Supporting information belonging to the publication

"A Diastereomerically Enriched, Dimeric Organolithium Compound and the Stereochemical Course of its Transformations"

Christian Unkelbach, Bors C. Abele, Klaus Lehmen, Benedikt Waerder, Kerstin Wild and Carsten Strohmann*
Anorganische Chemie, Technische Universität Dortmund, Otto-Hahn-Straße 6, 44227 Dortmund, Germany

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Experimental Details

General remarks

Trichloro(chloromethyl)silane was received by Wacker Chemie AG. (*S*)-2-methoxy-methylpyrrolidine was synthesized according to a literature procedure.[i] All manipulations were conducted under an atmosphere of dry argon using standard Schlenk techniques. THF, diethyl ether, toluene and *n*-pentane were purified by distillation from sodium/benzophenone and stored under an atmosphere of argon. NMR spectra were recorded with a Bruker Avance-400 DR X or Bruker Avance-300 DP X, chemical shifts are referred to TMS with the deuterium signal of the solvent serving as internal lock and the residual solvent signals as additional reference. GC/MS analyses were performed on an Agilent 6890 5972 GC MS system (temperature program: 50 °C (2 min) – 300 °C (5 min) with 40 °C/min and a HP Mass Selective Detector 5973 (EI(+)-MS, 70 eV). Elemental analyses were performed with a Leco CHNS-932/O VTF-900 analyzer. Powder diffraction spectra were recorded on a Siemens D500 diffractometer.

Synthesis of chloro(chloromethyl)diphenylsilane 2

The compound was synthesized according to a literature procedure[ii] in 63 % yield.

Synthesis of ethyl(chloromethyl)diphenylsilane 3

Following standard Grignard procedures, a solution of ethylmagnesium bromide was freshly prepared from magnesium turnings (2.00 g, 82.2 mmol) and bromoethane (8.97 g, 82.2 mmol) in diethyl ether (150 mL). The solution was filtrated and poured to a solution of **2** (11.0 g, 41.1 mmol) in diethyl ether (100 mL) at 0 °C and the reaction mixture stirred for 18 h at room temperature. After quenching of the reaction mixture by slow addition of water (100 mL) the organic phase was separated and dried over sodium sulfate and concentrated to dryness. Bulb-to-bulb destillation of the crude product under reduced pressure (144 °C, $2 \cdot 10^{-1}$ mbar) afforded **3** as a colorless oil (8.34 g, 32.0 mmol, 76 %). ^{1}H-NMR (400 MHz, C_6D_6): δ = 1.15 (t, 3H, ^{3}J(H,H) = 7.5 Hz; $SiCH_2CH_3$), 1.32 (q, 2H, ^{3}J(H,H) = 7.5 Hz; $SiCH_2CH_3$), 3.35 (s, 2H; $SiCH_2Cl$), 7.41-7.48 (m, 6H; *m*-H, *p*-H), 7.61-7.63 (m, 4H; *o*-H); {^{1}H}^{13}C-NMR (400 MHz, C_6D_6): δ = 3.2 ($SiCH_2CH_3$), 7.2 ($SiCH_2CH_3$), 27.5 ($SiCH_2Cl$), 128.0 (4C, *m*-Ph), 129.9 (2H, *p*-Ph), 133.3 (2C, *i*-Ph), 135.0 (4C, *o*-Ph); {^{1}H}^{29}Si-NMR (59.9 MHz,

C_6D_6): δ = –7.6; elemental analysis (%) calcd. for $C_{15}H_{17}ClSi$: C 69.07, H 6.57; exp.: C 69.4, H 6.7; GC/MS retention time: 6.71; EI-MS, *m/z* (%): 260 (1) [M^+], 211 (94) [$(M - CH_2Cl)^+$], 183 (100) [$(M - Ph)^+$].

Synthesis of ethyl(iodomethyl)diphenylsilane 4

To 8.00 g (30.7 mmol) **2** in acetone (50 mL) were added 9.14 g (61.3 mmol) of sodium iodide and the reaction mixture was heated under reflux for 48 h. The solvent was removed *in vacuo* and the residue dissolved in *n*-pentane and the salts separated by filtration. The filtrate was dried over sodium sulfate and concentrated to dryness. Bulb-to-bulb destillation of the crude product under reduced pressure (180 °C, $2 \cdot 10^{-1}$ mbar) afforded **4** as a light-yellow oil (9.56 g, 27.2 mmol, 88 %). ^{1}H-NMR (400 MHz, C_6D_6): δ = 1.09 (t, 3H, ^3J(H,H) = 7.8 Hz; $SiCH_2CH_3$), 1.31 (q, 2H, ^3J(H,H) = 7.8 Hz; $SiCH_2CH_3$), 2.52 (s, 2H; $SiCH_2I$), 7.38–7.46 (m, 6H; *m*-H, *p*-H), 7.56-7.59 (m, 4H; *o*-H); {^{1}H}^{13}C-NMR (400 MHz, C_6D_6): δ = –17.7 ($SiCH_2I$), 4.4 ($SiCH_2CH_3$), 7.1 ($SiCH_2CH_3$), 127.9 (4C, *m*-Ph), 129.8 (2H, *p*-Ph), 133.9 (2C, *i*-Ph), 135.0 (4C, *o*-Ph); {^{1}H}^{29}Si-NMR (59.9 MHz, $CDCl_3$): δ = –6.1; elemental analysis (%) calcd. for $C_{15}H_{17}ISi$: C 51.14, H 4.86; exp.: C 51.2, H 5.1; GC/MS retention time: 7.19; EI-MS, *m/z* (%): 352 (5) [M^+], 323 (100) [$(M - C_2H_4)^+$], 183 (51) [$(M - C_6H_6 - C_7H_7)^+$].

Synthesis of ethyl[(*S*)-2-(methoxymethyl)pyrrolidinomethyl]diphenylsilane (*S*)-5

To a solution of **4** (8.66g, 24.6 mmol) in toluene (50 mL) was added SMP (2.83 g, 24.6 mmol) and triethyl amine (2.48 g, 24.6 mmol) and the mixture was heated under reflux for 72 h. The reaction mixture was extracted with hydrochloric acid (1 M, 3 x 50 mL). The aqueous extracts were made basic by the slow addition of aqueous potassium hydroxide and extracted with diethyl ether (3 x 50 mL). The combined organic extracts were dried over sodium sulfate and concentrated to dryness. Bulb-to-bulb destillation of the crude product under reduced pressure (210 °C, $2 \cdot 10^{-1}$ mbar) afforded (*S*)-**5** as a light-yellow oil (6.26 g, 18.4 mmol, 75 %). ^{1}H-NMR (400 MHz, C_6D_6): δ = 1.00-1.25 (m, 5H; $SiCH_2CH_3$), 1.45-1.70, 1.75-1.88 (m, 4H; $CHCH_2CH_2CH_2$), 1.90-2.00, 2.73-2.84 (m, 2H; NCH_2CH_2), 2.31, 3.13 ["AB-system", 2H, ^2J(H,H) = 14.5 Hz; $SiCH_2N$], 2.35-2.50 [m, 1H; NC(C)*H*C], 3.20-3.30 (m, 2H; OCH_2C), 3.32 (s, 3H; OCH_3), 7.20-7.43 (m, 6H; *m*-H, *p*-H), 7.59-7.61 (m, 4H; *o*-H); {^{1}H}^{13}C-NMR (400 MHz, C_6D_6): δ = 5.4 ($SiCH_2CH_3$), 8.2 ($SiCH_2CH_3$), 24.1 (NCH_2CH_2), 29.2 ($CHCH_2CH_2$), 43.4 ($SiCH_2N$), 58.6 (NCH_2C), 59.1 (OCH_3), 68.1 [NC(C)HC], 77.7 (OCH_2C), 128.4 (2C), 128.5 (2C; *m*-Ph), 129.8, 129.9 (*p*-Ph), 135.8 (2C), 135.9 (2C; *o*-Ph), 136.9, 137.2 (*i*-Ph); {^{1}H}^{29}Si-NMR (59.9 MHz, C_6D_6): δ = –10.0; elemental analysis (%) calcd. for $C_{21}H_{29}NOSi$: C 74.28, H 8.61, N 4.12; exp.: C 74.2, H 8.8, N 3.9; GC/MS retention time: 7.76; EI-MS, *m/z* (%): 339 (1) [M^+], 294 (100) [$(M - CH_2OMe)^+$], 128 [$(SMP{=}CH_2)^+$]; $_D[\alpha]^{25}$ = –38° (1.1, *n*-hexane).

Crystallization of α-lithiated ethylsilane [(*R*,*S*)-6]$_2$

Ethylsilane (*S*)-**5** (220 mg, 650 µmol), was dissolved in *n*-pentane (2 mL) and cooled to –110 °C. *t*-BuLi (420 µL of a 1.7 M solution in *n*-pentane, 713 µmol) was added dropwise. The reaction mixture was stored at –78 °C for 4 d and the solution was separated. The precipitate was washed with *n*-pentane (3 x 2 mL), dissolved in toluene (2 mL) and *n*-pentane (2 mL) was added. After 3 d, [(*R*,*S*)-**6**]$_2$ was obtained as colorless, block-shaped crystals suitable for X-ray crystal structure determination (200 mg, 578 µmol, 89 %). Sufficiently resolved NMR spectra could not be recorded due to the low solubility of the lithiated compound in apolar solvents at low temperatures.

Synthesis of α-stannylated ethylsilane (*S*,*S*)-7

Ethylsilane (*S*)-**5** (500 mg, 1.47 mmol) was dissolved in *n*-pentane (10 mL) and upon cooling to –115 °C *t*-BuLi (950 µL of a 1.7 M solution in *n*-pentane, 1.62 mmol) was slowly added. The reaction mixture was allowed to warm to –78 °C over 3 h after which solid Me_3SnCl (323 mg, 1.62 mmol) was added and the mixture was allowed to warm to rt.

Note: For the other entries in the article's Table 1, the temperature at which *t*-BuLi was added ($T_{lithiation}$) and the temperature to which the reaction was allowed to warm prior to quenching (T_{max}) were changed accordingly, yielding the respective d.r.'s in the product indicated in the table. In case of entries 9 and 10, 5 min after the addition of *t*-BuLi at –40 °C, THF (0.2 mL; entry 9) or TMEDA (188 mg, 1.62 mmol; entry 10) were added and the solution allowed to warm to –20 °C.

Work up:
After warming to rt, the volatile components of the reaction mixture were removed *in vacuo* and the residue was taken up in *n*-pentane (30 mL) and washed with an aqueous saturated solution of sodium hydrogen carbonate (3 x 10 mL). The organic phase was dried over sodium sulfate and concentrated to dryness. Bulb-to-bulb destillation of the crude product under reduced pressure (260 °C, $2 \cdot 10^{-1}$ mbar) afforded (*S*,*S*)-**7** as a colorless oil in yields typically between 85 and 91 %. The d.r. was determined by ^{1}H NMR (via integration of the Sn(CH_3)$_3$ and SiCH_2N signals denoted below; D1 corresponds to (*S*,*S*)-**7** and D2 to (*R*,*S*)-**7**).

^{1}H-NMR (400 MHz, C_6D_6): δ = 0.05 [s, 9H, ^{2}J(H,^{119}Sn) = 49.2 Hz , ^{2}J(H,^{119}Sn) = 51.7 Hz; Sn(CH_3)$_3$, D1], 0.08 [s, 9H, ^{2}J(H,^{119}Sn) = 49.2 Hz , ^{2}J(H,^{119}Sn) = 51.7 Hz; Sn(CH_3)$_3$, D2], 0.98 [q, 1H, ^{2}J(H,H = 7.8 Hz); SiC(Sn)*H*], 1.10-1.55, 1.75-1.90 (m, 4H; CHCH_2CH_2CH$_2$), 1.48 [d, 3H, ^{2}J(H,H) = 7.8 Hz; C(Sn)CH_3]. 1.90-2.00, 2.80-2.89 (m, 2H; NCH_2CH$_2$), 2.30, 3.12 [“AB-system”, 2H, ^{2}J(H,H) = 14.3 Hz; SiCH_2N, D1], 2.43, 3.38 [“AB-system”, 2H, ^{2}J(H,H) = 14.6 Hz; SiCH_2N, D2], 2.49-2.56 [m, 1H; NC(C)*H*C], 3.24 (s, 3H; OCH_3), 3.43-3.50 (m, 2H; OCH_2C), 7.24-7.35 (m, 6H; *m*-Ph, *p*-Ph), 7.65-7.67 (m, 2H; *o*-Ph), 7.88-7.91 (m, 2H; *o*-Ph). {^{1}H}^{13}C-NMR (400 MHz, C_6D_6): δ = –8.8 [Sn(*C*H$_3$)$_3$, ^{1}J(C,^{117}Sn) = 304.2 Hz, ^{1}J(C,^{119}Sn) = 317.8 Hz], 1.2 [Si*C*HSn, ^{1}J(C,^{117}Sn) = 260.1 Hz, ^{1}J(C,^{119}Sn) = 273.1 Hz], 12.6 [CH(Sn)*C*H$_3$, ^{2}J(C,Sn) = 25.3 Hz], 24.0 (NCH$_2$*C*H$_2$), 29.0 (CH*C*H$_2$CH$_2$), 44.8 [Si*C*H$_2$N, ^{1}J(C,Si) = 9.7 Hz], 58.6 (N*C*H$_2$C), 59.2 (O*C*H$_3$), 68.3 [N*C*(C)HC], 77.8 (O*C*H$_2$C), 127.67 (2C), 127.72 (2C; *m*-Ph), 129.1, 129.2 (*p*-Ph), 135.0 (2C), 135.1 (2C; *o*-Ph), 136.1, 136.5 (*i*-Ph); {^{1}H}^{29}Si-NMR (59.9 MHz, C_6D_6): δ = –8.5; {^{1}H}^{119}Sn-NMR (60 MHz, C_6D_6): δ = 16.2 (D1), 17.0 (D2); elemental analysis (%) calcd. for $C_{24}H_{37}NOSiSn$: C 57.38, H 7.42, N 2.79; exp.: C 57.5, H 7.6, N 2.6; GC/MS retention time: 8.96; EI-MS, *m/z* (%): 502 (2) [M^{+}], 458 (71) [(M – CH$_2$OMe)$^{+}$], 338 (100) [(M – SnMe$_3$)$^{+}$].

Synthesis of methyl iodide adduct (*R*,*S*,*S*)-8
Stannane (*S*,*S*)-**7** (300 mg, 597 µmol, d.r. = 86:14) was dissolved in acetone (20 mL) and cooled to –78 °C. Iodomethane (100 mg, 705 µmol) was added and the solution warmed to rt. The volatile components were removed in vacuo upon which a microcrystalline, bright yellow solid remained which was washed with *n*-pentane (3 x 5 mL) and recrystallized from toluene/*i*-PrOH to yield (*R*,*S*,*S*)-**8** as pale yellow blocks suitable for X-ray crystal structure determination (369 mg, 573 µmol, 85 %). The homogenity of the crystalline sample was verified via powder diffraction. ^{1}H-NMR (400 MHz, C_6D_6): δ = –0.20 [s, 9H, ^{2}J(H,^{117}Sn) = 50.4 Hz, ^{2}J(H,^{119}Sn) = 53.0 Hz; Sn(CH_3)$_3$], 1.06 [q, 1H, ^{3}J(H,H) = 7.5 Hz; SiC(*H*)CH$_3$], 1.32 [d, 3H, ^{3}J(H,H) = 7.5 Hz, ^{3}J(H,^{117}Sn) = 62.7 Hz, ^{3}J(H,^{119}Sn) = 64.5 Hz; SnC(H)CH_3], 1.79-1.88 (m, 2H), 2.03-2.06 (m, 1H), 2.25-2.36 (m, 1H; NCH$_2$CH_2CH_2) 2.91 (s, 3H; NCH_3), 3.48 (s, 3H; OCH_3), 3.63-3.71 [m, 1H; NC(*H*)CH$_2$], 3.74-3.86 (m, 1H), 4.48-4.56 (m, 1H; NCH_2), 3.82, 4.39 [„AB-System“, 2H, ^{2}J(H,H) = 15.3 Hz; SiCH_2N], 7.45-7.56 (m, 6H; ar. H, *m*-C*H*, *p*-C*H*), 7.69-7.72 (m, 4H; ar. H, o-C*H*). {^{1}H}^{13}C-NMR (100 MHz, $CDCl_3$): –9.5 [3C, Sn(*C*H$_3$)$_3$], 0.1 [Si*C*(H)Sn], 10.8 [SiC(H)*C*H$_3$], 20.5, 23.6, 55.6, 59.4, 67.8, 69.7, 128.9, 130.9, 132.2, 131.7, 135.3, 135.6 (ar. *C*H); elemental analysis (%) calcd. for $C_{21}H_{29}NOSi$: C 46.60, H 6.26, N 2.17; exp.: C 46.9, H 6.3, N 2.0.

