

# Supporting Information

for the Communication Entitled

## Coplanar Oligo(*p*-phenylenedisilenyne)s Based on the Octaethyl-Substituted *s*-Hydrindacenyl Groups

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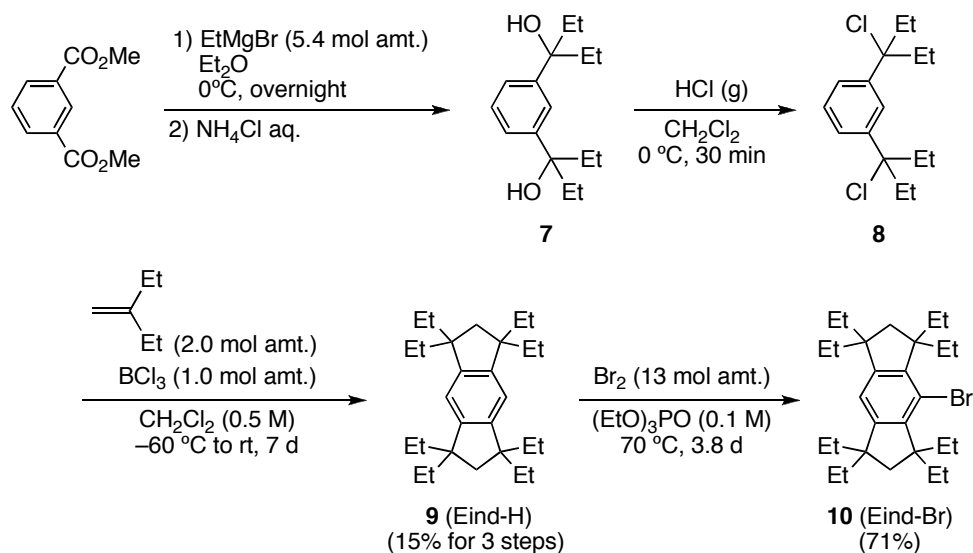
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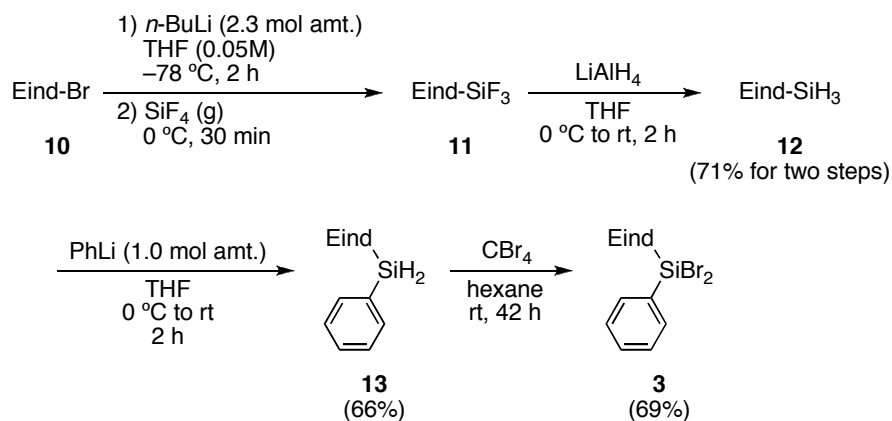
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## 1. Experimental detail

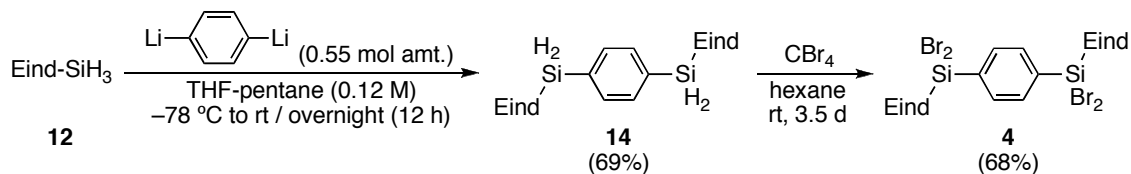
### Scheme S1. Preparation of Eind-Br (10).



### Scheme S2. Preparation of dibromosilane 3.



### Scheme S3. Preparation of bis(dibromosilane) 4.



**General.** Melting points (mp) were determined with a Yanaco MP-S3 or a Stanford Research Systems MPA100 OptiMelt instrument.  $^1\text{H}$  and  $^{13}\text{C}$  NMR were measured with a Varian Mercury (300 MHz for  $^1\text{H}$ ), JEOL EX-270 (67.9 MHz for  $^{13}\text{C}$ ) or a JEOL AL-400 spectrometer (100 MHz for  $^{13}\text{C}$ ) in  $\text{C}_6\text{D}_6$  and chemical shifts are reported in  $\delta$  ppm using  $\text{C}_6\text{HD}_5$  for  $^1\text{H}$  (7.20 ppm) and  $^{13}\text{C}$  (128.0 ppm) as an internal standard.  $^{29}\text{Si}$  NMR spectra were recorded with a JEOL EX-270 (53.6 MHz) or a JEOL AL-400 spectrometer (79.4 MHz) using tetramethylsilane (0.0 ppm) as an external standard. Elemental analyses and mass spectroscopy were performed at the Micro Analysis Division of Institute for Chemical Research, Kyoto University and the Mass Spectrum Division of Institute for Chemical Research, Kyoto University, respectively. Thin layer chromatography (TLC) was performed on plates coated with 0.25 mm thickness of Silica Gel 60 F-254 (Merck). Column chromatography was performed using Kieselgel 60 (70-230 mesh) (Merck) or neutral silica gel PSQ 100B (Fuji Silysia Chemical), respectively. Recycle preparative gel permeation chromatography (GPC) was performed using LC-908 with polystyrene gel column (JAIGEL 1H and 2H, Japan Analytical Industry) with toluene as eluent. All reactions were performed under an argon atmosphere, unless stated otherwise.

**1,3-Bis(1-ethyl-1-hydroxypropyl)benzene (7).** To a solution of dimethyl isophthalate (39.0 g, 0.201 mol) in dry  $\text{Et}_2\text{O}$  (Wako, 350 mL) was added ethylmagnesium bromide solution in dry  $\text{Et}_2\text{O}$  (2.0 M, 500 mL, 1.0 mol) at 0 °C over 3 h. After stirring for 23 h at ambient temperature, the reaction was quenched with 200 mL of sat.  $\text{NH}_4\text{Cl}$  aq. The resulting filtered through a plug of Celite<sup>®</sup> and washed with  $\text{Et}_2\text{O}$  (300 mL) and the organic layer was separated. The aqueous layer was extracted with  $\text{Et}_2\text{O}$  (150 mL  $\times$  3). Combined organic layer was washed with brine (200 mL  $\times$  2) and dried over  $\text{MgSO}_4$ . After concentration of organic layer, residual pale yellow solids (46.4 g) were recrystallized from hexane to afford 34.5 g of **7** (0.138 mol, 69% yield) as colorless solids: mp (MP-S3) 89.5–90.5 °C.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  0.73 (t,  $J$  = 7.5 Hz, 12H), 1.76–1.91 (m, 8H), 7.20–7.35 (m, 4H).  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 67.9 MHz)  $\delta$  8.07, 35.28, 77.70, 122.68, 123.50, 127.76, 145.32. MS (EI)  $m/z$ : 250 [ $M^+$ ], 221 [ $(M-29)^+$ ]. HRMS Calcd for  $\text{C}_{16}\text{H}_{26}\text{O}_2$ : 250.1933. Found: 250.1921.

**1,3-Bis(1-chloro-1-ethylpropyl)benzene (8).** To a solution of **7** (25.0 g, 99.9 mmol) in  $\text{CH}_2\text{Cl}_2$  (200 mL) was added  $\text{CaCl}_2$  powder (30 g), and then  $\text{HCl}$  gas was introduced into the mixture for 30 min at 0 °C. After the reaction was complete,  $\text{N}_2$  gas was bubbled for several hours, and the mixture was filtered. The filtrate was concentrated in vacuo to give

28.9 g of crude **8** as pale yellow oil (0.100 mol if pure). The crude product was used for the next reaction without further purification.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  0.86 (t,  $J$  = 7.5 Hz, 12H), 2.16 (q,  $J$  = 7.5 Hz, 4H), 7.27–7.38 (m, 3H), 7.54–7.55 (m, 1H).  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 67.9 MHz)  $\delta$  9.41, 37.70, 80.98, 125.24, 125.44, 127.84, 142.60.

