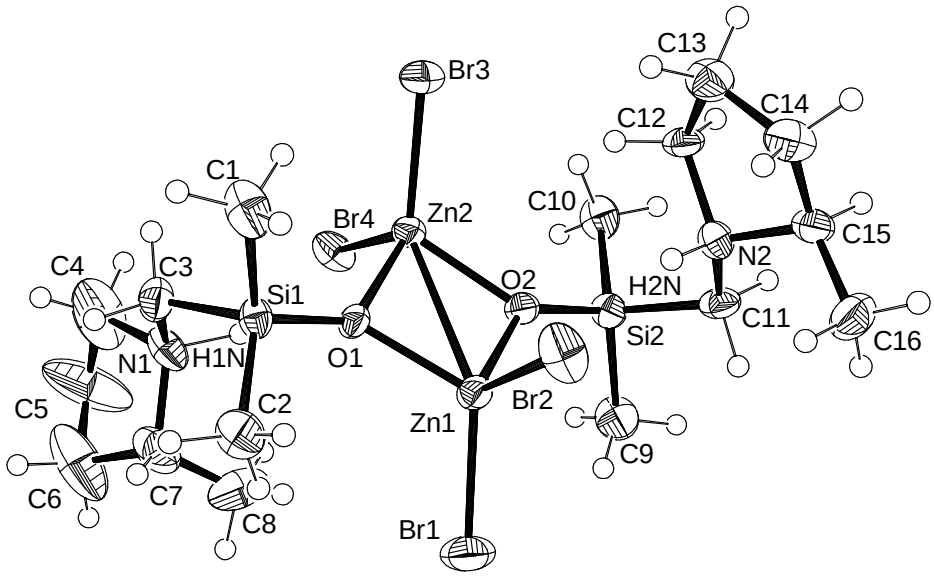

Abb. A.20 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von (*R*,*R*)-**176** im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber – mit Ausnahme der Wasserstoffatome an den Stickstoffen – weggelassen.

Tab. A.42 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*,*R*)-**176**.

Atom	x	y	z	U(eq)
Br(1)	5249(1)	8534(1)	8691(1)	56(1)
Br(2)	3789(1)	8099(1)	4960(1)	50(1)
Br(3)	18(1)	5778(1)	5815(1)	44(1)
Br(4)	1150(1)	5857(1)	9690(1)	37(1)
C(1)	–833(8)	8392(6)	5979(7)	49(2)
C(2)	1229(8)	9609(5)	7632(8)	46(2)
C(3)	–736(7)	8254(5)	8860(7)	36(2)
C(4)	–1043(11)	7609(6)	11072(8)	78(3)
C(5)	–339(15)	7738(8)	12363(9)	114(5)
C(6)	274(13)	8638(7)	12250(9)	96(4)
C(7)	931(9)	8637(6)	10881(9)	55(2)
C(8)	2344(10)	8336(7)	11046(11)	84(3)
C(9)	6238(7)	5868(6)	8822(6)	45(2)
C(10)	3959(8)	4528(5)	7645(7)	38(2)
C(11)	5748(7)	5672(5)	5923(6)	32(2)
C(12)	3524(7)	5298(5)	4414(6)	31(2)
C(13)	2959(8)	5485(5)	2997(7)	42(2)
C(14)	4213(7)	5957(5)	2383(7)	44(2)
C(15)	5504(7)	5871(5)	3435(6)	38(2)
C(16)	6615(7)	6577(5)	3359(7)	46(2)
N(1)	24(7)	7943(4)	10145(6)	39(2)
N(2)	4796(6)	5892(4)	4704(5)	28(1)
O(1)	1638(4)	7716(3)	7596(4)	25(1)
O(2)	3597(4)	6420(3)	7332(4)	26(1)
Si(1)	411(2)	8482(1)	7494(2)	27(1)
Si(2)	4808(2)	5641(1)	7458(2)	28(1)
Zn(1)	3638(1)	7746(1)	7212(1)	28(1)
Zn(2)	1539(1)	6379(1)	7561(1)	26(1)

Tab. A.43 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*,*R*)-**176**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	39(1)	45(1)	79(1)	–16(1)	–14(1)	–7(1)
Br(2)	76(1)	30(1)	47(1)	10(1)	24(1)	5(1)
Br(3)	34(1)	48(1)	46(1)	–16(1)	–7(1)	–3(1)
Br(4)	57(1)	24(1)	32(1)	2(1)	10(1)	–4(1)
C(1)	61(6)	51(5)	33(4)	3(4)	–1(4)	26(4)
C(2)	53(5)	24(4)	61(5)	5(4)	8(4)	3(4)
C(3)	31(4)	42(5)	37(4)	–1(4)	6(3)	8(3)
C(4)	125(9)	63(6)	56(6)	16(5)	52(7)	8(6)
C(5)	231(16)	73(8)	37(6)	–12(5)	19(8)	–68(9)
C(6)	168(12)	76(8)	46(6)	–6(6)	25(7)	46(8)

C(7)	63(6)	36(5)	63(6)	–13(4)	–8(5)	16(4)
C(8)	48(6)	87(8)	115(9)	–20(7)	–2(6)	–25(5)
C(9)	40(4)	54(5)	37(4)	–3(4)	–9(4)	12(4)
C(10)	42(4)	32(4)	41(5)	6(4)	2(4)	12(3)
C(11)	23(3)	25(4)	43(4)	–4(3)	–8(3)	1(3)
C(12)	26(4)	36(4)	29(4)	–5(3)	–4(3)	–7(3)
C(13)	39(4)	44(5)	39(4)	–2(4)	–7(4)	7(3)
C(14)	51(5)	40(5)	39(4)	–3(4)	1(4)	–8(4)
C(15)	39(4)	43(4)	31(4)	–11(4)	6(3)	–15(4)
C(16)	34(4)	49(5)	56(5)	1(4)	12(4)	–8(4)
N(1)	55(4)	35(4)	26(3)	–7(3)	3(3)	8(3)
N(2)	32(3)	24(3)	27(3)	0(3)	4(2)	3(3)
O(1)	17(2)	24(2)	35(3)	–1(2)	2(2)	2(2)
O(2)	23(2)	21(2)	34(3)	–2(2)	–1(2)	1(2)
Si(1)	28(1)	27(1)	27(1)	2(1)	4(1)	8(1)
Si(2)	28(1)	25(1)	30(1)	1(1)	–3(1)	7(1)
Zn(1)	24(1)	22(1)	38(1)	–1(1)	3(1)	0(1)
Zn(2)	25(1)	22(1)	30(1)	–2(1)	2(1)	–1(1)

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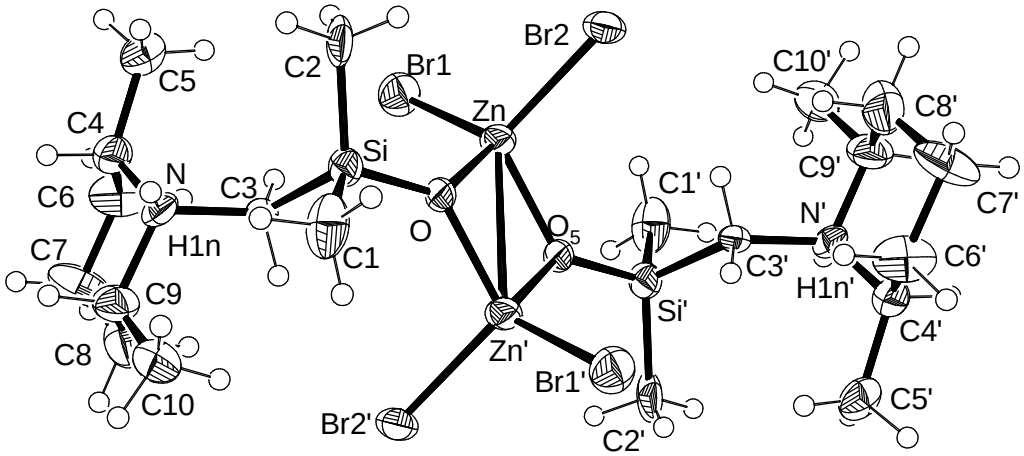

Abb. A.21 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von **177** im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber – mit Ausnahme der Wasserstoffatome an den Stickstoffen – weggelassen

Tab. A.44 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von **177**.

Atom	x	y	z	U(eq)
Br(1)	8473(1)	5111(1)	8125(1)	48(1)
Br(2)	8583(1)	4944(1)	12025(1)	37(1)
C(1)	10675(6)	2900(6)	9626(11)	54(3)
C(2)	9061(6)	3074(6)	9665(11)	51(3)
C(3)	9929(5)	3728(4)	7363(8)	30(2)

C(4)	9321(5)	3159(6)	5401(11)	39(3)
C(5)	8596(5)	3027(5)	6166(10)	42(3)
C(6)	9327(6)	3793(6)	4595(13)	52(4)
C(7)	10002(6)	3831(6)	3757(12)	69(3)
C(8)	10647(8)	3800(8)	4697(14)	75(5)
C(9)	10652(5)	3118(6)	5548(12)	45(3)
C(10)	11276(5)	3054(6)	6408(11)	49(3)
N	9950(4)	3148(3)	6314(7)	34(2)
O	9954(4)	4283(2)	9824(5)	29(1)
Si	9903(1)	3493(1)	9178(3)	32(1)
Zn	9223(1)	5036(1)	9974(1)	31(1)

Tab. A.45 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von **177**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	43(1)	54(1)	46(1)	–4(1)	–6(1)	3(1)
Br(2)	29(1)	38(1)	46(1)	–1(1)	11(1)	–3(1)
C(1)	90(9)	25(6)	48(8)	–2(5)	–8(7)	5(5)
C(2)	91(9)	31(6)	33(7)	–18(5)	16(6)	–23(6)
C(3)	22(5)	33(4)	35(6)	–10(4)	9(4)	–7(4)
C(4)	37(6)	48(7)	32(7)	–2(6)	–2(5)	–8(5)
C(5)	36(5)	52(7)	39(8)	4(5)	–17(5)	–1(5)
C(6)	46(7)	50(7)	60(9)	43(7)	–9(6)	5(5)
C(7)	58(7)	87(7)	62(9)	29(7)	31(8)	6(7)
C(8)	59(10)	106(13)	61(11)	–37(10)	5(8)	–1(7)
C(9)	42(7)	41(7)	52(8)	3(6)	14(6)	–10(5)
C(10)	40(6)	55(7)	52(8)	–3(6)	8(5)	5(5)
N	36(4)	32(4)	35(5)	–4(3)	0(4)	–16(4)
O	21(3)	29(3)	36(4)	–13(2)	2(3)	4(3)
Si	38(2)	23(1)	34(2)	–4(1)	5(1)	–3(1)
Zn	23(1)	28(1)	42(1)	–7(1)	5(1)	1(1)

(*R*,*R*,*R*,*R*)-182

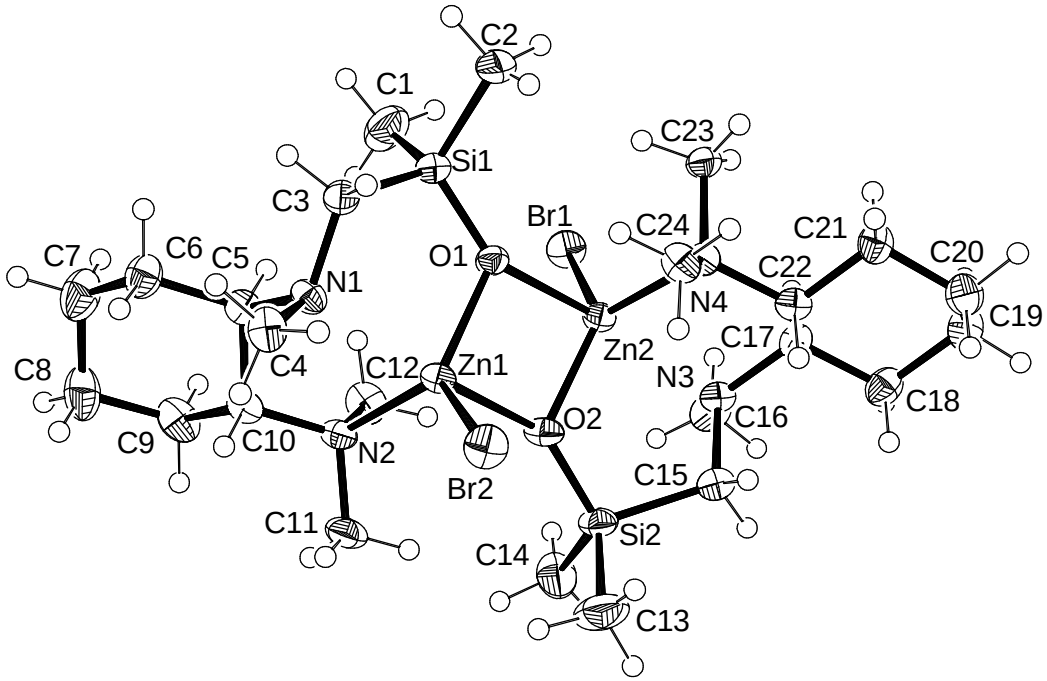

Abb. A.22 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von (*R*,*R*,*R*,*R*)-**182** im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.46 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*,*R*,*R*,*R*)-**182**.

Atom	x	y	z	U(eq)
Br(1)	8041(1)	–1647(1)	5413(1)	34(1)
Br(2)	3923(1)	3503(1)	4238(1)	35(1)
C(1)	7828(10)	1712(7)	8396(5)	55(2)
C(2)	4118(9)	1265(7)	8034(5)	55(2)
C(3)	5722(6)	4108(6)	7967(5)	32(1)
C(4)	5734(6)	6135(5)	7212(5)	31(1)
C(5)	8370(5)	5232(6)	7682(4)	26(1)
C(6)	8874(6)	6756(6)	8853(5)	35(1)
C(7)	10733(7)	7244(7)	9251(6)	49(2)
C(8)	11501(7)	7358(7)	8193(7)	48(2)
C(9)	11105(6)	5792(6)	7056(6)	38(1)
C(10)	9215(6)	5279(6)	6614(5)	26(1)
C(11)	8962(7)	4022(7)	4355(5)	37(1)
C(12)	9752(7)	2562(6)	5546(6)	35(1)
C(13)	5444(10)	1170(8)	1373(6)	57(2)
C(14)	8656(8)	43(7)	1864(6)	51(2)
C(15)	5256(6)	–1851(6)	1571(4)	30(1)
C(16)	7070(6)	–3359(6)	2216(5)	35(1)
C(17)	4170(6)	–3726(5)	2384(4)	26(1)
C(18)	3510(6)	–5007(6)	1073(5)	34(1)

C(19)	2016(7)	–6111(6)	1035(5)	39(1)
C(20)	652(7)	–5188(7)	1570(6)	37(1)
C(21)	1327(6)	–4002(6)	2889(5)	30(1)
C(22)	2765(6)	–2880(5)	2927(5)	24(1)
C(23)	3412(7)	–2170(6)	5215(5)	30(1)
C(24)	2348(7)	–394(6)	4430(5)	31(1)
N(1)	6537(5)	4808(5)	7218(4)	26(1)
N(2)	8760(5)	3782(5)	5482(4)	26(1)
N(3)	5585(5)	–2616(5)	2438(4)	24(1)
N(4)	3399(5)	–1618(5)	4199(4)	24(1)
O(1)	5860(4)	1326(4)	6020(3)	24(1)
O(2)	6470(4)	799(4)	3702(3)	28(1)
Si(1)	5931(2)	2017(2)	7518(1)	32(1)
Si(2)	6500(2)	125(2)	2219(1)	30(1)
Zn(1)	6245(1)	2819(1)	5256(1)	23(1)
Zn(2)	5925(1)	–674(1)	4432(1)	22(1)

Tab. A.47 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*,*R*,*R*,*R*)-**182**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	32(1)	36(1)	38(1)	21(1)	2(1)	12(1)
Br(2)	32(1)	36(1)	40(1)	19(1)	3(1)	13(1)
C(1)	84(5)	44(4)	34(3)	17(3)	–4(3)	10(3)
C(2)	84(5)	42(4)	30(3)	6(3)	25(3)	–16(3)
C(3)	32(3)	34(3)	26(2)	7(2)	13(2)	–2(2)
C(4)	25(2)	29(3)	38(3)	10(2)	7(2)	8(2)
C(5)	23(2)	28(2)	32(2)	15(2)	5(2)	7(2)
C(6)	29(3)	36(3)	34(3)	8(2)	2(2)	4(2)
C(7)	33(3)	53(4)	43(3)	6(3)	–2(2)	–2(3)
C(8)	28(3)	41(3)	58(4)	7(3)	1(3)	–5(3)
C(9)	18(2)	42(3)	58(4)	23(3)	13(2)	7(2)
C(10)	22(2)	26(3)	33(3)	17(2)	7(2)	8(2)
C(11)	41(3)	40(3)	38(3)	23(3)	16(3)	2(2)
C(12)	27(3)	33(3)	48(3)	15(3)	16(2)	15(2)
C(13)	94(5)	53(4)	37(3)	29(3)	12(3)	19(4)
C(14)	48(3)	47(4)	47(3)	4(3)	29(3)	–4(3)
C(15)	31(2)	34(3)	26(2)	14(2)	7(2)	8(2)
C(16)	26(2)	44(3)	35(3)	14(2)	9(2)	18(2)
C(17)	24(2)	28(2)	24(2)	7(2)	4(2)	7(2)
C(18)	28(3)	40(3)	28(3)	11(2)	4(2)	9(2)
C(19)	35(3)	36(3)	37(3)	8(2)	1(2)	2(2)
C(20)	26(3)	45(3)	39(3)	17(3)	3(2)	1(2)
C(21)	21(2)	34(3)	33(3)	12(2)	2(2)	5(2)
C(22)	21(2)	28(3)	28(2)	15(2)	6(2)	10(2)
C(23)	43(3)	26(3)	23(3)	11(2)	7(2)	2(2)
C(24)	30(3)	27(3)	39(3)	15(2)	10(2)	8(2)

N(1)	21(2)	27(2)	32(3)	14(2)	10(2)	4(2)
N(2)	32(2)	26(2)	29(2)	15(2)	13(2)	8(2)
N(3)	21(2)	30(2)	26(2)	15(2)	6(2)	9(2)
N(4)	24(2)	23(2)	25(2)	9(2)	6(2)	5(2)
O(1)	31(2)	23(2)	21(2)	11(1)	4(1)	4(1)
O(2)	32(2)	32(2)	28(2)	17(2)	14(2)	11(2)
Si(1)	41(1)	31(1)	23(1)	12(1)	7(1)	–1(1)
Si(2)	37(1)	34(1)	24(1)	14(1)	13(1)	8(1)
Zn(1)	23(1)	25(1)	26(1)	14(1)	8(1)	7(1)
Zn(2)	22(1)	24(1)	24(1)	13(1)	5(1)	6(1)

(*R*,*R*,*R*,*R*)-183

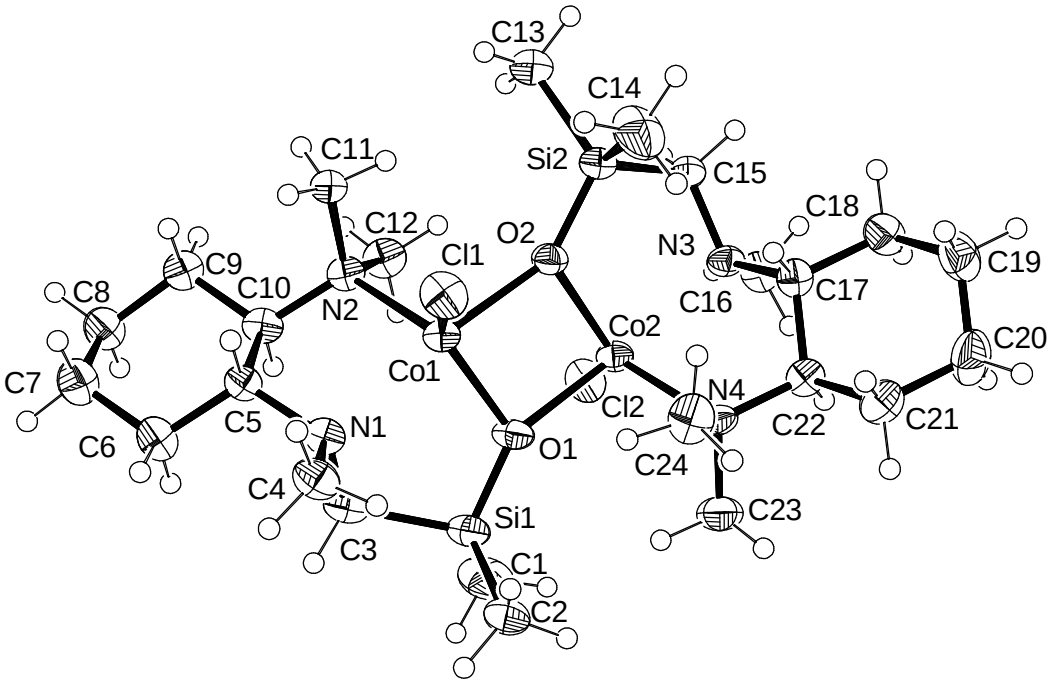

Abb. A.23 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von (*R*,*R*,*R*,*R*)-**183** im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.48 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*,*R*,*R*,*R*)-**183**.

