Supplementary Material (ESI) for Dalton Transactions
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Supporting Information for

Reactivity of an aryl-substituted silicon−silicon triple bond: 1,2-Disilabenzenes from the reaction of a 1,2-diaryldisilyne with alkynes

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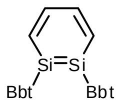
1



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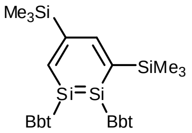

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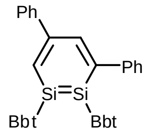

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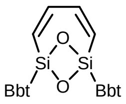

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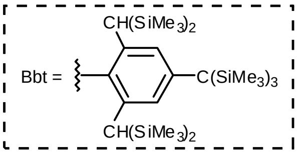

Experimental Section

General Procedure. All experiments were performed under an argon atmosphere unless otherwise noted. All solvents were purified by standard methods and/or The Ultimate Solvent System (Glass Contour Company)[S1] prior to use. NMR spectra were recorded on a JEOL JNM AL-300 spectrometer (300 MHz for ^{1}H; 75 MHz for ^{13}C NMR; 59 MHz for ^{29}Si NMR) using a C_6D_6 as a solvent. The chemical shifts are given in ppm relative to the standard as follows: residual C_6D_5H 7.16 ppm for ^{1}H NMR spectra, C_6D_6 central transition 128.0 ppm for ^{13}C NMR spectra, and external $SiMe_4$ 0.0 ppm for ^{29}Si spectra. Multiplicity of signals in ^{13}C NMR spectra was determined by DEPT technique. High-resolution mass spectral data were obtained on a JEOL JMS-700 spectrometer (FAB) or a Bruker micrOTOF (APPI-TOF). UV/Vis spectra were measured by a JASCO Ubest V-570. Melting points (uncorrected) were measured with a Yanaco micro melting point apparatus using sealed capillary tubes. Compound **1** was prepared according to the reported procedure.[S2]

Reaction of 1 with acetylene. Acetylene gas was generated by treating calcium carbide with degassed water under anaerobic condition, and dried through a column of phosphorus pentoxide. A valved NMR tube was charged with 20.2 mg (15.5 μmol) of **1** and 0.4 mL of *n*-hexane, and the solution was degassed by freeze-pump-thaw cycles. The solution was exposed to acetylene gas (1 atm) and shaken briefly at room temperature. The dark yellow color of the solution faded, and a light-yellow solution was obtained after 5 min. Volatiles were removed under vacuum, and the light-yellow residue was checked by NMR. The crude product was recrystallized from *n*-hexane. 13.2 mg (9.73 μmol, 63%) of **2** was afforded as light-yellow needles. **2**: Light-yellow crystals mp 317−318 °C (dec.); ^{1}H NMR (400 MHz, C_6D_6) δ 0.297, 0.301 (s, 72H, CH(Si*Me*$_3$)$_2$), 0.40 (s, 54H, C(Si*Me*$_3$)$_3$), 2.98 (s, 4H, C*H*Si), 7.05 (s, 4H, Bbt Ar*H*), 7.61−7.68 (m, 2H, CH=C*H*), 7.72−7.79 (m, 2H, C*H*=CH); ^{1}H NMR (300 MHz, C_6D_{12}) δ 0.10, 0.11 (s, 72H, CH(Si*Me*$_3$)$_2$), 0.33 (s, 54H, C(Si*Me*$_3$)$_3$), 2.77 (s, 4H, C*H*Si), 6.89 (s, 4H, Bbt Ar*H*), 7.46 (s, 4H, C*H*=C*H*); ^{13}C NMR (75 MHz, C_6D_6) δ 2.6, 3.1 (CH(Si*Me*$_3$)$_2$), 5.9 (C(Si*Me*$_3$)$_3$), 22.7 (*C*(SiMe$_3$)$_3$), 37.2 (*C*HSiMe$_3$), 127.2 (Bbt*C*(3,5)), 135.3 (Bbt*C*(1)), 135.8 (*C*H=CH), 146.3 (CH=*C*H), 148.0 (Bbt*C*(4)), 152.6 (Bbt*C*(2,6)); ^{13}C NMR (75 MHz, C_6D_{12}) δ 2.8, 3.3 (CH(Si*Me*$_3$)$_2$), 6.2 (C(Si*Me*$_3$)$_3$), 23.5 (*C*(SiMe$_3$)$_3$), 37.6 (*C*HSiMe$_3$), 127.7 (Bbt*C*(3,5)), 135.9 (Bbt*C*(1)), 136.0 (*C*H=CH), 146.7 (CH=*C*H), 148.3 (Bbt*C*(4)), 153.0 (Bbt*C*(2,6)); ^{29}Si NMR (59 MHz, C_6D_6) δ 1.0 (C(*Si*Me$_3$)$_3$), 1.5, 2.4 (CH(*Si*Me$_3$)$_2$), 57.1 (*Si*=*Si*); ^{29}Si NMR (59 MHz, C_6D_{12}) δ 0.9 (C(*Si*Me$_3$)$_3$), 1.4, 2.3 (CH(*Si*Me$_3$)$_2$), 56.8 (*Si*=*Si*); UV/Vis (*n*-hexane) λ_{max} (*n*-henxane)/nm 378 (ε/dm^3 mol^{-1} cm^{-1} 1.1 × 10^4); HRMS (ESI, [M+H]$^+$, *m/z*) Calcd for $C_{64}H_{139}Si_{16}$ 1355.7180, obsd: 1355.7129.

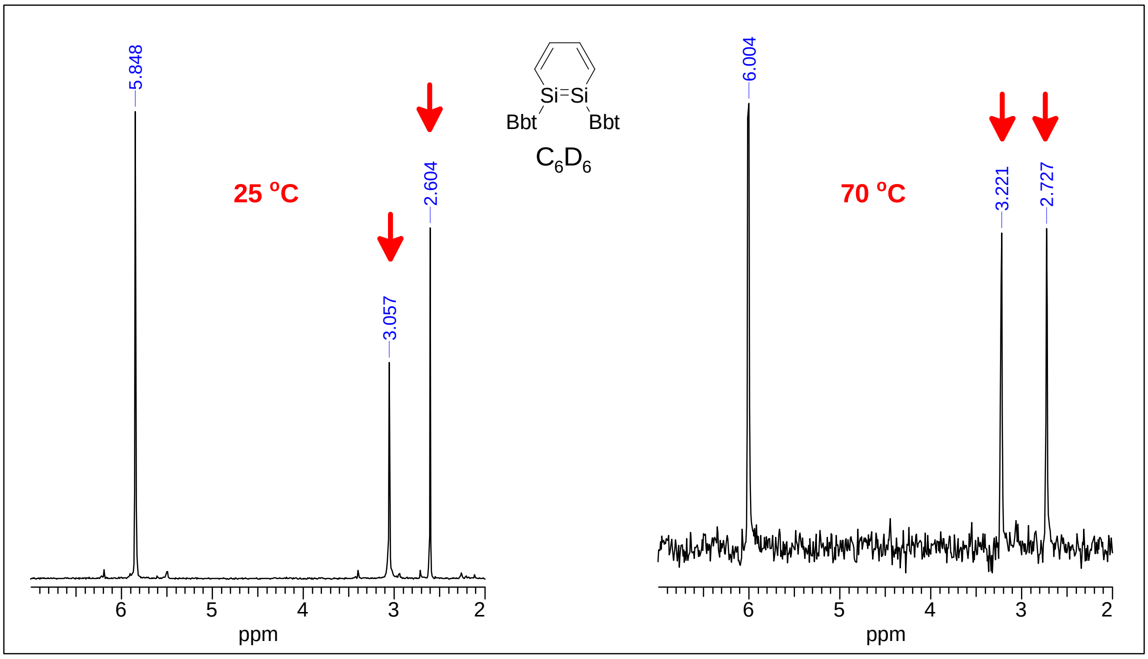

Fig. S-1. ^{13}C NMR spectra for **2** (trimethylsilyl regions) at room and elevated temperatures. The trimethylsilyl groups on *ortho* positions of Bbt groups were observed as two peaks due to the trans-bent character of **2**.