Crystal-Structure Determination

The crystals of (*R*,*S*)-**6** were mounted in an inert oil (perfluoropolyalkylether) at –80 °C (N_2 stream) using the X-TEMP 2 device.[v] Crystal structure determination of (*R*,*S*)-**6** was accomplished on a Stoe IPDS diffractometer; data collection: Expose in IPDS (Stoe & Cie, 1999); cell determination and –refinement: Cell in IPDS (Stoe & Cie, 1999); integration: Integrate in IPDS (Stoe & Cie, 1999); numerical absorption correction: Faceit in IPDS (Stoe & Cie, 1999). Crystal structure determination of (*R*,*S*,*S*)-**8** was accomplished on a Oxford Diffraction Xcalibur S diffractometer; data collection: CrysAlis CCD (Oxford Diffraction, 2006); cell refinement: CrysAlis RED (Oxford Diffraction, 2006); data reduction: CrysAlis RED; absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2006). The structures were solved by applying direct and Fourier methods, using SHELXS97[iii] and SHELXL-97.[iv] The non-hydrogen atoms were refined anisotropically. All of the H-atoms – except the ones located on the metalated carbon centres of (*R*,*S*)-**6** and (*R*,*S*,*S*)-**8** – were placed in geometrically calculated positions and each was assigned a fixed isotropic displacement parameter based on a riding-model. The hydrogen-atoms located at C4 on (*R*,*S*)-**6** and C1 on (*R*,*S*,*S*)-**8** were found and could be freely refined via Difference-Fourier-Synthesis. CCDC 836558 [(*R*,*S*)-**6**] and CCDC 836557 [(*R*,*S*,*S*)-**8**] contain the detailed crystallographic data for this publication. This data may be obtained free of charge from the Cambridge Crystallographic Data Center through www.ccdc.cam.ac.uk/data_request/cif.

Table 1 Crystal Data and Structural Refinement Details for compounds (*R*,*S*)-**6** and (*R*,*S*,*S*)-**8**

compound	(*R*,*S*)-**6**	(*R*,*S*,*S*)-**8**
empirical formula	$C_{42}H_{56}Li_2N_2O_2Si_2$	$C_{26}H_{37}INOSiSn$
molecular mass [g·mol^{-1}]	690.96	653.25
temperature [K]	173(2)	173(2)
wave length [Å]	0.71073	0.71073
crystal system	monoclinic	orthorhombic
space group (Nr.)	*C*2 (5)	$P2_12_12_1$ (19)
a [Å]	20.016(6)	10.3994(2)
b [Å]	11.190(2)	12.5653(2)
c [Å]	9.266(2)	21.0997(3)
α [°]		
β [°]	95.48(3)	
γ [°]		
cell volume V [Å^3]	2066.0(9)	2757.1 (1)
Z	2	4
calculated density *ρ* [g·cm^{-3}]	1.111	1.574
absorption coefficient *μ* [mm^{-1}]	0.121	2.107
F(000)	1120	1300
crystal size [mm^3]	0.40 x 0.40 x 0.20	0.30 x 0.20 x 0.20
range for data collection 2*θ* [°]	2.86 – 27.96	1.93 – 26.00
index ranges	$-26 \le h \le 26$	$-12 \le h \le 12$
	$-14 \le k \le 14$	$-15 \le k \le 15$
	$-12 \le l \le 12$	$-26 \le l \le 26$
reflections collected	11770	61579
independent reflections	4871 (R_{int} = 0.1016)	5405 (R_{int} = 0474)
refinement method	Full-matrix least-squares on F^2	
data / restraints / parameter	4871 / 1 / 230	5405 / 0 / 281
goodness-of-fit on F^2	1.058	1.009
final *R*-values [$I > 2\sigma(I)$]	*R1* = 0.0476, *wR2* = 0.1253	*R1* = 0.0207 *wR2* = 0.0417
R-values (all data)	*R1* = 0.0526, *wR2* = 0.1293	*R1* = 0.0253 *wR2* = 0.0421
absolute structure parameter	–0.13(11)	–0.03(1)
largest diff. peak and hole [e·Å^{-3}]	0.392 and –0.482	0.619 and –0.304

2.) Crystallographic data for compound (*R*,*S*)-**6**

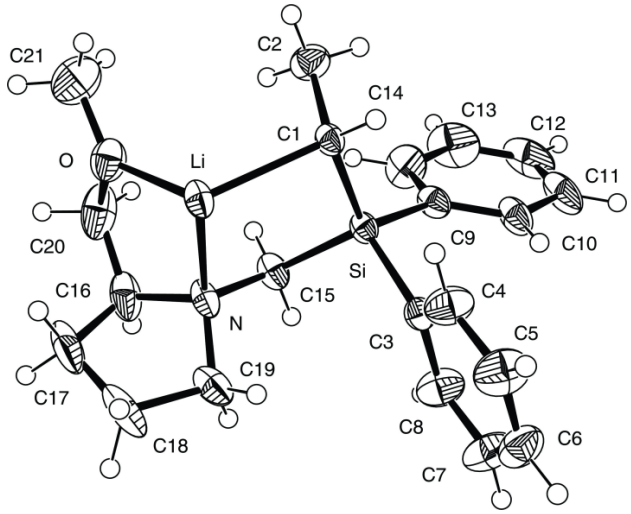


Fig. 2 ORTEP plot of (*R*,*S*)-**6** at 50% probability level

Table 2 Atomic coordinates ($\cdot 10^4$) and equivalent isotropic displacement parameters ($Å^2 \cdot 10^3$) for (*R*,*S*)-**6**.

Atom	x	y	z	U(eq)
Si	3602(1)	4746(1)	3683(1)	24(1)
O	4193(1)	7385(2)	6901(2)	41(1)
N	3728(1)	5084(2)	6728(2)	31(1)
Li	4574(2)	5936(3)	5893(3)	30(1)
C(1)	4289(1)	5783(2)	3457(2)	25(1)
C(2)	4041(1)	7053(2)	2995(3)	40(1)
C(3)	3869(1)	3130(2)	3687(2)	28(1)
C(4)	4488(1)	2788(2)	3282(3)	44(1)
C(5)	4663(2)	1583(3)	3167(4)	56(1)
C(6)	4218(1)	708(2)	3486(3)	48(1)
C(7)	3608(1)	1016(2)	3912(4)	54(1)
C(8)	3435(1)	2211(2)	4018(3)	45(1)
C(9)	2847(1)	4829(2)	2263(2)	32(1)
C(10)	2761(1)	3999(2)	1133(2)	40(1)
C(11)	2234(1)	4102(3)	23(2)	55(1)
C(12)	1788(1)	5051(3)	60(3)	66(1)
C(13)	1859(2)	5873(3)	1160(4)	69(1)
C(14)	2383(1)	5756(3)	2259(3)	52(1)
C(15)	3226(1)	5105(2)	5448(2)	31(1)
C(16)	3556(1)	5852(3)	7945(2)	47(1)
C(17)	4061(2)	5426(4)	9199(2)	60(1)
C(18)	4191(1)	4125(3)	8871(2)	57(1)
C(19)	3801(1)	3892(3)	7388(2)	42(1)
C(20)	3598(1)	7164(3)	7577(3)	54(1)
C(21)	4286(2)	8619(3)	6658(4)	63(1)

Table 3 Anisotropic Displacement parameters ($Å^2 \cdot 10^3$) for (*R*,*S*)-**6**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si	21(1)	31(1)	20(1)	0(1)	-3(1)	0(1)
O	36(1)	44(1)	42(1)	-11(1)	6(1)	0(1)
N	24(1)	50(1)	19(1)	-3(1)	2(1)	-5(1)
Li	26(1)	41(2)	21(1)	-4(1)	0(1)	-2(1)
C(1)	24(1)	31(1)	20(1)	0(1)	-2(1)	-1(1)
C(2)	40(1)	33(1)	44(1)	5(1)	-6(1)	-1(1)
C(3)	29(1)	31(1)	24(1)	1(1)	-4(1)	-1(1)
C(4)	37(1)	37(1)	60(1)	7(1)	11(1)	1(1)
C(5)	45(1)	46(1)	79(2)	5(1)	16(1)	13(1)
C(6)	52(1)	31(1)	58(1)	-1(1)	-12(1)	6(1)

C(7)	45(1)	33(1)	81(2)	8(1)	-8(1)	-8(1)
C(8)	31(1)	41(1)	64(2)	7(1)	2(1)	-5(1)
C(9)	26(1)	42(1)	26(1)	5(1)	-3(1)	-6(1)
C(10)	32(1)	61(1)	24(1)	1(1)	-3(1)	-14(1)
C(11)	45(1)	92(2)	24(1)	5(1)	-11(1)	-32(1)
C(12)	46(1)	102(3)	45(1)	31(2)	-26(1)	-19(1)
C(13)	49(2)	77(2)	75(2)	24(2)	-31(1)	8(1)
C(14)	43(1)	53(1)	55(1)	3(1)	-22(1)	8(1)
C(15)	20(1)	46(1)	25(1)	0(1)	0(1)	0(1)
C(16)	36(1)	76(2)	30(1)	-18(1)	15(1)	-13(1)
C(17)	56(2)	106(3)	19(1)	-7(1)	6(1)	-30(2)
C(18)	39(1)	112(3)	21(1)	12(1)	0(1)	-7(1)
C(19)	32(1)	64(1)	28(1)	10(1)	-1(1)	-8(1)
C(20)	35(1)	71(2)	58(2)	-34(1)	14(1)	0(1)
C(21)	65(2)	45(1)	80(2)	-7(1)	10(2)	7(1)

3.) Crystallographic data for compound (*R*,*S*,*S*)-**8**

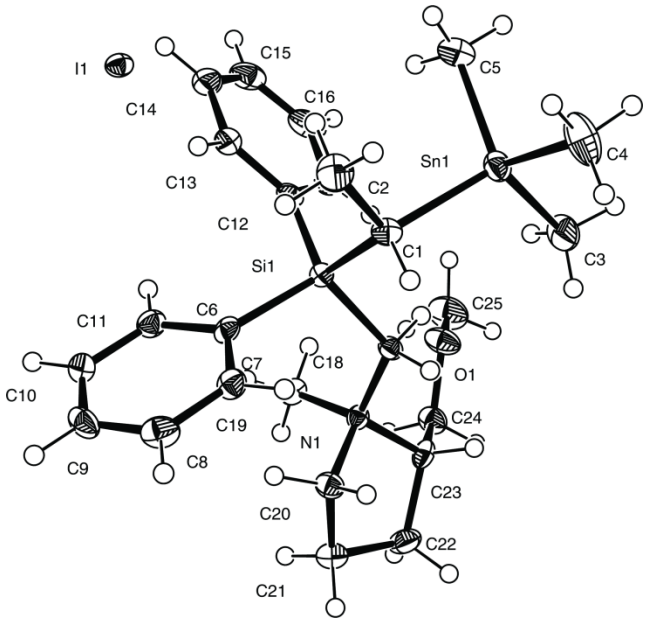


Fig. 3 ORTEP plot of (*R*,*S*,*S*)-**8** at 50% probability level

Table 4 Atomic coordinates ($\cdot 10^4$) and equivalent isotropic displacement parameters ($Å^2 \cdot 10^3$) for (*R*,*S*,*S*)-**8**.

Atom	x	y	z	U(eq)
Sn(1)	7003(1)	10834(1)	5330(1)	23(1)
I(1)	6717(1)	3627(1)	3709(1)	24(1)
Si(1)	7626(1)	10019(1)	3822(1)	15(1)
O(1)	3308(2)	9448(2)	3667(1)	31(1)
N(1)	5399(2)	10468(2)	2955(1)	16(1)
C(8)	9994(3)	11201(3)	2404(2)	29(1)
C(12)	7475(3)	8594(3)	4073(1)	18(1)
C(17)	6313(3)	8128(3)	4253(1)	22(1)
C(1)	8196(3)	10871(3)	4483(1)	20(1)
C(10)	9850(3)	9332(3)	2218(2)	27(1)
C(20)	6041(3)	11223(3)	2496(1)	22(1)
C(9)	10307(3)	10307(3)	2044(2)	28(1)
C(18)	5968(3)	10564(2)	3616(1)	17(1)
C(24)	3017(3)	9991(3)	3091(2)	25(1)
C(23)	3995(3)	10847(3)	2962(2)	21(1)
C(11)	9071(3)	9235(3)	2748(1)	23(1)
C(13)	8569(3)	7954(3)	4139(1)	24(1)
C(21)	5057(3)	11350(3)	1965(2)	26(1)

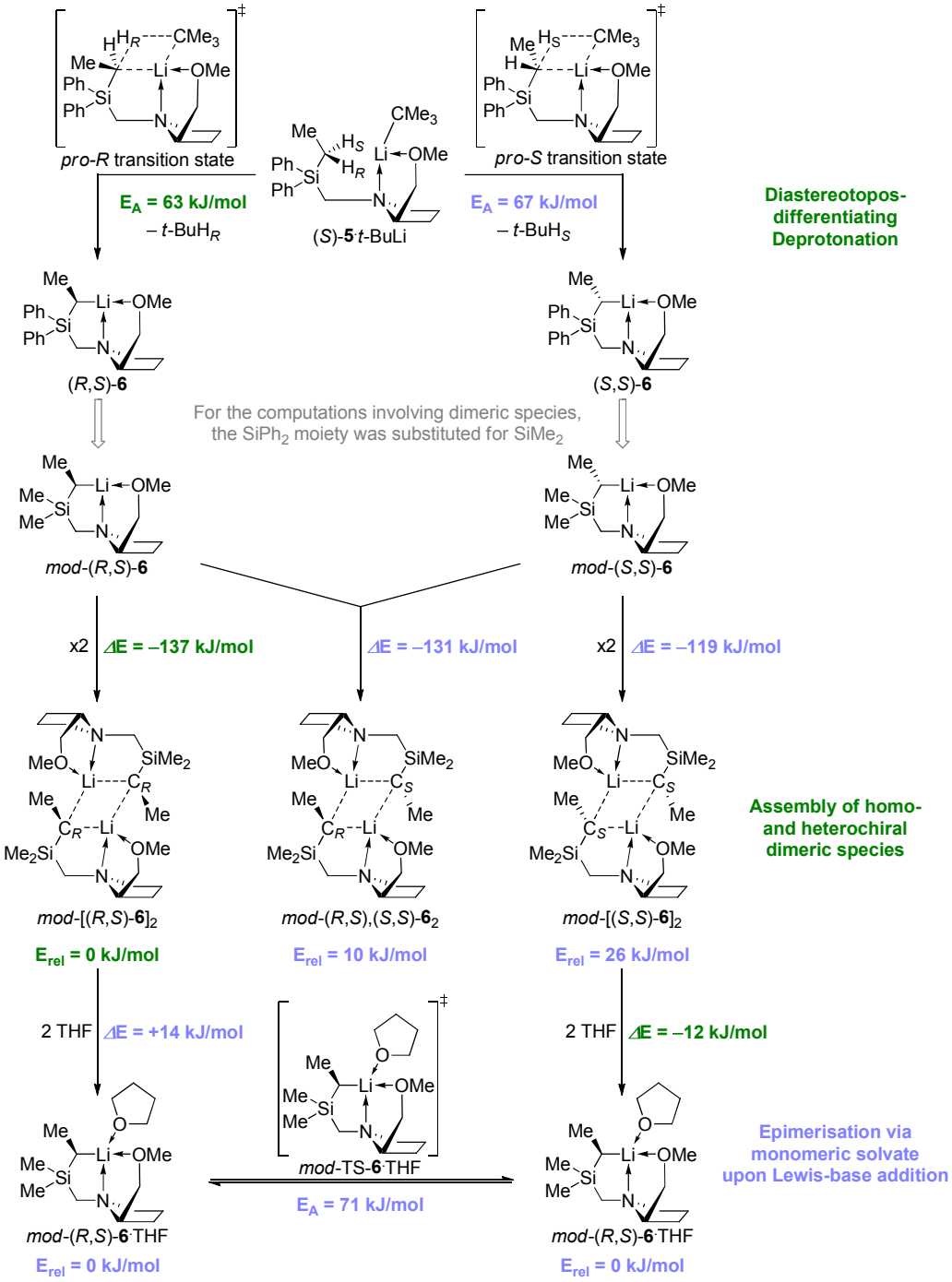
C(16)	6248(4)	7086(3)	4467(2)	30(1)
C(19)	5515(3)	9353(2)	2710(1)	21(1)
C(15)	7329(4)	6477(3)	4508(2)	33(1)
C(14)	8500(4)	6903(3)	4353(2)	32(1)
C(7)	9237(3)	11103(2)	2943(2)	23(1)
C(6)	8737(3)	10111(3)	3120(2)	19(1)
C(22)	3765(3)	11372(3)	2308(2)	29(1)
C(25)	2407(3)	8615(3)	3781(2)	44(1)
C(2)	9608(3)	10636(3)	4665(2)	32(1)
C(5)	7350(4)	9344(3)	5795(2)	39(1)
C(3)	4986(3)	11037(3)	5157(2)	36(1)
C(4)	7646(4)	12089(3)	5939(2)	46(1)