**1,1,3,3,5,5,7,7-Octaethyl-*s*-hydrindacene (9).** In 1981, Chang and Kennedy reported that 1,1,3,3,5,5,7,7-octamethyl-*s*-hydrindacene as an undesired byproduct during the preparation of telechelic polyisobutylenes.<sup>1</sup> The octaethyl-substituted *s*-hydrindacene was successfully synthesized by simple modification of the reported method as follows: To the solution of crude **8** (28.9 g, 0.100 mol if pure) and 2-ethyl-1-butene (25.0 mL, 0.204 mol) in dry  $\text{CH}_2\text{Cl}_2$  (distilled from  $\text{CaH}_2$ , 150 mL) was added  $\text{BCl}_3$  (1.0 M solution in  $\text{CH}_2\text{Cl}_2$ , 100 mL, 0.100 mol) at  $-60\text{ }^\circ\text{C}$  over 13 min. The resulting orange suspension was warmed to ambient temperature and stirred for 7 d, during which time the color of the solution became dark-brown. The reaction was then quenched with 1 M NaOH aq. (150 mL) at  $0\text{ }^\circ\text{C}$ . To the resulting mixture was added  $\text{CHCl}_3$  (50 mL), and the organic layer was separated. The aqueous layer was extracted with  $\text{CHCl}_3$  (25 mL  $\times$  3). The combined organic extracts were washed with brine (100 mL  $\times$  2), dried over  $\text{MgSO}_4$ , and filtered. The solution was concentrated on a rotary evaporator to reduce the volume to ca. 50 mL, and the residual solution was filtered through a plug of silica gel. The filtrate was concentrated in vacuo to give 37.4 g of pale yellow solids (37.4 g). After recrystallization from hexane (twice) 11.3 g of **9** (29.5 mmol, 30% yield) was obtained as colorless crystals: mp (MP-S3)  $83.0\text{--}84.0\text{ }^\circ\text{C}$ .  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  0.79 (t,  $J$  = 7.5 Hz, 24H), 1.48–1.69 (m, 16H), 1.77 (s, 4H), 6.63 (s, 2H).  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 300 MHz)  $\delta$  0.93 (t,  $J$  = 7.5 Hz, 24H), 1.60–1.81 (m, 16H), 1.85 (s, 4H), 6.89 (s, 2H).  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 67.9 MHz)  $\delta$  9.30, 33.16, 45.41, 48.91, 118.81, 147.58. MS (EI)  $m/z$ : 382 [ $M^+$ ], 353 [ $(M-29)^+$ ]. Anal. Calcd for  $\text{C}_{28}\text{H}_{46}$ : C, 87.88; H, 12.12. Found: C, 87.84; H, 12.09.

**4-Bromo-1,1,3,3,5,5,7,7-octaethyl-*s*-hydrindacene (10).** To the solution of **9** (11.7 g, 30.5 mmol) in triethyl phosphate (250 mL) was added bromine (20 mL, 0.389 mol). The reaction mixture, protected from moisture and from light, was stirred for 90 h at  $70\text{ }^\circ\text{C}$ . After completion of the reaction, the residual bromine was quenched with  $\text{Na}_2\text{SO}_3$  aq. The resulting yellow suspension was diluted with water (50 mL) and filtered to give the crude product as pale yellow powder (12.6 g). The crude material was purified by recrystallization from hexane to afford 10.1 g of pure **10** as colorless crystals (21.9 mmol, 72 % yield): mp (MP-S3)  $157.3\text{--}158.2\text{ }^\circ\text{C}$ .  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  0.76 (t,  $J$  = 7.5 Hz, 12H), 0.81 (t,  $J$

= 7.5 Hz, 12H), 1.07 (m, 8H), 1.82 (s, 4H), 1.95 (m,  $J$  = 7.5 Hz, 8H), 6.59 (s, 1H).  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 300 MHz)  $\delta$  0.89 (t,  $J$  = 7.5 Hz, 12H), 0.93 (t,  $J$  = 7.5 Hz, 12H), 1.52–1.73 (m, 8H), 1.85 (s, 4H), 2.00 (h,  $J$  = 7.5 Hz, 4H), 2.17 (hex,  $J$  = 7.5 Hz, 4H), 6.77 (s, 1H).  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 67.9 MHz)  $\delta$  9.25, 9.45, 31.12, 32.97, 43.15, 47.94, 53.25, 118.04, 118.55, 144.73, 151.76. MS (EI)  $m/z$ : 462  $[(M+2)^+]$ , 460  $[M^+]$ , 433  $[(M-27)^+]$ , 431  $[(M-29)^+]$ . Anal. Calcd for  $\text{C}_{28}\text{H}_{45}\text{Br}$ : C, 87.88; H, 12.12. Found: C, 87.84; H, 12.09.

**Trifluoro(1,1,3,3,5,5,7,7-octaethyl-*s*-hydindacen-4-yl)silane (11).** To a suspension of **10** (4.47 g, 9.03 mmol) in dry THF (Wako, 180 mL) was added *n*-BuLi in hexane (1.60 M, 13.0 mL, 20.8 mmol) dropwise over ca. 10 min at  $-78\text{ }^\circ\text{C}$  under an argon atmosphere. After stirring the suspension for 2 h,  $\text{SiF}_4$  gas was introduced into the mixture for 30 min at  $0\text{ }^\circ\text{C}$ . The reaction mixture was concentrated in vacuo. To the resulting yellow paste were added dry hexane (50 mL), the mixture was filtered through a plug of Celite<sup>®</sup> and rinsed with dry hexane (ca. 80 mL) under an argon atmosphere. After evaporation of the solvents, the crude **11** (5.19 g, containing 7 mol% of **9**) was obtained as a pale yellow solid. The solid was used for next reaction without further purification.  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 300 MHz)  $\delta$  0.84 (t,  $J$  = 7.5 Hz, 12H), 0.88 (t, overlapped), 1.50–1.70 (m, overlapped, 8H), 1.83 (s, 4H), 1.91–2.05 (m, 8H), 7.02 (s, 1H).  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 67.9 MHz)  $\delta$  9.42, 9.93, 32.05, 33.51, 43.52, 47.52, 53.36, 125.89, 150.46 (two signals were overlapped with that of benzene- $d_6$ ).  $^{19}\text{F}$  NMR ( $\text{C}_6\text{D}_6$ , 254.2 MHz)  $\delta$   $-120.62$ .  $^{29}\text{Si}$  NMR ( $\text{C}_6\text{D}_6$ , 53.6 MHz)  $\delta$   $-67.45$  (q,  $^1J_{\text{SiF}} = 271\text{ MHz}$ ). MS (EI)  $m/z$ : 437  $[(M-29)^+]$ . MS (EI)  $m/z$ : 382  $[M^+]$ , 353  $[(M-29)^+]$ .

**(1,1,3,3,5,5,7,7-Octaethyl-*s*-hydindacen-4-yl)silane (12).** To a suspension of lithium aluminum hydride (763 mg, 20.1 mmol) in dry THF (15 mL) was added a solution of the crude **11** (5.19 g, containing 7 mol% **9**) in dry THF (25 mL) over 10 min at  $0\text{ }^\circ\text{C}$ , and the mixture was stirred for 2 h at room temperature. The reaction was quenched with ethyl acetate (20 mL) at  $0\text{ }^\circ\text{C}$  and the mixture was concentrated in vacuo. To the residual mixture was added hexane (20 mL) and filtered through a plug of Celite<sup>®</sup>. The filtrate was evaporated to give 3.73 g of white solid. The crude solid was dissolved in hexane (50 mL) again and filtered through a plug of silica gel. After evaporation of solvent, 3.38 g of the residual solid (crude **12** containing ca. 10 mol% of **9**) was recrystallized from hexane to afford almost pure **12** as colorless crystals (2.66 g, 71% yield for 2 steps): mp (MPA100)  $123.5\text{--}124.5\text{ }^\circ\text{C}$ .  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 300 MHz)  $\delta$  0.899 (t,  $J$  = 7.5 Hz, 12H), 0.904 (t,  $J$  = 7.5 Hz, 12H), 1.58–1.77 (m, 8H), 1.84 (s, 4H), 1.97–2.08 (m, 8H), 4.71 (satellite,  $^1J_{\text{SiH}} = 198\text{ Hz}$ , 3H), 6.91 (s, 1H).  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 67.9 MHz)  $\delta$  9.57, 9.87, 33.07, 33.61, 43.57, 47.86,

53.41, 122.46, 149.05, 155.91 (one peak of the aromatic carbon was overlapped with that of benzene- $d_6$ ).  $^{29}\text{Si}$  NMR ( $\text{C}_6\text{D}_6$ , 53.6 MHz)  $\delta$  -74.34. MS (EI)  $m/z$ : 413 [ $M^+$ ], 383 [ $(M-29)^+$ ]. Anal. Calcd for  $\text{C}_{28}\text{H}_{48}\text{Si}$ : C, 81.47; H, 11.72. Found C, 81.48; H, 11.84.