Atom	x	y	z	U(eq)
C(1)	3473(9)	1795(7)	3120(5)	65(2)
C(2)	6711(7)	621(7)	3541(5)	56(1)
C(3)	3335(5)	–1319(5)	3274(4)	35(1)
C(4)	5196(5)	–2846(5)	3927(4)	39(1)
C(5)	2277(5)	–3244(5)	4070(4)	29(1)
C(6)	1640(5)	–4537(5)	2763(4)	38(1)
C(7)	150(6)	–5644(5)	2717(5)	44(1)
C(8)	–1247(6)	–4746(6)	3228(5)	41(1)

C(9)	–584(5)	–3552(5)	4568(4)	34(1)
C(10)	841(5)	–2398(5)	4599(4)	31(1)
C(11)	1525(6)	–1719(6)	6863(4)	37(1)
C(12)	407(6)	142(6)	6111(5)	37(1)
C(13)	2310(8)	1745(7)	9718(5)	61(2)
C(14)	6042(8)	2158(7)	10034(5)	62(2)
C(15)	3844(5)	4633(5)	9636(4)	37(1)
C(16)	3823(5)	6673(5)	8865(4)	37(1)
C(17)	6480(5)	5781(5)	9356(4)	31(1)
C(18)	6958(6)	7315(6)	10528(4)	40(1)
C(19)	8829(6)	7776(6)	10945(4)	52(1)
C(20)	9596(7)	7912(7)	9902(6)	55(2)
C(21)	9226(5)	6353(6)	8765(5)	42(1)
C(22)	7332(5)	5849(5)	8315(4)	30(1)
C(23)	7077(7)	4628(6)	6062(5)	46(1)
C(24)	7922(6)	3124(6)	7232(5)	44(1)
Cl(1)	6005(1)	–1238(1)	6973(1)	41(1)
Cl(2)	2111(1)	4090(1)	6047(1)	41(1)
Co(1)	4003(1)	–171(1)	6113(1)	26(1)
Co(2)	4388(1)	3362(1)	6942(1)	27(1)
N(1)	3672(4)	–2097(4)	4146(4)	29(1)
N(2)	1480(4)	–1117(4)	5871(4)	29(1)
N(3)	4641(4)	5334(4)	8881(4)	29(1)
N(4)	6882(5)	4350(4)	7185(4)	30(1)
O(1)	4554(4)	1339(4)	5388(3)	32(1)
O(2)	4022(4)	1835(3)	7704(3)	30(1)
Si(1)	4564(2)	690(2)	3913(1)	36(1)
Si(2)	4099(2)	2510(2)	9192(1)	38(1)

Tab. A.49 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*,*R*,*R*,*R*)-**183**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	99(5)	67(4)	42(3)	35(3)	14(3)	24(3)
C(2)	62(3)	52(3)	45(3)	3(2)	34(2)	2(2)
C(3)	36(2)	48(2)	25(2)	17(2)	10(2)	13(2)
C(4)	33(2)	45(2)	36(2)	13(2)	11(2)	16(2)
C(5)	25(2)	33(2)	29(2)	11(2)	5(1)	7(1)
C(6)	29(2)	40(2)	37(2)	9(2)	2(2)	9(2)
C(7)	40(2)	41(2)	45(3)	11(2)	5(2)	7(2)
C(8)	31(2)	46(3)	41(3)	12(2)	5(2)	5(2)
C(9)	25(2)	40(2)	39(2)	18(2)	3(2)	7(2)
C(10)	29(2)	37(2)	31(2)	18(2)	5(2)	13(2)
C(11)	47(3)	34(2)	29(2)	11(2)	13(2)	–1(2)
C(12)	30(2)	41(2)	47(3)	21(2)	14(2)	18(2)
C(13)	84(4)	55(3)	37(3)	12(2)	24(3)	–14(3)
C(14)	78(4)	60(3)	43(3)	25(3)	–13(3)	9(3)

C(15)	38(2)	38(2)	31(2)	8(2)	16(2)	–1(2)
C(16)	30(2)	37(2)	42(2)	12(2)	8(2)	12(2)
C(17)	26(2)	32(2)	35(2)	12(2)	5(2)	7(2)
C(18)	34(2)	46(3)	37(3)	13(2)	5(2)	8(2)
C(19)	38(2)	59(3)	43(3)	7(2)	–2(2)	2(2)
C(20)	32(3)	49(3)	70(4)	12(3)	6(3)	–3(2)
C(21)	27(2)	49(3)	52(3)	22(2)	11(2)	7(2)
C(22)	25(2)	30(2)	38(2)	16(2)	9(2)	11(2)
C(23)	61(3)	43(3)	41(3)	19(2)	26(2)	10(2)
C(24)	32(2)	39(3)	63(3)	17(2)	17(2)	18(2)
Cl(1)	41(1)	43(1)	41(1)	21(1)	0(1)	15(1)
Cl(2)	38(1)	41(1)	43(1)	16(1)	2(1)	14(1)
Co(1)	26(1)	30(1)	27(1)	14(1)	7(1)	8(1)
Co(2)	27(1)	31(1)	28(1)	15(1)	10(1)	9(1)
N(1)	25(2)	34(2)	31(2)	15(2)	6(2)	12(1)
N(2)	26(2)	32(2)	32(2)	15(2)	8(2)	9(2)
N(3)	23(2)	37(2)	30(2)	15(2)	11(1)	7(1)
N(4)	35(2)	29(2)	34(2)	16(2)	19(2)	11(2)
O(1)	43(2)	34(2)	27(2)	16(1)	16(1)	15(1)
O(2)	38(2)	30(2)	24(2)	13(1)	7(1)	5(1)
Si(1)	45(1)	40(1)	28(1)	16(1)	15(1)	13(1)
Si(2)	50(1)	37(1)	26(1)	13(1)	9(1)	–2(1)

(*R*,*R*,*R*,*R*)-184

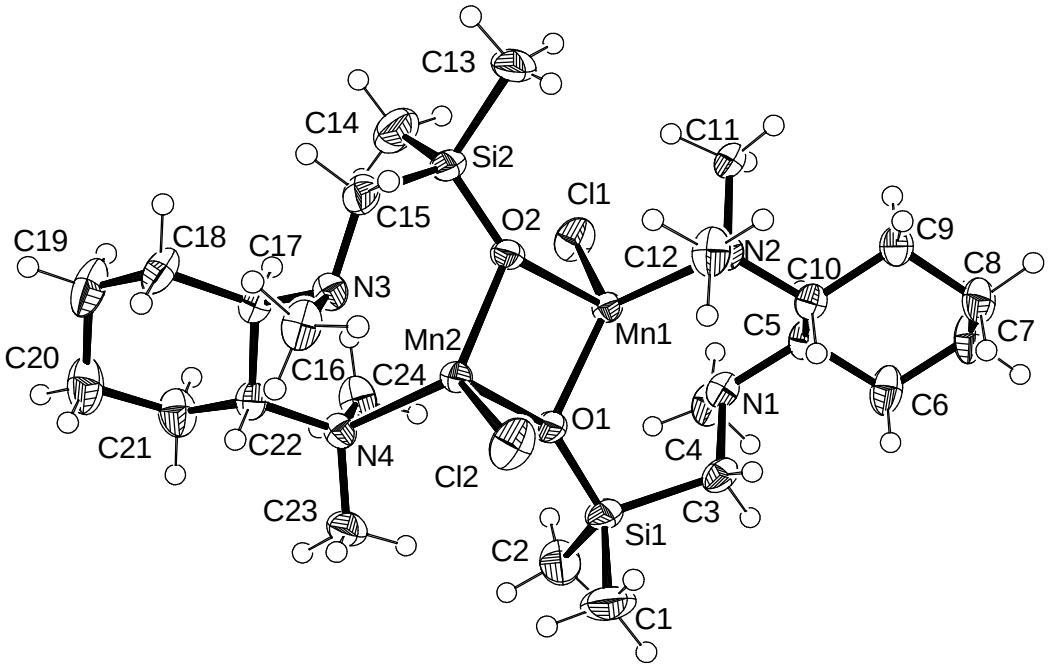

Abb. A.24 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von (*R*,*R*,*R*,*R*)-**184** im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.50 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*,*R*,*R*,*R*)-**184**.

Atom	x	y	z	U(eq)
C(1)	8059(5)	4358(10)	5715(2)	58(1)
C(2)	9674(6)	7451(6)	5889(2)	51(1)
C(3)	11130(4)	4097(5)	5859(2)	29(1)
C(4)	13008(5)	5830(5)	6148(2)	36(1)
C(5)	13351(4)	2935(5)	6276(2)	28(1)
C(6)	13848(5)	2538(6)	5611(2)	41(1)
C(7)	14888(5)	1160(6)	5604(2)	44(1)
C(8)	14284(5)	–335(5)	5914(2)	36(1)
C(9)	13831(4)	44(5)	6580(2)	30(1)
C(10)	12771(4)	1409(5)	6583(2)	25(1)
C(11)	13322(4)	1691(6)	7721(2)	31(1)
C(12)	11128(5)	630(5)	7383(2)	35(1)
C(13)	11130(6)	2029(9)	9191(2)	63(2)
C(14)	11005(6)	5688(8)	9235(2)	55(2)
C(15)	8357(5)	3549(6)	9078(2)	36(1)
C(16)	6059(4)	3482(5)	8630(2)	34(1)
C(17)	7150(4)	6126(5)	8850(2)	26(1)
C(18)	6229(5)	6298(6)	9428(2)	38(1)
C(19)	5995(7)	8083(7)	9596(3)	56(2)
C(20)	5350(6)	8973(6)	9040(3)	52(1)
C(21)	6335(5)	8876(6)	8487(2)	42(1)
C(22)	6597(4)	7112(5)	8293(2)	27(1)
C(23)	6696(5)	7295(7)	7143(2)	42(1)
C(24)	8707(5)	7999(6)	7771(2)	38(1)
Cl(1)	13038(1)	6249(2)	7755(1)	41(1)
Cl(2)	7072(1)	2249(2)	7176(1)	42(1)
Mn(1)	11456(1)	4363(1)	7320(1)	22(1)
Mn(2)	8313(1)	4410(1)	7639(1)	22(1)
N(1)	12333(3)	4286(5)	6293(1)	26(1)
N(2)	12230(3)	1779(4)	7224(2)	23(1)
N(3)	7359(3)	4389(5)	8655(2)	27(1)
N(4)	7479(3)	6946(4)	7735(2)	26(1)
O(1)	9600(3)	5049(4)	6886(1)	27(1)
O(2)	10187(3)	3947(4)	8101(1)	27(1)
Si(1)	9577(1)	5265(2)	6126(1)	32(1)
Si(2)	10217(1)	3865(2)	8863(1)	35(1)

Tab. A.51 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*,*R*,*R*,*R*)-**184**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	48(3)	89(4)	36(2)	1(3)	–18(2)	–1(4)
C(2)	69(4)	45(3)	41(3)	19(2)	17(3)	17(3)

C(3)	41(2)	26(2)	21(2)	1(2)	2(2)	–4(2)
C(4)	48(3)	24(2)	37(2)	–1(2)	12(2)	–5(2)
C(5)	26(2)	25(2)	31(2)	–6(2)	6(2)	–6(2)
C(6)	50(3)	32(2)	40(3)	–4(2)	23(2)	–4(2)
C(7)	46(3)	39(3)	47(3)	–10(2)	24(2)	3(2)
C(8)	48(2)	20(2)	42(2)	–8(2)	6(2)	1(2)
C(9)	31(2)	24(2)	34(2)	–5(2)	4(2)	–2(2)
C(10)	26(2)	22(2)	28(2)	–3(2)	2(2)	–4(2)
C(11)	35(2)	39(3)	19(2)	–3(2)	3(2)	5(2)
C(12)	34(2)	29(2)	43(3)	2(2)	19(2)	–11(2)
C(13)	58(3)	96(5)	33(3)	28(3)	10(2)	43(3)
C(14)	45(3)	84(4)	35(3)	–16(3)	–4(2)	–3(3)
C(15)	46(3)	34(2)	29(2)	10(2)	12(2)	8(2)
C(16)	39(2)	24(2)	40(2)	–2(2)	12(2)	–12(2)
C(17)	26(2)	25(2)	26(2)	–5(2)	4(2)	–7(2)
C(18)	58(3)	33(2)	25(2)	–3(2)	15(2)	–3(2)
C(19)	77(4)	48(3)	43(3)	–16(2)	26(3)	1(3)
C(20)	64(3)	29(3)	62(3)	–5(2)	24(3)	10(2)
C(21)	48(3)	28(2)	51(3)	3(2)	13(2)	3(2)
C(22)	26(2)	25(2)	30(2)	–2(2)	6(2)	–2(2)
C(23)	37(2)	54(3)	33(2)	12(2)	1(2)	13(2)
C(24)	31(2)	31(2)	53(3)	4(2)	15(2)	–7(2)
Cl(1)	38(1)	45(1)	41(1)	–11(1)	1(1)	–15(1)
Cl(2)	48(1)	37(1)	42(1)	–11(1)	5(1)	–16(1)
Mn(1)	20(1)	25(1)	21(1)	0(1)	2(1)	–2(1)
Mn(2)	20(1)	23(1)	22(1)	2(1)	1(1)	–1(1)
N(1)	32(2)	21(2)	24(2)	1(2)	5(1)	–6(2)
N(2)	19(2)	26(2)	25(2)	3(1)	6(1)	–6(1)
N(3)	24(1)	25(2)	31(2)	2(2)	5(1)	–1(2)
N(4)	22(2)	26(2)	30(2)	3(1)	4(1)	–1(1)
O(1)	24(1)	36(2)	21(1)	5(1)	4(1)	1(1)
O(2)	22(1)	35(2)	24(1)	4(1)	–1(1)	3(1)
Si(1)	35(1)	39(1)	20(1)	7(1)	1(1)	3(1)
Si(2)	32(1)	54(1)	20(1)	5(1)	1(1)	10(1)

(*R*,*R*,*R*,*R*)-185

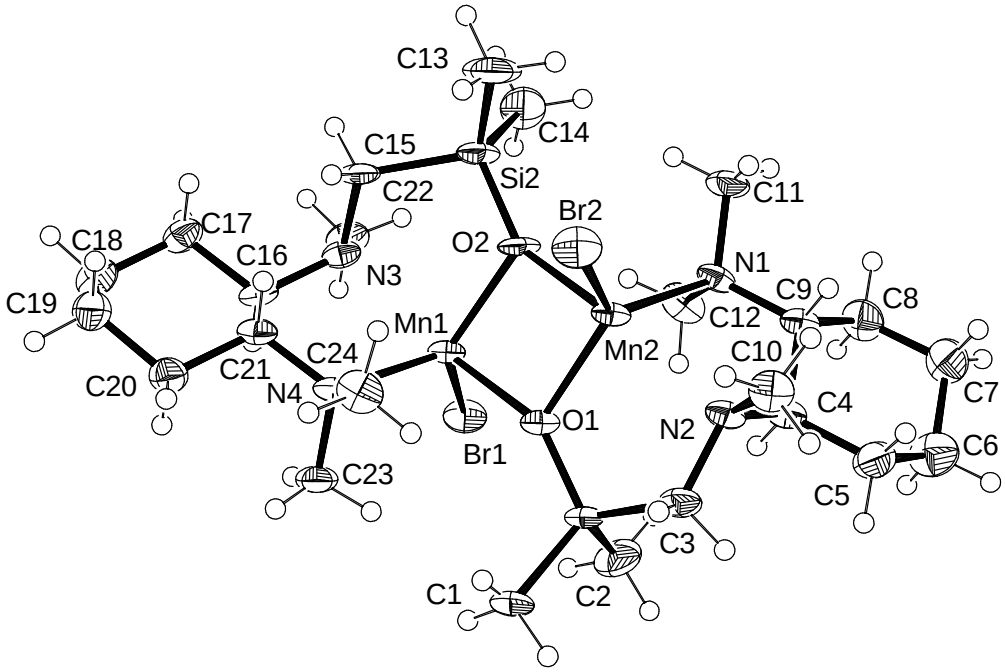

Abb. A.25 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von (*R*,*R*,*R*,*R*)-**185** im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.52 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*,*R*,*R*,*R*)-**185**.

Atom	x	y	z	U(eq)
Br(1)	11437(1)	598(1)	1375(1)	37(1)
Br(2)	7044(1)	5769(1)	78(1)	40(1)
C(1)	7342(15)	3634(12)	3941(9)	58(3)
C(2)	11024(15)	4026(13)	4298(9)	56(3)
C(3)	9033(10)	6438(9)	3859(7)	35(2)
C(4)	11673(9)	7534(9)	3599(7)	31(2)
C(5)	12146(11)	9034(11)	4766(8)	43(2)
C(6)	14000(11)	9498(13)	5219(9)	53(2)
C(7)	14820(11)	9597(11)	4165(9)	47(2)
C(8)	14426(10)	8089(11)	3050(9)	43(2)
C(9)	12564(9)	7569(8)	2570(7)	27(2)
C(10)	9088(10)	8396(9)	3082(8)	36(2)
C(11)	12417(11)	6358(11)	318(8)	40(2)
C(12)	13087(11)	4890(10)	1515(9)	40(2)
C(13)	8761(18)	3397(14)	–2732(10)	64(3)
C(14)	11901(14)	2292(13)	–2228(10)	57(3)
C(15)	8491(10)	412(9)	–2500(7)	33(2)
C(16)	7361(9)	–1468(9)	–1727(7)	29(1)
C(17)	6732(10)	–2718(10)	–3038(8)	36(2)
C(18)	5238(11)	–3809(10)	–3099(8)	44(2)

C(19)	3889(10)	–2973(11)	–2612(9)	43(2)
C(20)	4505(9)	–1767(10)	–1271(8)	35(2)
C(21)	5963(8)	–632(8)	–1198(7)	27(1)
C(22)	10235(10)	–1096(11)	–1880(8)	38(2)
C(23)	6529(11)	43(10)	1062(7)	36(2)
C(24)	5527(11)	1836(11)	297(9)	41(2)
Mn(1)	9220(1)	1594(1)	394(1)	24(1)
Mn(2)	9492(1)	5099(1)	1103(1)	25(1)
N(1)	12143(8)	6088(7)	1423(6)	28(1)
N(2)	9862(8)	7107(7)	3115(6)	29(1)
N(3)	8783(8)	–361(7)	–1648(6)	27(1)
N(4)	6561(7)	597(7)	70(6)	26(1)
O(1)	9089(6)	3603(6)	1951(5)	27(1)
O(2)	9771(7)	3100(6)	–408(5)	30(1)
Si(1)	9161(3)	4345(3)	3441(2)	34(1)
Si(2)	9766(3)	2377(3)	–1889(2)	35(1)

Tab. A.53 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*,*R*,*R*,*R*)-**185**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	39(1)	47(1)	38(1)	28(1)	7(1)	18(1)
Br(2)	38(1)	49(1)	43(1)	26(1)	8(1)	19(1)
C(1)	83(7)	59(6)	29(4)	14(4)	31(5)	–14(5)
C(2)	78(7)	61(6)	29(4)	23(4)	–4(4)	7(5)
C(3)	39(4)	43(4)	28(4)	16(3)	19(3)	8(3)
C(4)	32(4)	39(4)	29(4)	19(3)	12(3)	8(3)
C(5)	45(5)	49(5)	31(5)	13(4)	8(4)	4(4)
C(6)	38(5)	71(6)	47(5)	24(5)	2(4)	8(4)
C(7)	32(4)	54(5)	52(6)	19(5)	9(4)	0(4)
C(8)	31(4)	49(5)	50(5)	19(4)	17(4)	6(4)
C(9)	29(3)	36(4)	27(4)	19(3)	13(3)	13(3)
C(10)	30(4)	43(4)	42(4)	19(4)	13(3)	16(3)
C(11)	49(5)	48(4)	31(4)	22(4)	22(4)	7(4)
C(12)	38(4)	39(4)	59(6)	28(4)	26(4)	21(4)
C(13)	102(9)	74(7)	35(5)	38(5)	23(5)	17(6)
C(14)	60(6)	61(6)	45(6)	10(5)	33(5)	4(5)
C(15)	37(4)	50(4)	19(3)	21(3)	10(3)	7(3)
C(16)	35(4)	40(4)	17(3)	15(3)	5(3)	10(3)
C(17)	39(4)	41(4)	24(4)	6(3)	9(3)	9(3)
C(18)	49(5)	45(5)	30(4)	9(4)	6(4)	7(4)
C(19)	33(4)	56(5)	37(5)	20(4)	1(4)	–4(4)
C(20)	28(4)	46(4)	33(4)	18(4)	5(3)	3(3)
C(21)	27(3)	39(4)	24(3)	20(3)	8(3)	12(3)
C(22)	32(4)	54(5)	31(4)	14(4)	16(3)	15(4)
C(23)	48(5)	43(4)	24(4)	20(3)	11(3)	7(4)
C(24)	33(4)	46(5)	49(5)	24(4)	13(4)	15(4)

Mn(1)	27(1)	34(1)	20(1)	17(1)	10(1)	11(1)
Mn(2)	29(1)	33(1)	22(1)	18(1)	13(1)	12(1)
N(1)	30(3)	32(3)	35(4)	21(3)	19(3)	12(3)
N(2)	29(3)	37(3)	30(3)	20(3)	15(3)	9(3)
N(3)	27(3)	37(3)	21(3)	13(3)	8(2)	14(3)
N(4)	28(3)	37(3)	24(3)	19(3)	14(3)	14(3)
O(1)	33(3)	35(3)	21(3)	17(2)	10(2)	11(2)
O(2)	47(3)	37(3)	16(2)	17(2)	17(2)	17(2)
Si(1)	49(1)	39(1)	19(1)	16(1)	13(1)	3(1)
Si(2)	46(1)	45(1)	22(1)	19(1)	18(1)	12(1)

(*R*,*R*,*R*,*R*)-180·$(HgCl_2)_2$

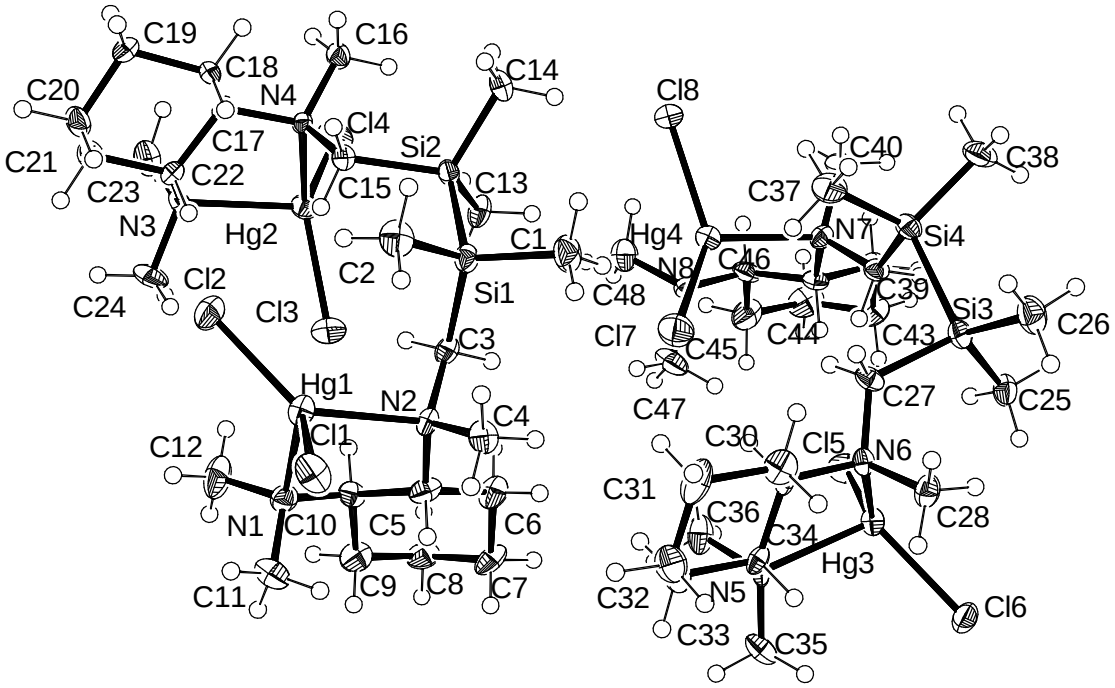

Abb. A.26 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von (*R*,*R*,*R*,*R*)-**180**·$(HgCl_2)_2$ im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.54 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*,*R*,*R*,*R*)-**180**·$(HgCl_2)_2$.

