

Supplementary Information for

**Inorganic salt-assisted assembly of anionic  $\pi$ -conjugated rings enabling  $^7\text{Li}$  NMR-based evaluation of antiaromaticity**

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## 1. General considerations

All manipulations were carried out under an argon atmosphere by using standard Schlenk techniques or a glovebox unless otherwise stated. Et<sub>2</sub>O, THF, toluene, toluene-*d*<sub>8</sub>, and THF-*d*<sub>8</sub> were distilled over potassium mirror. Me<sub>2</sub>SiCl<sub>2</sub> was purchased from Tokyo Chemical Industry (TCI). (*Z*)-2,2'-Dibromostilbene was synthesized according to the literature.<sup>[1]</sup> <sup>1</sup>H (500 MHz), <sup>13</sup>C{<sup>1</sup>H} (126 MHz), <sup>7</sup>Li{<sup>1</sup>H} (194 MHz), and <sup>29</sup>Si{<sup>1</sup>H} (99 MHz) NMR spectra were recorded on a JEOL ECZ-500 spectrometer at 20°C unless otherwise stated. Chemical shifts are reported in δ and referenced to residual <sup>1</sup>H and <sup>13</sup>C signals of deuterated solvents as internal standards or to the <sup>7</sup>Li{<sup>1</sup>H} and the <sup>29</sup>Si{<sup>1</sup>H} NMR signal of LiCl in D<sub>2</sub>O (δ = 0.00) and SiMe<sub>4</sub> in CDCl<sub>3</sub> (δ = 0.00), respectively, as external standards. Elemental analyses were performed on a Perkin Elmer 2400 series II CHN analyzer.

## X-ray diffraction analysis

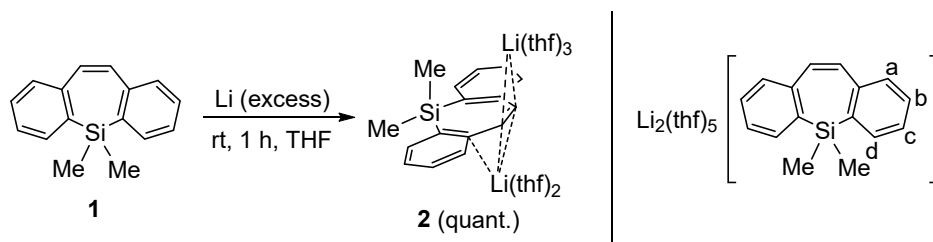
Diffraction data for **2**, **3-THF**, and **3-Et<sub>2</sub>O** were collected on a VariMax Saturn CCD diffractometer with graphite-monochromated Mo Kα radiation (λ = 0.71075 Å) at -180 °C. Intensity data were corrected for Lorenz-polarization effects and for empirical absorption (REQAB).<sup>[2]</sup> All calculations were performed using the CrystalStructure<sup>[3]</sup> crystallographic software package except for refinements, which were performed using SHELXL-2018/3.<sup>[4]</sup> The positions of the non-hydrogen atoms were determined by SHELXT.<sup>[5]</sup> All non-hydrogen atoms were refined on *F*<sub>o</sub><sup>2</sup> anisotropically by full-matrix least-square techniques. All hydrogen atoms were placed at the calculated positions with fixed isotropic parameters.

## Theoretical studies

Theoretical calculations were performed by using the *Gaussian* 16 Rev.C.<sup>[6]</sup> Structural optimization and NICS calculations were performed at the B3LYP<sup>[7]</sup> level of theory using 6-31+G(d)<sup>[8]</sup> basis sets, whereas <sup>1</sup>H and <sup>7</sup>Li NMR chemical shifts at the B3LYP/6-311+G(2d,p) level. The structural optimization has been carried out for **1**, **1<sup>2-</sup>**, **2**, and **3'**. The optimized structures of **2** and **3'** are in good agreement with the corresponding X-ray structures. All local minima were confirmed by the vibrational frequency calculations with zero imaginary frequency. The NICS values for **1** and **1<sup>2-</sup>**, and molecular orbitals for **1** and **2** and **3'** were calculated using the optimized structures, while the NICS values for 3,7-Bis([2,2'-bithiophen]-5-yl)-5,5-dimethyl-5*H*-dibenzo[*b,f*]silepin **A**,<sup>[9]</sup> **3-THF**, and **(1<sup>2-</sup>)<sub>3</sub>** were obtained by using the X-ray structures. The <sup>7</sup>Li NMR chemical shifts for the model compound [(**1**)<sub>3</sub>(Li<sub>9</sub>O<sub>2</sub>)]<sup>5+</sup> was calculated using the optimized structure of **3'**.

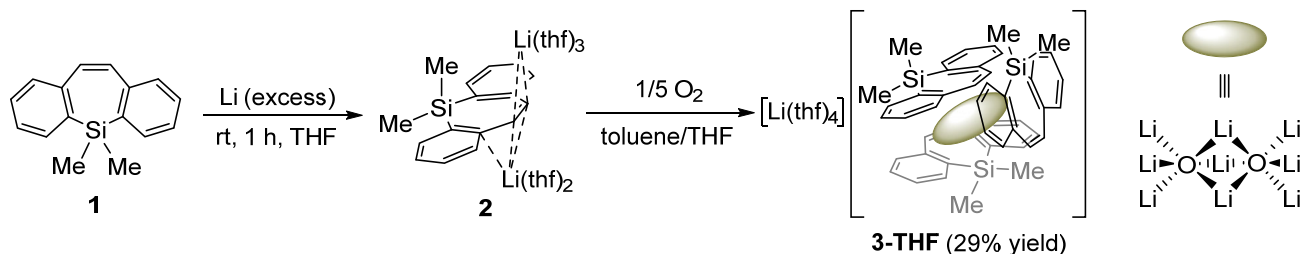
## 2. Synthesis and analytical data for the new compounds

### Synthesis of lithium salt of 5,5-dimethyldibenzo[*b,f*]silepinyll dianion **2**.



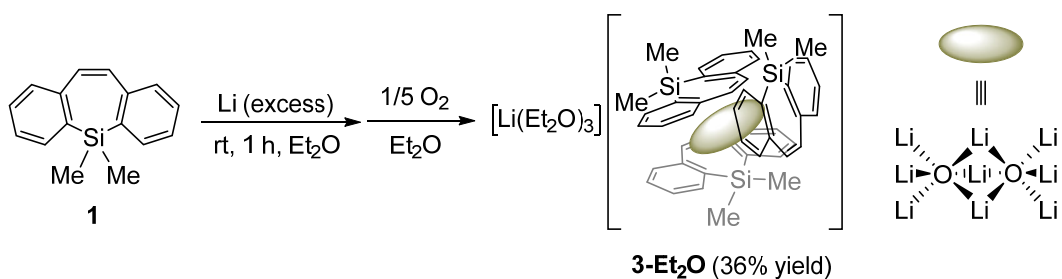
Lithium (16.0 mg, 2.30 mmol) was added to a solution of **1**<sup>8</sup> (50.0 mg, 0.212 mmol) in THF (2 mL) at room temperature. After 1 h, lithium was removed, and the solvent was removed in vacuo to yield **2** as a black-purple powder (130.3 mg, 0.213 mmol, quant.). m.p. > 82 °C (decomp.); <sup>1</sup>H NMR (500 MHz, THF-*d*<sub>8</sub>): δ = 5.80 (dd, <sup>3</sup>J<sub>H-H</sub> = 7 Hz, <sup>4</sup>J<sub>H-H</sub> = 1 Hz, 2H, *fused benzene-d*), 5.29 (ddd, <sup>3</sup>J<sub>H-H</sub> = 8 Hz, <sup>3</sup>J<sub>H-H</sub> = 6 Hz, <sup>4</sup>J<sub>H-H</sub> = 1 Hz, 2H, *fused benzene-b*), 4.92 (d, <sup>3</sup>J<sub>H-H</sub> = 9 Hz, 2H, *fused benzene-a*), 4.22 (t, <sup>3</sup>J<sub>H-H</sub> = 7 Hz, 2H, *fused benzene-c*), 2.81 (s, 2H, *vinyl*), -0.04 (s, 6H, *Me*); <sup>13</sup>C{<sup>1</sup>H} NMR (126 MHz, THF-*d*<sub>8</sub>): δ = 146.3 (*C*<sub>β</sub>), 138.4 (*fused benzene-d*), 127.7 (*fused benzene-b*), 119.1 (*fused benzene-a*), 109.3 (*C*<sub>α</sub>), 96.3 (*fused benzene-c*), 75.9 (*vinyl*), 0.0 (*Me*); <sup>7</sup>Li{<sup>1</sup>H} NMR (194 MHz, THF-*d*<sub>8</sub>): δ = 0.29; <sup>29</sup>Si{<sup>1</sup>H} NMR (99 MHz, THF-*d*<sub>8</sub>): δ = -24.7. Although satisfactory elemental analysis data could not be obtained because of its instability towards moisture and oxygen, the high purity of the sample is guaranteed by the NMR spectra (Figures S9–12).

