

## Supplementary Materials

### Approach to the “Missing” Diarylsilylene: Formation, Characterization, and Intramolecular C–H Bond Activation of Blue Diarylsilylenes Having Bulky Rind Groups

Kazuki Mochihara<sup>1</sup>, Tatsuto Morimoto<sup>1</sup>, Kei Ota<sup>1</sup>, Shinsuke Marumoto<sup>2</sup>,  
Daisuke Hashizume<sup>3</sup> and Tsukasa Matsuo<sup>1,\*</sup>

<sup>1</sup> Department of Applied Chemistry, Faculty of Science and Engineering, Kindai University, 3-4-1 Kowakae, Higashi-Osaka, Osaka 577-8502, Japan

<sup>2</sup> Joint Research Center, Kindai University, 3-4-1 Kowakae, Higashi-Osaka, Osaka 577-8502, Japan

<sup>3</sup> RIKEN Center for Emergent Matter Science (CEMS), 2-1 Hirosawa, Wako, Saitama 351-0198, Japan

E-mail: t-matsuo@apch.kindai.ac.jp

(submitted to International Journal of Molecular Sciences)

#### UV-vis spectra of **3a** and **3b**

The solution containing (EMind)<sub>2</sub>Si: (**3a**): Figure S1

The solution containing (Eind)<sub>2</sub>Si: (**3b**): Figure S2

#### NMR spectra of **3b**, **4b**, and **5b**

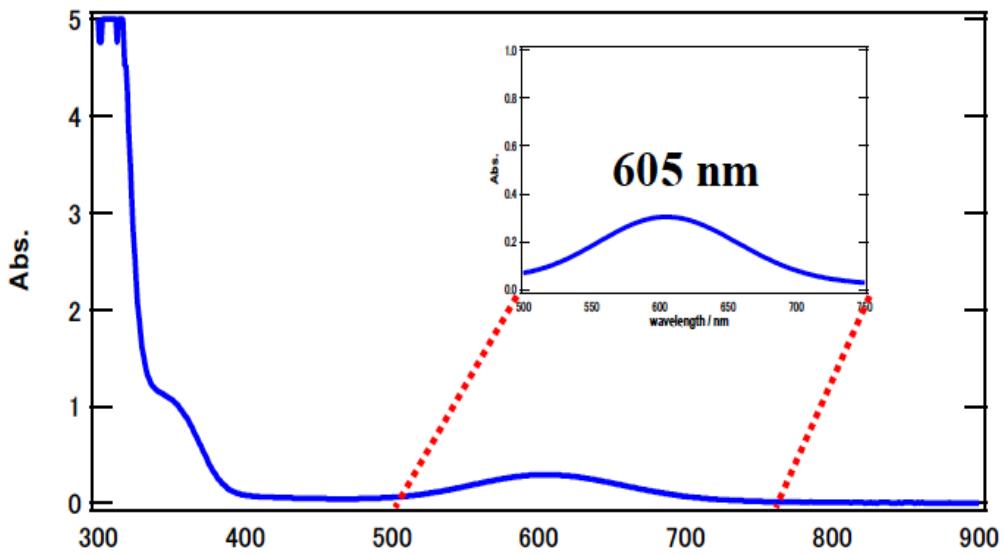
The solution containing (Eind)<sub>2</sub>Si: (**3b**): Figures S3 and S4

The cyclic hydrosilane (**4b**): Figures S5–S10.

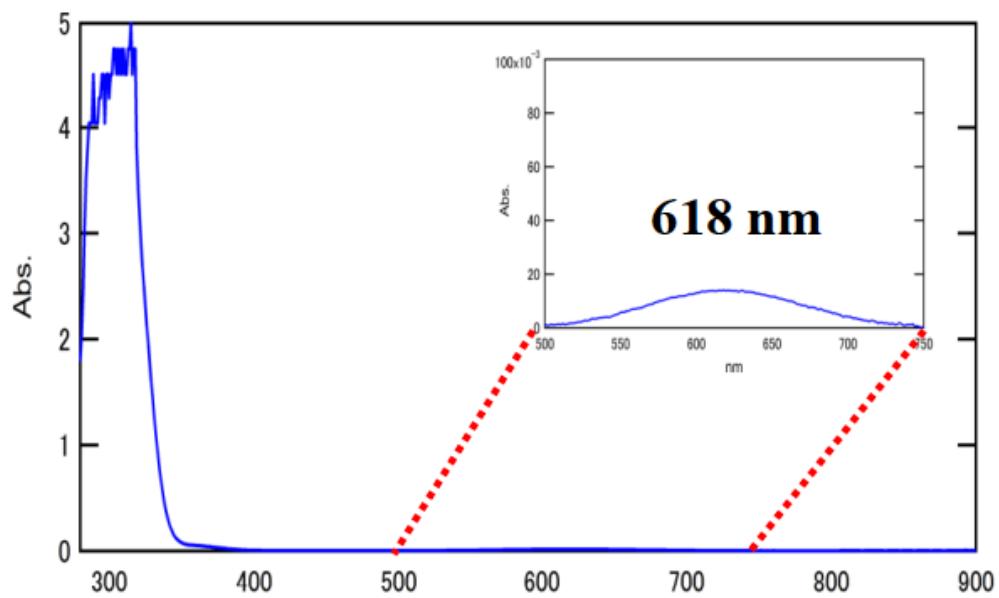
(Eind)<sub>2</sub>SiH(OH) (**4b**): Figures S11–S13

