Supporting Information

Opening the Silole Ring: Efficient and Specific Cleavage of the *endo*-C(sp^2)-Si Bond with AcOH/ROH System

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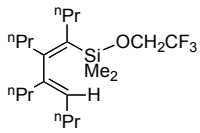
1. Experiment Section

1-1. General methods

All reactions were carried out under a slightly positive pressure of dry nitrogen by using standard Schlenk line techniques or under a nitrogen atmosphere in a Mikrouna Super (1220/750) Glovebox. The nitrogen in the glovebox was constantly circulated through a copper/molecular sieves catalyst unit. The oxygen and moisture concentrations in the glovebox atmosphere were monitored by an O_2/H_2O Combi-Analyzer to ensure both were always below 1 ppm. Unless otherwise noted, all starting materials were commercially available and were used without further purification. Solvents were distilled from sodium/benzophenone ketyl under a nitrogen atmosphere. Silole compounds were synthesized by reported methods.[1-5] NMR spectra were recorded on a JEOL-AL300 spectrometer (FT, 300 MHz for ^{1}H; 75 MHz for ^{13}C) or a Bruker-400 spectrometer (FT, 400 MHz for ^{1}H; 100 MHz for ^{13}C) at room temperature.

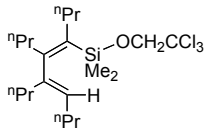
1-2. Experimental procedure and spectral data for all compounds

Typical procedure for ring-opening reaction of siloles 1 or 3 catalyzed by acetic acid: with magnetic stirring, a mixture of alcohol or phenol (neat, 10 mmol or more), silole **1** or **3** (1 mmol) and acetic acid (0.009 mL, 0.15 mmol, d 1.05) was maintained at room temperature for 2 hours. After that, water (10 mL) was added and the mixture was extracted by diethyl ether (30 mL in total) for three times. The combined organic solution was washed with brine and dried over Na_2SO_4. Solvent was removed in vacuum and the residue was purified by column chromatography (silicon gel., hexane) to give diene products **2** or **4**.



2aa

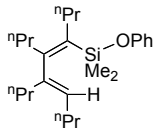
Colorless liquid, isolated yield 75% (284 mg); ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 0.19 (s, 6H, CH_3), 0.88-0.97 (m, 12H, CH_3), 1.29-1.47 (m, 8H, CH_2), 2.01-2.15 (m, 8H, CH_2), 3.87 (q, *J* = 8.7 Hz, 2H, CH_2), 5.15 (t, *J* = 7.2 Hz, 1H, CH); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 0.54 (2 CH_3), 14.11 (2 CH_3), 14.53 (1 CH_3), 14.97 (1 CH_3), 21.73 (1 CH_2), 22.19 (1 CH_2), 22.75 (1 CH_2), 24.17 (1 CH_2), 30.34 (1 CH_2), 32.78 (1 CH_2), 33.00 (1 CH_2), 33.30 (1 CH_2), 61.25 (q, *J* = 35 Hz, 1 CH_2), 124.55 (q, *J* = 277 Hz, 1 CF_3), 129.44 (1 CH), 132.65 (1 quat. C), 142.97 (1 quat. C), 158.89 (1 quat. C); HRMS calcd. for $C_{20}H_{37}F_3OSi$ $[M+Na]^+$: 401.2458, found 401.2466.



2ab

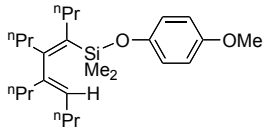
Colorless liquid, isolated yield 48% (205 mg); ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 0.18 (s, 6H, CH_3), 0.83-0.93 (m, 12H, CH_3), 1.29-1.42 (m, 8H, CH_2), 1.97-2.15 (m, 8H, CH_2), 4.07 (s, 2H, CH_2), 5.11 (t, *J* = 6.9 Hz, 1H, CH); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 0.84 (2 CH_3), 14.06 (2 CH_3), 14.56 (1 CH_3), 14.92 (1 CH_3), 21.56 (1 CH_2), 22.04 (1 CH_2), 22.62 (1 CH_2), 24.03 (1 CH_2), 30.22 (1 CH_2), 32.58

(1 CH_2), 32.90 (1 CH_2), 33.20 (1 CH_2), 76.28 (1 CH_2), 99.36 (1 CCl_3), 129.42 (1 CH), 133.11 (1 quat. C), 143.14 (1 quat. C), 158.46 (1 quat. C); HRMS calcd. for $C_{20}H_{37}Cl_3OSi$ $[M+H]^+$: 427.1768, found 427.1776.



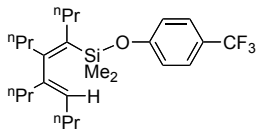
2ac

Colorless liquid, isolated yield 72% (268 mg); ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ = 0.25 (s, 6H, CH_3), 0.87-0.95 (m, 12H, CH_3), 1.35-1.43 (m, 8H, CH_2), 1.96-2.21 (m, 8H, CH_2), 5.14 (t, *J* = 7.2 Hz, 1H, CH), 6.80 (d, *J* = 8.4 Hz, 2H, CH), 6.90 (t, *J* = 7.2 Hz, 1H, CH), 7.18-7.22 (m, 2H, CH); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ºC): δ = 0.21 (2 CH_3), 14.15 (1 CH_3), 14.20 (1 CH_3), 14.67 (1 CH_3), 15.03 (1 CH_3), 21.69 (1 CH_2), 22.18 (1 CH_2), 22.66 (1 CH_2), 24.20 (1 CH_2), 30.30 (1 CH_2), 32.80 (1 CH_2), 33.08 (1 CH_2), 33.27 (1 CH_2), 119.96 (2 CH), 120.70 (1 CH), 129.23 (2 CH), 129.48 (1 CH), 133.20 (1 quat. C), 142.85 (1 quat. C), 155.85 (1 quat. C), 158.41 (1 quat. C); HRMS calcd. for $C_{20}H_{40}OSi$ $[M+Na]^+$: 395.2756, found 395.2764.



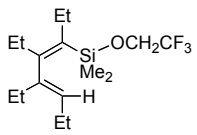
2ad

Colorless liquid, isolated yield 64% (258 mg); ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ = 0.25 (s, 6H, CH_3), 0.89-0.96 (m, 12H, CH_3), 1.37-1.41 (m, 8H, CH_2), 2.17-2.21 (m, 8H, CH_2), 3.76 (s, 3H, CH_3) , 5.14 (t, *J* = 7.2 Hz, 1H, CH), 6.72-6.78 (m, 4H, CH); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ºC): δ = 0.99 (2 CH_3), 14.11 (1 CH_3), 14.17 (1 CH_3), 14.65 (1 CH_3), 15.00 (1 CH_3), 21.67 (1 CH_2), 22.14 (1 CH_2), 22.65 (1 CH_2), 24.19 (1 CH_2), 30.28 (1 CH_2), 32.77 (1 CH_2), 33.10 (1 CH_2), 33.23 (1 CH_2), 55.48 (1 CH_3), 114.35 (2 CH), 120.40 (2 CH), 129.40 (1 CH), 133.22 (1 quat. C), 142.76 (1 quat. C), 149.57 (1 quat. C), 153.7 5 (1 quat. C), 158.29 (1 quat. C); HRMS calcd. for $C_{25}H_{42}O_2Si$ $[M+Na]^+$: 425.2954, found 425.2964.



2ae

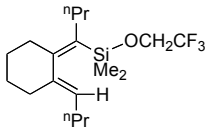
Colorless liquid, isolated yield 82% (361 mg); ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ = 0.28 (s, 6H, CH_3), 0.90-0.97 (m, 12H, CH_3), 1.38-1.47 (m, 8H, CH_2), 2.02-2.20 (m, 8H, CH_2), 5.15 (t, *J* = 7.2 Hz, 1H, CH), 6.88 (d, *J* = 8.4 Hz, 2H, CH), 7.48 (d, *J* = 8.4 Hz, 2H, CH); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ºC): δ = 0.57 (2 CH_3), 14.12 (1 CH_3), 14.18 (1 CH_3), 14.63 (1 CH_3), 15.00 (1 CH_3), 21.72 (1 CH_2), 22.23 (1 CH_2), 22.66 (1 CH_2), 24.22 (1 CH_2), 30.32 (1 CH_2), 32.84 (1 CH_2), 33.04 (1 CH_2), 33.29 (1 CH_2), 119.87 (2 CH), 122.87 (q, *J* = 32 Hz, 1 quat. C), 124.61 (q, *J* = 269 Hz, 1 CF_3), 126.72 (q, *J* = 3.7 Hz, 2 CH), 129.70 (1 CH), 132.63 (1 quat. C), 143.02 (1 quat. C), 158.82 (1 quat. C), 159.20 (1 quat. C); HRMS calcd. for $C_{25}H_{39}F_3OSi$ $[M+Na]^+$: 463.2598, found 463.2590.



2b

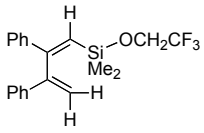
Colorless liquid, isolated yield 86% (277 mg); ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 0.22 (s, 6H, CH_3), 0.92-1.06 (m, 12H, CH_3), 2.10-2.22 (m, 8H, CH_2), 3.88 (q, *J* = 8.4 Hz, 2H, CH_2), 5.14 (t, *J* = 7.2 Hz, 1H, CH); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 0.54 (2 CH_3), 13.00 (1 CH_3), 13.05 (1 CH_3), 13.86 (1 CH_3), 15.34 (1 CH_3), 21.23 (1 CH_2), 23.08 (1 CH_2), 23.22 (1 CH_2), 23.45 (1 CH_2), 61.22 (q, *J* = 35 Hz, 1

CH_2), 124.54 (q, J = 277 Hz, 1 CF_3), 131.12 (1 CH), 133.55 (1 quat. C), 142.91 (1 quat. C), 159.76 (1 quat. C); HRMS calcd. for $C_{16}H_{29}F_3OSi$ [M+H]$^+$: 323.2012, found 323.2013.



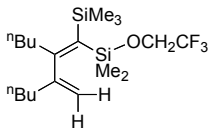
2c

Colorless liquid, isolated yield 81% (283 mg); ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 0.19 (s, 6H, CH_3), 0.90 (t, J = 7.2 Hz, 3H, CH_3), 0.93 (t, J = 7.2 Hz, 3H, CH_3), 1.27-1.67 (m, 8H, CH_2), 1.93-2.31 (m, 8H, CH_2), 3.87 (q, J = 8.7 Hz, 2H, CH_2), 5.19 (t, J = 7.2 Hz, 1H, CH); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 0.15 (2 CH_3), 14.03 (1 CH_3), 14.25 (1 CH_3), 22.70 (1 CH_2), 24.07 (1 CH_2), 27.91 (1 CH_2), 28.26 (1 CH_2), 29.83 (1 CH_2), 30.37 (1 CH_2), 32.32 (1 CH_2), 32.67 (1 CH_2), 61.21 (q, J = 35 Hz, 1 CH_2), 124.50 (q, J = 277 Hz, 1 CF_3), 125.42 (1 CH), 129.29 (1 quat. C), 144.15 (1 quat. C), 158.36 (1 quat. C); HRMS calcd. for $C_{18}H_{31}F_3OSi$ [M+H]$^+$: 349.2169, found 349.2164.



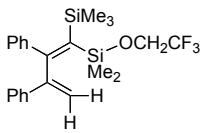
2d

Colorless liquid, isolated yield 82% (296 mg); ^{1}H NMR (400 MHz, $CDCl_3$, $SiMe_4$, 25 ºC): δ = 0.21 (s, 6H, CH_3), 3.90 (q, J = 8.7 Hz, 2H, CH_2), 5.35 (d, J = 1.4 Hz, 1H, CH_2), 5.85 (d, J = 1.4 Hz, 1H, CH_2), 6.27 (s, 1H, CH), 7.17-7.47 (m, 10H, CH); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = -0.55 (2 CH_3), 61.29 (q, J = 35 Hz, 1 CH_2), 116.15 (1 CH_2), 124.28 (q, J = 277 Hz, 1 CF_3), 126.47 (1 CH), 126.62 (2 CH), 126.72 (2 CH), 127.87 (1 CH), 128.23 (1 CH), 128.28 (2 CH), 128.36 (2 CH), 138.31 (1 quat. C), 140.50 (1 quat. C), 148.45 (1 quat. C), 159.11 (1 quat. C); HRMS calcd. for $C_{20}H_{21}F_3OSi$ [M+H]$^+$: 363.1386, found 363.1389.



4a

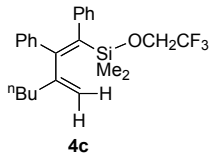
Colorless liquid, isolated yield 75% (296 mg); ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 0.01 (s, 3H, CH_3), 0.13 (s, 3H, CH_3), 0.17 (s, 9H, CH_3), 0.85-0.95 (m, 6H, CH_3), 1.27-1.38 (m, 8H, CH_2), 2.03-2.24 (m, 4H, CH_2), 3.81 (q, J = 8.7 Hz, 2H, CH_2), 4.75 (s, 2H, CH_2); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = - 0.55 (1 CH_3), - 0.01 (1 CH_3), 2.43 (3 CH_3), 14.03 (2 CH_3), 22.85 (1 CH_2), 22.96 (1 CH_2), 29.18 (1 CH_2), 31.22 (1 CH_2), 34.11 (1 CH_2), 37.27 (1 CH_2), 60.86 (q, J = 35 Hz, 1 CH_2), 122.95 (1 CH_2), 124.45 (q, J = 277 Hz, 1 CF_3), 133.99 (1 quat. C), 155.26 (1 quat. C), 174.24 (1 quat. C); HRMS calcd. for $C_{19}H_{37}F_3OSi_2$ [M+Na]$^+$: 417.2366, found 417.2369.



4b

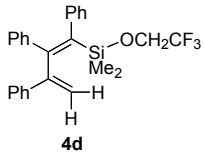
Colorless liquid, isolated yield 84% (365 mg); ^{1}H NMR (300 MHz, $CDCl_3$, $SiMe_4$, 25 ºC): δ = -0.10 (s, 9H, CH_3), 0.12 (s, 3H, CH_3), 0.36 (s, 3H, CH_3), 3.88 (q, J = 8.7 Hz, 2H, CH_2), 5.34 (d, J = 1.8 Hz, 1H, CH_2), 5.60 (d, J = 1.8 Hz, 1H, CH_2), 7.01-7.33 (m, 10H, CH); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = - 0.41 (1 CH_3), 2.06 (3 CH_3), 2.56 (1 CH_3), 61.00 (q, J = 35 Hz, 1 CH_2), 115.83 (1 CH_2), 124.44 (q, J = 277 Hz, 1 CF_3), 127.61 (2 CH), 127.71 (1 CH), 127.79 (4 CH), 127.85 (1 CH), 128.01 (2 CH),

137.94 (1 quat. C), 143.82 (1 quat. C), 144.67 (1 quat. C), 154.41 (1 quat. C), 169.85 (1 quat. C); HRMS calcd. for $C_{23}H_{29}F_3OSi_2$: 434.1709, found 434.1711.



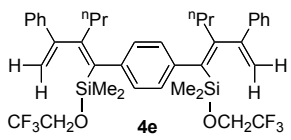
4c

Colorless liquid, isolated yield 88% (365 mg); ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 0.30 (s, 6H, CH_3), 0.82 (t, *J* = 7.2 Hz, 3H, CH_3), 1.19-1.41 (m, 4H, CH_2), 1.97 (t, *J* = 7.8 Hz, 2H, CH_2), 3.56 (q, *J* = 8.7 Hz, 2H, CH_2), 5.10 (d, *J* = 2.1 Hz, 1H, CH_2), 5.28 (d, *J* = 2.1 Hz, 1H, CH_2), 6.91-7.11 (m, 10H, CH); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 0.14 (2 CH_3), 13.94 (1 CH_3), 22.54 (1 CH_2), 29.23 (1 CH_2), 34.59 (1 CH_2), 61.27 (q, *J* = 35 Hz, 1 CH_2), 113.64 (1 CH_2), 124.18 (q, *J* = 277 Hz, 1 CF_3), 125.26 (1 CH), 126.48 (1 CH), 127.23 (2 CH), 127.46 (2 CH), 129.14 (2 CH), 129.80 (2 CH), 138.92 (1 quat. C), 140.09 (1 quat. C), 142.04 (1 quat. C), 151.92 (1 quat. C), 158.17 (1 quat. C); HRMS calcd. for $C_{24}H_{29}F_3OSi$ $[M+H]^+$: 419.2013, found 419.2005.



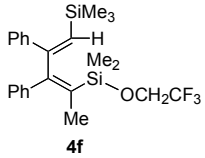
4d

Colorless liquid, isolated yield 75% (328 mg); ^{1}H NMR (400 MHz, $CDCl_3$, $SiMe_4$, 25 ºC): δ = 0.23 (s, 6H, CH_3), 3.52 (q, *J* = 8.7 Hz, 2H, CH_2), 5.51 (d, *J* = 1.1 Hz, 1H, CH_2), 5.82 (d, *J* = 1.1 Hz, 1H, CH_2), 6.89-7.52 (m, 15H, CH); ^{13}C NMR (75 MHz, $CDCl_3$, $SiMe_4$, 25 ºC): δ = 0.05 (2 CH_3), 61.29 (q, *J* = 35 Hz, 1 CH_2), 115.68 (1 CH_2), 124.17 (q, *J* = 277 Hz, 1 CF_3), 125.58 (1 CH), 126.62 (1 CH), 127.01 (2 CH), 127.23 (2 CH), 127.70 (2 CH), 127.92 (1 CH), 128.28 (2 CH), 129.48 (2 CH), 129.81 (2 CH), 138.08 (1 quat. C), 139.84 (1 quat. C), 142.09 (1 quat. C), 142.76 (1 quat. C), 149.90 (1 quat. C), 154.50 (1 quat. C); HRMS calcd. for $C_{26}H_{25}F_3OSi$ $[M+H]^+$: 439.1699, found 439.1705.



4e

Colorless liquid, isolated yield 65% (475 mg); ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 0.19 (s, 12H, CH_3), 0.63 (t, *J* = 7.2 Hz, 6H, CH_3), 1.20-1.26 (m, 4H, CH_2), 1.94 (t, *J* = 7.8 Hz, 4H, CH_2), 3.55 (q, *J* = 8.4 Hz, 4H, CH_2), 5.30 (d, *J* = 1.8 Hz, 2H, CH_2), 5.66 (d, *J* = 1.8 Hz, 2H, CH_2), 7.15-7.57 (m, 14H, CH); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = - 0.18 (4 CH_3), 13.67 (2 CH_3), 21.45 (2 CH_2), 35.04 (2 CH_2), 61.26 (q, *J* = 35 Hz, 2 CH_2), 114.42 (2 CH_2), 124.12 (q, *J* = 277 Hz, 2 CF_3), 126.85 (4 CH), 127.98 (2 CH), 128.43 (8 CH), 138.47 (2 quat. C), 140.26 (2 quat. C), 140.98 (2 quat. C), 149.68 (2 quat. C), 156.09 (2 quat. C); HRMS calcd. for $C_{40}H_{48}F_6O_2Si_2$ $[M+Na]^+$: 753.2989, found 753.2988.



4f

Colorless liquid, isolated yield 68% (305 mg); ^{1}H NMR (300 MHz, $CDCl_3$, $SiMe_4$, 25 ºC): δ = 0.06 (s, 9H, CH_3), 0.09 (s, 3H, CH_3), 0.19 (s, 3H, CH_3), 2.02 (s, 3H, CH_3), 3.79 (q, *J* = 8.4 Hz, 2H, CH_2), 6.32 (s, 1H, CH), 7.16-7.51 (m, 10H, CH); ^{13}C NMR (75 MHz, $CDCl_3$, $SiMe_4$, 25 ºC): δ = -1.10 (1 CH_3), - 0.52 (1 CH_3), - 0.27 (3 CH_3), 19.31 (1 CH_3), 61.28 (q, *J* = 35 Hz, 1 CH_2), 124.26 (q, *J* = 276 Hz, 1 CF_3),

126.95 (2 CH), 127.13 (1 CH), 127.63 (1 CH), 127.70 (2 CH), 128.15 (2 CH), 129.92 (2 CH), 129.96 (1 CH), 134.45 (1 quat. C), 140.48 (1 quat. C), 141.66 (1 quat. C), 151.20 (1 quat. C), 156.22 (1 quat. C); HRMS calcd. for $C_{24}H_{31}F_3OSi_2$ $[M+Na]^+$: 471.1758, found 471.1759.

Reference

1. Yamaguchi, S.; Endo, T.; Uchida, M.; Izumizawa, T.; Furukawa, K.; Tamao, K. *Chem. Eur. J.* **2000**, *6*, 1683.

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2. Calculation Section

2-1. Full/Detailed Citation

Gaussian 03: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkar, A.; Challacombe, A. M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03, Revision E.01*, Gaussian, Inc., Wallingford, CT, 2004.