Table 5 Anisotropic Displacement parameters ($Å^2 \cdot 10^3$) for (*R*,*S*,*S*)-**8**.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Sn(1)	22(1)	28(1)	19(1)	-4(1)	-1(1)	0(1)
I(1)	30(1)	20(1)	24(1)	1(1)	-4(1)	0(1)
Si(1)	14(1)	15(1)	16(1)	0(1)	0(1)	-1(1)
O(1)	24(1)	43(1)	24(1)	10(1)	-1(1)	-9(1)
N(1)	16(2)	16(1)	17(1)	-3(1)	-2(1)	1(1)
C(8)	24(2)	27(2)	36(2)	10(2)	0(2)	-7(2)
C(12)	25(2)	17(2)	12(1)	-1(1)	-2(1)	-3(1)
C(17)	20(2)	25(2)	21(2)	0(2)	-3(1)	-3(1)
C(1)	19(2)	21(2)	20(1)	-1(1)	-5(1)	-4(2)
C(10)	26(2)	31(2)	23(2)	1(2)	3(1)	8(2)
C(20)	21(2)	24(2)	20(2)	3(2)	1(1)	-3(1)
C(9)	17(2)	46(2)	20(2)	5(2)	4(1)	-2(2)
C(18)	18(2)	20(2)	14(2)	0(1)	-1(1)	0(1)
C(24)	20(2)	33(2)	23(2)	3(1)	2(2)	-2(2)
C(23)	14(2)	21(2)	26(2)	-4(2)	-1(1)	5(2)
C(11)	25(2)	18(2)	25(2)	2(2)	0(1)	1(2)
C(13)	23(2)	27(2)	21(2)	2(1)	2(1)	3(1)
C(21)	27(2)	26(2)	24(2)	4(2)	-4(1)	0(2)
C(16)	40(2)	28(2)	23(2)	5(2)	-3(2)	-18(2)
C(19)	23(2)	17(2)	23(2)	-4(1)	-6(1)	0(1)
C(15)	55(3)	19(2)	24(2)	3(2)	-4(2)	-4(2)
C(14)	48(3)	25(2)	24(2)	1(2)	0(2)	12(2)
C(7)	18(2)	23(2)	27(2)	2(1)	2(1)	0(1)
C(6)	11(2)	22(2)	23(2)	1(1)	-1(1)	3(1)
C(22)	27(2)	28(2)	32(2)	9(2)	-5(1)	7(2)
C(25)	38(2)	52(2)	40(2)	12(2)	3(2)	-12(2)
C(2)	22(2)	42(2)	32(2)	-7(2)	-9(2)	-2(2)
C(5)	46(2)	45(2)	24(2)	9(2)	0(2)	7(2)
C(3)	19(2)	59(3)	31(2)	0(2)	4(1)	7(2)
C(4)	50(3)	51(3)	36(2)	-24(2)	7(2)	-17(2)

Computational Details

If not otherwise mentioned, all calculations were performed without symmetry restrictions. Starting coordinates were obtained with Chem3D Ultra 10.0 (apart from [(*R*,*S*)-**6**]$_2$, where the crystal structure provided the starting coordinates), optimisation and frequency analyses were conducted with Gaussian *03* Revision B.04 at the M052X/6-31+G(d) and in case of [(*R*,*S*)-**6**]$_2$ and *mod*-[(*R*,*S*)-**6**]$_2$ (which features dimethyl- instead of diphenyl-subsituted silicon centers to decrease the size of the system for computational purposes) at the M052X/6-31G(d) level.[vi] For the quantum-chemical description of Sn, *Energy Consistent Pseudo Potentials* (ECP46MWB) were used.[vii] Harmonic vibrational frequency analyses (to establish the nature of stationary points on the potential energy surface) were performed on the same level. Table 1 lists the total (SCF) and zero-point energies (ZPE) of all compounds. The vibrational frequency of all compounds analyses showed no imaginary frequencies for ground state structures and exactly one imaginary frequence for transition states.



Scheme 1 Computed species and processes [M052X/6-31+G(d)].

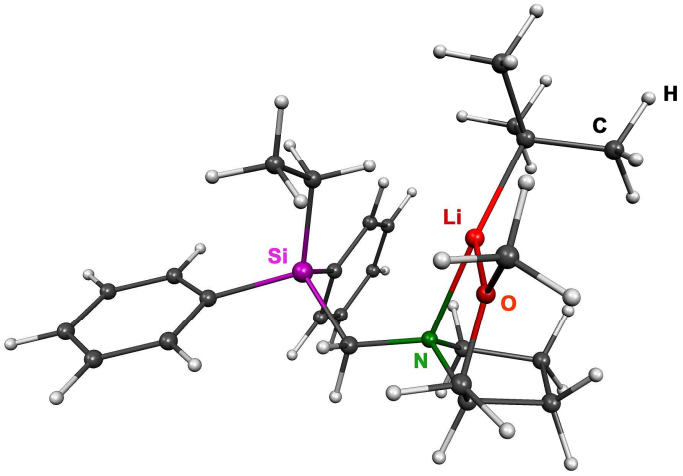


Fig. 4 Molekel plot of [(*S*)-**5**·*t*-BuLi] (ground state)

Table 6 Cartesian coordinates of [(*S*)-**5**·*t*-BuLi] (ground state) [M052X/6-31+G(d)]

atom	X	Y	Z
C	-5.258767	-1.424075	0.668290
C	-5.184990	-2.797471	0.448317
C	-4.110899	-0.639554	0.572540
C	-1.785809	3.994729	0.640906
C	-2.551372	4.340051	-0.470006
C	-1.426813	2.663871	0.852917
C	-3.959629	-3.381512	0.134798
C	-2.959646	3.352530	-1.366259
C	-2.866722	-1.205088	0.258331
C	-1.824903	1.657616	-0.036383
C	-2.816437	-2.590701	0.042158
C	-2.598859	2.025830	-1.147229
C	-0.262509	-0.345644	1.749885
C	0.239525	-1.787021	1.935990
Si	-1.311073	-0.135518	0.201375
C	3.271332	0.764212	1.774517
C	3.170687	0.169949	3.179024
C	2.848661	2.228226	1.878979
C	4.752846	0.746051	1.390316
C	-0.288254	-0.747616	-1.293873
Li	2.329678	-0.400042	0.342439
N	1.078796	-0.216605	-1.348533
C	1.129651	1.212215	-1.703840
O	3.095219	-1.923013	-0.589408
C	3.778057	-3.030097	-0.018898
C	2.600991	1.433701	-2.037216
C	1.911454	-0.895968	-2.366323
C	2.448988	-2.210306	-1.821459
C	3.025780	0.116341	-2.719004
H	-6.208327	-0.963226	0.912533
H	-6.076248	-3.409169	0.520475
H	-4.186370	0.429173	0.741861
H	-1.463728	4.757898	1.338924
H	-2.829659	5.373506	-0.637747
H	-0.820050	2.415141	1.716754
H	-3.894548	-4.449391	-0.036603
H	-3.557749	3.616675	-2.230218
H	-1.873356	-3.071269	-0.196686

H	-2.931612	1.265161	-1.847946
H	-0.852279	-0.048417	2.623189
H	0.595303	0.338604	1.708695
H	-0.592899	-2.480403	2.077697
H	0.897113	-1.861665	2.804101
H	0.808440	-2.139442	1.066613
H	3.506665	-0.875582	3.217637
H	2.145334	0.196506	3.571277
H	3.797982	0.728612	3.907815
H	1.807616	2.339007	2.212357
H	2.939684	2.764824	0.925253
H	3.471462	2.785366	2.612779
H	4.942698	1.206540	0.411189
H	5.160382	-0.273417	1.348870
H	5.376662	1.303243	2.123348
H	-0.820877	-0.537214	-2.237430
H	-0.231528	-1.837184	-1.210320
H	0.781273	1.826642	-0.873667
H	0.483538	1.407645	-2.574963
H	4.201151	-2.687429	0.922477
H	3.081293	-3.854004	0.163846
H	4.577262	-3.364298	-0.685824
H	3.160719	1.580800	-1.111471
H	2.753913	2.307838	-2.669749
H	1.300447	-1.115606	-3.255064
H	1.649518	-2.941753	-1.651201
H	3.167188	-2.642081	-2.527646
H	3.994708	-0.222734	-2.350102
H	3.097375	0.227215	-3.801506

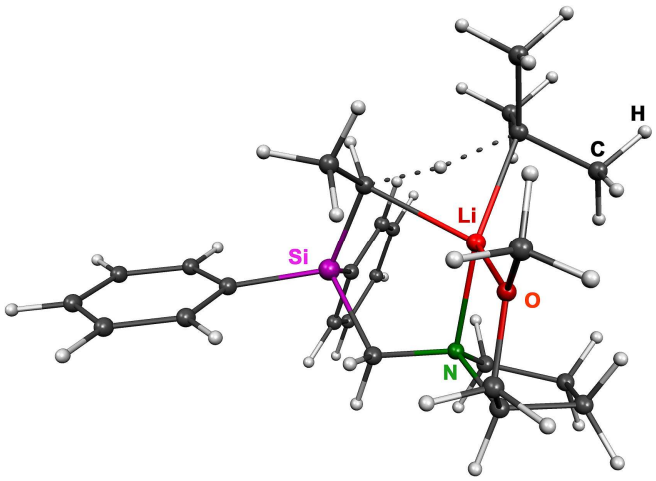


Fig. 5 Molekel plot of [(*S*)-**5**·*t*-BuLi] (pro-*R* transition state)

Table 7 Cartesian coordinates of [(*S*)-**5**·*t*-BuLi] (pro-*R* transition state) [M052X/6-31+G(d)]

atom	X	Y	Z
C	-5.106081	-1.462872	0.497349
C	-5.017547	-2.837267	0.287885
C	-3.959940	-0.671590	0.439175
C	-1.687672	3.953492	0.676772
C	-2.420216	4.307898	-0.453644
C	-1.312993	2.624524	0.876146
C	-3.776806	-3.413621	0.024133
C	-2.783323	3.328944	-1.378484
C	-2.699974	-1.226872	0.172028
C	-1.660824	1.627547	-0.042740
C	-2.636537	-2.614601	-0.030345

C	-2.407181	2.004454	-1.169384
C	0.009376	-0.400911	1.628121
C	0.371114	-1.879004	1.878257
Si	-1.122957	-0.165986	0.188246
C	2.598609	0.839506	2.086916
C	3.064008	0.082922	3.327450
C	2.066051	2.200554	2.518767
C	3.802493	1.076348	1.168122
C	-0.154225	-0.733040	-1.374512
Li	1.962361	-0.467312	0.451453
N	1.194964	-0.148879	-1.441016
C	1.182109	1.269790	-1.855682
O	2.957198	-1.938665	-0.405481
C	3.491167	-3.093293	0.228751
C	2.545263	1.523747	-2.534902
C	2.112417	-0.845833	-2.353432
C	2.562352	-2.171721	-1.755011
C	3.252478	0.156748	-2.534280
H	-6.066819	-1.006256	0.704681
H	-5.907092	-3.454395	0.331094
H	-4.048866	0.397104	0.603089
H	-1.405328	4.708711	1.400914
H	-2.710856	5.339564	-0.612533
H	-0.733509	2.362865	1.753600
H	-3.697615	-4.482533	-0.136883
H	-3.359433	3.597899	-2.256122
H	-1.681500	-3.091675	-0.227172
H	-2.707102	1.249930	-1.891524
H	-0.444956	0.017410	2.533579
H	1.229293	0.279301	1.724208
H	-0.417537	-2.439495	2.389669
H	1.278183	-1.963502	2.493616
H	0.575622	-2.427225	0.947235
H	3.547398	-0.869503	3.075517
H	2.224786	-0.141737	3.996032
H	3.797228	0.668325	3.911683
H	1.211306	2.096309	3.198260
H	1.735442	2.797015	1.660268
H	2.833809	2.787309	3.051603
H	3.529002	1.643018	0.268593
H	4.285266	0.144339	0.843691
H	4.585722	1.666542	1.679166
H	-0.710746	-0.535568	-2.305331
H	-0.054281	-1.820526	-1.301216
H	1.005499	1.906761	-0.987751
H	0.358100	1.443442	-2.559662
H	3.751000	-2.808577	1.245903
H	2.746418	-3.894428	0.250710
H	4.385125	-3.433752	-0.300312
H	3.129825	2.277511	-2.008231
H	2.393362	1.881295	-3.553958
H	1.622765	-1.051313	-3.319917
H	1.761637	-2.920007	-1.768981
H	3.412397	-2.567358	-2.322520
H	3.936060	0.077003	-1.686594
H	3.817680	-0.031656	-3.447974

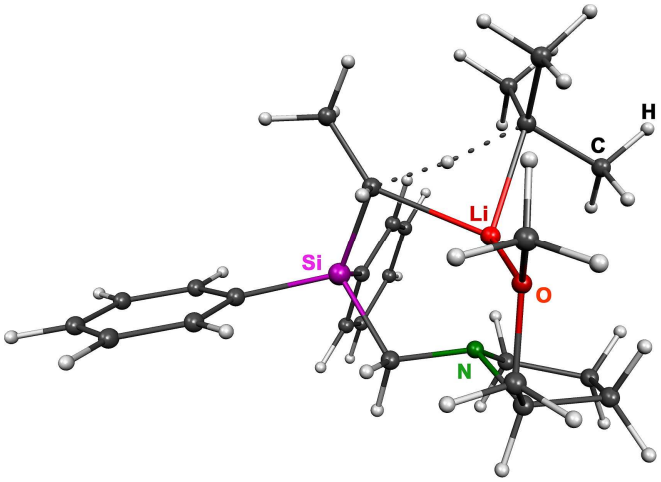


Fig. 6 Molekel plot of [(*S*)-**5**·*t*-BuLi] (pro-*S* transition state)

Table 8 Cartesian coordinates of [(*S*)-**5**·*t*-BuLi] (pro-*S* transition state) [M052X/6-31+G(d)]

atom	X	Y	Z
C	-5.13003200	-0.87303700	0.93958100
C	-5.38406200	-2.14832900	0.43804700
C	-3.86253200	-0.31090000	0.80419900
C	-0.58328600	3.89633700	-0.20357000
C	-1.51296600	4.27729700	-1.16889600
C	-0.49467300	2.56015100	0.18498800
C	-4.36429000	-2.85561500	-0.19467800
C	-2.35389700	3.32038200	-1.73727400
C	-2.81866800	-1.00448000	0.17207700
C	-1.32666000	1.58327300	-0.37653300
C	-3.09770900	-2.28677600	-0.32091900
C	-2.26074400	1.98787200	-1.34047700
C	-0.05208800	-0.38637200	1.62128600
C	-0.77377500	0.07581500	2.90019500
Si	-1.09321500	-0.22798700	0.09571800
C	-0.14135200	-1.14831700	-1.29441000
N	1.23286700	-0.63567800	-1.45677300
C	1.30428300	0.53477800	-2.35057900
O	2.70482500	-2.23236300	0.18022100
C	2.93242300	-3.25952500	1.13978700
C	2.78752800	0.63991700	-2.74760100
C	2.15826500	-1.60480600	-2.06490100
C	2.45764900	-2.75798700	-1.12019300
C	3.37970000	-0.74863600	-2.41504300
C	2.49495700	1.06604700	1.96783600
C	3.41517200	0.07868800	2.68505200
C	2.08717300	2.13800100	2.97288300
C	3.28055400	1.73814800	0.83964900
Li	1.90578400	-0.43746400	0.51017900
H	-5.91861600	-0.31649400	1.43226000
H	-6.36967400	-2.58685300	0.53868000
H	-3.68408900	0.68862300	1.18897400
H	0.07040500	4.63501800	0.24609100
H	-1.58651600	5.31428400	-1.47458100
H	0.23823100	2.26508400	0.92680500
H	-4.55510500	-3.84646200	-0.59029400
H	-3.08220100	3.61403100	-2.48426700
H	-2.32043100	-2.85879300	-0.81757200
H	-2.92885000	1.25500900	-1.78274600
H	0.21366900	-1.45322500	1.73146600
H	1.11715400	0.37480200	1.71175300
H	-1.03352200	1.13785700	2.84013500
H	-0.13041400	-0.04140300	3.77776100
H	-1.70080000	-0.47443800	3.09715100