**(1,1,3,3,5,5,7,7-Octaethyl-*s*-hyndacen-4-yl)phenylsilane (13).** To a solution of **12** (3.00 g, 7.27 mmol) in dry THF (35 mL) was added phenyllithium solution in  $\text{Et}_2\text{O}$  (2.01 M, 3.65 mL, 7.34 mmol) dropwise at 0 °C. After stirring for 2 h, the reaction mixture was concentrated in vacuo. To the residual paste was added hexane (20 mL) and the resulting mixture was filtered through a plug of silica gel. The filtrate was evaporated under reduced pressure to afford 2.46 g of crude oil. After purification of column chromatography (silica gel, hexane as eluent), 2.16 g of **13** was obtained as colorless oil ( $R_f$  = 0.58 (hexane), 4.81 mmol, 66% yield):  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 300 MHz)  $\delta$  0.80 (t,  $J$  = 7.5 Hz, 12H), 0.93 (t,  $J$  = 7.5 Hz, 12H), 1.89–1.81 (m, 8H), 1.86 (s, 4H), 1.56–1.99 (m, 4H), 2.08–2.22 (m, 4H), 5.70 (satellite,  $^1J_{\text{SiH}}$  = 196 Hz, 2H), 6.97 (s, 1H), 7.11–7.14 (m, 3H), 7.48–7.51 (m, 2H).  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 67.9 MHz)  $\delta$  9.61, 10.26, 33.81, 34.32, 43.98, 47.76, 53.97, 122.19, 129.33, 135.67, 149.66, 155.94 (3 aromatic peaks are overlapped).  $^{29}\text{Si}$  NMR (using INEPT technique,  $\text{C}_6\text{D}_6$ , 53.6 MHz)  $\delta$  -48.49. MS (EI)  $m/z$ : 488 [ $M^+$ ], 459 [ $(M-29)^+$ ], 381 [ $(M-107)^+$ ].

**Dibromo(1,1,3,3,5,5,7,7-octaethyl-*s*-hydrindacen-4-yl)phenylsilane (3).** To a solution of **13** (431.2 mg, 0.888 mmol) in dry hexane (7.0 mL) was added carbon tetrabromide<sup>2</sup> (891.6 mg, 2.69 mmol) in one portion at room temperature, and the mixture was stirred for 42 h. After removal of solvents, the resulting pale yellow paste was dried under reduced pressure for 4 h to sublime the residual carbon tetrabromide to give pale yellow powder. To the crude solid was added dry hexane (5 mL) and filtered through a plug of Celite<sup>®</sup>, and rinsed with dry hexane (3 mL) under an argon atmosphere. The filtrate was evaporated to give 565.2 mg of crude product (0.874 mmol, 98% crude yield) as colorless solid. The crude product was recrystallized from dry hexane to give 396.9 mg of **3** (0.614 mmol, 69% yield) as moisture-sensitive colorless crystals (*Note: compound 3 is found to be extremely sensitive toward moisture and acid. If only small portion of 3 is hydrolyzed, evolved HBr spontaneously causes the protodesilylation reaction to give Eind-H (9)*):  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 300 MHz)  $\delta$  0.80 (t,  $J$  = 7.5 Hz, overlapped, 12H), 0.85 (t,  $J$  = 7.5 Hz, overlapped, 12H), 1.58–1.77 (m, 8H), 1.77 (s, 4H), 2.19 (q,  $J$  = 7.5 Hz, 8H), 6.97 (s, 1H), 7.02–7.09 (m, 3H), 7.70 (m, 2H).  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 100.5 MHz)  $\delta$  9.24, 10.19, 33.64, 33.79, 43.99, 47.79, 54.93, 124.35, 126.08, 127.91, 130.44, 133.56, 143.05, 150.90, 157.39.

$^{29}\text{Si}$  NMR ( $\text{C}_6\text{D}_6$ , 79.4 MHz)  $\delta$  -11.33. Mass spectrometry did not yield satisfactory results presumably due to the moisture sensitivity of **3**.

**(E)-1,2-Bis(1,1,3,3,5,5,7,7-octaethyl-s-hydrindacen-4-yl)-1,2-diphenyldisilene (1).**

To a solution of **3** (169.4 mg, 0.262 mmol) in THF (distilled from sodium/benzophenone ketyl, 3.0 mL) was added a THF solution of lithium naphthalenide (1.0 M, 0.58 mL, 0.58 mmol) dropwise at  $-78^\circ\text{C}$ . After stirring for 4.5 h at  $0^\circ\text{C}$ , the reaction mixture was allowed to warm to ambient temperature and concentrated in vacuo to give yellow solid. In a glove box filled with argon, toluene (Wako, degassed by three freeze-pump-thaw cycles, 5.0 mL) was added to the crude product. The resulting orange suspension was filtered through a plug of Celite<sup>®</sup> and rinsed with toluene (ca. 15 mL). The filtrate was concentrated in vacuo and the crude solid was dried under reduced pressure for 3.5 h to remove naphthalene. The residual solid was washed with hexane (distilled from sodium/benzophenone ketyl) several times to give analytically pure **1** (96.9 mg, 99.5  $\mu\text{mol}$ , 76% yield) as orange powder: mp (MP-S3, in sealed tube)  $286\text{--}290^\circ\text{C}$  (dec).  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 300 MHz)  $\delta$  0.85–1.06 (t  $\times$  4, overlapped, 48H), 1.65–1.89 (m, 16H), 1.95 (s, 8H) 2.30–2.42 (m, 4H), 2.46–2.59 (m, 10H), 6.89–6.99 (m, 6H), 7.06 (s, 2H), 7.32–7.36 (m, 4H).  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 67.9 MHz)  $\delta$  9.65, 9.72, 11.30, 11.65, 33.40, 33.45, 34.01, 34.22, 40.97, 48.18, 54.62, 121.99, 122.93, 126.03, 126.90, 127.84, 128.20, 128.36, 135.36, 139.42, 150.45, 156.78 (one peak is overlapped with a peak of  $\text{C}_6\text{D}_6$ ).  $^{29}\text{Si}$  NMR ( $\text{C}_6\text{D}_6$ , 53.6 MHz)  $\delta$  63.19. MS (FAB)  $m/z$ : 972 [ $M^+$ ]. HRMS (FAB) Calcd for  $\text{C}_{68}\text{H}_{100}\text{Si}_2$ : 972.7364. Found: 972.7372. Anal. Calcd for  $\text{C}_{68}\text{H}_{100}\text{Si}_2$ : C, 83.88; H, 10.35. Found C, 83.73; H, 10.40. UV-vis (hexane)  $\lambda_{\text{max}}$  ( $\epsilon$ ): 461 nm ( $2.4 \times 10^4$ ), 293 nm ( $1.2 \times 10^4$ ).