Reaction of 1 with trimethylsilylacetylene. To a *n*-hexane solution (0.4 mL) of **1** (20.2 mg, 15.5 μmol) was added 8.7 μL (61.9 μmol) of trimethylsilylacetylene. After the solution was stood at room temperature for 4 hr, an orange-yellow solution was obtained. Volatiles were removed under vacuum and the residue was analyzed by NMR (C_6D_6). Its NMR spectra suggested the formation of **3** as a major product. The crude product was recrystallized from *n*-hexane. 57.0 mg (38.0 μmol, 25%) of pure **3** was afforded as orange-yellow crystals. **3**: Orange-yellow crystals slowly changed to a green solid over 179 °C; ^{1}H NMR (300 MHz, C_6D_6) δ 0.24 (s, 27H, CH(Si*Me*$_3$)$_2$, ring Si*Me*$_3$), 0.27 (s, 18H, CH(Si*Me*$_3$)$_2$), 0.38 (br s, 45H, CH(Si*Me*$_3$)$_2$, C(Si*Me*$_3$)$_3$), 0.40 (s, 18H, CH(Si*Me*$_3$)$_2$), 0.43 (s, 27H, C(Si*Me*$_3$)$_3$), 0.48 (br s, 9H, ring Si*Me*$_3$), 2.65 (br s, 2H, C*H*Si), 2.84 (br s, 2H, C*H*Si), 7.00 (s, 2H, Bbt Ar*H*), 7.02 (s, 2H, Bbt Ar*H*), 8.28 (s, 1H, ring C*H*), 8.35 (s, 1H, ring C*H*); ^{13}C NMR (75 MHz, C_6D_6) δ 0.6, 3.3, 3.5, 3.97, 4.01, 4.3, (CH(Si*Me*$_3$)$_2$, ring Si*Me*$_3$), 5.4, 6.0 (C(Si*Me*$_3$)$_3$), 22.1, 22.6 (*C*(SiMe$_3$)$_3$), 36.2 (*C*HSiMe$_3$), 127.2 (d, Bbt*C*(3,5)), 128.3 (d, Bbt*C*(3,5)), 128.7 (s), 133.9 (s), 134.8 (s), 144.8 (d, ring *C*H), 147.1 (s), 148.0 (s), 148.4 (s), 150.3 (s) , 153.0 (s), 153.3 (d, ring *C*H); ^{29}Si NMR (59 MHz, C_6D_6) δ 0.87, 0.93 (C(*Si*Me$_3$)$_3$), −2.2, 0.3, 0.8, 2.2, 2.5, 3.6 (CH(*Si*Me$_3$)$_2$, ring *Si*Me$_3$), 64.1, 65.4 (*Si*=*Si*); HRMS (ESI, $[M+H]^+$, *m/z*) Calcd for $C_{70}H_{155}Si_{18}$ 1499.7970, obsd: 1499.7985.

Reaction of 1 with phenylacetylene. To a *n*-hexane solution (0.4 mL) of **1** (15.9 mg, 12.2 μmol) was added 5.4 μL (48.7 μmol) of phenylacetylene. After the solution was stood at room temperature for 2 hr, an orange solution was obtained. Volatiles were removed under vacuum and the residue was analyzed by NMR (C_6D_6). Its NMR spectra suggested formation of 3,5-diphenyl-1,2-bis(Bbt)-1,2-

disilabenzene (**4**) as a major product. All attempts for isolation of the product by recrystallization were failed due to high solubility and low crystallinity. The NMR data of **4** were collected from the crude mixture. **4**: ^{1}H NMR (300 MHz, C_6D_6) δ 0.07, 0.25, 0.29, 0.34 (s×4, 18×4H, CH(Si*Me*$_3$)$_2$), 0.38, 0.40 (s×2, 27×2H, C(Si*Me*$_3$)$_3$), 2.83 (s, 2H, C*H*Si), 2.93 (br s, 2H, C*H*Si), 7.03 (s, 4H, Bbt Ar*H*), 6.96-7.13 (m, 4H, Ph*H*), 7.24−7.31 (m, 4H, Ph*H*), 7.51 (d, ^3J = 7.5 Hz, 2H, Ph*H*), 7.76 (d, ^3J = 7.2 Hz, 2H, Ph*H*), 8.21 (d, ^4J = 2.2 Hz, 1H, ring C*H*), 8.26 (d ^4J = 2.2 Hz, 1H, ring C*H*); ^{13}C NMR (75 MHz, C_6D_6) δ 2.7, 2.8, 3.7, 4.0 (CH(Si*Me*$_3$)$_2$), 5.8, 6.0 (C(Si*Me*$_3$)$_3$), 22.8, 22.9 (*C*(SiMe$_3$)$_3$), 35.8, 35.9 (*C*HSiMe$_3$), 126.4 (s), 126.6 (s), 127.8 (d), 128.8 (d) 129.1 (d), 131.4 (s), 131.7 (d), 132.5 (s), 134.0 (s), 139.5 (d), 145.7 (s), 146.2 (s), 147.7 (s), 148.0 (s), 148.2 (s), 148.5 (s), 152.6 (s), 153.3 (s), 157.3 (s); ^{29}Si NMR (59 MHz, C_6D_6) δ 0.8, 1.0 (C(*Si*Me$_3$)$_3$), 1.1, 1.3, 2.2, 3.4 (CH(*Si*Me$_3$)$_2$), 55.0, 61.7 (*Si*=*Si*).

Reaction of 1 with 1,7-octadiyne. To a *n*-hexane solution (0.4 mL) of **1** (29.6 mg, 22.7 μmol) was added 5.9 μL (45 μmol) of 1,7-octadiyne. After the solution was stood at 3 ºC for 12 hr, a light-yellow solution was obtained. Volatiles were removed under vacuum and the residue was analyzed by NMR (C_6D_6). Its NMR spectra suggested formation of a complex mixture.

Reaction of 1 with bis(trimethylsilyl)acetylene. By the similar procedure for **1** with trimethylsilylacetylene, a *n*-hexane solution of **1** was reacted with 4 equiv of bis(trimethylsilyl)acetylene. After 8 hr at room temperature, volatiles were removed under vacuum. No change was observed in ^{1}H NMR spectrum.

Reaction of 2 with oxygen. A valved NMR tube was charged with 10.5 mg (7.74 μmol) of **2** and 0.4 mL of C_6D_6, and the solution was degassed by freeze-pump-thaw cycles. The solution was exposed to dry oxygen gas (1 atm) and shaken briefly at room temperature. The dark yellow color of the solution faded immediately, and a colorless solution was obtained after 1 min. The reaction mixture was checked by NMR, and it was confirmed that **2** changed to **6** quantitatively. **6**: Colorless crystals mp 340−1 °C; ^{1}H NMR (300 MHz, C_6D_6) δ 0.33 (s, 27H, C(Si*Me*$_3$)$_3$), 0.37 (s, 27H, C(Si*Me*$_3$)$_3$), 0.38 (s, 72H, CH(Si*Me*$_3$)$_2$), 2.64 (s, 4H, C*H*Si), 6.12−6.19 (m, 2H, CH=C*H*), 6.64−6.71 (m, 2H, C*H*=CH), 6.97 (s, 4H, Ar*H*); ^{13}C NMR (75 MHz, C_6D_6) δ 2.2, 2.6 (CH(Si*Me*$_3$)$_2$), 5.8 (C(Si*Me*$_3$)$_3$), 22.8 (*C*(SiMe$_3$)$_3$), 29.8 (*C*H$_2$), 127.4 (Ar*C*(3,5)), 128.8 (Ar*C*(1)), 135.9 (CH=*C*H), 142.6 (*C*H=CH), 148.9 (Ar*C*(4)), 151.8 (Ar*C*(2,6)); ^{29}Si NMR (59 MHz, C_6D_6) δ −10.1 (*Si*O), 1.1 (C(*Si*Me$_3$)$_3$), 2.0, 2.7 (CH(*Si*Me$_3$)$_2$); HRMS (FAB, M$^+$, *m/z*) Calcd for $C_{64}H_{138}O_2Si_{16}$ 1386.7000, obsd: 1386.7007.

X-ray crystallographic analyses of 2 and 6. The intensity data were collected on a Rigaku/MSC Mercury CCD diffractometer with graphite monochromated Mo*Kα* radiation (λ = 0.71070 Å). Single crystals suitable for X-ray analysis were obtained by cooling down the concentrated solutions (toluene solution for **2**; toluene and hexane mixed solution for **6**). A single crystal suitable for X-ray analysis was mounted on a glass fiber. In the case of air-sensitive compound, mounting was made in a glove-box (Ar). The structures were solved by a direct method (SIR-97[S3]) and refined by full-matrix least-squares procedures on F^2 for all reflections (SHELXL-97[S4]). All hydrogen atoms were placed using AFIX instructions, while all other atoms were refined anisotropically.

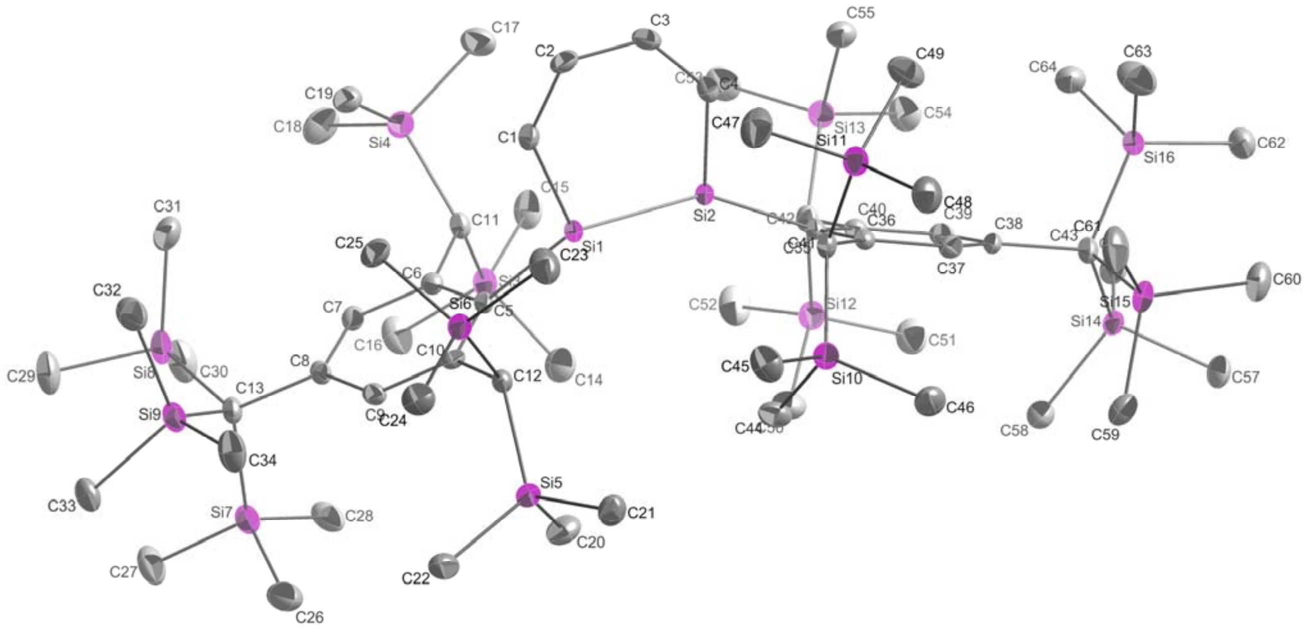

Figure S-2. Thermal ellipsoid (50%) drawing of [**2**·0.5(C_7H_8)]. Hydrogen atoms and solvate are omitted for clarity. Tris(trimethylsilyl)methyl group attached to C(38) is disordered, and one of them is shown.