### Synthesis of trimer **3**-THF.



Lithium (16.0 mg, 2.30 mmol) was added to a solution of **1** (50.1 mg, 0.212 mmol) in THF (2 mL) at room temperature. After 1 h, the solvent was removed in vacuo, and the resulting black-purple powder was dissolved in a mixed solvent of toluene (6 mL) and THF (0.06 mL). The solution and the lithium were charged into a 100 mL Schlenk flask, then O<sub>2</sub> gas (0.2 mL, 0.008 mmol at 1 atm, 298 K) was injected to the flask every 10–12 h for five times (total O<sub>2</sub> amount: 1.0 mL, 0.04 mmol at 1 atm, 298 K). Standing the solution at room temperature deposited black crystals of **3-THF** (23.3 mg, 0.0205 mmol, 29% yield). m.p. > 156 °C (decomp.); <sup>1</sup>H NMR (500 MHz, toluene-*d*<sub>8</sub>): δ = 5.93 (dd, <sup>3</sup>J<sub>H-H</sub> = 7 Hz, <sup>4</sup>J<sub>H-H</sub> = 1 Hz, 6H, *Ar*), 5.81 (brt, 6H, *Ar*), 4.89 (brs, 6H, *Ar*), 4.09 (t, <sup>3</sup>J<sub>H-H</sub> = 6 Hz, 6H, *Ar*), 3.52 (brs, 6H, *vinyl*), 1.27 (brs, 9H, *Me*), 0.09 (brs, 9H, *Me*); <sup>7</sup>Li{<sup>1</sup>H} NMR (194 MHz, toluene-*d*<sub>8</sub>): δ = 6.29 (3Li, *middle of the Li<sub>9</sub>O<sub>2</sub> cluster*), 4.44 (6Li, *edge of the Li<sub>9</sub>O<sub>2</sub> cluster*), 0.62 (1Li, *solvent separated lithium cation*). Satisfactory elemental analysis data could not be obtained because of its instability towards moisture and oxygen. <sup>13</sup>C{<sup>1</sup>H} and <sup>29</sup>Si{<sup>1</sup>H} NMR in toluene-*d*<sub>8</sub> could not be measured due to its low solubility. The <sup>1</sup>H, <sup>13</sup>C{<sup>1</sup>H}, and <sup>7</sup>Li{<sup>1</sup>H} NMR spectra of **3-THF** in THF-*d*<sub>8</sub> are identical to those of **2**, suggesting **3-THF** is dissociated into three dibenzosilepinyll dianions in THF solution.

### Synthesis of trimer 3-Et<sub>2</sub>O.



Lithium (19.7 mg, 2.83 mmol) was added to a solution of **1** (50.9 mg, 0.215 mmol) in Et<sub>2</sub>O (2 mL) at room temperature. After 1 h, the solution and the lithium were charged into a 100 mL Schlenk flask, then O<sub>2</sub> gas (0.2 mL, 0.008 mmol at 1 atm, 298 K) was injected to the flask every 10–12 h for five times (total O<sub>2</sub> amount: 1.0 mL, 0.04 mmol at 1 atm, 298 K). Standing the solution at room temperature deposited black crystals of **3-Et<sub>2</sub>O** (26.5 mg, 0.0257 mmol, 36% yield). The crystals are insoluble in C<sub>6</sub>D<sub>6</sub>. The <sup>1</sup>H, <sup>13</sup>C{<sup>1</sup>H}, and <sup>7</sup>Li{<sup>1</sup>H} NMR spectra of **3-Et<sub>2</sub>O** in THF-*d*<sub>8</sub> are identical to those of **2**, suggesting **3-Et<sub>2</sub>O** is dissociated into three dibenzosilolepinyne dianions in THF solution.

### 3. Crystal structure of 3-Et<sub>2</sub>O

Compound 3-Et<sub>2</sub>O crystallizes as trigonal with space group *R3c* and has a three-fold rotation axis. Metrical parameters of 3-Et<sub>2</sub>O are similar to those of 3-THF.

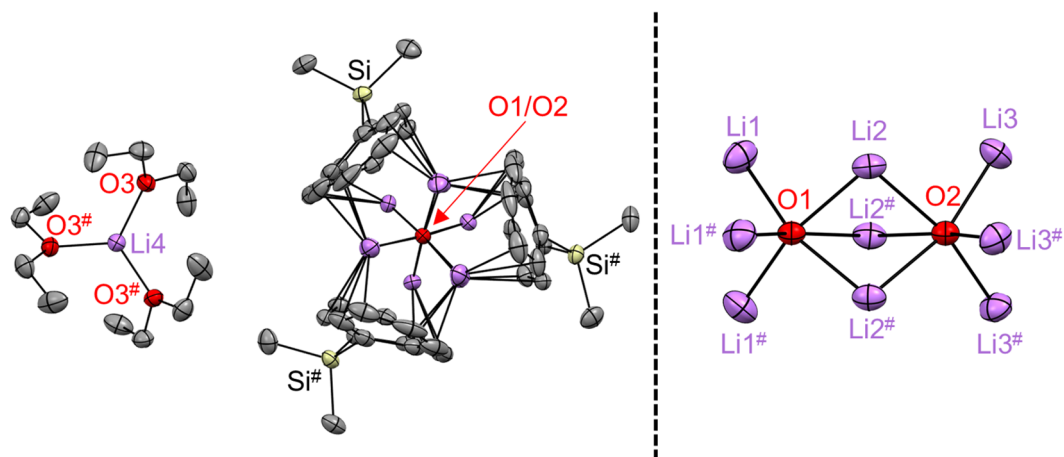
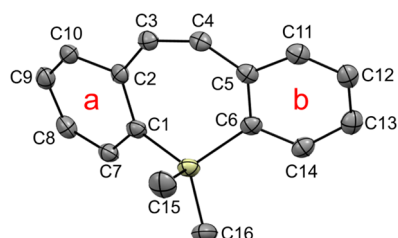


Figure S1. The crystal structure of 3-Et<sub>2</sub>O.

#### 4. Bond lengths of a selected neutral silepin **A**, **2**, and **3-THF**, and the optimized structures

**Table S1.** Comparison of the Si–C and C–C bond lengths (Å) of **A**, **2**, and **3-THF**.

	Selected neutral silepin <b>A</b> <sup>[9]</sup>	<b>2</b>	<b>3-THF</b>
Si–C1/Si–C6	1.872(3)/1.874(3)	1.848(4)/1.864(4)	1.868(3)/1.871(3)
Si–C15/Si–C16	1.860(3)/1.865(3)	1.884(4)/1.887(4)	1.878(3)/1.874(3)
C1–C2/C5–C6	1.404(4)/1.413(4)	1.474(5)/1.453(5)	1.487(3)/1.465(3)
C2–C3/C4–C5	1.470(4)/1.413(4)	1.404(5)/1.410(5)	1.395(3)/1.405(3)
C3–C4	1.343(4)	1.465(5)	1.461(3)
C1–C7/C6–C14	1.402(4)/1.391(4)	1.407(5)/1.388(5)	1.397(3)/1.409(3)
C7–C8/C14–C13	1.396(4)/1.406(4)	1.384(6)/1.393(5)	1.415(4)/1.405(4)
C8–C9/C13–C12	1.393(4)/1.397(4)	1.402(6)/1.412(5)	1.424(4)/1.416(4)
C9–C10/C12–C11	1.371(4)/1.377(4)	1.368(6)/1.361(5)	1.371(4)/1.379(4)
C10–C2/C5–C11	1.406(4)/1.401(4)	1.447(5)/1.446(5)	1.472(3)/1.461(4)

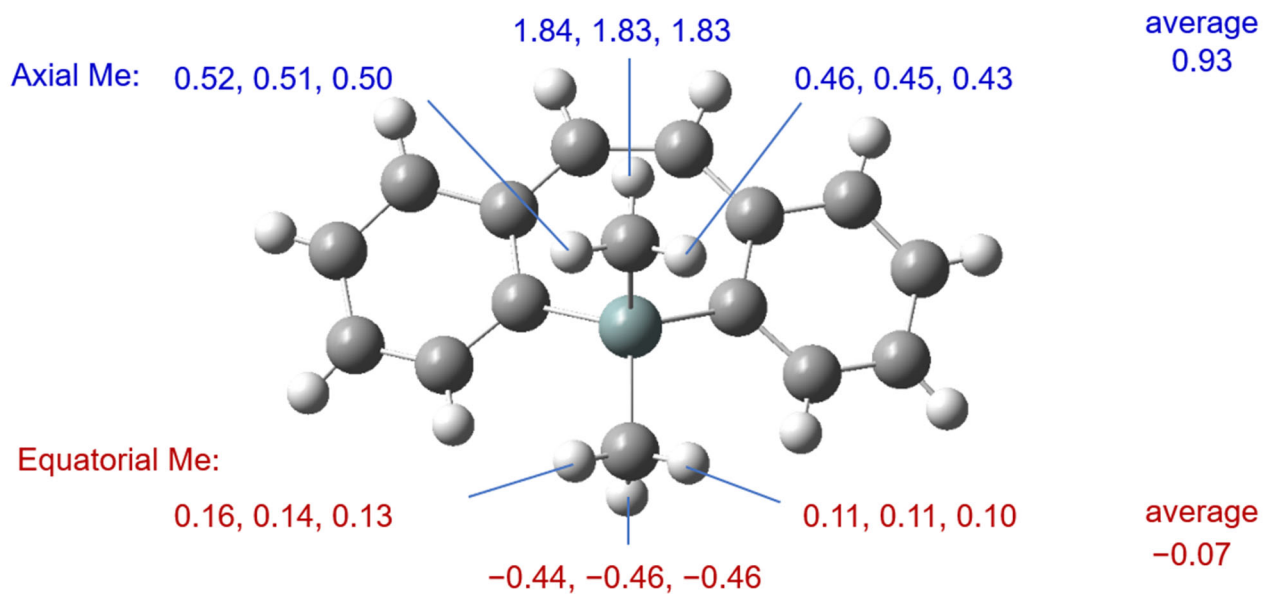


**Table S2.** Si–C<sub>α</sub> and Si–Me bonds (Å) in the optimized structures (**1**, **1**<sup>2-</sup>, **2** and **3**<sup>'</sup>).