#### IR spectra of **5b**

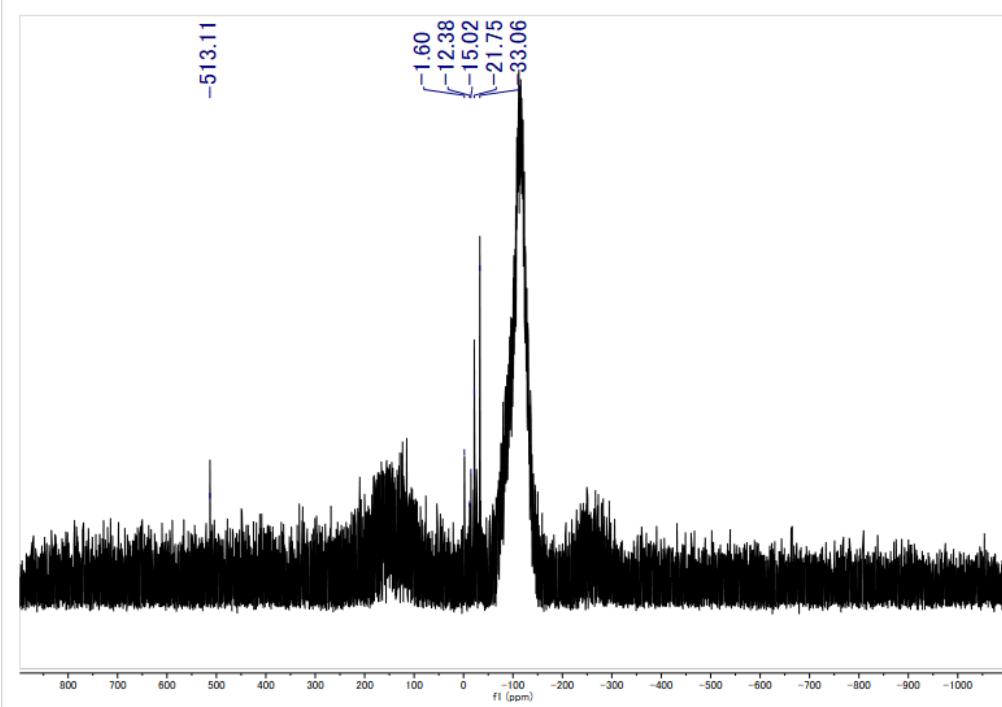
(Eind)<sub>2</sub>SiH(OH) (**4b**): Figure S14