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6-31+G* basic set: (a) Hariharan, P. C.; Pople, J. A. *Theoret. Chim. Acta* **1973**, 28, 213. (b) Francl, M.M.; Petro, W.J.; Hehre, W.J.; Binkley, J. S.; Gordon, M.S.; DeFrees D.J.; Pople, J. A. *J. Chem. Phys.* **1982**, 77, 3654-3665. (c) Clark, T.; Chandrasekhar, J.; Schleyer, P.v.R.; *J. Comp. Chem.* **1983**, *4*, 294. (d) Krishnam, R.; Binkley, J.S.; Seeger, R.; Pople, J.A. *J. Chem. Phys.* **1980**, *72*, 650-654. (e) Gill, P.M.W.; Johnson, B. G.; Pople P.M.W.; Frisch, M. J.; *Chem. Phys. Lett.* 1992, *197*, 499.

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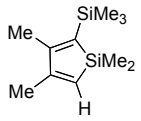
2-2 General Methods

All calculations were carried out with the Gaussian 03 programs. The global reaction route mapping method (GRRM) based on Gaussian 03 was utilized for locating all local equilibrium structures. Geometry optimization were carried put by using the method of the Becke three-parameter hybrid functional combined with Lee–Yang–Parr correlation functional (B3LYP/6–31+G*). All stationary points were optimized without any symmetry assumptions, and characterized by normal coordinate analysis at the same level of theory. The method of (B3LYP/STO-3G) is utilized for the orbital analysis and the natural charges calculation (by natural population analysis with the NBO 3.1 program package). Second-order perturbation theory analysis of fock matrix was also performed with NBO 5.G program package at the same level as used for geometry optimization.

2-3. Geometry optimization (Cartesian coordinates and total electron energies)



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C	1.214021775424	-0.548726195807	0.080526228023
C	0.306183032623	0.437223449330	-0.108413506421
H	0.613501137798	1.479191198904	-0.168249621369
Si	-1.391903603607	-0.341797321555	-0.226062710437
Si	-1.671507141108	-3.704451377741	0.053430276758
C	-2.556492587276	0.229731408654	1.158107030143
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C	-2.216601736401	-0.046652505777	-1.908873513771
H	-3.178105378242	-0.568406703165	-1.986913166309
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H	-3.923788921134	-2.707602878884	0.617607415692
H	-3.731878089433	-2.858258281379	-1.138620603310
H	-4.091609360892	-4.285417921269	-0.160597304660
C	-1.148522853246	-4.878211311446	-1.348822798816
H	-0.093829416935	-5.170977935461	-1.284732307287
H	-1.749497307375	-5.797363729100	-1.326598748943
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H	2.193117562641	-2.949493836848	1.293555307730
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H	3.076652051138	-0.680396854655	1.189791512469
H	3.270547833288	-0.841969624137	-0.553860232558
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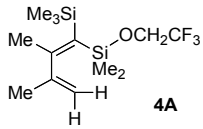

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Si	-1.829444379890	-0.410493876748	-0.392489667515
Si	-1.662193622638	-3.679709127969	-0.135821414860
C	-2.853679721574	0.108111550576	1.111556320219
H	-3.460632514480	0.998191925021	0.903524400040
H	-3.542286169087	-0.698667063849	1.392083852150
H	-2.226596541145	0.313377972851	1.987622047790
C	-2.932724643443	-0.617812783115	-1.909856094783
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H	-2.407589211725	-1.122900417205	-2.729933687289
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H	-1.955796835759	-5.607973131423	1.418849008917
H	-0.364614837209	-4.891297239651	1.708139679216
C	-3.553478383486	-3.562865887180	-0.307364710259

H	-4.019537608482	-2.860376791876	0.393896964641
H	-3.876600660219	-3.297953243540	-1.318916448731
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C	-1.066833218747	-4.681641212456	-1.638015509342
H	0.001231532498	-4.924690575206	-1.609756081294
H	-1.620801069604	-5.627837072506	-1.702969538075
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C	1.433973803908	-3.078934724012	0.528267926428
H	1.044630545153	-4.011229046353	0.119041059234
H	2.407327947239	-2.893222325919	0.058563559284
H	1.630932418585	-3.224000221575	1.599126303158
C	2.189986955296	-0.094920931246	-0.454330385844
H	2.910560220146	-0.864055565673	-0.759965657355
H	1.626174614783	0.193847728918	-1.349241464690
H	2.757473389315	0.772528364624	-0.099725324284
C	1.137567918779	-0.019233815739	1.813852579987
H	1.722384826737	0.861997049553	2.071702799701
H	0.472818780049	-0.408576279096	2.581684674981
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C	-0.615057405477	2.105268459580	-0.239079770101
H	0.455688203477	2.340905500373	-0.211134098438
H	-1.000720968757	2.150687467185	0.786839917449
C	-1.297585672239	3.221831985217	-1.024690706879
F	-0.835082024506	3.327229880437	-2.289160482062
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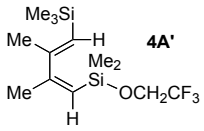

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C	1.437817983603	-0.536495766099	0.458094128896
Si	-1.829406786123	-0.293308469160	-0.388006311986
C	-2.532085718149	0.393981215997	1.225258333609
H	-3.235040011525	1.218026208447	1.049936728877
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H	-1.750240040800	0.742007220532	1.909914151539
C	-3.223394206664	-0.851088257788	-1.522813335717
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F	-1.425925181838	4.474591842777	-1.257480191113
H	0.696951812835	-0.393573727079	2.374562937730
Si	2.312126021873	1.517269765446	2.453434000288
C	3.562988128440	0.803791877286	3.689530912486
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H	4.335333861905	0.214122465828	3.179794050465
C	3.229418683147	2.680201130190	1.266479469228

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C	1.029673956531	2.534237732752	3.415790220910
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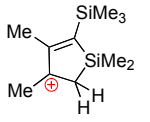

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C	0.387096376612	0.327333229135	-0.678804817032
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Si	-1.414890697376	-0.362743567160	-0.326910764198
Si	-1.689957007767	-3.759940333251	-0.060732921435
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H	-2.984997053404	-0.150439435676	1.595142739876
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C	-2.583312381315	-0.102460135634	-1.768933501074
H	-3.598251729834	-0.438786718657	-1.529438694260
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H	-2.255854384644	-0.628711344388	-2.673117131720
C	-1.433036382363	-4.571615010109	1.627863798996
H	-1.738813995948	-3.909989508153	2.447174784030
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H	-0.399052256648	-4.881509566650	1.810174866863
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H	-0.050900345215	-5.160503086784	-1.397413609619
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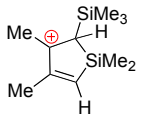

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C	0.236166754642	0.333297252580	0.351187554242
H	0.567445483262	1.346744131774	0.573541958034
Si	-1.480285898766	-0.250854652428	-0.165178484503
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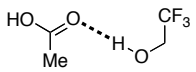
H	-1.901693120981	1.042480752478	-2.247321775644
H	-0.940436800930	-0.402116878171	-2.615900145906
C	1.402400268677	-3.092321544563	-0.464735154375
H	0.843476476672	-3.999684942765	-0.696839764783
H	1.946063793838	-2.768164140817	-1.364407408591
H	2.178155545932	-3.324040062191	0.277949313150
C	2.606707791071	-0.568281071760	0.671446932045
H	2.925228442965	-1.224687864368	1.490585962905
H	3.207422023299	-0.833939396078	-0.207501081357
H	2.856387282715	0.459310898589	0.946665136377
H	-1.279614643196	-2.864732517619	-0.581944681610
Si	-1.461402915793	-2.882953513423	1.868018442566
C	-0.842408736786	-1.801693330212	3.277094114698
H	-1.263474043295	-2.179587707815	4.218308314574
H	0.248786380503	-1.838067864791	3.375548505133
H	-1.136651066559	-0.750351351577	3.193863268743
C	-0.699156169910	-4.602443202857	1.950385287269
H	-1.061559146534	-5.105191193162	2.856920227073
H	-0.989985590729	-5.229661628670	1.099204759794
H	0.394919365465	-4.587630486973	2.008743386636
C	-3.335841464248	-3.009258843844	1.772755025818
H	-3.839351299721	-2.039010170016	1.814993450712
H	-3.664622316484	-3.529505532038	0.865125983092
H	-3.689830303497	-3.599139840738	2.628600755887

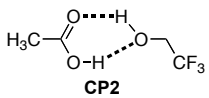
ENERGY = -1011.835772157685 a.u.



CP1

C	-0.183077419487	-2.131378176806	0.198896310535
O	-0.140801037957	-3.313495088145	0.472576622481
H	-1.286855158683	-4.530607448151	-0.278286466641
O	-1.923947516052	-5.113581619045	-0.744163085821
C	-1.246432048361	-5.882625524270	-1.700114700120
H	-1.848442316012	-6.769865952993	-1.919893929840
H	-0.253074824583	-6.207893686122	-1.362893875286
C	-1.054336252226	-5.132009515275	-3.016249709663
F	-0.330627802136	-3.990908226908	-2.849931600155
F	-0.385008802422	-5.901713461025	-3.912555853507
F	-2.225363009485	-4.772564078541	-3.587428611553
O	0.775282216367	-1.316337890330	0.700663372341
H	0.641684337499	-0.397632049004	0.412012980648
C	-1.233542978156	-1.479963079639	-0.674468091850
H	-0.770239129779	-1.068121749125	-1.579367150378
H	-1.980688139532	-2.217472123572	-0.969882196611
H	-1.727058859034	-0.659760581040	-0.138871634579

ENERGY = -681.880803841881 a.u.

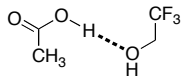


CP2

C	0.321708032153	-0.320492933091	0.091318179657
O	1.339868524962	-0.982673951754	-0.074525859742
O	0.336263769076	0.992472696194	0.366311335100
H	1.273127315629	1.303267567878	0.419077489560
C	-1.074266098439	-0.878401961118	0.014144389606
H	-1.573754591710	-0.756151550613	0.981697321659
H	-1.658622550468	-0.322777139347	-0.726957145313
H	-1.036196122627	-1.935137027483	-0.252623991834
H	2.859014603032	0.092356266615	0.136446281333
O	3.122202537487	1.037134042833	0.233705218029
C	4.288061929179	1.192203378866	1.008035619465

H	4.657928536448	2.209281179935	0.854755050774
H	5.072661142463	0.482252484691	0.719408662561
C	4.021461985508	1.012027460872	2.499828861216
F	3.102030521192	1.888110252955	2.963591271313
F	3.567313527578	-0.233132151086	2.781152451002
F	5.162751408519	1.201643763651	3.206969255616

ENERGY = -681.893879811408 a.u.



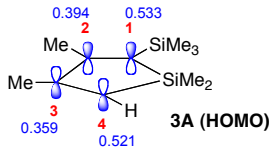
CP3

C	-0.506213679397	-2.455778588313	-0.022765332167
O	-0.443655808961	-3.642691464182	-0.244095720220
O	0.558285396000	-1.804877913078	0.512534175391
H	0.390273778754	-0.844903703854	0.621708931338
C	-1.733703428311	-1.601513882012	-0.291526137488
H	-2.154737505571	-1.237602736602	0.654205953274
H	-1.482527732249	-0.726441746920	-0.902141557202
H	-2.485725863431	-2.201933801466	-0.805551316103
O	0.614272081241	1.001280956720	0.718142531893
H	0.280320344894	1.540930969330	1.453604600257
C	1.901212660398	1.456663371065	0.330767472916
H	2.593941277713	1.507247009269	1.178854318809
H	2.285524946605	0.746230608071	-0.403759931195
C	1.827655013314	2.838022732190	-0.310522381623
F	1.095811733401	2.846135027206	-1.441179098796
F	1.262431902228	3.732711615911	0.544400587196
F	3.067715083372	3.283112016651	-0.610786186289

ENERGY = -681.878607877469 a.u.

2-4. HOMO orbital and NPA analysis for silole molecule

The result for the molecular orbital coefficients of HOMO (No. 58) of silole **3A** was showed below. According to the data, the double bond of C=C(TMS) contributed a little more than that of C=C(H), probably due to the donating effect from TMS group. Natural population analysis (NPA) showed the same trend, in which the C1 is bearing more negative charge. These results indicate the region-selectivity should have preferred the C=C(TMS) part kinetically if considering the classic reaction pathway. Yet, the mismatch between theoretical conclusions and experimental data imply that a new mechanism may be involved in this reaction.



3A (HOMO)

				58 (A)--O
EIGENVALUES --				-0.13638
1	1	C	1S	-0.00013
2			2S	0.00056
3			2PX	0.00044
4			2PY	-0.00014
5			2PZ	0.53312
6	2	C	1S	0.00003
7			2S	-0.00011
8			2PX	-0.00082
9			2PY	0.00021
10			2PZ	0.39412
11	3	C	1S	-0.00004
12			2S	0.00019
13			2PX	0.00107
14			2PY	-0.00033
15			2PZ	-0.35868
16	4	C	1S	-0.00006
17			2S	0.00028
18			2PX	0.00136
19			2PY	-0.00017
20			2PZ	-0.52105
21	5	H	1S	-0.00014
22	6	Si	1S	-0.00002
23			2S	0.00007
24			2PX	0.00013
25			2PY	-0.00014
26			2PZ	-0.00070
27			3S	-0.00022
28			3PX	-0.00032
29			3PY	0.00036
30			3PZ	0.00273
31	7	Si	1S	0.00002
32			2S	-0.00005
33			2PX	0.00009
34			2PY	0.00001

35			2PZ	0.00731	66			2PX	0.00000
36			3S	0.00019	67			2PY	-0.00020
37			3PX	-0.00023	68			2PZ	-0.00118
38			3PY	-0.00001	69	21	H	1S	-0.00381
39			3PZ	-0.00688	70	22	H	1S	0.00373
40	8	C	1S	-0.00007	71	23	H	1S	0.00002
41			2S	0.00067	72	24	C	1S	0.01476
42			2PX	0.00542	73			2S	-0.06890
43			2PY	-0.00238	74			2PX	0.04648
44			2PZ	0.00012	75			2PY	-0.05303
45	9	H	1S	-0.01530	76			2PZ	0.09178
46	10	H	1S	0.01449	77	25	H	1S	0.01258
47	11	H	1S	0.00023	78	26	H	1S	0.03272
48	12	C	1S	0.00005	79	27	H	1S	0.01590
49			2S	-0.00058	80	28	C	1S	0.00005
50			2PX	-0.00537	81			2S	-0.00022
51			2PY	0.00221	82			2PX	0.00013
52			2PZ	0.00002	83			2PY	-0.00032
53	13	H	1S	-0.01447	84			2PZ	-0.05362
54	14	H	1S	0.01511	85	29	H	1S	0.00015
55	15	H	1S	-0.00015	86	30	H	1S	-0.09872
56	16	C	1S	-0.01474	87	31	H	1S	0.09870
57			2S	0.06878	88	32	C	1S	0.00000
58			2PX	-0.04576	89			2S	-0.00001
59			2PY	0.05335	90			2PX	-0.00024
60			2PZ	0.09157	91			2PY	0.00004
61	17	H	1S	-0.01574	92			2PZ	0.05021
62	18	H	1S	-0.03273	93	33	H	1S	-0.09294
63	19	H	1S	-0.01263	94	34	H	1S	0.09256
64	20	C	1S	-0.00002	95	35	H	1S	0.00037
65			2S	0.00007					

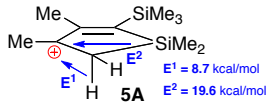
Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population			
			Core	Valence	Rydberg	Total
C	1	-0.39001	1.99980	4.39020	0.00000	6.39001
C	2	0.01383	1.99986	3.98630	0.00000	5.98617
C	3	0.01121	1.99985	3.98894	0.00000	5.98879
C	4	-0.26642	1.99985	4.26657	0.00000	6.26642
H	5	0.03443	0.00000	0.96557	0.00000	0.96557
Si	6	0.83556	9.99983	3.16460	0.00000	13.16444
Si	7	0.85501	9.99989	3.14510	0.00000	13.14499
C	8	-0.36913	1.99995	4.36918	0.00000	6.36913
H	9	0.05594	0.00000	0.94406	0.00000	0.94406
H	10	0.05477	0.00000	0.94523	0.00000	0.94523
H	11	0.05737	0.00000	0.94263	0.00000	0.94263
C	12	-0.36907	1.99995	4.36912	0.00000	6.36907
H	13	0.05472	0.00000	0.94528	0.00000	0.94528
H	14	0.05594	0.00000	0.94406	0.00000	0.94406
H	15	0.05738	0.00000	0.94262	0.00000	0.94262
C	16	-0.37205	1.99995	4.37210	0.00000	6.37205
H	17	0.05219	0.00000	0.94781	0.00000	0.94781
H	18	0.05182	0.00000	0.94818	0.00000	0.94818
H	19	0.05234	0.00000	0.94766	0.00000	0.94766
C	20	-0.37914	1.99995	4.37919	0.00000	6.37914
H	21	0.04968	0.00000	0.95032	0.00000	0.95032
H	22	0.04957	0.00000	0.95043	0.00000	0.95043
H	23	0.05227	0.00000	0.94773	0.00000	0.94773
C	24	-0.37202	1.99995	4.37207	0.00000	6.37202
H	25	0.05235	0.00000	0.94765	0.00000	0.94765
H	26	0.05181	0.00000	0.94819	0.00000	0.94819
H	27	0.05220	0.00000	0.94780	0.00000	0.94780
C	28	-0.20266	1.99997	4.20269	0.00000	6.20266
H	29	0.05552	0.00000	0.94448	0.00000	0.94448
H	30	0.06322	0.00000	0.93678	0.00000	0.93678
H	31	0.06321	0.00000	0.93679	0.00000	0.93679
C	32	-0.19822	1.99997	4.19825	0.00000	6.19822

H	33	0.06253	0.00000	0.93747	0.00000	0.93747
H	34	0.06251	0.00000	0.93749	0.00000	0.93749
H	35	0.06132	0.00000	0.93868	0.00000	0.93868
* Total *		0.00000	41.99875	74.00125	0.00000	116.00000

2-5. NBO analysis for donor-acceptor interaction

Note: The corresponding interactions between silyl groups and the cation centers were marked in red.



see: No. 9-1; No. 10-1

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

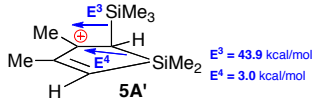
Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1- C 2	86. RY*(1) C 3	1.25	1.78	0.042
1. BD (1) C 1- C 2	254. BD*(1) C 1-Si 6	1.24	0.96	0.031
1. BD (1) C 1- C 2	255. BD*(1) C 1-Si 7	1.55	0.98	0.035
1. BD (1) C 1- C 2	256. BD*(1) C 2- C 3	2.72	1.20	0.051
1. BD (1) C 1- C 2	257. BD*(1) C 2- C28	2.60	1.12	0.048
1. BD (1) C 1- C 2	259. BD*(1) C 3- C32	3.15	1.13	0.053
1. BD (1) C 1- C 2	261. BD*(1) C 4-Si 6	0.73	0.93	0.023
2. BD (2) C 1- C 2	59. LP*(1) C 3	73.97	0.13	0.095
2. BD (2) C 1- C 2	92. RY*(7) C 3	0.64	1.71	0.033
2. BD (2) C 1- C 2	220. RY*(2) C28	0.77	1.21	0.030
2. BD (2) C 1- C 2	253. BD*(2) C 1- C 2	1.50	0.29	0.020
2. BD (2) C 1- C 2	263. BD*(1)Si 6- C 8	2.19	0.52	0.033
2. BD (2) C 1- C 2	264. BD*(1)Si 6- C12	1.38	0.53	0.026
2. BD (2) C 1- C 2	265. BD*(1)Si 7- C16	1.02	0.55	0.023
2. BD (2) C 1- C 2	267. BD*(1)Si 7- C24	1.18	0.55	0.025
2. BD (2) C 1- C 2	284. BD*(1) C28- H30	1.45	0.73	0.032
2. BD (2) C 1- C 2	285. BD*(1) C28- H31	2.56	0.72	0.042
3. BD (1) C 1-Si 6	73. RY*(1) C 2	1.56	1.67	0.046
3. BD (1) C 1-Si 6	74. RY*(2) C 2	1.46	1.41	0.041
3. BD (1) C 1-Si 6	252. BD*(1) C 1- C 2	1.18	1.05	0.032
3. BD (1) C 1-Si 6	254. BD*(1) C 1-Si 6	0.68	0.74	0.020
3. BD (1) C 1-Si 6	255. BD*(1) C 1-Si 7	1.29	0.75	0.028
3. BD (1) C 1-Si 6	256. BD*(1) C 2- C 3	0.71	0.98	0.024
3. BD (1) C 1-Si 6	257. BD*(1) C 2- C28	10.02	0.90	0.085
3. BD (1) C 1-Si 6	259. BD*(1) C 3- C32	0.73	0.91	0.023
3. BD (1) C 1-Si 6	261. BD*(1) C 4-Si 6	0.94	0.71	0.023
3. BD (1) C 1-Si 6	262. BD*(1) C 4- H36	1.45	0.95	0.033
3. BD (1) C 1-Si 6	263. BD*(1)Si 6- C 8	2.36	0.75	0.038
3. BD (1) C 1-Si 6	264. BD*(1)Si 6- C12	2.46	0.76	0.039
3. BD (1) C 1-Si 6	268. BD*(1) C 8- H 9	0.89	0.97	0.026
3. BD (1) C 1-Si 6	272. BD*(1) C12- H14	0.78	0.96	0.025
4. BD (1) C 1-Si 7	73. RY*(1) C 2	2.74	1.67	0.061
4. BD (1) C 1-Si 7	252. BD*(1) C 1- C 2	2.58	1.05	0.047
4. BD (1) C 1-Si 7	254. BD*(1) C 1-Si 6	1.01	0.74	0.024
4. BD (1) C 1-Si 7	256. BD*(1) C 2- C 3	6.38	0.98	0.071
4. BD (1) C 1-Si 7	265. BD*(1)Si 7- C16	2.09	0.78	0.036
4. BD (1) C 1-Si 7	266. BD*(1)Si 7- C20	2.13	0.79	0.037
4. BD (1) C 1-Si 7	267. BD*(1)Si 7- C24	2.11	0.78	0.036
4. BD (1) C 1-Si 7	275. BD*(1) C16- H18	0.92	0.98	0.027
4. BD (1) C 1-Si 7	279. BD*(1) C20- H23	0.80	0.99	0.025
4. BD (1) C 1-Si 7	281. BD*(1) C24- H26	0.93	0.98	0.027
5. BD (1) C 2- C 3	60. RY*(1) C 1	1.00	1.89	0.039
5. BD (1) C 2- C 3	99. RY*(1) C 4	1.31	1.63	0.041