	<b>1</b>	<b>1</b> <sup>2-</sup>	<b>2</b>	<b>3</b> <sup>'</sup>
Si–C <sub>endo</sub>	1.886, 1.886	1.872, 1.878	1.876, 1.878	1.876, 1.876
Si–Me	1.894, 1.893	1.917, 1.921	1.908, 1.914	1.901, 1.901

### 5. Calculated $^1\text{H}$ NMR chemical shifts of $\mathbf{3}'$

The  $^1\text{H}$  NMR chemical shifts of the Me groups in  $\mathbf{3}'$  calculated by GIAO method (B3LYP/6-311+G(2d,p) level of theory) are shown in Figure S2 (the chemical shift of TMS calculated at the same level of theory was set as 0 ppm). The average chemical shift for the axial Me protons (0.93 ppm) are in lower field by 1 ppm relative to that for the equatorial Me (-0.07 ppm). Thus, the experimental  $^1\text{H}$  NMR signals of  $\delta$  1.27 and 0.09 are assignable to the axial and equatorial Me groups, respectively. The downfield shifts of the axial Me can be reasonably explained by the paratropic ring current.



**Figure S2.** Calculated chemical shifts [ppm] of the Me groups in  $\mathbf{3}'$  (blue: axial Me, red: equatorial Me).

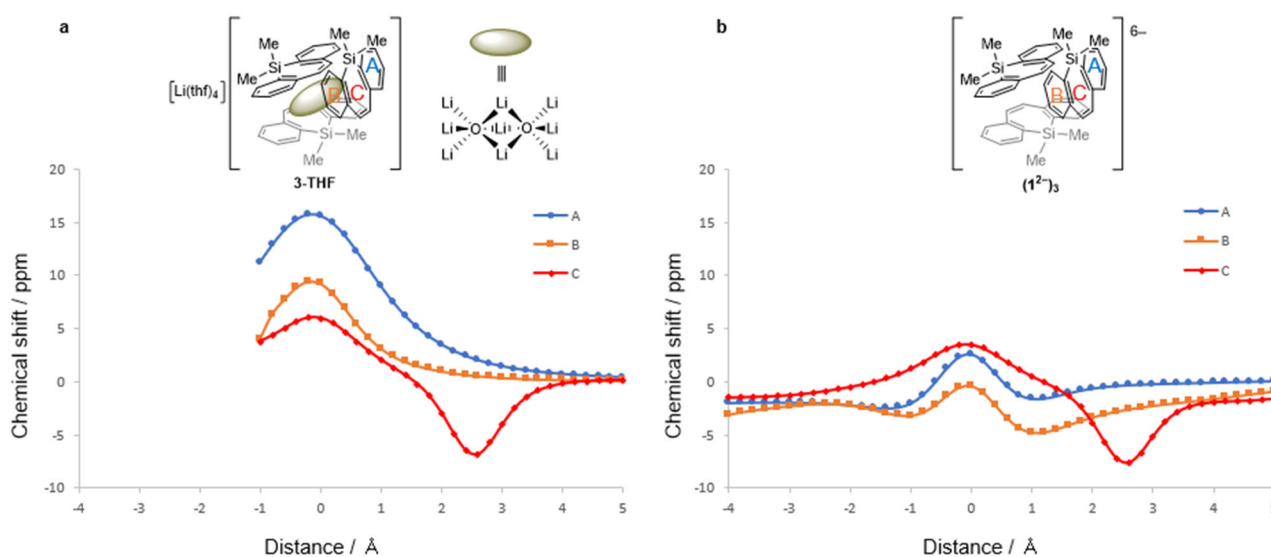
## 6. NICS calculations for **1**, **1<sup>2-</sup>**, **3-THF**, and **(1<sup>2-</sup>)<sub>3</sub>**

The NICS<sub>iso</sub>(0) values of **1**, lithium-free dianion **1<sup>2-</sup>**, and **3-THF** are shown in Table S2. The silepin ring and the benzene rings of neutral species **1** is nonaromatic and aromatic, respectively. In contrast, large positive NICS values of **1<sup>2-</sup>** are indicative of its antiaromaticity. The NICS values of **3-THF** are also positive and large, which is in line with the downfield shifted <sup>7</sup>Li{<sup>1</sup>H} NMR signals.

**Table S3.** NICS<sub>iso</sub>(0) values for **1**, **1<sup>2-</sup>**, and **3-THF**.

	NICS <sub>iso</sub> (0) / ppm	
	six-membered rings	seven-membered ring
<b>1</b>	-8.8/-8.8	1.7
<b>1<sup>2-</sup></b>	12.1/10.9	5.1
<b>3-THF</b>	15.6/9.2	6.0

The NICS<sub>iso</sub>-scan curves for lithium-free model structure **(1<sup>2-</sup>)<sub>3</sub>** are also shown in Figure S3. All NICS<sub>iso</sub> values of **(1<sup>2-</sup>)<sub>3</sub>** were calculated to be small (less than 5 ppm for NICS<sub>iso</sub>(0)). These NICS<sub>iso</sub> values smaller than those of **3-THF** indicate that the presence of the Li<sub>9</sub>O<sub>2</sub> core is essential for the antiaromatic character of the trimeric cluster, the reason for which is not clear at this point.

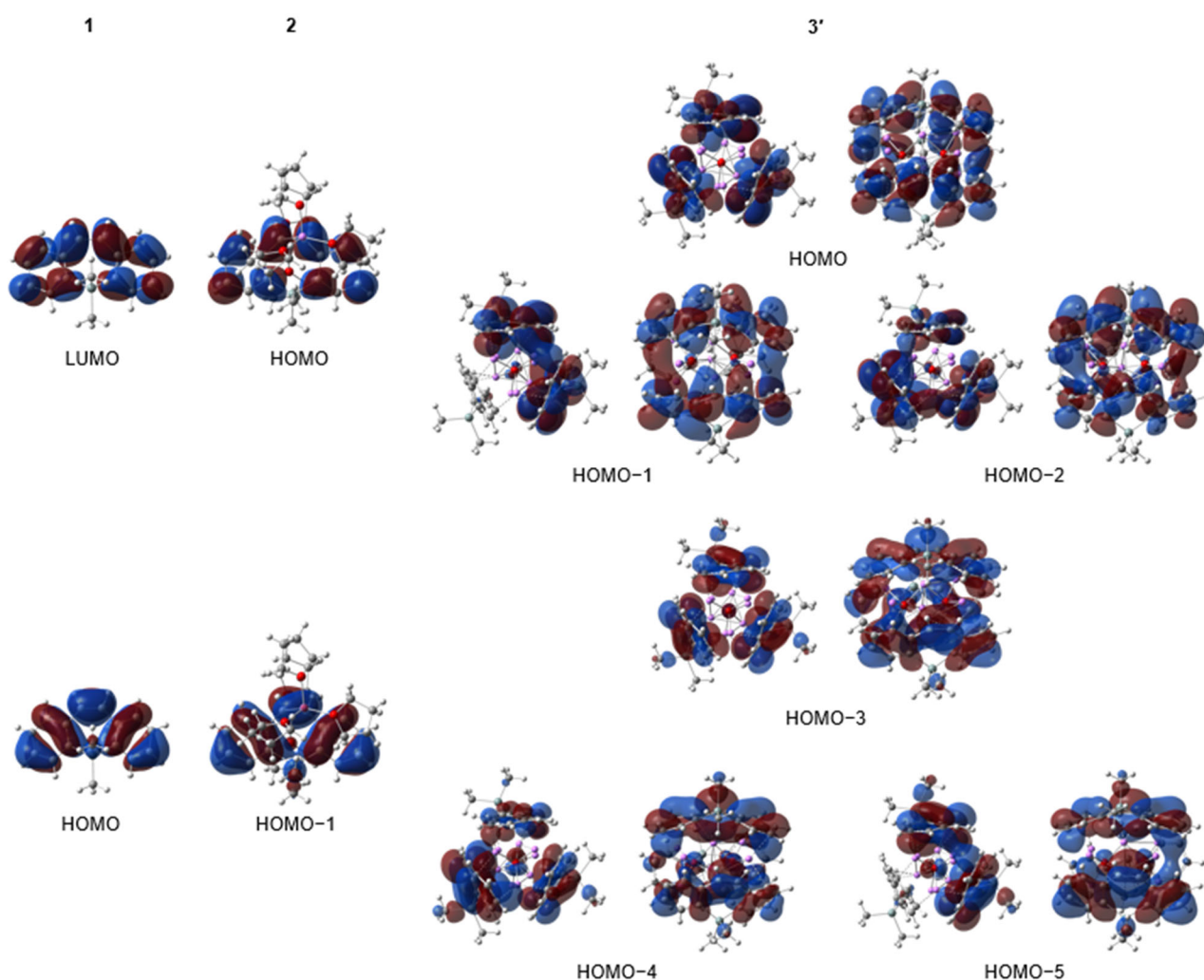


**Figure S3.** NICS<sub>iso</sub>-scan curves for a) **3-THF**, and b) **(1<sup>2-</sup>)<sub>3</sub>**.



## 7. Frontier molecular orbitals of **1**, **2**, and **3'** and their energy levels

Frontier molecular orbitals (MOs) of **1**, **2** and **3'** are shown in Figure 4S, and their energy levels in Figure S5. The LUMO and HOMO of **1** are similar to the HOMO and HOMO-1 of **2**, respectively, as expected from the fact that dilithiosilepin **2** is a doubly-reduced form of **1**. Since **3'** can be regarded as a trimeric cluster of **2**, the HOMO, HOMO-1, HOMO-2 in **3'** correspond to the HOMO of **2**, and the HOMO-3, HOMO-4, HOMO-5 to the HOMO-1 of **2**. Bonding interactions between the silepin rings are found only in the HOMO-1, HOMO-2, HOMO-4, and HOMO-5, but not in the HOMO nor HOMO-3, which led to the two sets of degenerated MO pairs (HOMO-1/HOMO-2, and HOMO-4/HOMO-5).