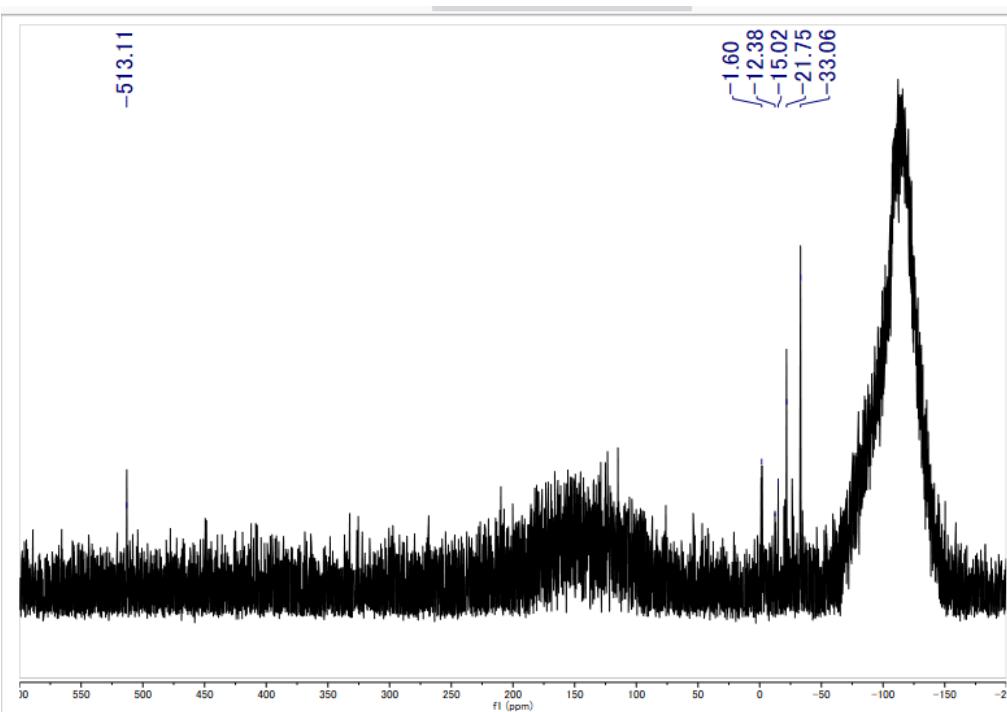
**Figure S1.** UV-vis spectrum of the solution containing (EMind)<sub>2</sub>Si: (3a) in toluene at -20 °C.



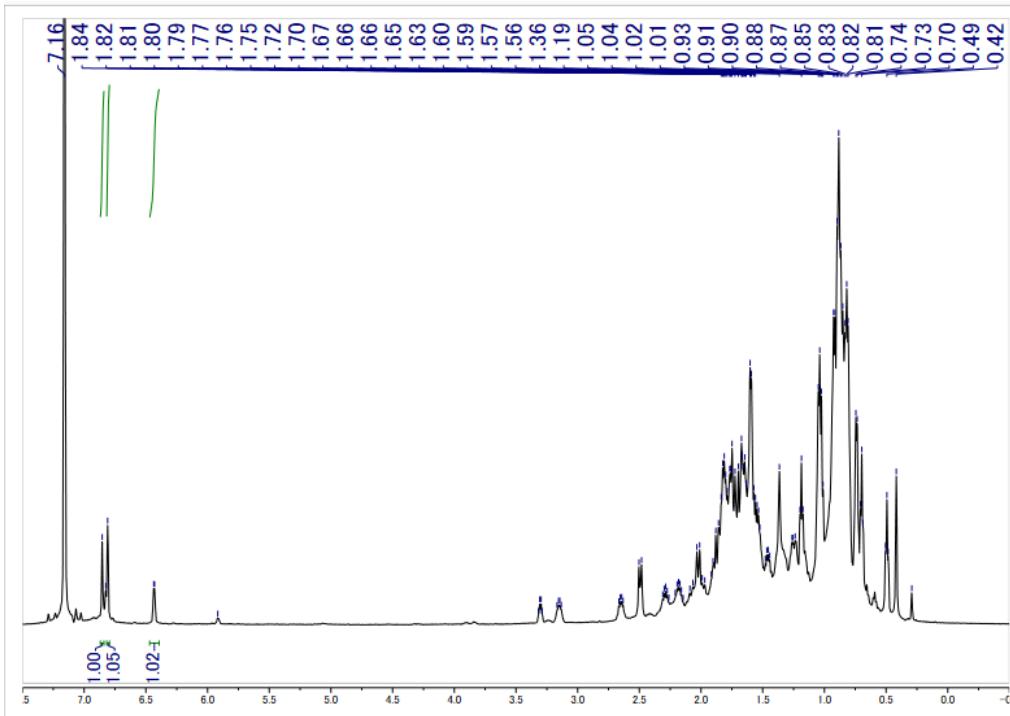
**Figure S2.** UV-vis spectrum of the solution containing (Eind)<sub>2</sub>Si: (3b) in toluene at -20 °C.