Atom	x	y	z	U(eq)
C(1)	994(6)	2237(5)	5934(4)	36(2)
C(2)	–250(5)	3848(5)	7843(4)	34(2)
C(3)	–31(5)	4941(5)	5557(4)	22(1)
C(4)	–1891(5)	4574(5)	5859(5)	26(2)
C(5)	–1878(6)	6387(5)	4946(5)	28(2)
C(6)	–995(6)	5918(5)	3801(4)	29(1)
C(7)	–1457(6)	6812(5)	2977(4)	32(2)
C(8)	–1401(6)	7934(5)	3107(4)	31(2)

C(9)	–2286(6)	8427(5)	4215(4)	32(2)
C(10)	–1975(6)	7594(5)	5121(5)	22(1)
C(11)	–4274(5)	8540(5)	6312(5)	37(2)
C(12)	–2668(7)	9001(5)	6480(5)	44(2)
C(13)	3378(5)	4201(5)	4620(4)	29(1)
C(14)	3914(5)	2265(5)	6229(4)	35(2)
C(15)	2156(5)	4816(5)	7103(4)	22(1)
C(16)	4289(5)	4509(5)	6937(4)	24(2)
C(17)	2428(5)	6106(5)	8081(4)	19(1)
C(18)	1950(5)	5448(5)	9105(4)	21(1)
C(19)	1523(5)	6137(5)	10112(4)	27(1)
C(20)	400(5)	7313(5)	10095(4)	28(2)
C(21)	857(5)	7992(5)	9113(4)	26(1)
C(22)	1392(5)	7329(5)	8067(4)	19(1)
C(23)	2760(5)	8405(5)	7175(5)	32(2)
C(24)	740(5)	9050(5)	6927(4)	32(2)
C(25)	3466(5)	–1202(5)	–125(4)	31(1)
C(26)	2919(5)	–2733(5)	1801(4)	38(2)
C(27)	1824(5)	–48(5)	2143(4)	22(1)
C(28)	67(5)	–142(5)	1855(4)	27(1)
C(29)	–310(6)	1593(5)	2743(4)	24(2)
C(30)	–1034(5)	1104(5)	3797(4)	31(2)
C(31)	–1909(6)	2060(6)	4656(4)	39(2)
C(32)	–2893(5)	3079(5)	4285(4)	38(2)
C(33)	–2229(5)	3585(5)	3267(4)	33(2)
C(34)	–1294(5)	2655(5)	2356(4)	20(1)
C(35)	–1507(5)	3874(5)	778(5)	38(2)
C(36)	–62(6)	3865(5)	1524(4)	33(2)
C(37)	4396(6)	–953(5)	3068(4)	36(2)
C(38)	6340(5)	–2865(5)	1375(4)	35(2)
C(39)	5204(5)	–244(5)	656(4)	21(1)
C(40)	7146(5)	–415(5)	831(4)	26(1)
C(41)	6066(5)	1191(5)	–251(4)	20(1)
C(42)	7167(5)	490(5)	–1225(4)	25(1)
C(43)	7252(6)	1217(6)	–2250(5)	35(2)
C(44)	7447(6)	2264(5)	–2070(4)	39(2)
C(45)	6389(6)	2964(5)	–1087(5)	39(2)
C(46)	6228(5)	2240(5)	–70(4)	27(1)
C(47)	3929(5)	3759(6)	692(5)	40(2)
C(48)	5532(6)	3650(5)	1295(5)	41(2)
Cl(1)	–4393(1)	6024(1)	8246(1)	36(1)
Cl(2)	–1616(1)	7019(1)	8397(1)	38(1)
Cl(3)	1296(1)	7392(1)	4875(1)	41(1)
Cl(4)	5207(1)	6340(1)	4748(1)	35(1)
Cl(5)	2828(1)	2056(1)	–667(1)	36(1)
Cl(6)	–34(1)	1034(1)	–617(1)	36(1)

Cl(7)	2344(1)	2402(1)	2939(1)	43(1)
Cl(8)	6131(1)	1148(1)	3169(1)	39(1)
Hg(1)	–2563(1)	6517(1)	7428(1)	26(1)
Hg(2)	2958(1)	6725(1)	5625(1)	25(1)
Hg(3)	1042(1)	1562(1)	230(1)	23(1)
Hg(4)	4656(1)	1640(1)	2253(1)	27(1)
N(1)	–2899(4)	8084(4)	6195(4)	26(1)
N(2)	–1452(4)	5490(4)	5777(3)	18(1)
N(3)	1851(4)	8015(4)	7120(4)	20(1)
N(4)	2964(4)	5390(4)	7092(3)	16(1)
N(5)	–647(4)	3166(4)	1354(3)	22(1)
N(6)	610(4)	635(4)	1912(3)	18(1)
N(7)	5893(4)	407(4)	731(4)	21(1)
N(8)	5145(4)	2967(4)	876(4)	26(1)
Si(1)	728(2)	3664(1)	6378(1)	24(1)
Si(2)	2703(1)	3727(1)	6024(1)	24(1)
Si(3)	3192(1)	–1388(1)	1325(1)	24(1)
Si(4)	4910(1)	–1401(1)	1663(1)	23(1)

Tab. A.55 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*,*R*,*R*,*R*)-**180**·$(HgCl_2)_2$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	47(4)	23(4)	43(4)	–2(3)	–17(3)	–16(3)
C(2)	46(4)	27(4)	31(4)	10(3)	–12(3)	–22(3)
C(3)	28(3)	27(4)	15(3)	0(3)	–8(2)	–14(3)
C(4)	34(4)	18(3)	30(4)	7(3)	–10(3)	–18(3)
C(5)	36(4)	32(4)	30(4)	11(3)	–21(3)	–21(3)
C(6)	46(4)	31(4)	16(3)	7(3)	–12(3)	–23(3)
C(7)	47(4)	44(4)	19(3)	8(3)	–20(3)	–28(3)
C(8)	41(4)	32(4)	28(4)	15(3)	–22(3)	–19(3)
C(9)	42(4)	28(4)	34(4)	12(3)	–20(3)	–21(3)
C(10)	24(3)	13(3)	34(4)	3(3)	–12(3)	–11(3)
C(11)	28(4)	29(4)	42(4)	3(3)	–12(3)	–4(3)
C(12)	74(5)	30(4)	39(4)	–1(3)	–21(4)	–31(4)
C(13)	38(4)	34(4)	15(3)	–6(3)	–5(3)	–17(3)
C(14)	33(4)	24(4)	37(4)	–13(3)	–12(3)	0(3)
C(15)	21(3)	21(3)	21(3)	–1(2)	–6(2)	–8(3)
C(16)	19(3)	24(4)	25(4)	–6(3)	–5(2)	–7(3)
C(17)	14(3)	28(4)	16(3)	–8(3)	–4(2)	–9(3)
C(18)	21(3)	14(3)	27(3)	–5(2)	–13(2)	–2(3)
C(19)	31(3)	31(4)	19(3)	–2(3)	–14(3)	–9(3)
C(20)	23(3)	27(4)	22(3)	–9(3)	–1(2)	–2(3)
C(21)	25(3)	22(3)	29(4)	0(3)	–7(3)	–11(3)
C(22)	22(3)	23(4)	17(3)	0(3)	–9(2)	–11(3)
C(23)	31(4)	27(4)	35(4)	–3(3)	–2(3)	–18(3)
C(24)	27(3)	24(4)	33(4)	12(3)	–13(3)	–2(3)

C(25)	32(4)	28(4)	32(4)	–11(3)	–9(3)	–9(3)
C(26)	36(4)	27(4)	49(4)	–4(3)	–11(3)	–15(3)
C(27)	19(3)	16(3)	30(3)	7(3)	–9(3)	–8(3)
C(28)	30(4)	28(4)	30(4)	–5(3)	–8(3)	–18(3)
C(29)	24(4)	28(4)	17(3)	–12(3)	–2(3)	–10(3)
C(30)	28(4)	40(4)	27(4)	0(3)	–3(3)	–21(3)
C(31)	56(5)	53(5)	18(4)	–4(3)	–4(3)	–38(4)
C(32)	29(4)	43(4)	26(4)	–11(3)	1(3)	–9(3)
C(33)	25(3)	34(4)	24(3)	–10(3)	0(3)	–6(3)
C(34)	29(3)	23(4)	20(3)	1(3)	–10(3)	–19(3)
C(35)	34(4)	18(4)	49(4)	1(3)	–17(3)	0(3)
C(36)	47(4)	29(4)	25(4)	–1(3)	–4(3)	–25(3)
C(37)	49(4)	29(4)	33(4)	14(3)	–22(3)	–18(3)
C(38)	34(4)	24(4)	49(4)	9(3)	–24(3)	–9(3)
C(39)	23(3)	18(3)	24(3)	5(3)	–12(2)	–10(3)
C(40)	26(3)	26(4)	23(3)	9(3)	–13(3)	–9(3)
C(41)	18(3)	21(4)	19(3)	5(3)	–8(2)	–7(3)
C(42)	27(3)	24(4)	28(4)	4(3)	–12(3)	–14(3)
C(43)	46(4)	47(5)	18(4)	11(3)	–14(3)	–26(4)
C(44)	53(4)	47(4)	32(4)	24(3)	–20(3)	–38(4)
C(45)	59(5)	36(4)	43(4)	12(3)	–28(3)	–33(4)
C(46)	24(3)	17(3)	42(4)	8(3)	–19(3)	–7(3)
C(47)	33(4)	25(4)	47(5)	4(3)	–18(3)	0(3)
C(48)	49(4)	27(4)	54(5)	–3(3)	–24(3)	–17(3)
Cl(1)	28(1)	29(1)	47(1)	–2(1)	–4(1)	–16(1)
Cl(2)	41(1)	42(1)	41(1)	–9(1)	–18(1)	–18(1)
Cl(3)	34(1)	44(1)	50(1)	–1(1)	–25(1)	–11(1)
Cl(4)	22(1)	36(1)	40(1)	6(1)	–6(1)	–12(1)
Cl(5)	31(1)	40(1)	40(1)	12(1)	–13(1)	–21(1)
Cl(6)	52(1)	27(1)	44(1)	1(1)	–31(1)	–18(1)
Cl(7)	27(1)	46(1)	51(1)	–7(1)	–11(1)	–12(1)
Cl(8)	42(1)	32(1)	47(1)	–5(1)	–31(1)	–5(1)
Hg(1)	31(1)	26(1)	23(1)	–1(1)	–9(1)	–15(1)
Hg(2)	22(1)	25(1)	24(1)	2(1)	–8(1)	–9(1)
Hg(3)	25(1)	21(1)	22(1)	–1(1)	–6(1)	–11(1)
Hg(4)	25(1)	24(1)	31(1)	–2(1)	–13(1)	–6(1)
N(1)	27(3)	26(3)	28(3)	0(2)	–11(2)	–14(2)
N(2)	28(3)	19(3)	12(3)	2(2)	–7(2)	–15(2)
N(3)	18(3)	13(3)	25(3)	–2(2)	–4(2)	–5(2)
N(4)	14(3)	19(3)	14(3)	–4(2)	–5(2)	–4(2)
N(5)	30(3)	13(3)	18(3)	–5(2)	–6(2)	–6(2)
N(6)	19(3)	16(3)	18(3)	–1(2)	–2(2)	–11(2)
N(7)	24(3)	23(3)	23(3)	0(2)	–11(2)	–13(2)
N(8)	30(3)	18(3)	40(3)	2(2)	–24(2)	–9(2)
Si(1)	34(1)	17(1)	22(1)	1(1)	–12(1)	–12(1)
Si(2)	29(1)	16(1)	22(1)	–4(1)	–10(1)	–4(1)

Si(3)	26(1)	17(1)	27(1)	0(1)	–8(1)	–10(1)
Si(4)	26(1)	18(1)	24(1)	4(1)	–9(1)	–8(1)

188·H_2ZnBr_4

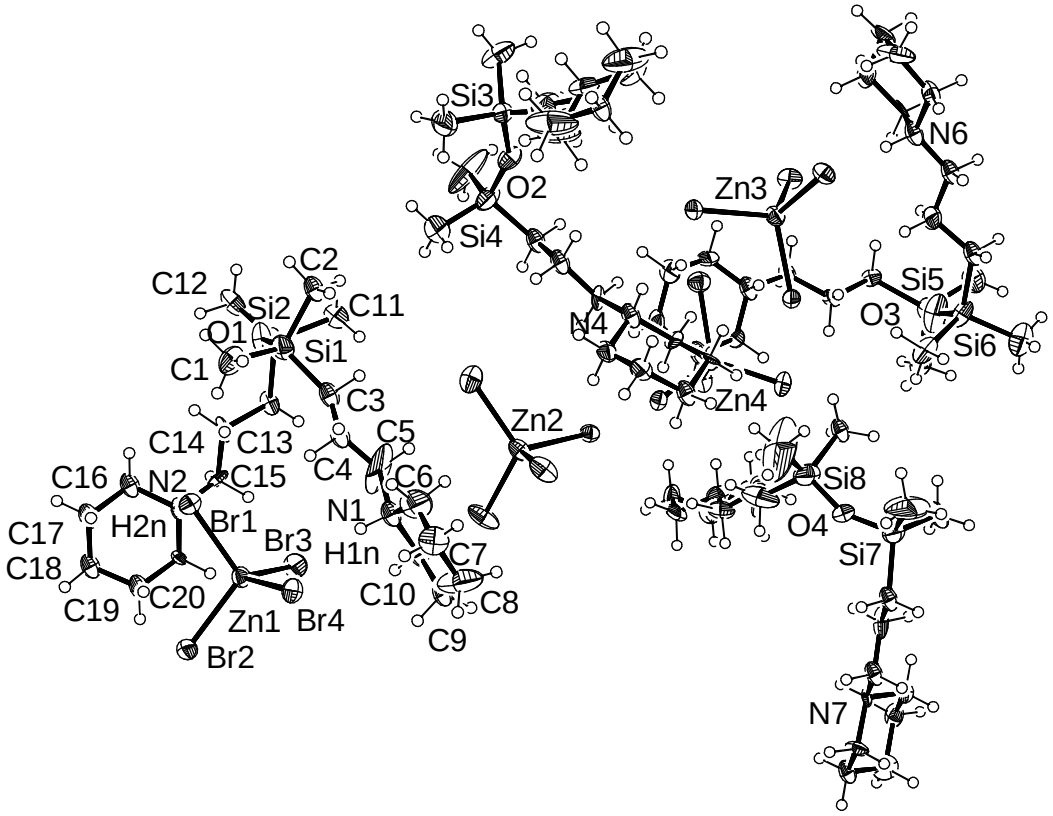

Abb. A.27 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von **188**·H_2ZnBr_4 im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome – mit Ausnahme der Wasserstoffatome an den Stickstoffen – sowie dem Großteil der Kohlenstoffatome wurde der Übersicht halber weggelassen.

Tab. A.56 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von **188**·H_2ZnBr_4.

Atom	x	y	z	U(eq)
Br(1)	2455(1)	526(1)	3289(1)	29(1)
Br(6)	3621(1)	3932(1)	6603(1)	31(1)
Br(7)	5570(1)	3007(1)	7088(1)	37(1)
Br(5)	5022(1)	3046(1)	5882(1)	41(1)
Br(8)	3082(1)	1002(1)	6489(1)	35(1)
Zn(2)	4323(1)	2752(1)	6516(1)	30(1)
Br(4)	1191(1)	–749(1)	4267(1)	46(1)
Br(2)	1615(1)	1935(1)	4101(1)	45(1)
Zn(1)	2333(1)	785(1)	4012(1)	34(1)
Br(3)	4083(1)	1358(2)	4307(1)	53(1)
Si(4)	559(3)	6688(4)	6723(2)	51(2)
Si(3)	2936(3)	7401(4)	6747(1)	35(2)

Si(2)	2911(3)	5641(4)	5066(1)	37(2)
Br(10)	918(1)	1745(1)	8398(1)	30(1)
Br(12)	2113(1)	194(1)	7868(1)	36(1)
Br(9)	3977(1)	2356(1)	8615(1)	35(1)
Zn(3)	2175(1)	1116(1)	8492(1)	32(1)
Br(11)	1777(1)	181(1)	9069(1)	40(1)
Br(16)	5343(1)	7698(1)	8199(1)	32(1)
Br(13)	6189(1)	9359(1)	9184(1)	39(1)
Br(14)	3972(1)	6593(1)	9183(1)	42(1)
Br(15)	6736(1)	6917(1)	9100(1)	43(1)
Zn(4)	5575(1)	7624(1)	8933(1)	33(1)
Si(8)	–396(4)	2169(4)	9971(1)	31(1)
Si(5)	8080(3)	4720(4)	8353(2)	49(2)
Si(1)	1262(4)	3911(4)	5460(1)	43(2)
Si(6)	7714(4)	2529(4)	8177(2)	63(2)
O(2)	1808(7)	7271(8)	6824(3)	39(3)
O(3)	7667(7)	3555(8)	8205(3)	50(4)
O(1)	2068(7)	5010(9)	5366(3)	37(3)
Si(7)	1341(4)	4035(4)	9616(1)	40(2)
O(4)	425(9)	3024(10)	9717(3)	67(4)
N(4)	555(8)	10243(10)	7031(3)	17(4)
C(34)	546(9)	8572(11)	6850(4)	17(4)
C(35)	41(10)	9154(12)	7050(4)	28(5)
C(16)	5750(10)	6724(11)	6488(4)	23(5)
C(36)	456(11)	10597(15)	6597(5)	48(7)
C(17)	6002(10)	6735(11)	6942(4)	24(5)
N(2)	5688(9)	5775(11)	6273(4)	29(5)
N(6)	4158(12)	–809(15)	8335(5)	55(6)
C(39)	733(12)	11910(15)	7299(4)	47(7)
C(38)	617(11)	12223(12)	6890(4)	30(5)
C(40)	189(10)	10780(12)	7318(4)	32(5)
C(55)	4710(12)	–54(14)	8071(5)	42(6)
C(60)	3875(11)	–422(13)	8699(5)	34(5)
C(19)	6901(10)	5720(12)	6811(4)	34(5)
C(18)	6986(10)	6639(12)	7034(4)	34(5)
C(37)	989(11)	11694(13)	6587(4)	42(6)
C(13)	4156(9)	5599(12)	5224(4)	30(5)
N(5)	4378(9)	4615(10)	7983(4)	27(5)
C(45)	5472(10)	5054(12)	7903(4)	29(5)
C(71)	1076(10)	4123(12)	9080(4)	37(5)
C(14)	4442(9)	5771(12)	5699(4)	33(6)
C(43)	7263(10)	5214(12)	8053(5)	42(5)
C(44)	6118(11)	4714(13)	8158(4)	44(6)
C(46)	3787(11)	4972(13)	7684(4)	33(5)
N(7)	–946(9)	–457(10)	8730(4)	26(4)
C(80)	3904(13)	1841(16)	9862(5)	58(7)