**Figure S4.** Frontier molecular orbitals of **1**, **2**, and **3'** (isovalues: 0.02 for **1**, **2**; 0.015 for **3'**).

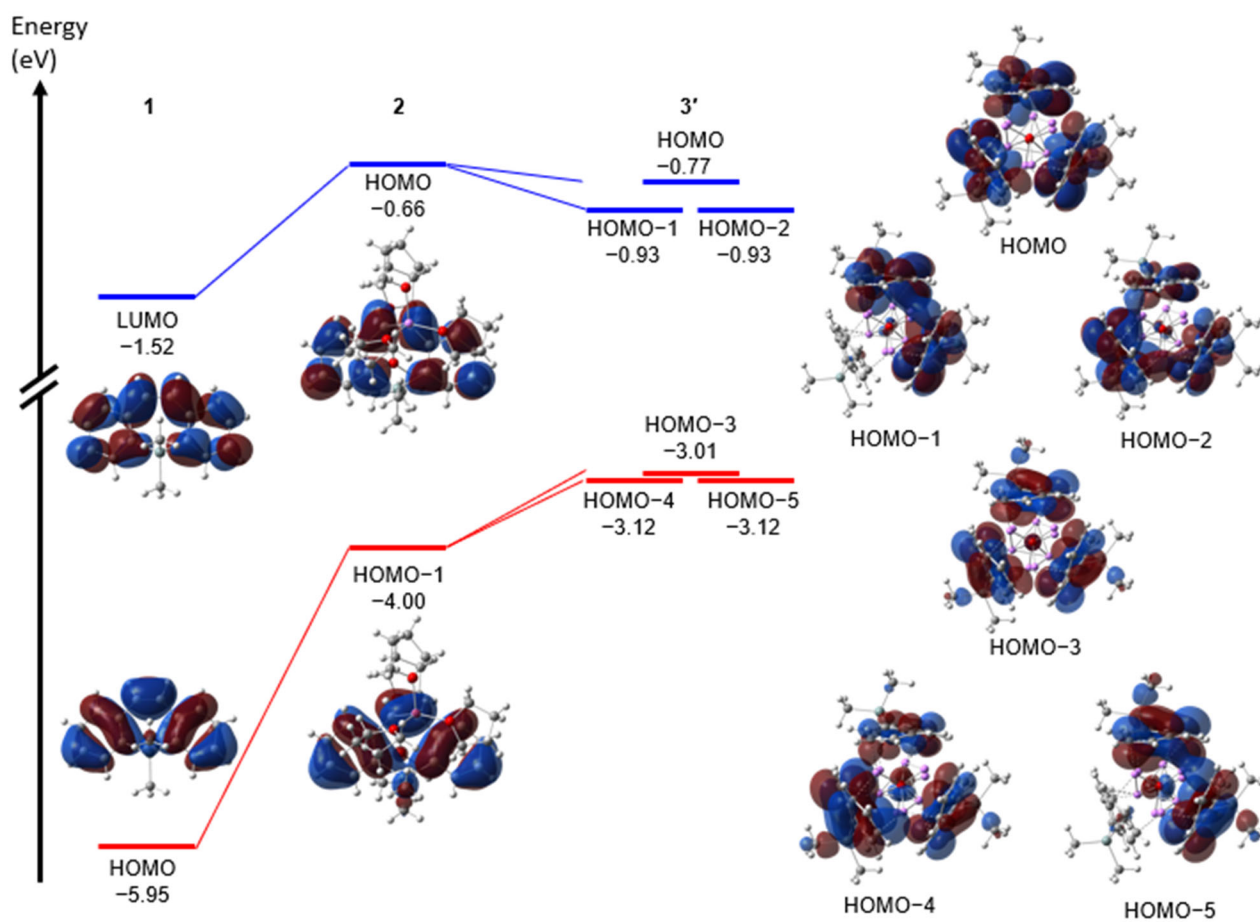


Figure S5. Energy diagrams for frontier molecular orbitals of **1**, **2**, and **3'** (isovalues: 0.02 for **1**, **2**; 0.015 for **3'**).

## 8. X-ray crystallographic data for 2, 3-THF, and 3-Et<sub>2</sub>O.

**Table S4.** X-ray crystallographic data for 2, 3-THF, and 3-Et<sub>2</sub>O.

	<b>2</b>	<b>3-THF</b>	<b>3-Et<sub>2</sub>O</b>
CCDC	2191231	2191232	2191233
formula	C <sub>36</sub> H <sub>56</sub> Li <sub>2</sub> O <sub>5</sub> Si	C <sub>68</sub> H <sub>85</sub> Li <sub>10</sub> O <sub>5</sub> Si <sub>3</sub>	C <sub>60</sub> H <sub>78</sub> Li <sub>10</sub> O <sub>5</sub> Si <sub>3</sub>
fw	610.77	1152.02	1032.89
crystal size	0.21 × 0.2 × 0.12	0.15 × 0.12 × 0.05	0.18 × 0.16 × 0.13
crystal system	monoclinic	triclinic	trigonal
space group	<i>Pc</i>	<i>P</i> -1	<i>R3c</i>
<i>a</i> [Å]	9.332(3)	11.117(6)	15.249(4)
<i>b</i> [Å]	10.610(3)	15.204(8)	15.249(4)
<i>c</i> [Å]	17.742(5)	19.765(10)	44.207(11)
$\alpha$ [deg]	90	85.97(2)	90
$\beta$ [deg]	95.085(5)	79.66(2)	90
$\gamma$ [deg]	90	79.45(2)	120
<i>V</i> [Å <sup>3</sup> ]	1749.7(8)	3228(3)	8902(5)
<i>Z</i>	2	2	6
$\rho_{\text{calcd}}$ [g cm <sup>-3</sup> ]	1.159	1.185	1.156
<i>F</i> (000)	664	1226	3300
$\mu$ [cm <sup>-1</sup> ]	1.06	1.23	1.25
transmission factors range	0.8715 – 1	0.8544 – 1	0.8544 – 1
index range	-12 ≤ <i>h</i> ≤ 11 -13 ≤ <i>k</i> ≤ 13 -22 ≤ <i>l</i> ≤ 23	-13 ≤ <i>h</i> ≤ 14 -19 ≤ <i>k</i> ≤ 19 -25 ≤ <i>l</i> ≤ 25	-19 ≤ <i>h</i> ≤ 15 -19 ≤ <i>k</i> ≤ 19 -57 ≤ <i>l</i> ≤ 45
no. reflections	13870	26145	22798
unique ( <i>R</i> <sub>int</sub> )	6403 (0.0364)	14088 (0.0419)	4195 (0.0565)
<i>I</i> > 2 $\sigma$ ( <i>I</i> )	5102	9201	3660
no. parameters	400	792	239
<i>R</i> <sub>1</sub> ( <i>I</i> > 2 $\sigma$ ( <i>I</i> )) <sup>a</sup>	0.0515	0.0611	0.0513
<i>wR</i> <sub>2</sub> (all data) <sup>b</sup>	0.1280	0.1887	0.1340
GOF <sup>c</sup>	1.038	1.025	1.066
max diff peak / hole [e Å <sup>-3</sup> ]	0.54/-0.314	0.803/-0.601	0.521/-0.613

<sup>a</sup>  $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$ . <sup>b</sup>  $wR_2 = [\sum \{w(F_o^2 - F_c^2)^2\} / \sum w(F_o^2)^2]^{1/2}$ ,  $w = 1 / [\sigma^2 F_o^2 + (aP)^2 + bP]$  (*a* and *b* are constants suggested by the refinement program;  $P = [\max(F_o^2, 0) + 2F_c^2] / 3$ ). <sup>c</sup>  $GOF = [\sum w(F_o^2 - F_c^2)^2 / (N_{\text{obs}} - N_{\text{params}})]^{1/2}$ .

## 9. NMR spectra for 1, 2, and 3-THF

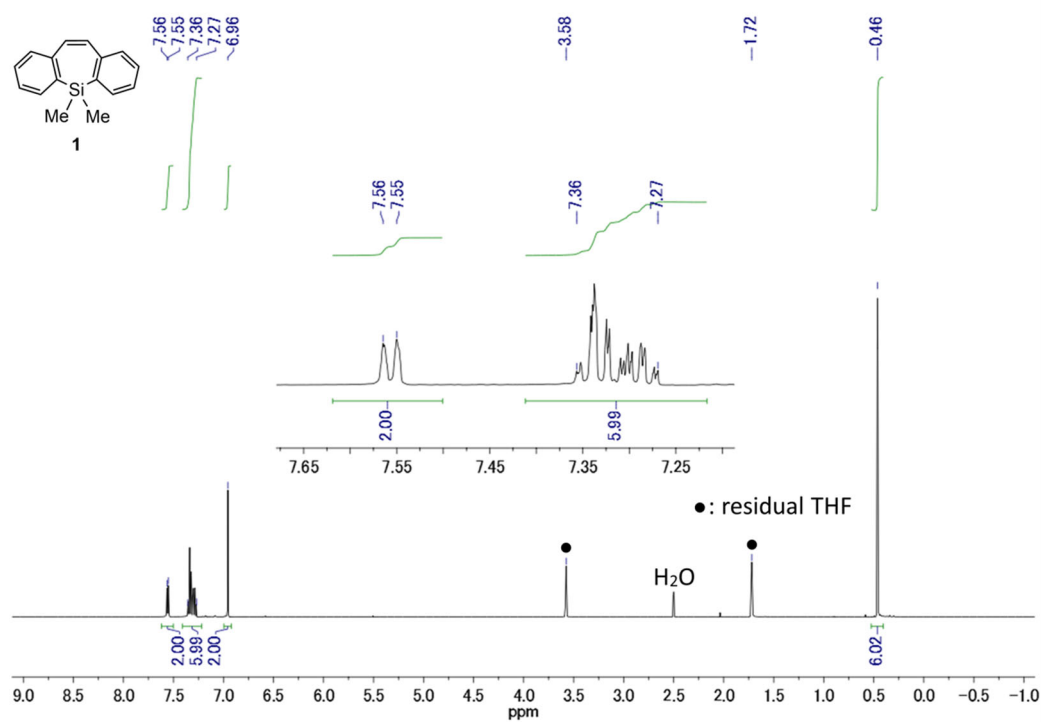


Figure S6.  $^1\text{H}$  NMR spectrum of **1** in  $\text{THF-}d_8$ .