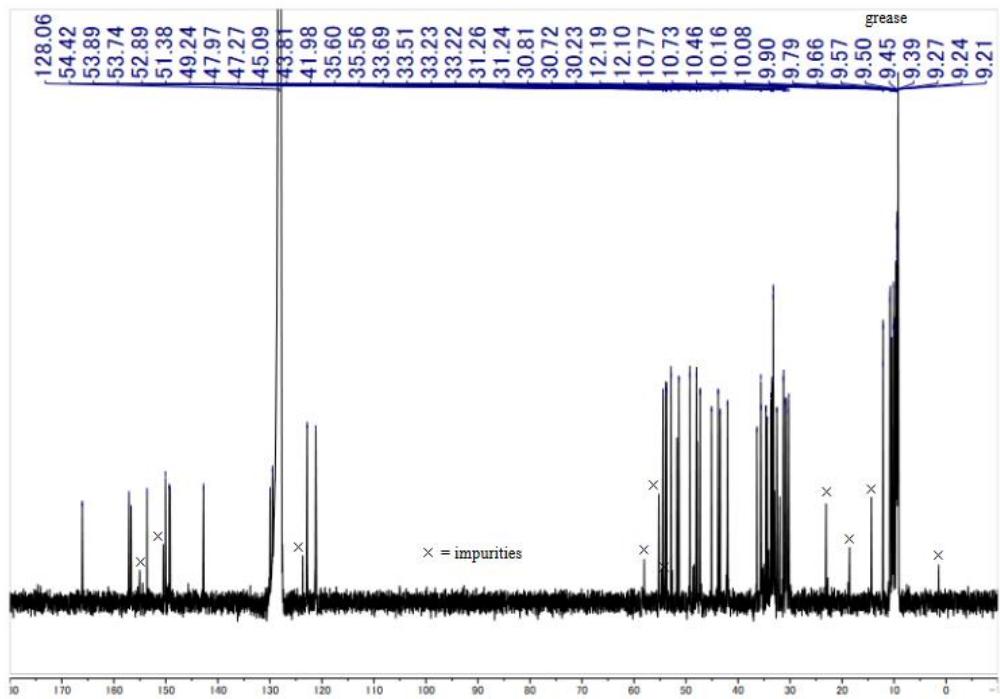
**Figure S3.**  $^{29}\text{Si}$  NMR spectrum of the solution containing  $(\text{Eind})_2\text{Si}$ : (**3b**) in  $\text{C}_7\text{D}_8$  at  $-20^\circ\text{C}$ , ranging from  $-1100$  to  $900$  ppm.



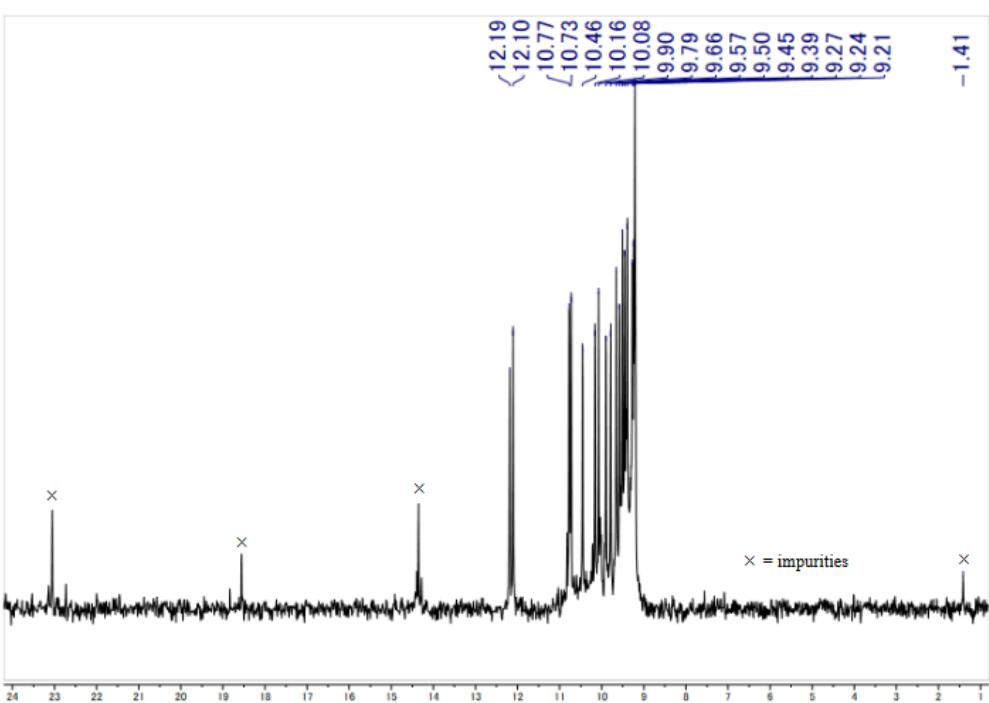
**Figure S4.**  $^{29}\text{Si}$  NMR spectrum of the solution containing  $(\text{Eind})_2\text{Si}$ : (**3b**) in  $\text{C}_7\text{D}_8$  at  $-20^\circ\text{C}$ , ranging from  $-200$  to  $600$  ppm.