5. BD (1) C 2- C 3	219. RY*(1) C28	0.62	1.55	0.028
5. BD (1) C 2- C 3	235. RY*(1) C32	0.86	1.48	0.032
5. BD (1) C 2- C 3	252. BD*(1) C 1- C 2	2.46	1.26	0.050
5. BD (1) C 2- C 3	255. BD*(1) C 1-Si 7	2.16	0.96	0.041
5. BD (1) C 2- C 3	257. BD*(1) C 2- C28	1.04	1.11	0.030
5. BD (1) C 2- C 3	258. BD*(1) C 3- C 4	0.89	1.14	0.029
5. BD (1) C 2- C 3	259. BD*(1) C 3- C32	0.87	1.12	0.028
5. BD (1) C 2- C 3	262. BD*(1) C 4- H36	1.40	1.16	0.036
5. BD (1) C 2- C 3	283. BD*(1) C28- H29	0.63	1.19	0.024
5. BD (1) C 2- C 3	288. BD*(1) C32- H35	0.88	1.15	0.029
6. BD (1) C 2- C28	60. RY*(1) C 1	0.59	1.81	0.029
6. BD (1) C 2- C28	86. RY*(1) C 3	0.86	1.69	0.034
6. BD (1) C 2- C28	252. BD*(1) C 1- C 2	2.87	1.18	0.052
6. BD (1) C 2- C28	254. BD*(1) C 1-Si 6	2.00	0.86	0.037
6. BD (1) C 2- C28	256. BD*(1) C 2- C 3	1.28	1.11	0.034
6. BD (1) C 2- C28	258. BD*(1) C 3- C 4	2.22	1.06	0.043
7. BD (1) C 3- C 4	74. RY*(2) C 2	1.34	1.60	0.041
7. BD (1) C 3- C 4	235. RY*(1) C32	0.85	1.47	0.032
7. BD (1) C 3- C 4	254. BD*(1) C 1-Si 6	0.99	0.93	0.027
7. BD (1) C 3- C 4	256. BD*(1) C 2- C 3	1.27	1.17	0.035
7. BD (1) C 3- C 4	257. BD*(1) C 2- C28	2.89	1.09	0.050
7. BD (1) C 3- C 4	259. BD*(1) C 3- C32	0.89	1.10	0.028
7. BD (1) C 3- C 4	260. BD*(1) C 4- H 5	0.56	1.10	0.022
7. BD (1) C 3- C 4	261. BD*(1) C 4-Si 6	1.31	0.90	0.031
7. BD (1) C 3- C 4	262. BD*(1) C 4- H36	0.94	1.14	0.029
7. BD (1) C 3- C 4	264. BD*(1)Si 6- C12	0.50	0.95	0.020
7. BD (1) C 3- C 4	286. BD*(1) C32- H33	1.22	1.14	0.033
8. BD (1) C 3- C32	73. RY*(1) C 2	0.90	1.85	0.037
8. BD (1) C 3- C32	74. RY*(2) C 2	0.57	1.58	0.027
8. BD (1) C 3- C32	99. RY*(1) C 4	0.70	1.60	0.030
8. BD (1) C 3- C32	252. BD*(1) C 1- C 2	2.32	1.23	0.048
8. BD (1) C 3- C32	256. BD*(1) C 2- C 3	1.05	1.16	0.031
8. BD (1) C 3- C32	258. BD*(1) C 3- C 4	0.87	1.11	0.028
8. BD (1) C 3- C32	260. BD*(1) C 4- H 5	0.56	1.09	0.022
8. BD (1) C 3- C32	261. BD*(1) C 4-Si 6	1.15	0.88	0.029
8. BD (1) C 3- C32	286. BD*(1) C32- H33	0.53	1.12	0.022
8. BD (1) C 3- C32	287. BD*(1) C32- H34	0.54	1.09	0.022
8. BD (1) C 3- C32	288. BD*(1) C32- H35	0.53	1.12	0.022
9. BD (1) C 4- H 5	59. LP*(1) C 3	8.73	0.38	0.061
9. BD (1) C 4- H 5	254. BD*(1) C 1-Si 6	0.61	0.76	0.019
9. BD (1) C 4- H 5	258. BD*(1) C 3- C 4	0.72	0.95	0.024
9. BD (1) C 4- H 5	259. BD*(1) C 3- C32	1.95	0.93	0.039
9. BD (1) C 4- H 5	261. BD*(1) C 4-Si 6	4.30	0.72	0.050
9. BD (1) C 4- H 5	263. BD*(1)Si 6- C 8	0.87	0.77	0.023
10. BD (1) C 4-Si 6	59. LP*(1) C 3	19.62	0.29	0.076
10. BD (1) C 4-Si 6	87. RY*(2) C 3	0.91	1.45	0.034
10. BD (1) C 4-Si 6	252. BD*(1) C 1- C 2	0.82	0.98	0.026
10. BD (1) C 4-Si 6	254. BD*(1) C 1-Si 6	2.96	0.67	0.041
10. BD (1) C 4-Si 6	255. BD*(1) C 1-Si 7	0.78	0.68	0.021
10. BD (1) C 4-Si 6	258. BD*(1) C 3- C 4	1.60	0.86	0.035
10. BD (1) C 4-Si 6	259. BD*(1) C 3- C32	4.64	0.84	0.058
10. BD (1) C 4-Si 6	261. BD*(1) C 4-Si 6	0.73	0.63	0.020
10. BD (1) C 4-Si 6	262. BD*(1) C 4- H36	1.79	0.88	0.037
10. BD (1) C 4-Si 6	263. BD*(1)Si 6- C 8	4.68	0.68	0.052
10. BD (1) C 4-Si 6	264. BD*(1)Si 6- C12	3.03	0.69	0.042
10. BD (1) C 4-Si 6	269. BD*(1) C 8- H10	1.08	0.89	0.029
10. BD (1) C 4-Si 6	271. BD*(1) C12- H13	0.89	0.90	0.026
11. BD (1) C 4- H36	86. RY*(1) C 3	0.51	1.58	0.025
11. BD (1) C 4- H36	256. BD*(1) C 2- C 3	4.26	1.00	0.059
11. BD (1) C 4- H36	258. BD*(1) C 3- C 4	0.97	0.95	0.027
12. BD (1)Si 6- C 8	253. BD*(2) C 1- C 2	1.34	0.52	0.024
12. BD (1)Si 6- C 8	254. BD*(1) C 1-Si 6	2.69	0.73	0.040
12. BD (1)Si 6- C 8	261. BD*(1) C 4-Si 6	0.63	0.70	0.019
12. BD (1)Si 6- C 8	264. BD*(1)Si 6- C12	2.80	0.76	0.041
12. BD (1)Si 6- C 8	268. BD*(1) C 8- H 9	0.66	0.96	0.023
12. BD (1)Si 6- C 8	269. BD*(1) C 8- H10	0.71	0.96	0.024
12. BD (1)Si 6- C 8	270. BD*(1) C 8- H11	0.71	0.96	0.023
12. BD (1)Si 6- C 8	273. BD*(1) C12- H15	1.08	0.96	0.029
13. BD (1)Si 6- C12	252. BD*(1) C 1- C 2	0.51	1.05	0.021
13. BD (1)Si 6- C12	253. BD*(2) C 1- C 2	0.62	0.53	0.016
13. BD (1)Si 6- C12	254. BD*(1) C 1-Si 6	2.90	0.74	0.042
13. BD (1)Si 6- C12	261. BD*(1) C 4-Si 6	1.02	0.71	0.024

13. BD (1)Si 6- C12	263. BD*(1)Si 6- C 8	2.74	0.75	0.041
13. BD (1)Si 6- C12	270. BD*(1) C 8- H11	1.06	0.97	0.029
13. BD (1)Si 6- C12	271. BD*(1) C12- H13	0.98	0.97	0.028
13. BD (1)Si 6- C12	272. BD*(1) C12- H14	0.82	0.97	0.025
13. BD (1)Si 6- C12	273. BD*(1) C12- H15	0.85	0.97	0.026
14. BD (1)Si 7- C16	253. BD*(2) C 1- C 2	1.15	0.49	0.021
14. BD (1)Si 7- C16	255. BD*(1) C 1-Si 7	2.58	0.72	0.039
14. BD (1)Si 7- C16	266. BD*(1)Si 7- C20	1.86	0.75	0.034
14. BD (1)Si 7- C16	267. BD*(1)Si 7- C24	2.16	0.74	0.036
14. BD (1)Si 7- C16	274. BD*(1) C16- H17	0.79	0.95	0.025
14. BD (1)Si 7- C16	275. BD*(1) C16- H18	0.68	0.95	0.023
14. BD (1)Si 7- C16	276. BD*(1) C16- H19	0.85	0.95	0.026
14. BD (1)Si 7- C16	278. BD*(1) C20- H22	1.18	0.95	0.030
14. BD (1)Si 7- C16	282. BD*(1) C24- H27	1.05	0.95	0.028
15. BD (1)Si 7- C20	252. BD*(1) C 1- C 2	1.89	1.02	0.039
15. BD (1)Si 7- C20	255. BD*(1) C 1-Si 7	2.11	0.72	0.035
15. BD (1)Si 7- C20	265. BD*(1)Si 7- C16	1.90	0.75	0.034
15. BD (1)Si 7- C20	267. BD*(1)Si 7- C24	1.87	0.75	0.033
15. BD (1)Si 7- C20	276. BD*(1) C16- H19	1.17	0.96	0.030
15. BD (1)Si 7- C20	277. BD*(1) C20- H21	0.92	0.94	0.026
15. BD (1)Si 7- C20	278. BD*(1) C20- H22	0.93	0.95	0.027
15. BD (1)Si 7- C20	279. BD*(1) C20- H23	0.93	0.95	0.027
15. BD (1)Si 7- C20	280. BD*(1) C24- H25	1.17	0.96	0.030
16. BD (1)Si 7- C24	253. BD*(2) C 1- C 2	1.28	0.49	0.023
16. BD (1)Si 7- C24	255. BD*(1) C 1-Si 7	2.52	0.72	0.038
16. BD (1)Si 7- C24	265. BD*(1)Si 7- C16	2.17	0.74	0.036
16. BD (1)Si 7- C24	266. BD*(1)Si 7- C20	1.87	0.75	0.034
16. BD (1)Si 7- C24	274. BD*(1) C16- H17	1.06	0.95	0.029
16. BD (1)Si 7- C24	277. BD*(1) C20- H21	1.21	0.94	0.030
16. BD (1)Si 7- C24	280. BD*(1) C24- H25	0.85	0.95	0.026
16. BD (1)Si 7- C24	281. BD*(1) C24- H26	0.68	0.95	0.023
16. BD (1)Si 7- C24	282. BD*(1) C24- H27	0.79	0.95	0.025
17. BD (1) C 8- H 9	254. BD*(1) C 1-Si 6	2.29	0.72	0.037
17. BD (1) C 8- H 9	263. BD*(1)Si 6- C 8	0.54	0.73	0.018
18. BD (1) C 8- H10	261. BD*(1) C 4-Si 6	2.55	0.69	0.038
19. BD (1) C 8- H11	263. BD*(1)Si 6- C 8	0.52	0.74	0.018
19. BD (1) C 8- H11	264. BD*(1)Si 6- C12	2.03	0.75	0.035
20. BD (1) C12- H13	261. BD*(1) C 4-Si 6	2.79	0.69	0.039
21. BD (1) C12- H14	254. BD*(1) C 1-Si 6	2.57	0.72	0.039
21. BD (1) C12- H14	264. BD*(1)Si 6- C12	0.55	0.74	0.018
22. BD (1) C12- H15	263. BD*(1)Si 6- C 8	2.18	0.73	0.036
22. BD (1) C12- H15	264. BD*(1)Si 6- C12	0.51	0.74	0.018
23. BD (1) C16- H17	265. BD*(1)Si 7- C16	0.50	0.74	0.017
23. BD (1) C16- H17	267. BD*(1)Si 7- C24	2.02	0.74	0.035
24. BD (1) C16- H18	255. BD*(1) C 1-Si 7	2.28	0.71	0.036
24. BD (1) C16- H18	265. BD*(1)Si 7- C16	0.62	0.74	0.019
25. BD (1) C16- H19	266. BD*(1)Si 7- C20	1.71	0.76	0.032
26. BD (1) C20- H21	267. BD*(1)Si 7- C24	1.81	0.75	0.033
27. BD (1) C20- H22	265. BD*(1)Si 7- C16	1.81	0.75	0.033
28. BD (1) C20- H23	255. BD*(1) C 1-Si 7	2.30	0.71	0.036
28. BD (1) C20- H23	266. BD*(1)Si 7- C20	0.63	0.75	0.020
29. BD (1) C24- H25	266. BD*(1)Si 7- C20	1.71	0.76	0.032
30. BD (1) C24- H26	255. BD*(1) C 1-Si 7	2.25	0.71	0.036
30. BD (1) C24- H26	267. BD*(1)Si 7- C24	0.62	0.74	0.019
31. BD (1) C24- H27	265. BD*(1)Si 7- C16	2.02	0.74	0.035
31. BD (1) C24- H27	267. BD*(1)Si 7- C24	0.51	0.74	0.017
32. BD (1) C28- H29	74. RY*(2) C 2	0.52	1.40	0.024
32. BD (1) C28- H29	256. BD*(1) C 2- C 3	4.28	0.97	0.058
32. BD (1) C28- H29	257. BD*(1) C 2- C28	0.70	0.89	0.022
32. BD (1) C28- H29	266. BD*(1)Si 7- C20	0.53	0.78	0.018
33. BD (1) C28- H30	252. BD*(1) C 1- C 2	3.69	1.04	0.055
33. BD (1) C28- H30	253. BD*(2) C 1- C 2	2.11	0.52	0.030
34. BD (1) C28- H31	75. RY*(3) C 2	0.82	1.43	0.031
34. BD (1) C28- H31	252. BD*(1) C 1- C 2	1.58	1.04	0.036
34. BD (1) C28- H31	253. BD*(2) C 1- C 2	4.08	0.51	0.042
35. BD (1) C32- H33	59. LP*(1) C 3	1.50	0.38	0.025
35. BD (1) C32- H33	87. RY*(2) C 3	0.69	1.54	0.029
35. BD (1) C32- H33	258. BD*(1) C 3- C 4	4.03	0.95	0.055
36. BD (1) C32- H34	59. LP*(1) C 3	12.77	0.37	0.072
36. BD (1) C32- H34	88. RY*(3) C 3	0.74	1.57	0.031
36. BD (1) C32- H34	256. BD*(1) C 2- C 3	0.74	0.98	0.024
37. BD (1) C32- H35	59. LP*(1) C 3	2.52	0.37	0.033

37. BD (1) C32- H35	86. RY*(1) C 3	0.74	1.57	0.031
37. BD (1) C32- H35	256. BD*(1) C 2- C 3	4.13	0.99	0.057
38. CR (1) C 1	74. RY*(2) C 2	2.47	10.95	0.147
38. CR (1) C 1	75. RY*(3) C 2	0.55	10.99	0.070
38. CR (1) C 1	120. RY*(8)Si 6	0.65	10.70	0.075
38. CR (1) C 1	133. RY*(8)Si 7	0.97	10.65	0.091
38. CR (1) C 1	256. BD*(1) C 2- C 3	0.69	10.53	0.077
38. CR (1) C 1	257. BD*(1) C 2- C28	1.18	10.45	0.100
39. CR (1) C 2	61. RY*(2) C 1	1.95	10.86	0.130
39. CR (1) C 2	87. RY*(2) C 3	2.29	11.09	0.142
39. CR (1) C 2	221. RY*(3) C28	1.28	10.88	0.105
39. CR (1) C 2	252. BD*(1) C 1- C 2	0.71	10.62	0.078
39. CR (1) C 2	254. BD*(1) C 1-Si 6	0.77	10.31	0.081
39. CR (1) C 2	255. BD*(1) C 1-Si 7	0.76	10.32	0.080
39. CR (1) C 2	259. BD*(1) C 3- C32	0.62	10.48	0.073
40. CR (1) C 3	73. RY*(1) C 2	1.08	11.29	0.099
40. CR (1) C 3	74. RY*(2) C 2	0.79	11.03	0.084
40. CR (1) C 3	101. RY*(3) C 4	1.67	10.85	0.120
40. CR (1) C 3	237. RY*(3) C32	1.17	11.00	0.101
40. CR (1) C 3	252. BD*(1) C 1- C 2	0.53	10.67	0.067
40. CR (1) C 3	257. BD*(1) C 2- C28	0.57	10.52	0.069
41. CR (1) C 4	86. RY*(1) C 3	1.80	11.11	0.126
41. CR (1) C 4	112. RY*(1) H 5	0.61	10.86	0.073
41. CR (1) C 4	251. RY*(1) H36	0.57	10.81	0.070
41. CR (1) C 4	256. BD*(1) C 2- C 3	0.53	10.53	0.067
41. CR (1) C 4	259. BD*(1) C 3- C32	0.67	10.46	0.075
43. CR (2)Si 6	156. RY*(2) C12	0.51	6.65	0.052
43. CR (2)Si 6	254. BD*(1) C 1-Si 6	0.74	6.14	0.061
43. CR (2)Si 6	255. BD*(1) C 1-Si 7	0.94	6.16	0.069
43. CR (2)Si 6	262. BD*(1) C 4- H36	0.53	6.36	0.052
43. CR (2)Si 6	263. BD*(1)Si 6- C 8	0.82	6.15	0.064
43. CR (2)Si 6	264. BD*(1)Si 6- C12	1.01	6.17	0.071
48. CR (2)Si 7	252. BD*(1) C 1- C 2	0.89	6.42	0.068
48. CR (2)Si 7	254. BD*(1) C 1-Si 6	0.72	6.10	0.060
48. CR (2)Si 7	255. BD*(1) C 1-Si 7	0.91	6.12	0.068
48. CR (2)Si 7	265. BD*(1)Si 7- C16	0.67	6.15	0.058
48. CR (2)Si 7	266. BD*(1)Si 7- C20	0.56	6.16	0.053
48. CR (2)Si 7	267. BD*(1)Si 7- C24	0.67	6.15	0.058
52. CR (1) C 8	118. RY*(6)Si 6	0.66	10.57	0.075
52. CR (1) C 8	152. RY*(1) H 9	0.60	10.81	0.072
52. CR (1) C 8	153. RY*(1) H10	0.61	10.82	0.073
52. CR (1) C 8	154. RY*(1) H11	0.60	10.83	0.072
53. CR (1) C12	116. RY*(4)Si 6	0.56	10.67	0.069
53. CR (1) C12	168. RY*(1) H13	0.64	10.83	0.075
53. CR (1) C12	169. RY*(1) H14	0.59	10.81	0.071
53. CR (1) C12	170. RY*(1) H15	0.59	10.82	0.071
54. CR (1) C16	132. RY*(7)Si 7	0.71	10.48	0.077
54. CR (1) C16	184. RY*(1) H17	0.57	10.83	0.070
54. CR (1) C16	185. RY*(1) H18	0.59	10.81	0.071
54. CR (1) C16	186. RY*(1) H19	0.63	10.83	0.074
55. CR (1) C20	131. RY*(6)Si 7	0.85	10.69	0.085
55. CR (1) C20	200. RY*(1) H21	0.57	10.83	0.070
55. CR (1) C20	201. RY*(1) H22	0.61	10.84	0.072
55. CR (1) C20	202. RY*(1) H23	0.59	10.81	0.071
56. CR (1) C24	132. RY*(7)Si 7	0.99	10.48	0.091
56. CR (1) C24	216. RY*(1) H25	0.64	10.83	0.074
56. CR (1) C24	217. RY*(1) H26	0.59	10.80	0.071
56. CR (1) C24	218. RY*(1) H27	0.58	10.82	0.070
57. CR (1) C28	73. RY*(1) C 2	1.07	11.21	0.098
57. CR (1) C28	232. RY*(1) H29	0.64	10.91	0.074
57. CR (1) C28	233. RY*(1) H30	0.53	10.85	0.067
57. CR (1) C28	234. RY*(1) H31	0.55	10.86	0.069
57. CR (1) C28	252. BD*(1) C 1- C 2	0.86	10.59	0.086
57. CR (1) C28	256. BD*(1) C 2- C 3	0.52	10.52	0.067
58. CR (1) C32	86. RY*(1) C 3	0.99	11.12	0.094
58. CR (1) C32	87. RY*(2) C 3	0.61	11.08	0.073
58. CR (1) C32	248. RY*(1) H33	0.58	10.85	0.071
58. CR (1) C32	249. RY*(1) H34	0.60	10.84	0.072
58. CR (1) C32	250. RY*(1) H35	0.57	10.83	0.070
58. CR (1) C32	256. BD*(1) C 2- C 3	0.59	10.54	0.071
58. CR (1) C32	258. BD*(1) C 3- C 4	0.57	10.49	0.069