H	-0.66595300	-1.16250300	-2.26258100
H	-0.07689800	-2.18611600	-0.95091600
H	0.92122800	1.42269200	-1.85141300
H	0.67878700	0.34830400	-3.23675300
H	3.06890900	-2.77861600	2.10429900
H	2.06972500	-3.93045900	1.18138200
H	3.82940800	-3.82638500	0.87708100
H	3.29059100	1.42452300	-2.18413100
H	2.88500700	0.87960400	-3.80641000
H	1.71392000	-2.02473700	-2.98340700
H	1.61914400	-3.46053400	-1.06448800
H	3.33959100	-3.30700200	-1.46953100
H	4.04221800	-0.69124800	-1.54793800
H	3.94669200	-1.18136900	-3.24001500
H	3.87764900	-0.64162500	1.99640300
H	2.87515400	-0.48951400	3.45298600
H	4.25203000	0.59286300	3.19170900
H	1.55637300	1.71243100	3.82948300
H	1.43662700	2.90293200	2.53501200
H	2.97446600	2.66586800	3.36839800
H	2.66490600	2.44548000	0.27126300
H	3.69621900	1.01553600	0.12069600
H	4.14811800	2.30411700	1.22926800

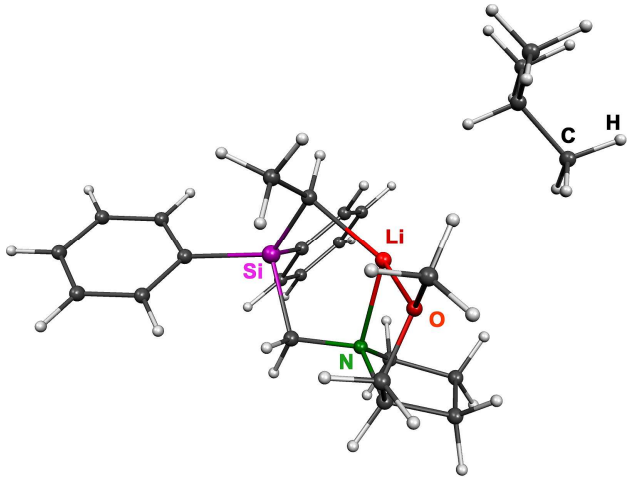


Fig. 7 Molekel plot of [(*R*,*S*)-**6**·*t*-BuH] (product)

Table 9 Cartesian coordinates of [(*R*,*S*)-**6**·*t*-BuH] (product) [M052X/6-31+G(d)]

atom	X	Y	Z
C	5.51592800	0.17686800	-0.69509600
C	5.95788700	-1.11214500	-0.40153600
C	4.15677800	0.47892500	-0.63773300
C	0.00585200	3.85748500	-0.34978900
C	0.68349300	4.42916900	0.72517400
C	0.22852700	2.52085700	-0.68341000
C	5.03138200	-2.09302500	-0.05560200
C	1.59139500	3.66268900	1.45573800
C	3.20392400	-0.48824800	-0.28591600
C	1.12817800	1.72914000	0.04274000
C	3.67388700	-1.77927500	-0.00117600
C	1.80736000	2.32934800	1.11335900
C	0.31720500	-0.65745500	-1.73116900
C	0.59526400	-2.09539800	-2.20560200
Si	1.33360600	-0.11929300	-0.32446700
C	-3.47347100	1.18476700	-1.34799000
C	-3.12242600	0.61708800	-2.72419900
C	-3.77499500	2.68023200	-1.44907600
C	-4.66107400	0.43331300	-0.74285900

C	0.64550600	-1.07020600	1.21740200
Li	-1.42762100	-0.80187400	-0.58197300
N	-0.79991400	-0.80385600	1.40222800
C	-1.06358600	0.34895400	2.27333800
O	-2.39773600	-2.44261300	-0.15716000
C	-2.74915500	-3.42379300	-1.12705500
C	-2.56390800	0.25883500	2.54236200
C	-1.55217500	-1.91095100	2.01707600
C	-1.80839700	-3.01993600	1.00965400
C	-2.84726500	-1.26008200	2.55156000
H	6.22965300	0.94594800	-0.96755400
H	7.01421300	-1.35006600	-0.44481600
H	3.83149600	1.48806300	-0.86990000
H	-0.69376900	4.45211300	-0.92625100
H	0.51069300	5.46607200	0.98835000
H	-0.30633000	2.08023100	-1.51896500
H	5.36483400	-3.09957100	0.16973500
H	2.12782800	4.10360400	2.28802500
H	2.97158200	-2.56405800	0.26397100
H	2.51722600	1.74346000	1.69039900
H	0.36023000	0.04431400	-2.57027100
H	-2.60145700	1.08453600	-0.68322900
H	1.59049500	-2.24647600	-2.64926600
H	-0.13337900	-2.42807400	-2.95644600
H	0.52858400	-2.81953500	-1.37860100
H	-2.90058500	-0.45384300	-2.68353800
H	-2.24591200	1.10979800	-3.14859700
H	-3.96614400	0.75827900	-3.40749000
H	-2.93542300	3.22029300	-1.89297700
H	-3.97539700	3.11131200	-0.46507800
H	-4.65466900	2.84475000	-2.07937500
H	-4.95231600	0.85327800	0.22333400
H	-4.43485500	-0.62703900	-0.59887600
H	-5.52474300	0.50643300	-1.41111700
H	1.19099100	-0.88582600	2.15549800
H	0.76821800	-2.13531100	0.99319900
H	-0.75676100	1.27611100	1.79249600
H	-0.49230400	0.24302000	3.21024800
H	-3.14997200	-2.89695900	-1.99025600
H	-1.86705400	-3.99487800	-1.42663800
H	-3.50955100	-4.09544300	-0.71975200
H	-3.11372700	0.74555200	1.73559400
H	-2.84189300	0.74680300	3.47649200
H	-0.97283200	-2.34225200	2.84925500
H	-0.88144700	-3.52774000	0.72145800
H	-2.49427400	-3.76163900	1.43381200
H	-3.69649400	-1.50642500	1.91200500
H	-3.06777100	-1.62814000	3.55408700

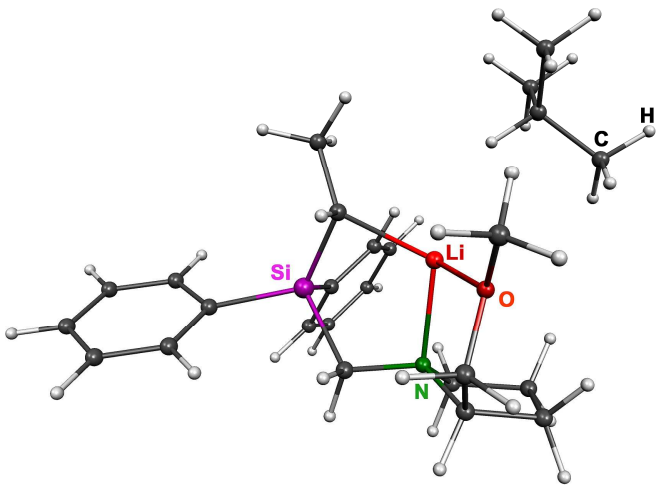


Fig. 8 Molekel plot of [(*S*,*S*)-**6**·*t*-BuH] (product)

Table 10 Cartesian coordinates of [(*S*,*S*)-**6**·*t*-BuH] (product) [M052X/6-31+G(d)]

atom	X	Y	Z
C	5.21523400	-0.20021800	-1.62200700
C	5.70289400	-1.45539200	-1.25978800
C	3.90747000	0.15727200	-1.30266900
C	0.40337400	3.70579200	0.94001800
C	1.40556500	3.97189200	1.87133100
C	0.38402100	2.48166600	0.27173800
C	4.87380500	-2.34487800	-0.58077200
C	2.38907000	3.01465000	2.11823800
C	3.05164300	-0.72091500	-0.61963000
C	1.35545600	1.50030900	0.51058200
C	3.56479800	-1.97694500	-0.26898700
C	2.36271100	1.79713400	1.43968400
C	-0.00271800	-0.25970700	-1.63293900
C	0.19520500	0.65191900	-2.85010000
Si	1.24172700	-0.21306200	-0.30661800
C	0.59002500	-1.45828300	1.01988800
N	-0.77423100	-1.09758900	1.46872100
C	-0.77215000	-0.22193300	2.64821500
O	-2.69746100	-2.11183500	-0.25346100
C	-3.09638400	-2.74490500	-1.46444800
C	-2.23472200	-0.21524100	3.09386700
C	-1.60571800	-2.24409000	1.87126400
C	-2.08513800	-3.02336400	0.65758400
C	-2.75174600	-1.61723800	2.69298000
C	-3.55613400	1.23094600	-1.81314200
C	-4.94866000	0.84964000	-2.31622700
C	-3.12234000	2.58163300	-2.38135600
C	-3.53804900	1.26566300	-0.28187000
Li	-1.61492600	-0.45360900	-0.31557100
H	5.85443800	0.49819500	-2.14975000
H	6.72044600	-1.73649700	-1.50442400
H	3.54601300	1.14222500	-1.58410700
H	-0.35711800	4.45037300	0.73260200
H	1.42552500	4.92035600	2.39506200
H	-0.39627100	2.27758900	-0.45368600
H	5.24563900	-3.32167500	-0.29291300
H	3.17675000	3.21891800	2.83426800
H	2.93855300	-2.68879900	0.25975600
H	3.14143800	1.06538700	1.63274100
H	-0.09704400	-1.31081300	-1.96130700
H	0.37695000	1.68967100	-2.54809200
H	-0.69091500	0.67416700	-3.49778400
H	1.04218200	0.36780400	-3.49091100
H	1.25014300	-1.59648000	1.88968500
H	0.53760000	-2.42472900	0.50639700
H	-0.37848400	0.76238300	2.39928400
H	-0.13058000	-0.66095700	3.42955200
H	-3.54447300	-1.98123400	-2.09593000
H	-2.22766200	-3.17282500	-1.97171500
H	-3.82972600	-3.52829000	-1.25400200
H	-2.78455200	0.56306500	2.56250600
H	-2.33231800	-0.01978300	4.16160600
H	-1.01746200	-2.93096800	2.50139200
H	-1.25408800	-3.52515300	0.15038600
H	-2.81494200	-3.78271500	0.96122200
H	-3.65765500	-1.54461300	2.08887700
H	-2.98060100	-2.23652100	3.56081800
H	-2.83220900	0.48283000	-2.16181700
H	-5.27731500	-0.10780200	-1.90174400
H	-4.96690500	0.77568200	-3.40625400
H	-5.67956200	1.60832700	-2.01859600
H	-3.13609700	2.56972900	-3.47368000
H	-2.10815300	2.83357400	-2.06361400

H	-3.79811300	3.37281900	-2.04043900
H	-2.55262600	1.55487800	0.10322600
H	-3.82764200	0.30045100	0.14848800
H	-4.24831100	2.01047300	0.09019100

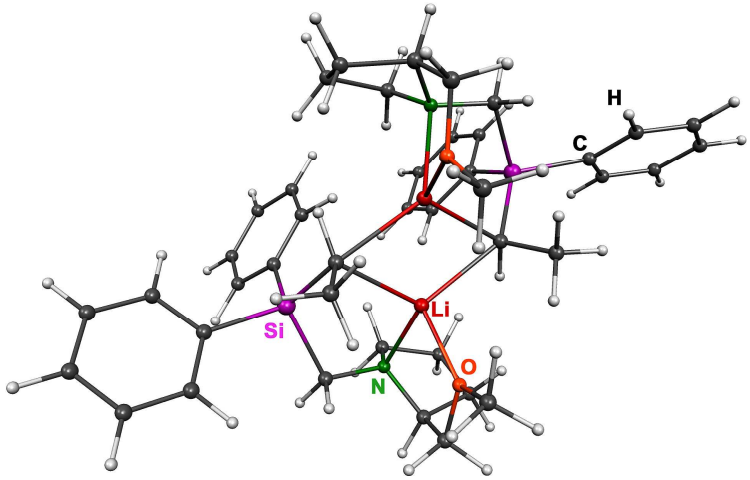


Fig. 9 Molekel plot of [(*R*,*S*)-**6**]$_2$

Table 11 Cartesian coordinates of [(*R*,*S*)-**6**]$_2$ [M052X/6-31G(d), *symm=loose* keyword used]

atom	x	y	z
H	4.72816600	0.38686500	1.68337700
H	5.40868800	0.25498000	-0.60247500
C	3.88375100	0.27640600	1.00363600
C	4.32679400	0.30479600	-0.47817500
H	3.38985000	-0.66421400	1.24389600
H	3.88204600	-0.52589600	-1.03059700
H	4.44894300	2.45160000	-0.77784800
H	3.44066600	2.34065200	1.56430900
C	3.75678700	1.62338300	-1.00864400
H	4.36356300	1.23300100	-3.03650100
C	2.91924200	1.46961500	1.13758300
H	2.04665500	1.27254000	1.75860300
C	3.49495500	1.63946600	-2.50476500
N	2.51415400	1.77163400	-0.24192700
H	3.32447200	2.65923600	-2.86835500
H	2.41496600	3.85813300	0.17744300
H	0.20735200	4.11518200	4.91997100
H	2.84748200	0.35959000	-4.72828400
H	0.56610300	4.56268500	2.52374800
O	2.34666100	0.85143400	-2.77983400
C	1.86731200	3.08563700	-0.38469200
C	-0.09163300	3.37858100	4.18382000
H	1.91618700	3.36909100	-1.44064500
C	0.11740600	3.62285600	2.82997100
C	2.04334700	0.84092200	-4.16406500
H	-0.86459500	2.00104400	5.64545600
Li	1.09296000	0.49378400	-1.16208300
C	-0.69477000	2.18988700	4.59241800
H	1.89842400	1.86125800	-4.53197300
H	1.12340800	0.27714700	-4.28986700
C	-0.26128900	2.68747600	1.85612000
C	-1.07420100	1.24594100	3.64362700
Si	-0.01200500	3.01784400	0.01218200
C	-0.84901900	1.49590500	2.29111000
H	0.69637400	5.21598200	-1.94703400
H	-1.52495200	0.31081800	3.95423600
C	-0.09163300	5.60195200	-1.30851800
C	-0.59661500	4.81133700	-0.26666400
H	-1.11876700	0.74724700	1.55490300
H	0.04510900	2.46325800	-2.97147700