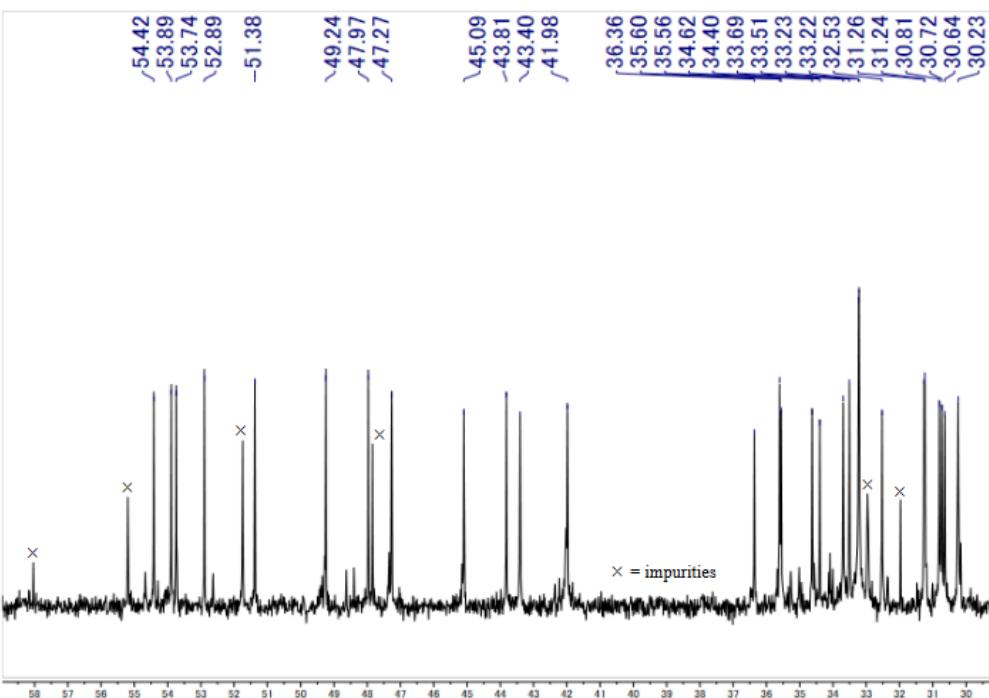
**Figure S5.**  $^1\text{H}$  NMR spectrum of the cyclic hydrosilane (**4b**) in  $\text{C}_6\text{D}_6$  at 20 °C.



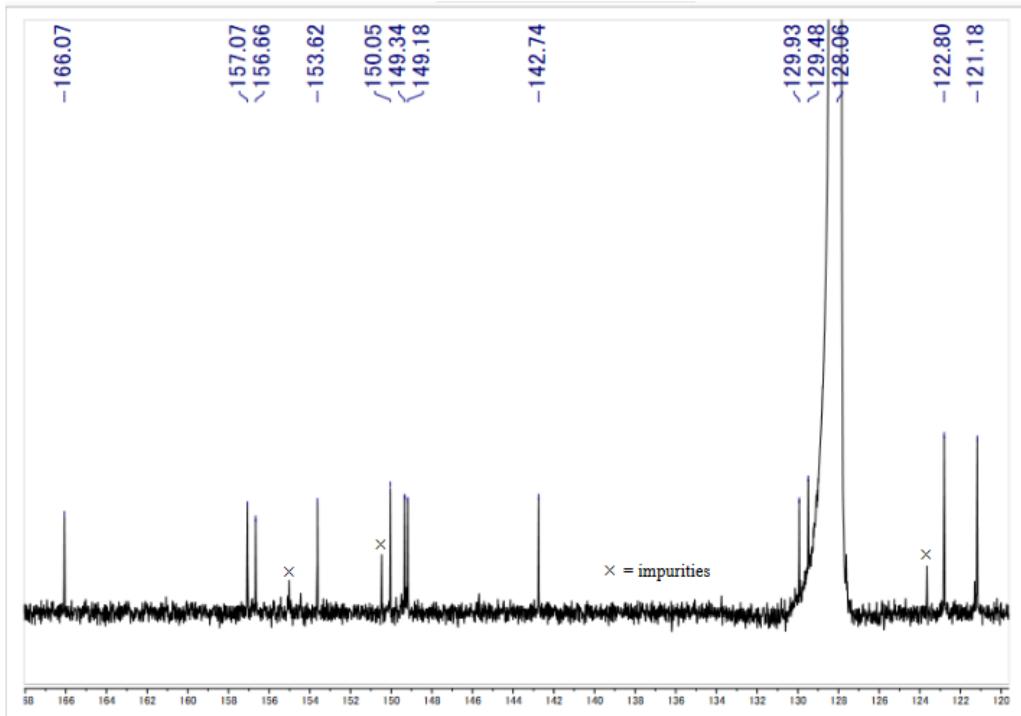
**Figure S6.**  $^{13}\text{C}$  NMR spectrum of the cyclic hydrosilane (**4b**) in  $\text{C}_6\text{D}_6$  at 20 °C, ranging from -10 to 180 ppm.



