Electronic Supplementary Information

Planar lithium silolide: Aromaticity, with significant contribution of a non-classical resonance structure

Csaba Fekete[a,b], Ilona Kovács[a], László Nyulászi[b*], Tamás Holczbauer[c]*

a. *Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, Szt. Gellért tér 4. Budapest, H-1111, Hungary. E-mail: ikovacs@mail.bme.hu*

b. *MTA-BME Computation Driven Chemistry Research Group. E-mail: nyulaszi@mail.bme.hu*

c. *Institute of Organic Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, POB. 206, H-1519 Budapest, Hungary.*

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Experimental section

General procedure: All reactions were performed in oven-dried glassware under dried nitrogen or argon using standard Schlenk techniques. Solvents were dried according to well-known procedures (THF, diethyl ether and C_6D_6 over sodium/benzophenone, hexane over $LiAlH_4$.) and distilled freshly before use. Solids were dried in vacuum. 12-crown-4 was dried over sodium chips and distillated before use. $CDCl_3$ was dried over activated molecular sieves. 1.6 M *n*-butyl lithium and 1.6 M *tert*-butyl lithium solution in hexane from Merck Ltd. were used directly. NMR spectra were recorded on a Bruker Avance 300 and a Bruker DRX-500 spectrometers (standard: external TMS, chemical shifts are given in ppm). HMBC, HMQC and DEPT measurements were carried out to interpret the signals of the phenyl- and silol-rings. X-ray crystallographic determinations were performed on a RIGAKU R-Axys Rapid diffractometer. High-resolution mass spectra were recorded with a Micromass GCT mass spectrometer (70eV; DIR-EI). Elemental analysis was performed with an Elemental vario EL analyser.

The single crystal of **3** was mounted on a loop. Intensity data were collected on a RAXIS-RAPID diffractometer (monochromator; Mo-Ka radiation, l Ľ 0.71073 Å) at 93(2) K. The structure was solved by direct methods[1] (and subsequent difference syntheses). Hydrogen atomic positions were calculated from assumed geometries. Hydrogen atoms were included in structure factor calculations but they were not refined. The isotropic displacement parameters of the hydrogen atoms were approximated from the U(eq) value of the atom they were bonded to. The molecular graphics were prepared using the software Mercury[2].

Computations: Quantum chemical calculations were carried out with the Gaussian09[3] package at the B3LYP/6-31+G(d, 2p) or M06-2X/6-31+G(d, 2p)[4] level of theory. Planar silolide anions were always (unless otherwise stated) first-order saddle points (the imaginary frequency being the out-of-the plane motion of the substituent on the silicon) and pyramidal silolide anions were always real minima. NMR chemical shifts and NICS(1)[5] values have been calculated by the B3LYP/pcS-2 method[6]. For the visualization of the structures the Molden program[7] was used. Bader analysis were carried out with Aimstudio program set.[8,9]

*1,1-Dichloro-3,4-diphenyl-2,5-bis(trimethylsilyl)-1-silacyclopentadiene (**1**)*

The synthesis was carried out according to Tamao's produce[10] The ^{1}H, ^{13}C, and ^{29}Si NMR data of the product were in agreement with the previously reported results. M.p. 78–81°C. ^{1}H NMR ($CDCl_3$): δ = 0.22 (s, 18H, $SiMe_3$), 6.67–6.96 (m, 10H, ArH). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$):

δ = 0.3 ($SiMe_3$), 127.0 (*p*Ph), 127.5, 128.4 (o/*m*Ph), 136.2 (C_α), 140.4 (*i*Ph), 169.8 (C_β). $^{29}Si\{^1H\}$ NMR (C_6D_6): δ = 19.3 (Si-*ring*), –7.9 ($SiMe_3$).

*1-Chloro-3,4-diphenyl-1-(2,4,6-trimethylphenyl)-2,5-bis(trimethylsilyl)-1-silacyclopentadiene (**2**)* 0.37 mL (2.41 mmol) mesityl bromide was dissolved in 10 mL diethyl ether and cooled to –80 °C. To this solution *tert*-BuLi (1.56 M in hexane, 1.55 mL, 2.41 mmol) was added dropwise. The resulting white suspension was stirred for another 1 hour at the same temperature. After that 900 mg (2.01 mmol) **1** in 10 mL THF was added dropwise to the reaction mixture and stirred for half hour at the same temperature. The resulted greenish mixture was allowed to warm to room temperature and was stirred overnight. The solvents were removed at reduced pressure resulting in a yellowish residue. After addition of 15 mL hexane the mixture was filtered. The volatiles were removed at reduced pressure at 100°C and the residue was distillated in vacuum (230-250°C / 10^{-3} Hgmm). Pure compound was obtained by recrystallization from hexane at –30 °C, yielded: 835 mg (78%). M.p. 143-145 °C. Anal. calcd. for $C_{31}H_{39}Si_3Cl$ (531.35): C, 70.07; H, 7.40%. Found: C, 69.02; H, 7.12. ^1H NMR ($CDCl_3$,): δ = –0.22 (s, 18H, $SiMe_3$), 2.32 (s, 3H, *p*Me), 2.57 (s, 3H, *o*Me) 2.81 (s, 3H, *o*Me), 6.83–6.96 (m, 6H, ArH), 7.03–7.12 (m, 6H, ArH). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ = 0.1 ($SiMe_3$), 20.2 (*o*Me) 21.1 (*p*Me) 25.8 (*o*Me), 125.0 (*i*Mes), 126.5 (*p*Ph) 127.1 (*m*Ph), 128.1 (br, *o*Ph) 129.2 (*m*Mes), 130.7 (*m*Mes), 140.1 (*p*Mes), 141.7 (PhC_i), 143.6 (C_α), 144.1 (*o*Mes), 146.0 (*o*Mes), 168.1 (C_β), $^{29}Si\{^1H\}$ NMR ($CDCl_3$): δ = 17.0 (Si-*ring*), –8.8 ($SiMe_3$) HRMS (EI): m/z (%) 530.2017 (calc. for $C_{31}H_{39}Si_3{}^{35}Cl$ 530.2048) (4.6), 532.2011 (calc. for $C_{31}H_{39}Si_3{}^{37}Cl$ 532.2019) (2.3) [M^+], 422.1794 (calc. for $C_{28}H_{30}Si_2$ 422.1886) (100) [M^+–$ClSiMe_3$], 303.0976 (calc. for $C_{19}H_{19}Si_2$ 303.10254) (66.9) [M^+–$ClSiMe_3$-Mes].

*η^5-Lithio- 3,4-diphenyl-1-(2,4,6-trimethylphenyl)-2,5-bis(trimethylsilyl)-1-silacyclopentadien (**3**)* 600 mg (1.13 mmol) **2** was dissolved in 8 mL THF and 15.8 mg granulated lithium (2.26 mmol) was added to the solution. The mixture was stirred for one day at room temperature while the colour slowly turned to deep red. THF was removed at reduced pressure and the residue was dissolved in diethyl ether followed by the filtration of the white precipitate (LiCl). Pure product was obtained by recrystallization from concentrated diethyl ether solution at –30 °C, yielded: 403 mg (62%) orange crystals. ^1H NMR (C_6D_6): δ = 0.16 (s, 18H, $SiMe_3$), 1.15 (m, 4.5H, OCH_2CH_2–), 2.13 (s, 3H, *p*Me), 2.71 (s, 3H, *o*Me) 2.88 (s, 3H, *o*Me), 3.36 (m,

4.5H, OC*H*$_2$CH$_2$–), 6.86 (s, 1H, MesC*H*), 6.95 (s, 1H, MesC*H*) 6.96 (m, 2H, Ph*pH*), 7.08 (t, 4H, Ph*mH*), 7.32 (d, 4H, Pho*H*). ^{13}C{^{1}H} NMR (C_6D_6): δ = 3.3 ($SiMe_3$), 21.5 (*p*Me), 25.3 (OCH$_2$*C*H$_2$–), 27.6 (*o*Me), 28.3 (*o*Me), 69.3 (OCH$_2$*C*H$_2$–), 103.1 (C_α), 125.0 (*p*Ph), 127.3 (*m*Ph), 127.9 (*m*Mes), 128.6 (*m*Mes), 132.0 (*o*Ph), 132.8 (*p*Mes), 135.0 (C_β), 140.2 (Mes*C*$_i$), 142.4 (*o*Mes), 145.7 (Ph*C*$_i$), 146.5 (*o*Mes). ^{29}Si{^{1}H} NMR (C_6D_6): δ = 65.7 (Si-*ring*), –11.6 ($SiMe_3$). ^{7}Li NMR (C_6D_6, external reference LiBr–D_2O (0.1M) = 0.00): –5.6

η^5-Lithio-3,4-diphenyl-1-(2,4,6-trimethylphenyl)-2,5-bis(trimethylsilyl)-1-silacyclopentadien with 12-crown-4: 46 mg (0.08 mmol) **3** was dissolved in 1 mL THF and 13 µl (0.08 mmol) 12-corown-4 was added to the solution. The mixture was stirred for an hour at room temperature. A part of the mixture was filled in an NMR tube containing C_6D_6. ^{1}H NMR (C_6D_6): δ = 0.03 (s, 18H, $SiMe_3$), 2.56 (s, 3H, *p*Me), 3.02 (s, 6H, *o*Me), 7.02 (m, 2H, Ph*pH*), 7.10 (s, 2H, MesC*H*) 7.15 (t, 4H, Ph*mH*), 7.36 (d, 4H, Pho*H*). ^{13}C{^{1}H} NMR (C_6D_6): δ = 3.5 ($SiMe_3$), 20.9 (*p*Me), 27.0 (*o*Me), 109.8 (C_α), 121.4 (*p*Ph), 125.7 (*m*Ph), 126.6 (*m*Mes), 132.1 (*o*Ph), 136.5 (*p*Mes), 136.8 (C_β), 139.6 (Mes*C*$_i$), 144.8 (*o*Mes), 150.1 (Ph*C*$_i$). ^{29}Si{^{1}H} NMR (C_6D_6): δ = 60.0 (Si-*ring*), –14.5 ($SiMe_3$). ^{7}Li NMR (C_6D_6, external reference LiBr–D_2O (0.1M) = 0.00): –0.2

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^{1}H, $^{13}C\{^{1}H\}$, DEPT, HSQC/HMBC and $^{29}Si\{^{1}H\}$ spectra of 2