C	-0.78596000	1.74586900	-1.06776700
H	-0.16580500	7.47165700	-2.36814200
C	-0.57801100	6.88320500	-1.55703800
C	-1.62432200	5.36027900	0.51399400
H	-2.03989600	4.77942100	1.33050500
C	-0.93589000	2.30373500	-2.50460900
H	-1.79388500	1.57112300	-0.65391700
C	-1.59335000	7.40626200	-0.76237300
C	-2.11772500	6.63964400	0.27464400
H	-1.47670400	1.61032200	-3.15541800
H	-1.46297700	3.26543900	-2.57116500
H	-1.97379500	8.40294900	-0.95015000
H	-2.90907300	7.03913200	0.89757700
H	-4.72816600	-0.38686500	1.68337700
H	-5.40868800	-0.25498000	-0.60247500
C	-3.88375100	-0.27640600	1.00363600
C	-4.32679400	-0.30479600	-0.47817500
H	-3.38985000	0.66421400	1.24389600
H	-3.88204600	0.52589600	-1.03059700
H	-4.44894300	-2.45160000	-0.77784800
H	-3.44066600	-2.34065200	1.56430900
C	-3.75678700	-1.62338300	-1.00864400
H	-4.36356300	-1.23300100	-3.03650100
C	-2.91924200	-1.46961500	1.13758300
H	-2.04665500	-1.27254000	1.75860300
C	-3.49495500	-1.63946600	-2.50476500
N	-2.51415400	-1.77163400	-0.24192700
H	-3.32447200	-2.65923600	-2.86835500
H	-2.41496600	-3.85813300	0.17744300
H	-0.20735200	-4.11518200	4.91997100
H	-2.84748200	-0.35959000	-4.72828400
H	-0.56610300	-4.56268500	2.52374800
O	-2.34666100	-0.85143400	-2.77983400
C	-1.86731200	-3.08563700	-0.38469200
C	0.09163300	-3.37858100	4.18382000
H	-1.91618700	-3.36909100	-1.44064500
C	-0.11740600	-3.62285600	2.82997100
C	-2.04334700	-0.84092200	-4.16406500
H	0.86459500	-2.00104400	5.64545600
Li	-1.09296000	-0.49378400	-1.16208300
C	0.69477000	-2.18988700	4.59241800
H	-1.89842400	-1.86125800	-4.53197300
H	-1.12340800	-0.27714700	-4.28986700
C	0.26128900	-2.68747600	1.85612000
C	1.07420100	-1.24594100	3.64362700
Si	0.01200500	-3.01784400	0.01218200
C	0.84901900	-1.49590500	2.29111000
H	-0.69637400	-5.21598200	-1.94703400
H	1.52495200	-0.31081800	3.95423600
C	0.09163300	-5.60195200	-1.30851800
C	0.59661500	-4.81133700	-0.26666400
H	1.11876700	-0.74724700	1.55490300
H	-0.04510900	-2.46325800	-2.97147700
C	0.78596000	-1.74586900	-1.06776700
H	0.16580500	-7.47165700	-2.36814200
C	0.57801100	-6.88320500	-1.55703800
C	1.62432200	-5.36027900	0.51399400
H	2.03989600	-4.77942100	1.33050500
C	0.93589000	-2.30373500	-2.50460900
H	1.79388500	-1.57112300	-0.65391700
C	1.59335000	-7.40626200	-0.76237300
C	2.11772500	-6.63964400	0.27464400
H	1.47670400	-1.61032200	-3.15541800
H	1.46297700	-3.26543900	-2.57116500
H	1.97379500	-8.40294900	-0.95015000
H	2.90907300	-7.03913200	0.89757700

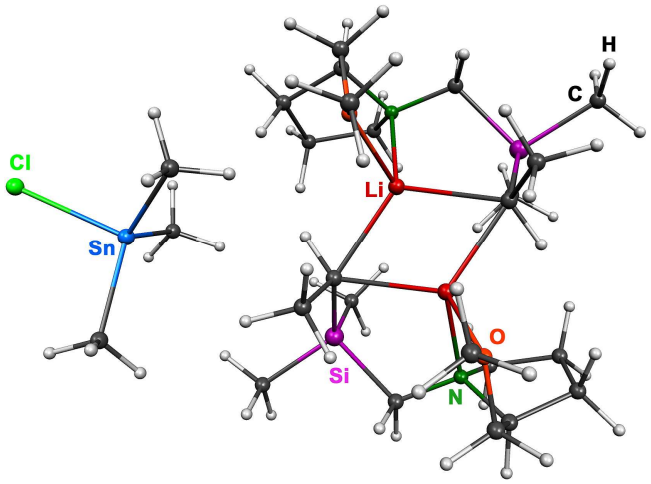


Fig. 10 Molekel plot of *mod*-[(*R*,*S*)-**6**]$_2$·Me$_3$SnCl (ground state)

Table 12 Cartesian coordinates of *mod*-[(*R*,*S*)-**6**]$_2$·Me$_3$SnCl (ground state) [C,H,Cl,Li,N,O,Si: M052X/6-31G(d), Sn: ECP46MWB]

atom	x	y	z
C	-0.79437800	2.49973300	-2.24406400
C	-1.44395500	2.96874400	-0.92046100
C	-0.29489200	3.62422300	-0.13807800
C	0.67778100	2.90348600	-2.10413200
C	-0.40693700	3.47488200	1.37092000
N	0.90003700	2.94812000	-0.65699300
O	-0.13077400	2.12584800	1.71808400
C	2.17636600	3.58496400	-0.29380000
C	-0.21564700	1.90724400	3.11690100
C	4.00873400	1.74422200	-2.07092200
Si	3.65916400	2.35650800	-0.30638600
C	5.13082000	3.46702900	0.17767300
C	3.23356600	0.98977500	0.85049600
C	3.32566400	1.44658600	2.32384000
H	-1.25243400	2.95620700	-3.12080700
H	-0.87937900	1.41945300	-2.34771900
H	-2.26565900	3.66879000	-1.07339400
H	-1.83009000	2.11591800	-0.36018200
H	-0.25170900	4.70233900	-0.36719400
H	0.85119900	3.90199600	-2.53626000
H	1.36602300	2.20688100	-2.57929500
H	-1.41935400	3.74345100	1.69561100
H	0.30212400	4.12907700	1.89059600
H	2.33743100	4.49720700	-0.89074700
H	2.11309600	3.90516600	0.75190000
H	-1.24304700	2.05145200	3.46306800
H	0.45245000	2.58808300	3.65209800
H	0.09327500	0.88102600	3.29982900
H	5.02833000	1.35465500	-2.13429300
H	3.92011300	2.54952700	-2.80456100
H	3.32729700	0.94040600	-2.35894200
H	6.05228900	2.88013900	0.21525600
H	4.98314100	3.90911200	1.16646500
H	5.27943300	4.28113700	-0.53699000
H	3.98752800	0.20142500	0.68794000
H	2.63492700	2.27623800	2.52399800
H	3.05120300	0.65124100	3.02733800
H	4.31870600	1.80077900	2.63560000
Li	1.03385500	1.11811200	0.39043500
Li	2.18136100	-0.93305700	0.56055000
C	-0.01888500	-0.83925700	0.00545900
C	-0.61987600	-1.56445300	1.22687100
Si	0.19201600	-1.95971000	-1.43789500
C	1.58910000	-3.20383100	-0.98705700

N	2.84842200	-2.55529400	-0.59238800
C	3.70831100	-2.23830000	-1.73532000
O	2.68163600	-2.17042100	2.10053000
C	2.16446200	-2.17233000	3.41956200
C	5.06842800	-1.89894400	-1.11029200
C	3.70219300	-3.35314000	0.29510100
C	3.09976000	-3.46286400	1.68662800
C	5.04481000	-2.60739000	0.26485000
C	-1.24595800	-3.14756600	-1.85348700
C	0.60810000	-1.02607300	-3.03870600
H	-0.67596000	-0.00436100	-0.29180100
H	-0.63215200	-0.94423700	2.13125200
H	-0.02551700	-2.45049200	1.48463500
H	-1.65112300	-1.93401000	1.10050700
H	1.77049200	-3.96430100	-1.76361800
H	1.19226700	-3.74030800	-0.11854300
H	3.28242700	-1.42394700	-2.31922300
H	3.79218100	-3.11990200	-2.39069400
H	1.79974900	-1.16895600	3.62395400
H	1.33912900	-2.88505000	3.50876500
H	2.94917500	-2.43052200	4.13644700
H	5.17429700	-0.82247200	-0.98420100
H	5.88721400	-2.24413600	-1.74068700
H	3.82375500	-4.37387400	-0.10470700
H	2.23914100	-4.14142100	1.70162400
H	3.85132200	-3.85272900	2.38306900
H	5.07059900	-1.87441400	1.07321800
H	5.87976000	-3.29425100	0.40300600
H	-2.14568300	-2.60146900	-2.14898600
H	-0.98535900	-3.82515900	-2.67143400
H	-1.49846300	-3.76042400	-0.98295000
H	1.27844700	-0.18554600	-2.84323700
H	1.08370500	-1.68132500	-3.77284200
H	-0.30276100	-0.63020400	-3.49613500
Sn	-4.24130800	-0.44732800	0.10819500
Cl	-6.53632900	0.31821200	0.14616500
C	-4.41984800	-2.55370000	0.50448500
C	-3.33061800	0.71815200	1.67050200
C	-3.59638000	0.04048900	-1.88333800
H	-5.39689100	-2.89242800	0.16231900
H	-4.33380400	-2.74446200	1.57338200
H	-3.64347200	-3.10713900	-0.02129100
H	-3.54531400	0.26552500	2.63845800
H	-3.74816800	1.72523500	1.65106800
H	-2.25270500	0.76685500	1.52444200
H	-3.75815900	1.10062900	-2.07573600
H	-4.16762500	-0.54009700	-2.60688400
H	-2.53701000	-0.18913800	-1.99509700

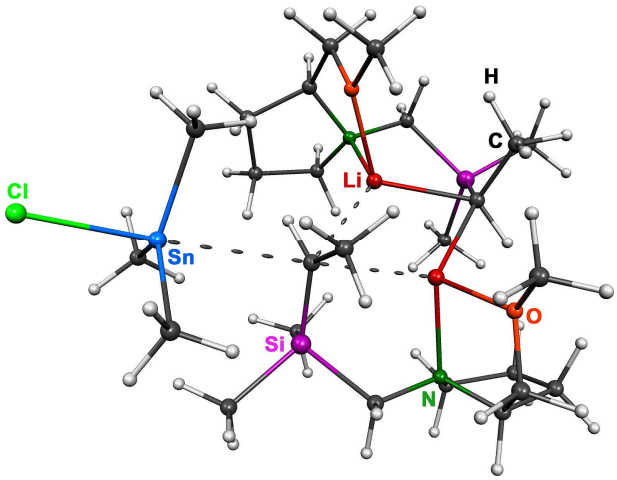


Fig. 11 Molekel plot of *mod*-[(*R*,*S*)-**6**]$_2$·Me_3SnCl (transition state)

Table 13 Cartesian coordinates of *mod*-[(*R*,*S*)-**6**]$_2$·Me_3SnCl (transition state) [C,H,Cl,Li,N,O,Si: M052X/6-31G(d), Sn: ECP46MWB]

atom	x	y	z
C	-0.67442700	2.89877700	-2.21167400
C	-1.22082600	3.44249400	-0.86979400
C	0.03029700	3.90090400	-0.10511000
C	0.84579200	3.05987600	-2.09077300
C	-0.07633200	3.77410300	1.40566100
N	1.09147400	3.04192500	-0.64585100
O	0.03265000	2.40271600	1.76848200
C	2.46119800	3.45043700	-0.28998700
C	-0.10039900	2.23099200	3.17364000
C	3.96094100	1.37559100	-2.09494700
Si	3.70318300	1.98085800	-0.31368500
C	5.34146700	2.79133600	0.21742700
C	3.03498100	0.68245100	0.82143900
C	3.21504800	1.11378200	2.29712400
Li	0.94397300	1.22853100	0.37576000
H	-1.06591100	3.43882100	-3.07281300
H	-0.93542600	1.84904400	-2.33067300
H	-1.92559700	4.26374500	-0.99834900
H	-1.72962500	2.65390800	-0.31262900
H	0.24392300	4.95722700	-0.33841300
H	1.16913900	4.02721400	-2.50629400
H	1.41037500	2.27421700	-2.58911300
H	-1.04246000	4.16781000	1.74132300
H	0.71525200	4.33702400	1.91197200
H	2.77871700	4.31324100	-0.89628400
H	2.45855500	3.78801500	0.75170200
H	-1.08975400	2.56015600	3.50171100
H	0.67179100	2.79950700	3.69912100
H	0.01892600	1.17243200	3.38573800
H	4.88028900	0.78820600	-2.16217000
H	4.06025200	2.21812800	-2.78436300
H	3.13812000	0.74779100	-2.44249600
H	6.14199200	2.04796200	0.25682400
H	5.25800900	3.23755100	1.21166300
H	5.64651800	3.57636100	-0.47960900
H	3.66046500	-0.21067100	0.65022500
H	2.70950400	2.06775600	2.49229300
H	2.77878300	0.39762600	3.00342700
H	4.25935400	1.25409300	2.60796400
Li	1.78866100	-1.09411100	0.59793100
C	-0.56928200	-0.59473400	0.01395100
C	-0.54333600	-1.05419700	1.47109600
Si	-0.41372500	-1.69762300	-1.43696500
C	0.81655300	-3.11614400	-0.99981700
N	2.17858300	-2.69485200	-0.64392900
C	3.01162100	-2.43094100	-1.82219900
O	2.32961300	-2.47100800	2.07755600
C	1.95364000	-2.48813100	3.44546000
C	4.44269800	-2.36545200	-1.27526900
C	2.94055700	-3.69059500	0.12196800
C	2.43187100	-3.78674000	1.54918900
C	4.39356300	-3.19844900	0.02664900
C	-1.84934900	-2.78255500	-2.08635700
C	0.17304300	-0.74935600	-2.97777000
H	-0.87375100	0.44146800	-0.15574900
H	0.23979300	-0.57036800	2.08657200
H	-0.33438500	-2.12819500	1.53359700
H	-1.47046000	-0.90337000	2.04016100
H	0.84471500	-3.87271900	-1.80132500
H	0.36839000	-3.61425900	-0.13260800
H	2.69480100	-1.51541000	-2.31665300
H	2.90747500	-3.26116300	-2.53828600

H	1.88388600	-1.45650200	3.77863100
H	0.98443500	-2.98046700	3.57252700
H	2.70786400	-3.01219500	4.03872300
H	4.71998600	-1.33524800	-1.05795400
H	5.15823300	-2.75954100	-1.99594500
H	2.84239700	-4.68352800	-0.34578800
H	1.45081200	-4.27345400	1.59985800
H	3.13380600	-4.37512700	2.15129300
H	4.62527800	-2.57365900	0.89059700
H	5.08958400	-4.03698500	0.01907200
H	-2.76032800	-2.22146400	-2.30053800
H	-1.52962800	-3.25669800	-3.01991500
H	-2.10621200	-3.57853000	-1.38419100
H	0.92691500	-0.00109400	-2.72471600
H	0.60096200	-1.43941700	-3.71019300
H	-0.65808900	-0.24004600	-3.47139600
Sn	-3.59814000	-0.33642900	0.10855900
Cl	-6.06523600	-0.08136400	0.30957200
C	-3.61022000	-2.40024100	0.72434700
C	-3.16258200	1.14435000	1.61960600
C	-3.53972300	0.36422300	-1.93036300
H	-4.16503900	-2.98141700	-0.01059000
H	-4.14010200	-2.45433000	1.67515500
H	-2.60648100	-2.80442100	0.82993900
H	-3.45971800	0.75768900	2.59486800
H	-3.77783400	2.01786200	1.40105100
H	-2.11185000	1.42114200	1.63426000
H	-3.73943900	1.43673000	-1.92174200
H	-4.33614300	-0.12571800	-2.48957100
H	-2.58463100	0.17550000	-2.41336700

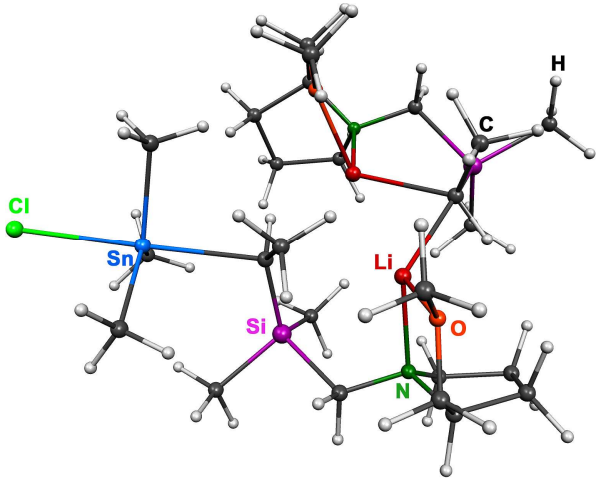


Fig. 11 Molekel plot of *mod*-[(*R*,*S*)-**6**]$_2$·Me_3SnCl (product)

Table 14 Cartesian coordinates of *mod*-[(*R*,*S*)-**6**]$_2$·Me_3SnCl (product) [C,H,Cl,Li,N,O,Si: M052X/6-31G(d), Sn: ECP46MWB]

atom	x	y	z
C	-0.71378600	3.01446500	-2.17664200
C	-1.24299700	3.50481400	-0.80786800
C	0.01654700	3.93917100	-0.04582500
C	0.81265900	3.12356200	-2.05415100
C	-0.07679000	3.79210600	1.46596400
N	1.06440700	3.07570600	-0.60960100
O	0.08906900	2.42068400	1.81403700
C	2.44056700	3.45875000	-0.25061500
C	-0.05207200	2.21848800	3.21533600
C	3.94468200	1.41946500	-2.11631500
Si	3.67423400	1.98477000	-0.32634700
C	5.31231900	2.75448100	0.25490900