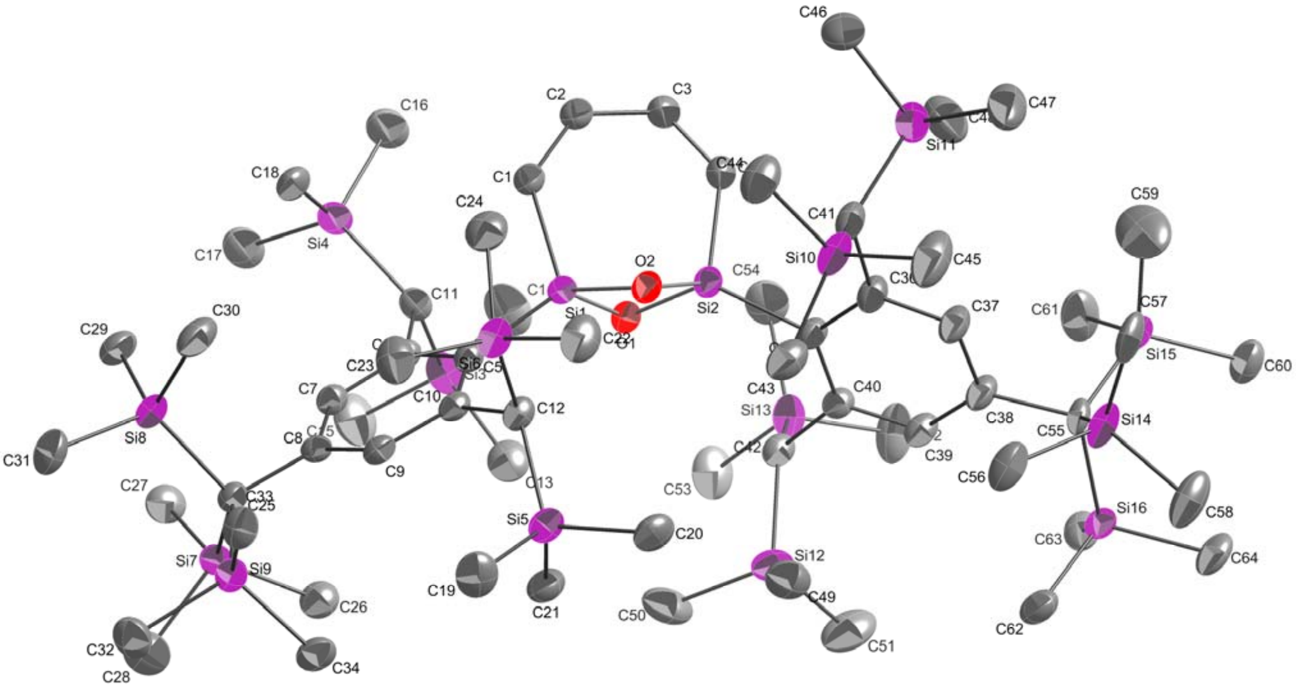

Figure S-3. Thermal ellipsoid (50%) drawing of [**6**·C_7H_8·C_6H_{14}]. Hydrogen atoms and solvates are omitted for clarity. Tris(trimethylsilyl)methyl group attached to C(38) is disordered, and one of them is shown.

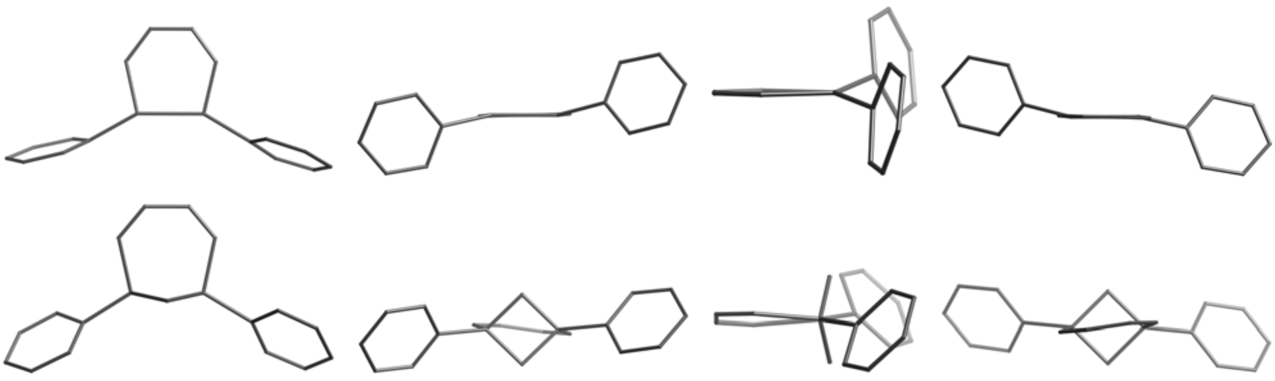

Figure S-4. Stick plots of **2** (top) and **6** (bottom) for geometrical comparison between the two compounds. Only skeletal structures were drawn for clarity.

Table S-1. Crystal data and structure refinement for [**2**·0.5(C_7H_8)].

Empirical formula	$C_{67.50}H_{142}Si_{16}$	
Formula weight	1403.25	
Temperature	103(2) K	
Wavelength	0.71075 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$ (#14)	
Unit cell dimensions	a = 18.524(2) Å	α = 90°.
	b = 12.0037(14) Å	β = 101.5916(14)°.
	c = 40.568(5) Å	γ = 90°.
Volume	8836.5(19) $Å^3$	
Z	4	
Density (calculated)	1.055 Mg/m^3	
Absorption coefficient	0.264 mm^{-1}	
$F(000)$	3084	
Crystal size	0.20 × 0.20 × 0.10 mm^3	
θ range for data collection	2.84 to 25.00°.	
Index ranges	$-22<=h<=22$, $-14<=k<=14$, $-47<=l<=48$	
Reflections collected	80148	
Independent reflections	15370 [R(int) = 0.0709]	
Completeness to θ = 25.00°	98.8 %	
Max. and min. transmission	0.9741 and 0.9492	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15370 / 0 / 879	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2σ(I)]	R_1 = 0.0441, wR_2 = 0.1243	
R indices (all data)	R_1 = 0.0492, wR_2 = 0.1284	
Largest diff. peak and hole	1.134 and −0.389 e.$Å^{-3}$	

Table S-2. Crystal data and structure refinement for [**6**·C_7H_8·C_6H_{14}].

Empirical formula	$C_{77}H_{160}O_2Si_{16}$	
Formula weight	1567.49	
Temperature	103(2) K	
Wavelength	0.71075 Å	
Crystal system	triclinic	
Space group	$P\overline{1}$ (#2)	
Unit cell dimensions	a = 16.8221(2) Å	α = 92.6933(4)°.
	b = 17.7685(2) Å	β = 111.9361(5)°.
	c = 18.7611(2) Å	γ = 107.5178(12)°.
Volume	4879.28(10) $Å^3$	
Z	2	
Density (calculated)	1.067 Mg/m^3	
Absorption coefficient	0.246 mm^{-1}	
F(000)	1724	
Crystal size	0.10 × 0.05 × 0.02 mm^3	
θ range for data collection	2.78 to 25.00°.	
Index ranges	$-19<=h<=19$, $-21<=k<=19$, $-22<=l<=22$	
Reflections collected	40744	
Independent reflections	16924 [R(int) = 0.0296]	
Completeness to θ = 25.00°	98.5 %	
Max. and min. transmission	0.9951 and 0.9758	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16924 / 108 / 1119	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2σ(I)]	R_1 = 0.0452, wR_2 = 0.1196	
R indices (all data)	R_1 = 0.0496, wR_2 = 0.1244	
Largest diff. peak and hole	0.498 and −0.543 e.$Å^{-3}$	

References

(S1) A. B. Pangborn, M. A. Giardello, R. H. Grubbs, R. K. Rosen and F. J. Timmers, *Organometallics*, 1996, **15**, 1518.

(S2) T. Sasamori, J. S. Han, K. Hironaka, N. Takagi, S. Nagase and N. Tokitoh, *Pure Appl. Chem.*, 2010, **82**, 603-612.

(S3) A. Altomare, M. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. Moliterni, G. Polidori and R. Spagna, *J. Appl. Cryst.*, 1999, **32**, 115.