C(70)	–894(10)	–1398(12)	8599(4)	37(5)
C(15)	5491(10)	5790(11)	5831(4)	26(5)
N(8)	4314(12)	2718(13)	9615(4)	45(6)
C(67)	–1830(10)	–447(11)	8058(4)	28(4)
C(63)	–516(10)	920(11)	9777(4)	27(5)
C(50)	4215(11)	4839(12)	8396(4)	36(5)
C(79)	4229(12)	1050(13)	9738(4)	52(6)
C(64)	–717(11)	748(12)	9315(4)	36(5)
C(20)	6665(10)	5690(11)	6370(4)	26(5)
C(66)	–1864(11)	–399(13)	8512(4)	50(7)
C(59)	3285(13)	–1246(17)	8947(5)	64(7)
C(65)	–897(10)	–305(11)	9178(4)	26(5)
C(77)	5866(14)	2431(19)	9531(5)	74(9)
C(68)	–1762(11)	–1375(13)	7901(4)	52(7)
C(57)	2629(12)	–2484(14)	8344(5)	46(6)
C(56)	3226(13)	–1653(16)	8088(5)	60(7)
C(76)	5463(11)	3146(13)	9653(4)	41(6)
C(54)	5795(12)	805(16)	8273(5)	61(8)
N(3)	3736(12)	9193(14)	3485(5)	55(6)
C(25)	4574(14)	9748(16)	3211(5)	65(7)
C(30)	2890(13)	8289(14)	3280(5)	48(6)
C(11)	2393(10)	5085(13)	4542(4)	38(5)
C(33)	58(10)	7490(12)	6956(5)	43(5)
C(12)	3108(10)	6948(12)	5095(4)	43(5)
C(73)	2634(11)	4090(12)	9744(4)	50(6)
C(2)	1097(11)	3955(13)	5977(4)	51(6)
C(62)	29(12)	2442(14)	10508(4)	69(7)
C(26)	4182(15)	8953(17)	3877(5)	68(7)
C(74)	2844(11)	3211(13)	9608(4)	41(6)
C(21)	2923(11)	7100(14)	6207(4)	66(7)
C(24)	5376(12)	10749(15)	3387(6)	58(7)
C(47)	2689(10)	4513(12)	7739(5)	50(7)
C(49)	3069(12)	4323(13)	8465(4)	41(6)
C(48)	2493(11)	4730(13)	8149(5)	50(6)
C(61)	–1666(11)	2151(13)	9888(5)	79(8)
C(58)	2329(12)	–2039(14)	8686(5)	66(7)
C(22)	3259(12)	6518(14)	7052(4)	65(6)
C(31)	176(12)	6499(15)	6190(5)	81(8)
N(1)	2318(11)	815(13)	5451(5)	60(6)
C(6)	1330(20)	–60(20)	5442(5)	79(9)
C(75)	3982(11)	3495(13)	9731(4)	38(5)
C(42)	7984(13)	4798(15)	8904(4)	93(9)
C(72)	1374(12)	5120(14)	9908(5)	71(7)
C(29)	2065(14)	7731(17)	3542(7)	87(9)
C(53)	6446(14)	1468(19)	7997(6)	108(10)
C(10)	3206(14)	581(17)	5282(5)	87(8)

C(23)	6149(12)	11301(16)	3087(6)	93(10)
C(28)	2485(15)	7468(18)	3935(7)	87(9)
C(4)	1823(11)	2271(16)	5455(4)	53(7)
C(69)	–838(11)	–1458(13)	8143(4)	48(6)
C(9)	2998(14)	–500(16)	5406(7)	75(8)
C(8)	1971(16)	–1280(20)	5444(6)	95(9)
C(41)	9393(11)	5411(15)	8236(6)	109(9)
C(3)	1630(30)	2940(20)	5322(5)	340(30)
C(27)	3337(17)	8390(20)	4133(6)	96(9)
C(52)	8069(16)	2341(17)	8707(7)	196(15)
C(32)	0(14)	5443(15)	6930(7)	114(9)
C(5)	2120(30)	1570(20)	5301(6)	230(20)
C(51)	8643(13)	2520(20)	7859(9)	250(30)
C(7)	1250(20)	–930(20)	5561(7)	164(18)
C(1)	28(12)	3610(20)	5144(6)	220(20)
C(78)	5400(14)	1503(18)	9770(5)	77(10)

Tab. A.57 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von **188**·H_2ZnBr_4.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	23(1)	31(1)	32(1)	4(1)	2(1)	12(1)
Br(6)	25(1)	24(1)	41(1)	5(1)	7(1)	7(1)
Br(7)	40(1)	33(1)	38(1)	–2(1)	–6(1)	17(1)
Br(5)	44(1)	45(2)	36(1)	9(1)	11(1)	19(1)
Br(8)	33(1)	28(1)	38(1)	1(1)	7(1)	7(1)
Zn(2)	29(1)	27(2)	29(1)	–1(1)	0(1)	9(1)
Br(4)	31(1)	48(2)	40(1)	16(1)	–1(1)	2(1)
Br(2)	40(1)	39(2)	52(1)	–1(1)	16(1)	12(1)
Zn(1)	21(1)	37(2)	31(1)	7(1)	1(1)	3(1)
Br(3)	24(1)	62(2)	47(1)	24(1)	–8(1)	–2(1)
Si(4)	34(3)	36(5)	82(4)	–10(4)	10(3)	17(3)
Si(3)	37(3)	38(4)	33(3)	2(3)	2(3)	21(3)
Si(2)	26(3)	44(5)	25(3)	–6(3)	3(3)	2(3)
Br(10)	27(1)	30(1)	32(1)	–3(1)	1(1)	13(1)
Br(12)	39(1)	45(2)	29(1)	–9(1)	–4(1)	25(1)
Br(9)	26(1)	44(2)	30(1)	5(1)	2(1)	11(1)
Zn(3)	28(1)	39(2)	26(1)	0(1)	2(1)	14(1)
Br(11)	36(1)	46(2)	39(1)	13(1)	9(1)	19(1)
Br(16)	36(1)	30(1)	30(1)	0(1)	5(1)	14(1)
Br(13)	42(1)	29(1)	41(1)	–7(1)	10(1)	10(1)
Br(14)	38(1)	40(2)	34(1)	5(1)	13(1)	4(1)
Br(15)	40(1)	41(2)	49(1)	9(1)	5(1)	18(1)
Zn(4)	34(1)	25(2)	33(1)	–2(1)	6(1)	7(1)
Si(8)	41(3)	28(4)	21(3)	5(3)	11(3)	14(3)
Si(5)	33(3)	28(4)	78(4)	–6(3)	–13(3)	10(3)
Si(1)	59(4)	34(5)	31(3)	8(3)	–1(3)	18(4)

Si(6)	41(3)	31(5)	107(5)	–2(4)	–19(4)	13(4)
O(2)	38(6)	40(10)	46(7)	6(6)	21(6)	20(7)
O(3)	54(7)	50(10)	56(7)	–9(7)	–13(7)	39(8)
O(1)	28(6)	33(11)	25(6)	1(7)	23(6)	–13(7)
Si(7)	53(3)	29(5)	44(3)	9(3)	30(3)	18(4)
O(4)	98(10)	41(13)	48(8)	8(9)	46(9)	11(9)
N(4)	0(6)	12(11)	26(8)	–1(7)	–2(7)	–8(8)
C(34)	0(7)	16(13)	14(8)	18(8)	19(8)	–18(9)
C(35)	23(9)	5(14)	38(11)	–9(10)	3(9)	–10(10)
C(16)	10(8)	0(13)	27(10)	4(9)	5(8)	–27(9)
C(36)	28(10)	80(20)	44(12)	–26(13)	–12(10)	33(13)
C(17)	20(9)	2(13)	38(11)	16(9)	14(9)	–9(9)
N(2)	27(8)	33(13)	20(9)	–5(9)	5(8)	9(9)
N(6)	59(12)	73(17)	55(11)	–4(11)	–2(11)	50(13)
C(39)	52(12)	110(20)	12(10)	–18(11)	–18(10)	67(14)
C(38)	32(10)	0(13)	49(11)	12(9)	24(10)	–5(10)
C(40)	38(10)	49(16)	26(10)	–6(10)	9(9)	35(11)
C(55)	45(13)	52(19)	36(11)	26(12)	8(12)	26(14)
C(60)	46(11)	12(14)	34(11)	–1(10)	20(10)	3(11)
C(19)	22(9)	0(13)	58(12)	–3(10)	8(10)	–14(9)
C(18)	18(9)	19(14)	48(11)	19(10)	20(9)	–11(10)
C(37)	41(11)	50(17)	34(11)	–3(11)	–4(10)	23(12)
C(13)	16(8)	38(15)	20(9)	3(9)	9(8)	–2(10)
N(5)	20(8)	36(12)	24(8)	–22(8)	–9(7)	14(9)
C(45)	21(9)	31(15)	39(10)	34(9)	20(9)	10(11)
C(71)	29(9)	31(15)	53(11)	12(10)	38(10)	8(10)
C(14)	18(9)	56(17)	12(9)	–11(10)	4(8)	6(11)
C(43)	42(11)	0(13)	55(12)	0(10)	7(11)	–15(10)
C(44)	42(11)	46(17)	28(10)	–17(11)	25(10)	4(12)
C(46)	36(10)	58(16)	17(9)	12(9)	2(9)	31(12)
N(7)	46(10)	1(11)	21(8)	5(8)	19(9)	–1(8)
C(80)	55(13)	90(20)	24(11)	–39(13)	–33(12)	38(15)
C(70)	25(9)	52(15)	44(11)	0(10)	1(9)	26(10)
C(15)	31(10)	10(13)	43(11)	10(9)	17(10)	13(10)
N(8)	67(13)	94(18)	0(7)	9(9)	3(9)	60(14)
C(67)	25(9)	0(13)	21(10)	8(8)	–1(9)	–29(9)
C(63)	25(9)	35(14)	27(10)	9(9)	13(9)	16(10)
C(50)	43(11)	39(15)	28(10)	–6(10)	0(10)	21(11)
C(79)	87(14)	60(17)	19(10)	–10(10)	1(11)	43(14)
C(64)	56(11)	60(16)	7(9)	2(9)	–2(9)	41(12)
C(20)	26(9)	22(13)	24(10)	–8(9)	–16(9)	12(10)
C(66)	49(11)	85(19)	35(11)	–28(12)	–7(10)	53(13)
C(59)	63(14)	100(20)	57(14)	4(15)	7(13)	65(16)
C(65)	38(9)	46(15)	0(8)	7(8)	21(8)	19(10)
C(77)	54(14)	150(30)	44(13)	22(15)	5(12)	73(19)
C(68)	53(11)	63(18)	39(11)	–26(12)	5(10)	26(12)

C(57)	60(13)	24(17)	45(12)	–8(11)	0(12)	12(12)
C(56)	52(13)	90(20)	51(13)	–26(14)	–29(12)	53(15)
C(76)	32(10)	53(17)	27(11)	–12(11)	–1(10)	10(11)
C(54)	44(13)	80(20)	59(15)	–16(14)	–3(12)	31(15)
N(3)	46(11)	66(17)	73(12)	2(12)	–1(11)	45(12)
C(25)	46(12)	100(20)	81(15)	1(15)	–7(13)	66(15)
C(30)	38(11)	19(16)	82(15)	10(13)	28(13)	3(12)
C(11)	28(9)	51(16)	30(10)	14(10)	15(9)	10(10)
C(33)	22(10)	0(14)	88(14)	34(11)	26(11)	–17(10)
C(12)	30(9)	62(17)	19(9)	16(9)	8(9)	4(10)
C(73)	72(13)	0(14)	48(11)	5(10)	0(11)	–9(11)
C(2)	54(11)	25(15)	67(13)	–1(11)	8(11)	13(11)
C(62)	97(14)	90(20)	31(11)	–11(12)	–11(11)	53(14)
C(26)	74(15)	100(20)	65(13)	59(14)	25(14)	67(18)
C(74)	57(12)	48(16)	23(10)	–6(10)	–2(10)	29(12)
C(21)	56(11)	100(20)	47(12)	–16(13)	–3(11)	47(13)
C(24)	31(11)	42(17)	97(17)	–7(14)	0(13)	15(12)
C(47)	36(11)	46(16)	49(13)	–46(12)	–31(10)	12(11)
C(49)	68(13)	34(16)	23(10)	4(10)	11(11)	23(13)
C(48)	20(9)	35(17)	82(14)	10(12)	11(11)	–2(11)
C(61)	67(13)	48(18)	117(17)	–36(14)	–37(13)	34(13)
C(58)	63(13)	70(20)	63(14)	–1(14)	15(13)	27(14)
C(22)	86(14)	62(18)	79(13)	26(12)	36(13)	56(14)
C(31)	75(13)	90(20)	75(15)	–29(15)	–25(13)	49(14)
N(1)	31(9)	25(13)	90(14)	–41(11)	–43(10)	–6(10)
C(6)	130(20)	120(30)	28(12)	23(15)	19(15)	100(30)
C(75)	46(11)	23(15)	14(9)	9(9)	34(10)	–18(11)
C(42)	126(16)	150(20)	33(11)	–52(14)	–44(13)	98(18)
C(72)	79(13)	56(18)	72(13)	–10(13)	18(12)	26(12)
C(29)	37(13)	60(20)	170(20)	38(19)	16(17)	24(16)
C(53)	85(18)	130(30)	120(20)	5(19)	–42(17)	70(20)
C(10)	138(19)	60(20)	15(11)	–1(13)	81(14)	–14(16)
C(23)	40(12)	120(30)	102(18)	–42(19)	19(14)	22(14)
C(28)	32(13)	40(20)	170(30)	81(18)	37(17)	–12(14)
C(4)	40(10)	150(20)	9(9)	6(12)	11(9)	76(14)
C(69)	48(11)	84(19)	24(10)	–12(11)	9(10)	42(13)
C(9)	42(13)	0(16)	140(20)	0(15)	–24(15)	–28(12)
C(8)	120(20)	160(30)	76(15)	64(17)	54(17)	120(20)
C(41)	41(12)	120(30)	180(20)	39(18)	2(15)	49(15)
C(3)	1000(100)	300(50)	7(12)	61(17)	100(30)	530(70)
C(27)	91(18)	160(30)	88(18)	80(19)	34(18)	90(20)
C(52)	190(20)	0(20)	270(30)	20(20)	–160(30)	–37(17)
C(32)	160(20)	30(20)	190(20)	39(18)	110(20)	54(16)
C(5)	590(60)	120(30)	77(17)	–15(18)	–40(30)	260(40)
C(51)	58(15)	250(40)	390(50)	–200(40)	40(20)	40(20)
C(7)	200(30)	200(40)	150(20)	–100(30)	–110(20)	170(30)

C(1)	16(12)	410(60)	90(20)	120(30)	18(14)	–40(20)
C(78)	77(17)	140(30)	36(13)	–46(16)	–40(14)	90(20)

(*R*,*R*,*R*,*R*)-189·$(ZnBr_2)_2$

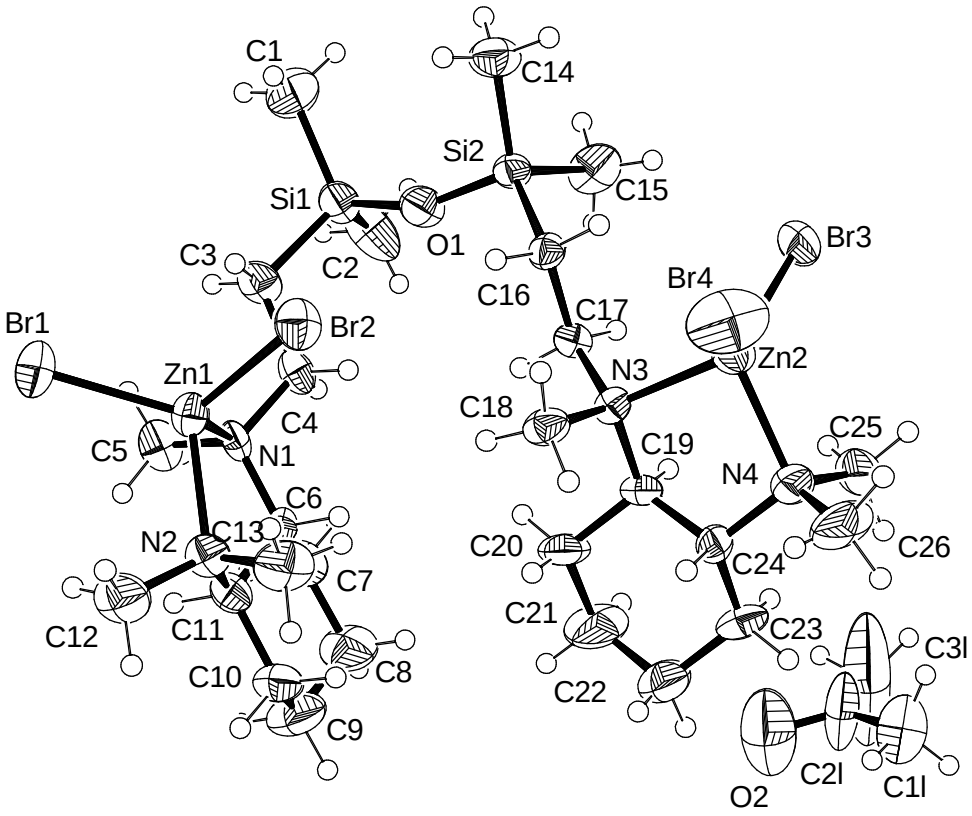

Abb. A.28 Thermische Auslenkungsellipsoide (50 % Aufenthaltwahrscheinlichkeit) der Molekülstruktur von (*R*,*R*,*R*,*R*)-**189**·$(ZnBr_2)_2$ im Kristall (ORTEP-Darstellung der asymmetrischen Einheit) mit Angabe des Nummerierungsschemas. Das Nummerierungsschema der Wasserstoffatome wurde der Übersicht halber weggelassen.

Tab. A.58 Atomkoordinaten ($\cdot 10^4$) und äquivalente isotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*,*R*,*R*,*R*)-**189**·$(ZnBr_2)_2$.

Atom	x	y	z	U(eq)
O(2)	5390(12)	1099(6)	5944(3)	140(4)
Br(1)	3097(1)	1518(1)	10332(1)	57(1)
Br(2)	825(1)	434(1)	9339(1)	48(1)
Br(3)	–496(1)	–2084(1)	7303(1)	63(1)
Br(4)	–3767(1)	–554(1)	7713(1)	90(1)
C(1)	4710(14)	–2036(6)	9761(3)	82(4)
C(2)	6897(11)	–1614(6)	8993(4)	79(3)
C(3)	5051(10)	–372(4)	9470(3)	45(2)
C(4)	5102(10)	194(4)	9090(3)	37(2)
C(5)	6430(9)	1202(5)	9524(3)	50(2)
C(6)	5038(10)	1524(5)	8820(2)	35(2)
C(7)	6645(10)	1547(5)	8574(3)	56(3)
C(8)	6542(13)	2058(6)	8157(3)	73(3)

C(9)	6034(14)	2856(6)	8290(3)	72(3)
C(10)	4411(11)	2837(5)	8520(3)	51(2)
C(11)	4447(10)	2316(5)	8931(3)	40(2)
C(12)	2670(12)	2959(5)	9469(3)	62(3)
C(13)	1455(11)	2230(6)	8874(3)	62(3)
C(14)	984(11)	–2525(5)	9022(3)	53(2)
C(15)	3175(12)	–2500(5)	8205(3)	61(3)
C(16)	862(9)	–1179(4)	8375(2)	32(2)
C(17)	1689(8)	–724(4)	8019(2)	30(2)
C(18)	–147(10)	357(4)	8071(3)	40(2)
C(19)	1538(9)	201(4)	7394(2)	32(2)
C(20)	2630(11)	838(5)	7561(3)	57(3)
C(21)	3586(13)	1190(7)	7180(4)	89(4)
C(22)	2510(13)	1483(6)	6817(3)	71(3)
C(23)	1432(11)	840(5)	6651(3)	47(2)
C(24)	467(9)	481(4)	7019(2)	33(2)
C(25)	29(18)	–619(6)	6516(3)	95(5)
C(26)	–2156(13)	225(7)	6687(4)	90(4)
N(1)	5045(7)	1019(3)	9223(2)	33(2)
N(2)	2870(8)	2289(4)	9176(2)	39(2)
N(3)	626(7)	–200(3)	7765(2)	28(1)
N(4)	–669(9)	–129(4)	6864(2)	48(2)
O(1)	3529(7)	–1465(3)	8930(2)	49(2)
Si(1)	5012(3)	–1385(1)	9278(1)	44(1)
Si(2)	2191(3)	–1918(1)	8642(1)	33(1)
Zn(1)	2910(1)	1272(1)	9556(1)	36(1)
Zn(2)	–1179(1)	–797(1)	7435(1)	41(1)

Tab. A.59 Anisotrope Auslenkungsparameter ($Å^2 \cdot 10^3$) von (*R*,*R*,*R*,*R*)-**189**·$(ZnBr_2)_2$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(2)	128(9)	163(10)	130(8)	–51(8)	–41(7)	21(8)
Br(1)	64(1)	71(1)	35(1)	–11(1)	1(1)	2(1)
Br(2)	34(1)	58(1)	52(1)	–4(1)	–3(1)	–3(1)
Br(3)	97(1)	35(1)	58(1)	–3(1)	–22(1)	–9(1)
Br(4)	31(1)	118(1)	121(1)	40(1)	5(1)	1(1)
C(1)	115(10)	66(7)	65(7)	18(6)	–25(7)	5(7)
C(2)	43(6)	60(7)	134(10)	–38(7)	5(7)	7(6)
C(3)	45(5)	32(5)	58(6)	–2(4)	–9(4)	11(4)
C(4)	29(5)	36(5)	46(5)	–14(4)	3(4)	2(4)
C(5)	36(5)	52(6)	62(6)	–11(5)	–10(4)	10(4)
C(6)	42(5)	36(5)	27(4)	–3(4)	–4(4)	1(4)
C(7)	45(6)	52(6)	70(6)	–6(5)	28(5)	1(5)
C(8)	81(8)	70(8)	67(7)	12(6)	35(6)	–11(6)
C(9)	85(8)	69(8)	62(7)	23(6)	19(6)	4(7)
C(10)	59(6)	36(5)	58(6)	9(4)	3(5)	2(5)