C	3.00745800	0.63347000	0.75447600
C	3.22949300	0.97050200	2.25047000
H	-1.08639100	3.61443600	-3.00567000
H	-1.01593000	1.98381500	-2.35332500
H	-1.95363900	4.32608500	-0.89541700
H	-1.74140600	2.69385100	-0.27433500
H	0.24093000	4.99549200	-0.26678800
H	1.16633800	4.08592200	-2.45443900
H	1.35171300	2.32887800	-2.56635500
H	-1.05613800	4.14113600	1.81049000
H	0.69532000	4.37824700	1.97578300
H	2.76469700	4.33631300	-0.83123100
H	2.44661500	3.76450600	0.80137500
H	-1.06371100	2.48075700	3.53306600
H	0.67854600	2.82445400	3.75843800
H	0.12914700	1.16544600	3.41237300
H	4.84945900	0.80855000	-2.17724000
H	4.08097100	2.27346300	-2.78466000
H	3.11421600	0.82130100	-2.49576900
H	6.10121200	1.99853000	0.28887200
H	5.21878500	3.17819200	1.25790500
H	5.64021700	3.55112700	-0.41781900
H	3.64349900	-0.23529700	0.50367300
H	2.71124000	1.89739700	2.52464400
H	2.83509000	0.19870500	2.92309700
H	4.28110100	1.11226900	2.53226800
Li	0.93911600	1.29083400	0.41873600
Li	1.86505700	-1.17188300	0.67730200
C	-0.86655400	-0.53545400	-0.04479900
C	-0.54419900	-0.90989600	1.40536400
Si	-0.49555400	-1.64466800	-1.48148400
C	0.70906700	-3.07040400	-0.99066200
N	2.08776800	-2.70072800	-0.63946500
C	2.91616400	-2.43680300	-1.82484100
O	2.24502500	-2.57066000	2.08698800
C	1.81720300	-2.60916400	3.44130900
C	4.36542700	-2.49032100	-1.31788300
C	2.82322800	-3.74510900	0.09224500
C	2.31700600	-3.87432700	1.51832700
C	4.28526800	-3.28724900	0.00408000
C	-1.90836700	-2.70558000	-2.18180300
C	0.17612500	-0.66638900	-2.96331200
H	-0.79067600	0.53282800	-0.27563200
H	-1.32619800	-0.62650200	2.12131700
H	0.37466000	-0.45819300	1.83221700
H	-0.42308600	-1.99253300	1.51347200
H	0.71301100	-3.83982500	-1.78025300
H	0.23895200	-3.53871400	-0.11870400
H	2.65034900	-1.48013300	-2.26826200
H	2.73919800	-3.22264600	-2.57394300
H	1.75596500	-1.58293400	3.79381700
H	0.83414100	-3.08255500	3.51843500
H	2.53771200	-3.16188800	4.04927100
H	4.75258700	-1.48768300	-1.14134100
H	5.01401400	-2.97089400	-2.04920700
H	2.69536100	-4.71816000	-0.40802200
H	1.32507300	-4.33768500	1.55763000
H	3.00661000	-4.49433600	2.10155300
H	4.51555500	-2.64365800	0.85524500
H	4.96684800	-4.13707700	0.03052200
H	-2.78551500	-2.11968900	-2.45843700
H	-1.54806400	-3.20847900	-3.08461500
H	-2.22911700	-3.47531400	-1.47724700
H	0.94629500	0.04504900	-2.65833600
H	0.59652300	-1.33324900	-3.72054400
H	-0.63056200	-0.10529300	-3.44087600
Sn	-3.38884000	-0.34426000	0.09809100
Cl	-5.95971500	-0.13979300	0.36328100

C	-3.55957700	-2.39902000	0.76612100
C	-3.16927800	1.20574400	1.60498400
C	-3.61583700	0.37146000	-1.93677900
H	-4.17270100	-2.94709900	0.05160600
H	-4.08608500	-2.39682000	1.72011900
H	-2.59258900	-2.89142300	0.87322000
H	-3.49826200	0.82211000	2.57159700
H	-3.84365100	2.01589000	1.32725500
H	-2.14796000	1.57385700	1.67932300
H	-3.96183200	1.40487200	-1.88059800
H	-4.39606600	-0.20702200	-2.43025500
H	-2.69979400	0.32720000	-2.52533400

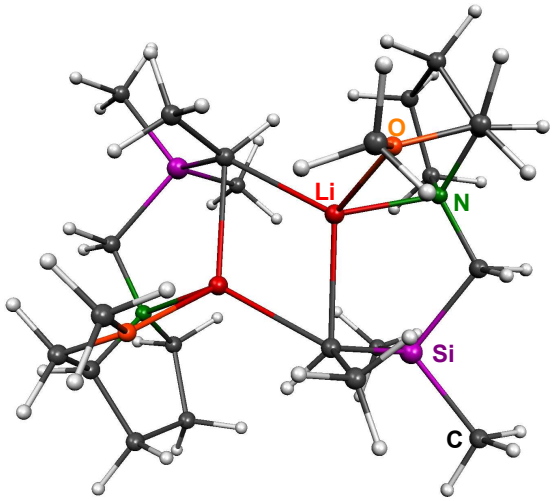


Fig. 12 Molekel plot of *mod*-[(*R*,*S*)-**6**]$_2$ (homochiral dimer)

Table 15 Cartesian coordinates of *mod*-[(*R*,*S*)-**6**]$_2$ (homochiral dimer) [M052X/6-31+G(d), *symm=loose*]

atom	x	y	z
H	3.70281200	2.68738400	-2.38335900
H	4.61199200	2.86787900	-0.18144400
C	3.07914300	2.20091400	-1.63298400
C	3.69218200	2.28256100	-0.21419300
H	2.09881800	2.67648200	-1.65528900
H	2.98168100	2.72753300	0.48529000
H	4.96076700	0.51162500	-0.14077800
H	3.83717100	0.32987100	-2.46436400
C	3.95012600	0.82072500	0.17920900
H	4.41036000	1.30266900	2.22790400
C	2.95820200	0.69465600	-1.90728100
H	2.06697300	0.42587000	-2.47209000
C	3.82909000	0.55703600	1.67147900
N	2.93368900	0.07949100	-0.57716400
H	4.20484300	-0.43755900	1.93839600
H	3.94802300	-1.63515500	-1.32010400
H	2.71561500	1.29331800	3.98220300
O	2.45811100	0.64769900	2.03277900
C	3.13916600	-1.37761100	-0.61524500
H	3.47894100	-1.70105300	0.37492400
C	2.25343500	0.47301400	3.42467200
Li	1.15467300	0.23031400	0.52940500
H	2.67307600	-0.48153300	3.75676100
H	1.17976400	0.47493800	3.59437200
Si	1.51215600	-2.37073600	-0.88872700
H	1.72684500	-2.17694700	2.11265400
C	0.33825300	-1.87517900	0.43699700

C	0.71956800	-2.48743600	1.80347400
H	-0.64956000	-2.26961900	0.14293200
H	0.04723100	-2.16813900	2.60937400
H	0.72240600	-3.58804800	1.82762100
H	-3.70232300	-2.68720800	-2.38428700
H	-4.61193100	-2.86788400	-0.18255900
C	-3.07881200	-2.20078300	-1.63375100
C	-3.69211900	-2.28255800	-0.21508200
H	-2.09847000	-2.67632300	-1.65590400
H	-2.98174700	-2.72759100	0.48449400
H	-4.96073000	-0.51164000	-0.14175400
H	-3.83673700	-0.32968300	-2.46509700
C	-3.95014600	-0.82075800	0.17839800
H	-4.41075800	-1.30287900	2.22696600
C	-2.95785300	-0.69449900	-1.90790000
H	-2.06653500	-0.42564800	-2.47253900
C	-3.82939800	-0.55718900	1.67071200
N	-2.93357500	-0.07945100	-0.57772500
H	-4.20522400	0.43737600	1.93763700
H	-3.94780700	1.63524900	-1.32067900
H	-2.71631600	-1.29361400	3.98160200
O	-2.45848600	-0.64785000	2.03226800
C	-3.13905700	1.37765300	-0.61571700
H	-3.47898500	1.70101300	0.37442700
C	-2.25407900	-0.47324800	3.42421000
Li	-1.15476300	-0.23036100	0.52913300
H	-2.67383600	0.48125400	3.75628600
H	-1.18043900	-0.47512200	3.59411000
Si	-1.51200400	2.37079800	-0.88886100
H	-1.72721200	2.17674900	2.11246000
C	-0.33832100	1.87511900	0.43701900
C	-0.71989100	2.48728500	1.80347100
H	0.64952700	2.26962300	0.14315600
H	-0.04768300	2.16795800	2.60946600
H	-0.72276100	3.58789500	1.82768200
C	-2.12685100	4.17663800	-0.87848600
H	-1.28819600	4.86504000	-1.01963200
H	-2.85187700	4.36183900	-1.67730900
H	-2.60262200	4.43022700	0.07369000
C	-0.82076600	2.05713400	-2.63125900
H	-0.27356200	1.11336500	-2.68686500
H	-1.61530600	2.03868900	-3.38313000
H	-0.12848100	2.85950100	-2.90429800
C	2.12702700	-4.17656700	-0.87841300
H	1.28841700	-4.86497700	-1.01977600
H	2.85220600	-4.36167900	-1.67711900
H	2.60263100	-4.43022900	0.07382800
C	0.82119400	-2.05689300	-2.63120100
H	0.27397700	-1.11312700	-2.68676800
H	1.61585000	-2.03833100	-3.38294400
H	0.12896900	-2.85923800	-2.90445500

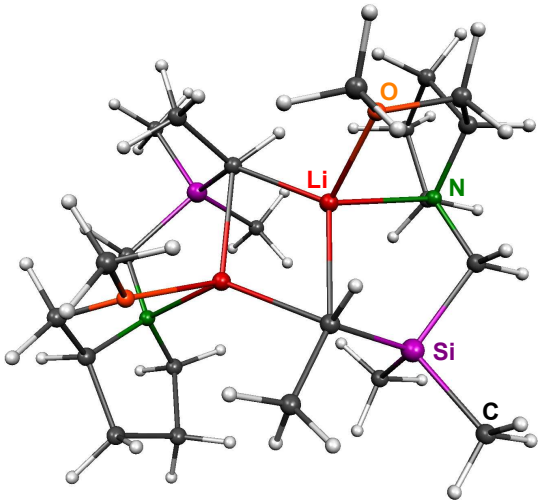


Fig. 13 Molekel plot of *mod*-(*R*,*S*),(*S*,*S*)-**6**$_2$ (heterochiral dimer)

Table 16 Cartesian coordinates of *mod*-(*R*,*S*),(*S*,*S*)-**6**$_2$ (heterochiral dimer) [M052X/6-31+G(d)]

atom	x	y	z
C	-3.35529400	-1.86015600	-1.66084400
C	-3.99701800	-1.94343000	-0.25482900
C	-4.00323900	-0.49228600	0.26041400
C	-3.14666100	-0.36052200	-1.88376100
C	-3.71670200	-0.37546500	1.74999400
N	-2.95952000	0.17328000	-0.53225600
O	-2.35591600	-0.71738600	1.95348700
C	-3.02809100	1.64481900	-0.48649700
C	-1.98976600	-0.82568600	3.31701300
Li	-1.09105900	-0.31227700	0.44748100
Si	-1.32108800	2.49186000	-0.72845400
C	-0.19454900	1.79621300	0.54570400
C	-0.59195700	2.25550000	1.96805600
C	3.04610400	2.26508000	-1.49127900
C	3.74901200	2.21679600	-0.11440800
C	4.00236600	0.72398500	0.14026300
C	2.85969400	0.79008800	-1.87808700
C	3.96088900	0.34045100	1.61067200
N	2.93079800	0.05581000	-0.60961500
O	2.62146100	0.46833600	2.07175100
C	3.13608100	-1.39071100	-0.80432600
C	2.47645200	0.06463500	3.42329500
Li	1.22608200	0.14429300	0.62476500
Si	1.50076300	-2.39046200	-0.91868000
C	0.49723900	-1.96961400	0.57244600
C	-0.50883600	-3.11214900	0.85279900
H	-3.98130300	-2.29986400	-2.43758000
H	-2.39523800	-2.37601400	-1.67262200
H	-5.00966800	-2.34794600	-0.28065600
H	-3.39836700	-2.57133200	0.40650000
H	-4.98054200	-0.02087900	0.06023500
H	-4.04268700	0.09280900	-2.34052300
H	-2.29004700	-0.12577300	-2.51477100
H	-4.36277700	-1.06628900	2.30600100
H	-3.89735100	0.63916300	2.12394900
H	-3.81197900	2.01196500	-1.16976100
H	-3.33882700	1.94321600	0.52028000
H	-2.56909200	-1.61631400	3.80420700
H	-2.15076400	0.12412500	3.83607300
H	-0.93156800	-1.08181700	3.33601100

H	0.81175100	2.19172600	0.32970500
H	-1.61921400	1.95546400	2.21136500
H	0.04027400	1.80671500	2.74525100
H	-0.54554200	3.34349300	2.12926700
H	3.63824100	2.79174000	-2.24013900
H	2.08424100	2.76971700	-1.41261700
H	4.68112400	2.78276300	-0.09257500
H	3.09383900	2.61249500	0.66386500
H	4.98734200	0.42928400	-0.26186800
H	3.67837200	0.45943400	-2.53782200
H	1.91667300	0.58922200	-2.38484000
H	4.61624100	1.00351600	2.18830900
H	4.29562100	-0.69144900	1.76665300
H	3.83187500	-1.57012400	-1.64033800
H	3.61990500	-1.79571700	0.09102000
H	3.09141700	0.69134400	4.07596900
H	2.76559900	-0.98461800	3.54098600
H	1.42788800	0.18580700	3.68483800
H	1.20251700	-1.93423000	1.42649700
H	-0.03255800	-4.07423600	1.09442900
H	-1.14307300	-3.30634700	-0.02176800
H	-1.19758400	-2.89080900	1.67494500
C	-0.72520300	2.22859000	-2.51452600
H	-1.53460300	2.42740700	-3.22369200
H	0.09299100	2.91508200	-2.75161500
H	-0.36644800	1.21150900	-2.68528000
C	-1.74436700	4.34728300	-0.59026100
H	-0.84288700	4.95351300	-0.72191900
H	-2.47155200	4.65754900	-1.34731600
H	-2.15932600	4.58602900	0.39359200
C	2.08861500	-4.19932200	-1.05775200
H	1.23360500	-4.87697700	-1.13764400
H	2.71913800	-4.35593100	-1.93866100
H	2.65865300	-4.49412800	-0.17143100
C	0.60311300	-2.03107900	-2.55591400
H	1.28531200	-2.08599500	-3.40975400
H	-0.18700600	-2.77029800	-2.72157800
H	0.13626500	-1.04296800	-2.54787600

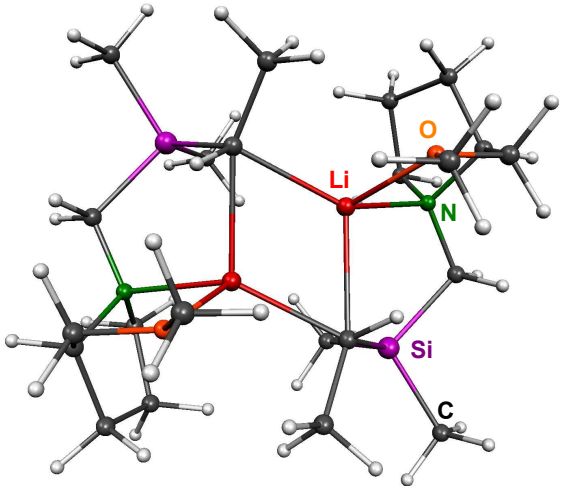


Fig. 14 Molekel plot of *mod*-[(*S*,*S*)-**6**]$_2$ (homochiral dimer)