(S4) (a) G. M. Sheldrick, *Acta Crystallogr. Sect. A* 1990, **46**, 467. (b) G. Sheldrick, SHELX-97 Program for Crystal Structure Solution and the Refinement of Crystal Structures, Institüt für Anorganische Chemie der Universität Göttingen, Tammanstrasse 4, D-3400 Göttingen, Germany, 1997.

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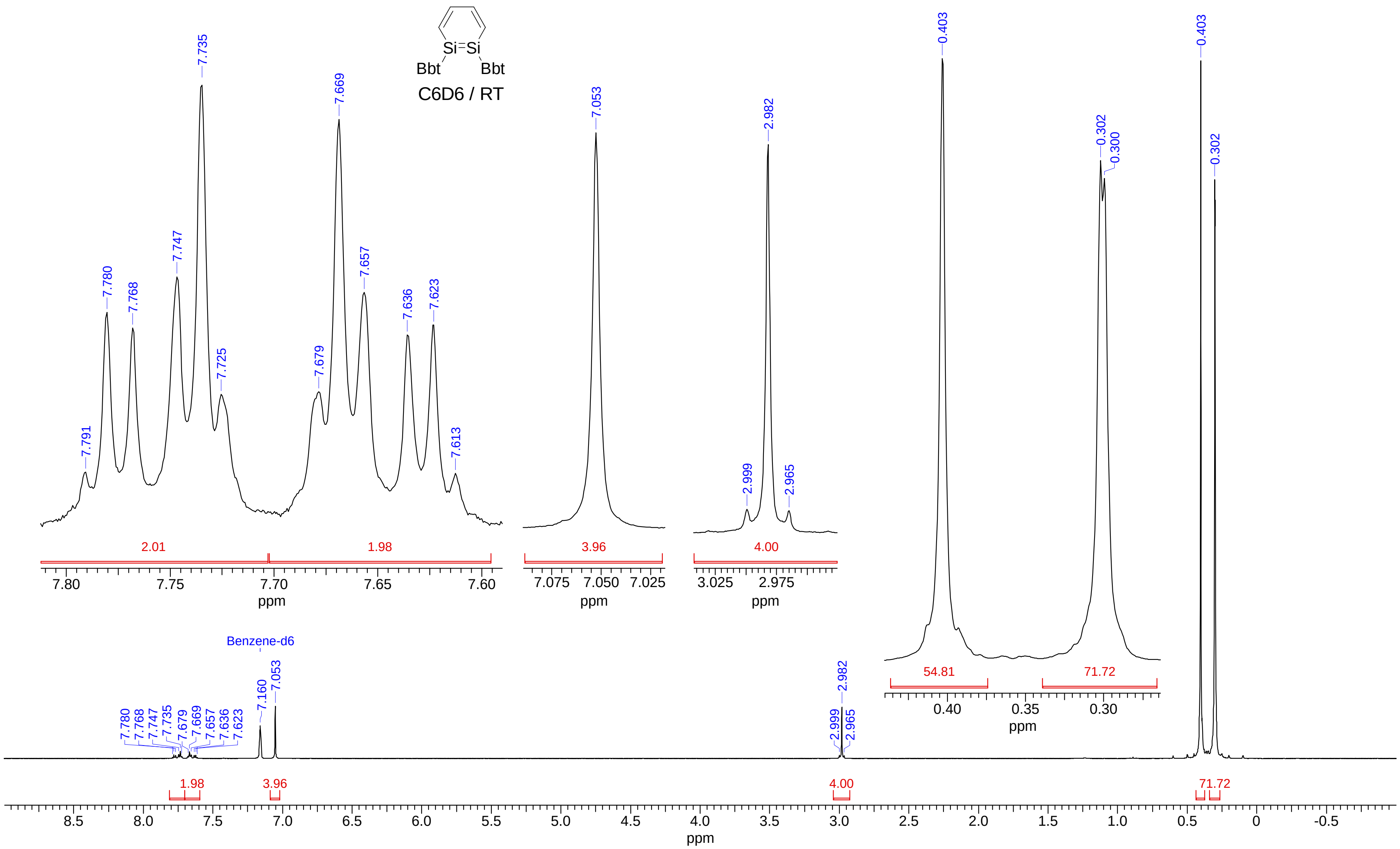

Fig. S-5. ^{1}H NMR spectrum of **2**.

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File Name	D:\HJS\KYOTO-U\NMR\091103-2-C2.DX			***Frequency (MHz)***	74.88	***Nucleus***	13C	***Origin***	JEOL
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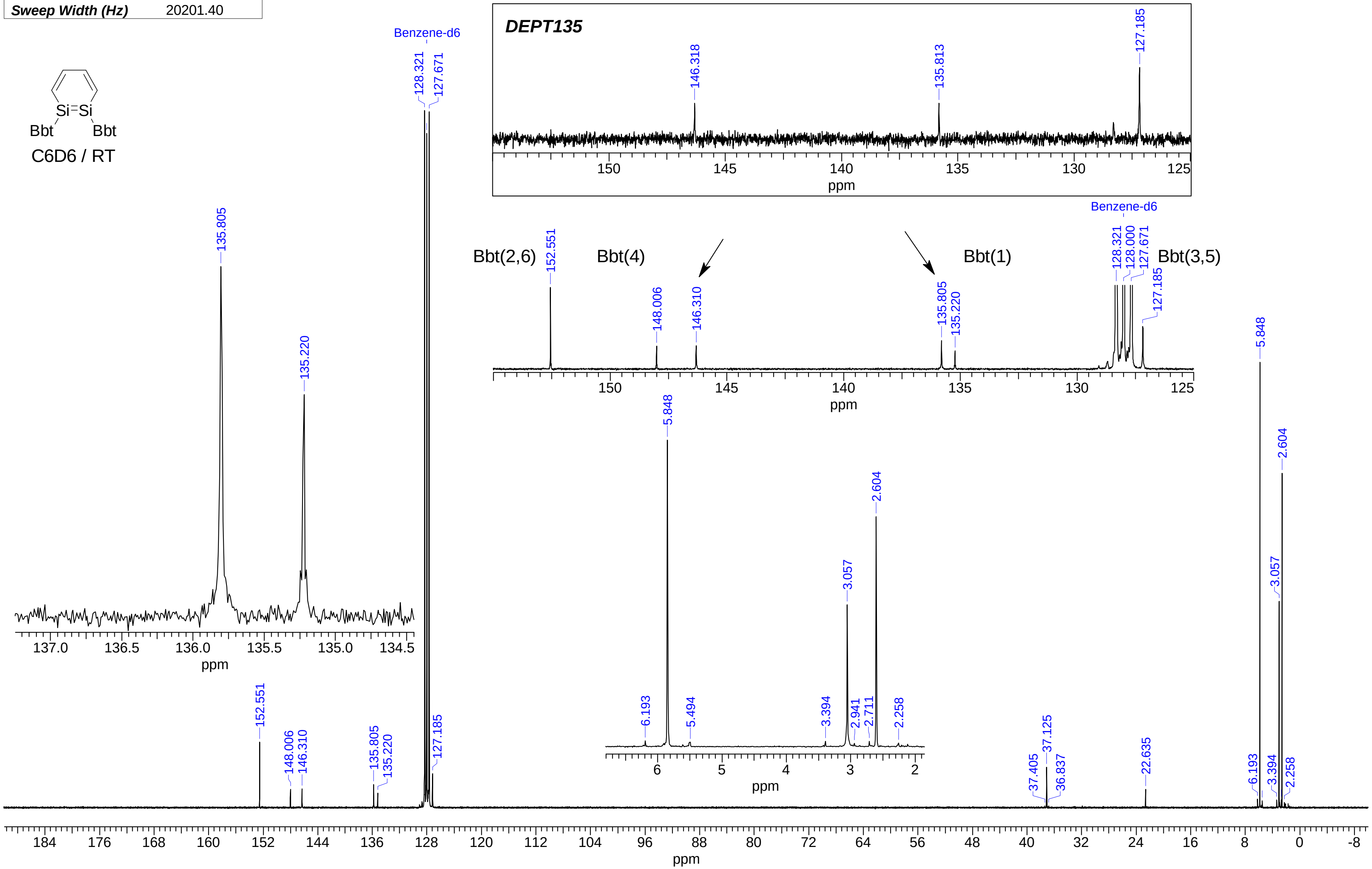

Fig. S-6. ^{13}C{^{1}H} and ^{13}C DEPT135 NMR spectra of **2**.