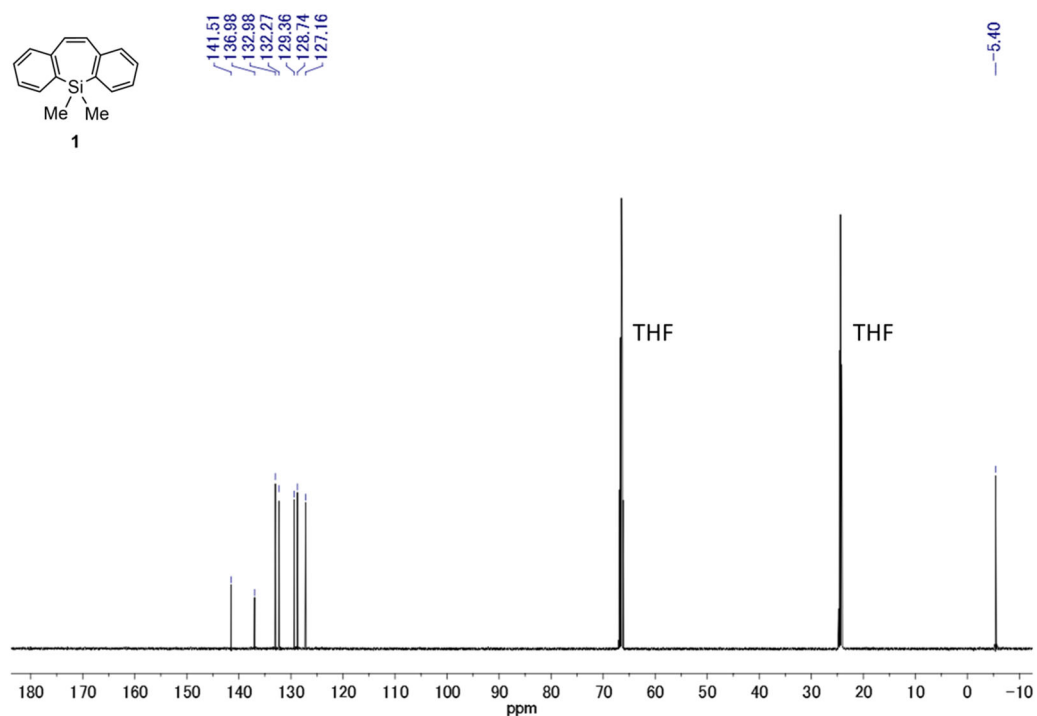


Figure S7.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1** in  $\text{THF-}d_8$ .

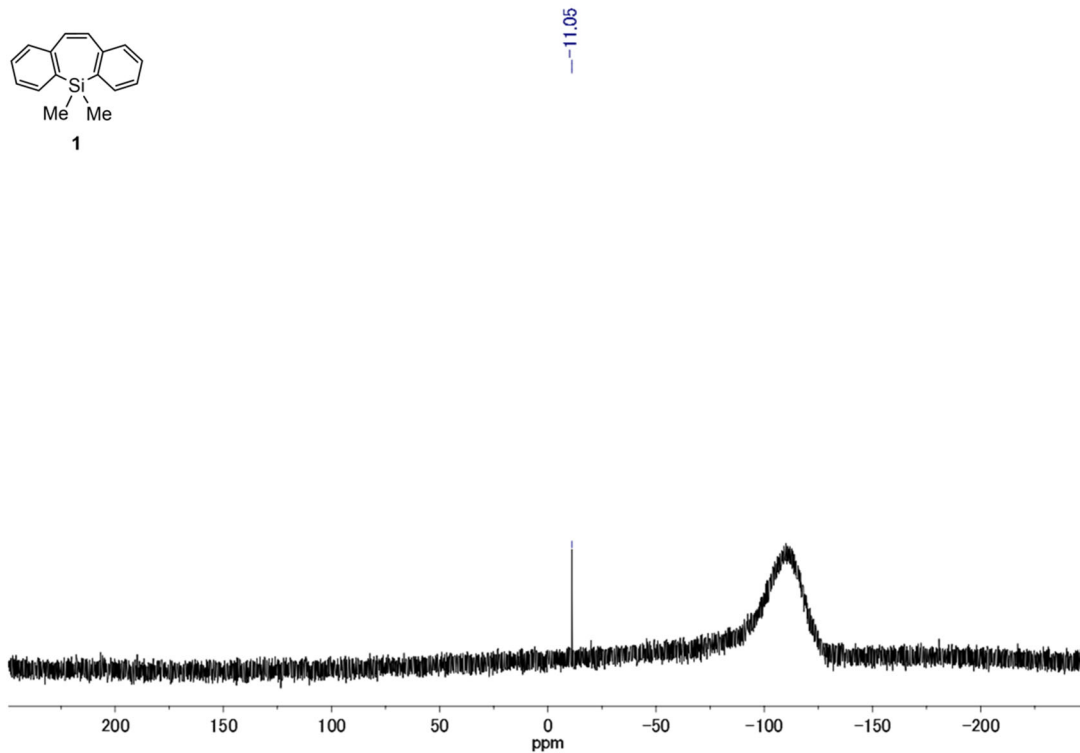


Figure S8.  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectrum of **1** in THF- $d_8$ .