Table 17 Cartesian coordinates of *mod*-[(*S*,*S*)-**6**]$_2$ (homochiral dimer) [M052X/6-31+G(d), *symm=loose*]

atom	x	y	z
C	-3.20655100	-1.97557900	-1.50307100

C	-4.01416200	-1.91237300	-0.18508500
C	-4.03918200	-0.41704600	0.19153200
C	-3.01217500	-0.50849800	-1.88399900
C	-3.83935600	-0.15859500	1.67603000
N	-2.94371700	0.17743400	-0.59057900
O	-2.52281500	-0.56824800	2.01025700
C	-3.03809600	1.64442400	-0.72161500
C	-2.19907500	-0.37524000	3.37547500
Li	-1.16107700	-0.27106500	0.54547100
Si	-1.32580500	2.50220600	-0.78613400
C	-0.37570000	1.89245700	0.67565100
C	0.58249400	2.99512200	1.19232900
C	3.20650300	1.97566700	-1.50295500
C	4.01418900	1.91237200	-0.18502100
C	4.03919100	0.41702500	0.19151600
C	3.01212500	0.50861400	-1.88398300
C	3.83939600	0.15850100	1.67600500
N	2.94370300	-0.17740200	-0.59060500
O	2.52286500	0.56814500	2.01028600
C	3.03807600	-1.64438200	-0.72174200
C	2.19917800	0.37509700	3.37551100
Li	1.16108700	0.27103700	0.54552400
Si	1.32578600	-2.50216700	-0.78626700
C	0.37569600	-1.89249500	0.67555500
C	-0.58250300	-2.99518600	1.19216400
H	-3.71564700	-2.53678200	-2.28695200
H	-2.23672000	-2.44048500	-1.32950300
H	-5.02945600	-2.29292000	-0.30272700
H	-3.52369800	-2.49263700	0.59749400
H	-4.99883400	0.03589700	-0.10899700
H	-3.87805500	-0.13600900	-2.45696100
H	-2.11175200	-0.32065000	-2.46858000
H	-4.56807200	-0.73400600	2.26008200
H	-3.96142500	0.90316300	1.92070500
H	-3.71078300	1.90745900	-1.55373200
H	-3.50108300	2.04512400	0.18619000
H	-2.87863700	-0.94810500	4.01400500
H	-2.25499900	0.68662900	3.63608900
H	-1.17999400	-0.73378900	3.51063800
H	-1.13170000	1.72938200	1.46867200
H	0.06658800	3.90814400	1.52523100
H	1.28107400	3.31969300	0.41184300
H	1.20799900	2.66737600	2.02929100
H	3.71554500	2.53694000	-2.28682100
H	2.23667500	2.44054600	-1.32929200
H	5.02948800	2.29289500	-0.30270400
H	3.52379000	2.49260800	0.59761900
H	4.99883200	-0.03591000	-0.10905800
H	3.87799300	0.13616700	-2.45699000
H	2.11168800	0.32079800	-2.46855200
H	4.56812800	0.73387800	2.26007000
H	3.96146500	-0.90327000	1.92062100
H	3.71073900	-1.90736500	-1.55389500
H	3.50108900	-2.04514100	0.18602300
H	2.87877000	0.94793800	4.01403100
H	2.25510600	-0.68678000	3.63609100
H	1.18010600	0.73364800	3.51072900
H	1.13169700	-1.72945900	1.46858300
H	-0.06660000	-3.90822900	1.52501600
H	-1.28107400	-3.31971000	0.41165100
H	-1.20801600	-2.66749200	2.02913900
C	0.52892900	-2.17341800	-2.48272800

H	1.23921200	-2.37634200	-3.29058400
H	-0.33761600	-2.82229600	-2.64105800
H	0.19039400	-1.13882900	-2.57581700
C	1.73515900	-4.36476000	-0.79243400
H	2.35792200	-4.63478200	-1.65092200
H	2.26487400	-4.65538000	0.11985600
H	0.82097400	-4.96335100	-0.84509300
C	-1.73515900	4.36480300	-0.79221500
H	-2.35793500	4.63486600	-1.65068000
H	-2.26485500	4.65539200	0.12009700
H	-0.82096900	4.96338600	-0.84486600
C	-0.52899200	2.17351300	-2.48262500
H	-1.23928700	2.37648100	-3.29046000
H	0.33756300	2.82237900	-2.64094900
H	-0.19048000	1.13892000	-2.57575700

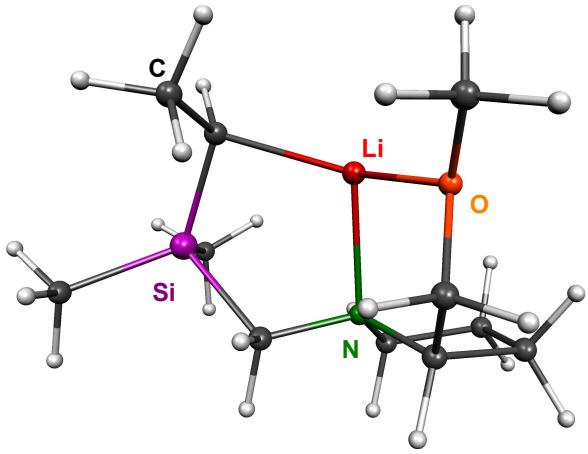


Fig. 15 Molekel plot of *mod*-(*R*,*S*)-**6** (monomer)

Table 18 Cartesian coordinates of *mod*-(*R*,*S*)-**6** (monomer) [M052X/6-31+G(d)]

atom	x	y	z
C	-1.66436000	1.20181300	-1.05814400
C	-1.66165400	2.55909900	-0.33128900
Si	-2.14896900	-0.22202400	-0.02415300
C	-0.58975600	-0.65218400	1.05429900
Li	0.32855900	0.63462700	-1.13737900
N	0.62387900	-0.85997700	0.23513200
C	0.78214000	-2.24214900	-0.21933300
O	1.90992600	1.49790700	-0.35899600
C	2.11038900	2.90664900	-0.41432700
C	2.18399200	-2.25302700	-0.82485000
C	1.89456800	-0.53473800	0.90159700
C	2.10156700	0.97120100	0.95445600
C	2.97203200	-1.27403200	0.07470000
H	-2.24383700	1.24519800	-1.98537700
H	-2.65778800	2.92206600	-0.03353400
H	-1.21281500	3.35812900	-0.93560300
H	-1.07481600	2.51977200	0.60018800
H	-0.72169400	-1.49179200	1.75607500
H	-0.43585700	0.24263500	1.66929100
H	-0.00649700	-2.50794000	-0.92205400
H	0.72166500	-2.93021100	0.64023000
H	1.90922900	3.22005800	-1.43596500
H	1.42102800	3.41487100	0.26456100
H	3.14296700	3.14830400	-0.14868100

H	2.14609800	-1.88263000	-1.85144000
H	2.61921700	-3.25204900	-0.84627700
H	1.88478000	-0.90923700	1.93755700
H	1.39019900	1.45131900	1.63537900
H	3.11744100	1.20053300	1.29576800
H	3.55576900	-0.57055000	-0.52057800
H	3.65981500	-1.79987100	0.73782800
C	-2.64941300	-1.73122100	-1.06620200
H	-2.58634700	-2.66571200	-0.50101200
H	-3.68549500	-1.61154300	-1.39556800
H	-2.03133400	-1.82197500	-1.96367700
C	-3.49869500	0.00932200	1.30528100
H	-4.46171500	0.21777200	0.83051300
H	-3.61664600	-0.87819600	1.93542900
H	-3.26490500	0.85769200	1.95615600

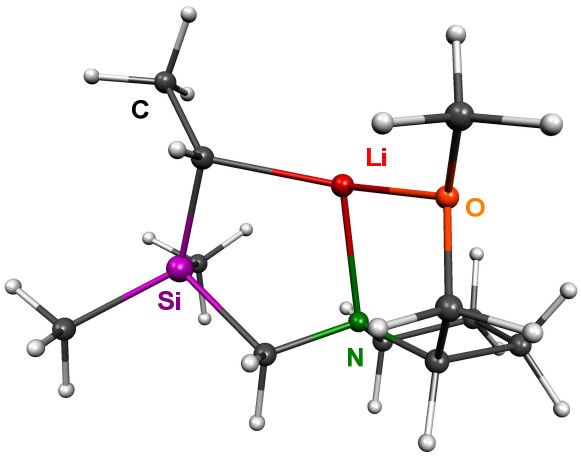


Fig. 16 Molekel plot of *mod*-(*S*,*S*)-**6** (monomer)

Table 19 Cartesian coordinates of *mod*-(*S*,*S*)-**6** (monomer) [M052X/6-31+G(d)]

atom	x	y	z
C	-1.67696600	1.41655800	-0.50274700
C	-2.68509600	1.91920500	-1.54771400
Si	-2.06743600	-0.17558500	0.30698300
C	-0.41065000	-0.74953900	1.13739300
Li	0.29942500	0.90065300	-0.87451100
N	0.71321600	-0.81299900	0.17993000
C	0.79980500	-2.09575300	-0.52003400
O	2.00958600	1.59231700	-0.16842900
C	2.20666600	2.99363000	-0.01222700
C	2.13526500	-2.00191400	-1.25310900
C	2.04888900	-0.60920600	0.76377900
C	2.29343600	0.86792600	1.02905700
C	3.02912300	-1.21897300	-0.26634300
H	-1.50709200	2.18819700	0.26769300
H	-2.86842400	1.15767900	-2.31447000
H	-2.31592800	2.80214500	-2.08195000
H	-3.67070800	2.19454800	-1.14121100
H	-0.47664100	-1.69041400	1.70778100
H	-0.19437000	0.04085500	1.86622400
H	-0.05825400	-2.23454400	-1.17616600
H	0.81153900	-2.92270300	0.20952900
H	1.96135800	3.46155200	-0.96241700
H	1.54757300	3.38421200	0.76773300
H	3.24945800	3.19966000	0.24356300

H	2.00776900	-1.44082800	-2.18137000
H	2.54085000	-2.98125800	-1.50682800
H	2.12623500	-1.14070900	1.72536200
H	1.64824400	1.24264100	1.83149900
H	3.33765800	1.03326300	1.31746300
H	3.59604100	-0.43874300	-0.77583400
H	3.74129500	-1.87444400	0.23604500
C	-2.66828900	-1.47323800	-0.94871900
H	-2.58977100	-2.49099900	-0.55510700
H	-3.72174100	-1.28824800	-1.17941200
H	-2.11561200	-1.41671700	-1.89057900
C	-3.30307200	-0.26047300	1.76018700
H	-2.98834600	0.39361400	2.57890400
H	-4.29117200	0.07672300	1.43418900
H	-3.40799900	-1.27613300	2.15590500

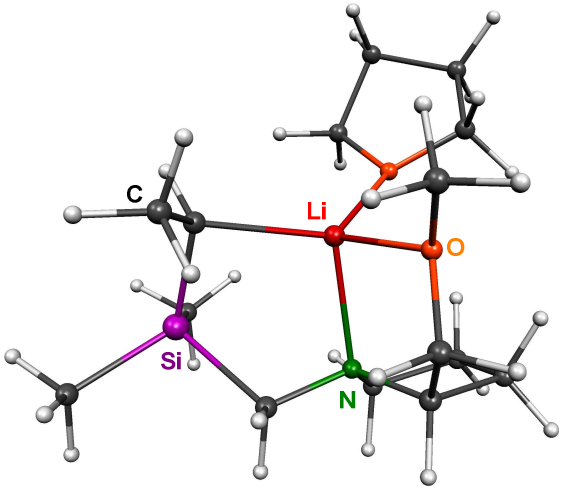


Fig. 17 Molekel plot of *mod*-(*R*,*S*)-**6**·THF (monomeric solvate)

Table 20 Cartesian coordinates of *mod*-(*R*,*S*)-**6**·THF (monomeric solvate) [M052X/6-31+G(d)]

atom	x	y	z
C	1.24613800	-1.53833300	1.15158800
C	1.74110000	-1.14128100	2.55298700
Si	2.38532700	-1.12727200	-0.21006500
C	2.21593500	0.78213900	-0.48368400
Li	-0.24474700	-0.16389800	0.47603200
N	0.81937000	1.17570300	-0.75990900
C	0.50028000	1.17763800	-2.18701300
O	-0.69380600	1.48563300	1.54396500
C	-0.91568600	1.38518400	2.94359100
C	-0.87143400	1.84849000	-2.25052500
C	0.44210700	2.51452100	-0.28879600
C	0.23262000	2.51683700	1.21655000
C	-0.83510100	2.86372200	-1.08470200
H	0.96487400	-2.59908500	1.12488600
H	2.61760900	-1.70449400	2.91196000
H	0.96552100	-1.26214200	3.32085400
H	2.03801000	-0.08174500	2.59083500
H	2.89123000	1.21701500	-1.23897400
H	2.51097000	1.21525400	0.47902900
H	0.51080700	0.16286700	-2.58336600
H	1.25052200	1.76896500	-2.73970600
H	-1.56453900	0.52684200	3.10673500
H	0.02838900	1.22406900	3.46961500

H	-1.39998900	2.29321100	3.31608500
H	-1.64697600	1.10130200	-2.08140600
H	-1.05308200	2.32144200	-3.21596700
H	1.24281500	3.23760800	-0.51787300
H	1.17253800	2.33233300	1.74829500
H	-0.16528200	3.48622700	1.54073000
H	-1.71792000	2.76810700	-0.45024400
H	-0.79022200	3.89390300	-1.44041800
O	-1.95498900	-0.74547400	-0.25217800
C	-2.05479500	-2.14681100	-0.58734100
C	-3.24642600	-0.22424700	0.11036300
C	-3.38435500	-2.59374200	0.00483500
C	-4.24263000	-1.34118700	-0.19639700
H	-1.17992100	-2.64097700	-0.16851500
H	-2.04946400	-2.24348500	-1.67714000
H	-3.42357900	0.68829700	-0.46001800
H	-3.23233600	0.02268700	1.17445400
H	-3.26676100	-2.81096500	1.06920600
H	-3.78695800	-3.47729700	-0.49048500
H	-4.57850200	-1.27799900	-1.23428600
H	-5.11764300	-1.30333200	0.45268900
C	1.92258200	-2.04977100	-1.81139500
H	2.40090600	-1.61560400	-2.69433200
H	2.24981200	-3.09093500	-1.73350600
H	0.84041700	-2.05698700	-1.97247100
C	4.26921500	-1.34848200	0.02018600
H	4.51360200	-2.40849600	0.13537800
H	4.83963000	-0.95819000	-0.82905100
H	4.61264800	-0.83416000	0.92338900

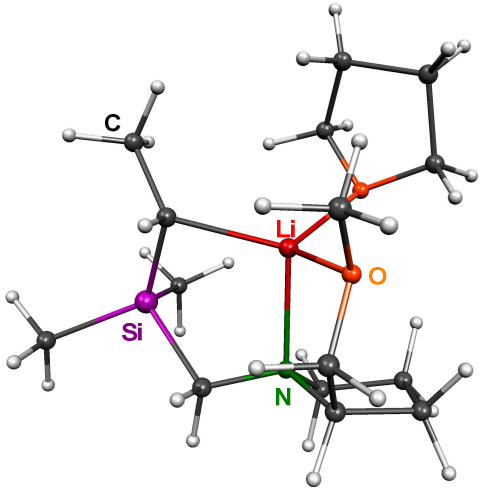


Fig. 18 Molekel plot of *mod*-(*S*,*S*)-**6**·THF (monomeric solvate)

Table 21 Cartesian coordinates of *mod*-(*S*,*S*)-**6**·THF (monomeric solvate) [M052X/6-31+G(d)]

atom	x	y	z
C	1.04854600	-1.58745800	0.97349000
C	0.90395400	-3.11582100	0.93748300
Si	2.44460400	-0.89501600	0.02296400
C	2.24317800	1.01800000	0.17023600
Li	-0.32613400	-0.14452400	0.20949100
N	0.91750200	1.47805300	-0.29305100
C	0.90284200	1.87832200	-1.69971000
O	-1.18946600	1.15837400	1.49781700
C	-1.70808500	0.57416700	2.68491800