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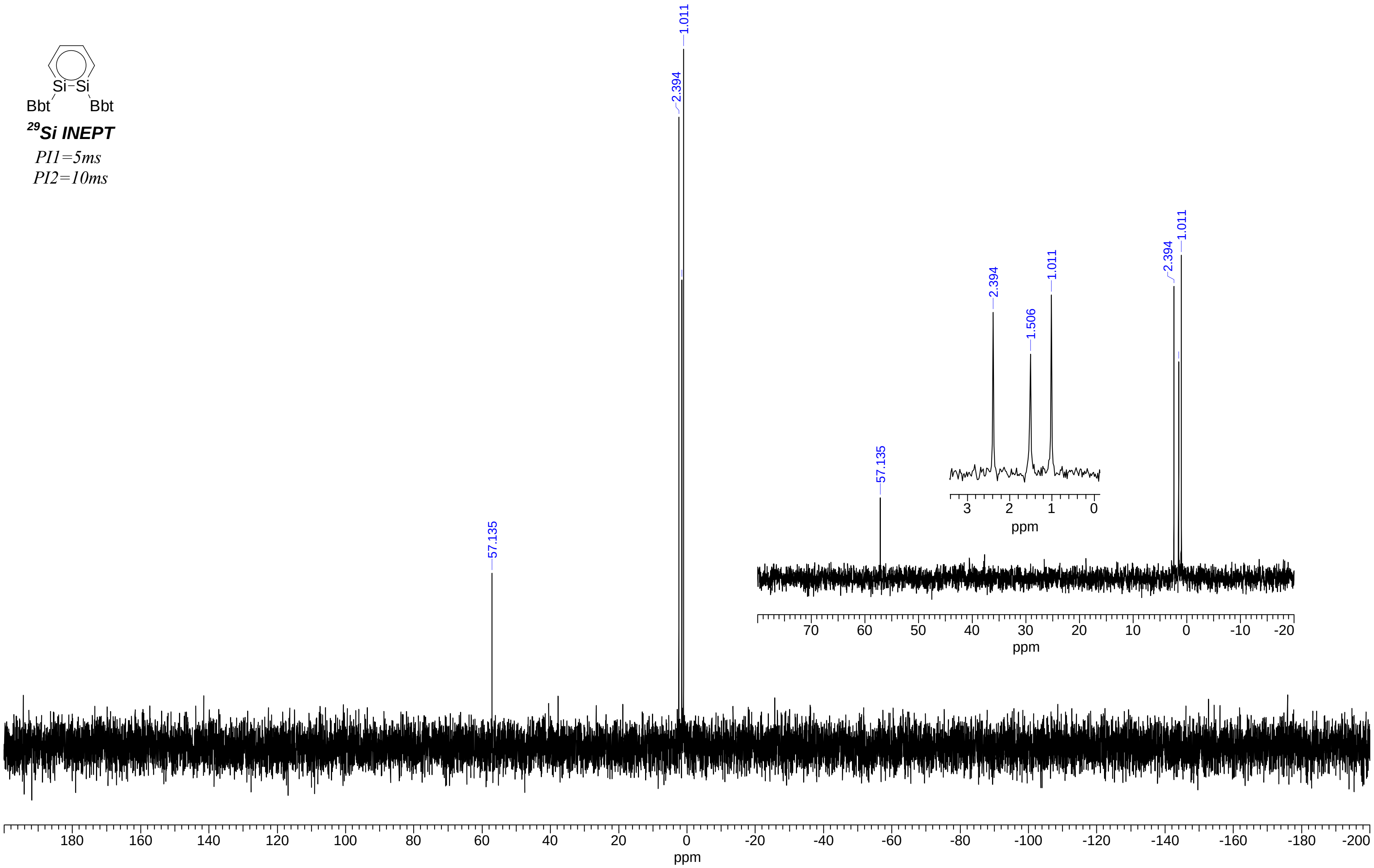

Fig. S-7. ^{29}Si INEPT NMR spectrum of **2**.

Origin	JASCO	**Owner**	icr	**File Name**	D:\HJS\KYOTO-U\UV\2-068 DISILABENZENE\2.4E4P.DX	**Date Stamp**	09/11/11 21:33:33
Date	11 Nov 2009 21:38:20			**Technique**	UV-Visible	**Instrument**	JASCO Corp., V-570, Rev. 1.00
Spectral Region	UV-Vis-NIR	**X Axis**	Wavelength (nanometers)	**Y Axis**	Absorbance	**Spectrum Range**	220.0000 - 800.0000
Points Count	581	**Data Spacing**	1.0000				

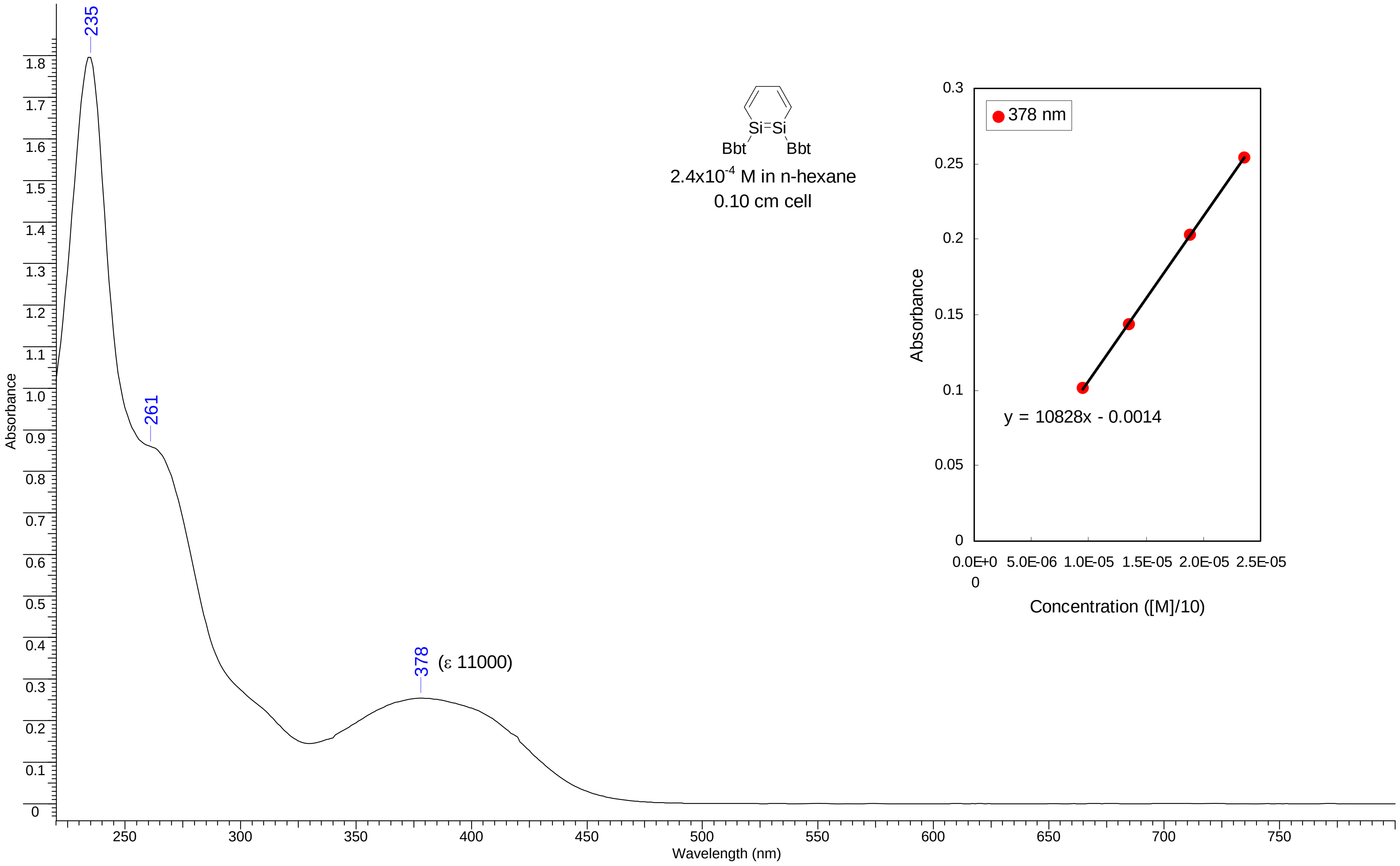

Fig. S-8. UV/Vis spectrum of **2**.