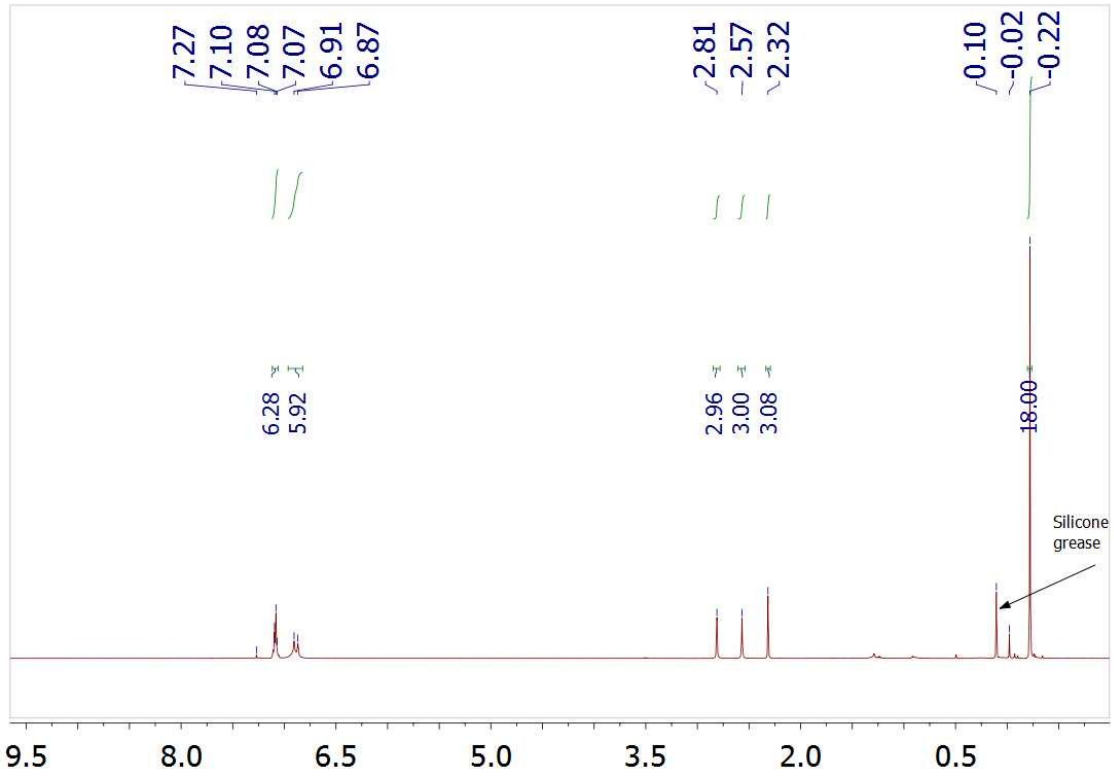


Fig. S1 ^{1}H spectrum of **2** at 298K in $CDCl_3$

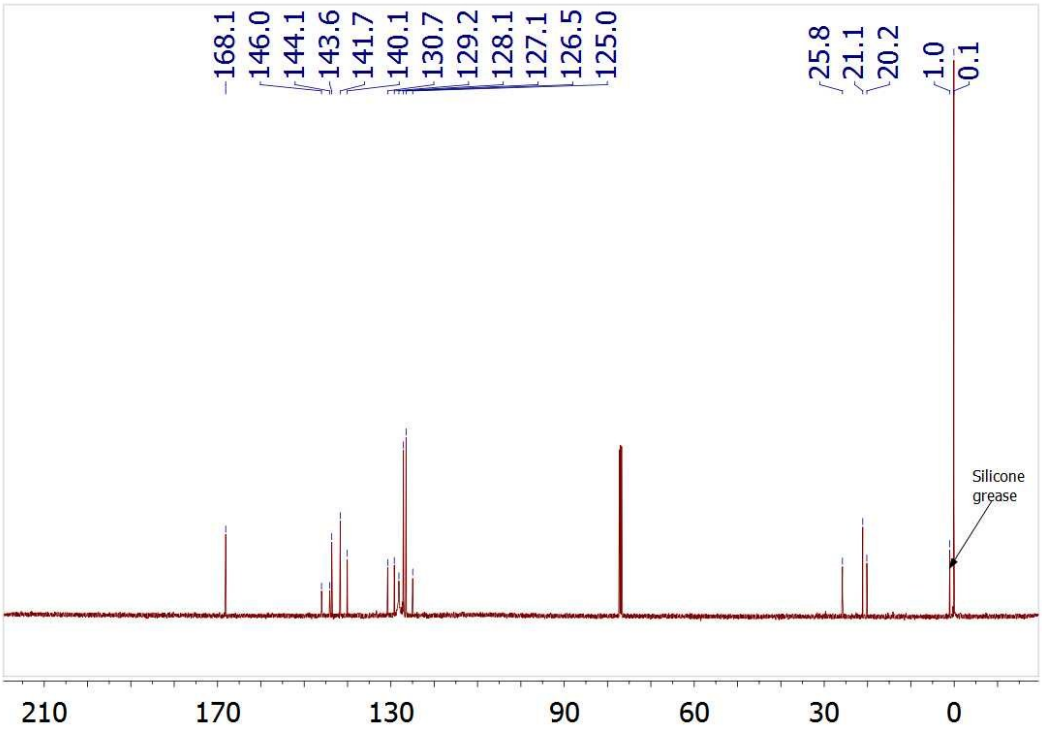


Fig. S2 $^{13}C\{^{1}H\}$ spectrum of **2** at 298K in $CDCl_3$

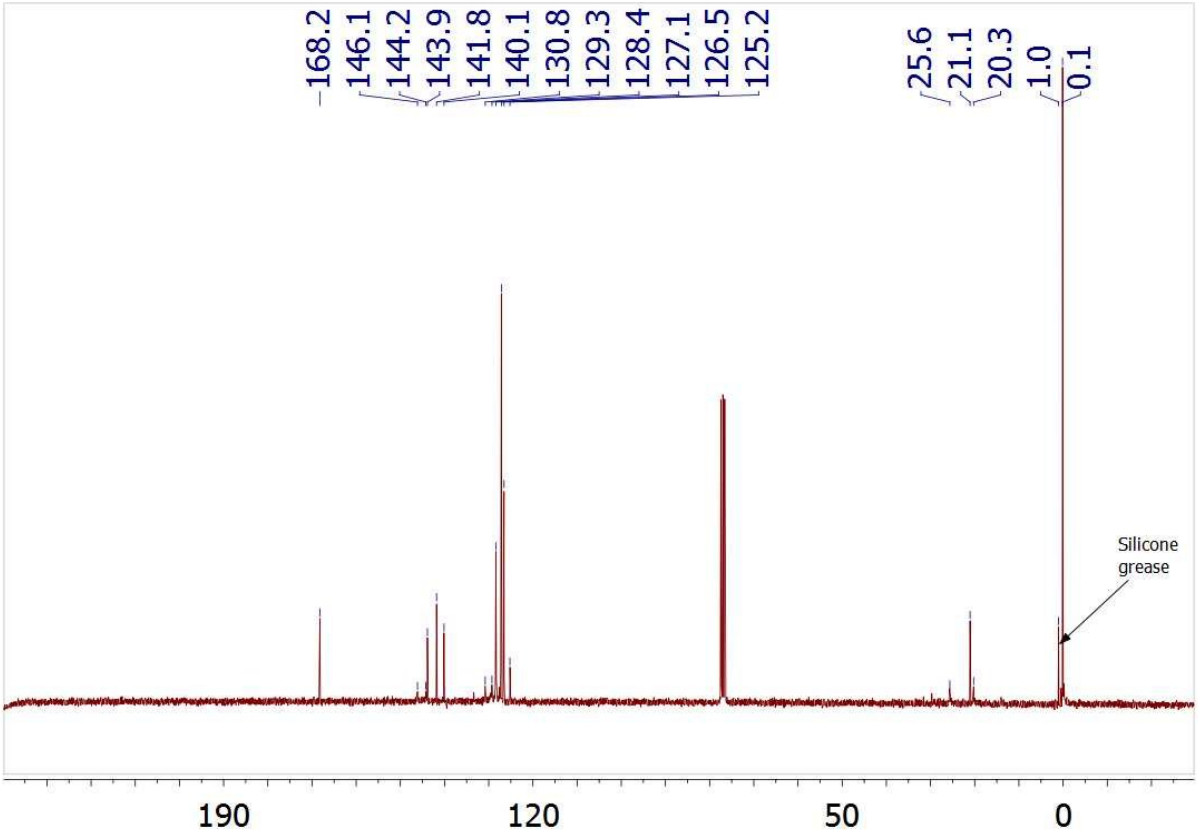


Fig. S3 $^{13}C\{^{1}H\}$ spectrum of **2** at 320K in $CDCl_3$

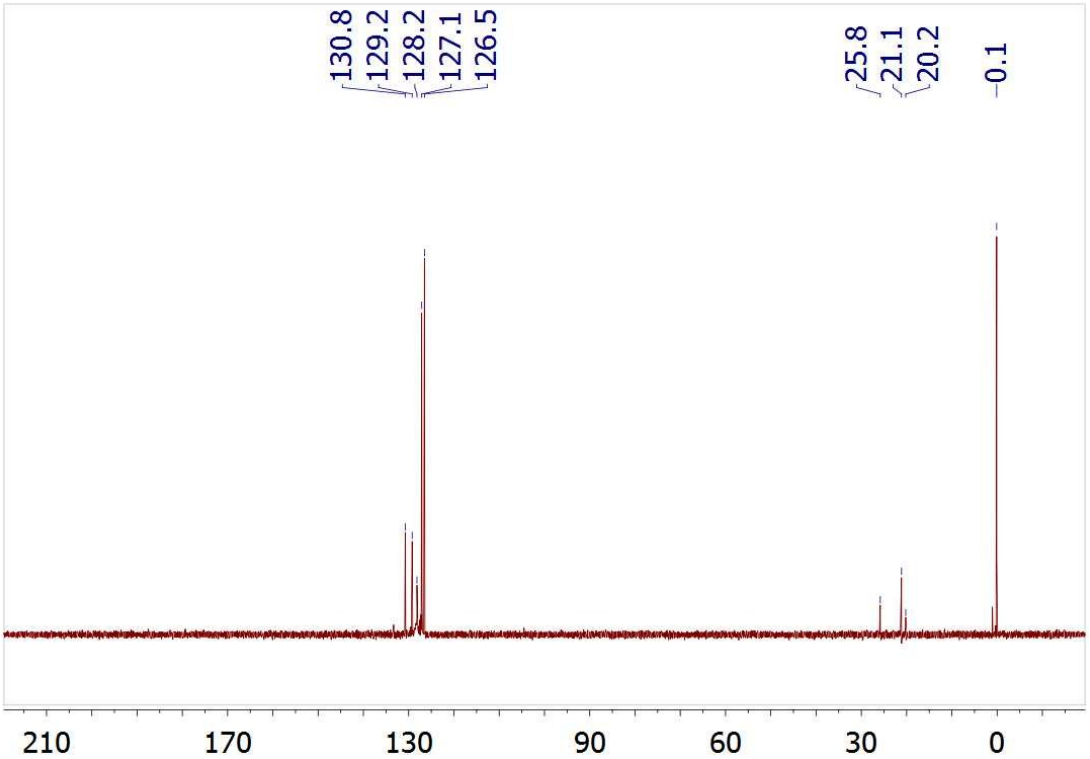


Fig. S4 DEPT spectrum of **2** in $CDCl_3$

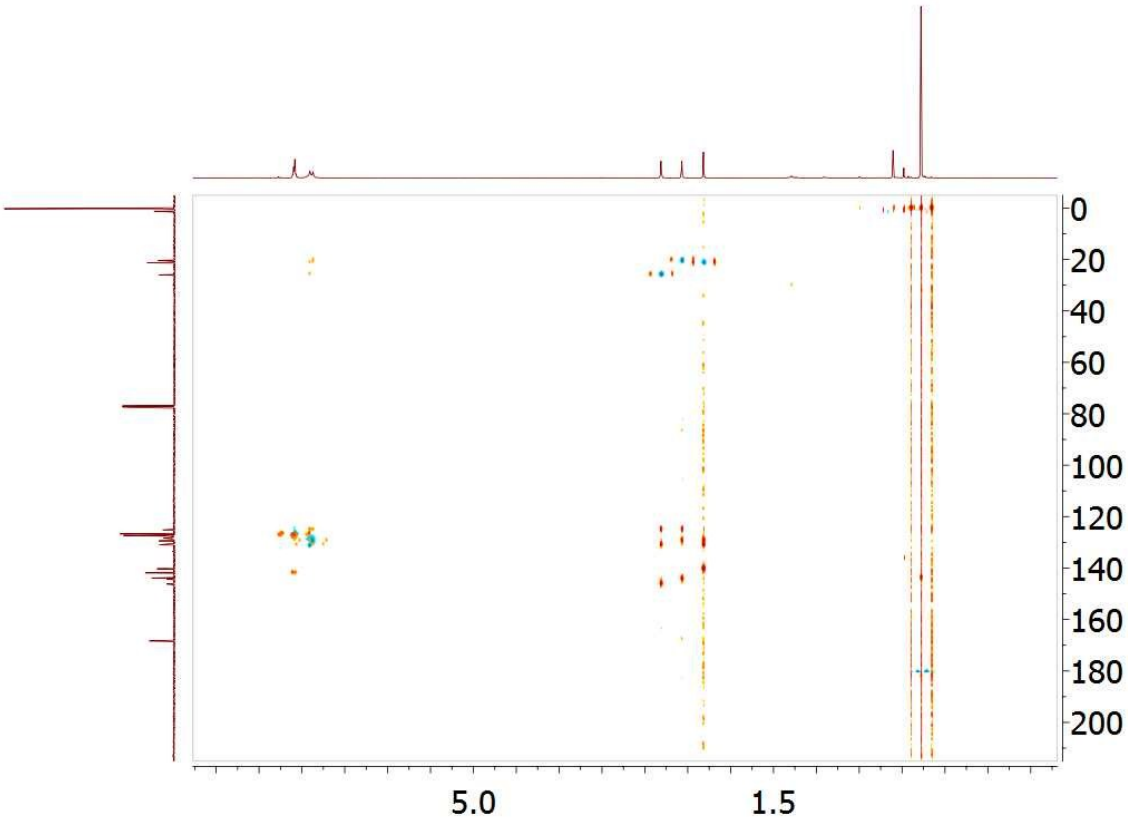


Fig. S5 HSQC/HMBC spectrum of **2** in $CDCl_3$

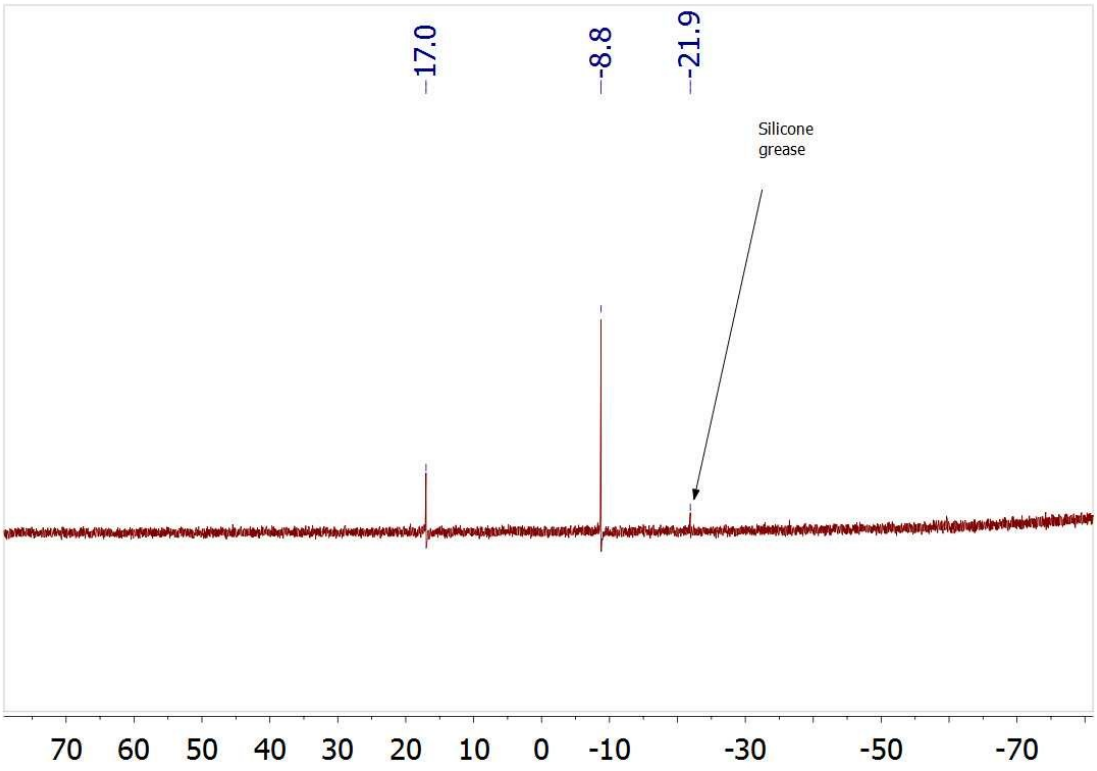


Fig. S6 $^{29}Si\{^{1}H\}$ spectrum of **2** in $CDCl_3$

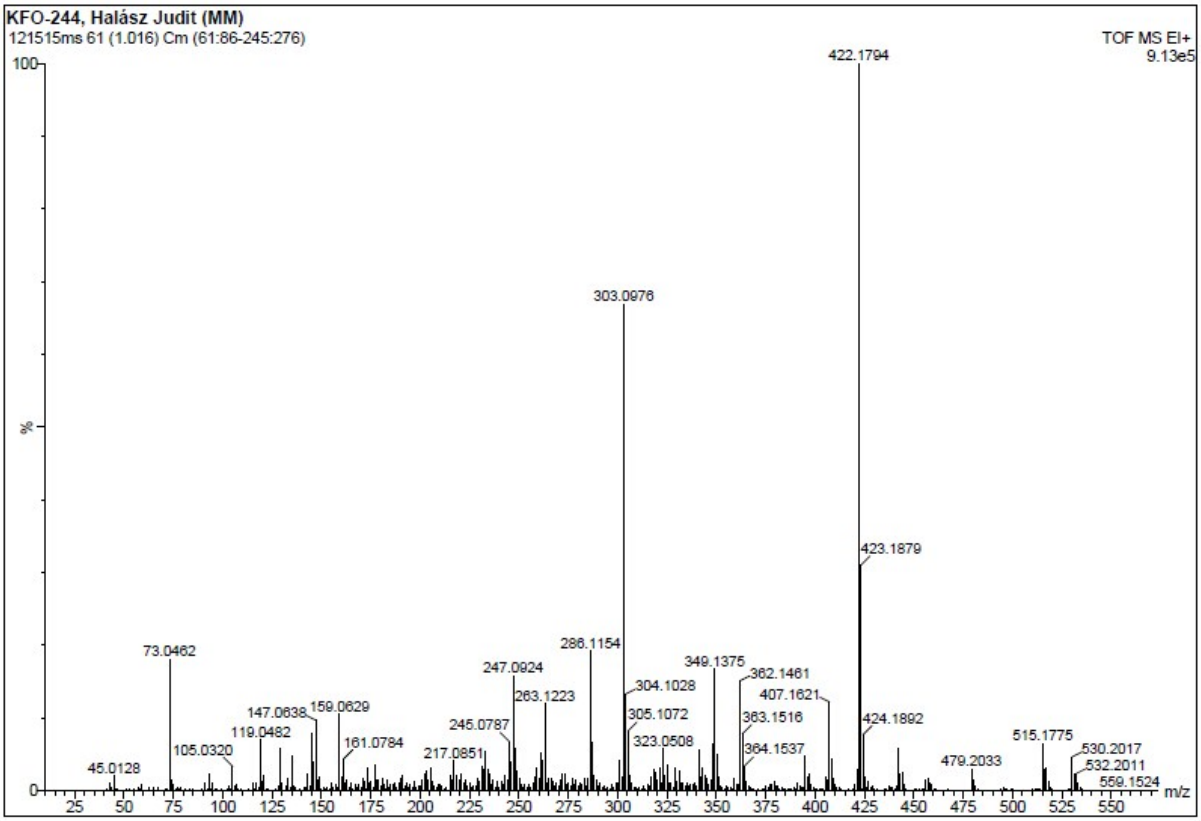


Fig. S7 HRMS (EI) spectrum of **2**

^{1}H, $^{13}C\{^{1}H\}$, DEPT, HSQC/HMBC, $^{29}Si\{^{1}H\}$ and $^{29}Si - ^{1}H$ corr. spectra of 3