C(11)	41(5)	31(5)	48(5)	–5(4)	3(4)	3(4)
C(12)	71(7)	47(6)	69(7)	–1(5)	13(5)	19(5)
C(13)	42(6)	62(7)	82(7)	17(6)	–22(5)	6(5)
C(14)	54(6)	44(6)	61(6)	16(5)	–5(5)	–3(5)
C(15)	79(7)	47(6)	58(6)	2(5)	7(6)	37(6)
C(16)	30(4)	38(5)	28(4)	2(3)	2(3)	–5(4)
C(17)	24(4)	28(5)	37(4)	2(3)	–1(3)	1(4)
C(18)	53(5)	32(5)	36(5)	5(4)	11(4)	10(4)
C(19)	36(5)	25(4)	36(4)	6(3)	7(4)	1(3)
C(20)	61(6)	43(5)	66(6)	28(5)	–17(5)	–19(5)
C(21)	77(8)	99(10)	91(8)	49(7)	–12(7)	–52(7)
C(22)	86(8)	69(7)	56(6)	25(6)	–9(6)	–21(7)
C(23)	55(6)	41(5)	46(5)	20(4)	2(4)	13(5)
C(24)	32(4)	32(5)	34(4)	1(4)	–8(4)	5(4)
C(25)	201(14)	48(7)	37(5)	–14(5)	5(7)	–33(8)
C(26)	77(8)	98(9)	96(9)	58(7)	–54(7)	–30(7)
N(1)	34(4)	27(4)	36(4)	–12(3)	–9(3)	4(3)
N(2)	36(4)	36(4)	46(4)	–2(3)	5(4)	13(3)
N(3)	26(3)	31(4)	25(3)	0(3)	6(3)	7(3)
N(4)	54(5)	42(5)	48(4)	12(4)	–17(4)	–4(4)
O(1)	46(4)	41(4)	59(4)	7(3)	–16(3)	–2(3)
Si(1)	45(2)	35(1)	52(1)	0(1)	–15(1)	7(1)
Si(2)	36(1)	28(1)	36(1)	3(1)	–2(1)	3(1)
Zn(1)	32(1)	41(1)	33(1)	–5(1)	1(1)	6(1)
Zn(2)	37(1)	40(1)	47(1)	8(1)	–9(1)	–7(1)

8.3 Daten der quantenchemischen Berechnungen – Kartesische Atomkoordinaten der energieoptimierten Strukturen

Quantenchemische Studien zur Reaktivität des Silagerman 93 und des Disilans 17

Tab. A.60 Standard Orientierung von PhH_2SiSiH_3 (**95**) [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.40636	–0.00058	0.40462
Si	–1.37117	–0.00162	1.03531
C	1.0867	–1.20612	0.14829
C	2.39348	–1.20794	–0.34692
C	3.04929	0.00105	–0.59577
Si	–2.94758	0.0009	–0.71836
C	2.39272	1.20924	–0.34499
C	1.08595	1.20581	0.15021
H	–1.58966	1.20631	1.88042
H	–1.58937	–1.21208	1.87687
H	0.59628	–2.15841	0.34157
H	2.89977	–2.15176	–0.53469
H	4.06668	0.00168	–0.979
H	–4.33631	0.00011	–0.17756
H	–2.78254	–1.20455	–1.57747
H	–2.78256	1.20887	–1.57393
H	2.89842	2.15368	–0.53122
H	0.59493	2.15748	0.34501

Tab. A.61 Standard Orientierung von $PhH_2SiSiH_3^{\bullet-}$ (**95**$^{\bullet-}$) [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.54198	–0.00041	0.41795
Si	–1.32552	–0.00098	0.78069
C	1.25909	–1.20538	0.17174
C	2.57593	–1.20776	–0.28085
C	3.25507	0.00088	–0.52311
Si	–3.40377	0.0003	–0.57456
C	2.5757	1.20886	–0.2782
C	1.25887	1.20524	0.17438
H	–1.52107	1.20935	1.65587
H	–1.52083	–1.2132	1.6533
H	0.7631	–2.161	0.34836
H	3.08791	–2.15759	–0.44196
H	4.28094	0.00138	–0.88651

H	–4.90646	–0.00005	–0.22199
H	–3.31182	–1.18547	–1.50128
H	–3.31182	1.18787	–1.49898
H	3.0875	2.15914	–0.43723
H	0.76269	2.16038	0.3531

Tab. A.62 Standard Orientierung von PhH_2SiGeH_3 (**96**) [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.97441	–0.00033	0.50668
Si	–0.77954	–0.00125	1.18408
C	1.65528	–1.20666	0.26023
C	2.97024	–1.20895	–0.21188
C	3.63045	0.00093	–0.44574
Ge	–2.37329	0.00021	–0.56173
C	2.97013	1.21018	–0.209
C	1.65525	1.20664	0.26333
H	–0.98851	1.21032	2.02584
H	–0.98815	–1.21462	2.02333
H	1.16168	–2.15811	0.44916
H	3.48034	–2.15225	–0.39156
H	4.65582	0.00141	–0.80717
H	–3.82868	–0.00048	–0.01722
H	–2.20497	–1.25075	–1.4683
H	–2.20523	1.25294	–1.4659
H	3.48016	2.15396	–0.38638
H	1.1616	2.1576	0.45465

Tab. A.63 Standard Orientierung von $PhH_2SiGeH_3^{\bullet-}$ (**96**$^{\bullet-}$) [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	1.13514	–0.00051	0.57657
Si	–0.6688	–0.00116	1.03661
C	1.8384	–1.21211	0.28423
C	3.13887	–1.21028	–0.20305
C	3.81504	0.00085	–0.46736
Ge	–2.62025	0.00029	–0.50513
C	3.13866	1.2113	–0.20044
C	1.8382	1.21185	0.28687
H	–0.91877	1.21136	1.88744
H	–0.91854	–1.21553	1.88486
H	1.3502	–2.16838	0.47613
H	3.64302	–2.16042	–0.38523
H	4.82901	0.00137	–0.86157
H	–4.19163	–0.00026	–0.13695

H	–2.5001	–1.22778	–1.48844
H	–2.50034	1.23048	–1.48581
H	3.64265	2.16191	–0.38056
H	1.34984	2.16762	0.48085

Quantenchemische Studien zur Reaktivität von Oligosilanen gegenüber elementarem Lithium: Si–Si- vs. Si–C-Bindungsspaltung

Tab. A.64 Standard Orientierung von **1** [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	0.3031228494	–0.3953201432	0.1120742207
C	0.1031566784	1.4876478657	0.2054422091
Si	–1.8963989169	–1.3168159805	–0.010492906
C	–2.7649553234	–0.6724306176	–1.5753692863
C	–2.8538164339	–0.7336697608	1.5235305929
N	2.3355431914	–0.0108607956	–1.9627734664
C	–1.9208948812	–3.221130153	–0.0474814947
C	2.8749044555	–0.4867688671	–3.2418870382
C	3.4045759024	0.2149832723	–0.9873843907
C	4.4345779596	1.2283770371	–1.4991611989
C	1.2897781949	–0.9099074646	–1.4683564331
C	3.8774669031	0.5048498061	–3.8403675635
C	5.0142575555	0.7974304853	–2.8524547799
C	0.0566015274	2.2836007597	–0.9568220511
C	–0.142101176	3.665282023	–0.8836076235
C	–0.2977605428	4.287919567	0.3583089128
C	–0.0567817696	2.1376842667	1.4450445695
C	–0.2526894395	3.5195308206	1.5245593057
C	–3.7934523208	0.3124411587	1.4507825907
C	–4.4682277064	0.7691866544	2.5874663943
C	–4.2159523405	0.1879843854	3.8323209375
C	–2.9873424664	–3.9459308125	0.5201374318
C	–3.0453061206	–5.3405886285	0.4423436998
C	–2.0326768721	–6.0499517021	–0.2090400998
C	–0.9642387027	–5.3545893973	–0.7812337308
C	–0.913161813	–3.9600055459	–0.6979471049
C	–3.2872657221	–0.8528316937	3.9314395285
C	–2.6175539272	–1.303777481	2.7910638937
C	1.1582185771	–1.0401329608	1.6848918306
H	–3.8221036151	–0.9664625427	–1.5871293567
H	–2.2969174734	–1.0952509672	–2.4728645493
H	–2.7107545081	0.4199379534	–1.6552068653
H	2.035109405	–0.6350730962	–3.9316226681

H	3.3658874007	–1.4768415049	–3.1142055401
H	3.9161565897	–0.7409882021	–0.7378277014
H	2.9555920818	0.5914515298	–0.0629095819
H	5.2312362955	1.3396014069	–0.7518998533
H	3.9444117057	2.2059135386	–1.6001991314
H	0.5618120215	–1.0348634941	–2.2815824732
H	1.6967388064	–1.9289630292	–1.2773222515
H	4.272274431	0.096982688	–4.7802816368
H	3.3509300154	1.4375161182	–4.0850079095
H	5.6844083825	1.5704568149	–3.2503016218
H	5.6226574987	–0.1100202419	–2.7177561705
H	0.2038992682	1.8247430469	–1.9309221109
H	–0.1688549929	4.2561597988	–1.796549712
H	–0.4498631865	5.3631308262	0.4166866945
H	–0.0313948594	1.5625498899	2.3681093334
H	–0.3721516197	3.9937647391	2.4960372555
H	–4.0080464681	0.7840911691	0.4945204282
H	–5.1896196598	1.5783265328	2.4991948024
H	–4.7396560401	0.5403908188	4.7177404067
H	–3.7845345338	–3.4169869136	1.0374555957
H	–3.8808646924	–5.8722669366	0.8920230207
H	–2.0749797261	–7.1348531515	–0.2688121893
H	–0.1697374718	–5.8964016644	–1.289402936
H	–0.0680617557	–3.4457540758	–1.1508939283
H	–3.0869396371	–1.3151748651	4.8954062221
H	–1.9064759643	–2.1218228213	2.8915014894
H	1.3413007956	–2.1189027167	1.6029829186
H	0.5335823701	–0.8820657399	2.5719833551
H	2.1225318167	–0.5496310063	1.8634297152

Tab. A.65 Standard Orientierung von **1**$^{\bullet-}$ [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	–0.4528690306	–0.3928116156	0.4294268101
C	–1.1185020297	–2.0572877357	–0.1170828141
Si	1.6407309409	0.2857124299	–0.6281195502
C	1.4311156496	–0.1851770911	–2.4653205697
C	3.121542325	–0.6628912874	0.0704795466
N	–3.1329036513	0.8238095517	0.0470162634
C	1.9321153373	2.1367808611	–0.5029115319
C	–3.860631569	2.0385406118	–0.3192728981
C	–3.6169058615	0.2759219034	1.311797835
C	–5.1147406765	–0.0483610152	1.2482115193
C	–1.6795778397	1.0514414625	0.0199095149
C	–5.3669158977	1.7849701797	–0.452904655
C	–5.935333654	1.1820008028	0.8387364931

C	–2.0940369917	–2.1975266289	–1.145953031
C	–2.4704821026	–3.4428167686	–1.6400926085
C	–1.8867832775	–4.624340946	–1.1397084248
C	–0.5518964376	–3.2697215196	0.3779838483
C	–0.9259578287	–4.5157726933	–0.1188224968
C	3.8888605217	–1.5327522784	–0.7428794518
C	4.9801842931	–2.2456208183	–0.2468016738
C	5.355908009	–2.123397898	1.1019080523
C	2.6492468517	2.7592677722	0.5589366269
C	2.7915467904	4.1393553862	0.6523164586
C	2.2145481991	4.9929103858	–0.3120065043
C	1.503139418	4.4089450026	–1.3738078294
C	1.3649320612	3.0258920123	–1.4672083145
C	4.6046205389	–1.2847551141	1.9363888576
C	3.507389952	–0.5828475256	1.4353776756
C	–0.1560719127	–0.4212895221	2.3208687376
H	2.3128755707	0.0869616299	–3.060570543
H	0.5628831001	0.3223338448	–2.9043652926
H	1.2536776191	–1.2626348483	–2.5679736492
H	–3.4554096821	2.4058525295	–1.270077164
H	–3.6887297213	2.8437772592	0.4313240638
H	–3.4285279763	0.9853861703	2.1502321395
H	–3.054978217	–0.6376938898	1.5253958724
H	–5.4451185614	–0.4274621072	2.2253685285
H	–5.2660559964	–0.8548655269	0.5180643985
H	–1.4346620042	1.4127028588	–0.9877004944
H	–1.3990708315	1.8880834755	0.6969353412
H	–5.8753478857	2.7278017722	–0.7001701567
H	–5.5370199629	1.09216429	–1.2888944675
H	–6.9955888907	0.920366749	0.7133183635
H	–5.8871148037	1.9351337117	1.6410749356
H	–2.576206205	–1.3062114818	–1.5419594614
H	–3.2295090628	–3.50191524	–2.4201387693
H	–2.1750056499	–5.5973840818	–1.5316962614
H	0.2009394499	–3.2302323856	1.164204199
H	–0.464498687	–5.414788228	0.2893525944
H	3.6308482553	–1.65044293	–1.7931472064
H	5.5426162409	–2.8998452222	–0.9115572455
H	6.2062402661	–2.677800742	1.4934886416
H	3.1250091504	2.1415270484	1.317255285
H	3.3614375784	4.562167696	1.4794148373
H	2.3178950824	6.0730081544	–0.2354641587
H	1.0539835126	5.0426464621	–2.1386522618
H	0.8137931364	2.6205616122	–2.3142824913
H	4.8685448909	–1.1875011819	2.9888141215
H	2.9311783918	0.0318151163	2.1235051405

H	0.2263330882	0.5498486336	2.6626913541
H	0.5890847157	–1.1790438818	2.5908882535
H	–1.0734316492	–0.6396461858	2.8825622446

Tab. A.66 Standard Orientierung von **102** [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	–0.2440031583	0.2363965553	–0.1751565416
C	–0.3009881089	2.1360953291	–0.2503434625
Si	–2.445420947	–0.6612803256	–0.2062201391
C	–3.2990150887	–0.2770584874	–1.8647492913
C	–3.4826614301	0.1116026826	1.1908175904
N	2.0013226527	0.132602039	–2.0003310886
C	–2.3921064535	–2.54675335	0.0390050383
C	2.3354403031	0.1604454221	–3.4298091333
C	3.013396771	–0.6163107168	–1.2495666578
C	4.4058309223	0.0053154677	–1.4018855633
C	0.6447377024	–0.3863141026	–1.7646467256
C	3.6993775487	0.8138198987	–3.6770509332
C	4.803950321	0.1061497913	–2.8804476502
H	–0.847504507	2.4948355524	–1.1316193467
H	0.7173120362	2.5403003161	–0.3092289082
H	–0.7836317918	2.5606709597	0.6387838076
H	–4.4829285627	–0.3390021563	1.2311555603
H	–3.6097881649	1.1885617682	1.0235178994
H	–3.0208612189	–0.0126349475	2.1777942378
C	–2.5863482201	–3.1313642367	1.305695245
C	–2.5194333142	–4.5157448872	1.4920149365
C	–2.2541930717	–5.3563443339	0.4079141524
C	–2.05918427	–4.8019465898	–0.8604468978
C	–2.1267038382	–3.4172134131	–1.0370198563
C	0.6110784367	–0.2767215731	1.4475902986
H	–4.3283031767	–0.6584318803	–1.8713201148
H	–2.7749306667	–0.7234732485	–2.7184547041
H	–3.3428180627	0.8058904239	–2.0374545384
H	1.5535402339	0.7233698002	–3.952789458
H	2.3344927468	–0.8683069549	–3.8528161373
H	3.0431775942	–1.6747600991	–1.5918253172
H	2.7253957258	–0.6353887829	–0.1951226473
H	5.1342794824	–0.5975524401	–0.8436152067
H	4.398334698	1.0072719872	–0.9512305093
H	0.0078753704	–0.0245026029	–2.5846785246
H	0.6168551919	–1.4937710522	–1.8364563558
H	3.9212837442	0.7930582	–4.752299892
H	3.6441651482	1.868910356	–3.3758563275
H	5.7596877325	0.6349090354	–2.9900148844

H	4.95370328	–0.9060156827	–3.2860896259
H	–2.7996583838	–2.5013735771	2.166737043
H	–2.6763778179	–4.9365050764	2.482722184
H	–2.2024726849	–6.4332466021	0.5490231694
H	–1.8558383882	–5.4472596918	–1.7120959588
H	–1.974110888	–3.0137776829	–2.0364384661
H	0.7900489601	–1.3576492051	1.4923011056
H	–0.0171965818	–0.0110966363	2.3078539987
H	1.5724921939	0.2349947503	1.5800545969

Tab. A.67 Standard Orientierung von **102**$^{\bullet-}$ [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	0.0179382392	–0.0244233883	0.1866192386
C	0.2381490814	1.8633509248	0.0124328564
Si	–2.2409013992	–0.7640601974	0.0657128862
C	–3.0536241378	–0.0267160813	–1.4951264764
C	–3.1914771178	–0.1510102333	1.6032928808
N	2.1143305671	–0.275864866	–1.8509286952
C	–2.2707019588	–2.6411561296	–0.0246426086
C	2.4704903242	–0.865522467	–3.1422287783
C	3.2488227035	–0.301742257	–0.9302768194
C	4.4592795665	0.4492777384	–1.4974997283
C	0.9065847604	–0.9033376527	–1.2898087228
C	3.6403187238	–0.127373036	–3.8015488725
C	4.861188889	–0.0977512498	–2.8730345837
H	–0.148778411	2.2261446962	–0.9491853752
H	1.3011230142	2.14521385	0.0721072794
H	–0.2951863557	2.3942743974	0.8120069553
H	–4.2421503955	–0.4721958418	1.5640050307
H	–3.1714004598	0.9472630227	1.6535875639
H	–2.756740383	–0.5302151	2.5386198829
C	–2.0573065619	–3.4444896873	1.1336759515
C	–2.0191199423	–4.8348499187	1.0706031978
C	–2.1871146824	–5.503436913	–0.1561305622
C	–2.3517288519	–4.7325560746	–1.3242551627
C	–2.3908761512	–3.3424083671	–1.2570548154
C	0.7667235565	–0.5769212602	1.8568068071
H	–4.0862606405	–0.3856796955	–1.6044539381
H	–2.5083492451	–0.2813273026	–2.41514992
H	–3.0829562341	1.0689962941	–1.4252836125
H	1.5868709351	–0.8209215387	–3.7919563629
H	2.7305010636	–1.9424286783	–3.0288633433
H	3.5413793584	–1.3499810702	–0.6932268661
H	2.9442053612	0.1603162779	0.0148028526
H	5.2959910395	0.374112081	–0.7880821918

H	4.2034442222	1.5142972772	–1.5845406947
H	0.1663046136	–0.9406797889	–2.1016120732
H	1.0939346577	–1.9648531699	–1.0185462264
H	3.8875085062	–0.6148243665	–4.7560519014
H	3.3256912058	0.9001855434	–4.0307846638
H	5.6701446096	0.5059224447	–3.310465165
H	5.2540966667	–1.1200330161	–2.7588034612
H	–1.9341529376	–2.9659531261	2.1047706126
H	–1.8664199665	–5.4083290755	1.9845877469
H	–2.1736602833	–6.5901451648	–0.2040042807
H	–2.4608516512	–5.2257798604	–2.289718855
H	–2.5330223855	–2.7832941434	–2.1810581882
H	0.7758804382	–1.6723421127	1.9472085747
H	0.1744007246	–0.1795146811	2.6916202999
H	1.7964773237	–0.2176370359	1.9898623274

Tab. A.68 Standard Orientierung von **92** [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	0.1788719554	–0.205713627	0.1302657184
C	–0.0331465067	1.6794478932	0.0773861979
Si	–1.9814822772	–1.1984536555	0.0205945493
C	–2.8848822863	–0.5389754824	–1.5321918438
C	–2.9666493604	–0.6232302001	1.5577161756
N	2.2785091318	–0.0089029432	–1.9094032118
Si	–1.9901626092	–3.5738963579	–0.0449849694
C	2.8460288109	–0.5956568096	–3.1286104284
C	3.3212100784	0.2732250696	–0.9207868394
C	4.387125796	1.2230639237	–1.4786637729
C	1.1935560878	–0.8405964635	–1.3825593116
C	3.8893798946	0.3235083916	–3.7716043035
C	5.000486374	0.6732717829	–2.7726675909
C	–0.0377036406	2.3905838869	–1.1392333353
C	–0.2504173341	3.7717615895	–1.1733239296
C	–0.4643762365	4.4800065187	0.0127007639
C	–0.2491998722	2.4157583794	1.2593947632
C	–0.4611483652	3.797432177	1.2321889621
C	–3.7925984096	–4.1917005685	–0.0024846111
C	–1.0727873256	–4.3217316491	1.4468337168
C	–1.179546197	–4.2284407061	–1.6389361029
C	1.0121816012	–0.6942120303	1.7734616915
H	–3.9218745134	–0.8979341829	–1.5600498876
H	–2.3984481393	–0.8619219036	–2.4608821227
H	–2.9124162599	0.5577797013	–1.5351028685
H	–4.0022199306	–0.9847530166	1.5158055961
H	–2.9999187008	0.4720591022	1.6147233317