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Origin	JEOL

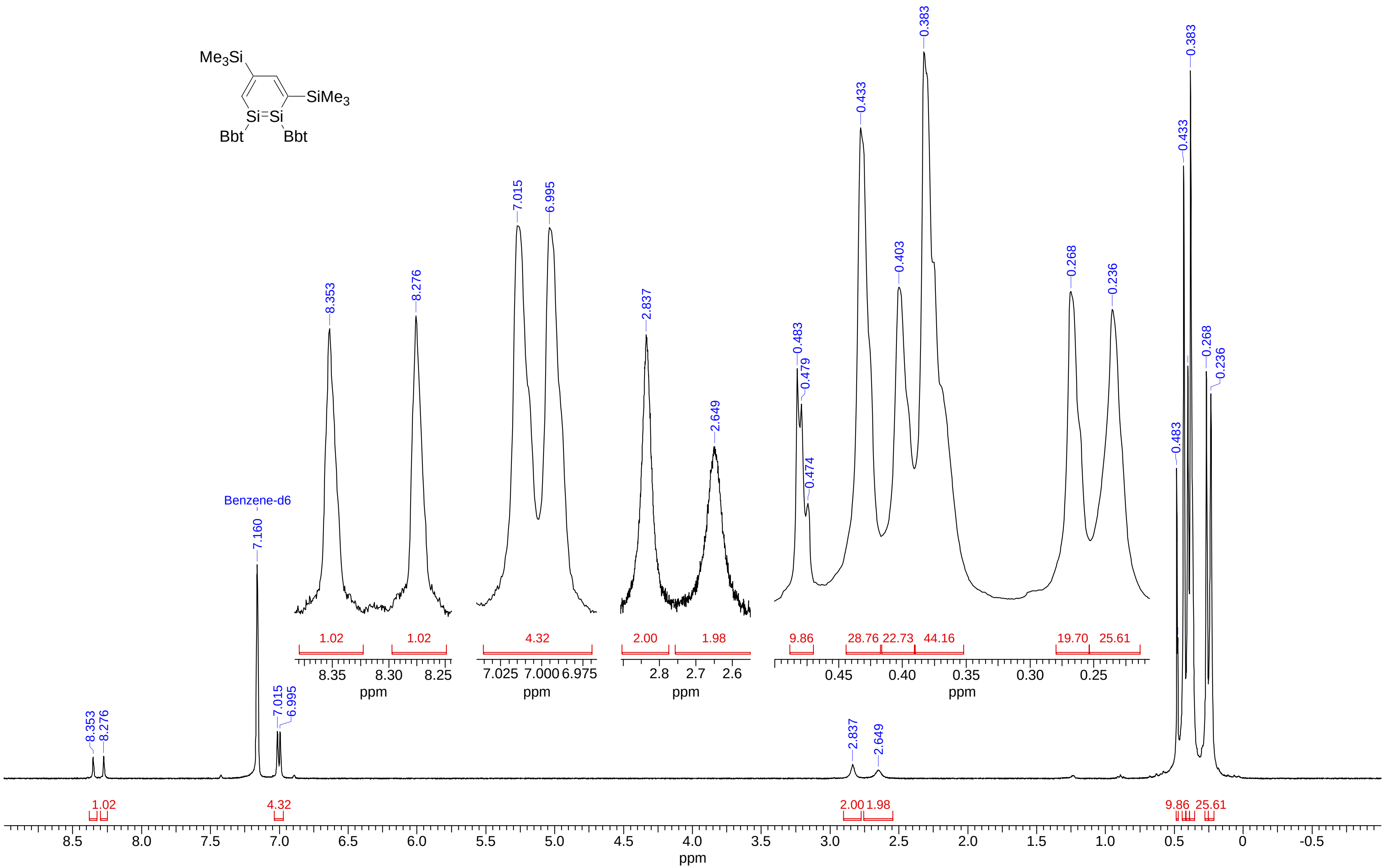

Fig. S-9. ^{1}H NMR spectrum of **3**.

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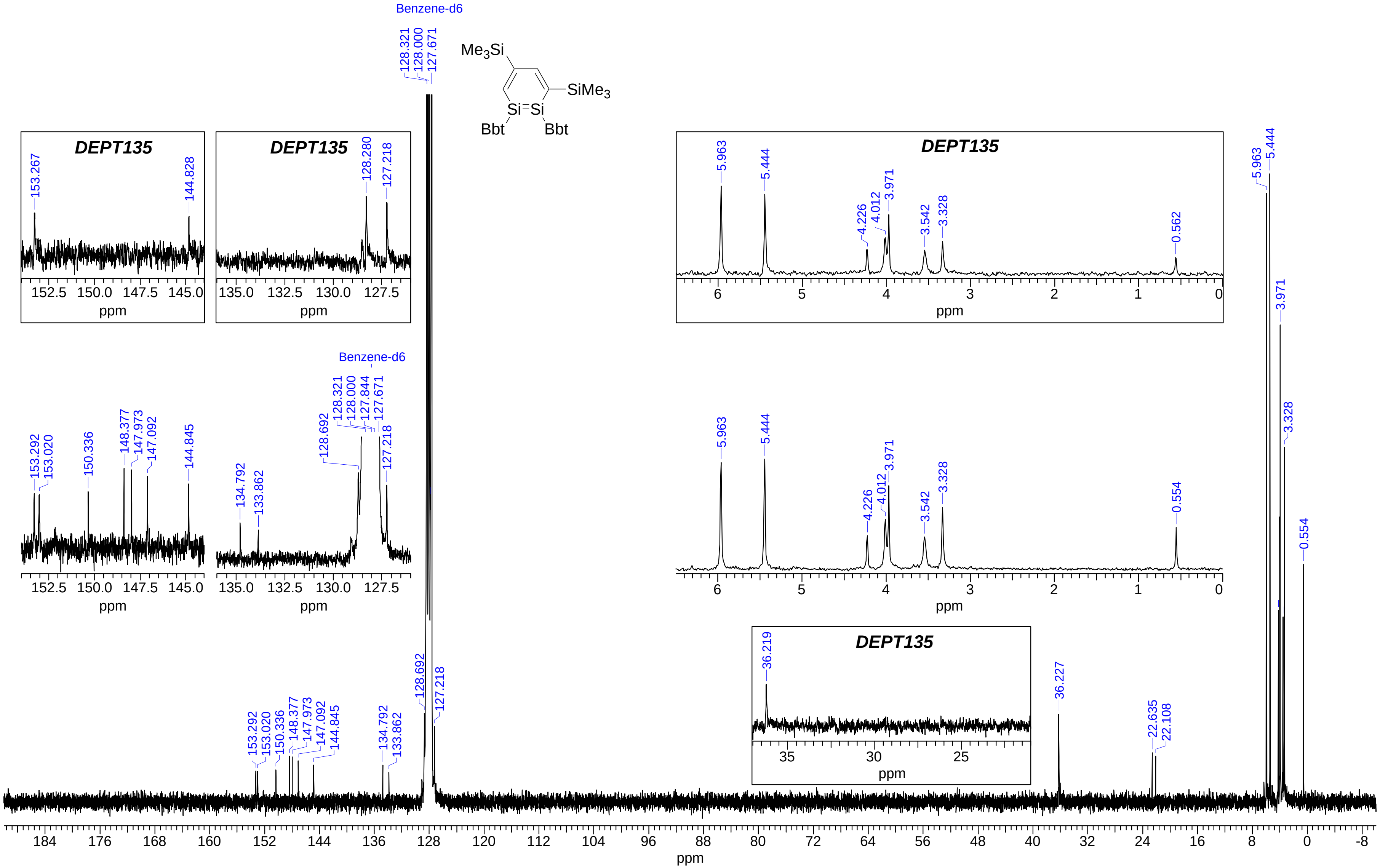

Fig. S-10. $^{13}C\{^{1}H\}$ and ^{13}C DEPT135 NMR spectra of **3**.

Acquisition Time (sec)	0.8192	**Comment**	C6D6, 40ms 40ms			**Date**	Sat Nov 21 12:29:07 2009		
Date Stamp	Sat Nov 21 12:29:07 2009			**File Name**	D:\HJS\KYOTO-U\NMR\091121-1-4040.DX			**Frequency (MHz)**	59.16
Nucleus	29Si	**Origin**	JEOL	**Original Points Count**	32768	**Owner**	GUEST	**Points Count**	32768
Solvent	BENZENE-D6	**Sweep Width (Hz)**	39998.78						

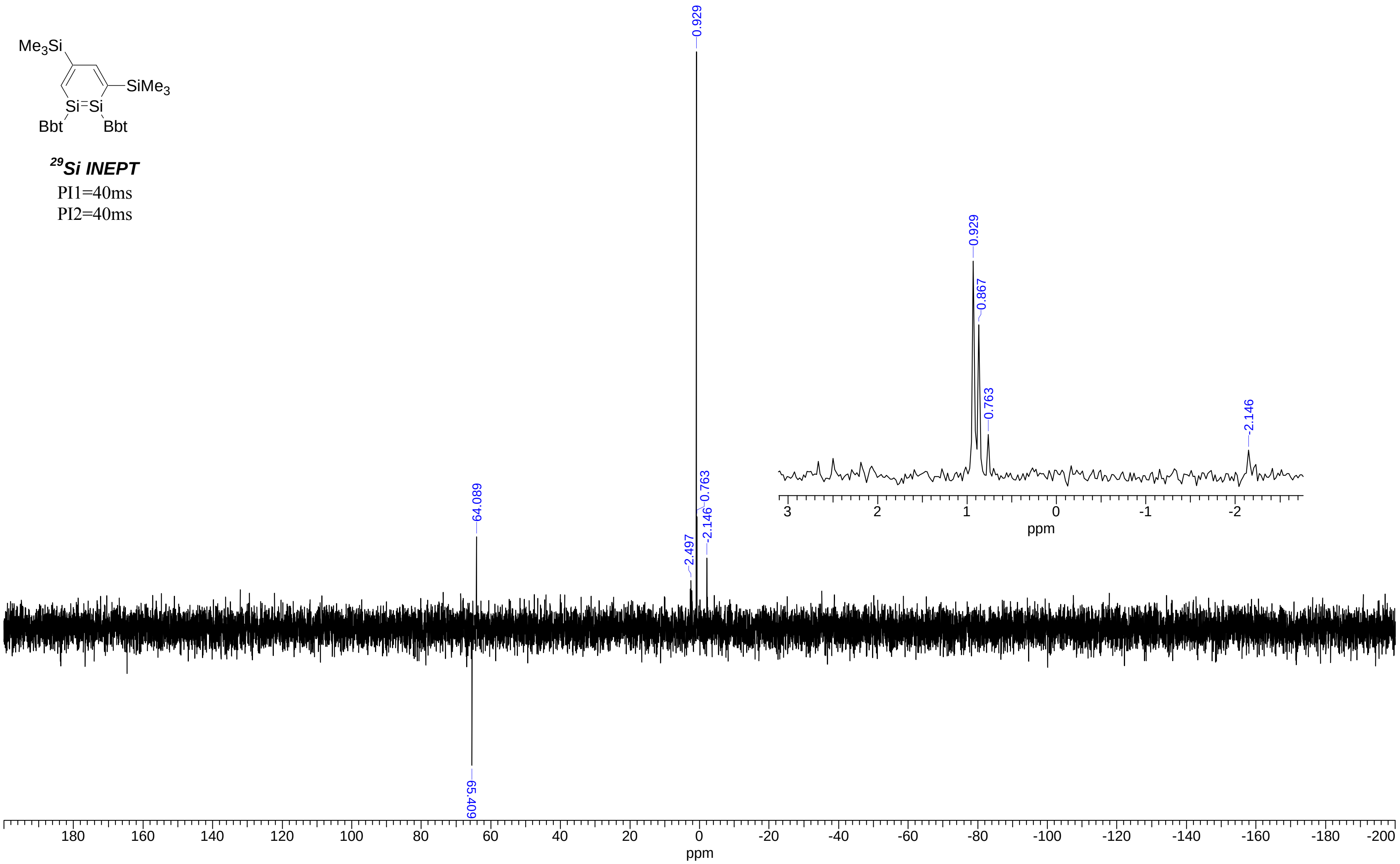

Fig. S-11. ^{29}Si INEPT NMR spectrum of **3**.