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see: No. 2-1; No. 4-1

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol

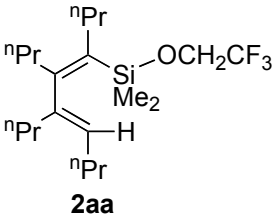
Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1- C 2	86. RY*(1) C 3	0.55	1.61	0.027
1. BD (1) C 1- C 2	87. RY*(2) C 3	0.89	1.86	0.037
1. BD (1) C 1- C 2	158. RY*(1) C15	0.66	1.52	0.028
1. BD (1) C 1- C 2	253. BD*(1) C 1-Si 6	1.43	0.92	0.033
1. BD (1) C 1- C 2	254. BD*(1) C 1- H23	0.93	1.15	0.029
1. BD (1) C 1- C 2	255. BD*(1) C 1-Si24	1.73	0.89	0.035
1. BD (1) C 1- C 2	256. BD*(1) C 2- C 3	1.62	1.17	0.039
1. BD (1) C 1- C 2	257. BD*(1) C 2- C15	1.35	1.12	0.035
1. BD (1) C 1- C 2	260. BD*(1) C 3- C19	2.85	1.12	0.051
1. BD (1) C 1- C 2	262. BD*(1) C 4-Si 6	0.91	0.97	0.027
1. BD (1) C 1- C 2	263. BD*(1)Si 6- C 7	1.05	0.98	0.029
1. BD (1) C 1- C 2	273. BD*(1) C15- H18	0.58	1.14	0.023
2. BD (1) C 1-Si 6	59. LP*(1) C 2	3.04	0.34	0.034
2. BD (1) C 1-Si 6	74. RY*(2) C 2	1.53	1.47	0.044
2. BD (1) C 1-Si 6	252. BD*(1) C 1- C 2	1.57	0.95	0.035
2. BD (1) C 1-Si 6	254. BD*(1) C 1- H23	0.89	0.91	0.026
2. BD (1) C 1-Si 6	255. BD*(1) C 1-Si24	8.56	0.65	0.067
2. BD (1) C 1-Si 6	257. BD*(1) C 2- C15	7.36	0.88	0.074
2. BD (1) C 1-Si 6	258. BD*(1) C 3- C 4	0.73	1.07	0.026
2. BD (1) C 1-Si 6	261. BD*(1) C 4- H 5	1.81	0.96	0.038
2. BD (1) C 1-Si 6	262. BD*(1) C 4-Si 6	1.80	0.74	0.033
2. BD (1) C 1-Si 6	263. BD*(1)Si 6- C 7	1.79	0.74	0.033
2. BD (1) C 1-Si 6	264. BD*(1)Si 6- C11	2.25	0.74	0.037
2. BD (1) C 1-Si 6	265. BD*(1) C 7- H 8	0.64	0.94	0.023
2. BD (1) C 1-Si 6	269. BD*(1) C11- H13	0.84	0.95	0.026
2. BD (1) C 1-Si 6	278. BD*(1)Si24- C29	0.67	0.74	0.020
2. BD (1) C 1-Si 6	279. BD*(1)Si24- C33	0.59	0.74	0.019
3. BD (1) C 1- H23	59. LP*(1) C 2	1.41	0.39	0.025
3. BD (1) C 1- H23	73. RY*(1) C 2	0.72	1.56	0.030
3. BD (1) C 1- H23	74. RY*(2) C 2	0.60	1.51	0.027
3. BD (1) C 1- H23	252. BD*(1) C 1- C 2	1.27	0.99	0.032
3. BD (1) C 1- H23	255. BD*(1) C 1-Si24	3.52	0.69	0.045
3. BD (1) C 1- H23	256. BD*(1) C 2- C 3	5.17	0.97	0.063
3. BD (1) C 1- H23	277. BD*(1)Si24- C25	0.88	0.78	0.023
4. BD (1) C 1-Si24	59. LP*(1) C 2	43.90	0.26	0.105
4. BD (1) C 1-Si24	73. RY*(1) C 2	0.65	1.44	0.029
4. BD (1) C 1-Si24	75. RY*(3) C 2	0.81	1.35	0.032
4. BD (1) C 1-Si24	116. RY*(4)Si 6	0.56	1.13	0.024
4. BD (1) C 1-Si24	252. BD*(1) C 1- C 2	2.76	0.86	0.047
4. BD (1) C 1-Si24	255. BD*(1) C 1-Si24	1.92	0.57	0.031
4. BD (1) C 1-Si24	256. BD*(1) C 2- C 3	0.57	0.85	0.021
4. BD (1) C 1-Si24	257. BD*(1) C 2- C15	0.60	0.80	0.021
4. BD (1) C 1-Si24	264. BD*(1)Si 6- C11	1.52	0.66	0.030
4. BD (1) C 1-Si24	277. BD*(1)Si24- C25	4.29	0.65	0.051
4. BD (1) C 1-Si24	278. BD*(1)Si24- C29	4.37	0.66	0.051
4. BD (1) C 1-Si24	279. BD*(1)Si24- C33	4.33	0.66	0.051
4. BD (1) C 1-Si24	280. BD*(1) C25- H26	0.88	0.86	0.027
4. BD (1) C 1-Si24	283. BD*(1) C29- H30	0.91	0.86	0.027
4. BD (1) C 1-Si24	288. BD*(1) C33- H36	0.77	0.86	0.025
5. BD (1) C 2- C 3	60. RY*(1) C 1	1.14	1.69	0.039
5. BD (1) C 2- C 3	99. RY*(1) C 4	1.21	1.92	0.043
5. BD (1) C 2- C 3	158. RY*(1) C15	0.92	1.50	0.033
5. BD (1) C 2- C 3	174. RY*(1) C19	0.66	1.48	0.028
5. BD (1) C 2- C 3	252. BD*(1) C 1- C 2	1.30	1.16	0.035
5. BD (1) C 2- C 3	254. BD*(1) C 1- H23	1.51	1.12	0.037
5. BD (1) C 2- C 3	257. BD*(1) C 2- C15	0.64	1.09	0.024
5. BD (1) C 2- C 3	258. BD*(1) C 3- C 4	1.93	1.28	0.044

5. BD (1) C 2- C 3	260. BD*(1) C 3- C19	1.00	1.10	0.030
5. BD (1) C 2- C 3	261. BD*(1) C 4- H 5	2.27	1.18	0.046
5. BD (1) C 2- C 3	271. BD*(1) C15- H16	1.16	1.14	0.033
5. BD (1) C 2- C 3	276. BD*(1) C19- H22	0.65	1.16	0.025
6. BD (1) C 2- C15	60. RY*(1) C 1	0.53	1.67	0.027
6. BD (1) C 2- C15	87. RY*(2) C 3	1.31	1.82	0.044
6. BD (1) C 2- C15	252. BD*(1) C 1- C 2	1.45	1.14	0.036
6. BD (1) C 2- C15	253. BD*(1) C 1-Si 6	1.90	0.88	0.037
6. BD (1) C 2- C15	256. BD*(1) C 2- C 3	0.78	1.12	0.027
6. BD (1) C 2- C15	258. BD*(1) C 3- C 4	1.80	1.26	0.043
6. BD (1) C 2- C15	271. BD*(1) C15- H16	0.52	1.13	0.022
6. BD (1) C 2- C15	272. BD*(1) C15- H17	0.53	1.10	0.022
6. BD (1) C 2- C15	273. BD*(1) C15- H18	0.59	1.10	0.023
7. BD (1) C 3- C 4	73. RY*(1) C 2	1.27	1.77	0.043
7. BD (1) C 3- C 4	253. BD*(1) C 1-Si 6	0.74	0.94	0.024
7. BD (1) C 3- C 4	256. BD*(1) C 2- C 3	2.35	1.18	0.047
7. BD (1) C 3- C 4	257. BD*(1) C 2- C15	3.12	1.13	0.053
7. BD (1) C 3- C 4	260. BD*(1) C 3- C19	2.54	1.14	0.048
7. BD (1) C 3- C 4	261. BD*(1) C 4- H 5	0.87	1.22	0.029
7. BD (1) C 3- C 4	262. BD*(1) C 4-Si 6	1.21	0.99	0.031
8. BD (2) C 3- C 4	59. LP*(1) C 2	58.13	0.14	0.090
8. BD (2) C 3- C 4	175. RY*(2) C19	0.71	1.25	0.029
8. BD (2) C 3- C 4	259. BD*(2) C 3- C 4	0.92	0.30	0.016
8. BD (2) C 3- C 4	263. BD*(1)Si 6- C 7	1.45	0.54	0.027
8. BD (2) C 3- C 4	264. BD*(1)Si 6- C11	2.67	0.53	0.036
8. BD (2) C 3- C 4	274. BD*(1) C19- H20	2.41	0.73	0.040
8. BD (2) C 3- C 4	275. BD*(1) C19- H21	2.32	0.73	0.039
9. BD (1) C 3- C19	73. RY*(1) C 2	0.90	1.68	0.035
9. BD (1) C 3- C19	99. RY*(1) C 4	0.65	1.86	0.031
9. BD (1) C 3- C19	252. BD*(1) C 1- C 2	2.07	1.10	0.043
9. BD (1) C 3- C19	256. BD*(1) C 2- C 3	1.27	1.09	0.033
9. BD (1) C 3- C19	258. BD*(1) C 3- C 4	2.66	1.22	0.051
9. BD (1) C 3- C19	262. BD*(1) C 4-Si 6	2.06	0.89	0.038
10. BD (1) C 4- H 5	87. RY*(2) C 3	1.49	1.68	0.045
10. BD (1) C 4- H 5	256. BD*(1) C 2- C 3	5.59	0.99	0.067
10. BD (1) C 4- H 5	258. BD*(1) C 3- C 4	1.45	1.12	0.036
11. BD (1) C 4-Si 6	86. RY*(1) C 3	3.77	1.40	0.065
11. BD (1) C 4-Si 6	252. BD*(1) C 1- C 2	0.60	0.97	0.022
11. BD (1) C 4-Si 6	253. BD*(1) C 1-Si 6	2.72	0.71	0.039
11. BD (1) C 4-Si 6	254. BD*(1) C 1- H23	1.28	0.94	0.031
11. BD (1) C 4-Si 6	256. BD*(1) C 2- C 3	0.53	0.96	0.020
11. BD (1) C 4-Si 6	257. BD*(1) C 2- C15	0.89	0.91	0.026
11. BD (1) C 4-Si 6	258. BD*(1) C 3- C 4	1.80	1.09	0.040
11. BD (1) C 4-Si 6	260. BD*(1) C 3- C19	9.07	0.92	0.082
11. BD (1) C 4-Si 6	263. BD*(1)Si 6- C 7	1.89	0.77	0.034
11. BD (1) C 4-Si 6	264. BD*(1)Si 6- C11	1.75	0.76	0.033
11. BD (1) C 4-Si 6	266. BD*(1) C 7- H 9	1.02	0.97	0.028
11. BD (1) C 4-Si 6	268. BD*(1) C11- H12	0.99	0.97	0.028
12. BD (1)Si 6- C 7	253. BD*(1) C 1-Si 6	3.50	0.71	0.045
12. BD (1)Si 6- C 7	259. BD*(2) C 3- C 4	0.61	0.53	0.016
12. BD (1)Si 6- C 7	262. BD*(1) C 4-Si 6	2.76	0.76	0.041
12. BD (1)Si 6- C 7	264. BD*(1)Si 6- C11	2.24	0.76	0.037
12. BD (1)Si 6- C 7	265. BD*(1) C 7- H 8	0.78	0.96	0.025
12. BD (1)Si 6- C 7	266. BD*(1) C 7- H 9	0.85	0.96	0.026
12. BD (1)Si 6- C 7	267. BD*(1) C 7- H10	0.97	0.97	0.028
12. BD (1)Si 6- C 7	270. BD*(1) C11- H14	1.09	0.97	0.029
13. BD (1)Si 6- C11	253. BD*(1) C 1-Si 6	2.00	0.69	0.033
13. BD (1)Si 6- C11	255. BD*(1) C 1-Si24	0.73	0.66	0.020
13. BD (1)Si 6- C11	259. BD*(2) C 3- C 4	1.25	0.52	0.023
13. BD (1)Si 6- C11	262. BD*(1) C 4-Si 6	2.24	0.75	0.037
13. BD (1)Si 6- C11	263. BD*(1)Si 6- C 7	2.07	0.75	0.035
13. BD (1)Si 6- C11	267. BD*(1) C 7- H10	1.30	0.96	0.032
13. BD (1)Si 6- C11	268. BD*(1) C11- H12	0.70	0.95	0.023
13. BD (1)Si 6- C11	269. BD*(1) C11- H13	0.62	0.96	0.022
13. BD (1)Si 6- C11	270. BD*(1) C11- H14	0.72	0.96	0.024
14. BD (1) C 7- H 8	253. BD*(1) C 1-Si 6	3.24	0.69	0.042
14. BD (1) C 7- H 8	263. BD*(1)Si 6- C 7	0.64	0.75	0.020
15. BD (1) C 7- H 9	117. RY*(5)Si 6	0.51	1.11	0.021
15. BD (1) C 7- H 9	262. BD*(1) C 4-Si 6	2.31	0.74	0.037
15. BD (1) C 7- H 9	263. BD*(1)Si 6- C 7	0.53	0.75	0.018
16. BD (1) C 7- H10	263. BD*(1)Si 6- C 7	0.52	0.75	0.018
16. BD (1) C 7- H10	264. BD*(1)Si 6- C11	1.84	0.75	0.033

17. BD (1) C11- H12	262. BD*(1) C 4-Si 6	2.17	0.74	0.036
17. BD (1) C11- H12	264. BD*(1)Si 6- C11	0.54	0.74	0.018
18. BD (1) C11- H13	253. BD*(1) C 1-Si 6	2.19	0.69	0.035
18. BD (1) C11- H13	264. BD*(1)Si 6- C11	0.56	0.74	0.018
19. BD (1) C11- H14	263. BD*(1)Si 6- C 7	1.98	0.75	0.035
19. BD (1) C11- H14	264. BD*(1)Si 6- C11	0.53	0.74	0.018
20. BD (1) C15- H16	73. RY*(1) C 2	0.59	1.56	0.027
20. BD (1) C15- H16	256. BD*(1) C 2- C 3	4.53	0.97	0.060
20. BD (1) C15- H16	257. BD*(1) C 2- C15	0.56	0.92	0.020
21. BD (1) C15- H17	59. LP*(1) C 2	8.70	0.37	0.061
21. BD (1) C15- H17	252. BD*(1) C 1- C 2	2.11	0.97	0.041
22. BD (1) C15- H18	59. LP*(1) C 2	6.56	0.37	0.053
22. BD (1) C15- H18	252. BD*(1) C 1- C 2	2.84	0.98	0.047
23. BD (1) C19- H20	88. RY*(3) C 3	0.52	1.43	0.025
23. BD (1) C19- H20	258. BD*(1) C 3- C 4	2.40	1.08	0.046
23. BD (1) C19- H20	259. BD*(2) C 3- C 4	3.65	0.52	0.039
24. BD (1) C19- H21	88. RY*(3) C 3	0.69	1.43	0.028
24. BD (1) C19- H21	258. BD*(1) C 3- C 4	2.24	1.08	0.044
24. BD (1) C19- H21	259. BD*(2) C 3- C 4	3.65	0.52	0.039
25. BD (1) C19- H22	256. BD*(1) C 2- C 3	5.61	0.94	0.065
25. BD (1) C19- H22	260. BD*(1) C 3- C19	0.65	0.90	0.022
26. BD (1)Si24- C25	255. BD*(1) C 1-Si24	1.29	0.67	0.027
26. BD (1)Si24- C25	278. BD*(1)Si24- C29	2.75	0.76	0.041
26. BD (1)Si24- C25	279. BD*(1)Si24- C33	2.85	0.76	0.042
26. BD (1)Si24- C25	280. BD*(1) C25- H26	0.87	0.96	0.026
26. BD (1)Si24- C25	281. BD*(1) C25- H27	0.92	0.96	0.027
26. BD (1)Si24- C25	282. BD*(1) C25- H28	1.05	0.97	0.029
26. BD (1)Si24- C25	284. BD*(1) C29- H31	1.12	0.96	0.029
26. BD (1)Si24- C25	287. BD*(1) C33- H35	1.02	0.96	0.028
27. BD (1)Si24- C29	255. BD*(1) C 1-Si24	0.77	0.66	0.020
27. BD (1)Si24- C29	277. BD*(1)Si24- C25	2.69	0.75	0.040
27. BD (1)Si24- C29	279. BD*(1)Si24- C33	2.47	0.75	0.039
27. BD (1)Si24- C29	282. BD*(1) C25- H28	1.21	0.97	0.031
27. BD (1)Si24- C29	283. BD*(1) C29- H30	0.88	0.96	0.026
27. BD (1)Si24- C29	284. BD*(1) C29- H31	0.96	0.96	0.027
27. BD (1)Si24- C29	285. BD*(1) C29- H32	1.00	0.96	0.028
27. BD (1)Si24- C29	286. BD*(1) C33- H34	1.19	0.97	0.030
28. BD (1)Si24- C33	252. BD*(1) C 1- C 2	1.13	0.96	0.029
28. BD (1)Si24- C33	255. BD*(1) C 1-Si24	0.70	0.66	0.019
28. BD (1)Si24- C33	277. BD*(1)Si24- C25	2.86	0.75	0.041
28. BD (1)Si24- C33	278. BD*(1)Si24- C29	2.61	0.75	0.040
28. BD (1)Si24- C33	281. BD*(1) C25- H27	1.11	0.96	0.029
28. BD (1)Si24- C33	285. BD*(1) C29- H32	1.22	0.96	0.031
28. BD (1)Si24- C33	286. BD*(1) C33- H34	1.01	0.97	0.028
28. BD (1)Si24- C33	287. BD*(1) C33- H35	0.90	0.96	0.026
28. BD (1)Si24- C33	288. BD*(1) C33- H36	0.79	0.96	0.025
29. BD (1) C25- H26	255. BD*(1) C 1-Si24	3.18	0.65	0.041
29. BD (1) C25- H26	277. BD*(1)Si24- C25	0.61	0.73	0.019
30. BD (1) C25- H27	277. BD*(1)Si24- C25	0.53	0.74	0.018
30. BD (1) C25- H27	279. BD*(1)Si24- C33	2.17	0.74	0.036
31. BD (1) C25- H28	194. RY*(4)Si24	0.75	1.03	0.025
31. BD (1) C25- H28	277. BD*(1)Si24- C25	0.52	0.74	0.018
31. BD (1) C25- H28	278. BD*(1)Si24- C29	1.75	0.74	0.032
32. BD (1) C29- H30	255. BD*(1) C 1-Si24	3.17	0.65	0.041
32. BD (1) C29- H30	278. BD*(1)Si24- C29	0.60	0.73	0.019
33. BD (1) C29- H31	277. BD*(1)Si24- C25	1.98	0.73	0.034
33. BD (1) C29- H31	278. BD*(1)Si24- C29	0.54	0.74	0.018
34. BD (1) C29- H32	278. BD*(1)Si24- C29	0.53	0.74	0.018
34. BD (1) C29- H32	279. BD*(1)Si24- C33	1.83	0.74	0.033
35. BD (1) C33- H34	278. BD*(1)Si24- C29	1.79	0.74	0.033
35. BD (1) C33- H34	279. BD*(1)Si24- C33	0.56	0.74	0.018
36. BD (1) C33- H35	277. BD*(1)Si24- C25	2.19	0.73	0.036
36. BD (1) C33- H35	279. BD*(1)Si24- C33	0.56	0.74	0.018
37. BD (1) C33- H36	255. BD*(1) C 1-Si24	2.96	0.65	0.040
37. BD (1) C33- H36	279. BD*(1)Si24- C33	0.59	0.73	0.019
38. CR (1) C 1	73. RY*(1) C 2	2.10	11.08	0.136
38. CR (1) C 1	79. RY*(7) C 2	0.53	12.13	0.071
38. CR (1) C 1	190. RY*(1) H23	0.60	10.88	0.072
38. CR (1) C 1	198. RY*(8)Si24	0.50	10.61	0.065
38. CR (1) C 1	252. BD*(1) C 1- C 2	0.67	10.50	0.075
38. CR (1) C 1	255. BD*(1) C 1-Si24	0.92	10.21	0.088
38. CR (1) C 1	256. BD*(1) C 2- C 3	0.64	10.49	0.074