**1,4-Bis{(1,1,3,3,5,5,7,7-octaethyl-s-hydrindacen-4-yl)silyl}benzene (14).** To a solution of 1,4-dibromobenzene (318 mg, 1.35 mmol) in dry THF (5.0 mL) was added *t*-BuLi (1.2 M solution in pentane, 4.65 mL, 5.58 mmol) dropwise at  $-78^\circ\text{C}$  over 15 min, and the resulting yellow suspension was stirred for 1 h at this temperature to give a suspension of 1,4-dilithiobenzene. To the suspension was added **12** (1.00 g, 2.43 mmol) in dry THF (10.0 mL) dropwise at  $-78^\circ\text{C}$ . After addition was complete, the reaction mixture was allowed to warm to ambient temperature and stirred for 12 h. The solvents were removed under reduced pressure to provide a pale yellow paste. Hexane (15 mL) and toluene (10 mL) was added, and the resulting suspension was filtered through a plug of Celite<sup>®</sup>. The filtrate was evaporated and the residue was subjected to short path column (silica gel, toluene as eluent) to give 1.14 g of colorless powder. The mixture was recrystallized from hexane to afford

487 mg of **14** (0.541 mmol, 45% yield). The residue was subjected to preparative GPC (eluted with toluene) to give **14** (270 mg, 0.300 mmol, 25% yield based on Eind-SiH<sub>3</sub>); total 756.9 mg, 0.841 mmol, 69% yield (based on **12**): mp (MPA100) 220.5 °C (dec). <sup>1</sup>H NMR (C<sub>6</sub>D<sub>6</sub>, 300 MHz) δ 0.80 (t, *J* = 7.5 Hz, 24H), 0.91 (t, *J* = 7.5 Hz, 24H), 1.59–1.76 (m, 16H), 1.85 (s, overlapped, 8H), 1.85–1.96 (m, overlapped, 8H), 2.04–2.15 (m, 8H), 5.62 (satellite, <sup>1</sup>*J*<sub>SiH</sub> = 196 Hz, 4H), 6.94 (s, 2H), 7.40 (s, 4H). <sup>13</sup>C{<sup>1</sup>H} NMR (C<sub>6</sub>D<sub>6</sub>, 67.9 MHz) δ 9.57, 10.28, 33.78, 34.29, 44.01, 47.73, 53.92, 122.21, 123.33, 134.94, 135.96, 149.62, 155.91. <sup>29</sup>Si NMR (INEPT, C<sub>6</sub>D<sub>6</sub>, 53.6 MHz) δ –48.54. MS (FAB) *m/z*: 899 [*M*<sup>+</sup>]. HRMS (FAB) Calcd for C<sub>62</sub>H<sub>98</sub>Si<sub>2</sub>: 898.7207. Found: 898.7252. Anal. Calcd for C<sub>62</sub>H<sub>98</sub>Si<sub>2</sub>: C, 82.78; H, 10.98. Found C, 82.59; H, 11.02.

**1,4-Bis{dibromo(1,1,3,3,5,5,7,7-octaethyl-*s*-hydrindacen-4-yl)silyl}benzene (4).** To a solution of **13** (401 mg, 0.446 mmol) in dry hexane (40 mL) was added carbon tetrabromide (604 mg, 1.82 mmol) in one portion at room temperature, and the mixture was stirred for 3.5 d. After removal of solvent, the resulting pale yellow paste was dried under reduced pressure for 3 h to sublime the residual carbon tetrabromide to give pale yellow powder. To the crude solid was added dry toluene (20 mL) and filtered through a plug of Celite®, and rinsed with dry toluene (3 mL) under an argon atmosphere. The filtrate was evaporated to give 557 mg of crude product as pale yellow powders. The crude product was recrystallized from dry hexane to give 369.9 mg of **4** (0.304 mmol, 68% yield) as moisture-sensitive colorless crystals (*Note: compound 4 is found to be extremely sensitive toward moisture as 3*): <sup>1</sup>H NMR (C<sub>6</sub>D<sub>6</sub>, 300 MHz) δ 0.81, 0.85 (t × 2, *J* = 7.2 Hz, 24H), 1.58–1.74 (m, 16H, overlapped), 1.77 (s, overlapped, 8H), 2.18 (q, *J* = 7.2 Hz, 16H), 6.96 (s, 2H), 7.65 (s, 4H). <sup>13</sup>C{<sup>1</sup>H} NMR (C<sub>6</sub>D<sub>6</sub>, 67.9 MHz) δ 9.44, 10.36, 33.89, 33.93, 44.13, 47.95, 54.99, 124.48, 125.40, 132.54, 145.56, 150.96. <sup>29</sup>Si NMR (C<sub>6</sub>D<sub>6</sub>, 53.6 MHz) δ –12.35. Anal. Calcd for C<sub>62</sub>H<sub>94</sub>Br<sub>4</sub>Si<sub>2</sub>: C, 61.28; H, 7.80. Found C, 61.11; H, 7.85. Mass spectrometry did not yield satisfactory results presumably due to the moisture sensitivity of **4**.

**Reductive cross-coupling reaction of 3 and 4.** To a solution of **3** (412.7 mg, 0.638 mmol) and **4** (150.3 mg, 0.124 mmol) in THF (distilled from sodium/benzophenone ketyl, 10.0 mL) was added a THF solution of lithium naphthalenide (1.0 M, 1.9 mL, 1.9 mmol) dropwise at –78 °C. Color of the reaction mixture was immediately changed to bright orange and later dark red. The resulting mixture was stirred for 30 min at –78 °C, and then stirred at 0 °C for 1.5 h. Then the reaction mixture was allowed to warm to ambient temperature and stirred 13.5 h and the resulting mixture was concentrated in vacuo. In a

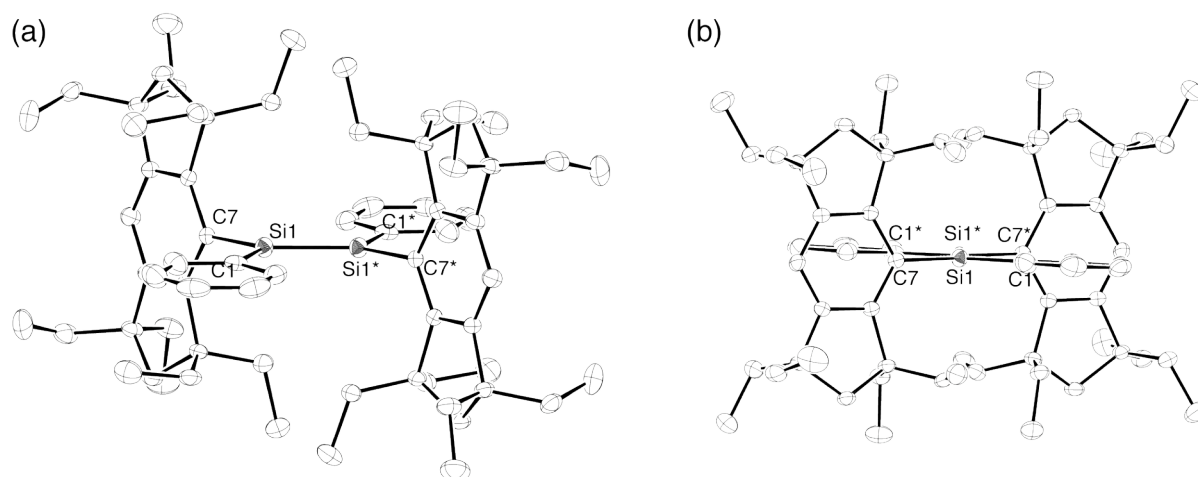


glove box filled with argon, hexane (Wako, degassed by three freeze-pump-thaw cycles, 15 mL) was added to the crude product. The resulting deep purple suspension was filtered through a membrane filter and washed with hexane (25 mL). The filtrate was concentrated in vacuo to give purple solids, which was subsequently subjected to column chromatography (silica gel, Fuji Silysia PSQ100: finely dried and degassed) in a glove box using degassed hexane as eluent to give the yellow fraction, followed by eluting with toluene to afford the red fraction. The first yellow fraction, after evaporation of hexane, was subjected to sublimation in vacuo to remove naphthalene. To the residue was added a small amount of hexane, and filtered to afford almost pure **1** (109.6 mg, 0.113 mmol, 35% yield based on **3**). The second red fraction after column chromatography was concentrated, followed by washing thoroughly with hexane (5 mL) to afford almost pure **2** (35.2 mg, 18.8  $\mu$ mol, 15% yield based on **4**) as purplish red powders. Recrystallization of this powder from hot toluene to afford analytically pure tetrasiladistyrylbenzene **2**: mp (MPA100, in sealed tube) > 255 °C. (The complete loss of color was observed at 255 °C without melting.) Anal. Calcd for C<sub>130</sub>H<sub>194</sub>Si<sub>4</sub>: C, 83.53; H, 10.46. Found C, 83.59; H, 10.56. UV-vis (hexane)  $\lambda_{\text{max}}$  ( $\epsilon$ ): 543 nm ( $3.0 \times 10^4$ ). NMR spectroscopy did not afford satisfactory resolution due to the pure solubility of **2**.