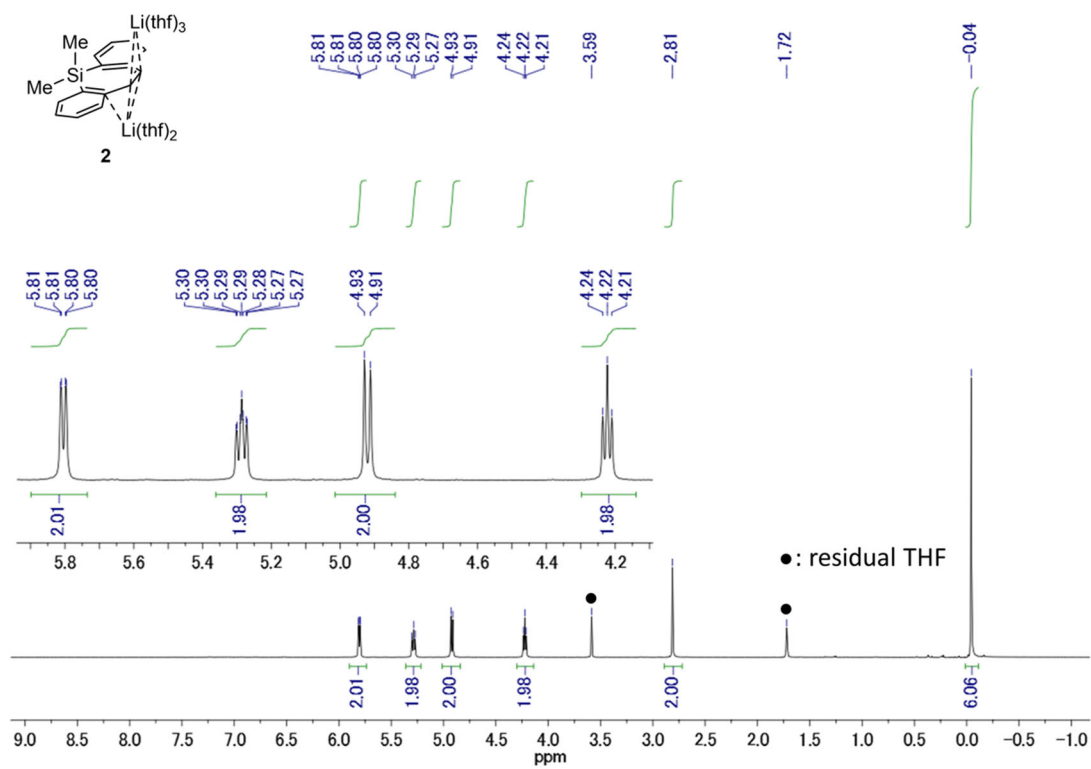
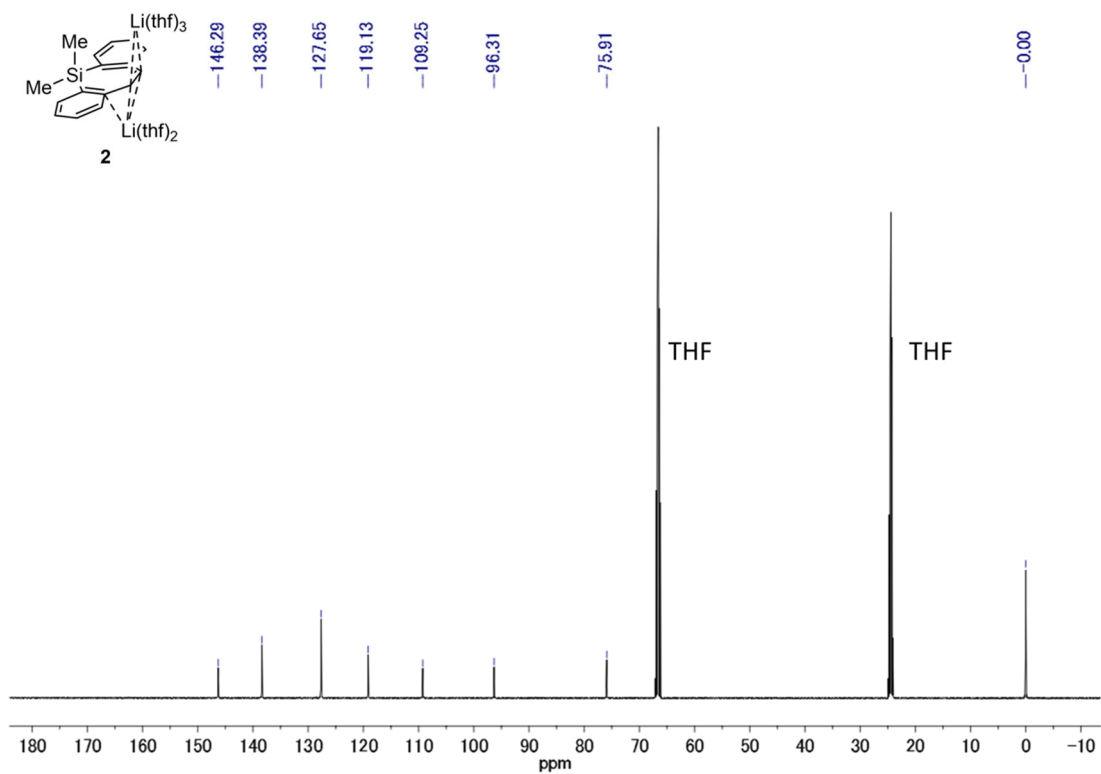
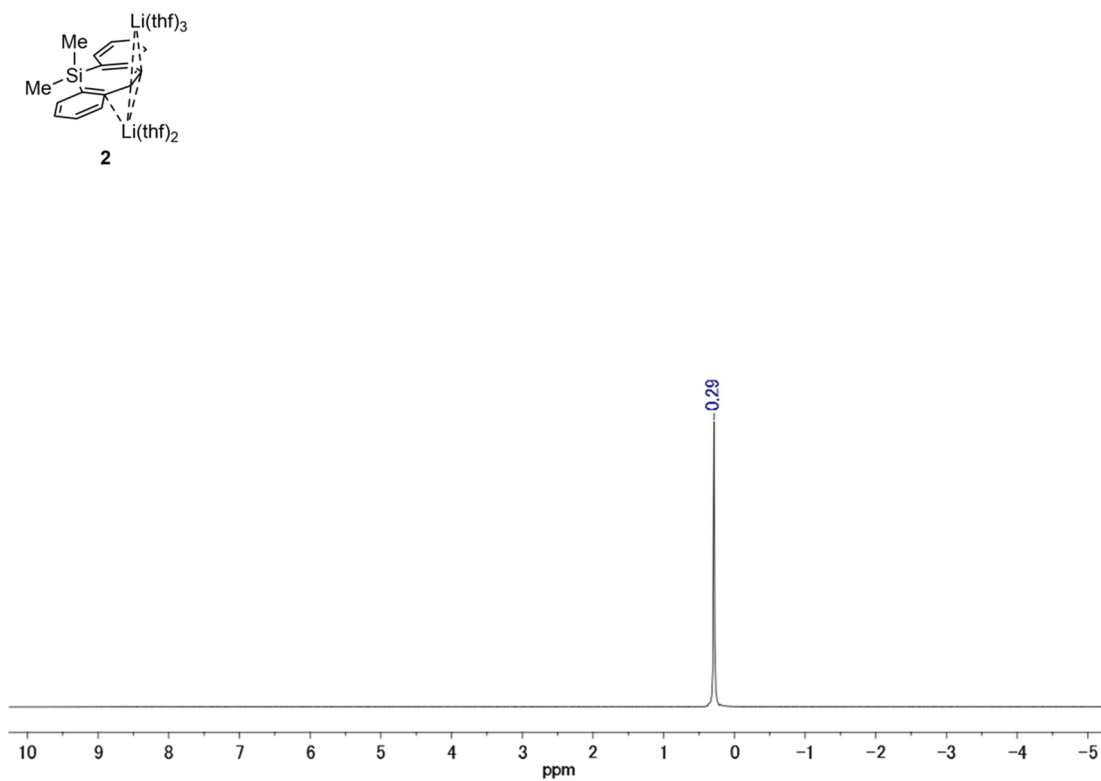


Figure S9.  $^1\text{H}$  NMR spectrum of **2** in THF- $d_8$ .



**Figure S10.** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of **2** in THF-*d*<sub>8</sub>.



**Figure S11.** <sup>7</sup>Li{<sup>1</sup>H} NMR spectrum of **2** in THF-*d*<sub>8</sub>.

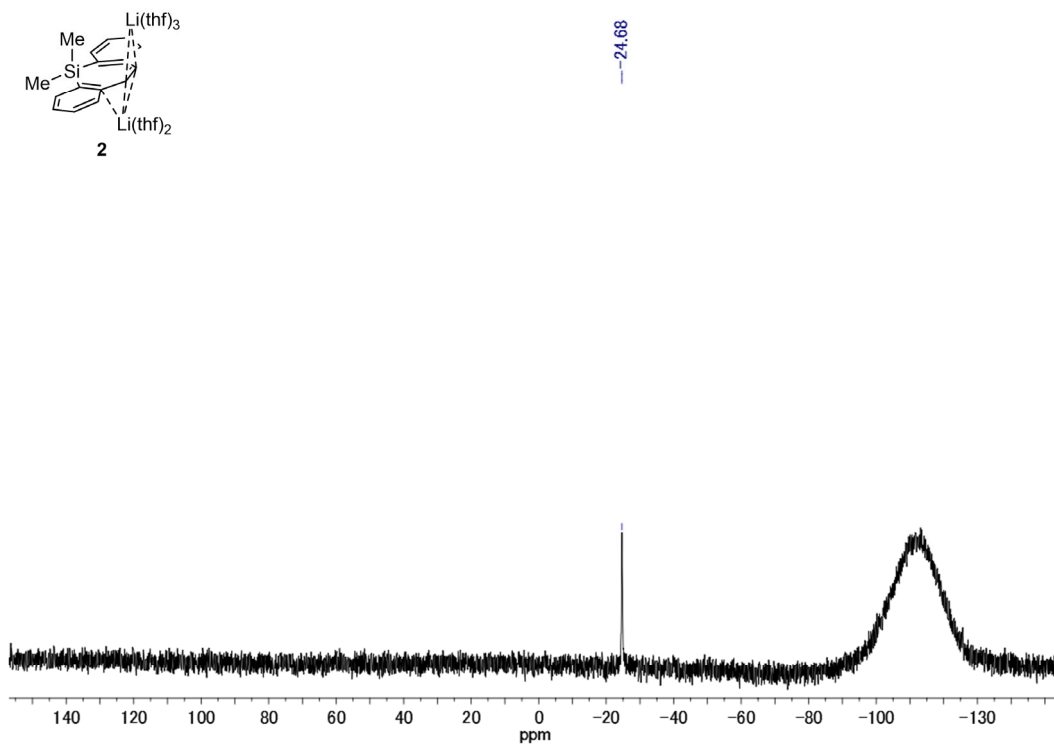


Figure S12.  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectrum of **2** in  $\text{THF-}d_8$ .