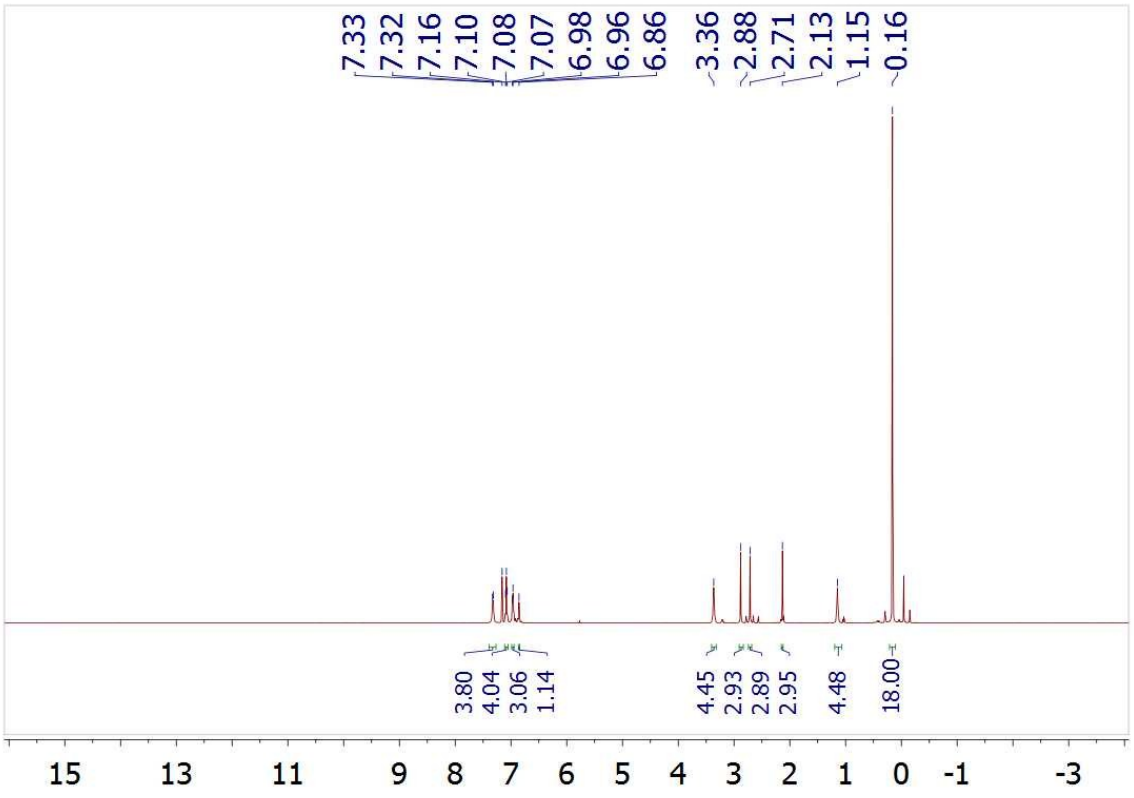


Fig. S8 ^{1}H spectrum of **3** at 298K in C_6D_6

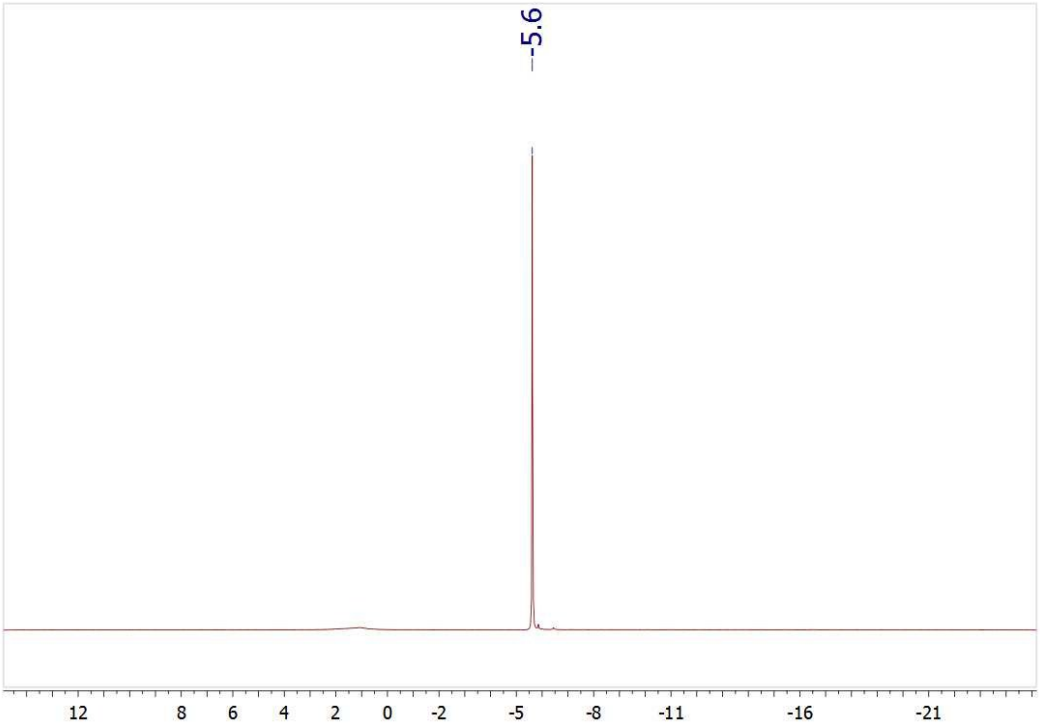


Fig. S9 ^{7}Li spectrum of **3** at 298K in C_6D_6

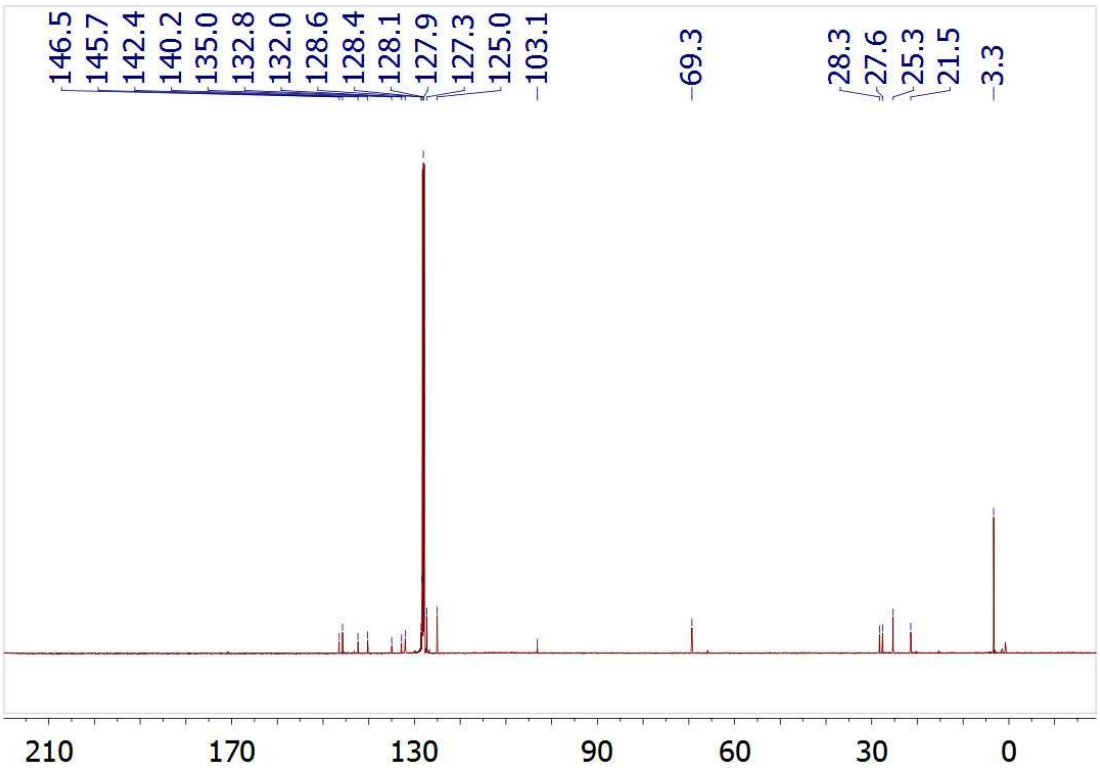


Fig. S10 $^{13}C\{^{1}H\}$ spectrum of **3** at 298K in C_6D_6

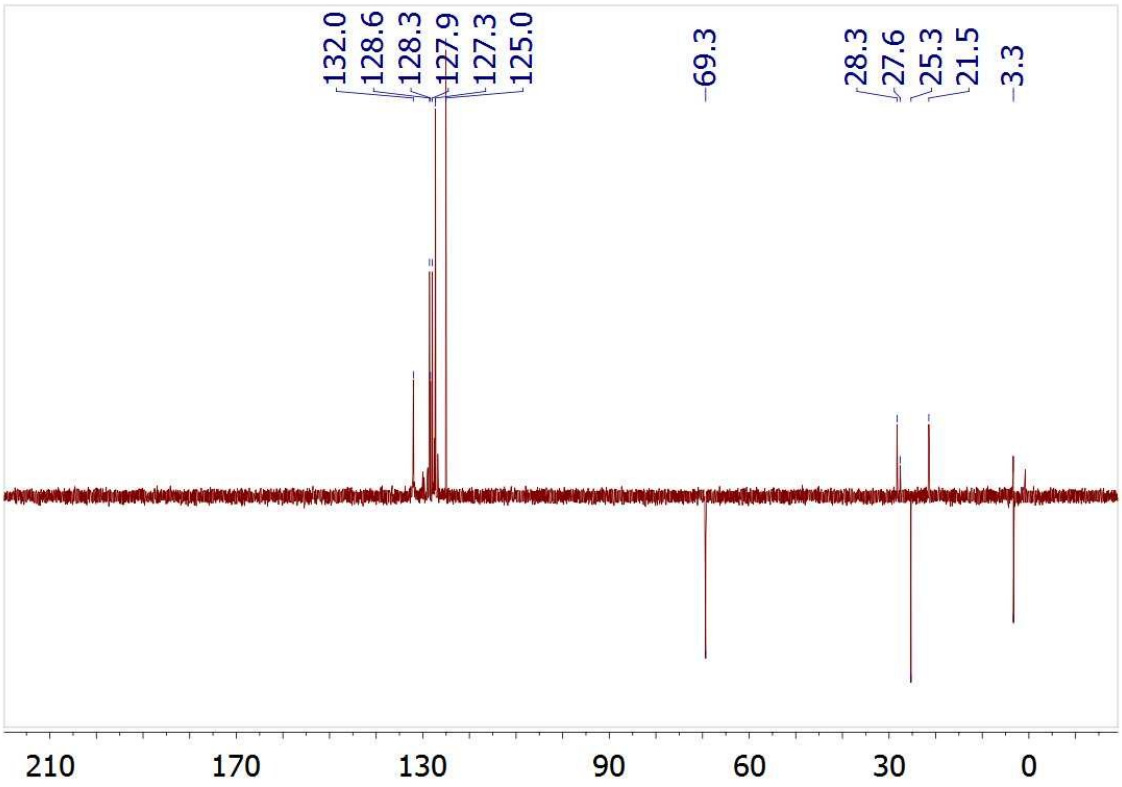


Fig. S11 DEPT spectrum of **3** in C_6D_6

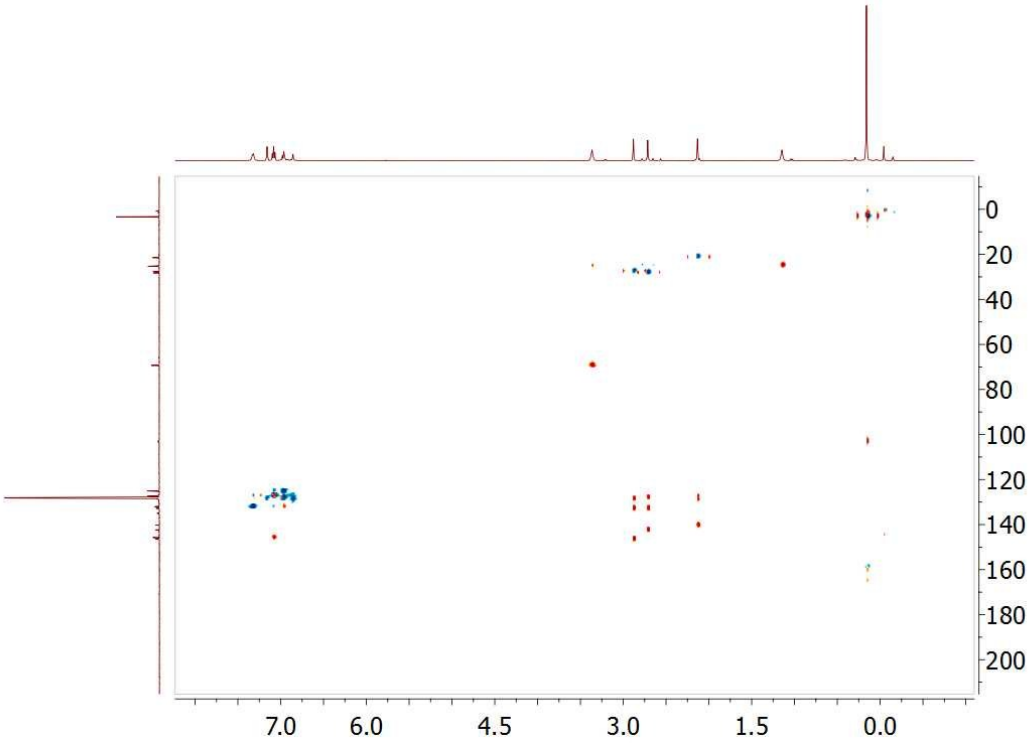


Fig. S12 HSQC/HMBC spectrum of **3** in C_6D_6

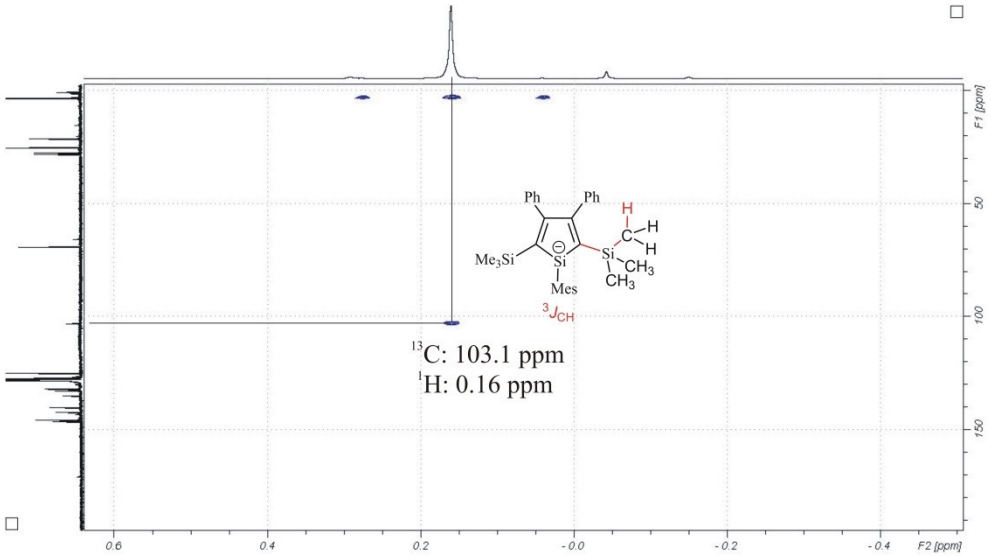


Fig. S13 Interpretation of C_α in HMBC spectrum of **3**

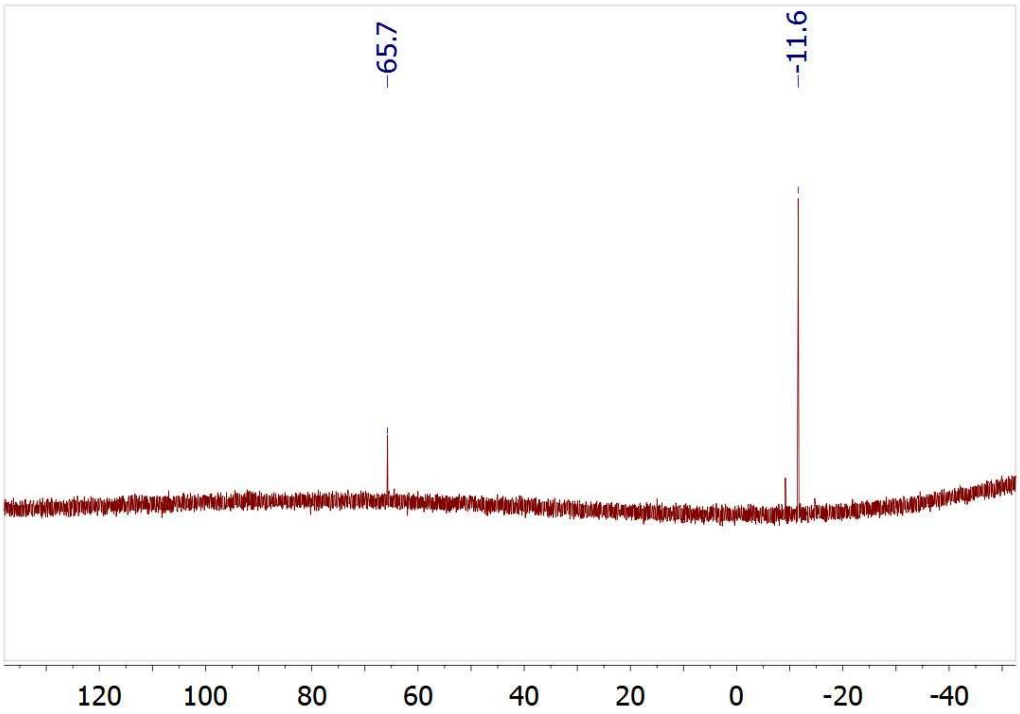


Fig. S14 $^{29}Si\{^{1}H\}$ spectrum of **3** in C_6D_6

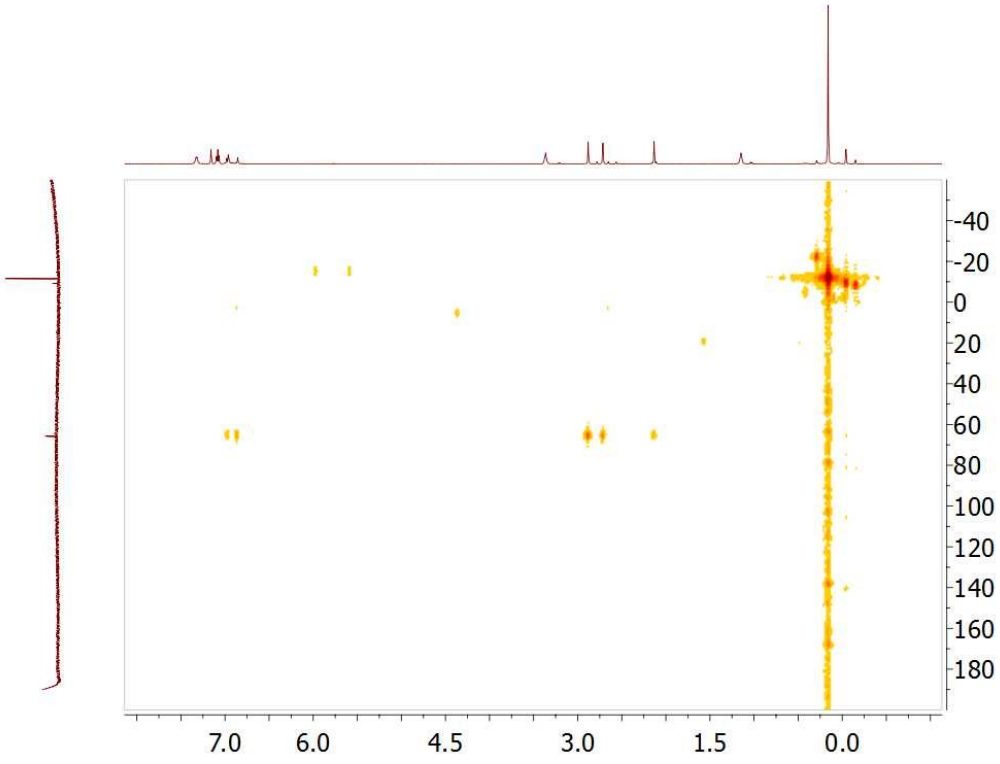


Fig. S15 $^{29}Si - {}^{1}H$ correlation spectrum of **3** in C_6D_6

^{1}H, $^{13}C\{^{1}H\}$, HSQC/HMBC, $^{29}Si\{^{1}H\}$ and $^{29}Si - ^{1}H$ corr. spectra of 3 with 12-crown-4

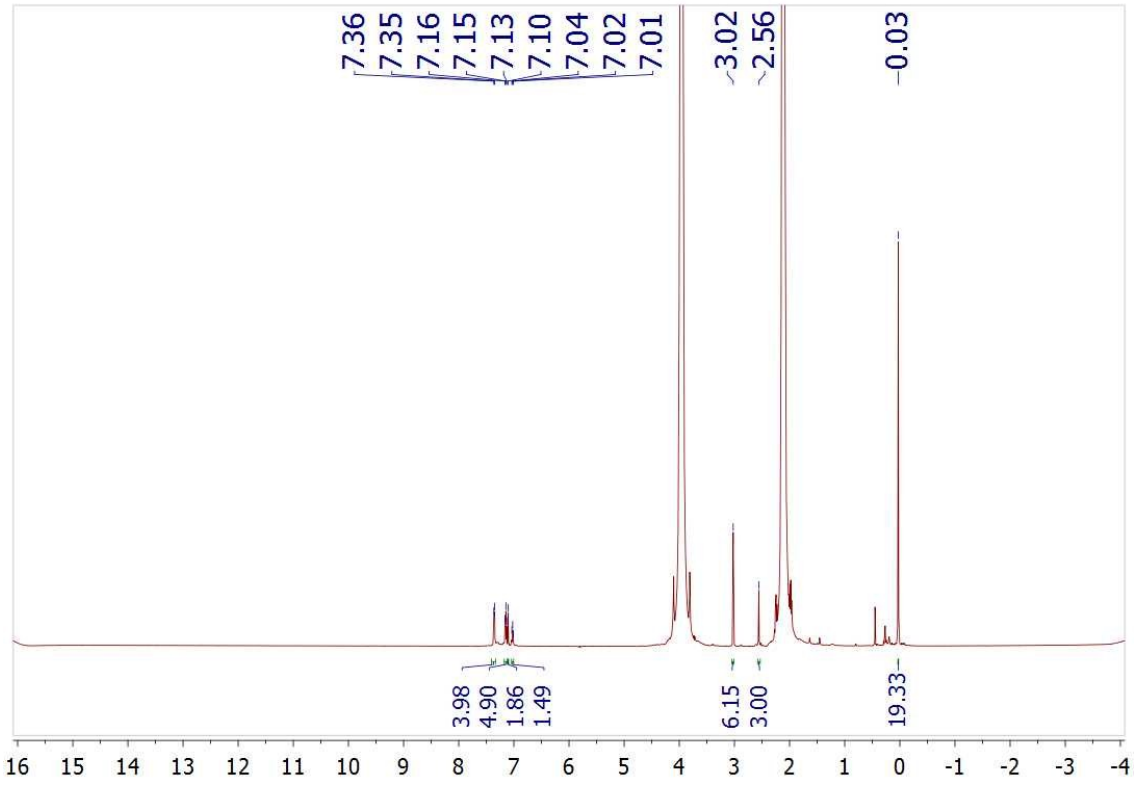


Fig. S16 ^{1}H spectrum of **3** with 12-crown-4 at 298K in C_6D_6/THF

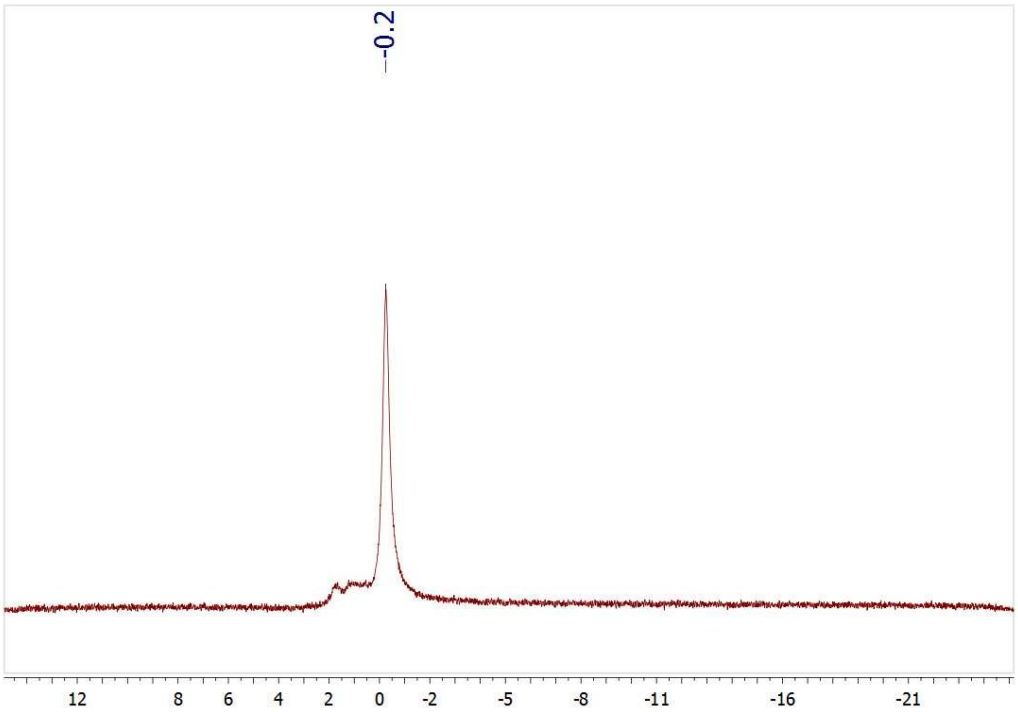


Fig. S17 ^{7}Li spectrum of **3** with 12-crown-4 at 298K in C_6D_6/THF

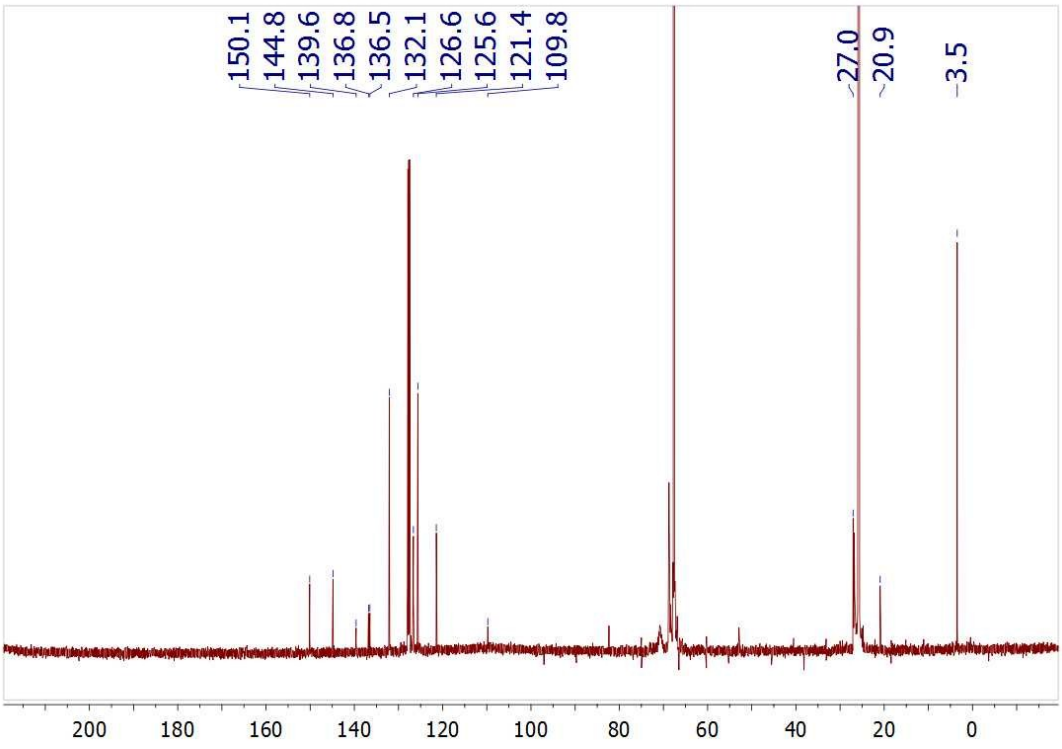


Fig. S18 $^{13}C\{^{1}H\}$ spectrum of **3** with 12-crown-4 at 298K in C_6D_6/THF

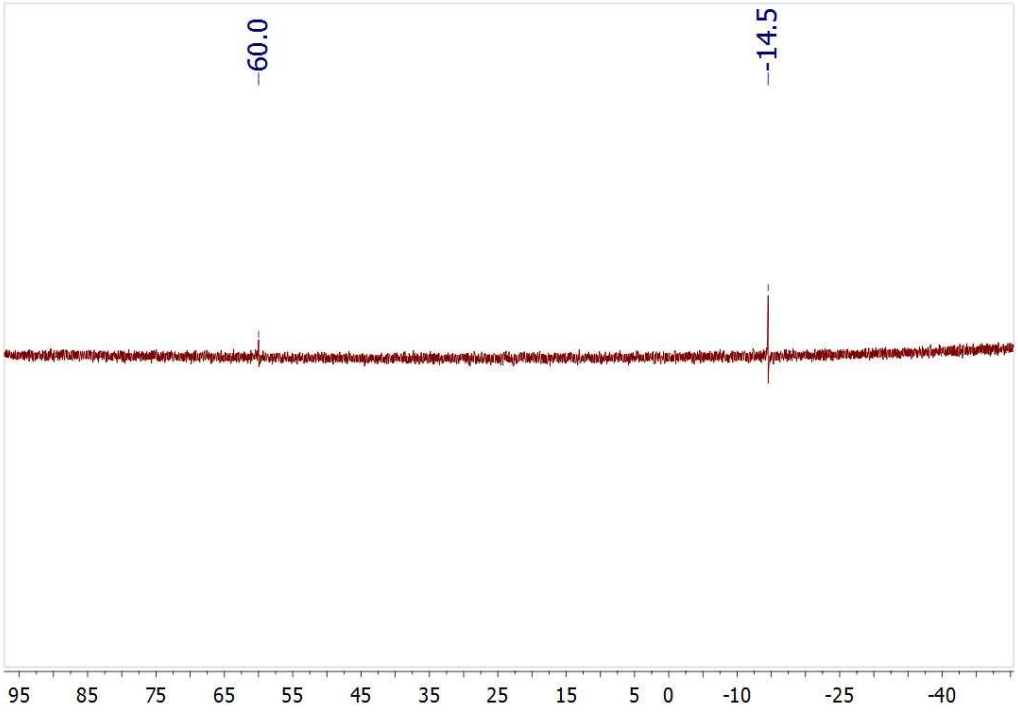


Fig. S19 $^{29}Si\{^{1}H\}$ spectrum of **3** with 12-crown-4 in C_6D_6/THF

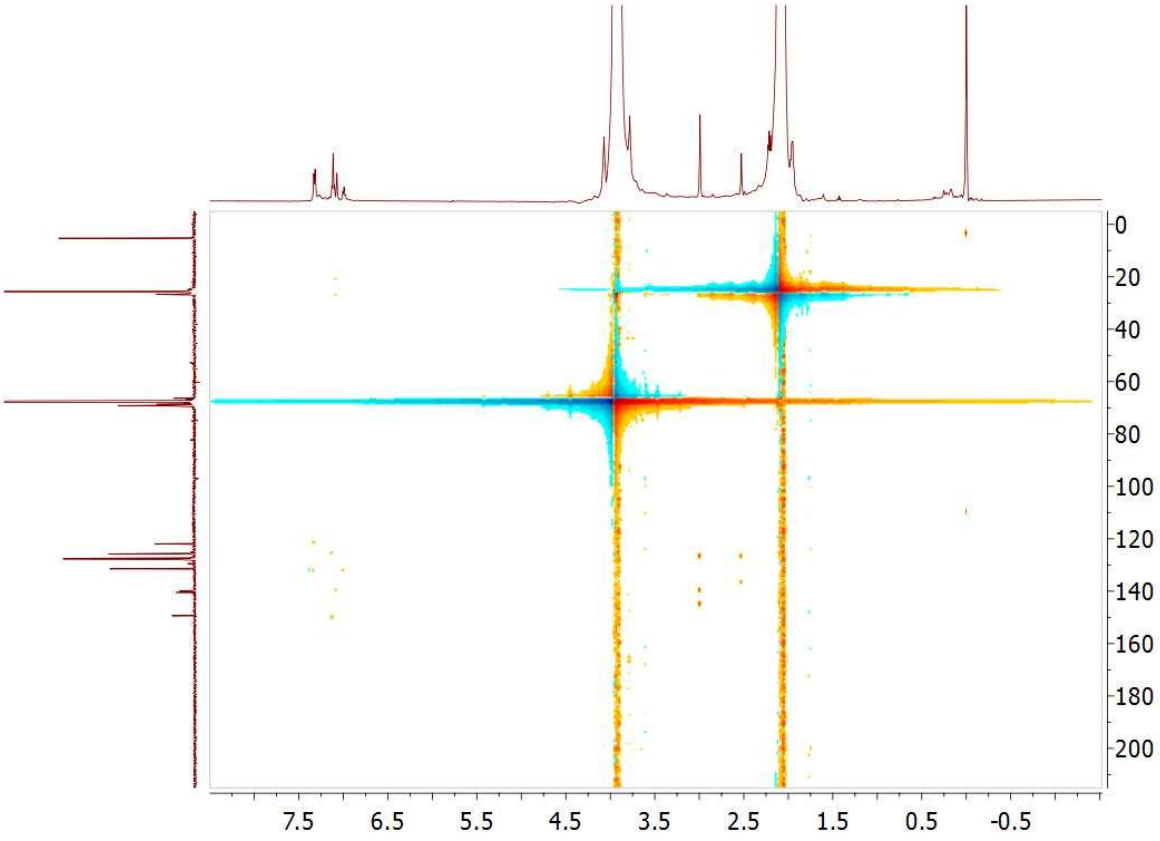


Fig. S20 HSQC/HMBC spectrum of **3** with 12-crown-4 in C_6D_6/THF

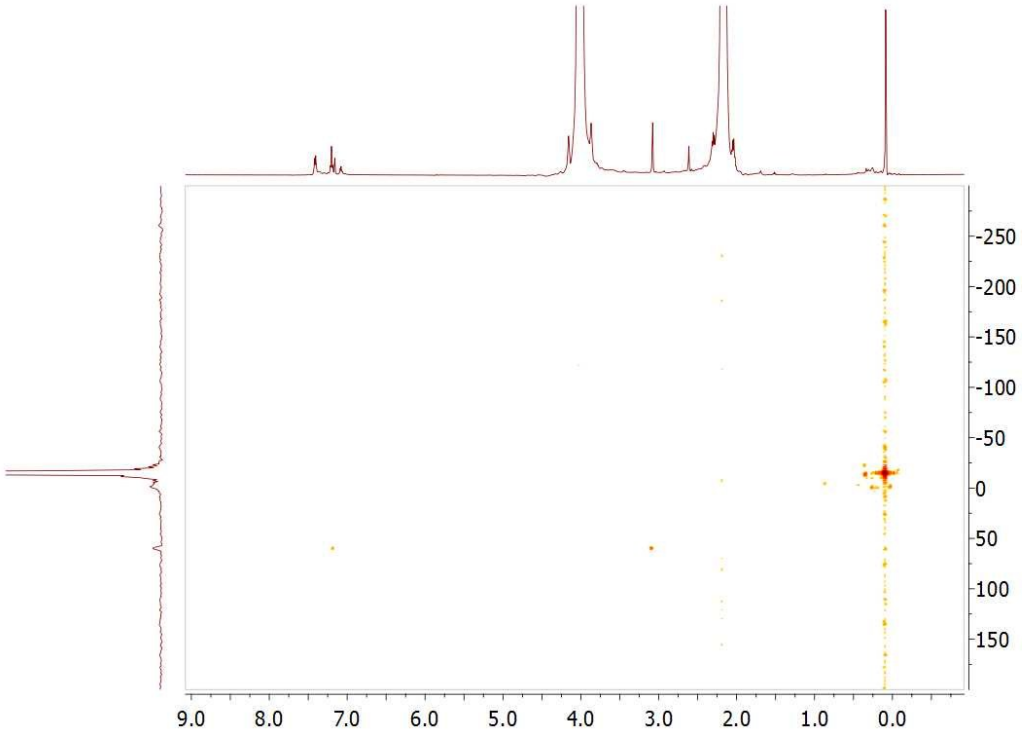
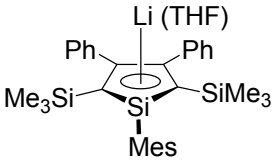
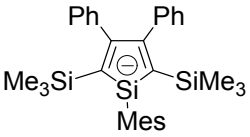
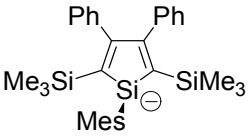


Fig. S21 ^{29}Si – ^{1}H correlation spectrum of **3** with 12-crown-4 in C_6D_6/THF

Calculated Structures

Table S1. Calculated bond length in the silolide rings **(3, 3pl⁻, 3⁻)**

		M06-2X/6-31+G(d,2p)	
	3_1[a]	**3_2**[b]	
Si_1C_α	1.797	1.798	
$Si_1C_{\alpha'}$	1.795	1.796	
$C_\alpha C_\beta$	1.444	1.443	
$C_{\alpha'}C_{\beta'}$	1.445	1.445	
$C_\beta C_{\beta,}$	1.418	1.421	
ASS	356.9	356.9	
Rel. E [kcal/mol]	+0.4	0	
	 **3**	 **3pl⁻**[c]	 **3⁻**
		B3LYP/6-31+G(d,2p)	
Si_1C_α	1.807	1.792	1.839
$Si_1C_{\alpha'}$	1.807	1.792	1.839
$C_\alpha C_\beta$	1.454	1.450	1.414
$C_{\alpha'}C_{\beta'}$	1.454	1.450	1.413
$C_\beta C_{\beta,}$	1.428	1.422	1.422
ASS	358.4	360	330.2
	3[d]	**3pl⁻**[e]	**3⁻**
		M06-2X/6-31+G(d,2p)	
Si_1C_α	1.798	1.780	1.839
$Si_1C_{\alpha'}$	1.796	1.780	1.834
$C_\alpha C_\beta$	1.443	1.443	1.403
$C_{\alpha'}C_{\beta'}$	1.445	1.443	1.402
$C_\beta C_{\beta,}$	1.421	1.411	1.443
ASS	356.2	360	324.0

[a] Calculation was started from the geometry of crystal structure **3_1**; [b] Calculation was started from the geometry of crystal structure **3_2**; [c] inversion barrier is 1.3 kcal/mol; [d] calculated structure of **3_2**; [e] **3pl⁻** at M06-2X/6-31+G(d,2p) is a real minimum.