H	–2.5243665549	–0.9932828377	2.4909413064
H	2.0242495632	–0.7808582009	–3.8309847937
H	3.309115368	–1.5827040868	–2.9074702128
H	3.8054751057	–0.6687823923	–0.5798821012
H	2.8526067821	0.7303210353	–0.0437201027
H	5.1622858325	1.3810305351	–0.7172408464
H	3.9202873034	2.1976725609	–1.6747812275
H	0.4798312758	–0.9971203237	–2.2032967068
H	1.5587736759	–1.8593190129	–1.1168027604
H	4.3045765943	–0.1678276902	–4.6615252005
H	3.3923949049	1.2434111052	–4.1089196006
H	5.7000073081	1.398334603	–3.2084113239
H	5.5834167831	–0.2322724657	–2.5450727866
H	0.1536354057	1.86422707	–2.0705325291
H	–0.2426592729	4.2959661505	–2.1264329023
H	–0.6282283928	5.5547269184	–0.0128533951
H	–0.2484968606	1.9093894207	2.2227991135
H	–0.6222370977	4.3391594995	2.161582128
H	–4.3714915397	–3.815927225	–0.8554756418
H	–4.308421608	–3.8779313544	0.913535919
H	–3.823890913	–5.2892608016	–0.039983948
H	–1.4909044103	–3.9741477961	2.3998750881
H	–0.0060623092	–4.0659666757	1.4395947741
H	–1.1493026592	–5.4174530033	1.4329448352
H	–0.1234501358	–3.940657066	–1.7097332037
H	–1.6876879016	–3.8520751743	–2.5355978306
H	–1.2267629183	–5.3254879572	–1.6692189746
H	0.342702316	–0.5295291643	2.6265420558
H	1.9305824455	–0.1246162453	1.958216792
H	1.2751501443	–1.7591982448	1.7707177387

Tab. A.69 Standard Orientierung von **92**$^{\bullet-}$ [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	0.122798125	–0.0357816729	0.1104865857
C	0.0488062984	1.8276858261	0.0913614631
Si	–1.9609802412	–1.2471540457	0.0057184347
C	–2.9132072209	–0.5916726164	–1.5323081803
C	–2.9584813458	–0.6815596713	1.5519319377
N	2.2655578102	0.0295131248	–1.9420097814
Si	–2.0711463194	–3.6351675093	–0.0593171976
C	2.8506797	–0.6432243276	–3.0988954817
C	3.2786366351	0.3425244534	–0.937869737
C	4.3840664158	1.2353324534	–1.5142665978
C	1.1221503208	–0.7197380852	–1.4067840505
C	3.9380872282	0.2080895589	–3.7656462415

C	5.0251119189	0.5972231754	–2.753801942
C	0.0017269747	2.5860284286	–1.1237523944
C	–0.2222455474	3.9564999188	–1.1318640088
C	–0.4180633123	4.6712284909	0.0710900628
C	–0.1245375527	2.5843466528	1.2962298156
C	–0.3481858745	3.9554344494	1.2863169467
C	–3.7984504822	–4.4797915764	–0.0212497179
C	–1.1092884277	–4.3798392978	1.4216694527
C	–1.2161139595	–4.2987386945	–1.6400622024
C	0.9672714108	–0.6017627186	1.7375271095
H	–3.9617303713	–0.9172019742	–1.5194590633
H	–2.4672342076	–0.9468396392	–2.4715606951
H	–2.8964365871	0.5060397781	–1.5496345792
H	–4.0015285617	–1.0200603571	1.4979501176
H	–2.9592972276	0.413982813	1.626913578
H	–2.527241739	–1.0802111254	2.4804679998
H	2.0467254809	–0.8533665421	–3.8152527787
H	3.2833611988	–1.6290737996	–2.807140548
H	3.733749303	–0.5896922377	–0.5292417072
H	2.7869026817	0.8580066478	–0.1087648222
H	5.1408065479	1.4220697664	–0.739465125
H	3.9434759052	2.2051587877	–1.7809827096
H	0.4052451329	–0.8414306128	–2.2311354834
H	1.4256316477	–1.7560303621	–1.1305966443
H	4.3713733143	–0.3474990523	–4.6097814829
H	3.4736556375	1.1163866365	–4.1739153008
H	5.7561125109	1.2790005385	–3.211174532
H	5.5789829883	–0.3062803869	–2.4528419958
H	0.1665484229	2.0766936214	–2.0718972879
H	–0.2377445409	4.4883542561	–2.0840246906
H	–0.6017547056	5.7433079877	0.0621869989
H	–0.0818342965	2.0740111499	2.2587337415
H	–0.4679022478	4.4838862604	2.2329130181
H	–4.4131469835	–4.1782157047	–0.8791301079
H	–4.3550298413	–4.2223144467	0.889273243
H	–3.6950316623	–5.580967911	–0.0520114573
H	–1.5338842007	–4.0578270802	2.3816775922
H	–0.052794813	–4.0828004003	1.4109607118
H	–1.1521735316	–5.4783541219	1.3929585963
H	–0.1654615255	–3.9876769996	–1.6982650744
H	–1.7194291	–3.9415856676	–2.547997526
H	–1.2448666628	–5.3981083327	–1.6567196956
H	0.3015153885	–0.4603433501	2.5986291183
H	1.8929898567	–0.048044052	1.9410623406
H	1.2127542348	–1.6708504038	1.6911619759

Tab. A.70 Standard Orientierung von **103** [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	–0.1178854713	0.1315880124	0.0328558462
C	–0.0829648283	2.0276130536	–0.0312488388
Si	–2.3809862198	–0.6037506085	–0.0552352652
C	–3.235595799	0.0870545281	–1.6065299745
C	–3.3254045041	0.009290641	1.4776927796
N	1.959256657	–0.0025157483	–2.0396111916
C	–2.439791767	–2.5048247913	–0.1037071766
C	2.3958668652	–0.6672941224	–3.2731499354
C	3.0542776677	0.087850203	–1.0716888413
C	4.2591010383	0.8438354176	–1.64434148
C	0.7638861353	–0.651349491	–1.4919657831
C	3.5684378122	0.0663250235	–3.9316702283
C	4.7429933296	0.2096179532	–2.9549550493
C	0.0846356128	2.725436562	–1.2440880714
C	0.0461473162	4.1223412363	–1.2899888679
C	–0.1589003479	4.8591484744	–0.1202046665
C	–0.2841063642	2.7927495976	1.1353503876
C	–0.3212114433	4.1895394642	1.0960254781
H	–4.3687972641	–0.3307689433	1.4509464848
H	–3.3310216596	1.1057699346	1.5103901851
H	–2.8838502021	–0.3456853278	2.4166651599
C	–2.5039069792	–3.2683864205	1.0786597274
C	–2.5184572638	–4.6660371384	1.0486253184
C	–2.4665434578	–5.3405098854	–0.1743401714
C	–2.4029153862	–4.606873943	–1.3622318894
C	–2.3888116742	–3.2096566221	–1.3225715104
C	0.6470598836	–0.4682679787	1.6708725243
H	–4.2821832356	–0.2409445847	–1.6517985095
H	–2.7477001815	–0.2310807563	–2.5356792791
H	–3.2255355499	1.1837637399	–1.5916272332
H	1.5420324064	–0.7034862778	–3.9608511064
H	2.6872513632	–1.7205888668	–3.0665236855
H	3.3741987936	–0.9262908865	–0.7448768495
H	2.6880464258	0.611473943	–0.1829962925
H	5.0636428115	0.8560088339	–0.8972748158
H	3.9667538507	1.8872380341	–1.8241183737
H	0.0207786787	–0.6904424567	–2.3006634088
H	0.9629263915	–1.7146706305	–1.23081937
H	3.8754487779	–0.4794492325	–4.8336720004
H	3.230420723	1.0613611145	–4.2521316304
H	5.5479474903	0.8081592508	–3.4007929948
H	5.1659525628	–0.7848424439	–2.7459077467
H	0.2752584842	2.1720018944	–2.159624238

H	0.1826562619	4.6351201661	–2.2395743064
H	–0.1878655949	5.9456600033	–0.1548754305
H	–0.4110086758	2.2966084579	2.0959359682
H	–0.4759383615	4.7536140019	2.0131110595
H	–2.5511571642	–2.7690082546	2.0443506191
H	–2.5722343051	–5.2270187572	1.978967626
H	–2.4786441868	–6.4274363426	–0.2015172665
H	–2.3659131895	–5.1219168026	–2.3195398805
H	–2.3433436112	–2.6638189791	–2.2628815081
H	0.717367228	–1.5630053353	1.6799758546
H	0.0315645842	–0.1752545358	2.5303361867
H	1.6533655363	–0.0651933776	1.8340136621

Tab. A.71 Standard Orientierung von **103**$^{\bullet-}$ [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	–0.0280214454	0.079600749	0.0050356719
C	0.0840629181	1.9453158241	–0.0069804056
Si	–2.2499238148	–0.8663538457	–0.0106116475
C	–3.2037553635	–0.056032571	–1.4564972027
C	–3.088532626	–0.2988149449	1.6133645688
N	1.979586353	–0.037850347	–2.1732550113
C	–2.396276193	–2.7297422471	–0.1505056474
C	2.4366084435	–0.7671484756	–3.3540588058
C	3.0770348423	0.1977949183	–1.23900313
C	4.2121805763	0.9932416844	–1.8958736783
C	0.814299025	–0.6923780127	–1.5611795772
C	3.5428465507	–0.0120870142	–4.10104777
C	4.7202931384	0.2970736065	–3.1660082002
C	0.0078058551	2.7066635163	–1.2158322906
C	–0.076785703	4.0939962894	–1.2116562763
C	–0.0936385391	4.8178363263	–0.0001512696
C	0.0835945023	2.7069306264	1.2035871472
C	–0.0005600352	4.0950878898	1.2076616435
H	–4.1500848319	–0.5821403664	1.6240766581
H	–3.0228143008	0.7919061213	1.7181852119
H	–2.6171451632	–0.7440633496	2.4988787396
C	–2.283021645	–3.588654112	0.9868899921
C	–2.2472190737	–4.9738366177	0.8732699829
C	–2.3154480959	–5.5989763759	–0.3899491755
C	–2.4394313244	–4.7789082957	–1.5309920944
C	–2.4759418361	–3.3938294861	–1.4142580048
C	0.8263839917	–0.5944095664	1.5821442187
H	–4.2567561102	–0.3700653785	–1.4562897974
H	–2.7796393589	–0.3172040151	–2.4347498244
H	–3.1693540549	1.0372098648	–1.3671000917

H	1.5753231846	–0.9211738233	–4.0159429669
H	2.8077725563	–1.7804586373	–3.0745357976
H	3.479907132	–0.7649658186	–0.8472938834
H	2.6845980827	0.7592123315	–0.3866328382
H	5.0292602862	1.1242844475	–1.1725808559
H	3.8348873823	1.9936807425	–2.1467726138
H	0.0425794154	–0.7590403584	–2.341084288
H	1.0463278686	–1.747830199	–1.2958445704
H	3.8751960904	–0.6085537383	–4.9628489923
H	3.1276679415	0.9271351236	–4.4923197218
H	5.4716440464	0.9159335996	–3.6769687171
H	5.2199607728	–0.6450917443	–2.8899898353
H	0.0377562667	2.1873228465	–2.1721919155
H	–0.1223707871	4.6288334149	–2.1608150101
H	–0.1668468268	5.9031691466	0.002007606
H	0.1532925054	2.1900833016	2.1606646049
H	0.0093253596	4.6286468124	2.158608883
H	–2.229566267	–3.1500377283	1.9832683153
H	–2.1699190562	–5.5826810881	1.7745685256
H	–2.2804534409	–6.6823473613	–0.4805510155
H	–2.5134782164	–5.2344250667	–2.5189396295
H	–2.5773390561	–2.801118151	–2.3231864599
H	0.8792299713	–1.690053763	1.5416408545
H	0.2582406368	–0.3312337829	2.4838020483
H	1.8458574699	–0.2074529009	1.7086443397

Tab. A.72 Standard Orientierung von **17** [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	0.0348412909	–0.066759064	0.1593340107
C	0.0818823891	1.8295860739	0.0985478619
Si	–2.2121088147	–0.8092755937	–0.0657819057
C	–2.9828113426	–0.1172589723	–1.661755614
C	–3.2517145256	–0.2185013877	1.4148397317
N	2.2369094997	–0.197504168	–1.7858455679
C	–2.2800733945	–2.7125318124	–0.1293640218
C	2.7643892216	–0.8844416467	–2.9708005241
C	3.2643242722	–0.0579323438	–0.7518570886
C	4.4870362334	0.7087432038	–1.2691384774
C	1.0173120739	–0.8518685439	–1.3036474954
C	3.9632404719	–0.1452152396	–3.5735484436
C	5.0677358201	0.0498182661	–2.5268673317
C	0.3087816251	2.5287193831	–1.1036568374
C	0.277541449	3.9257926565	–1.1487104064
C	0.0191679416	4.6615048341	0.0112836354
C	–0.1730828526	2.5934555478	1.2552615795

C	–0.2043256817	3.9904505219	1.2169116275
C	0.7101242987	–0.6689485286	1.8381295568
H	–4.0322308607	–0.4297759909	–1.7491059459
H	–2.4582533335	–0.4723499413	–2.5578296453
H	–2.9584522063	0.9791593075	–1.6753809294
H	–4.2929808909	–0.5520652972	1.30882956
H	–3.2606536094	0.8756576771	1.492152987
H	–2.8733616681	–0.6181256322	2.3641163508
H	–3.3184566003	–3.0582559242	–0.223848433
H	–1.8633083311	–3.1631337921	0.7801967235
H	–1.7201072489	–3.1119997897	–0.9842712498
H	1.9569246857	–0.9565504322	–3.7096066485
H	3.0624694352	–1.925736999	–2.7173064056
H	3.5828777918	–1.0556073618	–0.3765376516
H	2.8308803582	0.4825604806	0.0954848276
H	5.2416281314	0.7613070381	–0.4733145876
H	4.1833994368	1.739165502	–1.498007625
H	0.3251600734	–0.9076547476	–2.1557727902
H	1.2131981076	–1.9110288669	–1.0187456359
H	4.3390387928	–0.7097910083	–4.4371152796
H	3.6281336042	0.8329992554	–3.9446360609
H	5.8879334198	0.6536627348	–2.9363359063
H	5.496618927	–0.9290036789	–2.2629369206
H	0.5390920264	1.9757547759	–2.0101897803
H	0.4611138765	4.4398882904	–2.0896373345
H	–0.0039449572	5.7481807029	–0.0228312751
H	–0.3485066562	2.0955502418	2.20720691
H	–0.4016443115	4.5533800932	2.1264932137
H	0.0584010945	–0.3633840345	2.665837116
H	1.7143527765	–0.2826146476	2.0486756141
H	0.7640081609	–1.7650211415	1.8564825129

Tab. A.73 Standard Orientierung von **17**$^{\bullet-}$ [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	–0.7189991774	–0.3982822655	0.6131388016
C	–0.6564497282	1.4161717075	0.1574515895
Si	–2.6882250398	–1.3908633448	–0.3056634155
C	–2.6351988785	–1.3150162476	–2.212514169
C	–4.2160681274	–0.4007491517	0.2674692432
N	2.0903605549	–0.7733786396	–0.2236363483
C	–2.9626884326	–3.2125666807	0.2003353423
C	3.0444592132	–1.6687183212	–0.8780854393
C	2.6001298886	–0.2976416575	1.060250228
C	3.9348251598	0.4395181621	0.8968954622
C	0.7609438644	–1.3906141289	–0.1356352375

C	4.3933029761	–0.9832383691	–1.1232754689
C	4.9750911152	–0.4369255069	0.1872315307
C	–0.0093342176	1.8796925326	–1.0245397347
C	–0.0295816329	3.2228948842	–1.391784742
C	–0.7053054265	4.1755468283	–0.6055565755
C	–1.3726313571	2.3921309679	0.908528602
C	–1.3961115974	3.7343681955	0.5400577848
C	–0.8113110571	–0.623026502	2.5095855827
H	–3.5736400216	–1.7040959837	–2.6342274444
H	–1.8151229741	–1.9212625472	–2.6201545995
H	–2.5030487065	–0.2859656207	–2.5736329256
H	–5.1271517428	–0.8049831744	–0.1981594385
H	–4.1376040913	0.6605269409	–0.0039844094
H	–4.3477961676	–0.4594789845	1.356192678
H	–3.8990974577	–3.592424923	–0.2430327054
H	–3.0402349871	–3.3216848288	1.2908259488
H	–2.1451956084	–3.8622176268	–0.1412720429
H	2.6082418307	–1.9939882657	–1.8315586723
H	3.2037719801	–2.5887953817	–0.2709432788
H	2.7272816422	–1.1418245308	1.775530533
H	1.85753799	0.3820676695	1.491569066
H	4.2989901847	0.7507958661	1.8861734663
H	3.7592388408	1.3526200979	0.3120202683
H	0.4706644274	–1.6707413654	–1.1601577531
H	0.8035945849	–2.3521882314	0.4246822766
H	5.0860306776	–1.6986816583	–1.5896035647
H	4.2475028872	–0.1581103659	–1.8342530857
H	5.8985442132	0.1297403736	–0.0027462822
H	5.249362947	–1.279630452	0.8411792671
H	0.5448322899	1.1753984131	–1.6408736968
H	0.4954819821	3.538508379	–2.2930267972
H	–0.7094519516	5.2265149445	–0.8866289219
H	–1.9092088796	2.0915712341	1.807866589
H	–1.9467189307	4.448751081	1.15150655
H	–1.7555418415	–0.2271662068	2.9100780003
H	0.011793078	–0.1211697532	3.0346190766
H	–0.7768243732	–1.6914947006	2.7657152791

Tab. A.74 Standard Orientierung von **104** [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	–0.0486360076	0.0663129609	–0.0507008795
C	–0.1131583044	1.9604530463	–0.191159887
H	–0.5954313922	2.4127810721	0.6844881064
Si	–2.2383904012	–0.8547439215	0.0241214792
C	–3.230975045	–0.3698232576	–1.5280293438

C	–3.1685819257	–0.2061203521	1.5550257297
N	2.0183018953	0.0264520679	–2.1053831943
C	–2.1726820112	–2.7562983957	0.1231032153
C	2.2924759858	–0.2919795406	–3.5120400928
C	3.1807790643	–0.2760919598	–1.267560256
C	4.4211192577	0.5082947862	–1.7113507993
C	0.7978682787	–0.6395028373	–1.631680961
C	3.4938541627	0.4936736934	–4.0477102722
C	4.7405267454	0.2450857628	–3.188618025
H	–0.6656581355	2.2802351453	–1.0831235699
C	0.8552150373	–0.4018754226	1.5641506534
H	–4.2473858116	–0.783665553	–1.4806008301
H	–2.7639630235	–0.748869214	–2.4458505822
H	–3.3223348393	0.7189924226	–1.6277145854
H	–4.1800978065	–0.6319202007	1.6020249573
H	–3.271086431	0.8861432387	1.533631696
H	–2.6551696803	–0.4732969027	2.4872518483
H	–3.1864371187	–3.1762867149	0.1742584679
H	–1.6289663886	–3.0979971794	1.012850751
H	–1.6786076037	–3.1918120475	–0.754551366
H	1.3973479381	–0.0494806635	–4.0967653359
H	2.4768887018	–1.3817697667	–3.6382613287
H	3.4059740987	–1.3658221643	–1.2927628057
H	2.9377623667	–0.029002925	–0.2303746015
H	5.2710171214	0.2305258567	–1.0739793596
H	4.2356287965	1.5803575766	–1.5583305475
H	0.0431710376	–0.5274443781	–2.4231869639
H	0.9498639716	–1.7363043488	–1.5243624649
H	3.6769993145	0.2072823443	–5.091811158
H	3.247405949	1.5642450363	–4.0414202248
H	5.574539607	0.875461644	–3.5233720325
H	5.0641972747	–0.799865077	–3.3103597246
H	0.900352129	2.3718820925	–0.2724125468
H	0.2291594924	–0.1679977328	2.4349691636
H	1.7974836935	0.1457701315	1.6892186129
H	1.0849300064	–1.4741783223	1.6035790577

Tab. A.75 Standard Orientierung von **104**$^{\bullet-}$ [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	0.8595217752	0.7036961374	0.1841930644
C	0.5754451298	1.1883531226	2.0020034327
H	1.3489085722	1.8858957772	2.3509788121
Si	2.9343128586	–0.423689302	–0.0836564435
C	2.9685907682	–2.0283936197	0.9451792008
C	4.361247451	0.698847705	0.4940406465

N	–1.8885498351	–0.32656532	0.0713640106
C	3.215092843	–0.8721204966	–1.9159116654
C	–2.7112128996	–1.5198977121	–0.1349335365
C	–2.4931209812	0.8465807851	–0.5574260894
C	–3.9029492382	1.1179424804	–0.0197991732
C	–0.4992695189	–0.5557799845	–0.3525045544
C	–4.1231066761	–1.3424859816	0.4327098039
C	–4.8068667448	–0.1110040128	–0.1741980275
H	0.5966696475	0.3059531957	2.6570412597
C	0.8839973683	2.2691309818	–0.9103654255
H	3.9413744506	–2.5296451854	0.84215552
H	2.1944565383	–2.738983338	0.6211233835
H	2.8107057524	–1.8267086183	2.0144088201
H	5.327589827	0.1901828341	0.3608229424
H	4.2643039051	0.9581039663	1.557903128
H	4.3962370969	1.6375350357	–0.0771498469
H	4.1945474081	–1.3518746051	–2.0496403503
H	3.1905512155	0.0201265093	–2.557825257
H	2.4499835215	–1.5706982296	–2.2838586843
H	–2.2132056507	–2.3658480239	0.3575022223
H	–2.7774720586	–1.7734664735	–1.2171644053
H	–2.5357950612	0.723753691	–1.6631627864
H	–1.8556434311	1.7155503547	–0.3632052963
H	–4.3279750669	1.9844955302	–0.5465343215
H	–3.8287891183	1.390491752	1.0421472719
H	–0.1895029745	–1.5144819606	0.0907903665
H	–0.4356834181	–0.7068803876	–1.4537611704
H	–4.7104995099	–2.2519290026	0.2376857748
H	–4.0533685683	–1.2263573913	1.5230989842
H	–5.7856274419	0.064409976	0.2973224174
H	–4.9976908457	–0.2919094799	–1.2433822339
H	–0.4002087483	1.6750691577	2.1306286587
H	1.7992219696	2.8500490571	–0.726421007
H	0.0346595222	2.9365692656	–0.7150712569
H	0.8691295604	2.0093834109	–1.9790128844

Quantenchemische Studien bezüglich des Mechanismus bei der Reaktion von Lithiosilanen mit Chlor- und Brombenzol

Tab. A.76 Standard Orientierung von **TS-PhCl-at** [stationärer Punkt, B3LYP/6-31+G(d), CPCM].