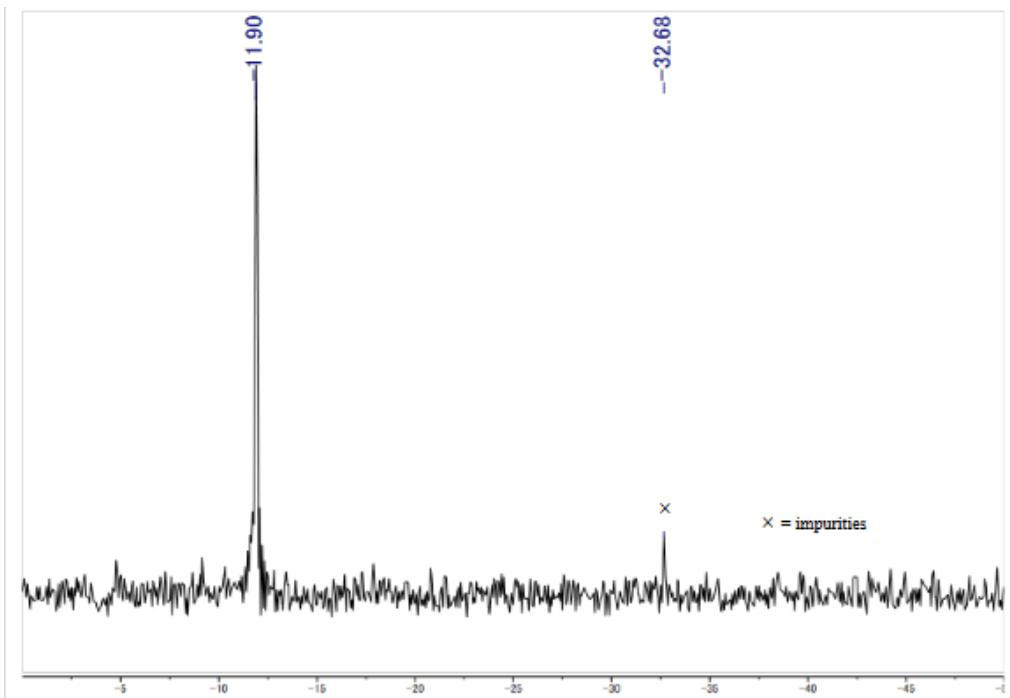
**Figure S7.** <sup>13</sup>C NMR spectrum of the cyclic hydrosilane (**4b**) in C<sub>6</sub>D<sub>6</sub> at 20 °C, ranging from 1 to 24 ppm.