## 2. X-ray Crystallographic analysis

### X-ray Data Collection of 1.

Crystal data: Formula  $C_{68}H_{100}Si_2$ , MW = 973.66, space group  $P2_1/n$  (#14),  $a = 12.639(5)$  Å,  $b = 14.481(5)$  Å,  $c = 16.752(7)$  Å,  $\beta = 105.982(6)^\circ$ ,  $V = 2948(2)$  Å<sup>3</sup>,  $Z = 2$ ,  $D_{\text{cald}} = 1.097$  g cm<sup>-3</sup>,  $\mu = 0.099$  mm<sup>-1</sup>;  $R_1(I > 2\sigma(I)) = 0.0779$ ,  $wR_2$  (all data) = 0.1835, GOF = 1.228 for 5485 reflections and 324 parameters. Orange and prismatic single crystals of **1** were grown by the slow evaporation of its benzene solution in a glove box filled with argon at room temperature. The intensity data were collected on a Rigaku Saturn CCD diffractometer with graphite monochromator MoK $\alpha$  radiation ( $\lambda = 0.71070$  Å) to  $2\theta_{\text{max}} = 51^\circ$  at 173 K. The structure was solved by direct methods (SIR97)<sup>3</sup> and refined by full-matrix least-squares procedures on  $F^2$  for all reflections (SHELX-97)<sup>4</sup>. All hydrogen atoms were placed using AFIX instructions, while all the other atoms were refined anisotropically.

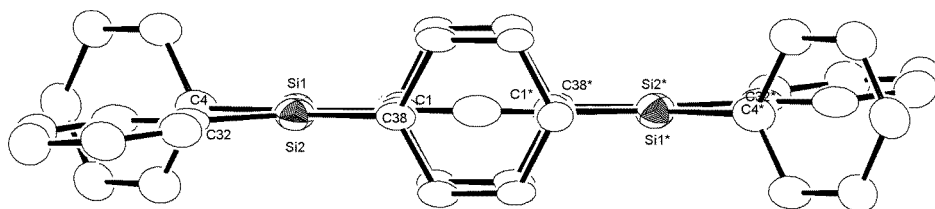


**Figure S1.** ORTEP drawing of compound **1** (50% probability for thermal ellipsoids): (a) side view and (b) Newman projection. The Si=Si axis is perpendicular to the plane of the paper. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and bond angles ( $^\circ$ ): Si1–Si1\* = 2.1593(16), Si1–C1 = 1.873(3), Si1–C7 = 1.910(3), C1–Si1–Si1\* = 119.07(10), C1–Si1–C7 = 118.14(12), C7–Si1–Si1\* = 127.71(10). The twist angle and the *trans*-bent angle are 3.26 $^\circ$  and 2.7 $^\circ$ , respectively.

### X-ray Data Collection of 2.

Crystal data: Formula  $C_{130}H_{194}Si_4$ , MW = 1869.21, space group  $P-1$  (#2),  $a = 11.6011(6)$  Å,  $b = 16.1550(8)$  Å,  $c = 17.1708(9)$  Å,  $\alpha = 114.6710(10)^\circ$ ,  $\beta = 99.850(2)^\circ$ ,  $\gamma = 95.161(2)^\circ$ ,  $V = 1834.0(3)$  Å<sup>3</sup>,  $Z = 1$ ,  $D_{\text{cald}} = 1.095$  g cm<sup>-3</sup>,  $\mu = 0.101$  mm<sup>-1</sup>;  $R_1(I > 2\sigma(I)) = 0.1055$ ,  $wR_2$  (all data) = 0.3108, GOF = 1.024 for 17935 reflections and 610 parameters with 2 restraints. Red and platelet single crystals of **2** were grown by the slow evaporation of its benzene solution in a glove

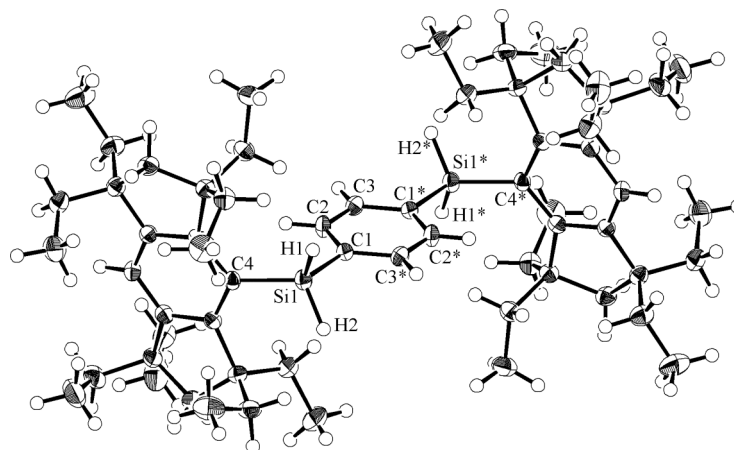
box filled with argon at room temperature. The intensity data were collected on a Rigaku Saturn CCD diffractometer with graphite monochromator MoK $\alpha$  radiation ( $\lambda = 0.71070$  Å) to  $2\theta_{\max} = 50^\circ$  at 100 K. The structure was solved by direct methods (SIR97) and refined by full-matrix least-squares procedures on  $F^2$  for all reflections (SHELX-97). All hydrogen atoms were placed using AFIX instructions, while all the other atoms except for disordered part were refined anisotropically.



**Figure S2.** Newman projection of compound **2**. The fused cyclopentene rings of Eind group as well as hydrogen atoms are omitted for clarity. Two Si=Si axes are perpendicular to the plane of the paper.

#### X-ray Data Collection of **14**.

Crystal data: Formula C<sub>62</sub>H<sub>98</sub>Si<sub>2</sub> MW = 899.58, space group  $P2_1/n$  (#14),  $a = 15.219(9)$  Å,  $b = 10.322(6)$  Å,  $c = 18.063(11)$  Å,  $\beta = 91.762(13)^\circ$ ,  $V = 2836(3)$  Å<sup>3</sup>,  $Z = 2$ ,  $D_{\text{calc}} = 1.053$  g cm<sup>-3</sup>,  $\mu = 0.098$  mm<sup>-1</sup>;  $R_1(I > 2\sigma(I)) = 0.0717$ ,  $wR_2$  (all data) = 0.1398, GOF = 1.189 for 4957 reflections and 305 parameters. Colorless and prismatic single crystals of **14** were grown by the slow evaporation of its benzene solution at room temperature. The intensity data were collected on a Rigaku Saturn CCD diffractometer with graphite monochromator MoK $\alpha$  radiation ( $\lambda = 0.71070$  Å) to  $2\theta_{\max} = 50^\circ$  at 173 K. The structure was solved by direct methods (SIR97) and refined by full-matrix least-squares procedures on  $F^2$  for all reflections (SHELX-97). All hydrogen atoms were placed using AFIX instructions, while all the other atoms were refined anisotropically.