Geometry optimizations were carried out at M06-2X/6-31+G(d,2p) using **3_1** and **3_2** structures as starting geometries. However the optimized geometries of **3_1** and **3_2** were virtually the same, and only differ by 0.4 kcal/mol, the observable difference was the orientation of the THF molecule. In both cases the mesityl group is slightly out of the perpendicular plane (by 7-8^{o} respectively). For further calculations the optimized structure of **3_2** was used as **3** at M06-2X/6-31+G(d,2p).

Bader analysis, EPS and HOMO of 3

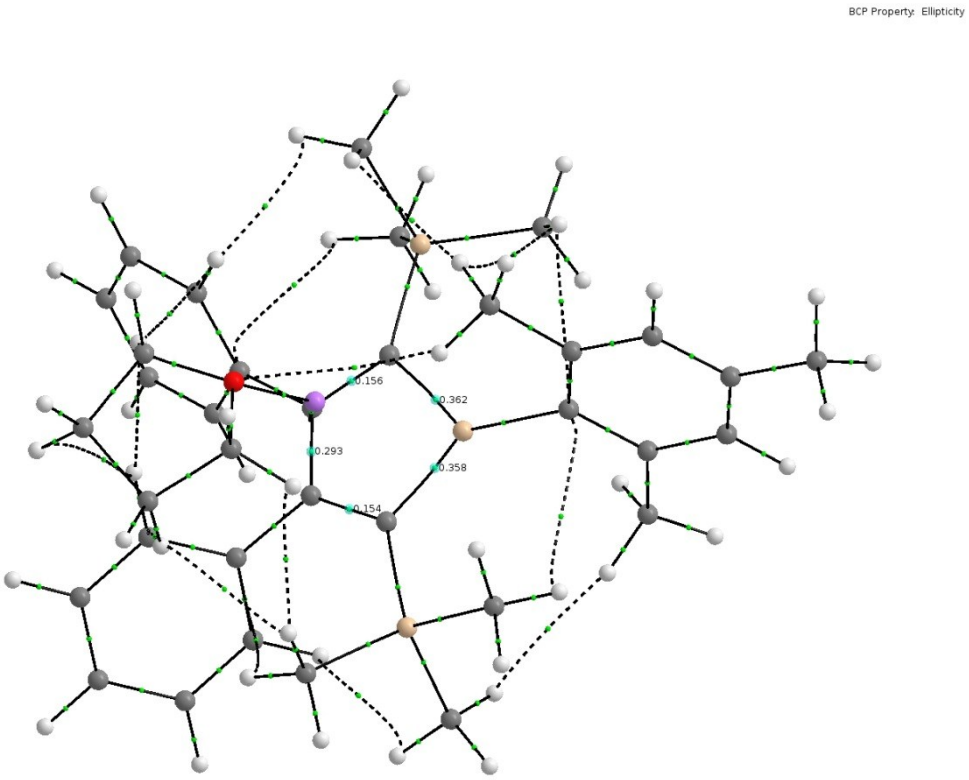


Fig. S22 Ellipticity (ε) values in bond critical points in **3** at M06-2X/6-31+G(d,2p) (ε (Si-C_α) :0.362, 0.358; ε (C_α-C_β) :0.156, 0.154; ε (C_β-C_β) :0.293).

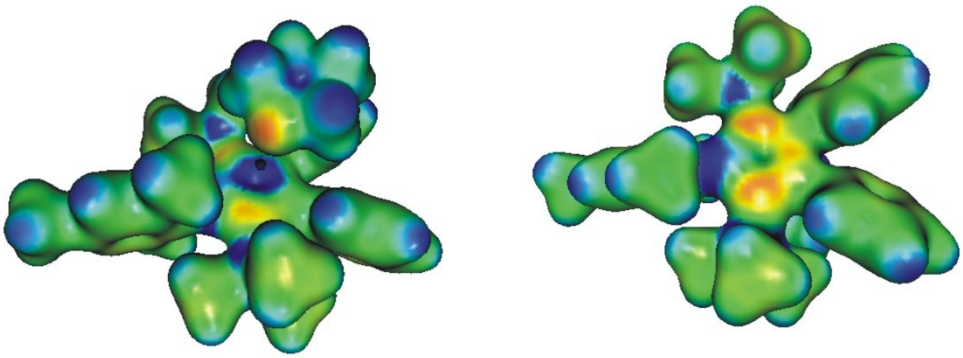


Fig. S23 Electrostatic potential surface map of **3** at M06-2X/6-31+G(d,2p) (blue:0.15; green:0.05; yellow: 0.00; red:-0.05).

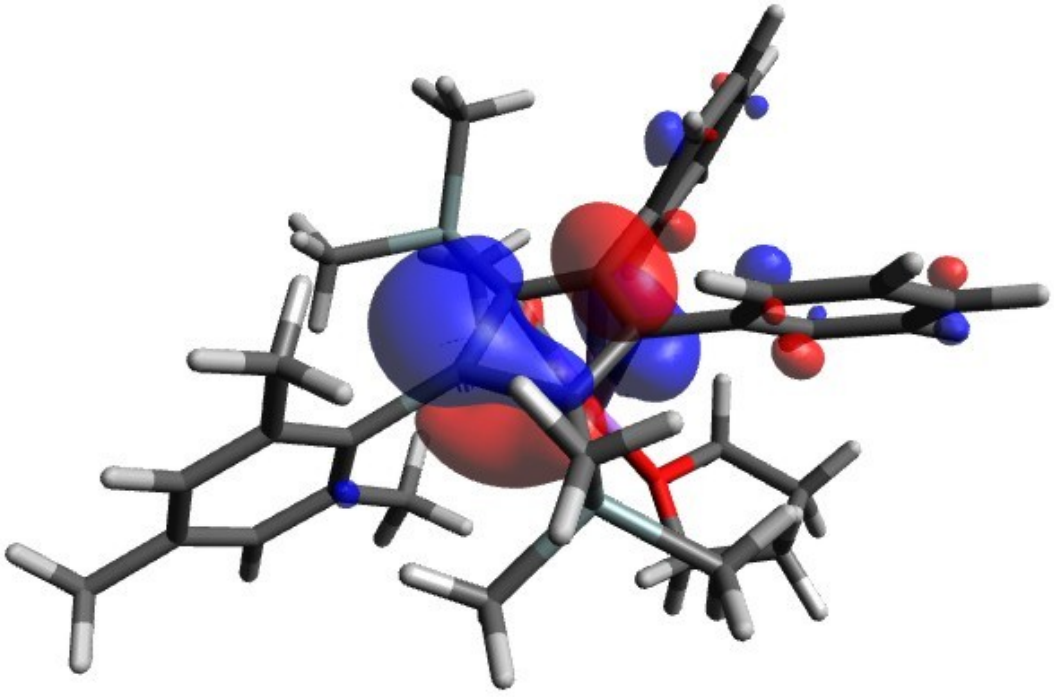


Fig. S24 The HOMO of **3** with C_{β}-$C_{\beta'}$ bonding character at M06-2X/6-31+G(d,2p).

NMR calculations

Nuclear magnetic shielding constants calculations were carried out at B3LYP/pcS-2// B3LYP/6-31+G(d,2p) and B3LYP/pcS-2// M06-2X/6-31+G(d,2p) for all structures (**3, 3**$^{-}$**, 3pl**$^{-}$).

Instead of using only TMS as reference for chemical shift calculations, we used **3** itself as a reference molecule to determine a calibration line for ^{13}C chemical shifts. For ring Si chemical shifts we used $SiMe_3$ group of **3** as an internal reference for calculations.

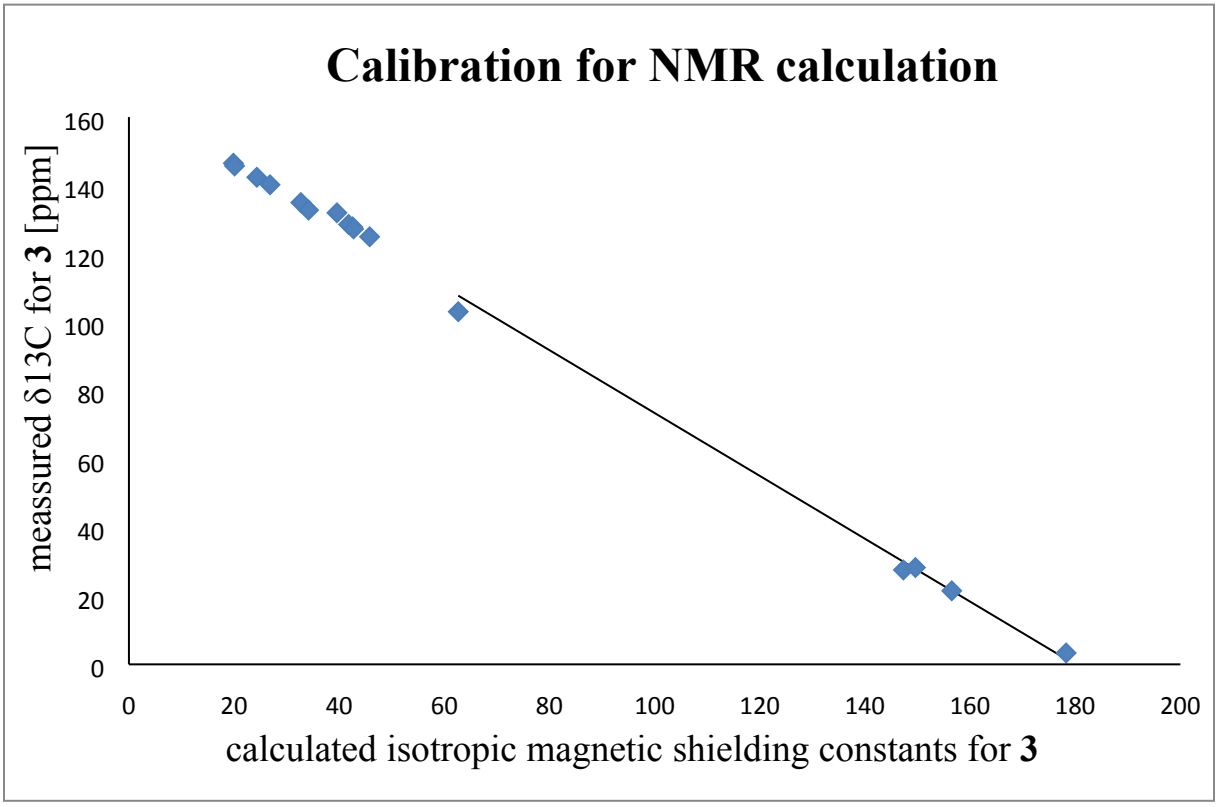


Fig. S25 Calibration line for ^{13}C NMR calculation on B3LYP/pcS-2// B3LYP/6-31+G(d,2p).

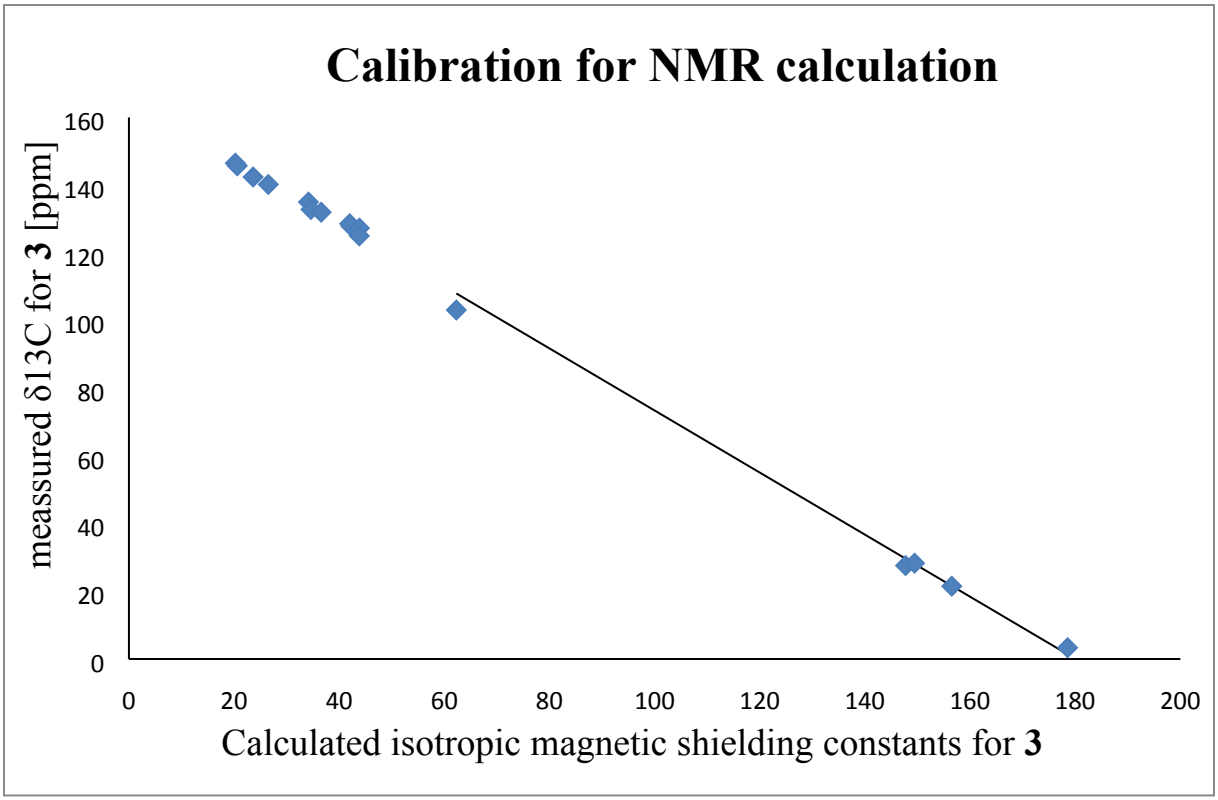


Fig. S26 Calibration line for ^{13}C NMR calculation on B3LYP/pcS-2// M06-2X/6-31+G(d,2p).

Table S2. Calculated and measured ^{29}Si and ^{13}C NMR chemical shifts for **3** and **3$^-$ and 3pl$^-$** [in ppm] at B3LYP/pcS-2// M06-2X/6-31+G(d,2p)

	Calculated **3**	Measured[a]	Calculated **3$^-$**	Calculated **3pl$^-$**	Measured[b]
δ ^{29}Si					
Si *ring*	66.6	65.7	37.3	73.8	60.0
$SiMe_3$	-11.7[c]	-11.7	-15.0	-15.4	–14.5
δ ^{13}C					
C_α	108.0	103.1	144.7	99.9	109.4
C_β	133.8	135.0	144.5	134.7	136.8
C(*p*Me)	21.6	21.5	21.8	21.6	20.9
C(*o*Me1)	28.1	27.6	25.9	29.1	27.0
C(*o*Me2)	29.6	28.3			
C(*i*Ph)	146.2	145.7	152.6	152.2	150.1
C(*o*Ph)	131.6	132.0	131.8	132.9	132.1
C(*m*Ph)	124.9	127.3	123.9	123.9	125.7
C(*p*Ph)	124.9	125.0	119.0	117.4	121.4
C(*i*Mes)	133.4	132.8	148.6	140.9	139.6
C(*o*Mes1)	143.4	142.4	147.9	145.6	144.8
C(*o*Mes2)	146.5	146.5			
C(*m*Mes1)	126.4	127.9	124.0	124.4	126.6
C(*m*Mes2)	126.6	128.6			
C(*p*Mes)	140.8	140.2	133.1	133.9	136.5
$SiMe_3$	1.4	3.3	1.7	2.2	3.5

[a] in C_6D_6 solution, where ^{7}Li NMR showed η^5-coordination; [b] in THF solution containing 12-crown-4, where ^{7}Li NMR showed no coordination to the silolide ring [c] Used as an internal reference for calculated ^{29}Si chemical shifts.

Table S3. Calculated and measured ^{29}Si and ^{13}C NMR chemical shifts for **3** and **3$^-$ and 3pl$^-$** [in ppm] at B3LYP/pcS-2// B3LYP/6-31+G(d,2p)

	Calculated **3**	Measured[a]	Calculated[b] **3$^-$**	Calculated[b] **3pl$^-$**	Measured[c]
δ ^{29}Si					
Si *ring*	68.6	65.7	37.4	75.9	60.0
$SiMe_3$	-11.7[d]	-11.7	-15.1	-15.5	–14.5
δ ^{13}C					
C_α	104.9	103.1	138.1	100.2	109.4
C_β	135.6	135.0	144.0	135.3	136.8
C(*p*Me)	21.9	21.5	21.6	21.5	20.9
C(*o*Me1)	28.1	27.6	29.0	29.0	27.0
C(*o*Me2)	29.8	28.3			
C(*i*Ph)	146.8	145.7	152.4	152.4	150.1
C(*o*Ph)	131.5	132.0	131.0	131.9	132.1
C(*m*Ph)	125.6	127.3	124.7	124.9	125.7
C(*p*Ph)	123.2	125.0	120.7	118.9	121.4
C(*i*Mes)	133.5	132.8	146.2	139.1	139.6
C(*o*Mes1)	143.3	142.4	147.5	145.9	144.8
C(*o*Mes2)	147.8	146.5			
C(*m*Mes1)	126.2	127.9	124.7	125.0	126.6
C(*m*Mes2)	126.6	128.6			
C(*p*Mes)	140.6	140.2	136.3	137.9	136.5
$SiMe_3$	2.4	3.3	2.2	2.5	3.5

[a] in C_6D_6 solution, where ^7Li NMR showed η^5-coordination; [b] PCM solvent model were used during NMR calculations (solvent=THF) [c] in THF solution containing 12-crown-4, where ^7Li NMR showed no coordination to the silolide ring;[d] Used as an internal reference for calculated ^{29}Si chemical shifts.

Bird Index calculations[11]

Table S4. Calculated bond length to be used for the calculation of the bond order (N) for I_5 calculations

	N	R[a]		N	R[a]
H_3C-CH_3	1	1.527	H_3Si-CH_3	1	1.880
$H_2C=CH_2$	2	1.329	$H_2Si=CH_2$	2	1.702
$HC\equiv CH$	3	1.204	$HSi\equiv CH$	3	1.613[b]

[a] Bond length form calculated structures at M06-2X/6-31+G(d,2p) in Å

[b] Bond length belongs to the linear structure (in minimum: H-Si-C 146.6°)

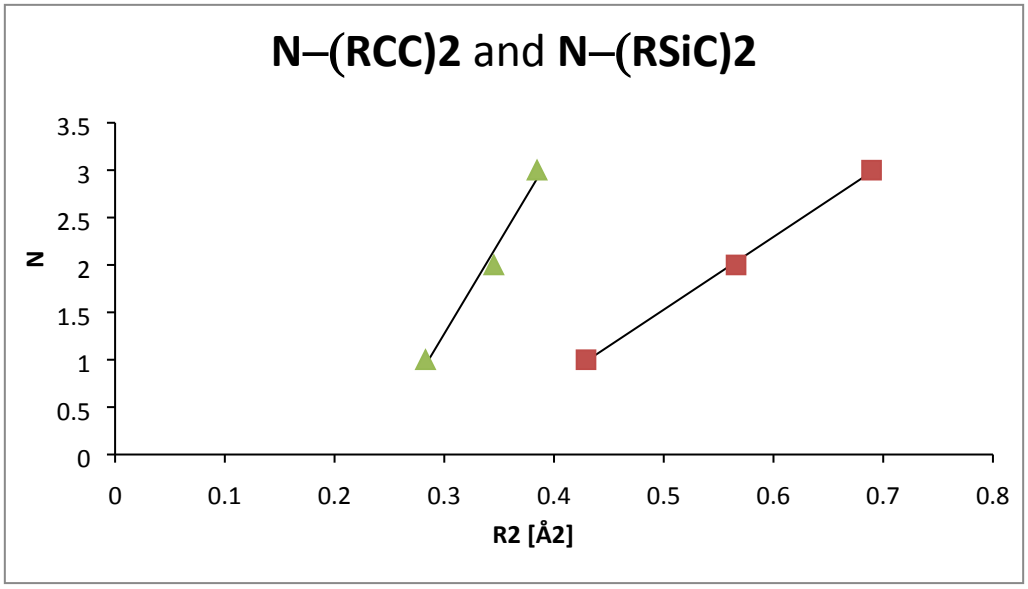
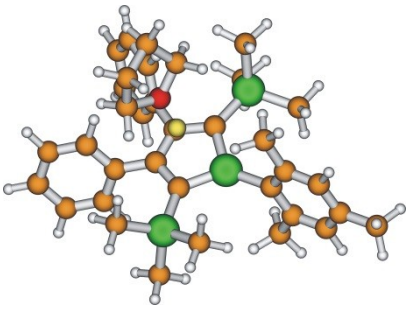


Fig. S27 Gordy equation for CC and SiC bonds[12] ■ $(R_{CC})^2$ calculated from Table S4 ▲($R_{SiC})^2$ calculated from Table S4

11 C. W. Bird, *Tetrahedron,* 1985, **41**, 1409.

12 W. J. Gordy, *Chem. Phys.* 1947, **15**, 305.

Atomic coordinates of 3, 3pl^{-}, 3^{-}



Aromaticity measures of **3** at B3LYP/6-31+G(d,2p)

NICS(1): −8.1 ppm

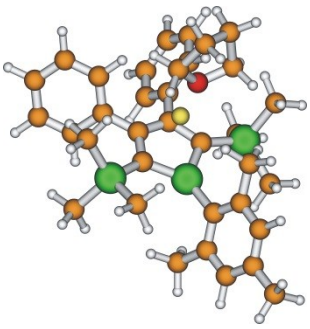
(NICS values calculated at B3LYP/pcS-2)

Atomic coordinates of **3** at B3LYP/6-31+G(d,2p)

Energy -2313.517211

C	-1.132271	0.703129	4.024078
O	-0.876364	-0.300094	3.010634
C	-1.151255	-1.629432	3.536175
C	-1.473567	-1.431619	5.020226
C	-2.011617	0.008265	5.059757
Li	-0.364786	-0.019405	1.197501
C	-1.184569	0.787322	-0.616399
C	0.109525	1.429540	-0.476451
Si	1.301177	0.086123	-0.698670
C	3.173716	0.067581	-0.394358
C	3.732903	0.118792	0.908482
C	5.125107	0.104102	1.068647
C	5.972455	0.039513	-0.035714
C	5.430670	-0.010264	-1.317855
C	4.042629	0.004068	-1.514821
C	2.871530	0.185793	2.150271
C	3.515940	-0.044349	-2.934046
C	-1.179329	-0.637738	-0.713161
C	0.117810	-1.283501	-0.640191
Si	0.517815	-3.114167	-0.672234
C	2.160654	-3.426390	0.231331
C	-2.445811	-1.396906	-0.955194
C	-3.489195	-1.432411	-0.014168
C	-4.666620	-2.142491	-0.259789
C	-4.831525	-2.838114	-1.460453
C	-3.809067	-2.807012	-2.413033
C	-2.634796	-2.094427	-2.161307
C	-2.448707	1.574734	-0.788123
C	-3.051889	1.675879	-2.053950
C	-4.218344	2.418697	-2.244205
C	-4.813361	3.084449	-1.168418
C	-4.231363	2.992930	0.098060
C	-3.065252	2.244582	0.280828
Si	0.473390	3.264973	-0.370656
C	-0.464456	4.313575	-1.642561
C	0.085819	3.962998	1.360703
C	2.321480	3.572200	-0.672242
C	-0.772577	-4.197360	0.206662