C	-0.46327800	2.53968600	-1.86068300
C	0.36962200	2.62655400	0.44461700
C	-0.21711300	2.16469500	1.76819700
C	-0.67135700	3.25875600	-0.50982700
O	-1.78404200	-0.63414300	-0.99894000
C	-1.82546000	-2.05949700	-1.17935600
C	-3.13767200	-0.19692800	-0.79960900
C	-2.83265100	-2.51250100	-0.13294400
C	-3.90007600	-1.40331800	-0.20409900
H	1.10625200	-1.23504300	2.01794100
H	0.95435200	-3.49505700	-0.09216200
H	-0.05920400	-3.46065100	1.33826000
H	1.67821100	-3.66557600	1.49470300
H	3.03960700	1.61358200	-0.30402400
H	2.31606600	1.20825100	1.24741800
H	1.05200300	1.01287800	-2.34523300
H	1.71345800	2.60017800	-1.89831900
H	-2.43412100	-0.17808400	2.38105700
H	-0.90779700	0.09261600	3.25290700
H	-2.20020700	1.33481500	3.29894500
H	-1.22152200	1.76961900	-2.00575600
H	-0.49832500	3.22135500	-2.71094100
H	1.16953100	3.35093000	0.66742000
H	0.56014600	1.74257000	2.41573900
H	-0.69144400	3.00328900	2.29159200
H	-1.68598300	3.11970200	-0.13401400
H	-0.49369400	4.33141000	-0.59793300
H	-0.81702000	-2.43390700	-1.02293200
H	-2.16670400	-2.28117000	-2.19714600
H	-3.55543100	0.10281200	-1.76442200
H	-3.09895800	0.66903200	-0.14088900
H	-2.34000900	-2.52355200	0.84175200
H	-3.23709700	-3.50504600	-0.33183400
H	-4.72063100	-1.69585400	-0.86067600
H	-4.32455300	-1.17701900	0.77433100
C	2.36964500	-1.42552700	-1.80708700
H	3.03263300	-0.81960200	-2.43211300
H	2.68913600	-2.46776600	-1.90388800
H	1.35367900	-1.35415400	-2.20770100
C	4.25600500	-1.19944900	0.55327100
H	4.43491200	-0.82302600	1.56502400
H	4.47111500	-2.27225800	0.56188800
H	4.97249300	-0.71979500	-0.12199800

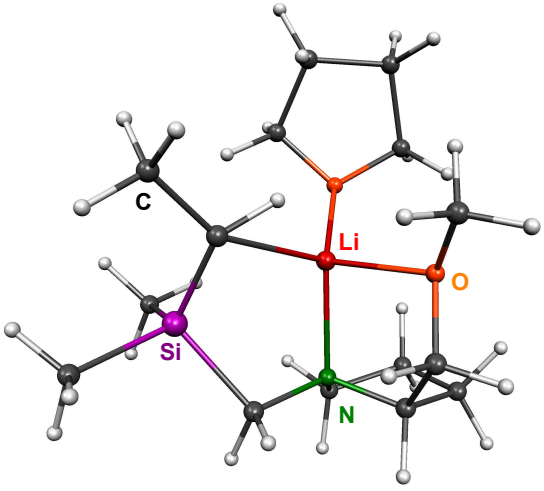


Fig. 18 Molekel plot of *mod*-TS-**6**·THF (transition state)

Table 22 Cartesian coordinates of *mod*-TS-**6**·THF (transition state) [M052X/6-31+G(d)]

atom	x	y	z
C	0.83654600	-1.65816300	0.97785500
C	0.95173700	-3.08236800	1.52331200
Si	2.11617500	-1.10644400	-0.17690200
C	2.32860800	0.80965200	-0.08337000
Li	-0.32050100	0.06708000	0.10889600
N	1.03519300	1.49561000	-0.34548500
C	0.93396400	2.08256500	-1.68282600
O	-0.96096000	1.21880600	1.59950000
C	-1.43653700	0.53894100	2.75834100
C	-0.35972600	2.88714300	-1.60324900
C	0.70807400	2.59096700	0.58460400
C	0.18853500	2.01870700	1.89230900
C	-0.32326600	3.46390700	-0.17141400
H	-0.20170200	-1.34163400	1.09399700
H	0.47817000	-3.86517300	0.90421700
H	0.50220900	-3.16994300	2.52109400
H	1.99704300	-3.38376900	1.64304200
H	3.09752700	1.20856300	-0.76102500
H	2.64749200	1.03719000	0.93794500
H	0.92643400	1.30306500	-2.44476700
H	1.79547900	2.74377200	-1.87280800
H	-2.30415800	-0.04481900	2.45308600
H	-0.65960700	-0.12799900	3.14183900
H	-1.73411700	1.26399400	3.52142400
H	-1.21175900	2.21499400	-1.72603000
H	-0.42162200	3.66012100	-2.36965800
H	1.61347700	3.17539000	0.80797900
H	0.94281800	1.38029400	2.36596400
H	-0.09564600	2.82284800	2.58097200
H	-1.30296700	3.41981100	0.30558300
H	0.00155500	4.50513300	-0.17445300
O	-1.79734300	-0.48008300	-0.99876100
C	-1.85883700	-1.88717300	-1.30575300
C	-3.14399700	-0.03839900	-0.75922100
C	-2.88728700	-2.41541700	-0.31639600
C	-3.92445100	-1.27598000	-0.26307600
H	-0.85644200	-2.28916100	-1.16490300
H	-2.18553100	-2.00642300	-2.34439700
H	-3.55647200	0.34752000	-1.69464000
H	-3.09184500	0.77124200	-0.03238200
H	-2.40390900	-2.55399900	0.65312100
H	-3.32035100	-3.36637300	-0.62661300
H	-4.76616800	-1.48337200	-0.92482700
H	-4.32075300	-1.13167400	0.74212300
C	1.93236200	-1.44359100	-2.06651400
H	2.76465800	-1.03322600	-2.65033900
H	1.89990500	-2.52430400	-2.24171400
H	1.00108500	-1.02686900	-2.46601700
C	3.80052600	-1.85399200	0.26903100
H	3.83486200	-2.92237000	0.04101200
H	4.59117900	-1.36787300	-0.31052100
H	4.01677500	-1.72582600	1.33232100

Table 23 Cartesian coordinates of THF (solvent) [M052X/6-31+G(d)]

atom	x	y	z

O	-0.00000100	-1.24544800	-0.00006700
C	-1.16420300	-0.42523800	-0.13741500
C	1.16419600	-0.42523400	0.13749600
C	-0.72743300	0.99010500	0.23780200
C	0.72745600	0.99007300	-0.23784200
H	-1.94542500	-0.82386300	0.51031000
H	-1.50962300	-0.46827100	-1.17550200
H	1.94551200	-0.82394000	-0.51006200
H	1.50937300	-0.46823700	1.17566900
H	-0.77014000	1.12633300	1.32136600
H	-1.34071300	1.75855300	-0.23390900
H	0.77018500	1.12623200	-1.32141500
H	1.34074200	1.75853700	0.23382900
H	-0.31345978	-0.92997314	-0.00000010
C	-0.67011420	0.07883686	-0.00000010
H	-0.31344136	0.58323505	0.87365140
H	-0.31344136	0.58323505	-0.87365160
H	-1.74011420	0.07885004	-0.00000010

Table 24 SCF and Zero-Point-Energies for the computed compounds

Structure	Properties	SCF energy	Zero-Point-Energy
[(*S*)-**5**·*t*-BuLi]	starting material	-1402.41882168	-1401.829354
[(*S*)-**5**·*t*-BuLi]	pro-*R* transition state	-1402.39074720	-1401.805201
[(*S*)-**5**·*t*-BuLi]	pro-*S* transition state	-1402.38916314	-1401.803689
[(*R*,*S*)-**6**·*t*-BuH]	product	-1402.43870264	-1401.848360
[(*S*,*S*)-**6**·*t*-BuH]	product	-1402.43886873	-1401.848659
[(*R*,*S*)-**6**]$_2$	dimeric crystal	-2488.02414005	-2487.108221
mod-[(*R*,*S*)-**6**]$_2$·Me_3SnCl	starting material	-2304.39630710	-2303.589364
mod-[(*R*,*S*)-**6**]$_2$·Me_3SnCl	transition state	-2304.39311842	-2303.583695
mod-[(*R*,*S*)-**6**]$_2$·Me_3SnCl	product	-2304.39535761	-2303.585688
mod-[(*R*,*S*)-**6**]$_2$	homochiral dimer	-1720.452789	-1720.452789
mod-(*R*,*S*),(*S*,*S*)-**6**$_2$	heterochiral dimer	-1721.13991081	-1720.448944
mod-[(*S*,*S*)-**6**]$_2$	homochiral dimer	-1721.13465375	-1720.442824
mod-(*R*,*S*)-**6**	monomer	-860.544890652	-860.200255
mod-(*S*,*S*)-**6**	monomer	-860.543359244	-860.198855
mod-(*R*,*S*)-**6**·THF	monomeric solvate	-1092.98796456	-1092.522721
mod-(*S*,*S*)-**6**·THF	monomeric solvate	-1092.98838460	-1092.522731
mod-TS-**6**·THF	transition state	-1092.96083597	-1092.495581
THF	solvent	-232.418147485	-232.298971

Additional perspectives of [(*R*,*S*)-6]$_2$

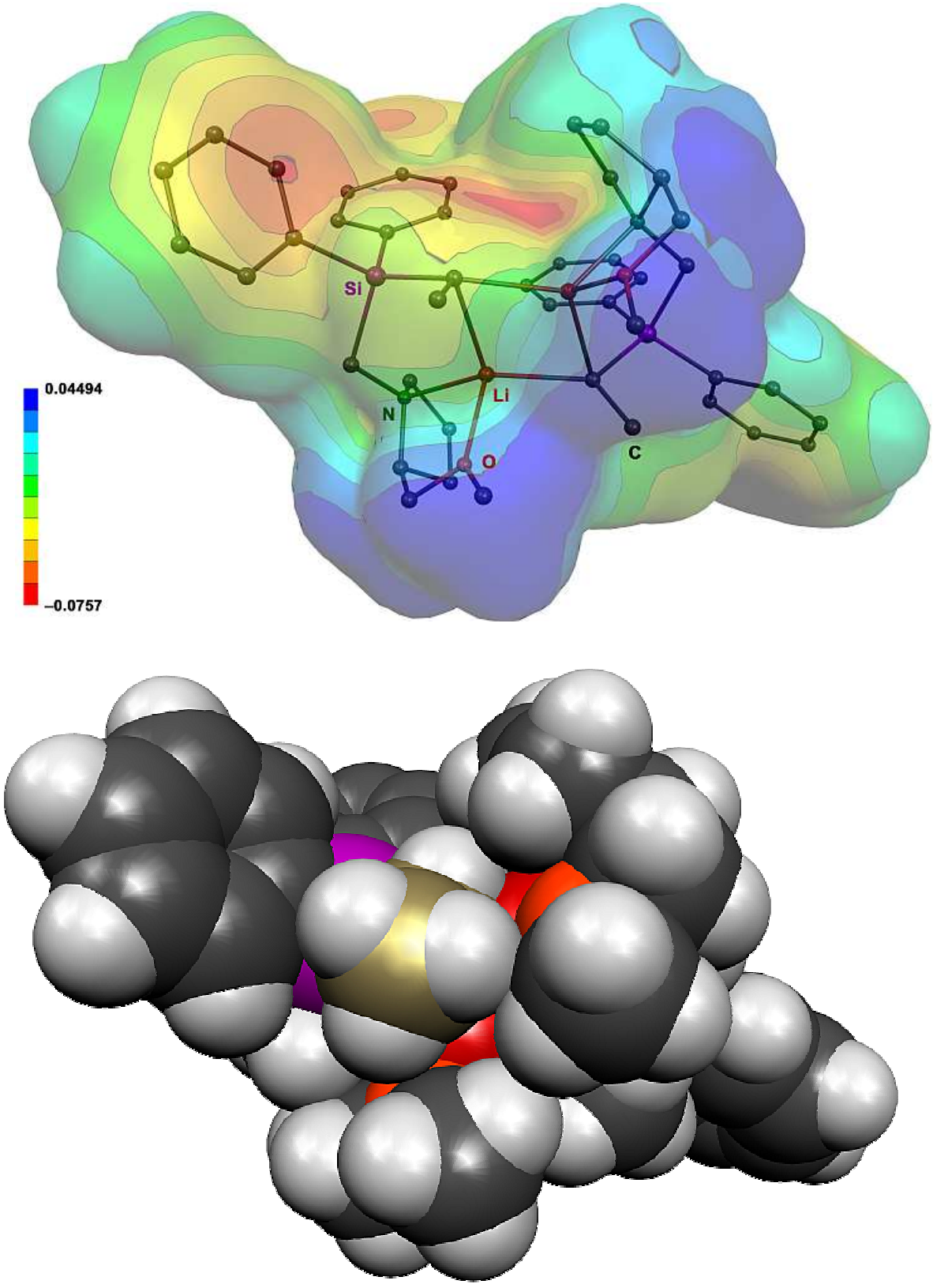


Fig. 19 Additional perspective and visualisation of [(*R*,*S*)-**6**]: Top: Conolly surface (probe radius 1.4 Å) mapped with electrostatic potential (hydrogens omitted for the sake of clarity); bottom: space-filling model, the exposed metalated ethyl side-chain is highlighted in gold.

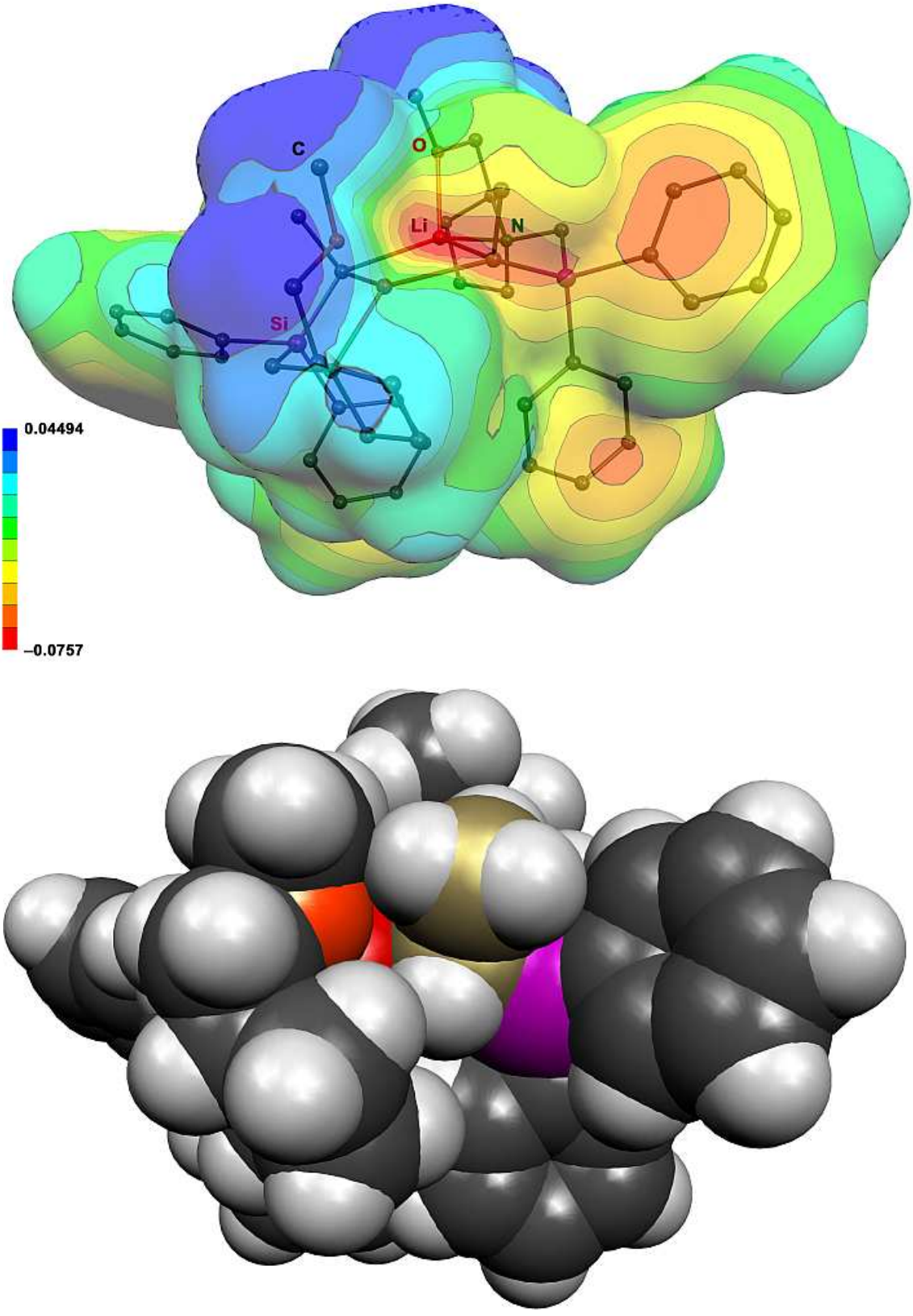


Fig. 20 Additional perspective and visualisation of [(*R*,*S*)-**6**]: Top: Conolly surface (probe radius 1.4 Å) mapped with electrostatic potential (hydrogens omitted for the sake of clarity); bottom: space-filling model, the exposed metalated ethyl side-chain is highlighted in gold.

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