38. CR (1) C 1	257. BD*(1) C 2- C15	0.81	10.44	0.082
39. CR (1) C 2	61. RY*(2) C 1	1.24	10.87	0.104
39. CR (1) C 2	62. RY*(3) C 1	0.53	10.95	0.068
39. CR (1) C 2	86. RY*(1) C 3	1.61	11.00	0.119
39. CR (1) C 2	160. RY*(3) C15	1.39	11.01	0.110
39. CR (1) C 2	253. BD*(1) C 1-Si 6	0.73	10.32	0.078
39. CR (1) C 2	260. BD*(1) C 3- C19	0.58	10.52	0.070
40. CR (1) C 3	74. RY*(2) C 2	2.16	11.06	0.138
40. CR (1) C 3	100. RY*(2) C 4	2.26	10.85	0.140
40. CR (1) C 3	176. RY*(3) C19	1.33	10.88	0.107
40. CR (1) C 3	257. BD*(1) C 2- C15	0.57	10.47	0.069
40. CR (1) C 3	258. BD*(1) C 3- C 4	0.77	10.65	0.081
40. CR (1) C 3	262. BD*(1) C 4-Si 6	0.86	10.32	0.085
41. CR (1) C 4	86. RY*(1) C 3	1.94	10.94	0.130
41. CR (1) C 4	87. RY*(2) C 3	0.84	11.20	0.087
41. CR (1) C 4	88. RY*(3) C 3	0.59	10.99	0.072
41. CR (1) C 4	112. RY*(1) H 5	0.66	10.76	0.075
41. CR (1) C 4	120. RY*(8)Si 6	0.78	10.58	0.081
41. CR (1) C 4	256. BD*(1) C 2- C 3	0.72	10.50	0.079
41. CR (1) C 4	258. BD*(1) C 3- C 4	0.91	10.64	0.088
41. CR (1) C 4	260. BD*(1) C 3- C19	1.20	10.46	0.101
43. CR (2)Si 6	253. BD*(1) C 1-Si 6	0.90	6.11	0.067
43. CR (2)Si 6	255. BD*(1) C 1-Si24	0.91	6.08	0.068
43. CR (2)Si 6	261. BD*(1) C 4- H 5	1.00	6.39	0.072
43. CR (2)Si 6	262. BD*(1) C 4-Si 6	0.60	6.16	0.055
43. CR (2)Si 6	263. BD*(1)Si 6- C 7	0.86	6.17	0.066
43. CR (2)Si 6	264. BD*(1)Si 6- C11	0.55	6.16	0.052
47. CR (1) C 7	117. RY*(5)Si 6	0.68	10.64	0.076
47. CR (1) C 7	139. RY*(1) H 8	0.59	10.82	0.071
47. CR (1) C 7	140. RY*(1) H 9	0.61	10.83	0.072
47. CR (1) C 7	141. RY*(1) H10	0.66	10.86	0.076
48. CR (1) C11	155. RY*(1) H12	0.59	10.81	0.071
48. CR (1) C11	156. RY*(1) H13	0.60	10.81	0.072
48. CR (1) C11	157. RY*(1) H14	0.60	10.83	0.072
49. CR (1) C15	73. RY*(1) C 2	1.09	11.10	0.098
49. CR (1) C15	74. RY*(2) C 2	0.60	11.05	0.073
49. CR (1) C15	171. RY*(1) H16	0.57	10.86	0.070
49. CR (1) C15	172. RY*(1) H17	0.60	10.85	0.072
49. CR (1) C15	173. RY*(1) H18	0.60	10.88	0.072
49. CR (1) C15	252. BD*(1) C 1- C 2	0.71	10.52	0.078
50. CR (1) C19	87. RY*(2) C 3	1.15	11.18	0.101
50. CR (1) C19	187. RY*(1) H20	0.53	10.85	0.068
50. CR (1) C19	188. RY*(1) H21	0.55	10.84	0.069
50. CR (1) C19	189. RY*(1) H22	0.56	10.81	0.069
50. CR (1) C19	256. BD*(1) C 2- C 3	0.66	10.49	0.075
50. CR (1) C19	258. BD*(1) C 3- C 4	0.75	10.63	0.080
52. CR (2)Si24	255. BD*(1) C 1-Si24	1.15	6.05	0.076
52. CR (2)Si24	277. BD*(1)Si24- C25	0.93	6.13	0.068
52. CR (2)Si24	278. BD*(1)Si24- C29	0.79	6.13	0.063
52. CR (2)Si24	279. BD*(1)Si24- C33	0.78	6.13	0.062
56. CR (1) C25	192. RY*(2)Si24	0.51	10.90	0.066
56. CR (1) C25	194. RY*(4)Si24	0.92	10.56	0.088
56. CR (1) C25	217. RY*(1) H26	0.59	10.82	0.072
56. CR (1) C25	218. RY*(1) H27	0.58	10.85	0.071
56. CR (1) C25	219. RY*(1) H28	0.65	10.87	0.075
57. CR (1) C29	195. RY*(5)Si24	1.18	10.56	0.100
57. CR (1) C29	233. RY*(1) H30	0.59	10.81	0.071
57. CR (1) C29	234. RY*(1) H31	0.57	10.82	0.070
57. CR (1) C29	235. RY*(1) H32	0.59	10.85	0.071
58. CR (1) C33	195. RY*(5)Si24	0.60	10.56	0.071
58. CR (1) C33	249. RY*(1) H34	0.66	10.87	0.076
58. CR (1) C33	250. RY*(1) H35	0.56	10.82	0.070
58. CR (1) C33	251. RY*(1) H36	0.58	10.81	0.071

3. Copies for NMR spectrums for all compounds



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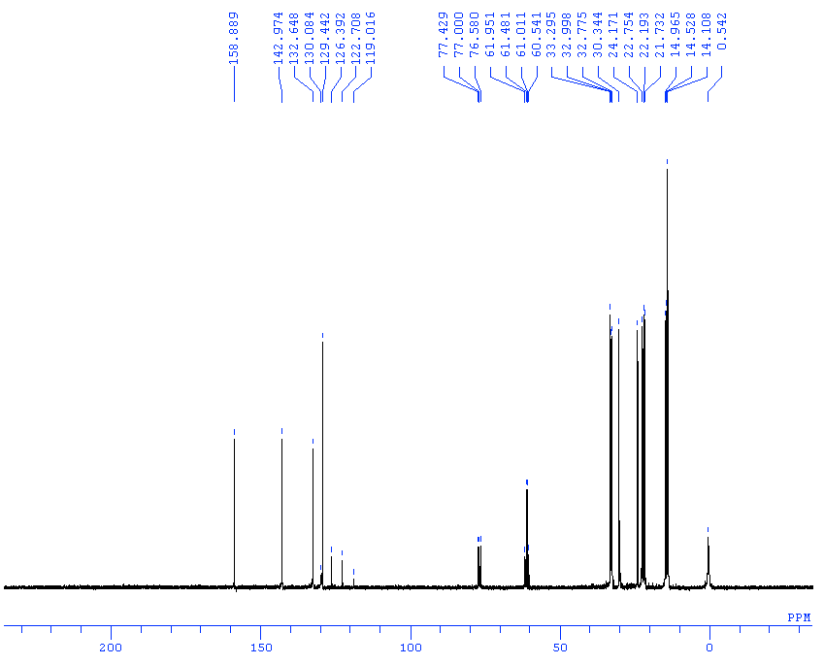
OBSET       130.00 KHz
OBFIN       1150.0 Hz
POINT        32768
FREQU       6013.2 Hz
SCANS            8
ACQTM        5.449 sec
PD           1.551 sec
PW1            5.8 us
IRNUC  1H
CTEMP         20.7 c
SLVNT  CDCL3
EXREF         7.25 ppm
BF            0.09 Hz
RGAIN            8
```

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DFILE  D:\NMR_Users\Xi Zhe
COMNT
DATIM  Mon Sep 21 14:08:28
OBNUC  13C
EXMOD  BCM
OBFRQ        75.45 MHz
OBSET       124.00 KHz
OBFIN       1840.0 Hz
POINT        32768
FREQU      20408.1 Hz
SCANS            512
ACQTM        1.606 sec
PD           1.394 sec
PW1            5.0 us
IRNUC  1H
CTEMP         20.7 c
SLVNT  CDCL3
EXREF        77.00 ppm
BF            0.62 Hz
RGAIN           27
```
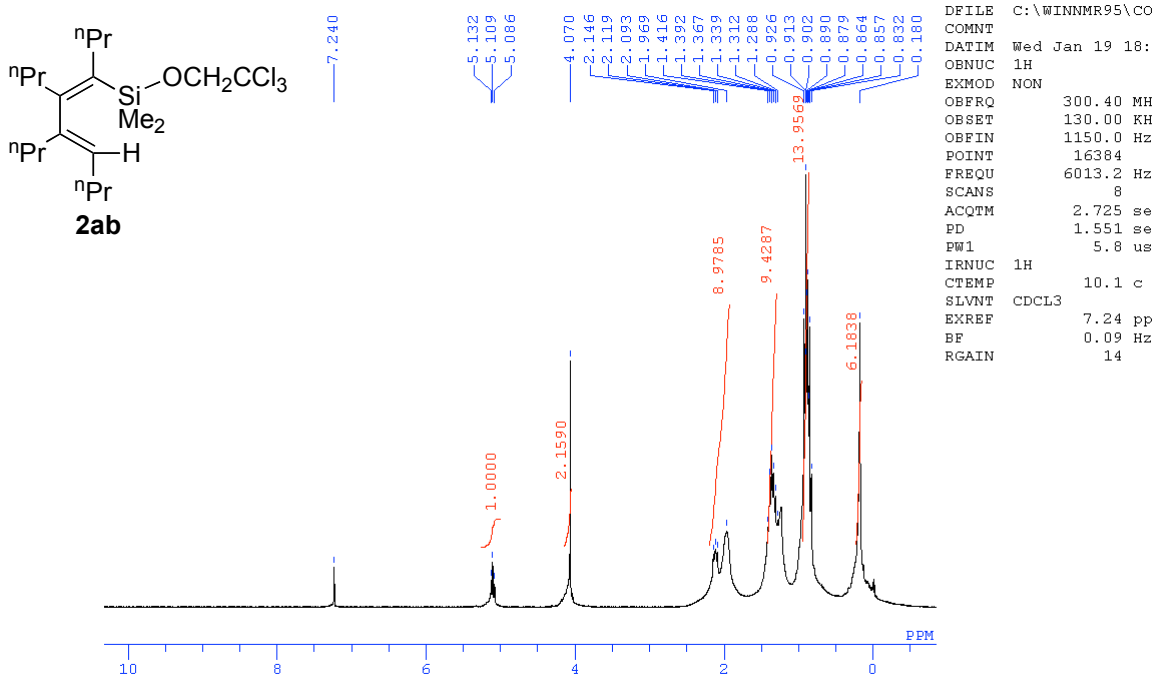
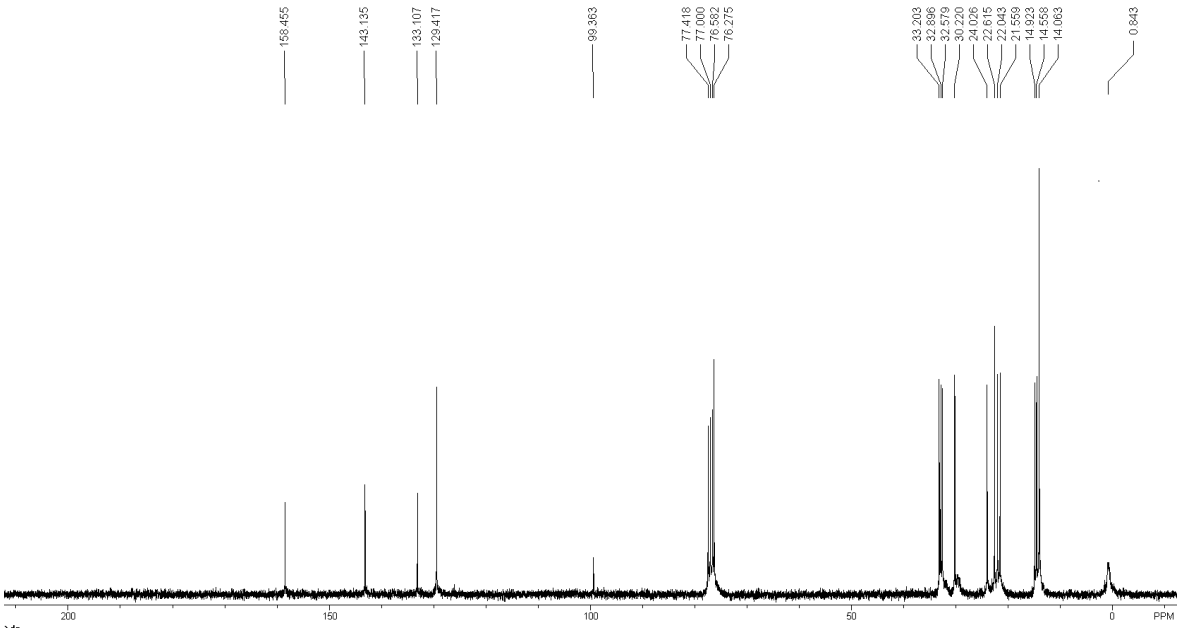
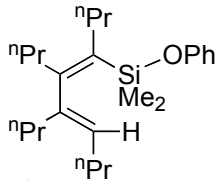
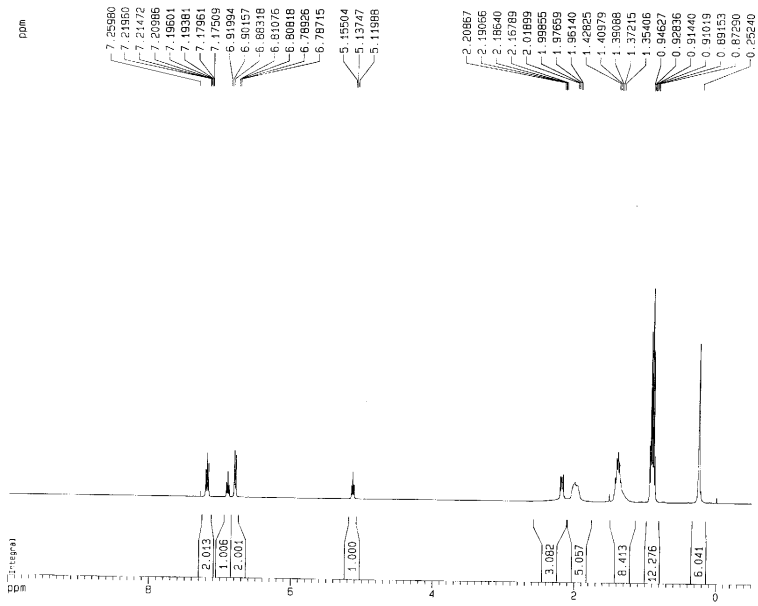


nPr
nPr
Si
OCH2CCl3
Me2
nPr
H
nPr
2ab
7.240
5.132
5.109
5.086
4.070
2.146
2.119
2.093
1.969
1.416
1.392
1.367
1.339
1.312
1.288
0.926
0.913
0.902
0.890
0.879
0.864
0.857
0.832
0.180
13.9569
8.9785
9.4287
6.1838
1.0000
2.1590
DFILE C:\WINNMR95\CO
COMNT
DATIM Wed Jan 19 18:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MH
OBSET 130.00 KH
OBFIN 1150.0 Hz
POINT 16384
FREQU 6013.2 Hz
SCANS 8
ACQTM 2.725 se
PD 1.551 se
PW1 5.8 us
IRNUC 1H
CTEMP 10.1 c
SLVNT CDCL3
EXREF 7.24 pp
BF 0.09 Hz
RGAIN 14
PPM
10
8
6
4
2
0


158.455
143.135
133.107
129.417
99.363
77.418
77.000
76.582
76.275
33.203
32.896
32.579
30.220
24.026
22.615
22.043
21.559
14.923
14.558
14.063
0.843
200
150
100
50
0
PPM



2ac

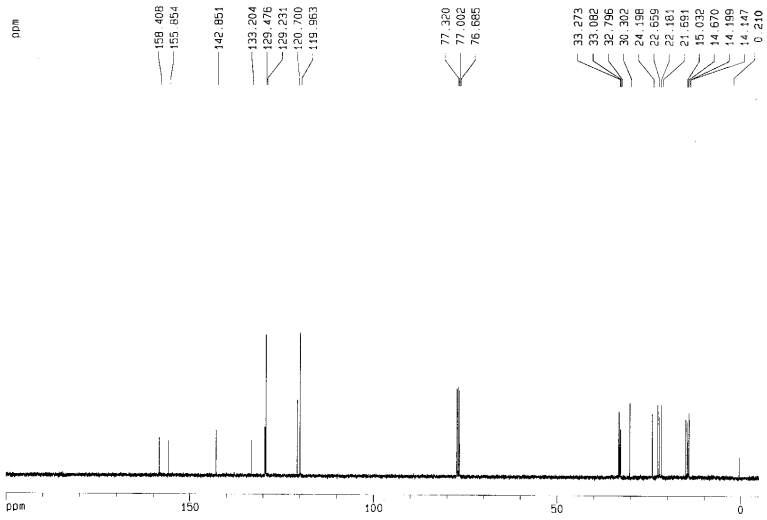


Current Data Parameters
NAME h05733
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100421
Time 16.47
INSTRUM ARX400
PROBHD 5 mm Multinu
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 32
DW 78.000 usec
DE 111.43 usec
TE 300.0 K
D1 2.00000000 sec
P1 3.00 usec
DE 111.43 usec
SFO1 400.1317143 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 32768
SF 400.1300255 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.52500 ppm/cm
HZCM 210.06827 Hz/cm

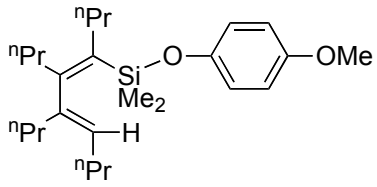


Current Data Parameters
NAME c05733
EXPNO 1
PROCNO 1

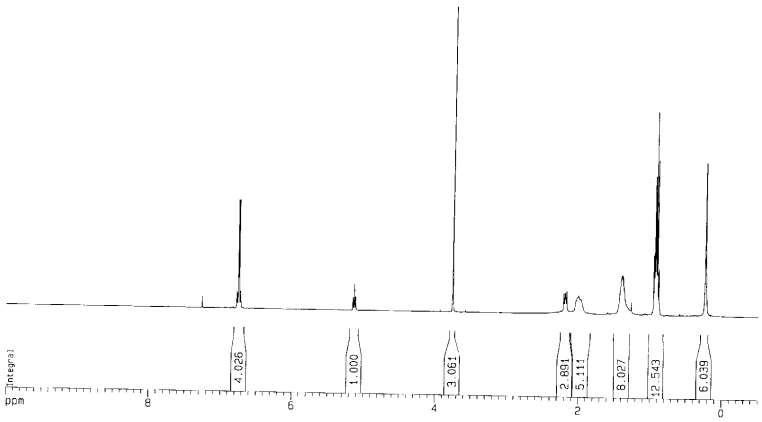
F2 - Acquisition Parameters
Date_ 20100421
Time 16.51
INSTRUM ARX400
PROBHD 5 mm Multinu
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 133
DS 2
SWH 25000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554100 sec
RG 256
DW 20.000 usec
DE 25.00 usec
TE 300.0 K
D12 0.00002000 sec
DL5 22.20 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.00000000 sec
P1 3.50 usec
DE 25.00 usec
SFO1 100.6233660 MHz
NUCLEUS 13C
D11 0.03000000 sec