**Figure S3.** ORTEP drawing of compound **11** (50% probability for thermal ellipsoids).

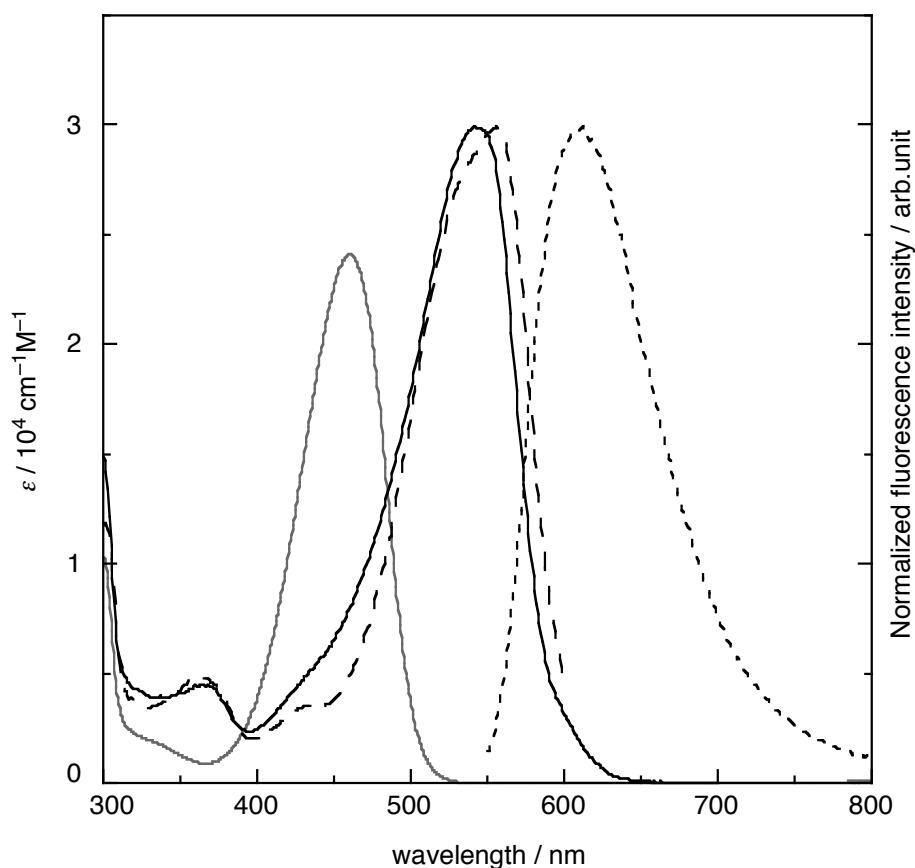
### 3. Photophysical Data

**Measurements.** UV-vis absorption spectra of Si-OPVs **1** and **2** were recorded on a Perkin Elmer Lambda 900 UV/VIS/NIR Spectrometer or a Shimadzu UV-3150 Spectrometer with a resolution of 0.5 nm. Ca.  $10^{-5}$  M of the sample solutions in a 1 cm square quartz cell were used for room temperature measurements. Fluorescence spectra of **2** were recorded on a HITACHI F-4500 Spectrophotometer. Absolute fluorescence quantum yield was determined by a calibrated integrating sphere system C-9920-02 (Hamamatsu Photonics). Fluorescence lifetime was measured on a Picosecond Fluorescence Lifetime Measurement System C4780 (Hamamatsu Photonics) equipped with a dye laser (coumarin 307 in ethanol, 510 nm). Dry hexane (purchased from Kanto Chemicals) was degassed by three freeze-pump-thaw cycles before preparation of sample solution. Electronic spectra of **1** and **2** are shown in Figure S4, and the data are summarized in Table 1 and S1. The pictures of photoluminescence of compound **2** are shown in Figure S5.

The radiative rate constant  $k_r$  is known to be related to the extinction coefficient for absorption by the following equation<sup>5</sup>:

$$k_e^0 = 3 \times 10^{-9} \nu_{\max}^2 \int \epsilon d\nu$$

where  $\nu_{\max}$  is the energy corresponding to the absorption maximum, and the integral  $\int \epsilon d\nu$  is the quantity of area under a curve of the molecular extinction coefficient plotted against wavenumber. The integral  $\int \epsilon d\nu$  can be approximated by  $\epsilon_{\max} \Delta\nu_{1/2}$ , where  $\epsilon_{\max}$  is the molar extinction coefficient at the absorption maximum, and  $\Delta\nu_{1/2}$  is the half maximum full-width of the lowest energy absorption band in energy unit.



**Figure S4.** Electronic spectra of Si-OPVs **1** and **2** in *n*-hexane at ambient temperature. UV-vis absorption of **1** (gray) and **2** (black solid line), luminescence spectrum of **2** (black dotted line, excited at 460 nm), and excitation spectrum of **2** (black broken line, observed at 620 nm).

**Table S1.** Summary of UV-vis absorption spectra of **1** and **2**.

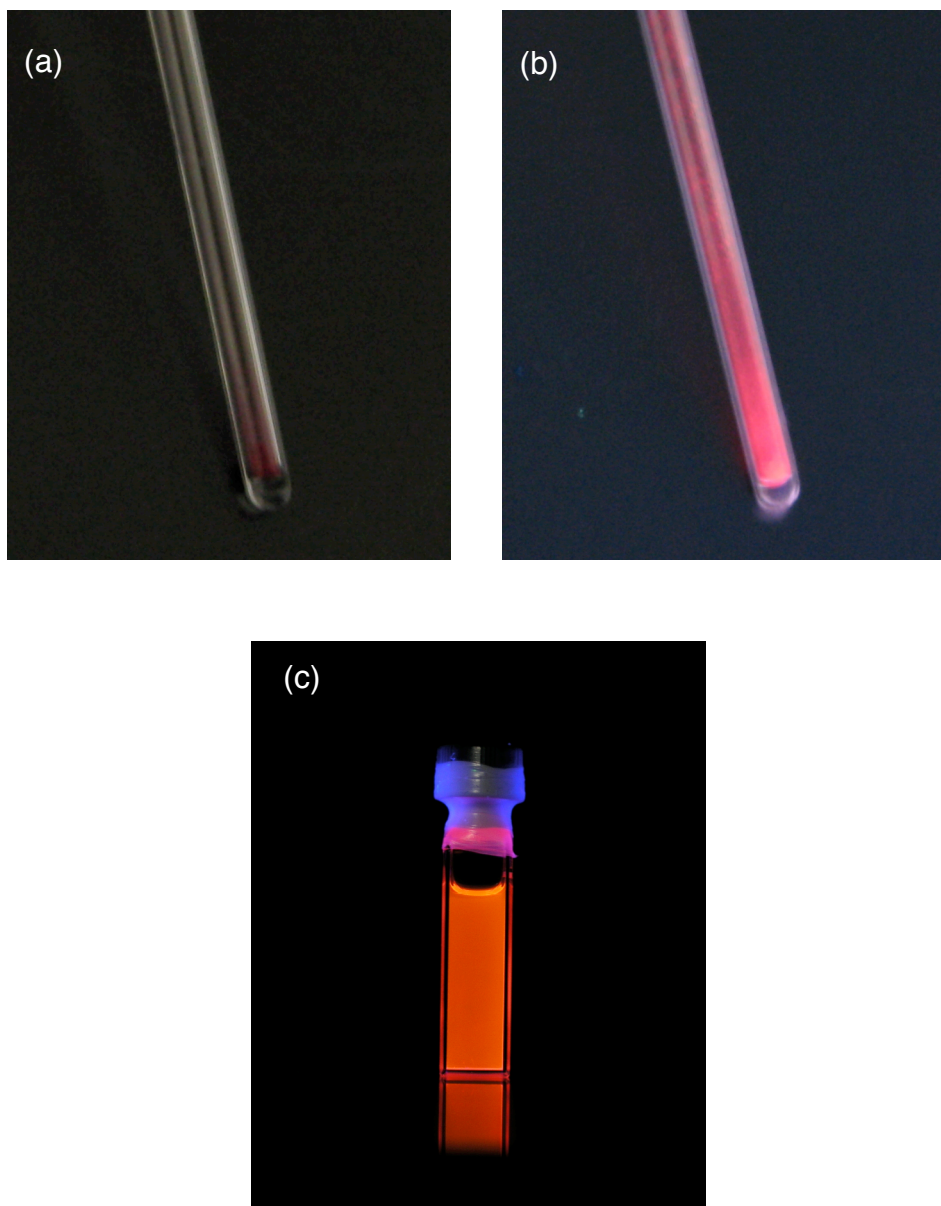
| compd    | $\lambda_{\max}/\text{nm}$ ( $\nu_{\max}/\text{cm}^{-1}$ ) | $\epsilon_{\max}/\text{cm}^{-1}\text{M}^{-1}$ | $\Delta\nu_{1/2}/\text{cm}^{-1}$ <sup>a</sup> | $\int \epsilon d\nu$ <sup>b</sup> | $k_{\text{e}}^0/\text{s}^{-1}$ <sup>c</sup> |
|----------|--|---|---|-----------------------------------|---|
| <b>1</b> | 461 (21700)  | $2.4 \times 10^4$                             | 3000  | $7.2 \times 10^7$                 | $1.0 \times 10^8$                           |
| <b>2</b> | 543 (18400)  | $3.0 \times 10^4$                             | 2800  | $8.4 \times 10^7$                 | $8.5 \times 10^7$                           |

<sup>a</sup> Half maximum full-width of the lowest energy absorption band.