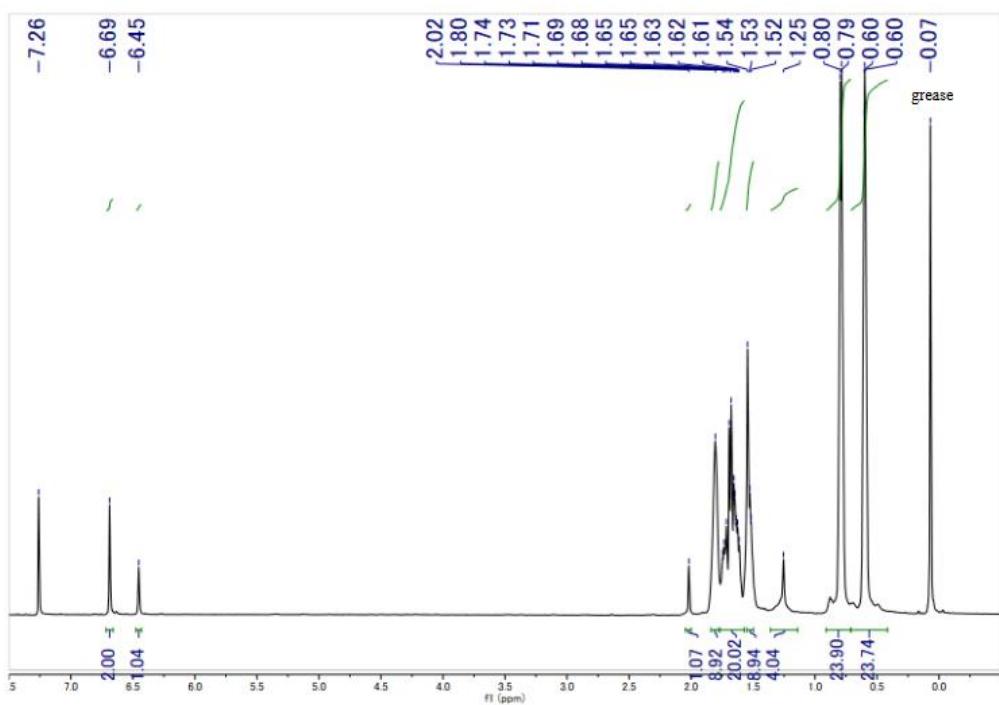
**Figure S8.** <sup>13</sup>C NMR spectrum of the cyclic hydrosilane (**4b**) in C<sub>6</sub>D<sub>6</sub> at 20 °C, ranging from 29 to 59 ppm.



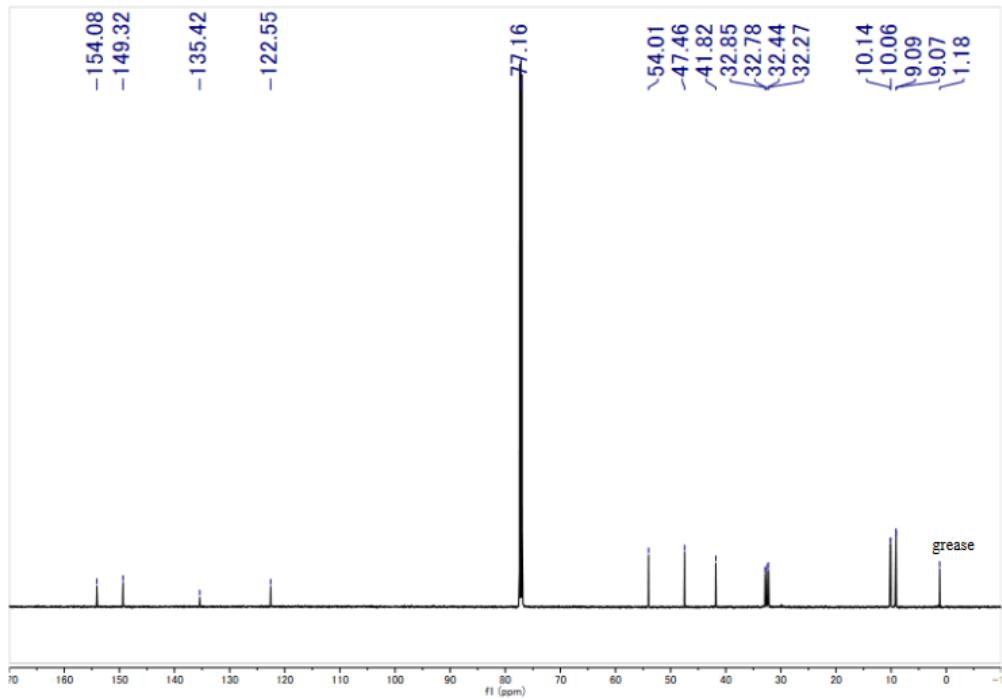
**Figure S9.**  $^{13}\text{C}$  NMR spectrum of the cyclic hydrosilane (**4b**) in  $\text{C}_6\text{D}_6$  at 20 °C, ranging from 120 to 166 ppm.