F2 - Processing parameters
SI 32768
SF 100.6127726 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 10.25000 ppm/cm
HZCM 1031.28101 Hz/cm



2ad

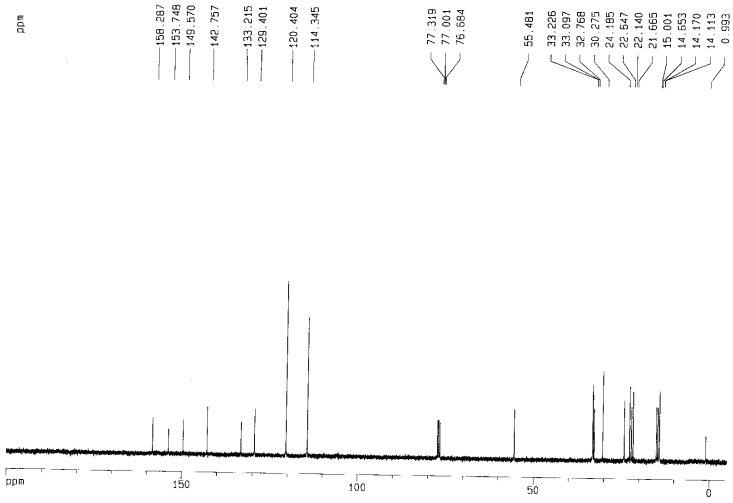


Current Data Parameters
NAME h05828
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100428
Time 9.08
INSTRUM ARX400
PROBHD 5 mm Multinu
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 64
DW 78.000 usec
DE 97.50 usec
TE 300.0 K
D1 2.00000000 sec
P1 3.00 usec
DE 97.50 usec
SFO1 400.1316187 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.52500 ppm/cm
HZCM 210.06825 Hz/cm

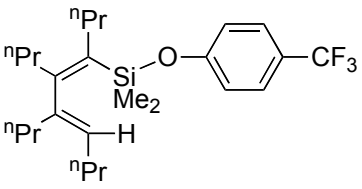


Current Data Parameters
NAME c05828
EXPNO 1
PROCNO 1

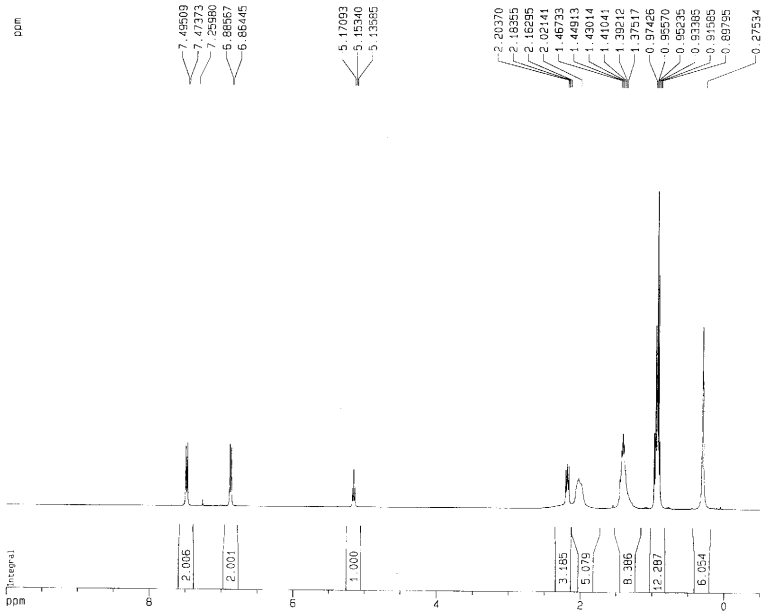
F2 - Acquisition Parameters
Date_ 20100428
Time 9.00
INSTRUM ARX400
PROBHD 5 mm Multinu
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 141
DS 2
SWH 25000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554100 sec
RG 256
DW 20.000 usec
DE 25.00 usec
TE 300.0 K
D12 0.00002000 sec
DL5 22.20 dB
CPDPRG waltz16
P31 100.00 usec
D1 2.00000000 sec
P1 3.50 usec
DE 25.00 usec
SFO1 100.6233680 MHz
NUCLEUS 13C
D11 0.03000000 sec

F2 - Processing parameters
SI 32768
SF 100.6127751 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 0.50

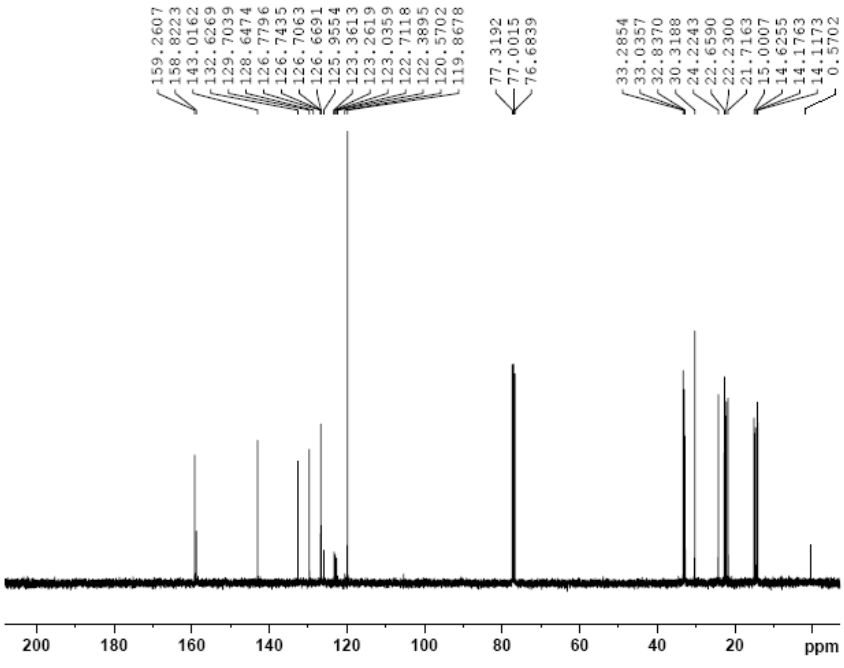
1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 20122.56 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 10.25000 ppm/cm
HZCM 1031.28101 Hz/cm



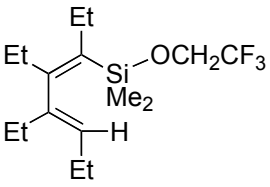
2ae



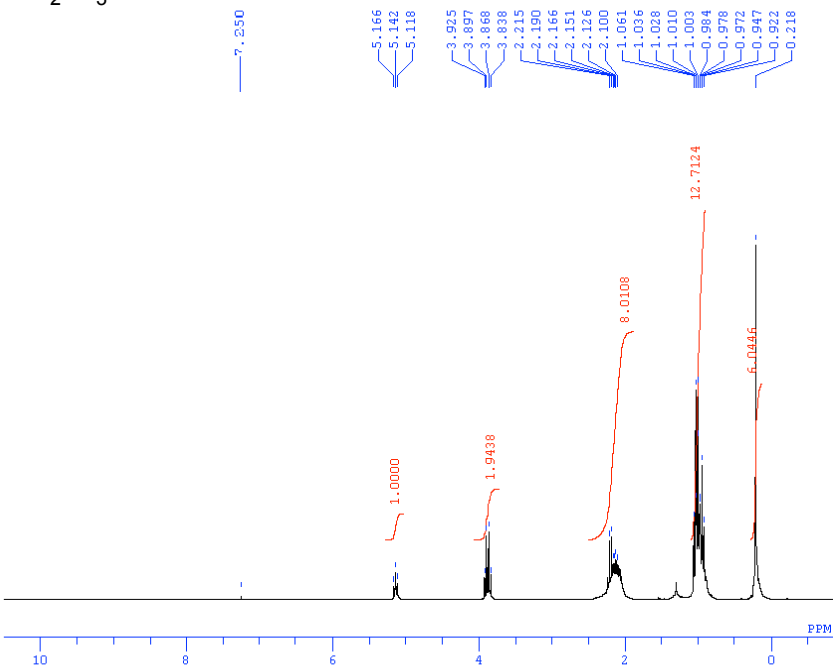

```
Current Data Parameters
NAME                  h05925
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20100430
Time                  16.57
INSTRUM              ARX400
PROBHD     5 mm Multinu
PULPROG                zg
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      0
SWH              6410.256 Hz
FIDRES           0.195625 Hz
AQ               2.5559540 sec
RG                     45
DW                78.000 usec
DE                97.50 usec
TE                300.0 K
D1             2.00000000 sec
P1                 3.00 usec
DE                97.50 usec
SFO1          400.1317143 MHz
NUCLEUS               1H

F2 - Processing parameters
SI                  32768
SF           400.1300093 MHz
WDW                    EM
SSB                     0
LB                 0.50 Hz
GB                      0
PC                   4.00

1D NMR plot parameters
CX                  20.00 cm
F1P                10.000 ppm
F1               4001.30 Hz
F2P                -0.500 ppm
F2               -200.07 Hz
PPMCM             0.52500 ppm/cm
HZCM            210.06825 Hz/cm
```



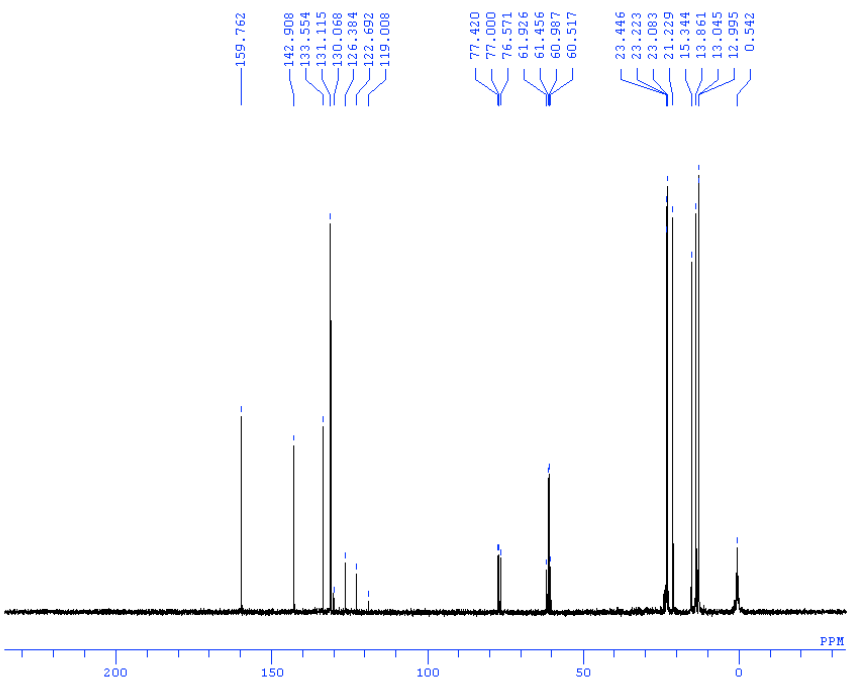

```
Current Data Parameters
NAME                  c05925
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20100430
Time                  16.58
INSTRUM              ARX400
PROBHD     5 mm Multinu
PULPROG             zgdc
TD                  32768
SOLVENT             CDCl3
NS                    301
DS                      2
SWH             25000.000 Hz
FIDRES           0.762939 Hz
AQ               0.6554100 sec
RG                    256
DW                20.000 usec
DE                25.00 usec
TE                300.0 K
D12            0.00002000 sec
DL5                22.20 dB
CPDPRG            waltz16
P31               100.00 usec
D1             2.00000000 sec
P1                 3.50 usec
DE                25.00 usec
SFO1          100.6233680 MHz
NUCLEUS               13C
D11            0.03000000 sec

F2 - Processing parameters
SI                  32768
SF           100.6127674 MHz
WDW                    EM
SSB                     0
LB                 0.50 Hz
GB                      0
PC                   0.50

1D NMR plot parameters
CX                  20.00 cm
F1P                33.438 ppm
F1               3364.25 Hz
F2P                14.004 ppm
F2               1408.95 Hz
PPMCM             0.97169 ppm/cm
HZCM             97.76487 Hz/cm
```



2b




```
DFILE   D:\NMR_Users\Xi Zhe
COMNT
DATIM   Mon Nov 16 10:01:09
OBNUC   1H
EXMOD   NON
OBFRQ       300.40 MHz
OBSET       130.00 KHz
OBFIN       1150.0 Hz
POINT        32768
FREQU       6013.2 Hz
SCANS           16
ACQTM        5.449 sec
PD           1.551 sec
PW1            5.8 us
IRNUC   1H
CTEMP         16.5 c
SLVNT   CDCL3
EXREF         7.25 ppm
BF            0.09 Hz
RGAIN            8
```




```
DFILE   D:\NMR_Users\Xi Zhe
COMNT
DATIM   Mon Nov 16 09:54:31
OBNUC   13C
EXMOD   BCM
OBFRQ        75.45 MHz
OBSET       124.00 KHz
OBFIN       1840.0 Hz
POINT        32768
FREQU      20408.1 Hz
SCANS          201
ACQTM        1.606 sec
PD           1.394 sec
PW1            5.0 us
IRNUC   1H
CTEMP         16.8 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             0.62 Hz
RGAIN            24
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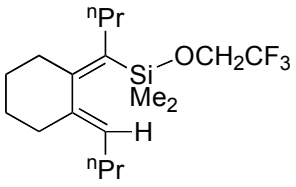
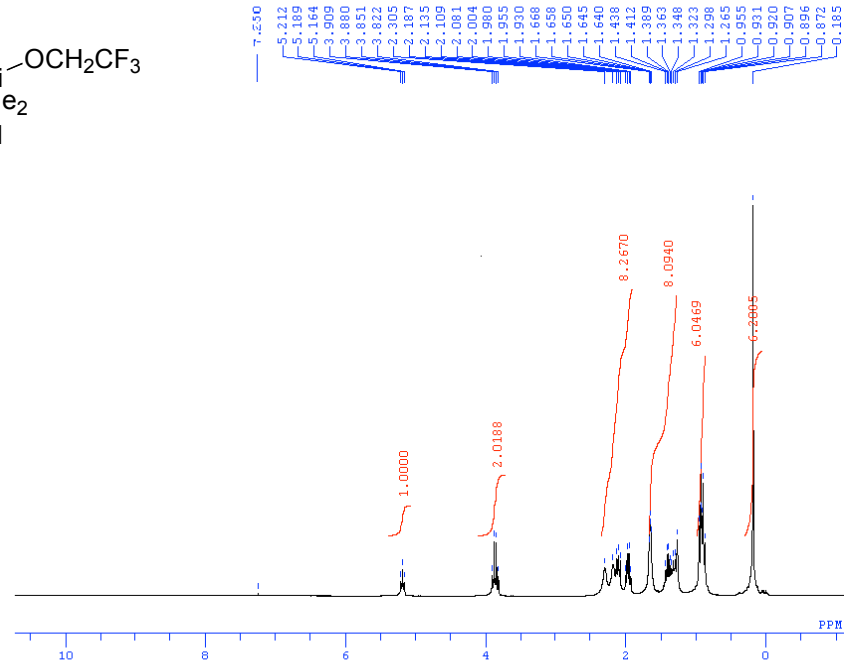
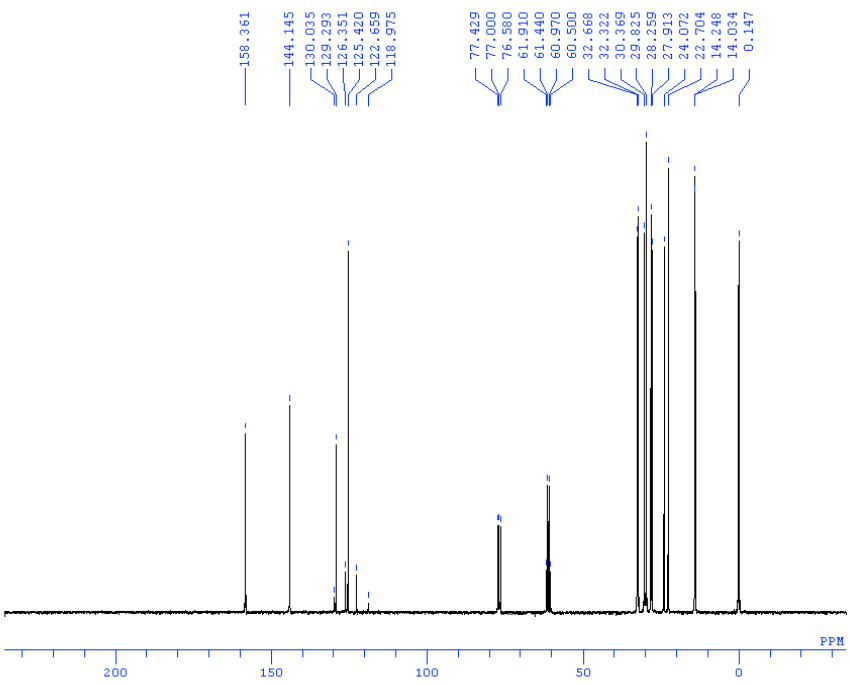


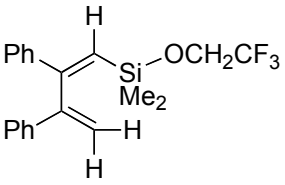
2c



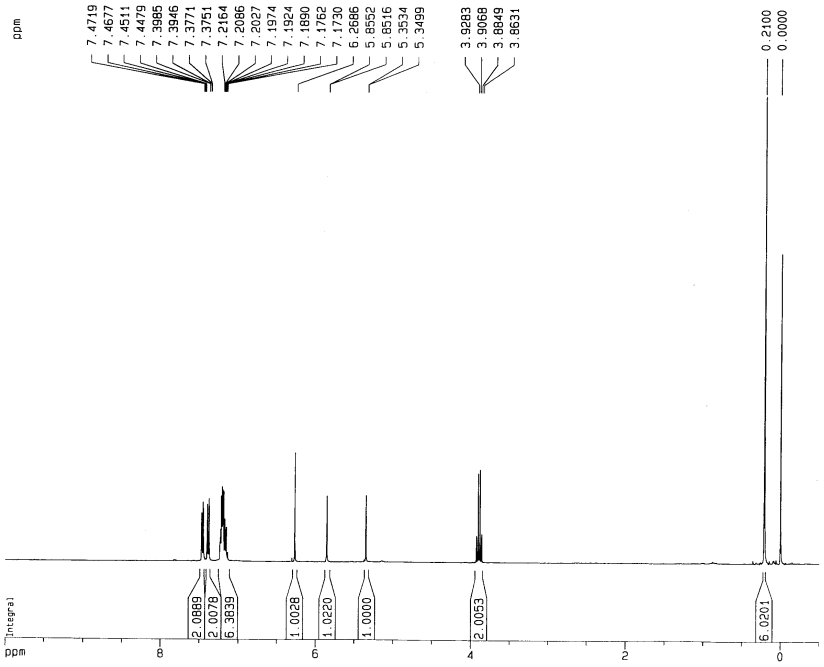
DFILE D:\NMR_Users\Xi Zhe
COMNT
DATIM Mon Aug 31 21:24:52
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 6013.2 Hz
SCANS 16
ACQTM 5.449 sec
PD 1.551 sec
PW1 5.8 us
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 7.25 ppm
BF 0.09 Hz
RGAIN 10



DFILE D:\NMR_Users\Xi Zhe
COMNT
DATIM Mon Aug 31 21:18:33
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 368
ACQTM 1.606 sec
PD 1.394 sec
PW1 5.0 us
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.62 Hz
RGAIN 26



2d

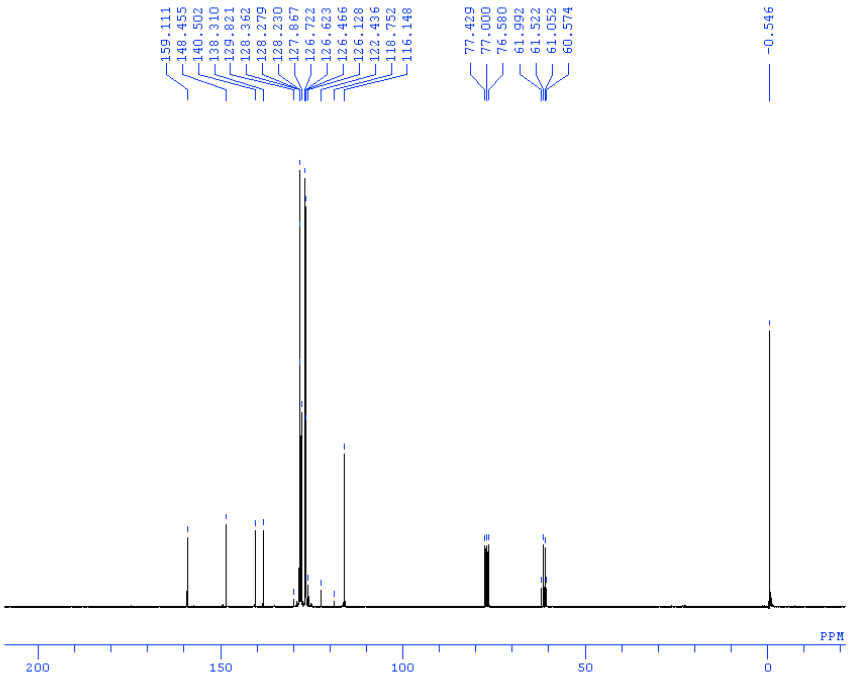