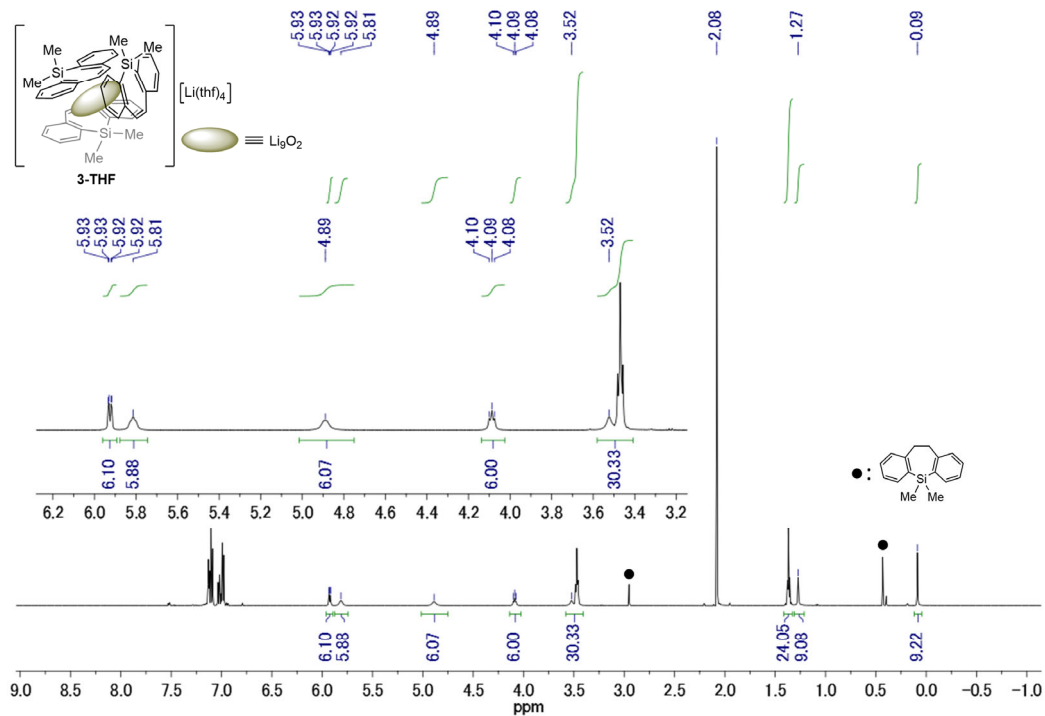
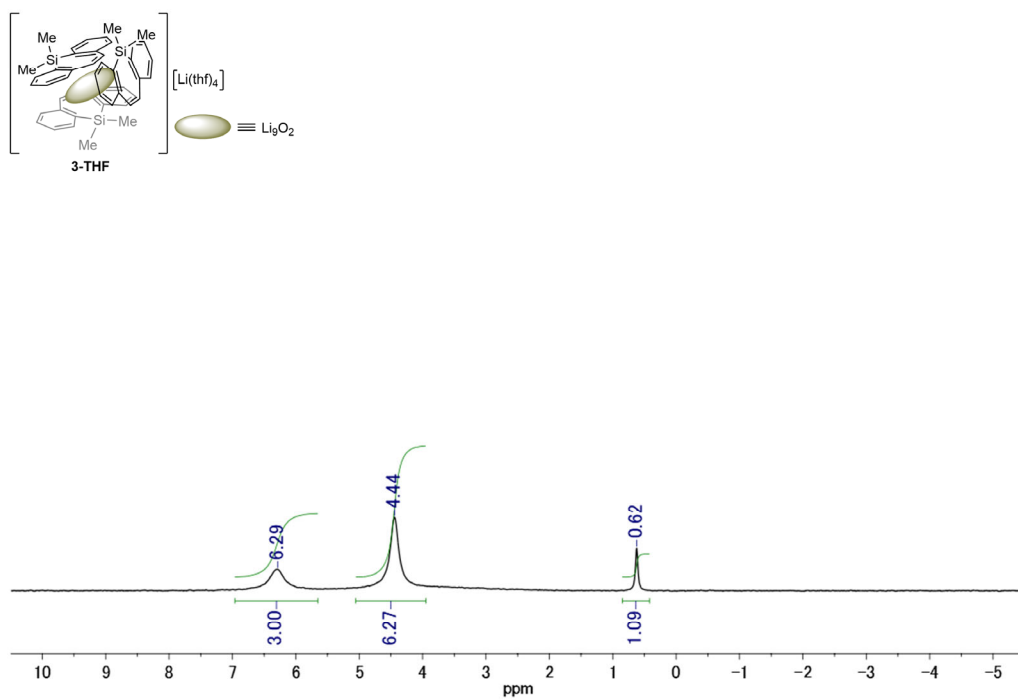


Figure S13.  $^1\text{H}$  NMR spectrum of **3-THF** in  $\text{toluene-}d_8$



**Figure S14.** <sup>7</sup>Li{<sup>1</sup>H} NMR spectrum of **3-THF** in toluene-*d*<sub>8</sub>



## 10. Energies and Cartesian coordinates for the optimized structures of **1**, **1<sup>2-</sup>**, **2**, and **3'**

**Table S5.** Uncorrected and thermal-corrected (298 K) energies of stationary points (Hartree).<sup>a</sup>

	<i>E</i>	<i>E</i> + <i>ZPE</i>	<i>H</i>	<i>G</i>
<b>1</b>	-908.884940588	-908.615189	-908.598765	-908.657002
<b>1<sup>2-</sup></b>	-908.533589338	-908.516127	-908.498745	-908.559477
<b>2</b>	-2086.330730	--2085.469107	-2085.416059	-2085.566126
<b>3'</b>	-2945.40776963	-2944.586003	-2944.520783	-2944.677978

a) *E*: electronic energy; *ZPE*: zero-point energy; *H* (= *E* + *ZPE* + *E*<sub>vib</sub> + *E*<sub>rot</sub> + *E*<sub>trans</sub> + *RT*): sum of electronic and thermal enthalpies; *G* (= *H* – *TS*): sum of electronic and thermal free energies.

### Cartesian coordinates for **1**

Si	0.0000022	1.2513694	0.5149221
C	-1.5184272	0.3059846	-0.0823376
C	1.5184347	0.3059875	-0.0823282
C	-2.5539054	0.9724229	-0.7625782
H	-2.4473955	2.0298742	-0.9928136
C	1.6805074	-1.0771364	0.1969272
C	-1.6805021	-1.0771385	0.1969207
C	2.5539152	0.9724281	-0.7625628
H	2.4474074	2.0298812	-0.9927912
C	3.7311138	0.3249288	-1.1427156
H	4.5128254	0.8729772	-1.6630292
C	-2.8901356	-1.7105887	-0.1625731
H	-3.0221946	-2.7648536	0.0721667
C	2.8901393	-1.7105874	-0.1625705
H	3.0221969	-2.7648536	0.0721646
C	-3.9015308	-1.0265435	-0.8308417
H	-4.8170634	-1.5443184	-1.1061245
C	0.6784533	-1.9316704	0.8528002
H	1.1231883	-2.7861574	1.3637977
C	-0.6784499	-1.9316717	0.8527974
H	-1.1231854	-2.7861591	1.3637939
C	3.9015358	-1.0265410	-0.8308361
H	4.8170672	-1.5443166	-1.1061212
C	-3.7311049	0.3249240	-1.1427290
H	-4.5128149	0.8729717	-1.6630457
C	-0.0000352	1.3688837	2.4054385
H	0.8875945	1.9083758	2.7600146

H	-0.8875917	1.9085501	2.7599356
H	-0.0001552	0.3783034	2.8727744
C	0.0000049	3.0046862	-0.1991368
H	-0.8809651	3.5626147	0.1420016
H	0.8809377	3.5626393	0.1420573
H	0.0000390	3.0150904	-1.2957365

Cartesian coordinates for  $1^{2-}$

Si	0.0016242	1.1559235	0.3283051
C	-1.5755044	0.2673802	-0.1713003
C	1.5844409	0.2827932	-0.1570548
C	-2.7060927	1.0267374	-0.4903550
H	-2.5919017	2.1061107	-0.5994414
C	1.7553197	-1.1587667	0.0679584
C	-1.7181340	-1.1803848	0.0096508
C	-0.6944116	-2.1071635	0.3052241
H	-1.0862354	-3.1161786	0.4724878
C	0.7399207	-2.1005493	0.3086791
H	1.1403928	-3.0962885	0.5303302
C	-4.0029127	0.4955502	-0.6539769
H	-4.8449322	1.1294687	-0.9282843
C	3.1350479	-1.6197938	0.0664906
H	3.3302276	-2.6486525	0.3819676
C	2.6746446	1.0248707	-0.6244336
H	2.5328356	2.0883488	-0.8327553
C	-3.0675004	-1.6939223	-0.1464887
H	-3.2154554	-2.7684127	-0.0133708
C	4.1817383	-0.8428526	-0.3857436
H	5.1906976	-1.2658239	-0.4039562
C	-4.1512007	-0.9036939	-0.4706390
H	-5.1351100	-1.3680167	-0.5831290
C	3.9654110	0.4924948	-0.8211202
H	4.7857882	1.1184706	-1.1698190
C	-0.0726984	1.3423671	2.2385857
H	0.8193165	1.8410977	2.6373997
H	-0.9613936	1.9207475	2.5417208
H	-0.1454174	0.3480611	2.7002634
C	-0.0136158	2.9397783	-0.3739298

H	-0.0664002	2.9454224	-1.4720851
H	-0.8733229	3.5083562	0.0085038
H	0.8914573	3.4852901	-0.0753847

Cartesian coordinates for 2

Si	0.4865336	-2.1304967	-1.5456197
O	-3.3348426	-0.9162772	1.0570443
O	-3.2229669	0.8484031	-1.4234232
O	3.6843021	-0.7304471	0.6173149
O	3.1151431	2.1883286	0.7788707
O	-2.7039610	2.2123630	1.3218287
C	0.2576300	-2.3342379	0.3077919
C	0.2216199	-3.6513481	0.8056248
H	0.2948386	-4.4760120	0.0963824
C	0.1098744	0.9792409	-0.2861815
H	-0.1205879	2.0279403	-0.0757073
C	0.7027032	0.7897259	-1.5576061
C	0.0742472	-1.6022304	2.6469215
H	0.0394249	-0.7991892	3.3853871
C	0.1418484	-1.2264196	1.2483506
C	-1.1898532	-2.3382896	-2.4467982
H	-1.8851211	-1.5308994	-2.1887601
H	-1.6717602	-3.2903808	-2.1852334
H	-1.0440349	-2.3208916	-3.5353445
C	0.0878095	0.1633298	0.9486210
H	-0.0166378	0.7866637	1.8417176
C	2.8630817	3.4710792	0.1612524
H	2.0235325	3.9572267	0.6797757
H	2.5806423	3.2848788	-0.8772517
C	1.5684757	-3.5582052	-2.2045692
H	1.6675492	-3.5090750	-3.2961380
H	1.1217605	-4.5321238	-1.9699235
H	2.5777454	-3.5482218	-1.7749978
C	-4.6471676	0.7222622	-1.5453076
H	-5.1081282	1.7198068	-1.4552963
H	-4.9919545	0.0978039	-0.7192517
C	1.9830031	-0.4608035	-3.2578553
H	2.3754121	-1.4040964	-3.6374990