Atomsymbol	x	y	z
C	–0.0294204913	–0.0011072347	–0.0010934282
Cl	2.2271896303	0.0639939629	0.0257090295
C	–0.7111242469	–1.2019426537	0.2251863009
C	–2.1156041257	–1.2491107149	0.2099035751
C	–2.8526127787	–0.0827559075	–0.0339283044
C	–2.1787620461	1.1244239789	–0.2612139608
C	–0.7739315852	1.1586065666	–0.243398968
Si	4.738938599	0.1359819174	0.0545639098
H	–0.1546567435	–2.1232240125	0.4173802952
H	–2.6346706332	–2.1930995443	0.3877902597
H	–3.9420840611	–0.1142951669	–0.0467793667
H	–2.7472397166	2.0369509128	–0.4517862816
H	–0.2673388633	2.1106693211	–0.4231061755
H	5.3695730385	0.4273954604	1.3975481132
H	5.3719103031	1.1746084856	–0.8436062683
H	5.4312777208	–1.1395773713	–0.3693007299

Tab. A.77 Standard Orientierung von **TS-PhCl-Meisenheimer** [stationärer Punkt, B3LYP/6-31+G(d), CPCM].

Atomsymbol	x	y	z
C	–0.0377584155	0.0035134442	0.1223287953
Cl	1.7849882439	–0.5674494881	0.1648953848
C	–0.7985921549	–0.4570468345	1.2370857015
C	–2.1415843542	–0.7753414076	1.0840998204
C	–2.7652708376	–0.7399567317	–0.178693622
C	–1.9871307752	–0.4039644414	–1.2931330863
C	–0.6333186417	–0.0831445091	–1.1666571595
Si	0.3510094704	2.4784146036	0.2098676534
H	–0.3377352372	–0.4867536092	2.2220312035
H	–2.7138598053	–1.0698813334	1.9647705027
H	–3.8169483102	–0.9977394079	–0.2883078694
H	–2.4297805393	–0.4104253795	–2.2901198871
H	–0.044419044	0.1545685453	–2.0493750695
H	–1.1159820819	2.8655762079	0.2779591489
H	0.6268920151	2.6690683358	–1.2730946176
H	0.9718264676	3.7860320055	0.7520551007

Tab. A.78 Standard Orientierung von **TS-PhBr-at** [stationärer Punkt, B3LYP/6-31+G(d), CPCM].

Atomsymbol	x	y	z
C	–0.0644307295	–0.0033753809	–0.0009545909
Br	2.3133516413	0.0650146774	0.0267823415
C	–0.7648736856	–1.1986424251	0.2235860719
C	–2.1687121919	–1.2489200146	0.2089985683
C	–2.9074151328	–0.0838273801	–0.034653791
C	–2.2302028676	1.1213343557	–0.2615122136
C	–0.8258234459	1.1505714602	–0.2426517704
Si	4.8723397921	0.1401964546	0.0557765638
H	–0.2149698837	–2.1246109552	0.4165195402
H	–2.6865319111	–2.1936953385	0.3870670848
H	–3.9969986454	–0.1146559171	–0.0475935245
H	–2.7962604616	2.0354360062	–0.4524222302
H	–0.3247274282	2.1062778959	–0.423128726
H	5.4867545341	0.4328155832	1.4021802102
H	5.4886851978	1.1817134858	–0.8448113169
H	5.5512592179	–1.1381145075	–0.3693142171

Tab. A.79 Standard Orientierung von **TS-PhCl-Meisenheimer** [stationärer Punkt, B3LYP/6-31+G(d), CPCM].

Atomsymbol	x	y	z
C	0.193762	–0.082775	–0.049350
Br	–1.709539	–0.802568	0.064126
C	0.916296	–0.546668	–1.186340
C	2.296421	–0.655357	–1.135398
C	3.004018	–0.453209	0.064230
C	2.270477	–0.172883	1.220932
C	0.880433	–0.060920	1.192320
Si	–0.473194	2.354387	–0.224665
H	0.393777	–0.695504	–2.125939
H	2.833040	–0.929979	–2.041802
H	4.085271	–0.549961	0.096788
H	2.780052	–0.070217	2.177364
H	0.335682	0.148318	2.107363
H	0.873851	3.058528	3.058528
H	–0.886659	2.575005	1.219016
H	–1.324881	3.423129	–0.933532

Quantenchemische Studien bezüglich des Mechanismus bei der Reaktion von Lithiosilanen mit *p*-Chlor- und *p*-Bromanisol

Tab. A.80 Standard Orientierung von **TS-*p*-Chloranisol-at** [stationärer Punkt, B3LYP/6-31+G(d), CPCM].

Atomsymbol	x	y	z
C	–0.0200539097	0.0418265483	0.0005839389
Cl	2.2337145585	0.010136393	–0.0189716876
C	–0.7589440323	–1.1451368934	0.0934562778
C	–2.1594086897	–1.1349971777	0.1080308376
C	–2.8493881262	0.0843946254	0.028687173
C	–2.1327934026	1.2836251576	–0.0645662366
C	–0.7236512229	1.2431352906	–0.0770094073
Si	4.7478379873	–0.0196427897	–0.0420839171
O	–4.2283760758	–0.0015703546	0.0502692007
C	–4.9772803726	1.2062611168	–0.0326990502
H	–0.2489833979	–2.1097821223	0.1565609452
H	–2.7322751764	–2.0605240289	0.1801961317
H	–2.6414533967	2.2425640482	–0.1271669701
H	–0.1886435379	2.1935132187	–0.1504148066
H	5.4174780592	0.0346192197	1.3126667138
H	5.4026143679	1.1251327842	–0.7817951423
H	5.3847512801	–1.2344628642	–0.6786549367
H	–6.0278087668	0.9094306528	–0.0014478841
H	–4.7753084139	1.7378575077	–0.9720056548
H	–4.7597457315	1.8703386679	0.8142774745

Tab. A.81 Standard Orientierung von **TS-*p*-Chloranisol-Meisenheimer** [stationärer Punkt, B3LYP/6-31+G(d), CPCM].

Atomsymbol	x	y	z
C	0.0247819237	0.0201933492	0.0206007693
Cl	1.669420088	–1.0208010506	0.0869403879
C	–0.7557437486	–0.1073435916	1.2056590218
C	–2.1392991954	–0.1320940325	1.1422958858
C	–2.8101962675	–0.1140632507	–0.0968511067
C	–2.056936714	–0.1002883189	–1.2715909843
C	–0.6539156361	–0.0785350656	–1.2165189174
Si	1.0416219196	2.2743610125	–0.2066093283
O	–4.1935294444	–0.1314566662	–0.0371337401
C	–4.907998288	–0.1277323533	–1.2662299147
H	–0.2622148096	–0.1193150089	2.1748093166
H	–2.7263695539	–0.1745443034	2.0596189603
H	–2.5294102384	–0.123830464	–2.2498351352

H	–0.0895323954	–0.0891616449	–2.1456925246
H	–0.2796448634	3.018804888	–0.1235009385
H	1.2322089044	2.1933392242	–1.7120795456
H	1.9979910447	3.4534370478	0.1008239906
H	–5.967121133	–0.1297112095	–0.9995450359
H	–4.6804373926	–1.0207597601	–1.8643887255
H	–4.6813132	0.7703671984	–1.8569534353

Tab. A.82 Standard Orientierung von **TS-*p*-Bromanisol-at** [stationärer Punkt, B3LYP/6-31+G(d), CPCM].

Atomsymbol	x	y	z
C	0.031158416	0.0154107276	–0.0142276685
Br	2.3949379118	–0.0075230365	–0.2745530579
C	–0.7183270031	–1.1618601565	0.1501216672
C	–2.1099566827	–1.1482617636	0.305492318
C	–2.7960609108	0.074973602	0.2986425293
C	–2.0844837044	1.2691941793	0.1370764337
C	–0.6845670775	1.2166147206	–0.0162245747
Si	4.9398153613	–0.0163734282	–0.548140406
O	–4.167569115	–0.0017476226	0.4584973109
C	–4.9101322066	1.2120158575	0.4570134724
H	–0.2154890175	–2.1332332599	0.1599952205
H	–2.6778820823	–2.0709808628	0.4324058037
H	–2.5907583343	2.2314491095	0.1279575483
H	–0.1583274134	2.167561588	–0.1402811414
H	5.7169511833	0.0231109238	0.7442430465
H	5.4998916191	1.1465362908	–1.3289964774
H	5.5035866198	–1.2210077653	–1.2600634233
H	–5.9548085512	0.9240734487	0.5938224522
H	–4.800479801	1.7470143866	–0.4956690374
H	–4.6020372116	1.8705580611	1.2799819839

Tab. A.83 Standard Orientierung von **TS-*p*-Bromanisol-Meisenheimer** [stationärer Punkt, B3LYP/6-31+G(d), CPCM].

Atomsymbol	x	y	z
C	0.0068013948	0.0227486736	0.0273856478
Br	1.8116271459	–1.0396477164	0.0794931619
C	–0.7683463432	–0.1299041002	1.2089122179
C	–2.1524920145	–0.1451442554	1.1477030321
C	–2.8220402705	–0.1229115153	–0.0924874116
C	–2.0697278466	–0.0966668029	–1.2674931917
C	–0.6663243272	–0.080348038	–1.2083407456
Si	1.0351430262	2.2962997753	–0.1944408528

O	–4.203922815	–0.1424390748	–0.0337211419
C	–4.9180419823	–0.1199052857	–1.2633816908
H	–0.2762825057	–0.1427542702	2.1787934131
H	–2.7393406735	–0.1941422506	2.0647261271
H	–2.5409126365	–0.1151275834	–2.2463717095
H	–0.102082404	–0.0724413636	–2.137719125
H	–0.2856870973	3.0512989937	–0.2224895263
H	1.3019749689	2.1446106276	–1.6829692199
H	1.9798163849	3.4900733835	0.0975
H	–5.9771681441	–0.1237426838	–0.9969803766
H	–4.6917763469	–1.0050045325	–1.8735256136
H	–4.6888565134	0.786014019	–1.8407739944

Quantenchemische Studien zur Selektivität der Lithiierung im Disilan 17

Tab. A.84 Standard Orientierung des Modellsystems **SiMe-ED** [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
H	3.4637685668	–0.0220858901	–2.2202994292
H	3.9709113679	1.5625018878	–1.6275125932
H	–0.8032627993	–0.5192691382	–2.9557596034
H	5.4161053014	–0.344413312	–0.7432327953
H	–0.7204047699	2.3140261676	–3.9229598481
H	–2.538378276	–0.383621984	–2.7048607603
C	3.5415267086	0.6000142325	–1.319731285
H	0.2556041679	–4.8167994889	–3.0097691858
H	–1.2093802355	–4.0782707887	–2.3499641218
C	–1.5918599305	–0.6146960135	–2.2001895407
H	–3.5342708385	2.7203545571	–2.5557949623
H	1.4958031128	1.2989369307	–1.509753632
H	–1.6265194048	–1.6656973158	–1.8873343302
C	4.4450116748	–0.0985476827	–0.29561099
Li	1.1679258561	–2.0708947671	–1.6086020853
H	–0.4308988101	4.015595174	–3.5388371487
C	–0.3131577072	–4.6601877841	–2.0792274581
C	–0.3158861609	2.9909137108	–3.1600935554
H	3.6817978838	–2.1141283929	–0.5662613505
C	2.1404312911	0.8459539999	–0.749563966
H	0.7602338398	2.7972536522	–3.073057055
H	4.6454719694	0.5850307157	0.5428979167
H	–3.0790031157	4.3857582222	–2.1625644195
C	–3.0426288085	3.3486695868	–1.8025285891

C	0.516812143	–3.9831077617	–0.97624197
H	–0.6820033522	–5.6692882679	–1.7740535106
C	3.7518758839	–1.3609030415	0.2310732827
H	–3.8804210128	–1.0480707774	–0.6595528872
H	2.2087642646	1.570833413	0.0856051777
H	2.3651419044	–5.0847229574	–1.4957938784
N	1.4914292662	–0.3934504047	–0.2741070594
H	4.3331846918	–1.8192618576	1.040798252
H	–1.2776392016	–3.3032775801	0.1207950805
Si	–1.3024518821	0.5535351688	–0.7298669242
Si	–1.2437587541	2.8111567597	–1.5028704691
H	–3.6387681166	3.2883058216	–0.8846669664
C	1.6888787747	–4.9186777694	–0.6401261293
C	–0.3763164757	–3.9193367109	0.272222096
C	–3.8593536796	–0.430467087	0.235218207
C	2.3501047612	–1.041258475	0.7558456692
H	–5.7574288631	–1.1909474889	0.9187813711
H	2.3108324597	–4.5346520384	0.1847289194
C	0.1717602963	–0.0951637008	0.3359364809
H	0.1471162824	–3.5101864067	1.1518701862
H	1.3476028444	–5.9338360583	–0.3228858509
H	1.8466158017	–1.9567859812	1.0784513639
H	–0.7436760908	–4.9273000678	0.5819531204
C	–2.7675370823	0.424851389	0.4762779856
H	2.4267575892	–0.3733805093	1.6354939373
C	–4.9301571553	–0.517753968	1.1308734575
H	0.3048900618	0.5909017685	1.1954379114
H	–0.2056816589	–1.0340768994	0.759528209
H	–0.4890775537	5.0289749737	–0.6217402885
C	–0.4573451943	3.9992327695	–0.2406873234
H	0.59245457	3.7549525833	–0.0375466501
H	–0.9934660316	3.9885350705	0.7162604096
C	–2.7956757322	1.1902496219	1.6599315056
C	–4.9335030975	0.2508967513	2.2969843227
H	–1.9742274911	1.8671909528	1.8905767613
H	–5.7637555312	0.1828162897	2.9956391605
C	–3.8599235992	1.1064451075	2.561153785
H	–3.8512182765	1.7071990659	3.4677294426
O	1.8950296111	–1.8174349341	–3.4800992634
C	1.7569652163	–0.7493072839	–4.4109737979
H	2.7204609913	–0.5259076163	–4.8905422978
H	1.417530416	0.1299561799	–3.8602821614
H	1.0193704288	–1.0029195821	–5.1851581212
C	2.3704562418	–3.018019063	–4.0987913921
H	3.3683936232	–2.8509834406	–4.527415288
H	1.6791867389	–3.3406779598	–4.8881756472

H	2.415330086	–3.7813742765	–3.3224774305

Tab. A.85 Standard Orientierung des Modellsystems **SiMe-TS** [Übergangszustand, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
H	3.3826180646	–0.0778330387	–2.5229668694
H	3.8898266399	1.5850039424	–2.227104995
H	–0.6046637733	–0.3998080565	–2.8600580969
H	5.5364178248	–0.1293363464	–1.2969233774
H	–0.3615946926	2.526416702	–3.5880417362
H	–2.116445638	–1.0620650786	–2.2793083131
C	3.554598644	0.6640138799	–1.7328218133
H	0.2639182883	–4.301632338	–3.1413150805
H	–1.4659754673	–3.9785830581	–2.942187676
C	–1.1006306822	–0.7975672499	–1.9585965467
H	–3.4327913503	2.3207461901	–2.6711777811
H	1.4699941642	1.2529903651	–1.7369121851
H	–0.6492481952	–2.056509104	–1.566812952
C	4.6222547958	0.150996672	–0.7582039921
Li	0.9714513597	–1.7203945391	–1.6799847684
H	–0.5912016193	4.2244579095	–3.146374844
C	–0.5667847581	–4.3385708675	–2.4200055243
C	–0.2762104764	3.2444447163	–2.7624760497
H	3.9367331801	–1.9046218376	–0.6213506422
C	2.2316517534	0.9469531573	–1.0139516782
H	0.7839742526	3.3271866651	–2.4939335042
H	4.9001845889	0.9565452926	–0.0625540327
H	–3.3613922933	4.0123104013	–2.1468466191
C	–3.1821987282	2.9764593788	–1.8277599284
C	–0.2790092488	–3.5122995034	–1.1645550161
H	–0.73774527	–5.4107349025	–2.1918680227
C	4.0743385793	–1.038471459	0.0408888955
H	–3.8676571239	–0.7485728358	–0.7920085241
H	2.3678484628	1.7924009981	–0.3117292636
H	1.8956471247	–3.9607973149	–1.1650098388
N	1.7178317285	–0.2286998087	–0.2738199211
H	4.7839331203	–1.3488436051	0.8184440564
H	–2.3836443507	–3.3484544536	–0.5825356736
Si	–1.1133270508	0.4778272003	–0.5932787144
Si	–1.3730351979	2.7497957676	–1.2785467962
H	–3.8807610375	2.749622432	–1.0136526868
C	1.0134266145	–4.0222886243	–0.5049294437
C	–1.4253197695	–3.6913364194	–0.167240027
C	–3.7534700434	–0.4015169144	0.2323879078
C	2.7392990653	–0.687267201	0.7011914092

H	–5.7406552042	–1.038974904	0.7752906644
H	1.2544019594	–3.4783094172	0.4211990694
C	0.4782229745	0.1380496384	0.4699671331
H	–1.2596602279	–3.1218991583	0.7591142665
H	0.939272406	–5.0930429151	–0.2161277887
H	2.3323669108	–1.5553342236	1.2297259841
H	–1.5628861355	–4.7511319241	0.1266320901
C	–2.5441686039	0.194813687	0.637208115
H	2.902961169	0.1052086337	1.4563479896
C	–4.8215125539	–0.5695727218	1.1190277979
H	0.7025713514	0.9677127254	1.1660576166
H	0.2171006203	–0.7247568747	1.0968703534
H	–1.2219030361	5.0127045008	–0.1905424336
C	–1.0251359106	3.9820519315	0.1355724168
H	0.0184107664	3.9365841464	0.4730821983
H	–1.6651881745	3.7815228924	1.003613134
C	–2.4565958862	0.6210350695	1.9780316144
C	–4.7068800917	–0.1421321873	2.4443827508
H	–1.5448896296	1.093547517	2.3403425719
H	–5.5347029204	–0.2741005846	3.1370949203
C	–3.5180341038	0.4551428349	2.8726705128
H	–3.4166416652	0.7917256442	3.902230904
O	1.9354408014	–2.0143681276	–3.4747162529
C	1.2539995164	–1.8387450599	–4.7203597509
H	1.916136864	–1.3458083979	–5.4451182244
H	0.3815374899	–1.2139465955	–4.5316255993
H	0.9268800726	–2.8080632479	–5.1177943129
C	3.0872328135	–2.8444520823	–3.6191775037
H	3.7887176567	–2.4025534966	–4.3403103873
H	2.799709628	–3.8490806875	–3.9563050911
H	3.5692496581	–2.9159937293	–2.6429540933

Tab. A.86 Standard Orientierung des Modellsystems **$SiMe_3$-ED** [lokales Minimum, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
H	–0.0883092651	–0.0318230426	–0.4062131795
H	–0.2549501942	–0.3495077438	1.3221218326
H	7.1343931829	–0.0656063768	–0.0008677466
H	–1.0470080242	1.9826270554	0.6485678875
H	5.8898467593	–4.3621009369	–1.8906129815
H	7.2687986941	–1.7661808517	0.4758852877
C	0.2829133012	0.2601901517	0.5844408839
H	2.1328256367	0.8897654468	–5.5763417967
H	3.8275509135	0.7177401974	–5.1031210409
C	6.6174056988	–0.8851358773	0.5136392442

H	3.3376545142	–3.1181345743	–3.2771964155
H	1.9493024046	–1.1254824496	0.4879014763
H	6.5130310411	–0.5968852957	1.5673959788
C	0.0143579597	1.7530674546	0.8063206881
Li	2.0835619752	0.7030943013	–2.3717957364
H	6.7871694067	–3.8885226406	–3.3437563531
C	2.998575696	1.4392291518	–5.1727338038
C	6.4633156279	–3.5485181296	–2.3506118247
H	0.5702538291	2.4413975743	–1.1781473106
C	1.7777588576	–0.0645344378	0.6828474535
H	7.3659385908	–3.3972593044	–1.7458956383
H	0.2449288571	2.0178118877	1.8491283487
H	4.3386589723	–2.605793531	–4.6413640889
C	3.9665411265	–2.3020889661	–3.6534516396
C	2.7014717787	2.1252219523	–3.8287543692
H	3.2919217486	2.1708154641	–5.963827856
C	0.8962568954	2.5783162572	–0.1375584218
H	4.6836051544	–1.8249380931	2.6486312927
H	2.1242576489	0.1262096562	1.7172989953
H	0.6659950944	2.7523908178	–4.4442287565
N	2.5993034651	0.7292396351	–0.262283666
H	0.8050864959	3.6510608539	0.0743068435
H	4.8321692464	2.2280552983	–3.2468759707
Si	4.9251740053	–1.2482615076	–0.2917461874
Si	5.444418252	–1.9469208915	–2.5123762894
H	3.3328834677	–1.4210103026	–3.8049513695
C	1.6163416703	3.1840336405	–4.0879238906
C	3.9734276331	2.8923086991	–3.4339964801
C	4.1646441376	–2.6302626397	2.1325234005
C	2.3680080262	2.1800448554	–0.0044235184
H	3.6361299364	–3.6027022842	3.982844731
H	1.3786602649	3.773640863	–3.1881648812
C	4.0465361592	0.4639442007	–0.054339066
H	3.8376459762	3.5033664629	–2.5274134373
H	1.9226822593	3.9209692825	–4.869083187
H	2.9790705477	2.7455189663	–0.7121994295
H	4.3026930323	3.6031204606	–4.2296124835
C	4.1051534717	–2.6391174563	0.7241395572
H	2.7235256473	2.4244763224	1.0152237695
C	3.5717178906	–3.63782094	2.8977059853
H	4.3162431191	0.7653850483	0.9787886447
H	4.5959585555	1.1527729182	–0.7103708205
H	6.8828343448	–0.9747005004	–4.3035627648
C	6.5398785973	–0.6242990565	–3.3206730229
H	7.4313619863	–0.4097261172	–2.718720842
H	6.0031697803	0.3176178909	–3.4784367917