```
Current Data Parameters
NAME                  h04671
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20100204
Time                  13.37
INSTRUM              ARX400
PROBHD     5 mm Multinu
PULPROG                zg
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      0
SWH              8064.516 Hz
FIDRES           0.246110 Hz
AQ               2.0316660 sec
RG                     64
DW                62.000 usec
DE                88.57 usec
TE                300.0 K
D1             2.00000000 sec
P1                 3.00 usec
DE                88.57 usec
SFO1           400.1320153 MHz
NUCLEUS               1H

F2 - Processing parameters
SI                  16384
SF             400.1300479 MHz
WDW                    no
SSB                     0
LB                 0.00 Hz
GB                      0
PC                 4.00

1D NMR plot parameters
CX                20.00 cm
F1P               10.000 ppm
F1                4001.30 Hz
F2P               -0.500 ppm
F2                -200.07 Hz
PPMCM             0.52500 ppm/cm
HZCM          210.06827 Hz/cm
```

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DFILE   D:\NMR_Users\Xi Zhe
COMNT
DATIM   Sat Jan 30 12:24:33
OBNUC   13C
EXMOD   BCM
OBFRQ         75.45 MHz
OBSET       124.00 KHz
OBFIN       1840.0 Hz
POINT        32768
FREQU      20408.1 Hz
SCANS         2024
ACQTM         1.606 sec
PD            1.394 sec
PW1             5.0 us
IRNUC   1H
CTEMP          19.0 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             0.62 Hz
RGAIN            27
```
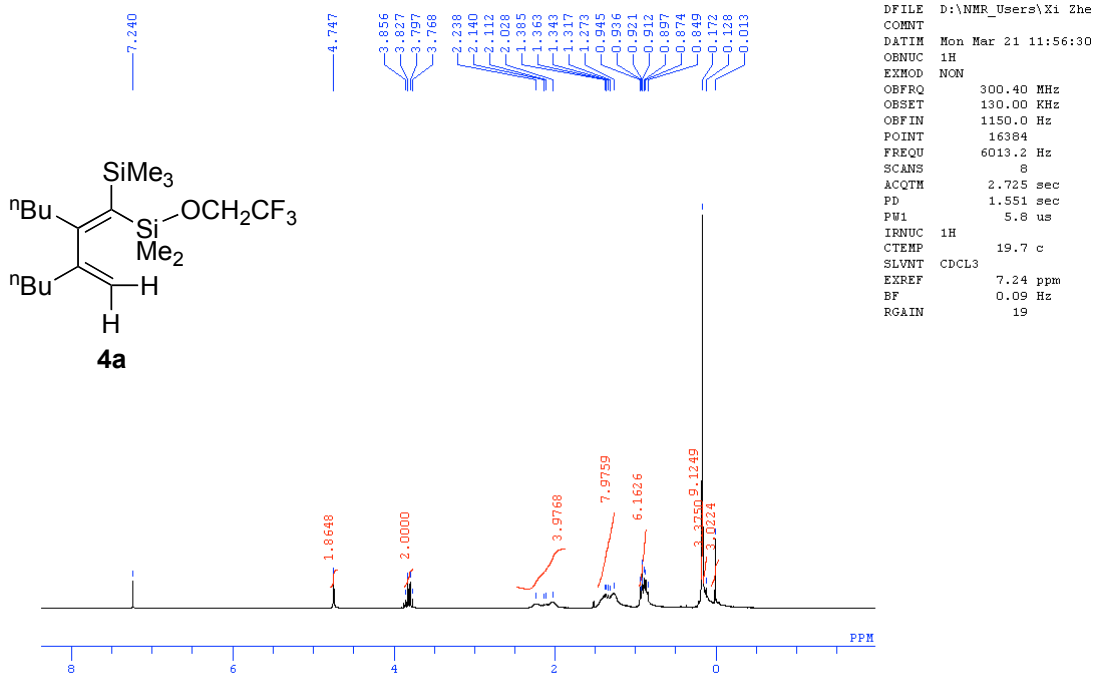
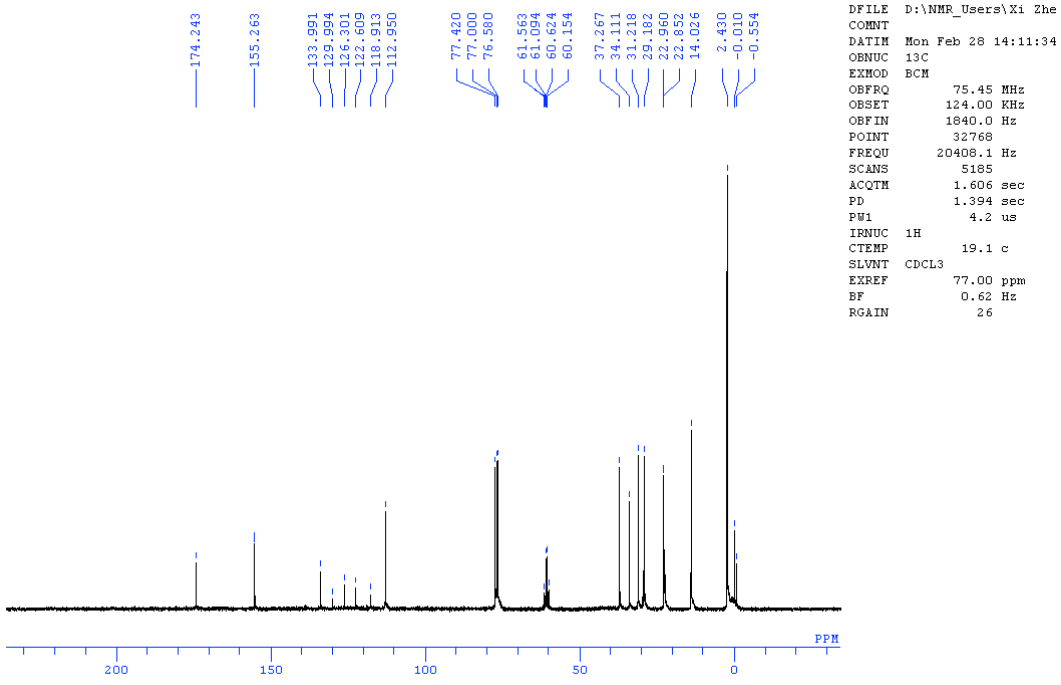
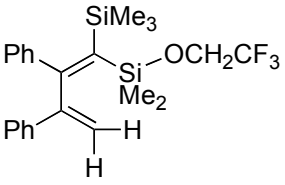
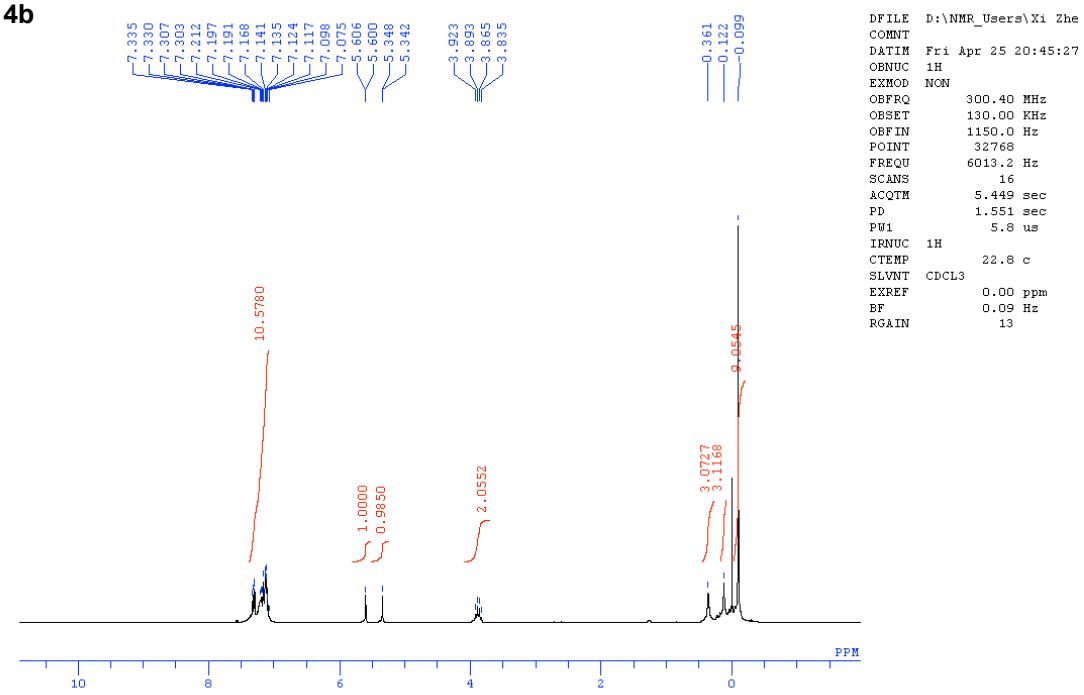


7.240
4.747
3.856
3.827
3.797
3.768
2.238
2.140
2.112
2.028
1.385
1.363
1.343
1.317
1.273
0.945
0.936
0.921
0.912
0.897
0.874
0.849
0.172
0.128
0.013
SiMe3
nBu
OCH2CF3
Si
Me2
nBu
H
H
4a
1.8648
2.0000
3.9768
7.9759
6.1626
3.3750
9.1249
3.0224
PPM
8
6
4
2
0
DFILE D:\NMR_Users\Xi Zhe
COMNT
DATIM Mon Mar 21 11:56:30
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 16384
FREQU 6013.2 Hz
SCANS 8
ACQTM 2.725 sec
PD 1.551 sec
PW1 5.8 us
IRNUC 1H
CTEMP 19.7 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.09 Hz
RGAIN 19

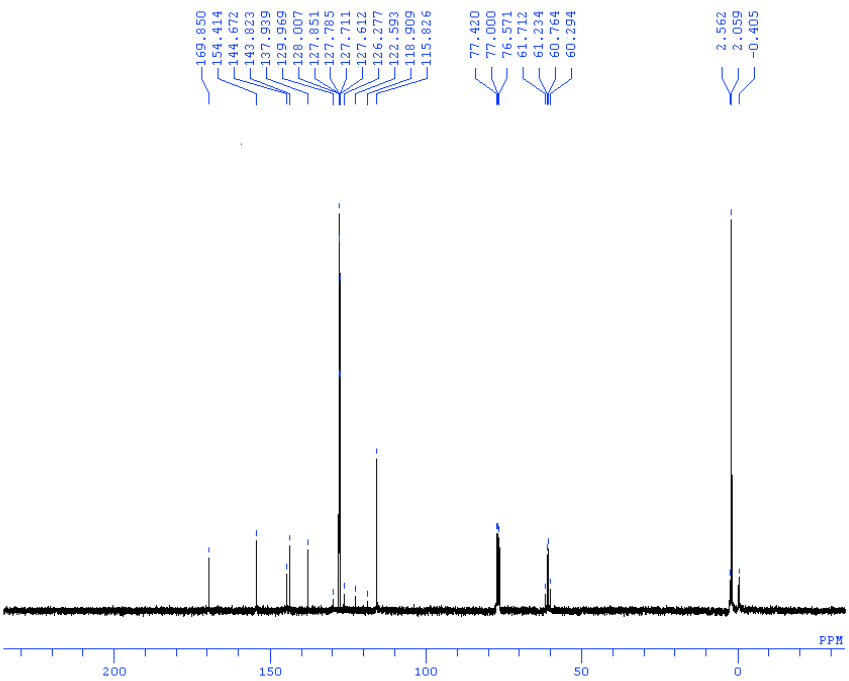

174.243
155.263
133.991
129.994
126.301
122.609
118.913
112.950
77.420
77.000
76.580
61.563
61.094
60.624
60.154
37.267
34.111
31.218
29.182
22.960
22.852
14.026
2.430
-0.010
-0.554
PPM
200
150
100
50
0
DFILE D:\NMR_Users\Xi Zhe
COMNT
DATIM Mon Feb 28 14:11:34
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 5185
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRNUC 1H
CTEMP 19.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.62 Hz
RGAIN 26



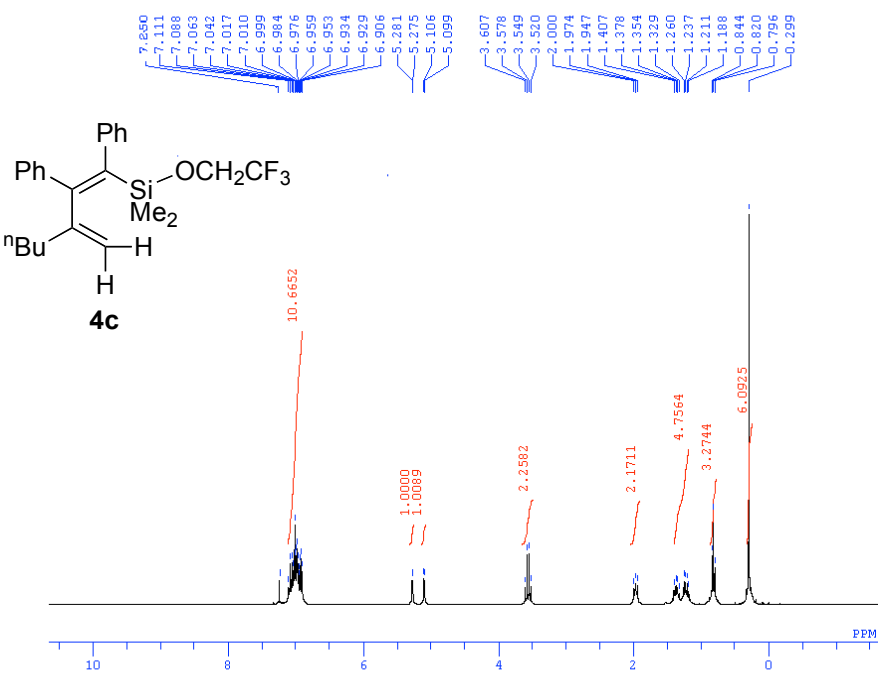
4b



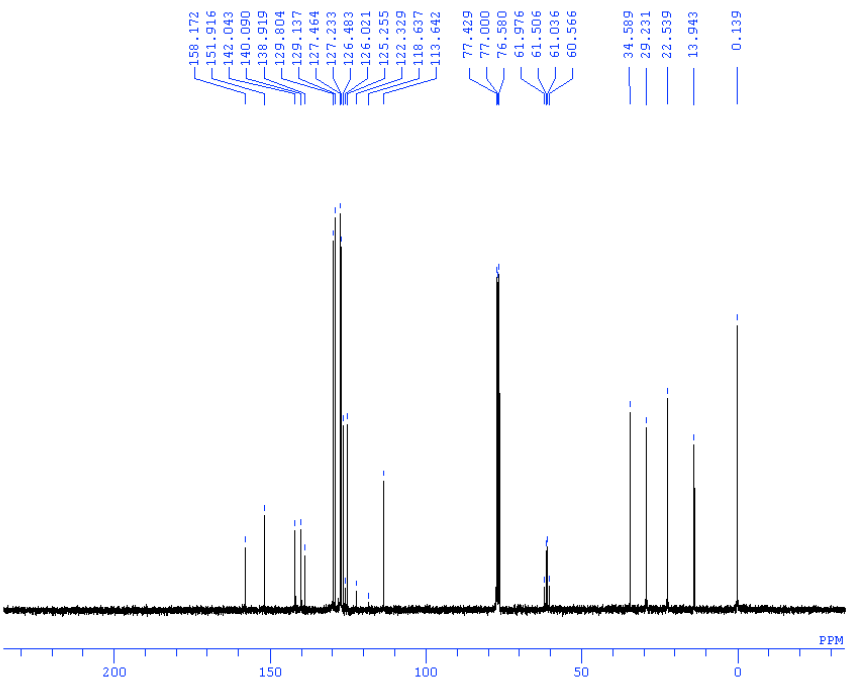

```
DFILE  D:\NMR_Users\Xi Zhe
COMNT
DATIM  Fri Apr 25 20:45:27
OBNUC  1H
EXMOD  NON
OBFRQ       300.40 MHz
OBSET       130.00 KHz
OBFIN       1150.0 Hz
POINT        32768
FREQU       6013.2 Hz
SCANS           16
ACQTM        5.449 sec
PD           1.551 sec
PW1            5.8 us
IRNUC  1H
CTEMP         22.8 c
SLVNT  CDCL3
EXREF         0.00 ppm
BF            0.09 Hz
RGAIN           13
```



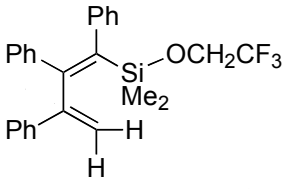

```
DFILE  D:\NMR_Users\Xi Zhe
COMNT
DATIM  Fri Apr 25 20:15:39
OBNUC  13C
EXMOD  BCM
OBFRQ        75.45 MHz
OBSET       124.00 KHz
OBFIN       1840.0 Hz
POINT        32768
FREQU       20408.1 Hz
SCANS          336
ACQTM        1.606 sec
PD           1.394 sec
PW1            5.0 us
IRNUC  1H
CTEMP         23.2 c
SLVNT  CDCL3
EXREF         77.00 ppm
BF            0.62 Hz
RGAIN           26
```



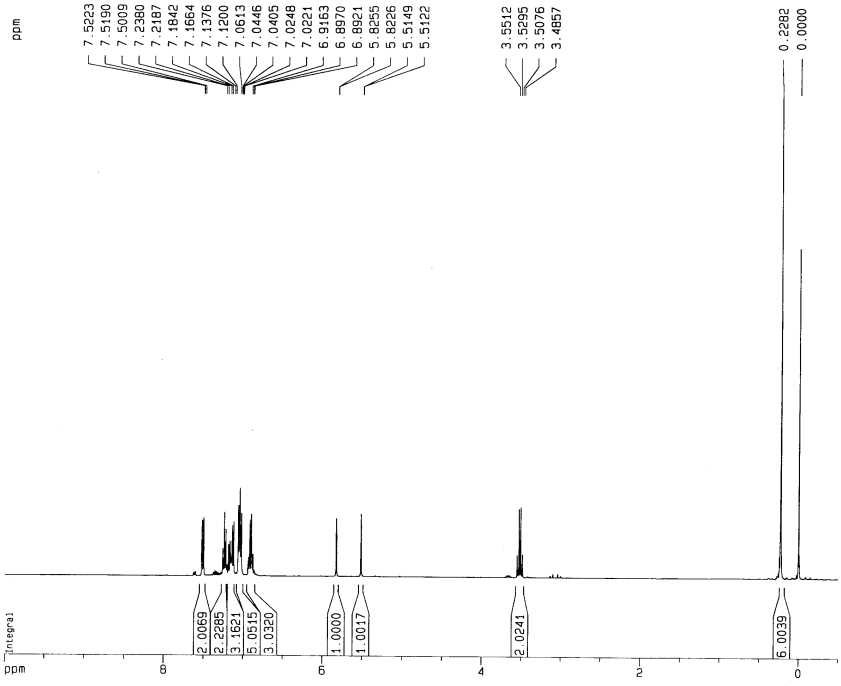

```
DFILE   D:\NMR_Users\Xi Zhe
COMNT
DATIM   Mon Dec 14 14:17:01
OBNUC   1H
EXMOD   NON
OBFRQ       300.40 MHz
OBSET       130.00 KHz
OBFIN       1150.0 Hz
POINT        32768
FREQU        6013.2 Hz
SCANS           16
ACQTM         5.449 sec
PD            1.551 sec
PW1             5.8 us
IRNUC   1H
CTEMP          15.7 c
SLVNT   CDCL3
EXREF          7.25 ppm
BF             0.09 Hz
RGAIN            17
```