<sup>b</sup> Peak area calculated with the following approximation formula:  $\int \epsilon d\nu \sim \epsilon_{\max} \Delta\nu_{1/2}$ .

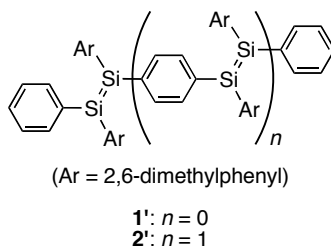
<sup>c</sup> Theoretical radiative rate constants are given from the following equation:

$$k_{\text{e}}^0 = 3 \times 10^{-9} \nu_{\max}^2 \int \epsilon d\nu$$



**Figure S5.** Photographs of compound **2**. (a) solid in sealed tube in the dark, (b) solid under irradiation at 254 nm, (c) solution in hexane under irradiation at 254 nm.

#### 4. Theoretical Calculations



Two model Si-OPVs, **1'** and **2'**, in which all of the Eind groups in **1** and **2** are replaced by 2,6-dimethylphenyl groups, were investigated.

The geometry optimizations of **1'** and **2'** were performed using Spartan 04 program<sup>6</sup> at the B3LYP/6-31G(d) level, with constraint where all disilene moieties and phenyl rings adopt coplanar geometry. The Cartesian coordinates of **1'** and **2'** are shown in Table S2 and S3, respectively. The plots of selected molecular orbitals of **1'** and **2'** are shown in Figure S6 and S7, respectively.

**Table S2.** Coordinates (Å) of the optimized structure for **1'** calculated at the B3LYP/6-31G(d) level with constraint.

| atom | <i>x</i>  | <i>y</i>  | <i>z</i>  | atom | <i>x</i>  | <i>y</i>  | <i>z</i>  |
|------|-----------|-----------|-----------|------|-----------|-----------|-----------|
| C    | 2.634394  | 0.085768  | -0.014811 | C    | -0.607236 | 3.150940  | 0.290392  |
| Si   | 0.838244  | 0.680476  | -0.102252 | C    | -0.721576 | 4.536301  | 0.377869  |
| Si   | -0.838244 | -0.680476 | 0.102252  | C    | 1.654579  | 4.759738  | 0.024575  |
| C    | 0.644384  | 2.534956  | 0.080066  | H    | 2.750795  | 2.933350  | -0.232444 |
| C    | -0.644384 | -2.534956 | -0.080066 | H    | -1.503087 | 2.542419  | 0.379637  |
| C    | -2.634394 | -0.085768 | 0.014811  | H    | -1.697250 | 4.985271  | 0.546940  |
| C    | -5.315666 | 0.762304  | -0.099724 | H    | 2.540144  | 5.381337  | -0.083028 |
| C    | -3.330475 | -0.076247 | -1.221784 | H    | 0.318242  | 6.428320  | 0.320132  |
| C    | -3.309378 | 0.319191  | 1.195521  | C    | 5.315666  | -0.762304 | 0.099724  |
| C    | -4.642604 | 0.741248  | 1.118488  | C    | 3.309378  | -0.319191 | -1.195521 |
| C    | -4.662642 | 0.352068  | -1.258891 | C    | 3.330475  | 0.076247  | 1.221784  |
| C    | -2.672052 | -0.518574 | -2.510339 | C    | 4.662642  | -0.352068 | 1.258891  |
| C    | -2.629130 | 0.319530  | 2.549449  | C    | 4.642604  | -0.741248 | -1.118488 |
| H    | -5.156294 | 1.048799  | 2.026151  | C    | 2.629130  | -0.319530 | -2.549449 |
| H    | -5.191043 | 0.361578  | -2.209278 | C    | 2.672052  | 0.518574  | 2.510339  |
| H    | -6.351086 | 1.090662  | -0.145116 | H    | 5.191043  | -0.361578 | 2.209278  |
| C    | 0.409412  | 5.347598  | 0.249249  | H    | 5.156294  | -1.048799 | -2.026151 |
| C    | 1.770059  | 3.371748  | -0.063324 | H    | 6.351086  | -1.090662 | 0.145116  |

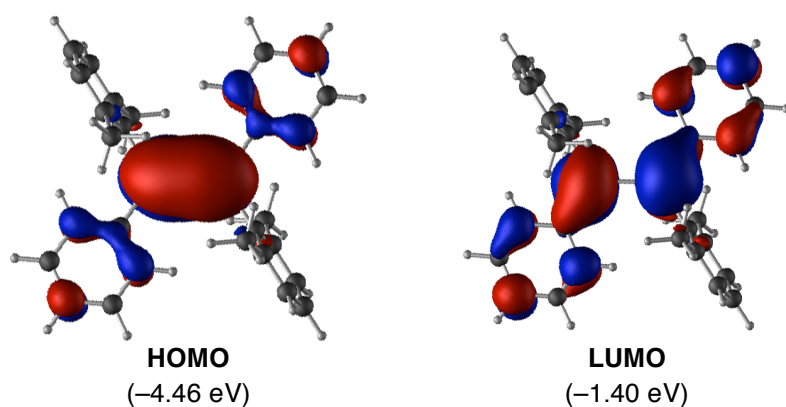
| (Table S2 continued) |           |           |           |   |           |           |           |
|----------------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C                    | -0.409412 | -5.347598 | -0.249249 | H | 1.855004  | -1.093818 | -2.613358 |
| C                    | 0.607236  | -3.150940 | -0.290392 | H | 3.354561  | -0.508298 | -3.347625 |
| C                    | -1.770059 | -3.371748 | 0.063324  | H | 2.240196  | 1.521826  | 2.416582  |
| C                    | -1.654579 | -4.759738 | -0.024575 | H | 3.395369  | 0.539175  | 3.332023  |
| C                    | 0.721576  | -4.536301 | -0.377869 | H | 1.855072  | -0.154251 | 2.797655  |
| H                    | 1.503087  | -2.542419 | -0.379637 | H | -2.138126 | -0.637284 | 2.762163  |
| H                    | -2.750795 | -2.933350 | 0.232444  | H | -3.354561 | 0.508298  | 3.347625  |
| H                    | -2.540144 | -5.381337 | 0.083028  | H | -1.855004 | 1.093818  | 2.613358  |
| H                    | 1.697250  | -4.985271 | -0.546940 | H | -2.240196 | -1.521826 | -2.416582 |
| H                    | -0.318242 | -6.428320 | -0.320132 | H | -1.855072 | 0.154251  | -2.797655 |
| H                    | 2.138126  | 0.637284  | -2.762163 | H | -3.395369 | -0.539175 | -3.332023 |

**Table S3.** Coordinates (Å) of the optimized structure for **2'** calculated at the B3LYP/6-31G(d) level with constraint.