C	0.743853	-3.780228	-2.438794
H	2.891845	-0.926644	-3.106824
H	2.201522	-0.678223	2.215622
H	3.488860	0.199785	3.052175
H	2.246945	1.084928	2.157685
H	4.339348	-0.072338	-3.651924
H	2.898554	0.829762	-3.165139
H	6.089109	-0.058912	-2.180022
C	7.410509	0.025099	0.149470
H	5.545935	0.142532	2.069080
H	-0.151879	5.361260	-1.558270
H	-0.244461	3.981544	-2.662636
H	-1.547930	4.272636	-1.506448
H	0.353065	5.024425	1.418632
H	-0.977525	3.879047	1.603859
H	0.655774	3.437188	2.135403
H	2.533392	4.643782	-0.581659
H	2.964043	3.045869	0.039508
H	2.619856	3.261292	-1.678612
H	2.428639	-4.486860	0.158309
H	2.988993	-2.846355	-0.185336
H	2.088517	-3.178933	1.296327
H	-0.433483	-5.240144	0.198295
H	-0.895056	-3.902305	1.254498
H	-1.756091	-4.159673	-0.267125
H	1.049234	-4.832783	-2.417148
H	-0.177191	-3.713610	-3.024724
H	1.518798	-3.219656	-2.972579
H	-2.594506	1.166685	-2.895721
H	-4.660808	2.479977	-3.233616
H	-5.719237	3.663863	-1.314569
H	-4.685407	3.499507	0.944410
H	-2.629288	2.174741	1.272970
H	-1.853187	-2.062981	-2.912730
H	-3.927387	-3.332405	-3.355814
H	-5.745093	-3.391251	-1.653076
H	-5.454915	-2.151444	0.486863
H	-3.379131	-0.888240	0.918821
H	-1.997107	-2.043253	2.978704
H	-0.273865	-2.256383	3.360895
H	-0.567083	-1.517482	5.627811
H	-2.191260	-2.170166	5.383354
H	-1.933773	0.470836	6.046063
H	-3.061775	0.037769	4.752041
H	-0.175411	1.023740	4.453946
H	-1.603379	1.560326	3.538719
H	7.901015	-0.027617	-0.821379
H	7.719458	0.934147	0.663378
H	7.691081	-0.842059	0.745488



Aromaticity measures of **3(3_2)** at M06-2X/6-31+G(d,2p)

I_5: 90

NICS(1): −8.2 ppm

(NICS values calculated at B3LYP/pcS-2)

Atomic coordinates of **3 (3_2)** at M06-2X/6-31+G(d,2p)

Energy : -2312.7456908

C	-0.078605	1.281108	3.798310
O	-0.275467	0.102589	2.991679
C	0.270319	-1.059992	3.650349
C	1.124151	-0.509426	4.785354
C	0.358000	0.762085	5.163570
Li	-0.431063	0.081729	1.138191
C	-1.414044	-0.746702	-0.553540
C	-2.649603	-1.574952	-0.496306
C	-3.580284	-1.461224	0.544333
C	-4.698728	-2.289530	0.596742
C	-4.910147	-3.248721	-0.393555
C	-4.001824	-3.360478	-1.445206
C	-2.886828	-2.526995	-1.495632
C	-1.447877	0.669899	-0.601114
C	-2.722777	1.439344	-0.599284
C	-2.993498	2.360632	0.419821
C	-4.151341	3.134886	0.405545
C	-5.070511	2.991170	-0.632466
C	-4.824197	2.063126	-1.644149
C	-3.662310	1.295107	-1.627365
C	-0.168432	1.339305	-0.665009
Si	0.140903	3.152031	-0.947888
C	-1.028203	3.887324	-2.232682
C	0.016973	4.207540	0.625108
C	1.911370	3.348116	-1.580162
Si	1.026805	0.010607	-0.854276
C	2.901655	0.036471	-0.766305
C	3.589094	0.528934	0.362485
C	4.985197	0.533508	0.376337
C	5.730548	0.058548	-0.701815
C	5.042629	-0.436674	-1.809325
C	3.648438	-0.452490	-1.859767
C	2.852847	1.051040	1.572909
C	7.236531	0.100940	-0.686347
C	2.967279	-1.011899	-3.086465
C	-0.103544	-1.353347	-0.562554

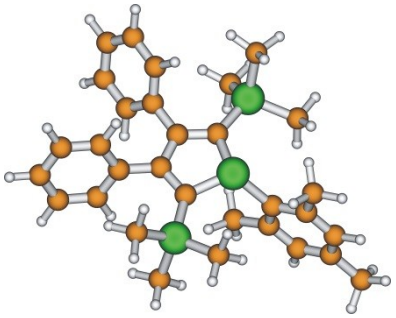
Si	0.323456	-3.139747	-0.276661
C	2.126549	-3.225973	0.295718
C	-0.760100	-3.925388	1.059887
C	0.209612	-4.234322	-1.816693
H	5.504793	0.914733	1.252187
H	5.606668	-0.818332	-2.657190
H	2.169561	0.290483	1.969607
H	2.244579	1.927058	1.322206
H	3.552928	1.334093	2.362606
H	7.660666	-0.792615	-1.149866
H	7.619889	0.174907	0.333175
H	7.601951	0.968278	-1.244617
H	2.395073	-1.913918	-2.845027
H	3.699604	-1.270559	-3.853390
H	2.262436	-0.291396	-3.513049
H	0.492304	5.180027	0.458875
H	0.524599	3.730314	1.470239
H	-1.022510	4.390882	0.909908
H	2.120157	4.401497	-1.793259
H	2.064931	2.779516	-2.503289
H	2.654731	3.000678	-0.855032
H	-0.714762	4.904033	-2.492061
H	-2.058370	3.930440	-1.866635
H	-1.022131	3.285345	-3.146285
H	-2.278691	2.470023	1.231692
H	-4.336754	3.846806	1.203149
H	-5.972355	3.592923	-0.650400
H	-5.537695	1.941307	-2.451966
H	-3.469870	0.578384	-2.419650
H	-3.422215	-0.716000	1.319540
H	-5.404973	-2.189553	1.414029
H	-5.777966	-3.897365	-0.349282
H	-4.163108	-4.094354	-2.227951
H	-2.183105	-2.602591	-2.319129
H	-0.366120	-4.910736	1.330978
H	-1.790237	-4.053810	0.713801
H	-0.792030	-3.314310	1.967521
H	0.774877	-5.158805	-1.657956
H	0.624614	-3.731925	-2.695735
H	-0.824102	-4.510154	-2.040203
H	2.385148	-4.252969	0.574034
H	2.319123	-2.580987	1.160265
H	2.817235	-2.912183	-0.494271
H	0.830392	-1.637440	2.908362
H	-0.562582	-1.666242	4.021111
H	1.222466	-1.218167	5.608290
H	2.124579	-0.257091	4.421438
H	-0.514286	0.514313	5.774893
H	0.965393	1.488451	5.704655
H	0.700996	1.893526	3.330728
H	-1.015241	1.841290	3.814161

Atomic coordinates of **3_1** at M06-2X/6-31+G(d,2p)

Energy : -2312.7450154

Si	1.369674	0.126965	-0.545168
C	0.131216	-1.174935	-0.617398
C	-1.128421	-0.474894	-0.698392
C	-1.073725	0.936256	-0.541222
C	0.238141	1.505498	-0.332264
Si	0.709435	3.307840	-0.315735
C	2.574323	3.426427	-0.598555
H	2.871938	4.478156	-0.664626
H	3.147166	2.969631	0.215228
Li	-0.351562	0.037303	1.218474
H	2.874851	2.932543	-1.528285
C	-0.157459	4.268979	-1.688284
H	-1.238545	4.320993	-1.528101
H	0.015489	3.789815	-2.656683
H	-0.659701	4.548198	1.397799
H	1.033617	5.046434	1.440973
C	0.368741	4.182897	1.334963
H	-2.701153	0.767447	2.573907
H	0.547403	3.519250	2.187919
H	-2.150513	0.724163	4.265035
C	-2.299780	0.125029	3.362156
C	-3.157752	-1.127861	3.630614
H	-3.373184	-1.218857	4.697389
H	-2.431094	-3.209272	3.718692
C	-2.274249	-2.291367	3.149983
H	-2.453702	-2.500101	2.091420
C	-0.876281	-1.720418	3.324115
H	-0.113248	-2.177121	2.688014
O	-1.015942	-0.352244	2.912730
H	2.276173	1.541419	2.070066
H	2.128408	-0.171841	2.462691
H	3.443734	0.781692	3.164492
C	2.849830	0.628873	2.261361
C	3.735361	0.272726	1.090827
C	3.207540	0.013163	-0.191841
C	5.114438	0.198615	1.295665
H	5.513927	0.405487	2.285649
C	5.993840	-0.133696	0.265781
H	7.779074	0.385949	1.358866
C	7.476078	-0.237709	0.515473
H	7.755095	-1.270206	0.747259
H	8.046515	0.069660	-0.363567
H	6.131636	-0.652096	-1.812858
H	4.401177	-0.798910	-3.320485
C	3.575292	-0.627358	-2.627921
H	2.968177	0.197188	-3.015125
H	2.941276	-1.520661	-2.629342
C	4.089163	-0.325913	-1.239999
C	5.461371	-0.394449	-0.996355

H	2.344009	-4.386962	0.191178
C	2.170869	-3.310700	0.086608
H	-0.596395	-5.112391	0.057812
Si	0.469310	-3.002978	-0.680603
H	1.158373	-4.598178	-2.464779
H	0.949585	-2.976806	-3.147516
C	0.531002	-3.700880	-2.442049
H	-0.463139	-3.984202	-2.798920
C	-2.546446	-2.022106	-2.057098
H	-2.889725	1.116266	-2.561919
C	-3.493031	-1.103240	-0.051815
C	-4.665098	-1.822356	-0.271141
C	-4.778594	-2.655555	-1.383827
C	-3.715225	-2.746195	-2.280994
H	-3.796818	-3.377856	-3.159464
H	-1.725251	-2.078724	-2.764844
H	-5.689255	-3.218751	-1.554757
H	-5.491321	-1.732476	0.426849
H	-3.415801	-0.444894	0.809616
C	-2.406895	-1.200105	-0.931673
C	-0.771968	-4.055549	0.286970
H	-0.545197	-1.749461	4.369837
H	-4.109306	-1.090770	3.097289
H	-0.650165	-3.935156	1.367861
H	-1.809515	-3.823492	0.027327
H	2.981898	-2.901624	-0.524547
H	2.254612	-2.854460	1.079167
C	-2.287260	1.795433	-0.614249
C	-3.122114	1.785371	-1.739463
C	-2.603874	2.669584	0.433523
H	-1.962817	2.691783	1.310894
C	-3.708609	3.515532	0.361951
H	-3.928461	4.188520	1.184392
H	-5.388007	4.153293	-0.827676
C	-4.527730	3.496167	-0.765706
H	-4.860380	2.605131	-2.696629
C	-4.230552	2.624885	-1.813721
H	0.230079	5.291827	-1.739831



Aromaticity measures of **3**$^{-}$ at B3LYP/6-31+G(d,2p)

NICS(1): −6.6/−8.0 ppm

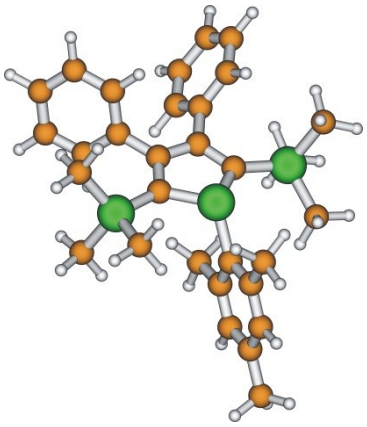
(NICS values calculated at B3LYP/pcS-2)

Atomic coordinates of **3**$^{-}$ at B3LYP/6-31+G(d,2p)

Energy : -2073.502149

C	2.741250	-2.307751	1.251370
C	2.534871	-1.504995	0.114865
C	3.554850	-1.483955	-0.854924
C	4.722349	-2.233677	-0.700703
C	4.905158	-3.031233	0.433885
C	3.906365	-3.063284	1.411092
C	1.272119	-0.718501	-0.055505
C	1.299104	0.727963	-0.071904
C	2.586543	1.460519	0.119934
C	3.298190	1.386440	1.333418
C	4.492418	2.084223	1.522848
C	5.016160	2.881293	0.499518
C	4.329350	2.962575	-0.715882
C	3.135837	2.260074	-0.900190
C	0.071964	1.383744	-0.334210
Si	-0.300628	3.203790	-0.324704
C	-2.177207	3.500438	-0.200461
Si	-1.080930	0.042688	-0.848759
C	0.029127	-1.336340	-0.331649
Si	-0.345537	-3.145827	-0.535195
C	-0.593344	-4.039609	1.136538
C	-2.869722	0.027647	-0.116270
C	-3.087539	-0.001623	1.286337
C	-4.394764	-0.021993	1.799786
C	-5.516556	-0.011956	0.968833
C	-5.301245	0.021169	-0.412393
C	-4.011145	0.040922	-0.960347
C	-1.936003	-0.006459	2.266695
C	-3.887237	0.070149	-2.471184
C	-6.918261	-0.033007	1.536716
C	-1.980937	-3.380413	-1.480243
C	0.953786	-4.150143	-1.505340
C	0.477374	4.104519	1.165064
C	0.230882	4.162500	-1.892114
H	-1.299594	-0.884431	2.122737
H	-3.447655	-0.856683	-2.852960
H	-4.870006	0.197963	-2.936984
H	-3.234728	0.880637	-2.807017
H	-2.300704	0.001282	3.298671
H	-1.285154	0.859589	2.114425
H	-4.535850	-0.044070	2.878862
H	-6.158964	0.033499	-1.082957
H	0.180529	5.160985	1.172628
H	0.143602	3.655651	2.107321
H	1.570056	4.058938	1.145535
H	-0.211816	5.167060	-1.894405
H	1.316927	4.275802	-1.956390
H	-0.108298	3.641386	-2.794196
H	-2.381776	4.578449	-0.191990
H	-2.715950	3.065684	-1.048362
H	-2.602805	3.065834	0.709082
H	-2.234159	-4.446394	-1.540749
H	-2.811567	-2.863885	-0.989153

H	-1.902774	-2.993314	-2.501537
H	0.601807	-5.179414	-1.653555
H	1.123042	-3.706306	-2.492600
H	1.918240	-4.192013	-0.991703
H	-0.895385	-5.082509	0.977145
H	0.323268	-4.044305	1.734513
H	-1.376479	-3.550029	1.726003
H	2.898015	0.776795	2.136771
H	5.013114	2.009258	2.473662
H	5.943513	3.427357	0.646059
H	4.727326	3.568442	-1.525725
H	2.618911	2.314557	-1.852330
H	1.976976	-2.326324	2.021720
H	4.035374	-3.672815	2.301467
H	5.812610	-3.615625	0.555222
H	5.490292	-2.197582	-1.468583
H	3.420857	-0.872309	-1.741029
H	-7.667824	-0.018854	0.740350
H	-7.093018	-0.931905	2.139539
H	-7.103058	0.835064	2.180373



Aromaticity measures of **3**$^{-}$ at M06-2X/6-31+G(d,2p)

I_5: 65

NICS(1): –6.7/–7.7 ppm

(NICS values calculated at B3LYP/pcS-2)

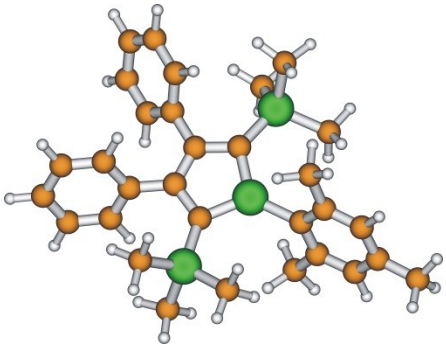
Atomic coordinates of **3**$^{-}$ at M06-2X/6-31+G(d,2p)

Energy -2072.835524

C	3.580265	-1.493656	-0.760263
C	2.485016	-1.518473	0.114326
C	2.557975	-2.360442	1.232265
C	3.668733	-3.170898	1.457875
C	4.741993	-3.148107	0.568477
C	4.694218	-2.299724	-0.538816
C	1.254819	-0.714211	-0.131380
C	1.289024	0.727744	-0.165054
C	2.556346	1.466696	0.074065
C	3.276526	1.306489	1.267611
C	4.434642	2.037839	1.514270
C	4.907005	2.950048	0.569038

C	4.211485	3.110941	-0.628795
C	3.054091	2.373375	-0.872592
C	0.079179	1.373156	-0.460732
Si	-0.311424	3.175311	-0.375491
C	0.476035	3.997661	1.141027
Si	-1.070357	0.045270	-0.989454
C	0.025625	-1.320061	-0.426562
Si	-0.352343	-3.120154	-0.603330
C	-1.956216	-3.311384	-1.590522
C	-2.800368	0.035694	-0.147662
C	-3.990721	-0.003573	-0.901816
C	-5.236101	-0.024584	-0.262375
C	-5.344417	-0.005888	1.125230
C	-4.167055	0.036882	1.872173
C	-2.908682	0.061844	1.264570
C	-3.964420	-0.021041	-2.413531
C	-1.686904	0.149352	2.146225
C	-6.689016	-0.015120	1.809403
C	0.982293	-4.123216	-1.503526
C	-0.677197	-3.976432	1.062321
C	0.193184	4.207350	-1.892035
C	-2.187673	3.394387	-0.229817
H	-0.930260	-0.583688	1.849512
H	-3.441701	-0.905414	-2.789525
H	-4.980468	-0.019525	-2.817714
H	-3.428919	0.847544	-2.807607
H	-1.953845	-0.002888	3.195531
H	-1.210404	1.130240	2.043557
H	-4.229600	0.052471	2.959288
H	-6.141731	-0.056820	-0.865231
H	0.125581	5.031140	1.242139
H	0.210156	3.456235	2.054710
H	1.568098	4.009266	1.066414
H	-0.333806	5.168399	-1.886769
H	1.267303	4.412425	-1.904099
H	-0.066865	3.678767	-2.814492
H	-2.446171	4.459015	-0.203410
H	-2.704648	2.939823	-1.082263
H	-2.582208	2.919828	0.674460
H	-2.251351	-4.364337	-1.659526
H	-2.770723	-2.758609	-1.108061
H	-1.835663	-2.918565	-2.604836
H	0.638454	-5.149935	-1.675298
H	1.200707	-3.667230	-2.474551
H	1.917083	-4.163122	-0.935376
H	-1.116689	-4.967282	0.901186
H	0.242257	-4.107042	1.639687
H	-1.378783	-3.386761	1.661609

H	2.905363	0.605602	2.009346
H	4.966888	1.901655	2.450554
H	5.806872	3.524412	0.763652
H	4.573736	3.809029	-1.377674
H	2.518995	2.484640	-1.810959
H	1.726367	-2.364213	1.931128
H	3.697406	-3.817127	2.329865
H	5.608602	-3.778714	0.738684
H	5.527043	-2.270128	-1.234500
H	3.543318	-0.838549	-1.625653
H	-6.650154	0.520062	2.761183
H	-7.020448	-1.037298	2.014690
H	-7.450167	0.464835	1.185872



Aromaticity measures of **3pl**$^{-}$ at B3LYP/6-31+G(d,2p)

NICS(1): –6.9 ppm

(NICS values calculated at B3LYP/pcS-2)

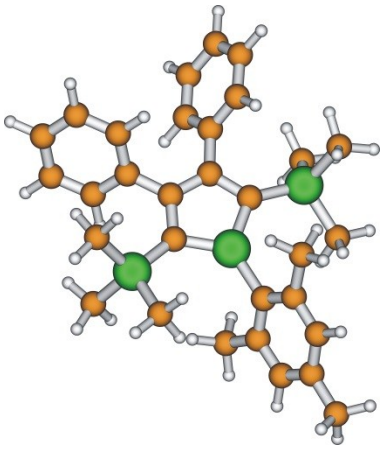
Atomic coordinates of **3pl**$^{-}$ at B3LYP/6-31+G(d,2p)

Energy : -2073.499954

Si	1.052689	0.004379	-0.000763
C	-0.092240	-1.373744	-0.017926
C	-1.383410	-0.713249	-0.008818
C	-1.387235	0.708726	0.009459
C	-0.099795	1.376216	0.017420
C	2.949764	0.007359	-0.001635
C	3.681805	-0.422826	-1.140495
C	5.082551	-0.412277	-1.122176
C	5.804802	0.011864	-0.002554
C	5.082299	0.437890	1.114840
C	3.680442	0.441698	1.135003
Si	0.280560	3.166999	-0.252520
Si	0.296917	-3.162106	0.254894
C	-2.657101	1.486033	-0.016446
C	-2.649196	-1.497035	0.016639
C	-3.592107	-1.361953	1.056479
C	-2.963039	2.410915	1.002240
C	-3.598064	1.347466	-1.057522
C	-2.949638	-2.424315	-1.001537

C	-4.139601	3.163011	0.982448
C	-4.768826	-2.112369	1.078249
C	-4.122745	-3.181831	-0.982442
C	-4.778254	2.092422	-1.080009
C	-5.058165	3.009910	-0.061409
C	-5.043301	-3.032045	0.060137
H	-5.957079	-3.618947	0.078238
H	-5.974603	3.592630	-0.080114
H	-4.322986	-3.883551	-1.788126
H	-5.471621	-1.983474	1.897169
H	-5.479488	1.961006	-1.899863
H	-4.344024	3.863164	1.788441
H	-3.389602	0.646654	-1.858700
H	-2.252637	-2.530767	-1.825758
H	-3.387827	-0.659644	1.857415
H	-2.267330	2.519978	1.827212
H	0.583174	-5.263538	-1.105407
H	-0.880503	-4.409141	-1.615499
H	0.705499	-3.832569	-2.144525
C	0.158419	-4.270525	-1.301787
H	2.284788	-2.859711	1.775947
H	2.305765	-4.451046	0.995193
H	2.828558	-3.013321	0.106126
C	2.100400	-3.385248	0.833279
H	-1.829415	-4.005951	1.340726
H	-0.441823	-5.026891	1.763733
H	-0.668366	-3.453588	2.551770
H	2.813991	3.019994	-0.122445
H	2.283553	4.465338	-0.994726
C	2.079883	3.398115	-0.840345
H	0.553768	5.268232	1.111328
H	-0.893155	4.392955	1.633959
C	0.144176	4.269097	1.308786
H	0.705449	3.835720	2.144491
H	-0.469388	5.033615	-1.752788
H	-1.853745	4.011985	-1.321767
C	-0.794094	3.997531	-1.591027
C	7.316311	-0.018667	0.006976
H	7.691973	-1.018277	0.259081
H	7.724385	0.679429	0.743869
H	7.727471	0.244510	-0.972876
C	2.986931	-0.900824	-2.397640
H	2.173526	-0.227325	-2.684405
H	3.694814	-0.974168	-3.229265
H	2.538651	1.912056	2.248398
H	2.167225	0.254294	2.674405
H	3.691885	0.990100	3.224619
C	2.985753	0.922983	2.390975