Acquisition Time (sec)	0.8192	***Comment***	C6D6, 5ms 10ms			***Date***	Sat Nov 21 00:05:17 2009		
Date Stamp	Sat Nov 21 00:05:17 2009			***File Name***	D:\HJS\KYOTO-U\NMR\091120-2-0510.DX			***Frequency (MHz)***	59.16
Nucleus	29Si	***Origin***	JEOL	***Original Points Count***	32768	***Owner***	GUEST	***Points Count***	32768
Solvent	BENZENE-D6	***Sweep Width (Hz)***	39998.78						

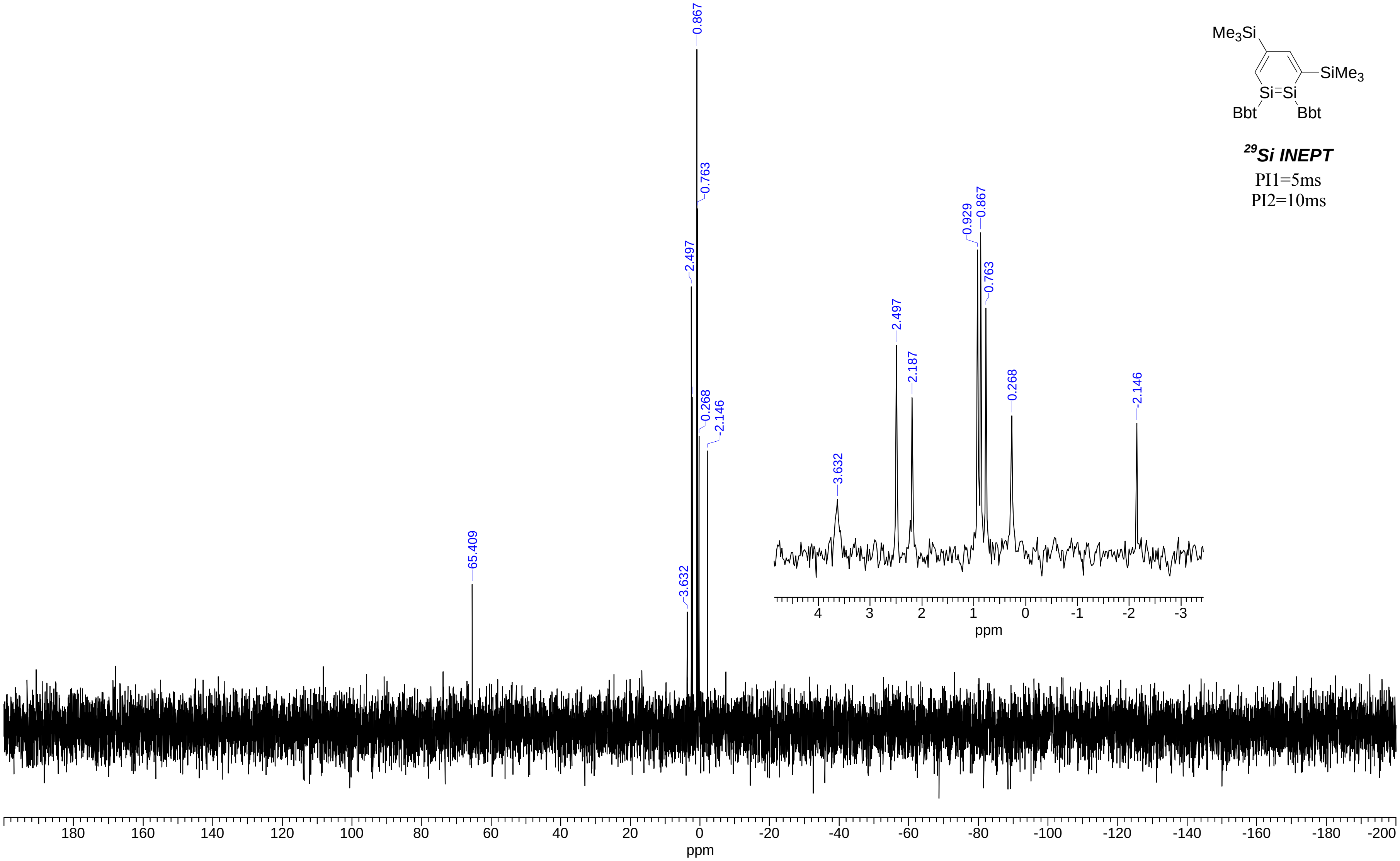

Fig. S-12. ^{29}Si INEPT NMR spectrum of **3**.

Acquisition Time (sec)	5.5052	***Date***	Thu Nov 05 17:10:59 2009	***Date Stamp***	Thu Nov 05 17:10:59 2009		
File Name	D:\HJS\KYOTO-U\NMR\091105-1.DX	***Frequency (MHz)***	297.78	***Nucleus***	1H	***Origin***	JEOL
Original Points Count	32768	***Owner***	GUEST	***Points Count***	32768	***Sweep Width (Hz)***	5952.20

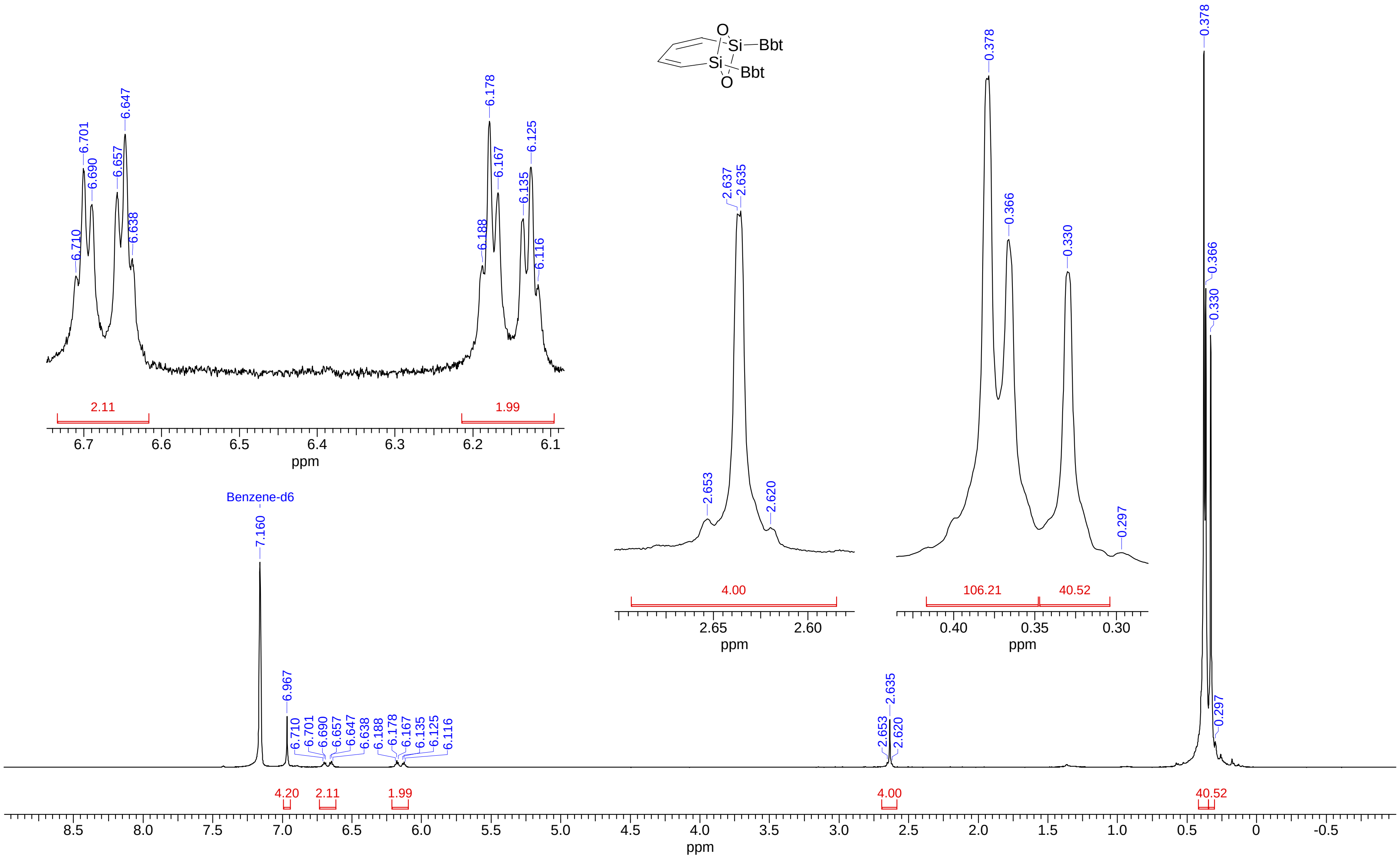

Fig. S-13. ^{1}H NMR spectrum of **6**.