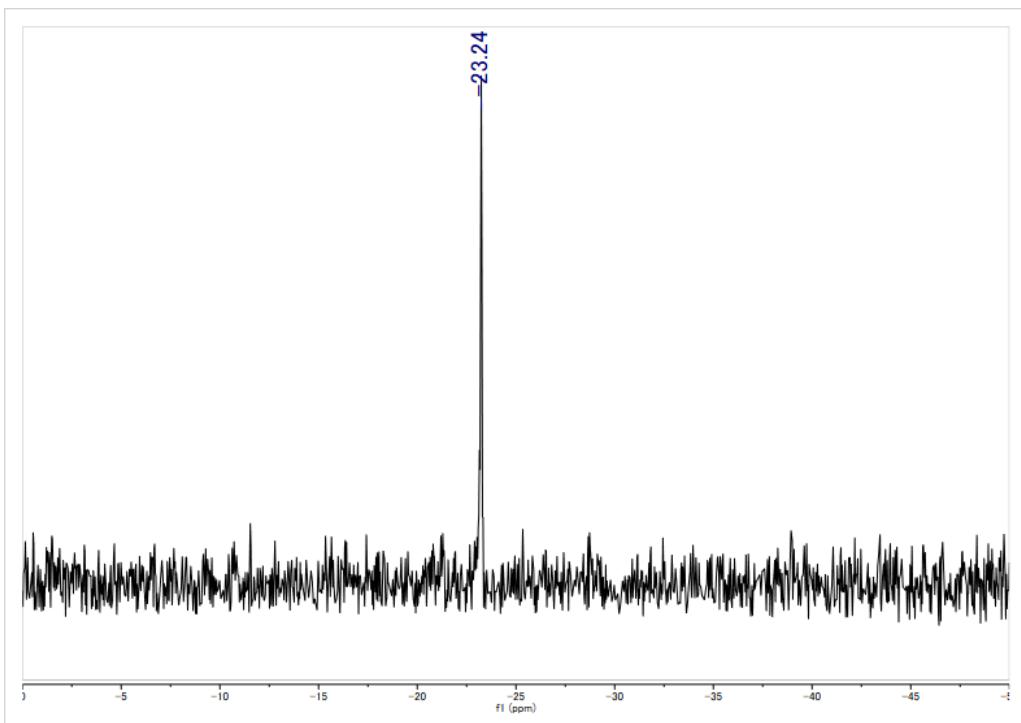
**Figure S10.**  $^{29}\text{Si}$  NMR spectrum of the cyclic hydrosilane (**4b**) in  $\text{C}_6\text{D}_6$  at 20 °C.



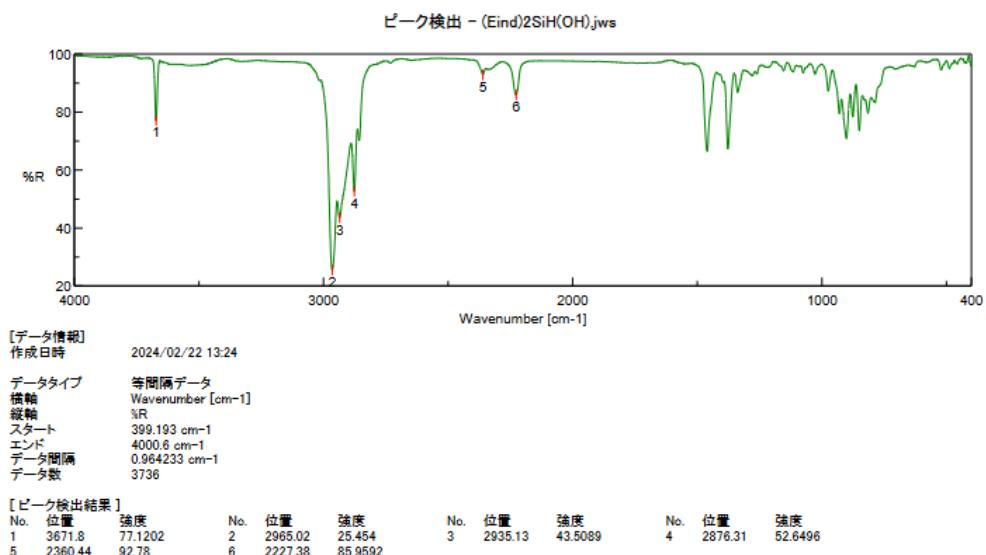
**Figure S11.**  $^1\text{H}$  NMR spectrum of  $(\text{Eind})_2\text{SiH}(\text{OH})$  (**5b**) in  $\text{CDCl}_3$  at 20 °C.



**Figure S12.**  $^{13}\text{C}$  NMR spectrum of  $(\text{Eind})_2\text{SiH}(\text{OH})$  (**5b**) in  $\text{CDCl}_3$  at 20 °C.



**Figure S13.**  $^{29}\text{Si}$  NMR spectrum of  $(\text{Eind})_2\text{SiH}(\text{OH})$  (**5b**) in  $\text{CDCl}_3$  at  $20^\circ\text{C}$ .



**Figure S14.** IR spectrum of (Eind)<sub>2</sub>SiH(OH) (**5b**) in KBr at ambient temperature.