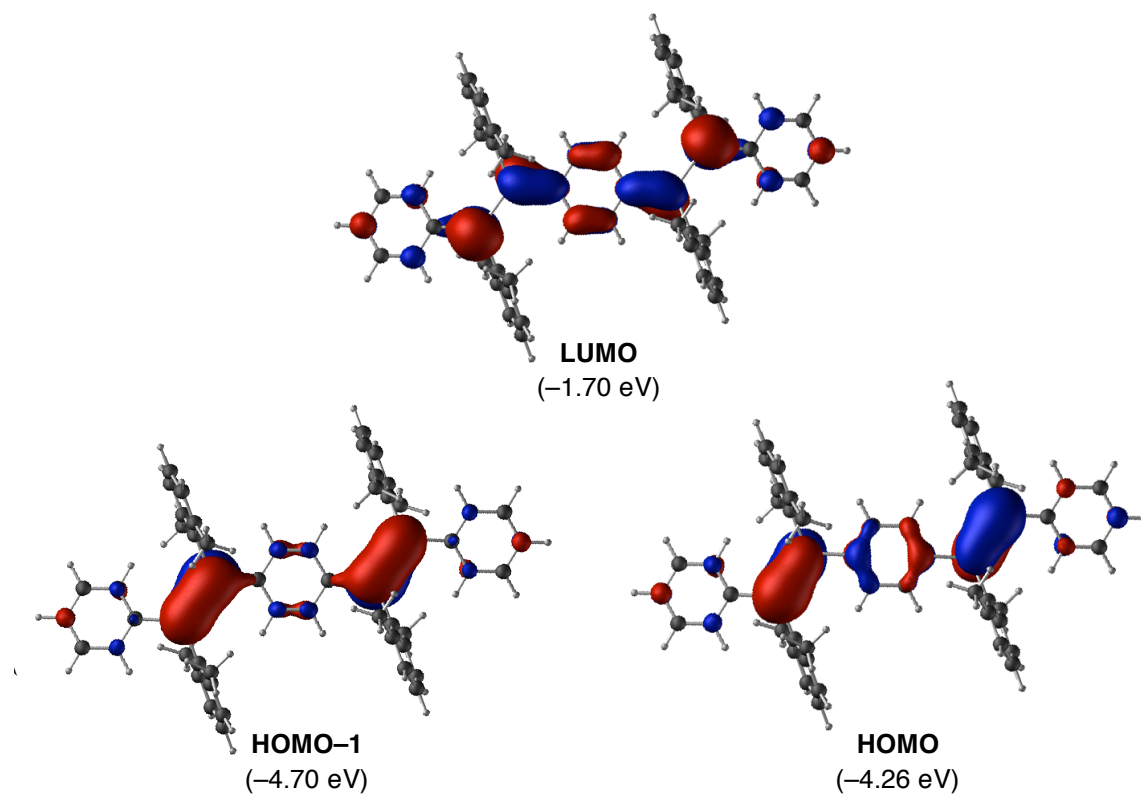
| atom | x        | y         | z         | atom | x         | y         | z         |
|------|----------|-----------|-----------|------|-----------|-----------|-----------|
| C    | 4.488222 | -2.467746 | 0.339152  | C    | 8.386776  | 1.522229  | 0.212550  |
| Si   | 4.802958 | -0.636832 | -0.030160 | C    | 8.952448  | -0.823318 | 0.178371  |
| Si   | 3.192467 | 0.818696  | -0.046792 | H    | 7.300923  | -2.192870 | 0.095088  |
| C    | 6.605524 | -0.143645 | 0.121798  | H    | 6.301076  | 2.003035  | 0.145237  |
| C    | 3.502328 | 2.651649  | -0.409507 | H    | 8.690116  | 2.565809  | 0.245200  |
| C    | 3.926376 | 5.377984  | -0.965904 | H    | 9.695777  | -1.616818 | 0.183560  |
| C    | 3.414398 | 3.134609  | -1.741310 | H    | 10.409194 | 0.766612  | 0.263824  |
| C    | 3.794772 | 3.559190  | 0.640832  | C    | 4.066221  | -5.192687 | 0.905095  |
| C    | 4.003976 | 4.912324  | 0.343277  | C    | 4.190836  | -3.378423 | -0.707148 |
| C    | 3.629472 | 4.493206  | -1.999168 | C    | 4.579274  | -2.946659 | 1.672379  |
| C    | 3.092357 | 2.213379  | -2.897795 | C    | 4.365434  | -4.304569 | 1.934808  |
| C    | 3.900018 | 3.115682  | 2.085818  | C    | 3.983277  | -4.730773 | -0.405056 |
| H    | 4.224903 | 5.605843  | 1.151239  | C    | 4.073563  | -2.938079 | -2.152059 |
| H    | 3.561032 | 4.857689  | -3.021415 | C    | 4.900528  | -2.021255 | 2.825534  |
| H    | 4.090291 | 6.431220  | -1.180017 | H    | 4.436171  | -4.665870 | 2.958032  |
| C    | 9.353230 | 0.512393  | 0.222926  | H    | 3.758184  | -5.426464 | -1.209970 |
| C    | 7.596106 | -1.146803 | 0.125248  | H    | 3.903298  | -6.245320 | 1.122873  |
| C    | 7.032611 | 1.199928  | 0.160535  | H    | 4.903579  | -2.289897 | -2.454951 |



| (Table S3 continued) |           |           |           |   |            |           |           |
|----------------------|-----------|-----------|-----------|---|------------|-----------|-----------|
| H                    | 3.149758  | -2.373329 | -2.328443 | H | -3.561032  | -4.857689 | -3.021415 |
| H                    | 4.061803  | -3.805118 | -2.820868 | H | -4.090291  | -6.431220 | -1.180017 |
| H                    | 5.843642  | -1.487524 | 2.660423  | C | -9.353230  | -0.512393 | 0.222926  |
| H                    | 4.987820  | -2.577702 | 3.764145  | C | -7.596106  | 1.146803  | 0.125248  |
| H                    | 4.122426  | -1.259187 | 2.953008  | C | -7.032611  | -1.199928 | 0.160535  |
| H                    | 3.065529  | 2.469616  | 2.380709  | C | -8.386776  | -1.522229 | 0.212550  |
| H                    | 3.907827  | 3.981606  | 2.756126  | C | -8.952448  | 0.823318  | 0.178371  |
| H                    | 4.820893  | 2.548564  | 2.269827  | H | -7.300923  | 2.192870  | 0.095088  |
| H                    | 2.149059  | 1.679438  | -2.733832 | H | -6.301076  | -2.003035 | 0.145237  |
| H                    | 3.869812  | 1.451371  | -3.029281 | H | -8.690116  | -2.565809 | 0.245200  |
| H                    | 3.004235  | 2.773422  | -3.834209 | H | -9.695777  | 1.616818  | 0.183560  |
| C                    | 1.393032  | 0.326633  | -0.168955 | H | -10.409194 | -0.766612 | 0.263824  |
| C                    | -1.393032 | -0.326633 | -0.168955 | C | -4.066221  | 5.192687  | 0.905095  |
| C                    | 0.954951  | -1.013469 | -0.171234 | C | -4.190836  | 3.378423  | -0.707148 |
| C                    | 0.399271  | 1.329727  | -0.174086 | C | -4.579274  | 2.946659  | 1.672379  |
| C                    | -0.954951 | 1.013469  | -0.171234 | C | -4.365434  | 4.304569  | 1.934808  |
| C                    | -0.399271 | -1.329727 | -0.174086 | C | -3.983277  | 4.730773  | -0.405056 |
| H                    | 1.679092  | -1.823773 | -0.161402 | C | -4.073563  | 2.938079  | -2.152059 |
| H                    | 0.693457  | 2.376684  | -0.178193 | C | -4.900528  | 2.021255  | 2.825534  |
| H                    | -1.679092 | 1.823773  | -0.161402 | H | -4.436171  | 4.665870  | 2.958032  |
| H                    | -0.693457 | -2.376684 | -0.178193 | H | -3.758184  | 5.426464  | -1.209970 |
| C                    | -4.488222 | 2.467746  | 0.339152  | H | -3.903298  | 6.245320  | 1.122873  |
| Si                   | -4.802958 | 0.636832  | -0.030160 | H | -4.903579  | 2.289897  | -2.454951 |
| Si                   | -3.192467 | -0.818696 | -0.046792 | H | -3.149758  | 2.373329  | -2.328443 |
| C                    | -6.605524 | 0.143645  | 0.121798  | H | -4.061803  | 3.805118  | -2.820868 |
| C                    | -3.502328 | -2.651649 | -0.409507 | H | -5.843642  | 1.487524  | 2.660423  |
| C                    | -3.926376 | -5.377984 | -0.965904 | H | -4.987820  | 2.577702  | 3.764145  |
| C                    | -3.414398 | -3.134609 | -1.741310 | H | -4.122426  | 1.259187  | 2.953008  |
| C                    | -3.794772 | -3.559190 | 0.640832  | H | -3.065529  | -2.469616 | 2.380709  |
| C                    | -4.003976 | -4.912324 | 0.343277  | H | -3.907827  | -3.981606 | 2.756126  |
| C                    | -3.629472 | -4.493206 | -1.999168 | H | -4.820893  | -2.548564 | 2.269827  |
| C                    | -3.092357 | -2.213379 | -2.897795 | H | -2.149059  | -1.679438 | -2.733832 |
| C                    | -3.900018 | -3.115682 | 2.085818  | H | -3.869812  | -1.451371 | -3.029281 |
| H                    | -4.224903 | -5.605843 | 1.151239  | H | -3.004235  | -2.773422 | -3.834209 |



**Figure S6.** Plots of selected MOs of **1'** (isosurface at  $\pm 0.03$  a.u.).



**Figure S7.** Plots of selected MOs of **2'** (isosurface at  $\pm 0.03$  a.u.).

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## 5. References and Notes

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