H	5.622039	0.773689	1.998108
H	5.622909	-0.738334	-2.008876
H	2.532663	-1.886446	-2.254373
H	-0.701501	3.461996	-2.542444
H	2.257120	2.880726	-1.788914
C	-0.767798	-3.991196	1.602185



Aromaticity measures of **3pl**$^{-}$ at M06-2X/6-31+G(d,2p)

I_5: 81

NICS(1): −6.8 ppm

(NICS values calculated at B3LYP/pcS-2)

Atomic coordinates of **3pl**$^{-}$ at M06-2X/6-31+G(d,2p)

Energy -2072.835097

C	-1.388369	0.704082	0.010836
C	-1.384369	-0.706411	-0.015228
C	-0.100346	-1.363746	-0.027416
Si	1.036716	0.004951	-0.002161
C	-0.107426	1.367653	0.023057
C	2.922826	0.007827	-0.002168
Si	0.262490	3.137909	-0.301429
Si	0.276013	-3.133026	0.295273
C	-2.632627	-1.506727	0.000135
C	-3.610958	-1.353229	0.995999
C	-4.746739	-2.158281	1.021061
C	-4.937541	-3.144181	0.051261
C	-3.982374	-3.302605	-0.953093
C	-2.851462	-2.489838	-0.978177
H	-2.113694	-2.601005	-1.767119
H	-4.121008	-4.057554	-1.721473
H	-5.819170	-3.776343	0.076335
H	-5.483669	-2.022663	1.806748
C	-2.640798	1.497559	0.000461
H	-3.461521	-0.596780	1.760209
H	-3.479017	0.575979	-1.749391
C	-3.626411	1.334387	-0.986754
H	-5.508426	1.990928	-1.786202

C	-4.766632	2.133334	-1.006311
C	-4.955461	3.122133	-0.039066
H	-5.839984	3.750365	-0.060732
H	-4.129349	4.047952	1.722801
C	-3.993089	3.290066	0.956883
C	-2.857647	2.483588	0.976459
H	-2.114437	2.602084	1.759191
C	0.147395	4.299830	1.206301
H	-0.890940	4.548884	1.443738
H	0.678212	5.236884	1.001988
H	0.596225	3.841214	2.093440
C	2.052078	3.312683	-0.910847
H	2.271504	4.361178	-1.142834
H	2.779796	2.974953	-0.165324
H	2.216280	2.718596	-1.815935
C	-0.841683	3.901358	-1.640751
H	-0.794348	3.303180	-2.556162
H	-1.888735	3.943745	-1.324100
H	-0.511489	4.919808	-1.876524
H	0.618654	-3.837523	-2.097643
H	-0.874981	-4.538595	-1.455406
C	0.163229	-4.294196	-1.212884
H	0.688912	-5.233563	-1.005895
H	-1.870008	-3.955846	1.315767
H	-0.484383	-4.915314	1.876339
H	-0.785722	-3.298597	2.547901
C	-0.824285	-3.901347	1.635098
H	2.228798	-2.711180	1.810057
H	2.792672	-2.959406	0.158130
H	2.290333	-4.351130	1.131019
C	2.066734	-3.302673	0.902881
H	2.395963	-2.002610	-2.047965
H	3.656959	-1.321706	-3.093662
H	2.197264	-0.384624	-2.689763
C	2.940633	-1.087731	-2.301948
C	3.646182	-0.515834	-1.095454
C	5.043834	-0.509357	-1.077221
C	5.760169	0.007704	-0.000017
C	5.041578	0.530171	1.074885
C	3.645398	0.535074	1.091841
H	5.582200	0.942166	1.925053
H	5.585435	-0.913906	-1.930073
C	7.267960	-0.021508	0.020265
H	7.675017	0.889332	0.467067
H	7.674196	-0.118441	-0.989291
H	7.633434	-0.869580	0.608720
C	2.936843	1.112645	2.293854
H	3.651598	1.354918	3.084446

H	2.388093	2.023227	2.033441
H	2.196431	0.408725	2.685878

Crystal structure and refinement details for 3

$2xC_{35}H_{47}LiOSi_3$, *Fwt.*: 574.93, yellow, block, size: 0.28 x 0.25 x 0.23 mm, monoclinic, space group $P\,2_1$, a = 11.8347(3)Å, b = 19.7159(5)Å, c = 14.9148(4)Å, $\alpha = 90°$, $\beta = 91.806(7)°$, $\gamma = 90°$, V = 3478.37(16)Å^3, T = 112(2)K, Z= 4, $F(000)$ = 1240, D_x = 1.098 Mg/m^3, μ 1.426mm^{-1}.

A crystal of **3** was mounted on a fiber. Cell parameters were determined by least-squares using 45071 ($2.97 \leq \theta \leq 68.28°$) reflections.

Intensity data were collected on a Rigaku R-AXIS RAPID II conversion diffractometer (monochromator; Cu-$K\alpha$ radiation, λ = 1.54178Å) at 112(2) K in the range $2.964 \leq \theta \leq 68.232$.[13] A total of 52455 reflections were collected of which 12555were unique [R(int) = 0.0451, $R(\sigma)$ = 0.0536]; intensities of 11275 reflections were greater than $2\sigma(I)$. Completeness to θ = 0.997.

A numerical absorption correction was applied to the data (the minimum and maximum transmission factors were 0.9248 and 1.0000).[14]

The structure was solved by direct methods (and subsequent difference syntheses).

Anisotropic full-matrix least-squares refinement on F^2 for all non-hydrogen atoms yielded R_1 = 0.0469 and wR^2 = 0.0988 for 1332 [$I>2\sigma(I)$] and R_1 = 0.0558 and wR^2 = 0.1061 for all (12555) intensity data, (number of parameters = 739, goodness-of-fit = 1.045, the maximum and mean shift/esd is 0.002 and 0.000).[15] The absolute structure parameter is 0.040(6). (Friedel coverage: 0.919, Friedel fraction max.: 0.976, Friedel fraction full: 0.979).

The maximum and minimum residual electron density in the final difference map was 0.457 and -0.387e.Å^{-3}.

The weighting scheme applied was $w = 1/[\sigma^2(F_o^2)+(0.0315P)^2+2.7635P]$ where $P = (F_o^2+2F_c^2)/3$.

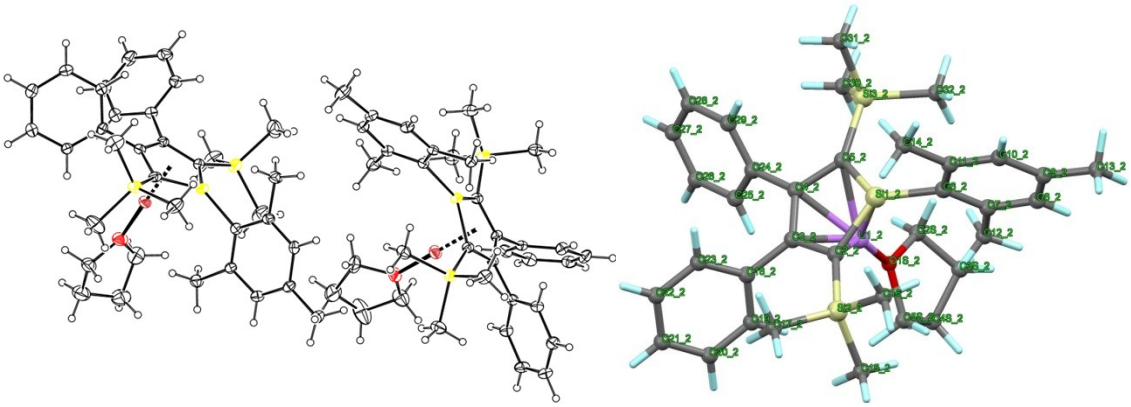
Hydrogen atomic positions were calculated from assumed geometries (but hydrogens were located in difference maps also). Hydrogen atoms were included in structure factor calculations but they were not refined. The isotropic displacement parameters of the hydrogen atoms were approximated from the U(eq) value of the atom they were bonded to. ORTEP style molecular structure diagram[16] can be found in Figure 1, simulated powder diffraction in Figure 4, while crystallographic data are in Table 1 – 2 (more information in table 3-7).

Crystallographic data (including structure factors) for the crystal structure of **3** has been deposited with the Cambridge Crystallographic Data Centre as supplementary publication number CCDC 1561388.

Table S6. Summary of crystallographic data, data collections, structure determination and refinement for **3**

crystal structure	**3**
CCDC	1561388
Empirical formula	$C_{35}H_{47}LiOSi_3$
Formula weight	574.93
Temperature	112(2)
Radiation and wavelength (Å)	Cu-Kα, λ =1.54178
Crystal system	monoclinic
Space group	$P\,2_1$
Unit cell dimensions: a (Å)	11.8347(3)
b (Å)	19.7159(5)
c (Å)	14.9148(4)
α (°)	90
β (°)	91.806(7)
γ (°)	90
Volume (Å^3)	3478 (1)
Z, Z'	4, 2
Density (calculated) (Mg/m^3)	1.098
Absorption coefficient, μ (mm^{-1})	1.426
F(000)	1240
Crystal colour, description	yellow, block
Crystal size (mm)	0.28 x 0.25 x 0.23
Absorption correction	numerical
Max. and min. transmission	0.9248 and 1.0000
θ–range for data collection (°)	2.964 ≤ θ ≤ 68.232
Index ranges	-14 ≤ *h* ≤13; -22≤ *k* ≤23; -17 ≤ *l* ≤17
Reflections collected	52455
Completeness to 2θ	0.998
Absolute structure parameters:[17]	
Flack Parameter	0.040(6)
Hooft parameter	0.031(6)
Parsonz Parameter	0.043(6)
Friedel coverage	0.919
Friedel fraction max.	0.976
Friedel fraction full	0.979
Independent reflections	12555 [*R*(int) =0.0451]
Reflections *I*>2σ(*I*)	11275
Refinement method	full-matrix least-squares on F^2
Data / restraints / parameters	12555 /1 /739
Goodness-of-fit on F^2	1.045
Final *R* indices [*I*>2σ(*I*)]	R_1 =0.0469, wR^2 =0.0988

R indices (all data)	R_1 =0.0558,
	wR^2 =0.1061
Max. and mean shift/esd	0.002 and 0.001
Largest diff. peak and hole (e.Å^{-3})	0.46;-0.39



a. b.

Fig. S28 a: The crystallographically independent molecule in the asymmetric unit of the crystal **3** without the atomic labelling. Displacement ellipsoids are drawn at the 30% probability level for clarity. b: The numbering of the molecules in the crystal structure **3**.

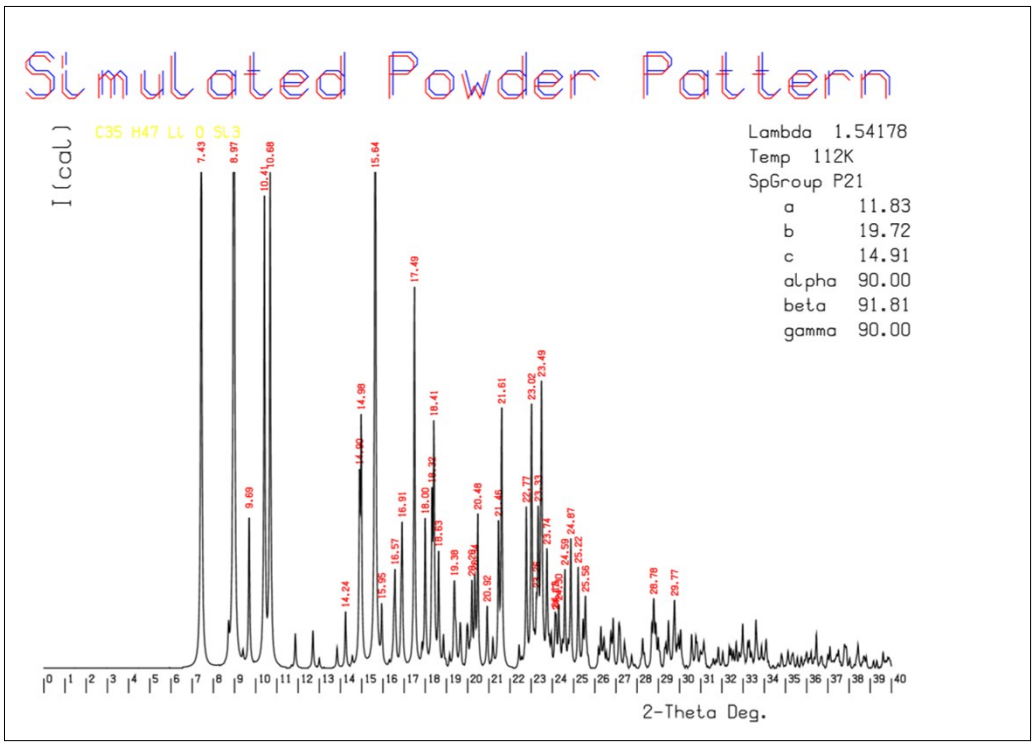


Fig. S29 The simulated powder diffractogram of the final crystal structure of **3**.

Comparison of the two independent molecules in the asymmetric unit of 3 (3_1 and 3_2)

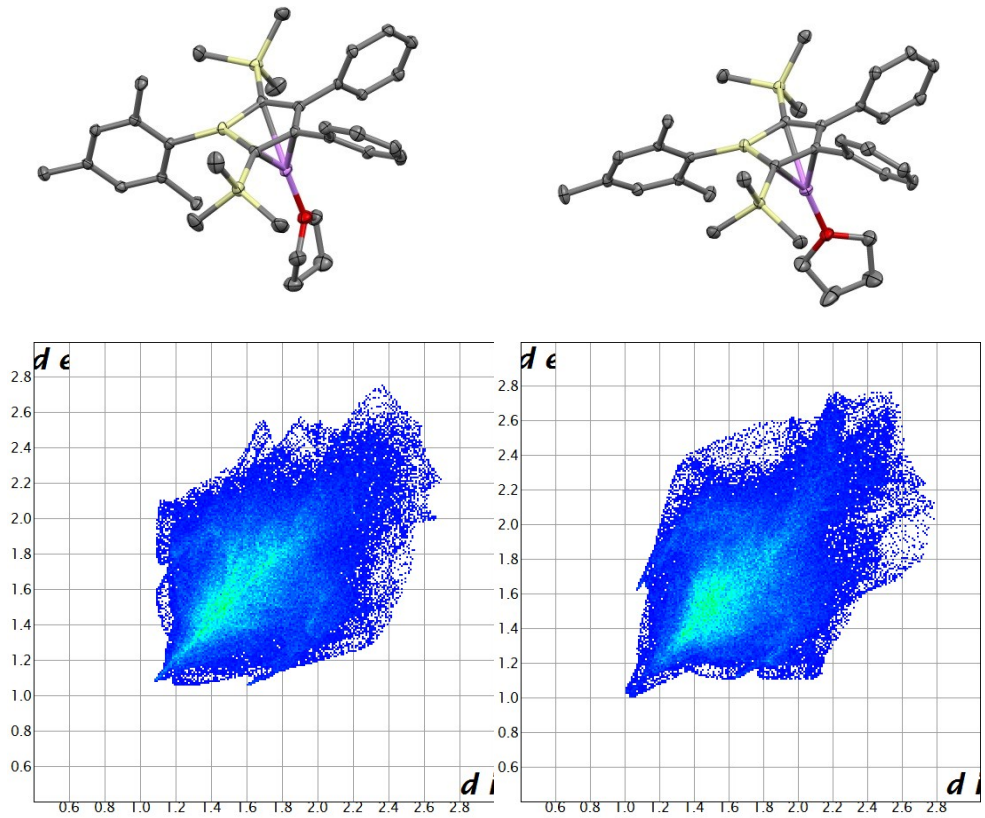


Fig. S30 Two independent molecules are observed within the asymmetric unit in structure **3**.[18] The intermolecular interactions of the molecules are different.[19–20]

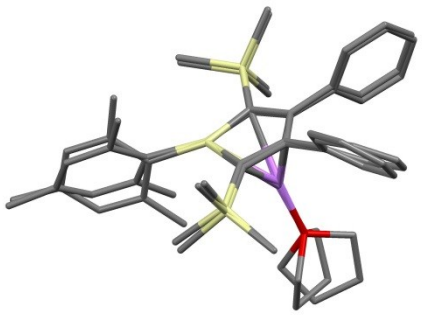


Fig. S31 The two conformations in structure **3**, the orientation of the tetrahydrofuran and the phenyl rings are different. The Root-mean-square deviation of atomic positions is 0.5417 Å and the biggest distance is 1.4508 Å (tetrahydrofuran methylene group).

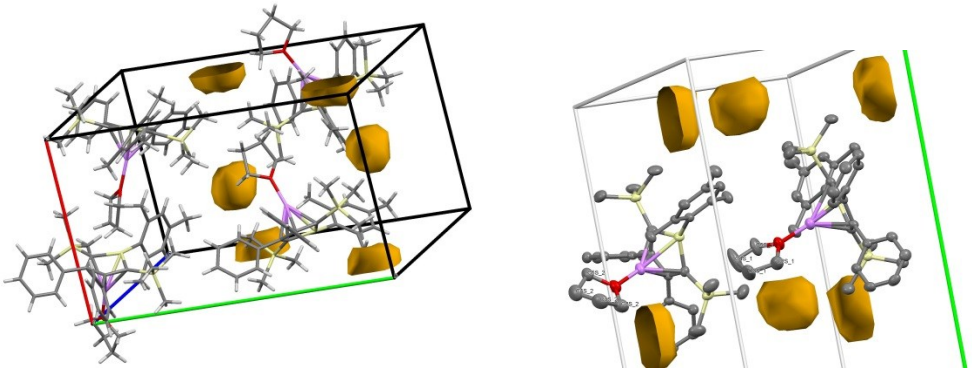


Fig. S32 The K.P.I. packing-index is 65,5%.[21] However small voids are observed in the crystal lattice (brownish-orange), the biggest void is just 30 Å^3. These voids are not enough for smaller molecules (water needed 40 Å^3), but the tetrahydrofuran molecules nearby the void can oscillate. The U_{ISO} parameter of THF methylene atoms (C3S_1, C4S_1, C5S_1) is bigger than the other ones.

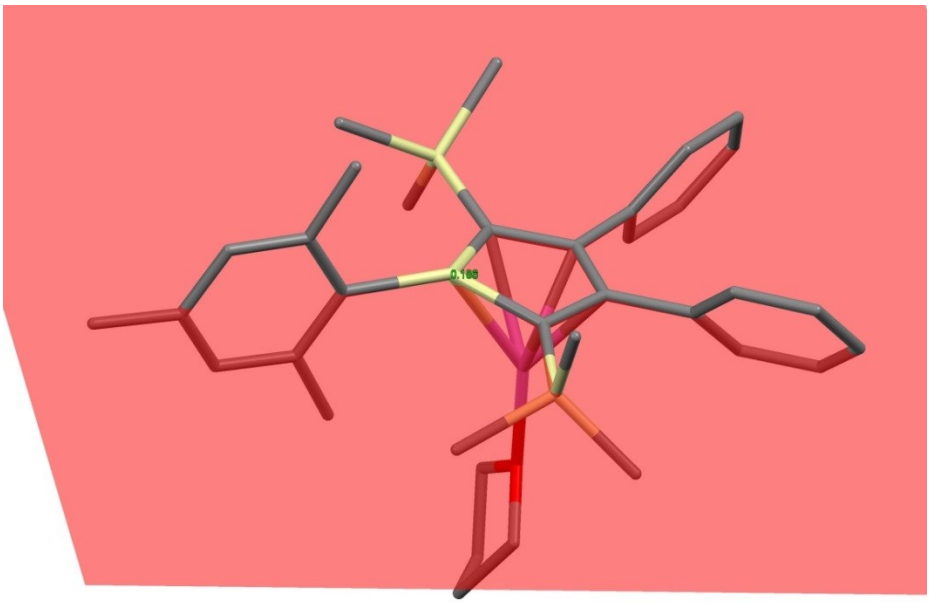


Fig. S33 The Si1 is hang out of the central C2 C3C4C5 ring with 0.2 Å. The Si and C2C3C4C5 plane distances are 0.1742 (0.0063) Å and 0.1862 (0.0064) Å calculated by the program platon. (The Puckering-parameters[19] of the ring is Q(2) = 0.099(4) Ang., Phi(2) = 350(3) Deg).