Acquisition Time (sec)	1.6221	***Comment***	auto	***Date***	Thu Nov 05 18:04:38 2009			***Date Stamp***	Thu Nov 05 18:04:38 2009
File Name	D:\HJS\KYOTO-U\NMR\091105-1-C.DX			***Frequency (MHz)***	74.88	***Nucleus***	13C	***Origin***	JEOL
Original Points Count	32768	***Owner***	GUEST	***Points Count***	32768	***Sweep Width (Hz)***	20201.40		

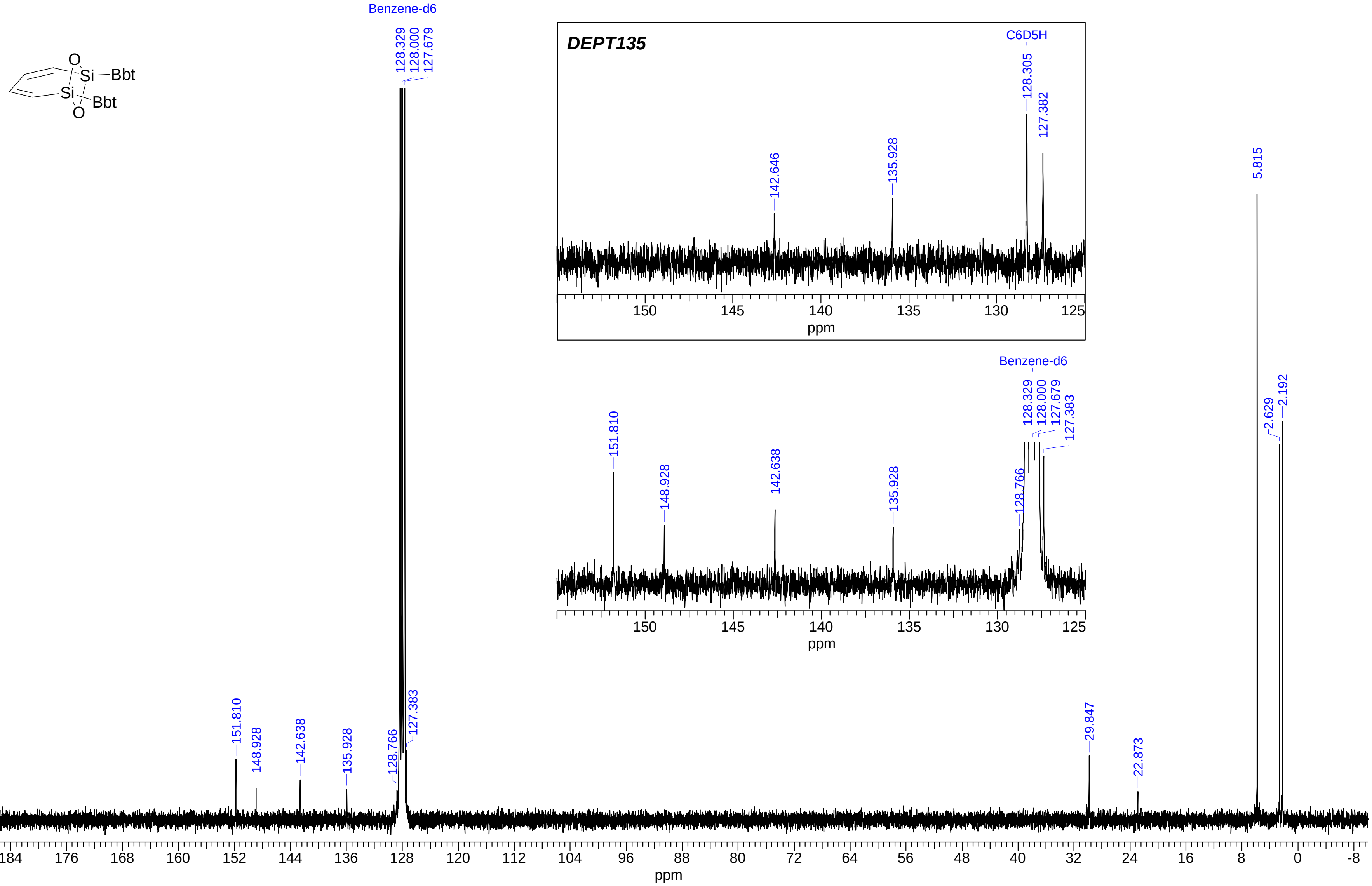

Fig. S-14. $^{13}C\{^1H\}$ and ^{13}C DEPT135 NMR spectra of **6**.

Acquisition Time (sec)	0.8192	**Comment**	C6D6, 5ms 10ms			**Date**	Thu Nov 05 19:44:59 2009		
Date Stamp	Thu Nov 05 19:44:59 2009			**File Name**	D:\HJS\KYOTO-U\NMR\091105-1-0510.DX			**Frequency (MHz)**	59.16
Nucleus	29Si	**Origin**	JEOL	**Original Points Count**	32768	**Owner**	GUEST	**Points Count**	32768
Solvent	BENZENE-D6	**Sweep Width (Hz)**	39998.78						

^{29}Si INEPT

PI1 = 5 ms
PI2 = 10 ms

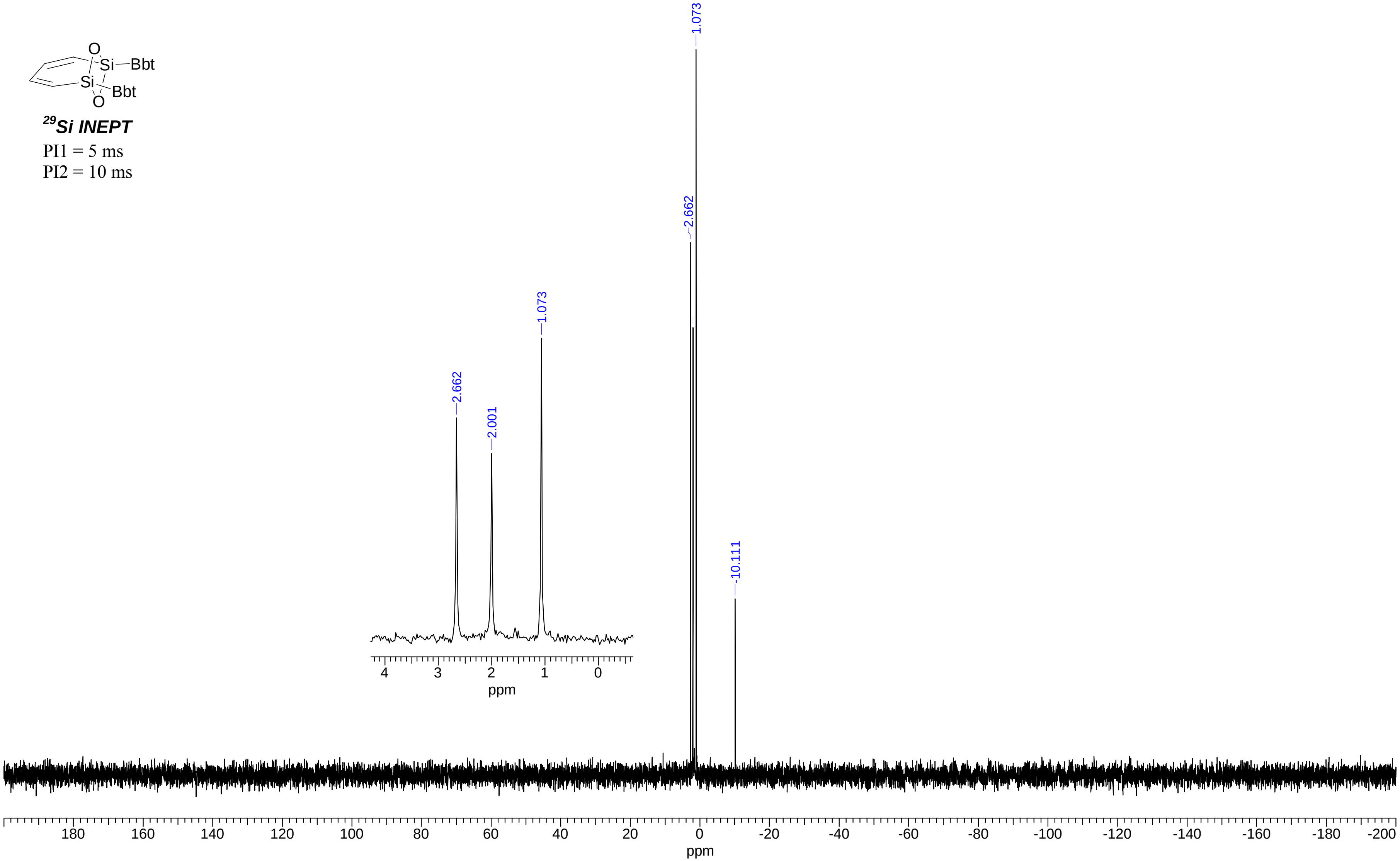

Fig. S-15. ^{29}Si INEPT NMR spectrum of **6**.