C	0.1202706	-3.9809905	2.1616313
H	0.1230476	-5.0161887	2.4922688
C	1.2069091	-0.4824645	-2.0803032
C	-3.4612038	-2.2558995	0.5128711
H	-2.4670597	-2.7102389	0.4468168
H	-3.8819194	-2.1587626	-0.4918119
C	0.0634374	-2.9106569	3.0832318
H	0.0154978	-3.1140478	4.1533814
C	0.8629414	1.9361589	-2.4361575
H	0.3893323	2.8751964	-2.1443443
C	-2.0625895	3.9960757	2.7409740
H	-2.2421139	4.4490348	3.7214234
H	-1.0053853	4.1368808	2.4858496
C	1.6177419	1.8911884	-3.5897296
H	1.7239277	2.7946202	-4.1907277
C	2.2467981	0.6925617	-4.0023401
H	2.8512680	0.6541600	-4.9044886
C	3.7026178	-1.8274880	1.5730752
H	2.8377612	-2.4706333	1.3837978
H	3.6081282	-1.3961136	2.5737578
C	4.1601210	4.2557395	0.3443131
H	4.0075191	5.3388786	0.2949897
H	4.8853213	3.9764336	-0.4296320
C	-4.3572024	-2.9936577	1.5028655
H	-4.2394348	-4.0799996	1.4384917
H	-5.4130149	-2.7483291	1.3282521
C	-2.7510743	1.3246392	-2.7029400
H	-1.6898698	1.0864680	-2.7713448
H	-2.8730311	2.4181612	-2.7347362
C	4.2032906	2.2955826	1.7280729
H	5.0075139	1.6324859	1.3912533
H	3.8501417	1.9466423	2.7045451
C	-3.5314309	-0.9614405	2.4938411
H	-4.3485404	-0.2691199	2.7321233
H	-2.6127636	-0.6238777	2.9830332
C	-2.9540720	3.4381373	0.5910134
H	-3.9021508	3.3320478	0.0552983
H	-2.1486087	3.5653446	-0.1419795

C	-4.8732038	0.1341768	-2.9463587
H	-4.8870214	-0.9596390	-2.9024327
H	-5.8257480	0.4622158	-3.3757095
C	4.6259539	3.7722330	1.7285401
H	4.1019687	4.3236755	2.5188842
H	5.7016366	3.8938182	1.8915095
C	4.6763762	-0.9469973	-0.4186792
H	5.4589139	-0.1835019	-0.3049543
H	4.1892471	-0.8163663	-1.3892741
C	-3.8710146	-2.4187721	2.8440708
H	-2.9674159	-2.9442856	3.1695694
H	-4.6197336	-2.4884629	3.6402863
C	-2.9671603	4.5622821	1.6341672
H	-2.6081549	5.5115508	1.2238778
H	-3.9824104	4.7225122	2.0175109
C	-3.6424068	0.6324362	-3.7550137
H	-3.1160848	-0.2052890	-4.2204597
H	-3.9244794	1.3299865	-4.5503204
C	-2.4231792	2.5111309	2.7068825
H	-1.6179006	1.8495785	3.0355705
H	-3.3221455	2.3026339	3.3044818
C	5.0294452	-2.5460406	1.3292023
H	5.8428589	-2.0623155	1.8855402
H	4.9888799	-3.5976951	1.6302492
C	5.2252674	-2.3579445	-0.1847047
H	4.6330985	-3.0948674	-0.7386008
H	6.2688539	-2.4537474	-0.5022583
Li	-2.1115153	0.5127328	0.2644598
Li	2.1565453	0.5043183	0.3206826

Cartesian coordinates for **3'**

Si	-2.1893510	-3.9531480	0.1465170
Si	4.5211480	0.0817420	0.1131360
Si	-2.3309660	3.8732750	0.1111540
O	-0.0028700	-0.0055490	-1.2913800
O	0.0050670	0.0094340	1.5109250
C	-1.2056390	-3.2540950	1.5827890
C	0.2715020	-3.2729150	1.5271730

C	-1.6776750	-3.1143900	-1.4515380
C	-3.4429680	0.7573870	0.3793540
H	-4.0284340	-0.1329760	0.6161270
C	1.0671840	-3.3580670	0.3805950
H	2.1332720	-3.4190310	0.6072560
C	-0.2792290	-3.1944800	-1.8923910
C	0.8434980	-3.3504130	-1.0614230
H	1.7787080	-3.4874130	-1.6092860
C	-3.3262080	0.9321390	-1.0646930
H	-3.9123030	0.1845430	-1.6042520
C	-1.8372320	-2.8925430	2.7759750
H	-2.9275940	-2.9081900	2.8126750
C	-2.9710960	1.4167680	1.5185420
C	-2.6396130	-2.6088530	-2.3344740
H	-3.6749510	-2.5480760	-1.9997540
C	2.7137160	1.8805950	1.4991800
C	-2.6310120	1.8177590	-1.9055310
C	-3.2136600	0.8075940	2.8335740
H	-3.9657210	0.0208030	2.9077950
C	0.2587290	-2.7702140	3.9684550
H	0.8057490	-2.6811910	4.9067690
C	-1.1436540	-2.5118910	3.9506690
H	-1.6788830	-2.2716150	4.8646370
C	0.9330010	-3.1722730	2.8355620
H	1.9909420	-3.4303880	2.9010260
C	-2.2164240	2.6872820	1.5601810
C	-2.3474310	-2.1910500	-3.6497480
H	-3.1278340	-1.8189230	-4.3069100
C	-0.0712750	-3.0106300	-3.3243880
H	0.9005490	-3.2660350	-3.7460140
C	3.4354150	0.5915390	1.5554030
C	2.8922820	1.3461520	-1.9188610
C	2.3073100	2.4103480	2.8082000
H	2.0038430	3.4563400	2.8708990
C	-1.8163790	-5.8113760	-0.0037990
H	-0.7467470	-5.9672620	-0.1862000
H	-2.3701500	-6.2612150	-0.8383970
H	-2.0831260	-6.3456270	0.9176030

C	-1.5866180	3.0660070	2.7490770
H	-1.0549200	4.0184140	2.7754240
C	-1.8614970	2.9933000	-1.4775320
C	5.2683980	-1.6402040	0.4159190
H	4.5049950	-2.4203600	0.5248500
H	5.8830340	-1.6437390	1.3250970
H	5.9224940	-1.9282110	-0.4168920
C	-1.0512690	-2.4894860	-4.1455130
H	-0.8259700	-2.3218320	-5.1980650
C	3.5255500	0.0970600	-1.4766190
C	-4.0542610	-3.7366830	0.4467490
H	-4.3653680	-4.2621490	1.3586130
H	-4.6306400	-4.1632140	-0.3840250
H	-4.3472790	-2.6846760	0.5499420
C	3.5611280	-0.9933020	-2.3540870
H	4.0293870	-1.9184770	-2.0187980
C	2.4733910	2.4010660	-1.0902010
H	2.1197610	3.2763980	-1.6400320
C	-2.5780210	1.5315790	-3.3350320
H	-3.2873300	0.8154340	-3.7490560
C	2.3804290	2.6065030	0.3515460
H	1.9030480	3.5618940	0.5772000
C	2.3045980	1.6310310	3.9450830
H	1.9623160	2.0654800	4.8840480
C	-1.6356500	2.1090600	-4.1623770
H	-1.6041350	1.8194690	-5.2120860
C	-0.9426180	3.5630180	-2.3670140
H	-0.3719290	4.4329230	-2.0424860
C	-1.6032060	2.2878030	3.9320920
H	-1.1253910	2.6399810	4.8415710
C	3.0413640	-0.9563320	-3.6650870
H	3.1045440	-1.8215030	-4.3184490
C	-2.5275700	1.2024230	3.9619750
H	-2.7232010	0.6938700	4.9057460
C	3.4472920	-0.1300580	2.7523450
H	4.0056320	-1.0667570	2.7893160
C	2.6483740	0.3129420	-4.1644910
H	2.3817410	0.4187160	-5.2154170

C	2.6176260	1.4267020	-3.3491900
H	2.3500520	2.3939610	-3.7738890
C	-0.7269980	3.0857330	-3.6769860
H	-0.0151740	3.5685460	-4.3400400
C	5.9426200	1.3329800	-0.0550890
H	6.6011660	1.0750980	-0.8949570
H	6.5473400	1.3724830	0.8604990
H	5.5410770	2.3365530	-0.2375080
C	2.7808480	0.2869370	3.9302480
H	2.8457430	-0.2928010	4.8463170
C	-1.2107520	5.3832570	0.3941080
H	-1.5064950	5.9226030	1.3029810
H	-1.2966580	6.0887810	-0.4420790
H	-0.1523750	5.1130580	0.4945190
C	-4.1268180	4.4777900	-0.0441070
H	-4.7965950	3.6273740	-0.2169820
H	-4.2403170	5.1733930	-0.8860180
H	-4.4554470	4.9855970	0.8722350
Li	-1.1489540	0.7312320	0.0992730
Li	0.4617790	1.5413770	-2.2060970
Li	-0.0554160	-1.3587780	0.1054400
Li	-1.5840750	-0.3830320	-2.1904230
Li	-1.4051960	-0.6319950	2.4943200
Li	0.1560590	1.5605800	2.4793440
Li	1.2075670	0.6328590	0.0932170
Li	1.2729330	-0.8873420	2.4880740
Li	1.1064680	-1.1910070	-2.1934700



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