13 CrystalClear SM 1.4.0 (Rigaku/MSC Inc., 2008).

14 NUMABS: T. Higashi, (1998), rev. 2002. (Rigaku/MSC Inc.)

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Atomic information of structure 3

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3). *U*(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	*U*(eq)
Si1_1	8445(1)	1365.3(6)	4921.2(8)	25(1)
Si2_1	9383(1)	-183.5(6)	4835.0(8)	28(1)
Si3_1	7091(1)	2574.3(6)	5944.6(8)	28(1)
C2_1	8579(4)	517(2)	5342(3)	25(1)
C3_1	8225(4)	563(2)	6263(3)	24(1)
C4_1	7821(3)	1202(2)	6543(3)	23(1)
C5_1	7770(4)	1732(2)	5863(3)	25(1)
C6_1	8607(3)	1726(2)	3776(3)	25(1)
C7_1	8035(4)	1463(2)	3007(3)	27(1)
C8_1	8139(4)	1787(2)	2190(3)	32(1)
C9_1	8746(4)	2378(2)	2093(3)	29(1)
C10_1	9332(4)	2627(2)	2851(3)	30(1)
C11_1	9282(4)	2312(2)	3677(3)	24(1)
C12_1	7268(4)	854(3)	3042(3)	41(1)
C13_1	8762(5)	2741(3)	1209(3)	48(1)
C14_1	9948(4)	2616(2)	4461(3)	30(1)
C15_1	8462(5)	-894(3)	4400(4)	44(1)
C16_1	10165(4)	153(3)	3858(3)	40(1)
C17_1	10469(4)	-534(3)	5641(3)	36(1)
C18_1	8339(3)	-26(2)	6888(3)	25(1)
C19_1	7701(4)	-607(2)	6764(3)	32(1)
C20_1	7833(4)	-1159(2)	7338(4)	37(1)
C21_1	8619(4)	-1134(2)	8042(3)	36(1)
C22_1	9259(4)	-561(3)	8172(3)	36(1)
C23_1	9122(4)	-10(2)	7609(3)	31(1)
C24_1	7474(3)	1349(2)	7474(3)	25(1)
C25_1	6586(4)	1027(2)	7894(3)	30(1)

C26_1	6219(4)	1238(3)	8718(3)	36(1)
C27_1	6751(4)	1773(3)	9156(3)	37(1)
C28_1	7652(4)	2088(3)	8772(3)	34(1)
C29_1	8020(4)	1878(2)	7944(3)	28(1)
C30_1	5748(4)	2552(3)	6575(4)	42(1)
C31_1	8010(4)	3257(2)	6471(3)	38(1)
C32_1	6710(4)	2857(3)	4765(3)	38(1)
Li2_1	6677(7)	788(4)	5480(6)	35(2)
O1S_1	5242(3)	428(2)	5203(2)	39(1)
C2S_1	4704(5)	-96(3)	5714(4)	54(2)
C3S_1	3566(5)	-200(4)	5294(6)	83(2)
C4S_1	3503(6)	221(5)	4478(5)	91(3)
C5S_1	4641(5)	495(4)	4354(4)	59(2)
Si1_2	3334(1)	1329.8(6)	536.6(8)	28(1)
Si2_2	2388(1)	2568.4(6)	-734.5(9)	30(1)
Si3_2	3975(1)	-260.9(7)	854.1(9)	35(1)
C2_2	2714(4)	1672(2)	-471(3)	28(1)
C3_2	2799(4)	1125(2)	-1120(3)	25(1)
C4_2	3226(3)	498(2)	-791(3)	24(1)
C5_2	3496(4)	470(2)	164(3)	26(1)
C6_2	3320(4)	1682(2)	1706(3)	26(1)
C7_2	2368(4)	1641(2)	2244(3)	25(1)
C8_2	2421(4)	1910(2)	3116(3)	30(1)
C9_2	3391(4)	2217(2)	3460(3)	27(1)
C10_2	4330(4)	2255(2)	2921(3)	28(1)
C11_2	4306(4)	1997(2)	2058(3)	27(1)
C12_2	1278(4)	1324(3)	1914(3)	35(1)
C13_2	3423(4)	2529(3)	4388(3)	41(1)
C14_2	5343(4)	2069(3)	1505(3)	38(1)
C15_2	828(5)	2736(3)	-805(5)	59(2)
C16_2	3009(5)	3108(3)	188(3)	45(1)
C17_2	2993(5)	2878(3)	-1794(4)	49(1)
C18_2	2489(4)	1237(2)	-2083(3)	24(1)
C19_2	1364(3)	1339(2)	-2364(3)	26(1)
C20_2	1056(4)	1442(2)	-3255(3)	34(1)
C21_2	1879(4)	1452(3)	-3883(3)	36(1)
C22_2	3000(4)	1358(3)	-3628(3)	33(1)
C23_2	3299(4)	1253(2)	-2733(3)	29(1)
C24_2	3399(4)	-90(2)	-1400(3)	26(1)
C25_2	2512(4)	-354(2)	-1935(3)	32(1)
C26_2	2673(5)	-898(2)	-2491(3)	38(1)
C27_2	3712(5)	-1202(3)	-2530(3)	43(1)
C28_2	4611(4)	-949(3)	-2014(4)	40(1)
C29_2	4453(4)	-392(2)	-1461(3)	32(1)
C30_2	3378(6)	-1092(3)	477(4)	55(2)
C31_2	5548(5)	-317(3)	933(4)	60(2)
C32_2	3529(6)	-135(3)	2042(3)	56(2)
Li1_2	1658(6)	714(4)	-153(6)	33(2)
O1S_2	237(3)	349(2)	55(2)	43(1)
C2S_2	41(5)	-202(3)	640(4)	55(2)

C3S_2	-1100(5)	-44(3)	1038(4)	62(2)
C4S_2	-1714(5)	316(4)	277(4)	62(2)
C5S_2	-820(4)	763(3)	-89(4)	44(1)

Table S8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3).

	x	*y*	*z*	*U*(iso)
H8_1	7775	1594	1673	38
H10_1	9777	3025	2798	36
H12A_1	7486	573	3562	61
H12B_1	7335	587	2492	61
H12C_1	6484	1005	3096	61
H13A_1	9525	2913	1111	71
H13B_1	8228	3120	1213	71
H13C_1	8543	2425	727	71
H14A_1	10284	2251	4827	44
H14B_1	9442	2886	4826	44
H14C_1	10548	2907	4237	44
H15A_1	8929	-1232	4104	66
H15B_1	7898	-714	3968	66
H15C_1	8078	-1106	4900	66
H16A_1	10582	-217	3580	60
H16B_1	10697	505	4066	60
H16C_1	9626	348	3417	60
H17A_1	10994	-822	5318	54
H17B_1	10096	-804	6098	54
H17C_1	10887	-160	5930	54
H19_1	7164	-630	6278	39
H20_1	7383	-1554	7245	44
H21_1	8715	-1511	8434	43
H22_1	9803	-543	8654	43
H23_1	9566	385	7713	37
H25_1	6224	652	7606	36
H26_1	5602	1015	8984	43
H27_1	6495	1923	9719	45
H28_1	8025	2452	9076	41
H29_1	8652	2096	7691	33
H30A_1	5357	2988	6508	64
H30B_1	5924	2467	7212	64
H30C_1	5261	2189	6336	64
H31A_1	7730	3703	6278	57
H31B_1	8790	3199	6281	57
H31C_1	7989	3223	7125	57
H32A_1	6192	3243	4785	57
H32B_1	6344	2482	4436	57
H32C_1	7398	2991	4462	57
H2S1_1	4642	46	6347	64
H2S2_1	5149	-521	5697	64

H3S1_1	3453	-684	5138	100
H3S2_1	2975	-63	5712	100
H4S1_1	3260	-56	3953	110
H4S2_1	2953	594	4549	110
H5S1_1	5029	238	3884	71
H5S2_1	4598	978	4173	71
H8_2	1776	1882	3477	36
H10_2	5003	2463	3152	34
H12A_2	1400	842	1791	53
H12B_2	1013	1552	1363	53
H12C_2	708	1372	2373	53
H13A_2	4068	2346	4738	62
H13B_2	2721	2421	4689	62
H13C_2	3500	3022	4338	62
H14A_2	5557	1624	1272	56
H14B_2	5967	2251	1881	56
H14C_2	5181	2379	1004	56
H15A_2	695	3225	-862	88
H15B_2	479	2568	-261	88
H15C_2	494	2503	-1330	88
H16A_2	2718	3571	128	68
H16B_2	3834	3113	151	68
H16C_2	2801	2921	770	68
H17A_2	2883	3369	-1842	73
H17B_2	2611	2653	-2305	73
H17C_2	3803	2774	-1793	73
H19_2	794	1338	-1929	32
H20_2	284	1505	-3431	40
H21_2	1676	1524	-4497	43
H22_2	3566	1365	-4066	39
H23_2	4072	1192	-2563	35
H25_2	1784	-152	-1914	38
H26_2	2059	-1065	-2852	46
H27_2	3815	-1583	-2908	51
H28_2	5334	-1156	-2039	48
H29_2	5077	-215	-1119	38
H30A_2	3633	-1449	894	83
H30B_2	3636	-1195	-125	83
H30C_2	2551	-1068	466	83
H31A_2	5772	-696	1326	89
H31B_2	5858	106	1181	89
H31C_2	5842	-392	334	89
H32A_2	3804	-514	2413	84
H32B_2	2703	-115	2054	84
H32C_2	3849	290	2277	84
H2S1_2	642	-230	1115	66
H2S2_2	13	-636	306	66
H3S1_2	-1499	-464	1206	75
H3S2_2	-1014	253	1571	75
H4S1_2	-2001	-10	-181	74

H4S2_2	-2354	586	496	74
H5S1_2	-769	1198	242	53
H5S2_2	-968	857	-734	53

Table S9. Anisotropic displacement parameters (Å^2 x 10^3). The anisotropic displacement factor exponent takes the form: $-2\pi^2(h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12})$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si1_1	29(1)	24(1)	23(1)	1(1)	4(1)	-1(1)
Si2_1	32(1)	25(1)	28(1)	-3(1)	6(1)	1(1)
Si3_1	29(1)	24(1)	31(1)	1(1)	4(1)	2(1)
C2_1	24(2)	25(2)	27(2)	-3(2)	4(2)	-5(2)
C3_1	27(2)	22(2)	22(2)	-4(2)	2(2)	-5(2)
C4_1	20(2)	25(2)	24(2)	-3(2)	3(2)	-4(2)
C5_1	24(2)	25(2)	25(2)	-1(2)	3(2)	-4(2)
C6_1	21(2)	28(2)	25(2)	1(2)	3(2)	2(2)
C7_1	27(2)	27(3)	27(2)	0(2)	5(2)	-1(2)
C8_1	31(3)	40(3)	23(2)	-4(2)	2(2)	-1(2)
C9_1	36(3)	29(3)	23(2)	0(2)	7(2)	3(2)
C10_1	36(2)	25(2)	29(2)	1(2)	8(2)	-1(2)
C11_1	22(2)	22(2)	27(2)	-2(2)	4(2)	3(2)
C12_1	39(3)	50(3)	33(3)	-2(2)	5(2)	-15(2)
C13_1	73(4)	44(3)	26(3)	9(2)	6(3)	-4(3)
C14_1	33(2)	30(2)	26(2)	0(2)	1(2)	-7(2)
C15_1	50(3)	38(3)	44(3)	-8(2)	-1(3)	2(2)
C16_1	40(3)	40(3)	41(3)	3(2)	16(2)	6(2)
C17_1	36(3)	33(3)	38(3)	-6(2)	8(2)	0(2)
C18_1	24(2)	25(2)	26(2)	-3(2)	6(2)	1(2)
C19_1	26(2)	30(3)	41(3)	-1(2)	2(2)	-2(2)
C20_1	33(3)	26(3)	50(3)	0(2)	7(2)	-5(2)
C21_1	38(3)	31(3)	38(3)	11(2)	12(2)	6(2)
C22_1	46(3)	39(3)	22(3)	3(2)	0(2)	2(2)
C23_1	34(3)	29(3)	29(2)	-1(2)	2(2)	-4(2)
C24_1	26(2)	23(2)	26(2)	2(2)	2(2)	4(2)
C25_1	32(3)	27(2)	32(3)	-1(2)	5(2)	-4(2)
C26_1	36(3)	40(3)	33(3)	0(2)	14(2)	-5(2)
C27_1	40(3)	44(3)	28(3)	-5(2)	10(2)	3(2)
C28_1	36(3)	33(3)	34(3)	-10(2)	1(2)	-1(2)
C29_1	29(2)	24(2)	30(2)	0(2)	6(2)	-1(2)
C30_1	36(3)	43(3)	49(3)	6(3)	10(2)	8(2)
C31_1	51(3)	25(3)	38(3)	-6(2)	3(2)	-1(2)
C32_1	35(3)	32(3)	46(3)	5(2)	2(2)	6(2)
Li2_1	28(4)	38(5)	38(5)	3(4)	-1(4)	-3(4)
O1S_1	30(2)	46(2)	41(2)	2(2)	-2(2)	-10(2)
C2S_1	43(3)	48(4)	70(4)	12(3)	1(3)	-6(3)
C3S_1	50(4)	59(4)	140(7)	31(5)	-23(4)	-26(4)
C4S_1	47(4)	175(9)	52(4)	-17(5)	-1(3)	-44(5)
C5S_1	47(3)	92(5)	37(3)	2(3)	-13(3)	-14(3)
Si1_2	31(1)	26(1)	27(1)	-6(1)	4(1)	1(1)

Si2_2	34(1)	23(1)	34(1)	-2(1)	7(1)	0(1)
Si3_2	46(1)	29(1)	30(1)	-1(1)	0(1)	7(1)
C2_2	29(2)	28(2)	27(2)	-7(2)	7(2)	-2(2)
C3_2	21(2)	27(2)	28(2)	-1(2)	4(2)	0(2)
C4_2	23(2)	25(2)	25(2)	-5(2)	3(2)	-1(2)
C5_2	24(2)	30(2)	24(2)	2(2)	2(2)	3(2)
C6_2	27(2)	23(2)	27(2)	-2(2)	1(2)	0(2)
C7_2	28(2)	23(2)	25(2)	-3(2)	2(2)	0(2)
C8_2	32(3)	29(3)	29(3)	-1(2)	8(2)	-2(2)
C9_2	37(3)	23(2)	22(2)	2(2)	3(2)	0(2)
C10_2	28(2)	29(2)	28(3)	-1(2)	-5(2)	-2(2)
C11_2	30(2)	24(2)	27(2)	-1(2)	4(2)	3(2)
C12_2	28(2)	42(3)	36(3)	-9(2)	2(2)	-6(2)
C13_2	49(3)	46(3)	28(3)	-6(2)	4(2)	-8(3)
C14_2	27(3)	48(3)	39(3)	-12(2)	5(2)	-6(2)
C15_2	41(3)	37(3)	99(5)	-3(3)	2(3)	11(3)
C16_2	69(4)	29(3)	38(3)	-10(2)	5(3)	2(3)
C17_2	72(4)	28(3)	46(3)	-1(2)	11(3)	-9(3)
C18_2	32(2)	20(2)	21(2)	-4(2)	-2(2)	-1(2)
C19_2	27(2)	28(2)	24(2)	-1(2)	3(2)	-1(2)
C20_2	30(2)	33(3)	38(3)	2(2)	-3(2)	1(2)
C21_2	42(3)	35(3)	29(3)	3(2)	-3(2)	0(2)
C22_2	35(3)	35(3)	28(2)	0(2)	9(2)	-1(2)
C23_2	26(2)	34(3)	27(2)	-1(2)	0(2)	3(2)
C24_2	29(2)	20(2)	28(2)	-1(2)	4(2)	-1(2)
C25_2	31(3)	27(3)	38(3)	0(2)	-1(2)	-2(2)
C26_2	50(3)	28(3)	36(3)	-4(2)	-10(2)	0(2)
C27_2	65(4)	29(3)	34(3)	-11(2)	-2(3)	6(2)
C28_2	43(3)	35(3)	43(3)	-2(2)	10(2)	12(2)
C29_2	30(3)	31(3)	34(3)	-2(2)	3(2)	1(2)
C30_2	84(5)	35(3)	47(4)	6(3)	10(3)	-4(3)
C31_2	59(4)	59(4)	60(4)	-6(3)	-13(3)	23(3)
C32_2	88(5)	47(4)	33(3)	9(3)	2(3)	18(3)
Li1_2	23(4)	41(5)	35(5)	-6(4)	1(3)	-3(3)
O1S_2	35(2)	48(2)	46(2)	-5(2)	8(2)	-10(2)
C2S_2	61(4)	49(4)	55(4)	4(3)	2(3)	-11(3)
C3S_2	61(4)	63(4)	64(4)	6(3)	17(3)	-15(3)
C4S_2	45(4)	74(5)	67(4)	-5(4)	12(3)	-2(3)
C5S_2	33(3)	50(3)	49(4)	-6(3)	2(2)	-3(2)

Table S10. Bond lengths (Å) and angles (°) to be deposited

Si1_1-C5_1	1.790(4)	Si1_1-C2_1	1.791(5)
Si1_1-C6_1	1.867(4)	Si1_1-Li2_1	2.546(8)
Si2_1-C2_1	1.853(4)	Si2_1-C17_1	1.864(5)
Si2_1-C16_1	1.873(5)	Si2_1-C15_1	1.878(5)
Si3_1-C5_1	1.851(4)	Si3_1-C30_1	1.872(5)
Si3_1-C32_1	1.886(5)	Si3_1-C31_1	1.886(5)
C2_1-C3_1	1.451(6)	C2_1-Li2_1	2.329(9)
C3_1-C4_1	1.415(6)	C3_1-C18_1	1.492(6)

C3_1-Li2_1	2.187(9)	C4_1-C5_1	1.455(6)
C4_1-C24_1	1.489(6)	C4_1-Li2_1	2.209(9)
C5_1-Li2_1	2.326(9)	C6_1-C7_1	1.413(6)
C6_1-C11_1	1.415(6)	C7_1-C8_1	1.385(6)
C7_1-C12_1	1.507(6)	C8_1-C9_1	1.379(6)
C9_1-C10_1	1.397(6)	C9_1-C13_1	1.499(6)
C10_1-C11_1	1.381(6)	C11_1-C14_1	1.513(6)
C18_1-C19_1	1.381(6)	C18_1-C23_1	1.398(6)
C19_1-C20_1	1.391(7)	C20_1-C21_1	1.383(7)
C21_1-C22_1	1.371(7)	C22_1-C23_1	1.378(6)
C24_1-C25_1	1.394(6)	C24_1-C29_1	1.403(6)
C25_1-C26_1	1.380(6)	C26_1-C27_1	1.383(7)
C27_1-C28_1	1.374(7)	C28_1-C29_1	1.385(6)
Li2_1-O1S_1	1.875(8)	O1S_1-C5S_1	1.438(6)
O1S_1-C2S_1	1.445(6)	C2S_1-C3S_1	1.481(8)
C3S_1-C4S_1	1.47(1)	C4S_1-C5S_1	1.469(8)
Si1_2-C2_2	1.784(5)	Si1_2-C5_2	1.796(5)
Si1_2-C6_2	1.879(5)	Si1_2-Li1_2	2.517(8)
Si2_2-C2_2	1.849(5)	Si2_2-C17_2	1.858(5)
Si2_2-C16_2	1.872(5)	Si2_2-C15_2	1.876(5)
Si3_2-C5_2	1.850(5)	Si3_2-C30_2	1.864(6)
Si3_2-C31_2	1.865(6)	Si3_2-C32_2	1.881(5)
C2_2-C3_2	1.455(6)	C2_2-Li1_2	2.322(9)
C3_2-C4_2	1.417(6)	C3_2-C18_2	1.488(6)
C3_2-Li1_2	2.164(9)	C4_2-C5_2	1.451(6)
C4_2-C24_2	1.491(6)	C4_2-Li1_2	2.154(9)
C5_2-Li1_2	2.262(9)	C6_2-C7_2	1.406(6)
C6_2-C11_2	1.408(6)	C7_2-C8_2	1.404(6)
C7_2-C12_2	1.502(6)	C8_2-C9_2	1.382(6)
C9_2-C10_2	1.394(6)	C9_2-C13_2	1.514(6)
C10_2-C11_2	1.383(6)	C11_2-C14_2	1.507(6)
C18_2-C23_2	1.384(6)	C18_2-C19_2	1.398(6)
C19_2-C20_2	1.382(6)	C20_2-C21_2	1.372(6)
C21_2-C22_2	1.381(6)	C22_2-C23_2	1.385(6)
C24_2-C29_2	1.388(6)	C24_2-C25_2	1.400(6)
C25_2-C26_2	1.372(6)	C26_2-C27_2	1.370(7)
C27_2-C28_2	1.386(7)	C28_2-C29_2	1.390(7)
Li1_2-O1S_2	1.865(8)	O1S_2-C2S_2	1.417(7)
O1S_2-C5S_2	1.503(6)	C2S_2-C3S_2	1.526(8)
C3S_2-C4S_2	1.506(9)	C4S_2-C5S_2	1.493(8)

C5_1-Si1_1-C2_1	97.9(2)	C5_1-Si1_1-C6_1	128.7(2)
C2_1-Si1_1-C6_1	131.8(2)	C5_1-Si1_1-Li2_1	62.1(2)
C2_1-Si1_1-Li2_1	62.1(2)	C6_1-Si1_1-Li2_1	125.4(2)
C2_1-Si2_1-C17_1	111.4(2)	C2_1-Si2_1-C16_1	109.0(2)
C17_1-Si2_1-C16_1	106.6(2)	C2_1-Si2_1-C15_1	113.4(2)
C17_1-Si2_1-C15_1	109.1(2)	C16_1-Si2_1-C15_1	106.9(2)
C5_1-Si3_1-C30_1	112.9(2)	C5_1-Si3_1-C32_1	107.1(2)
C30_1-Si3_1-C32_1	107.1(2)	C5_1-Si3_1-C31_1	115.0(2)
C30_1-Si3_1-C31_1	107.2(2)	C32_1-Si3_1-C31_1	107.2(2)

C3_1-C2_1-Si1_1	104.4(3)	C3_1-C2_1-Si2_1	126.9(3)
Si1_1-C2_1-Si2_1	126.4(2)	C3_1-C2_1-Li2_1	66.0(3)
Si1_1-C2_1-Li2_1	75.0(3)	Si2_1-C2_1-Li2_1	135.9(3)
C4_1-C3_1-C2_1	116.4(4)	C4_1-C3_1-C18_1	122.3(4)
C2_1-C3_1-C18_1	121.2(4)	C4_1-C3_1-Li2_1	72.1(3)
C2_1-C3_1-Li2_1	76.7(3)	C18_1-C3_1-Li2_1	123.3(4)
C3_1-C4_1-C5_1	116.1(4)	C3_1-C4_1-C24_1	123.6(4)
C5_1-C4_1-C24_1	120.3(4)	C3_1-C4_1-Li2_1	70.4(3)
C5_1-C4_1-Li2_1	75.7(3)	C24_1-C4_1-Li2_1	124.1(4)
C4_1-C5_1-Si1_1	104.3(3)	C4_1-C5_1-Si3_1	127.3(3)
Si1_1-C5_1-Si3_1	128.3(2)	C4_1-C5_1-Li2_1	67.0(3)
Si1_1-C5_1-Li2_1	75.1(3)	Si3_1-C5_1-Li2_1	119.6(3)
C7_1-C6_1-C11_1	118.3(4)	C7_1-C6_1-Si1_1	122.9(3)
C11_1-C6_1-Si1_1	118.8(3)	C8_1-C7_1-C6_1	119.4(4)
C8_1-C7_1-C12_1	118.0(4)	C6_1-C7_1-C12_1	122.6(4)
C9_1-C8_1-C7_1	122.9(4)	C8_1-C9_1-C10_1	117.3(4)
C8_1-C9_1-C13_1	121.0(4)	C10_1-C9_1-C13_1	121.6(4)
C11_1-C10_1-C9_1	122.0(4)	C10_1-C11_1-C6_1	120.0(4)
C10_1-C11_1-C14_1	118.4(4)	C6_1-C11_1-C14_1	121.6(4)
C19_1-C18_1-C23_1	117.9(4)	C19_1-C18_1-C3_1	121.6(4)
C23_1-C18_1-C3_1	120.6(4)	C18_1-C19_1-C20_1	121.1(5)
C21_1-C20_1-C19_1	119.9(4)	C22_1-C21_1-C20_1	119.5(5)
C21_1-C22_1-C23_1	120.6(5)	C22_1-C23_1-C18_1	120.9(4)
C25_1-C24_1-C29_1	117.2(4)	C25_1-C24_1-C4_1	124.4(4)
C29_1-C24_1-C4_1	118.3(4)	C26_1-C25_1-C24_1	121.7(4)
C25_1-C26_1-C27_1	120.0(4)	C28_1-C27_1-C26_1	119.7(4)
C27_1-C28_1-C29_1	120.5(5)	C28_1-C29_1-C24_1	120.9(4)
O1S_1-Li2_1-C3_1	141.1(5)	O1S_1-Li2_1-C4_1	146.0(5)
C3_1-Li2_1-C4_1	37.5(2)	O1S_1-Li2_1-C5_1	148.2(5)
C3_1-Li2_1-C5_1	65.2(3)	C4_1-Li2_1-C5_1	37.3(2)
O1S_1-Li2_1-C2_1	139.9(5)	C3_1-Li2_1-C2_1	37.3(2)
C4_1-Li2_1-C2_1	64.9(3)	C5_1-Li2_1-C2_1	70.9(3)
O1S_1-Li2_1-Si1_1	147.7(4)	C3_1-Li2_1-Si1_1	65.3(2)
C4_1-Li2_1-Si1_1	65.0(2)	C5_1-Li2_1-Si1_1	42.8(2)
C2_1-Li2_1-Si1_1	42.8(2)	C5S_1-O1S_1-C2S_1	108.5(4)
C5S_1-O1S_1-Li2_1	125.3(4)	C2S_1-O1S_1-Li2_1	124.5(4)
O1S_1-C2S_1-C3S_1	106.6(5)	C4S_1-C3S_1-C2S_1	107.1(5)
C5S_1-C4S_1-C3S_1	106.8(6)	O1S_1-C5S_1-C4S_1	106.6(5)
C2_2-Si1_2-C5_2	98.1(2)	C2_2-Si1_2-C6_2	128.9(2)
C5_2-Si1_2-C6_2	129.8(2)	C2_2-Si1_2-Li1_2	62.7(2)
C5_2-Si1_2-Li1_2	60.6(2)	C6_2-Si1_2-Li1_2	121.9(2)
C2_2-Si2_2-C17_2	114.3(2)	C2_2-Si2_2-C16_2	108.2(2)
C17_2-Si2_2-C16_2	106.6(2)	C2_2-Si2_2-C15_2	112.3(2)
C17_2-Si2_2-C15_2	107.4(3)	C16_2-Si2_2-C15_2	107.7(3)
C5_2-Si3_2-C30_2	114.2(2)	C5_2-Si3_2-C31_2	111.7(3)
C30_2-Si3_2-C31_2	109.6(3)	C5_2-Si3_2-C32_2	109.3(2)
C30_2-Si3_2-C32_2	106.6(3)	C31_2-Si3_2-C32_2	104.9(3)
C3_2-C2_2-Si1_2	104.2(3)	C3_2-C2_2-Si2_2	125.8(3)
Si1_2-C2_2-Si2_2	128.2(3)	C3_2-C2_2-Li1_2	65.3(3)
Si1_2-C2_2-Li1_2	74.3(3)	Si2_2-C2_2-Li1_2	135.3(3)