C	3.4294832474	–3.715535467	0.1182884317
C	2.9007160369	–4.6917104705	2.2698481863
H	3.3684602598	–3.7745241456	–0.9662357045
H	2.4413894605	–5.4788917624	2.8626146587
C	2.8329002995	–4.729421872	0.8751903574
H	2.3224311009	–5.5498338026	0.3757737426
O	0.6817283157	–0.6719716008	–2.8618847781
C	0.4481330038	–1.9934408268	–2.3845233181
H	–0.5959076508	–2.1089808118	–2.0607875966
H	1.1113545344	–2.1617366792	–1.5346754027
H	0.6665474279	–2.7297421241	–3.1697594798
C	–0.1391651769	–0.3512843534	–3.9895554077
H	–1.201023893	–0.4082954369	–3.7122110561
H	0.0619747646	–1.0442280539	–4.817257165
H	0.1162379795	0.6633877392	–4.2923164371

Tab. A.87 Standard Orientierung des Modellsystems **$SiMe_3$-TS** [Übergangszustand, B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
H	0.0022543912	0.0069469499	0.0078327809
H	0.005644717	0.0120684858	1.7736193814
H	6.9047414449	–0.0189491119	–1.2647047928
H	–1.1236113396	2.0752863315	0.7894669567
H	2.9391679284	–3.8860096311	0.6142655906
H	7.4949109632	–0.9101549399	0.1457153475
C	0.4050586049	0.5244350718	0.8891217834
H	1.5606736654	–0.121952159	–5.1771003657
H	2.7786656715	–1.3954465559	–5.3218842629
C	6.7884379117	–0.1376936677	–0.1809767522
H	2.0175788902	–1.8369578074	–1.486417534
H	2.2256979211	–0.6501799589	0.878341831
H	7.0917675929	0.806607178	0.2898971976
C	–0.0318388887	1.9945873365	0.8660596082
Li	2.0636437534	0.1594591402	–2.1936367734
H	3.6598235143	–4.8785431136	–0.6545898434
C	2.6430885501	–0.3069954267	–5.2409527983
C	3.8525592475	–4.0366414291	0.0254277524
H	0.2408986332	2.3451920292	–1.2490906197
C	1.9312253758	0.4034914801	0.8995242917
H	4.6538128423	–4.3434635827	0.7109092409
H	0.2567044408	2.4755287227	1.8123816173
H	2.6692561273	–2.6950654727	–2.877620486
C	2.9149826748	–1.9268643971	–2.1277670355
C	3.4024854539	0.2624548074	–4.0384707703
H	2.9829141598	0.1308715556	–6.201288296

C	0.6484853862	2.7190418496	–0.3020070153
H	6.0979894962	1.0432412165	2.5007746518
H	2.3282289769	0.8278571198	1.8393154652
H	2.1065006718	2.0538035612	–3.8047858315
N	2.5600294145	1.078216373	–0.2620696307
H	0.441061764	3.796467884	–0.2701776157
H	5.1318543275	–1.0370127929	–4.3558482336
Si	4.9995037245	–0.6208195343	0.2782869922
Si	4.3104791004	–2.5058255359	–1.0311266863
H	3.1819192946	–0.8111859344	–2.9629725854
C	3.1634179026	1.7805564732	–3.962715129
C	4.9005142446	0.0316218362	–4.2483763034
C	5.5973490906	0.202012867	2.9769518736
C	2.1653662539	2.5119604851	–0.2715109617
H	6.0925704601	0.9125421717	4.9519819535
H	3.7478481531	2.2568315868	–3.1616574586
C	4.046903448	1.0103992794	–0.1739923509
H	5.4996081039	0.4116567917	–3.4069551634
H	3.4611865891	2.2948221372	–4.9018904795
H	2.6384336463	2.9857959966	–1.1383684106
H	5.2782770354	0.5340341561	–5.1610383497
C	4.9722836449	–0.7841345954	2.1857360785
H	2.5778102029	3.0055497786	0.6289555538
C	5.599878321	0.1346027328	4.372742639
H	4.3950930875	1.7497498571	0.5735089557
H	4.4484540069	1.3479212082	–1.1376545363
H	5.5420180152	–3.8657865863	–2.7281434774
C	5.8299238049	–3.0568092634	–2.0422315588
H	6.6220000643	–3.4454654013	–1.3894138895
H	6.2562016791	–2.2494869841	–2.6459626632
C	4.3527671799	–1.8480543204	2.8668734095
C	4.9737898964	–0.9333147506	5.022700029
H	3.8642978054	–2.6372888671	2.3036728508
H	4.9759744306	–0.9916839335	6.1085737393
C	4.3505811894	–1.9263859667	4.2639742212
H	3.8642566965	–2.7653398463	4.7569375641
O	0.0673121911	0.0080760261	–2.8176524342
C	–0.5446046263	–1.2801505345	–2.9286285662
H	–1.5780047126	–1.2409292621	–2.5572596666
H	0.0385676453	–1.9767966621	–2.3267687635
H	–0.5422614834	–1.6152023926	–3.9741893178
C	–0.64565906	0.9863467194	–3.5738582631
H	–1.6734008788	1.0849854942	–3.1973441257
H	–0.6708829478	0.7102606285	–4.6362164069
H	–0.1248795494	1.9385392132	–3.4649649666

Rechnungen zur Stabilitat des experimentell vorgefundenen Silanolats 172 und seinem hypothetischem Silanol 173

Tab. A.88 Standard Orientierung des experimentell gefundenen Zinksilanolats **172** [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Br	1.1390070692	1.1115952179	–3.0395266697
H	2.2850534083	–2.3212740647	–2.6161953161
H	4.5280927896	1.5901831474	–2.2723941549
H	–5.0401666375	0.4888797629	–2.175739334
H	0.9010438499	–3.3579880081	–2.2675682822
Br	–2.0036687148	–1.4738534719	–2.1979606263
H	2.5392374437	–3.9513933951	–1.9526666215
C	1.8950557594	–3.0625698317	–1.9091965053
H	–6.6190741644	–1.3542476679	–1.5166977442
H	–0.9039044155	3.3386223799	–2.0022959805
H	4.8035891549	–0.768455498	–1.5301284109
H	–3.5571704671	2.166929579	–1.6123080232
H	–4.9329408332	–1.8713261113	–1.5219955158
H	3.087967217	–0.2743242405	–1.5288764932
C	4.4533882562	1.3648383041	–1.2030491996
Zn	–0.1840902561	–0.0656974622	–1.4795976253
C	–5.231695986	0.2237690377	–1.1326770624
H	–1.8160418348	4.5757367089	–1.1009606622
H	6.5967343564	1.140429259	–0.9585464738
C	–5.6590520318	–1.2389746937	–0.9982752722
C	4.0617163755	–0.1040466758	–1.0708582402
H	–5.9909924699	0.9039717663	–0.7297715495
H	3.6372355256	1.9860041198	–0.8151153346
H	5.9939950627	2.7407770503	–0.5295769105
C	–1.1109030573	3.7384650363	–1.0029416266
C	5.7646909212	1.6705789067	–0.4705866155
H	–3.2142978025	–0.0677554643	–0.8159394088
C	–3.5395962856	1.9634391966	–0.5352131531
H	–0.1684287708	4.1442995225	–0.6149757813
N	–3.9570143557	0.5210755856	–0.3772130395
H	–4.3297707717	2.5723461386	–0.0788308458
Si	1.7659932063	–2.4045567657	–0.1485493802
O	0.9285420482	–0.9940101874	–0.0765942666
H	4.3297707717	–2.5723461386	0.0788308458
O	–0.9285420482	0.9940101874	0.0765942666
Si	–1.7659932063	2.4045567657	0.1485493802
C	–5.7646909212	–1.6705789067	0.4705866155
H	–5.9939950627	–2.7407770503	0.5295769105

N	3.9570143557	–0.5210755856	0.3772130395
H	0.1684287708	–4.1442995225	0.6149757813
H	–6.5967343564	–1.140429259	0.9585464738
H	5.9909924699	–0.9039717663	0.7297715495
C	3.5395962856	–1.9634391966	0.5352131531
C	5.6590520318	1.2389746937	0.9982752722
H	3.2142978025	0.0677554643	0.8159394088
H	–3.6372355256	–1.9860041198	0.8151153346
C	1.1109030573	–3.7384650363	1.0029416266
C	5.231695986	–0.2237690377	1.1326770624
C	–4.0617163755	0.1040466758	1.0708582402
H	6.6190741644	1.3542476679	1.5166977442
H	1.8160418348	–4.5757367089	1.1009606622
C	–4.4533882562	–1.3648383041	1.2030491996
H	4.9329408332	1.8713261113	1.5219955158
H	–4.8035891549	0.768455498	1.5301284109
H	3.5571704671	–2.166929579	1.6123080232
H	–3.087967217	0.2743242405	1.5288764932
Zn	0.1840902561	0.0656974622	1.4795976253
H	0.9039044155	–3.3386223799	2.0022959805
H	–2.5392374437	3.9513933951	1.9526666215
H	5.0401666375	–0.4888797629	2.175739334
C	–1.8950557594	3.0625698317	1.9091965053
H	–4.5280927896	–1.5901831474	2.2723941549
H	–0.9010438499	3.3579880081	2.2675682822
Br	2.0036687148	1.4738534719	2.1979606263
H	–2.2850534083	2.3212740647	2.6161953161
Br	–1.1390070692	–1.1115952179	3.0395266697

Tab. A.89 Standard Orientierung des hypothetischen Zinksilanols **173** [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
H	0.0008734164	–0.0041398116	–0.0131899107
H	–0.0009492587	4.5495874899	0.0094486568
H	–0.4528892967	–1.715581798	0.0140662885
H	–0.6074359691	–0.7410858631	1.4787546702
C	–0.7255308729	–0.7201111529	0.3875959931
H	–1.3263790539	2.9956547456	1.3480230522
H	–0.7537531089	2.1796161852	–0.120783331
C	–1.0079828923	4.3110531347	–0.3562919046
H	–1.8227950525	–0.1506066579	–2.321530013
H	–1.9300876745	5.6691137842	1.0652115092
C	–1.4196741131	2.964212342	0.2482947831
H	–0.9278535369	4.20189255	–1.442730845
H	–1.7267892513	6.3483938522	–0.5502229298
C	–1.9929197808	5.4332179264	–0.0079413377

Si	–2.5007328086	–0.3085121851	–0.0825093653
O	–2.6051104651	–0.01375547	–1.7595272282
H	–3.0018702333	1.422297186	1.702856729
N	–2.8229417843	2.5775025726	–0.0865833046
H	–3.3215248241	–2.6583927597	–0.0451583802
H	–3.6972947567	3.7764215767	1.4264250132
C	–3.2090247091	1.3200639798	0.623674784
C	–3.4232082236	4.9976137574	–0.3463465812
C	–3.6681371581	–1.7041165484	0.3694439731
C	–3.7581289109	3.6701863836	0.3295141333
H	–4.1527679784	5.747988749	–0.0170853179
H	–3.7523278564	–1.8259620912	1.4573452581
H	–3.5539221508	4.8939163541	–1.4322294484
H	–4.2982102308	1.2262847964	0.5249712681
Zn	–3.1094351861	2.0872109529	–2.2043485067
H	–4.6715122313	–1.5115950815	–0.0283978092
H	–4.7702167577	3.3498711777	0.0724829818
Br	–1.1857815652	2.3275833331	–3.5282691899
Br	–5.4122857243	2.15047659	–2.5063636904

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Tab. A.90 Standard Orientierung des Disiloxans **A** [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	0.0397433134	0.0018923968	0.0327407012
O	–0.3927165879	–0.0110316034	1.6195234838
H	1.5209373391	0.0465243833	–0.0752269922
H	–0.4624126212	–1.2254295918	–0.6382459406
H	–0.5354184043	1.1966206013	–0.6384501452
C	0.4681066265	–0.0100667934	4.4477313701
Si	–0.9407013229	–0.0286859794	3.1760621179
H	–1.8067926044	1.1625086088	3.4072456946
H	–1.7644788028	–1.2518198825	3.3948482719
H	–0.5666935407	–0.8524102326	6.0457407147
H	–0.5946177277	0.7877304137	6.0503038003
N	–0.0112105393	–0.0220917729	5.8483324446
H	1.1309443981	–0.8735251844	4.3076934164
H	1.1030090495	0.8749581147	4.3129410996

Tab. A.91 Standard Orientierung von $ZnBr_2(H_2O)_2$ (**B**) [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Zn	–0.061739491	–0.02987879	0.0795121856
Br	–0.1096343771	2.2830745033	0.1387092481
O	–2.1894845352	–0.4420464721	0.1750984293
Br	0.6761288342	–2.0083632467	–0.8675472167
H	–2.7187793243	0.337691576	–0.0654157229
O	0.3700862399	–0.440348422	2.1654388152
H	–2.4426744698	–1.1694290184	–0.4188723649
H	0.7330759757	0.3397526327	2.6189472398
H	1.008442911	–1.1673863177	2.2650062253

Tab. A.92 Standard Orientierung des Startsystems **C** [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	0.3365623868	–0.1351556735	0.1122650109
O	–0.0917762605	0.1027557191	3.0358615298
H	1.6695216374	–0.2563862062	0.7383052664
H	–0.3538403691	1.1210947037	0.4526255248
H	0.4887420068	–0.2356216722	–1.3661138063
H	–3.7401954759	–2.5036623538	0.9235839256
N	–3.0251929198	–2.9381321222	1.5085617419
H	0.2393509697	–0.4144446405	3.7942764482
H	–0.5381431975	0.8869336683	3.3989904875
H	–3.5139977479	–3.456673197	2.2398347452
Zn	–1.9036233219	–1.3741358141	2.5456882386
C	–2.1424248897	–3.8422926524	0.7239363732
H	0.1826552804	–3.5353422706	–0.8017574892
Si	–1.0327265499	–2.789335874	–0.3942841151
H	–1.763728113	–2.3272760577	–1.6023187858
O	–0.6353931928	–1.4600878123	0.5626142226
H	–2.7072902538	–4.5951460613	0.1561313043
H	–1.5070889252	–4.3741963998	1.440503952
Br	–3.3651420583	0.4395472801	2.2520853989
Br	–0.8645989101	–2.8274033415	4.1132589974

Tab. A.93 Standard Orientierung von H_2O [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
O	–0.1150625973	–0.0225357265	0.0000000000
H	0.6085684465	–0.6666767432	0. 0000000000
H	0.3119323316	0.8469625549	0. 0000000000

Tab. A.94 Standard Orientierung des Übergangszustandes **TS** [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	–0.1017937815	0.0615868846	0.1532040557
O	0.1524134528	1.8623334833	–0.0220102391
H	–1.5180031209	–0.3154127686	0.0156034563
H	0.1509681889	0.0687076744	1.6236810748
H	1.0081524765	–0.7150777392	–0.42085723
H	0.0734680481	1.1058185863	–5.4211069686
N	–0.7204517508	1.4869427365	–4.9041040221
H	–0.6086480225	2.3881739301	–0.4400519208
H	0.9567401666	2.129211361	–0.5756751223
H	–1.1012434697	2.2400505847	–5.4786234925
Zn	–0.1108096148	2.1152530128	–3.0047358134
C	–1.7503090946	0.4143211615	–4.6675303659
H	–2.3260056772	–1.43765353	–2.6750352587
Si	–1.1489668289	–0.705406795	–3.2212845408
H	–0.1913015884	–1.7119184215	–3.771098089
O	–0.4526217801	0.3318981363	–2.1572727232
H	–1.9785033977	–0.1250973014	–5.5956352811
H	–2.6643000364	0.9238299821	–4.3431970144
Br	2.1010249618	2.760047677	–2.3858635609
Br	–1.7515091315	3.5333913452	–1.9482069439

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Die Standard Orientierung von **172** findet sich bereits in Tab. A.88 wieder.

Tab. A.95 ^{29}Si- und ^{13}C-Verschiebungen der Zinksilanolate **172** und **175**; Referenz: TMS [GAIO/B3LYP-IGLO-II//B3LYP/6-31+G(d)].

Spektrum [Atom(e)]	**172** [ppm]	**175** [ppm]
^{29}Si (Si)	–1 (2 Si)	1.1 (1 Si)
^{13}C (Si*C*H$_3$)	2.9, 3.2 (je 2 C)	0.9, 2.6 (je 1 C)
^{13}C (H$_3$*C*CO$_2$)	-	23.9, 24.8, 24.9, 25.3 (je 1 C)
^{13}C (NCH$_2$CH$_2$*C*H$_2$)	26.0 (2 C)	26.1 (1 C)
^{13}C (NCH$_2$*C*H$_2$CH$_2$)	27.1, 27.8 (je 2 C)	26.2, 27.5 (je 1 C)
^{13}C (NCH$_2$CH$_2$CH$_2$)	60.6, 64.2 (je 2 C)	63.1, 64.3 (je 1 C)
^{13}C (Si*C*H$_2$N)	55.1 (2 C)	54.0 (1 C)
^{13}C (H$_3$C*C*O$_2$)	-	187.39, 187.40, 189.4, 189.6 (je 1 C)

Tab. A.96 Standard Orientierung von **175** [B3LYP/6-31+G(d)].

Atomsymbol	x	Y	z
H	–3.6970373694	0.9006996887	–4.6158529796
H	–4.1437415559	–0.7867164498	–4.3128140044
C	–3.5878619408	0.0647961715	–3.9133510044
H	–2.5230554279	–0.1664783512	–3.8313444983
C	–4.1480391398	0.4955210095	–2.5717575511
O	–5.3760626552	0.252379869	–2.3492053013
H	–6.8393164508	5.2393619942	–2.2473064774
H	–9.7420384259	–1.9969362091	–1.816467306
O	–3.3590332594	1.0826505519	–1.7729608251
H	–4.1865556558	–5.0570552838	–1.3719877573
H	–4.7745519959	–2.6463040662	–1.4317725052
H	–5.7048455282	5.921083661	–1.0413039434
C	–6.4880658223	5.1804901661	–1.2113768749
H	–10.340310339	–1.4396188284	–0.2563597872
C	–9.54304975	–2.0151767043	–0.7389091649
O	–8.1227630932	–0.1206435339	–0.788068276
H	–3.0208241903	–2.7945101621	–1.530983587
O	–6.8137554026	2.8313257701	–1.1025029832
C	–5.9814088916	3.7794410674	–0.9303724166
C	–8.1998000236	–1.360694592	–0.4643513488
Zn	–6.4747044326	0.8995744263	–0.8053109967
O	–4.7804864743	3.6508815412	–0.5485934348
C	–3.8833837095	–2.9612038465	–0.8747708703
H	–7.3484520666	5.392339549	–0.567063362
O	–7.2728211518	–2.033659266	0.0470822335
C	–3.9965523546	–4.4412461408	–0.4851601056
H	–6.0945613045	–4.4260289598	0.072347735
H	–9.5580524704	–3.0464152971	–0.3805109966
Zn	–3.7494902466	2.0069714161	–0.0241616511
H	–3.0429555633	–4.7846571877	–0.0573003103
C	–5.1240134754	–4.6328665773	0.5390716162
H	–5.1522806376	–5.6665263124	0.9058429739
H	–3.6837282714	–1.011368293	0.1037171194
C	–3.7084118103	–2.0699311209	0.3522137371
H	–5.7313860881	–2.0323921761	0.8254613143
O	–5.2484951335	0.9202250568	0.7669981253
O	–2.0998269329	2.4907966436	0.8447895716
H	–2.7872449607	–2.3002629613	0.8968692581
N	–4.8445131655	–2.2630628064	1.3329728966
O	–1.9700937238	0.3576318403	1.5274002335
C	–1.4862168151	1.4982952801	1.4157267413
C	–4.9537091862	–3.7093186185	1.7458630005
H	0.5517711366	2.116365963	1.1268260959

H	–5.8100509478	–3.7793083635	2.4220103059
H	–7.8341592544	–0.4343252616	2.198856092
C	–0.1049001769	1.8293299789	1.9562414735
H	–4.04261554	–3.9394778071	2.3105065936
H	–7.7929380075	1.2879880806	2.6021645612
Si	–5.4655179132	0.4262534997	2.3291752094
H	–0.1631331761	2.6902589271	2.6312239466
C	–7.2967978058	0.3246355827	2.7761965485
C	–4.7016103476	–1.3422715803	2.5283499284
H	0.3222838823	0.9718499983	2.4804809634
H	–3.6313042647	–1.2595593015	2.740274177
H	–5.1776803411	–1.8450463914	3.3780808783
H	–3.5157128314	1.5604661003	3.4165528668
H	–7.415001784	0.0842015306	3.8417494218
H	–4.9877292282	2.5436900515	3.5463774482
C	–4.5952175149	1.5197173187	3.5887627542
H	–4.7639889928	1.1477397158	4.6086344988