C4_2-C3_2-C2_2	116.6(4)	C4_2-C3_2-C18_2	122.5(4)
C2_2-C3_2-C18_2	120.9(4)	C4_2-C3_2-Li1_2	70.5(3)
C2_2-C3_2-Li1_2	77.1(3)	C18_2-C3_2-Li1_2	124.0(4)
C3_2-C4_2-C5_2	116.0(4)	C3_2-C4_2-C24_2	121.5(4)
C5_2-C4_2-C24_2	122.5(4)	C3_2-C4_2-Li1_2	71.2(3)
C5_2-C4_2-Li1_2	74.9(3)	C24_2-C4_2-Li1_2	124.0(4)
C4_2-C5_2-Si1_2	104.2(3)	C4_2-C5_2-Si3_2	129.1(3)
Si1_2-C5_2-Si3_2	126.7(3)	C4_2-C5_2-Li1_2	66.8(3)
Si1_2-C5_2-Li1_2	75.7(3)	Si3_2-C5_2-Li1_2	123.9(3)
C7_2-C6_2-C11_2	118.9(4)	C7_2-C6_2-Si1_2	122.6(3)
C11_2-C6_2-Si1_2	118.5(3)	C8_2-C7_2-C6_2	119.5(4)
C8_2-C7_2-C12_2	118.3(4)	C6_2-C7_2-C12_2	122.2(4)
C9_2-C8_2-C7_2	121.4(4)	C8_2-C9_2-C10_2	118.5(4)
C8_2-C9_2-C13_2	120.9(4)	C10_2-C9_2-C13_2	120.6(4)
C11_2-C10_2-C9_2	121.5(4)	C10_2-C11_2-C6_2	120.1(4)
C10_2-C11_2-C14_2	118.7(4)	C6_2-C11_2-C14_2	121.2(4)
C23_2-C18_2-C19_2	117.4(4)	C23_2-C18_2-C3_2	121.7(4)
C19_2-C18_2-C3_2	120.9(4)	C20_2-C19_2-C18_2	121.9(4)
C21_2-C20_2-C19_2	119.2(4)	C20_2-C21_2-C22_2	120.4(4)
C21_2-C22_2-C23_2	120.0(4)	C18_2-C23_2-C22_2	121.1(4)
C29_2-C24_2-C25_2	117.5(4)	C29_2-C24_2-C4_2	121.0(4)
C25_2-C24_2-C4_2	121.4(4)	C26_2-C25_2-C24_2	121.2(5)
C27_2-C26_2-C25_2	120.6(5)	C26_2-C27_2-C28_2	119.6(5)
C27_2-C28_2-C29_2	119.9(5)	C24_2-C29_2-C28_2	121.1(5)
O1S_2-Li1_2-C4_2	142.3(5)	O1S_2-Li1_2-C3_2	147.2(5)
C4_2-Li1_2-C3_2	38.3(2)	O1S_2-Li1_2-C5_2	138.6(5)
C4_2-Li1_2-C5_2	38.3(2)	C3_2-Li1_2-C5_2	66.6(3)
O1S_2-Li1_2-C2_2	147.3(5)	C4_2-Li1_2-C2_2	66.0(3)
C3_2-Li1_2-C2_2	37.6(2)	C5_2-Li1_2-C2_2	72.3(3)
O1S_2-Li1_2-Si1_2	145.2(4)	C4_2-Li1_2-Si1_2	66.3(2)
C3_2-Li1_2-Si1_2	65.9(2)	C5_2-Li1_2-Si1_2	43.8(2)
C2_2-Li1_2-Si1_2	43.0(2)	C2S_2-O1S_2-C5S_2	110.7(4)
C2S_2-O1S_2-Li1_2	124.3(4)	C5S_2-O1S_2-Li1_2	121.2(4)
O1S_2-C2S_2-C3S_2	104.3(5)	C4S_2-C3S_2-C2S_2	102.4(5)
C5S_2-C4S_2-C3S_2	102.9(5)	C4S_2-C5S_2-O1S_2	102.9(4)

Table S11. Torsion angles (°) to be deposited

C5_1-Si1_1-C2_1-C3_1	-7.3(3)	C6_1-Si1_1-C2_1-C3_1	-173.8(3)
Li2_1-Si1_1-C2_1-C3_1	-59.8(3)	C5_1-Si1_1-C2_1-Si2_1	-171.0(3)
C6_1-Si1_1-C2_1-Si2_1	22.6(4)	Li2_1-Si1_1-C2_1-Si2_1	136.5(4)
C5_1-Si1_1-C2_1-Li2_1	52.5(3)	C6_1-Si1_1-C2_1-Li2_1	-113.9(3)
C17_1-Si2_1-C2_1-C3_1	-37.2(4)	C16_1-Si2_1-C2_1-C3_1	-154.6(4)
C15_1-Si2_1-C2_1-C3_1	86.4(4)	C17_1-Si2_1-C2_1-Si1_1	122.9(3)
C16_1-Si2_1-C2_1-Si1_1	5.5(4)	C15_1-Si2_1-C2_1-Si1_1	-113.6(3)
C17_1-Si2_1-C2_1-Li2_1	-129.7(4)	C16_1-Si2_1-C2_1-Li2_1	112.9(4)
C15_1-Si2_1-C2_1-Li2_1	-6.2(5)	Si1_1-C2_1-C3_1-C4_1	4.2(5)
Si2_1-C2_1-C3_1-C4_1	167.7(3)	Li2_1-C2_1-C3_1-C4_1	-61.9(4)
Si1_1-C2_1-C3_1-C18_1	-172.8(3)	Si2_1-C2_1-C3_1-C18_1	-9.3(6)
Li2_1-C2_1-C3_1-C18_1	121.1(5)	Si1_1-C2_1-C3_1-Li2_1	66.1(3)

Si2_1-C2_1-C3_1-Li2_1	-130.4(4)	C2_1-C3_1-C4_1-C5_1	2.2(6)
C18_1-C3_1-C4_1-C5_1	179.2(4)	Li2_1-C3_1-C4_1-C5_1	-62.2(4)
C2_1-C3_1-C4_1-C24_1	-177.1(4)	C18_1-C3_1-C4_1-C24_1	-0.1(6)
Li2_1-C3_1-C4_1-C24_1	118.5(5)	C2_1-C3_1-C4_1-Li2_1	64.4(4)
C18_1-C3_1-C4_1-Li2_1	-118.6(5)	C3_1-C4_1-C5_1-Si1_1	-7.4(4)
C24_1-C4_1-C5_1-Si1_1	172.0(3)	Li2_1-C4_1-C5_1-Si1_1	-66.7(3)
C3_1-C4_1-C5_1-Si3_1	169.9(3)	C24_1-C4_1-C5_1-Si3_1	-10.8(6)
Li2_1-C4_1-C5_1-Si3_1	110.6(4)	C3_1-C4_1-C5_1-Li2_1	59.3(4)
C24_1-C4_1-C5_1-Li2_1	-121.4(4)	C2_1-Si1_1-C5_1-C4_1	8.4(3)
C6_1-Si1_1-C5_1-C4_1	175.5(3)	Li2_1-Si1_1-C5_1-C4_1	61.0(3)
C2_1-Si1_1-C5_1-Si3_1	-168.8(3)	C6_1-Si1_1-C5_1-Si3_1	-1.7(4)
Li2_1-Si1_1-C5_1-Si3_1	-116.2(4)	C2_1-Si1_1-C5_1-Li2_1	-52.5(3)
C6_1-Si1_1-C5_1-Li2_1	114.5(3)	C30_1-Si3_1-C5_1-C4_1	-37.0(5)
C32_1-Si3_1-C5_1-C4_1	-154.6(4)	C31_1-Si3_1-C5_1-C4_1	86.4(4)
C30_1-Si3_1-C5_1-Si1_1	139.6(3)	C32_1-Si3_1-C5_1-Si1_1	21.9(4)
C31_1-Si3_1-C5_1-Si1_1	-97.0(3)	C30_1-Si3_1-C5_1-Li2_1	45.4(4)
C32_1-Si3_1-C5_1-Li2_1	-72.3(4)	C31_1-Si3_1-C5_1-Li2_1	168.8(3)
C5_1-Si1_1-C6_1-C7_1	-110.7(4)	C2_1-Si1_1-C6_1-C7_1	51.9(5)
Li2_1-Si1_1-C6_1-C7_1	-30.4(5)	C5_1-Si1_1-C6_1-C11_1	65.7(4)
C2_1-Si1_1-C6_1-C11_1	-131.6(3)	Li2_1-Si1_1-C6_1-C11_1	146.1(4)
C11_1-C6_1-C7_1-C8_1	-0.9(6)	Si1_1-C6_1-C7_1-C8_1	175.6(3)
C11_1-C6_1-C7_1-C12_1	-178.2(4)	Si1_1-C6_1-C7_1-C12_1	-1.7(6)
C6_1-C7_1-C8_1-C9_1	-2.5(7)	C12_1-C7_1-C8_1-C9_1	174.9(4)
C7_1-C8_1-C9_1-C10_1	4.0(7)	C7_1-C8_1-C9_1-C13_1	-175.3(5)
C8_1-C9_1-C10_1-C11_1	-2.1(7)	C13_1-C9_1-C10_1-C11_1	177.2(5)
C9_1-C10_1-C11_1-C6_1	-1.2(6)	C9_1-C10_1-C11_1-C14_1	179.7(4)
C7_1-C6_1-C11_1-C10_1	2.7(6)	Si1_1-C6_1-C11_1-C10_1	-173.9(3)
C7_1-C6_1-C11_1-C14_1	-178.3(4)	Si1_1-C6_1-C11_1-C14_1	5.1(5)
C4_1-C3_1-C18_1-C19_1	115.6(5)	C2_1-C3_1-C18_1-C19_1	-67.6(6)
Li2_1-C3_1-C18_1-C19_1	26.7(6)	C4_1-C3_1-C18_1-C23_1	-66.0(6)
C2_1-C3_1-C18_1-C23_1	110.8(5)	Li2_1-C3_1-C18_1-C23_1	-154.8(4)
C23_1-C18_1-C19_1-C20_1	0.0(7)	C3_1-C18_1-C19_1-C20_1	178.5(4)
C18_1-C19_1-C20_1-C21_1	-0.5(7)	C19_1-C20_1-C21_1-C22_1	0.3(7)
C20_1-C21_1-C22_1-C23_1	0.3(7)	C21_1-C22_1-C23_1-C18_1	-0.8(7)
C19_1-C18_1-C23_1-C22_1	0.6(6)	C3_1-C18_1-C23_1-C22_1	-177.9(4)
C3_1-C4_1-C24_1-C25_1	-62.2(6)	C5_1-C4_1-C24_1-C25_1	118.5(5)
Li2_1-C4_1-C24_1-C25_1	25.6(7)	C3_1-C4_1-C24_1-C29_1	122.4(5)
C5_1-C4_1-C24_1-C29_1	-56.9(6)	Li2_1-C4_1-C24_1-C29_1	-149.8(4)
C29_1-C24_1-C25_1-C26_1	3.1(7)	C4_1-C24_1-C25_1-C26_1	-172.4(4)
C24_1-C25_1-C26_1-C27_1	-1.3(7)	C25_1-C26_1-C27_1-C28_1	-0.8(8)
C26_1-C27_1-C28_1-C29_1	0.9(8)	C27_1-C28_1-C29_1-C24_1	1.0(7)
C25_1-C24_1-C29_1-C28_1	-2.9(7)	C4_1-C24_1-C29_1-C28_1	172.8(4)
C3_1-Li2_1-O1S_1-C5S_1	-145.4(7)	C4_1-Li2_1-O1S_1-C5S_1	149.5(8)
C5_1-Li2_1-O1S_1-C5S_1	77(1)	C2_1-Li2_1-O1S_1-C5S_1	-85.0(8)
Si1_1-Li2_1-O1S_1-C5S_1	-10(1)	C3_1-Li2_1-O1S_1-C2S_1	18(1)
C4_1-Li2_1-O1S_1-C2S_1	-47(1)	C5_1-Li2_1-O1S_1-C2S_1	-119.2(8)
C2_1-Li2_1-O1S_1-C2S_1	78.4(8)	Si1_1-Li2_1-O1S_1-C2S_1	153.8(7)
C5S_1-O1S_1-C2S_1-C3S_1	-17.3(7)	Li2_1-O1S_1-C2S_1-C3S_1	176.9(6)
O1S_1-C2S_1-C3S_1-C4S_1	5.7(8)	C2S_1-C3S_1-C4S_1-C5S_1	8(1)
C2S_1-O1S_1-C5S_1-C4S_1	22.2(7)	Li2_1-O1S_1-C5S_1-C4S_1	-172.2(6)

C3S_1-C4S_1-C5S_1-O1S_1	-18.1(9)	C5_2-Si1_2-C2_2-C3_2	-8.0(3)
C6_2-Si1_2-C2_2-C3_2	-169.1(3)	Li1_2-Si1_2-C2_2-C3_2	-58.7(3)
C5_2-Si1_2-C2_2-Si2_2	-173.3(3)	C6_2-Si1_2-C2_2-Si2_2	25.6(4)
Li1_2-Si1_2-C2_2-Si2_2	135.9(4)	C5_2-Si1_2-C2_2-Li1_2	50.8(3)
C6_2-Si1_2-C2_2-Li1_2	-110.3(3)	C17_2-Si2_2-C2_2-C3_2	-35.7(5)
C16_2-Si2_2-C2_2-C3_2	-154.3(4)	C15_2-Si2_2-C2_2-C3_2	86.9(4)
C17_2-Si2_2-C2_2-Si1_2	126.6(3)	C16_2-Si2_2-C2_2-Si1_2	8.0(4)
C15_2-Si2_2-C2_2-Si1_2	-110.7(4)	C17_2-Si2_2-C2_2-Li1_2	-125.6(4)
C16_2-Si2_2-C2_2-Li1_2	115.8(4)	C15_2-Si2_2-C2_2-Li1_2	-2.9(5)
Si1_2-C2_2-C3_2-C4_2	4.9(4)	Si2_2-C2_2-C3_2-C4_2	170.6(3)
Li1_2-C2_2-C3_2-C4_2	-60.1(4)	Si1_2-C2_2-C3_2-C18_2	-173.0(3)
Si2_2-C2_2-C3_2-C18_2	-7.2(6)	Li1_2-C2_2-C3_2-C18_2	122.1(5)
Si1_2-C2_2-C3_2-Li1_2	65.0(3)	Si2_2-C2_2-C3_2-Li1_2	-129.3(4)
C2_2-C3_2-C4_2-C5_2	1.8(6)	C18_2-C3_2-C4_2-C5_2	179.6(4)
Li1_2-C3_2-C4_2-C5_2	-61.9(4)	C2_2-C3_2-C4_2-C24_2	-177.3(4)
C18_2-C3_2-C4_2-C24_2	0.5(6)	Li1_2-C3_2-C4_2-C24_2	119.0(4)
C2_2-C3_2-C4_2-Li1_2	63.7(4)	C18_2-C3_2-C4_2-Li1_2	-118.5(5)
C3_2-C4_2-C5_2-Si1_2	-7.4(4)	C24_2-C4_2-C5_2-Si1_2	171.7(3)
Li1_2-C4_2-C5_2-Si1_2	-67.3(3)	C3_2-C4_2-C5_2-Si3_2	175.6(3)
C24_2-C4_2-C5_2-Si3_2	-5.3(6)	Li1_2-C4_2-C5_2-Si3_2	115.7(4)
C3_2-C4_2-C5_2-Li1_2	59.9(4)	C24_2-C4_2-C5_2-Li1_2	-121.0(5)
C2_2-Si1_2-C5_2-C4_2	8.9(3)	C6_2-Si1_2-C5_2-C4_2	169.7(3)
Li1_2-Si1_2-C5_2-C4_2	61.1(3)	C2_2-Si1_2-C5_2-Si3_2	-174.0(3)
C6_2-Si1_2-C5_2-Si3_2	-13.2(4)	Li1_2-Si1_2-C5_2-Si3_2	-121.9(4)
C2_2-Si1_2-C5_2-Li1_2	-52.2(3)	C6_2-Si1_2-C5_2-Li1_2	108.6(3)
C30_2-Si3_2-C5_2-C4_2	-33.5(5)	C31_2-Si3_2-C5_2-C4_2	91.5(4)
C32_2-Si3_2-C5_2-C4_2	-152.8(4)	C30_2-Si3_2-C5_2-Si1_2	150.2(3)
C31_2-Si3_2-C5_2-Si1_2	-84.8(3)	C32_2-Si3_2-C5_2-Si1_2	30.9(4)
C30_2-Si3_2-C5_2-Li1_2	52.8(4)	C31_2-Si3_2-C5_2-Li1_2	177.8(4)
C32_2-Si3_2-C5_2-Li1_2	-66.5(4)	C2_2-Si1_2-C6_2-C7_2	76.7(4)
C5_2-Si1_2-C6_2-C7_2	-78.6(4)	Li1_2-Si1_2-C6_2-C7_2	-2.1(5)
C2_2-Si1_2-C6_2-C11_2	-103.6(4)	C5_2-Si1_2-C6_2-C11_2	101.1(4)
Li1_2-Si1_2-C6_2-C11_2	177.5(4)	C11_2-C6_2-C7_2-C8_2	-0.2(6)
Si1_2-C6_2-C7_2-C8_2	179.5(3)	C11_2-C6_2-C7_2-C12_2	178.9(4)
Si1_2-C6_2-C7_2-C12_2	-1.5(6)	C6_2-C7_2-C8_2-C9_2	0.0(7)
C12_2-C7_2-C8_2-C9_2	-179.1(4)	C7_2-C8_2-C9_2-C10_2	0.0(7)
C7_2-C8_2-C9_2-C13_2	177.7(4)	C8_2-C9_2-C10_2-C11_2	0.3(7)
C13_2-C9_2-C10_2-C11_2	-177.4(4)	C9_2-C10_2-C11_2-C6_2	-0.5(7)
C9_2-C10_2-C11_2-C14_2	178.6(4)	C7_2-C6_2-C11_2-C10_2	0.4(6)
Si1_2-C6_2-C11_2-C10_2	-179.2(3)	C7_2-C6_2-C11_2-C14_2	-178.7(4)
Si1_2-C6_2-C11_2-C14_2	1.7(6)	C4_2-C3_2-C18_2-C23_2	-68.3(6)
C2_2-C3_2-C18_2-C23_2	109.4(5)	Li1_2-C3_2-C18_2-C23_2	-155.5(4)
C4_2-C3_2-C18_2-C19_2	112.7(5)	C2_2-C3_2-C18_2-C19_2	-69.6(6)
Li1_2-C3_2-C18_2-C19_2	25.5(6)	C23_2-C18_2-C19_2-C20_2	1.1(7)
C3_2-C18_2-C19_2-C20_2	-179.8(4)	C18_2-C19_2-C20_2-C21_2	-0.7(7)
C19_2-C20_2-C21_2-C22_2	0.2(8)	C20_2-C21_2-C22_2-C23_2	0.0(8)
C19_2-C18_2-C23_2-C22_2	-0.9(7)	C3_2-C18_2-C23_2-C22_2	-180.0(4)
C21_2-C22_2-C23_2-C18_2	0.4(7)	C3_2-C4_2-C24_2-C29_2	122.6(5)
C5_2-C4_2-C24_2-C29_2	-56.5(6)	Li1_2-C4_2-C24_2-C29_2	-149.8(4)
C3_2-C4_2-C24_2-C25_2	-56.8(6)	C5_2-C4_2-C24_2-C25_2	124.1(5)

Li1_2-C4_2-C24_2-C25_2	30.8(6)	C29_2-C24_2-C25_2-C26_2	0.9(7)
C4_2-C24_2-C25_2-C26_2	-179.6(4)	C24_2-C25_2-C26_2-C27_2	0.6(7)
C25_2-C26_2-C27_2-C28_2	-1.1(8)	C26_2-C27_2-C28_2-C29_2	0.2(8)
C25_2-C24_2-C29_2-C28_2	-1.9(7)	C4_2-C24_2-C29_2-C28_2	178.7(4)
C27_2-C28_2-C29_2-C24_2	1.4(7)	C4_2-Li1_2-O1S_2-C2S_2	70.8(9)
C3_2-Li1_2-O1S_2-C2S_2	139.6(8)	C5_2-Li1_2-O1S_2-C2S_2	9.1(9)
C2_2-Li1_2-O1S_2-C2S_2	-147.2(8)	Si1_2-Li1_2-O1S_2-C2S_2	-64.5(9)
C4_2-Li1_2-O1S_2-C5S_2	-133.2(7)	C3_2-Li1_2-O1S_2-C5S_2	-64(1)
C5_2-Li1_2-O1S_2-C5S_2	165.1(6)	C2_2-Li1_2-O1S_2-C5S_2	9(1)
Si1_2-Li1_2-O1S_2-C5S_2	91.4(8)	C5S_2-O1S_2-C2S_2-C3S_2	-12.4(6)
Li1_2-O1S_2-C2S_2-C3S_2	145.8(5)	O1S_2-C2S_2-C3S_2-C4S_2	33.0(6)
C2S_2-C3S_2-C4S_2-C5S_2	-41.2(6)	C3S_2-C4S_2-C5S_2-O1S_2	33.4(6)
C2S_2-O1S_2-C5S_2-C4S_2	-13.2(6)	Li1_2-O1S_2-C5S_2-C4S_2	-172.2(5)