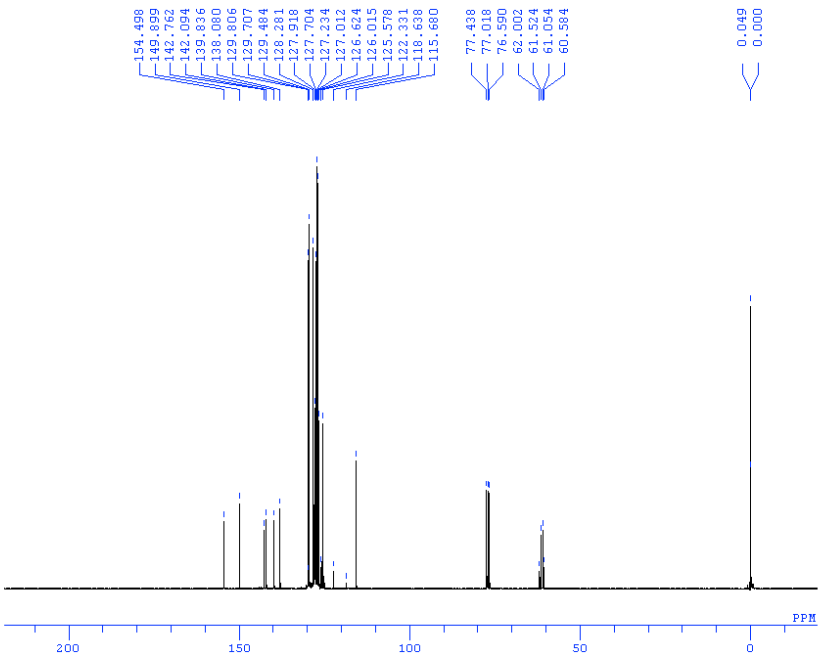

```
DFILE   D:\NMR_Users\Xi Zhe
COMNT
DATIM   Mon Dec 14 13:37:36
OBNUC   13C
EXMOD   BCM
OBFRQ        75.45 MHz
OBSET       124.00 KHz
OBFIN       1840.0 Hz
POINT        32768
FREQU       20408.1 Hz
SCANS         2292
ACQTM        1.606 sec
PD           1.394 sec
PW1            5.0 us
IRNUC   1H
CTEMP         14.9 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             0.62 Hz
RGAIN            27
```



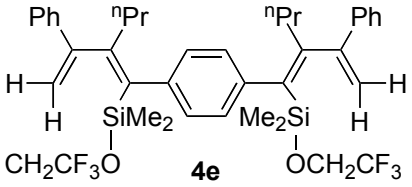
4d



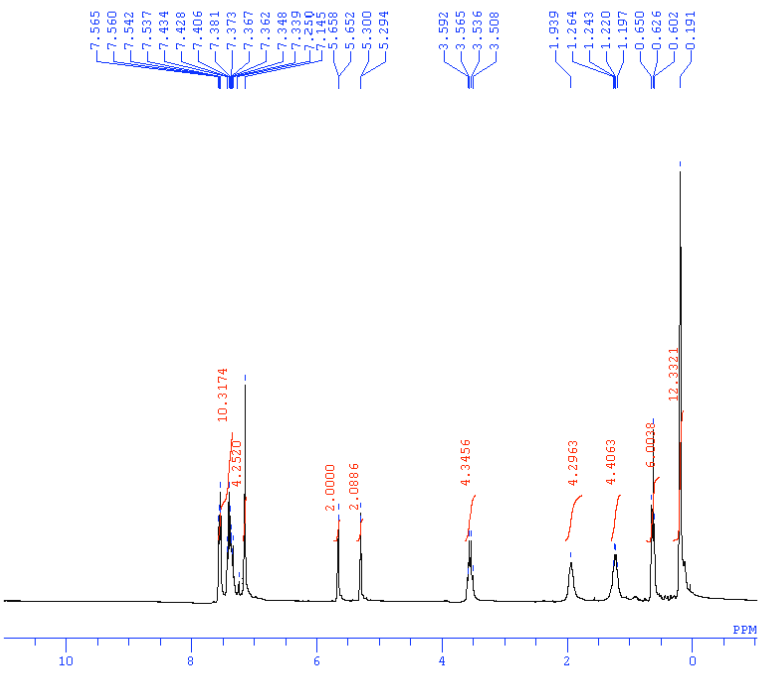

```
Current Data Parameters
NAME                  h04672
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20100204
Time                  13.54
INSTRUM              ARX400
PROBHD     5 mm Multinu
PULPROG                 zg
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               8064.516 Hz
FIDRES            0.246110 Hz
AQ                2.0316660 sec
RG                      64
DW                 62.000 usec
DE                 88.57 usec
TE                 300.0 K
D1                2.00000000 sec
P1                 3.00 usec
DE                 88.57 usec
SFO1           400.1320153 MHz
NUCLEUS                1H

F2 - Processing parameters
SI                   16384
SF              400.1300415 MHz
WDW                     no
SSB                      0
LB                0.00 Hz
GB                       0
PC                4.00

1D NMR plot parameters
CX                20.00 cm
F1P               10.000 ppm
F1                4001.30 Hz
F2P               -0.500 ppm
F2                -200.07 Hz
PPMCM             0.52500 ppm/cm
HZCM              210.06827 Hz/cm
```



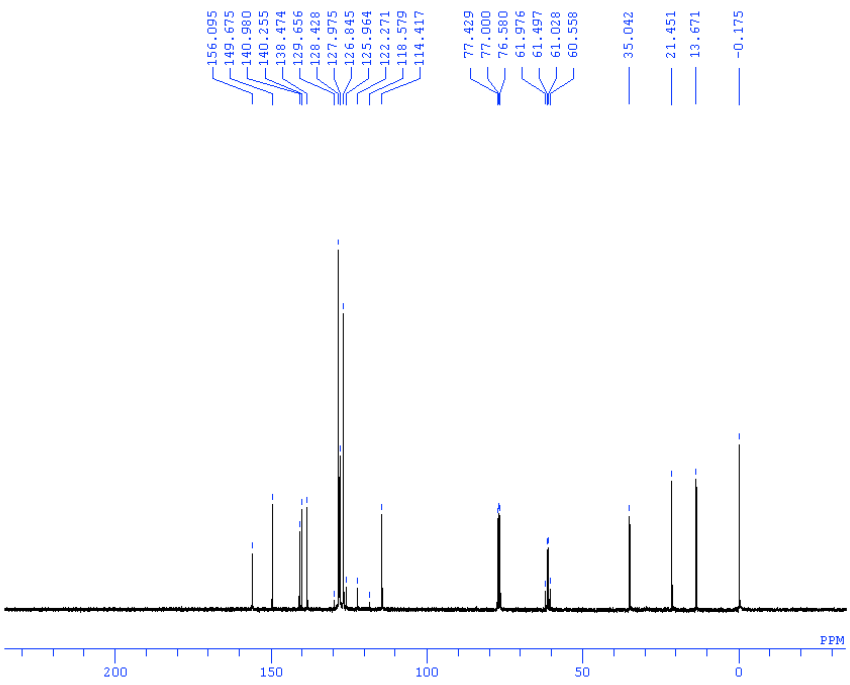

```
DFILE  D:\NMR_Users\Xi Zhe
COMNT
DATIM  Thu Feb 04 10:32:14
OBNUC  13C
EXMOD  BCM
OBFRQ        75.45 MHz
OBSET       124.00 KHz
OBFIN       1840.0 Hz
POINT        32768
FREQU      20408.1 Hz
SCANS          1017
ACQTM        1.606 sec
PD           1.394 sec
PW1            5.0 us
IRNUC  1H
CTEMP         20.7 c
SLVNT  CDCL3
EXREF         0.00 ppm
BF            0.62 Hz
RGAIN           26
```



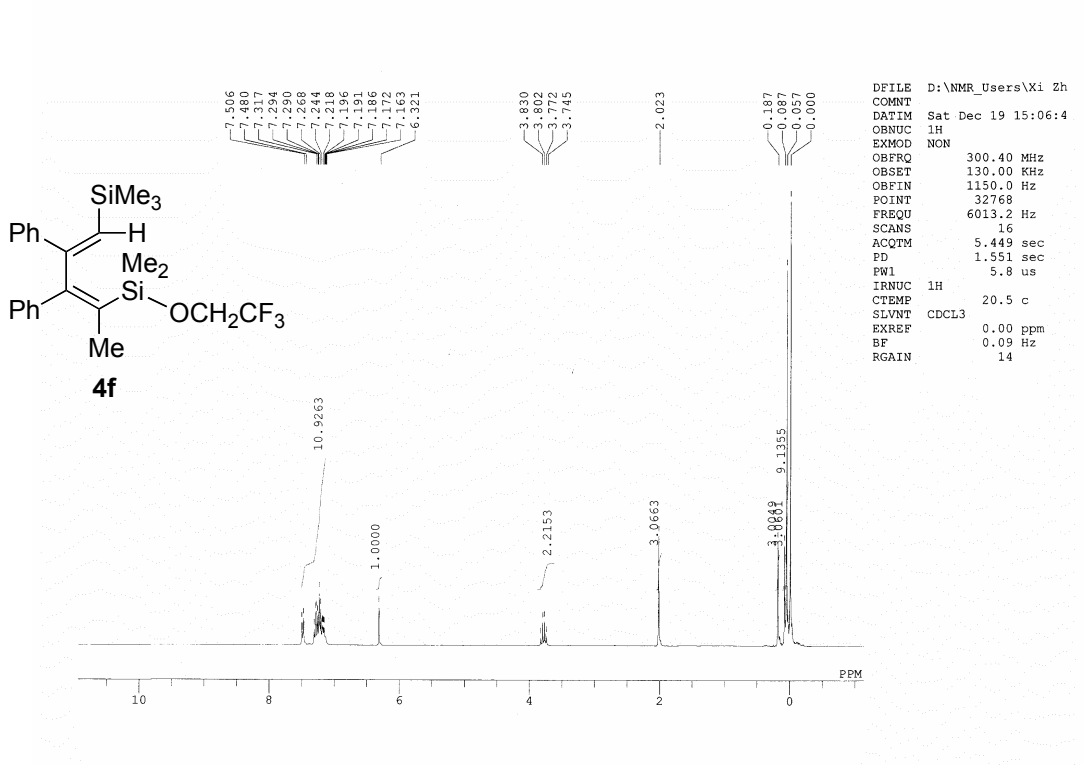
4e

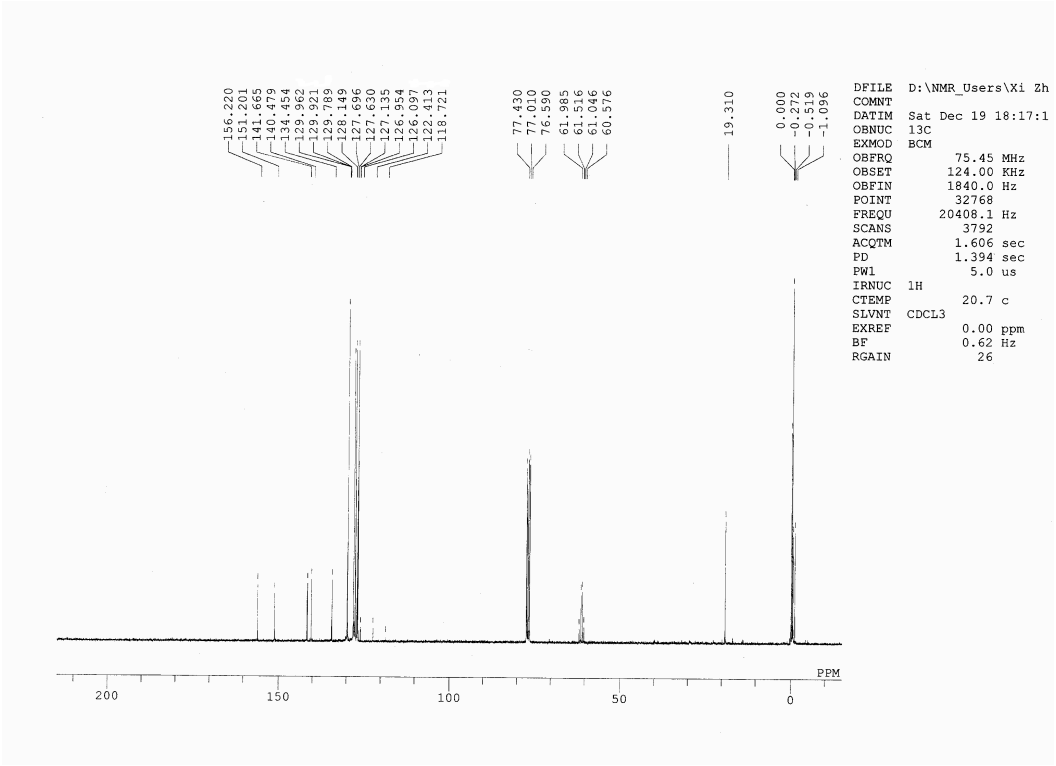


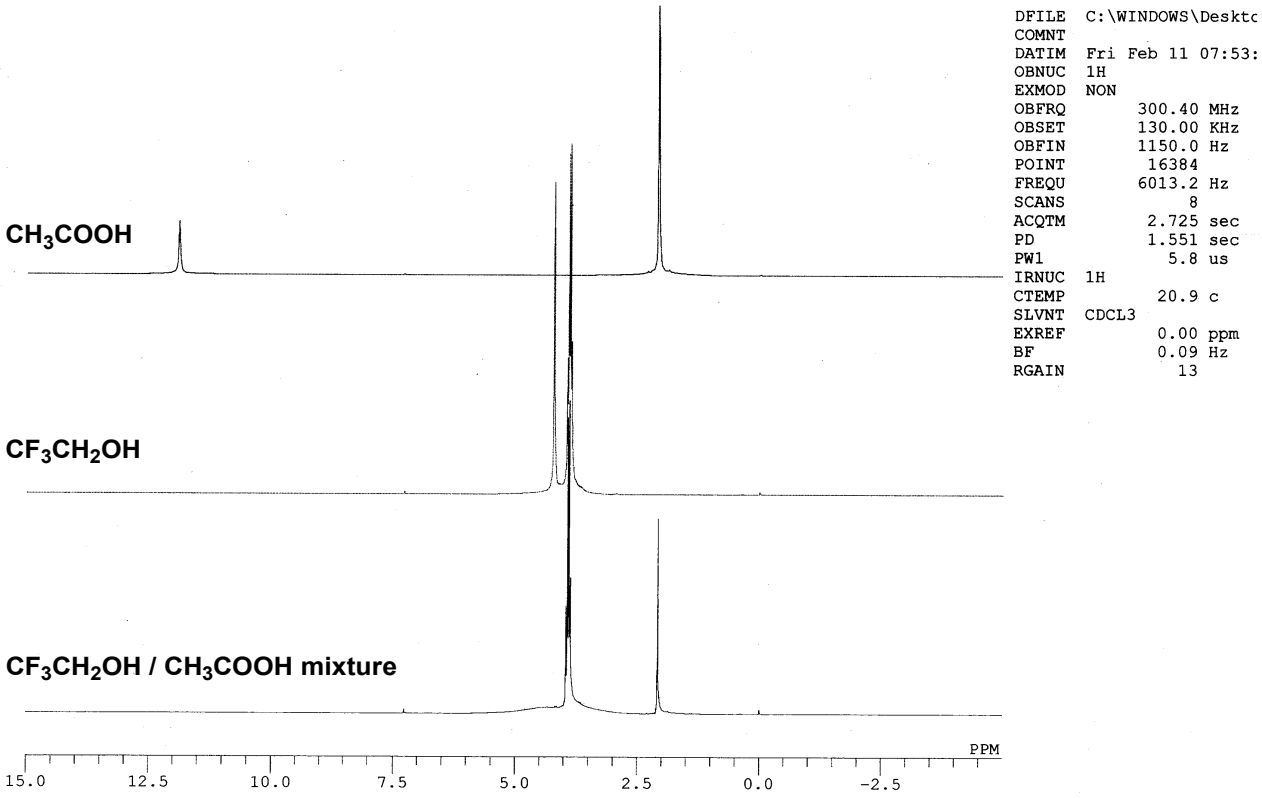

```
DFILE  D:\NMR_Users\Xi ZhenFeng\LUO
COMNT
DATIM  Fri Dec 04 18:05:31 2009
OBNUC  1H
EXMOD  NON
OBFRQ       300.40 MHz
OBSET       130.00 KHz
OBFIN       1150.0 Hz
POINT        32768
FREQU       6013.2 Hz
SCANS           16
ACQTM        5.449 sec
PD           1.551 sec
PW1            5.8 us
IRNUC  1H
CTEMP         14.2 c
SLVNT  CDCL3
EXREF         7.25 ppm
BF            0.09 Hz
RGAIN           12
```



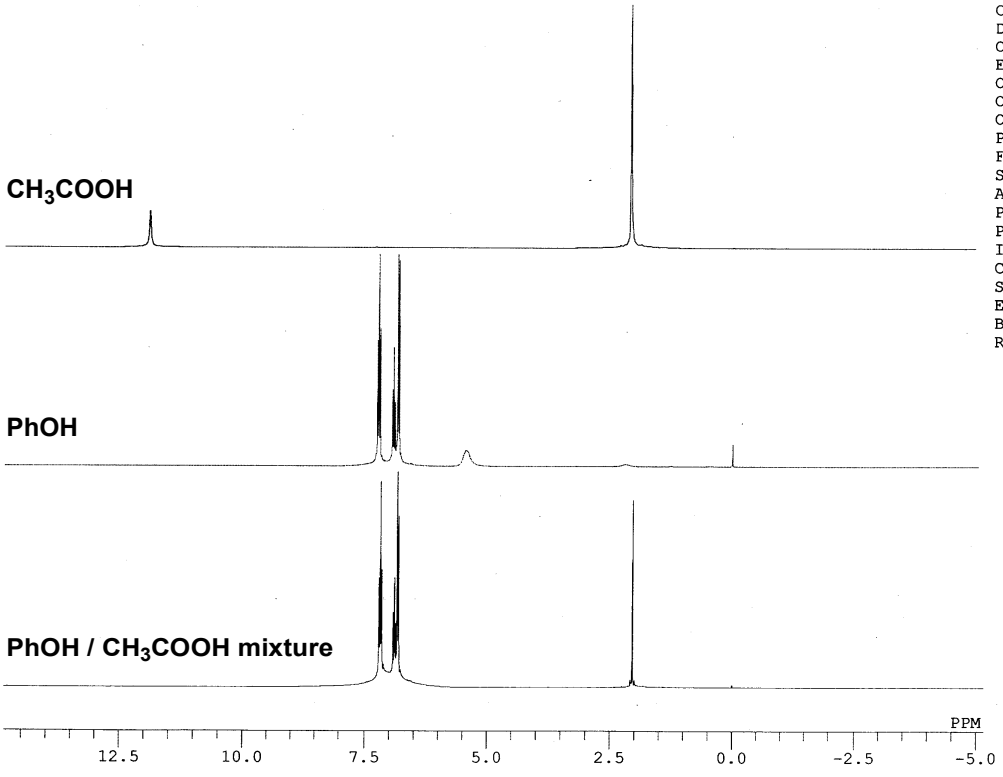

```
DFILE  D:\NMR_Users\Xi Zhe
COMNT
DATIM  Fri Dec 04 18:01:23
OBNUC  13C
EXMOD  BCM
OBFRQ        75.45 MHz
OBSET       124.00 KHz
OBFIN       1840.0 Hz
POINT        32768
FREQU      20408.1 Hz
SCANS          800
ACQTM        1.606 sec
PD           1.394 sec
PW1            5.0 us
IRNUC  1H
CTEMP         14.6 c
SLVNT  CDCL3
EXREF        77.00 ppm
BF            0.62 Hz
RGAIN           25
```


7.506
7.480
7.317
7.294
7.290
7.268
7.244
7.218
7.196
7.191
7.186
7.172
7.163
6.321
3.830
3.802
3.772
3.745
2.023
0.187
0.087
0.057
0.000
DFILE D:\NMR_Users\Xi Zh
COMNT
DATIM Sat Dec 19 15:06:4
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 6013.2 Hz
SCANS 16
ACQTM 5.449 sec
PD 1.551 sec
PW1 5.8 us
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.09 Hz
RGAIN 14
SiMe3
Ph
H
Me2
Si
Ph
OCH2CF3
Me
4f
10.9263
1.0000
2.2153
3.0663
9.1355
3.0049
3.0801
PPM
10
8
6
4
2
0


156.220
151.201
141.665
140.479
134.454
129.962
129.921
129.789
128.149
127.696
127.630
127.135
126.954
126.097
122.413
118.721
77.430
77.010
76.590
61.985
61.516
61.046
60.576
19.310
0.000
-0.272
-0.519
-1.096
DFILE D:\NMR_Users\Xi Zh
COMNT
DATIM Sat Dec 19 18:17:1
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 3792
ACQTM 1.606 sec
PD 1.394 sec
PW1 5.0 us
IRNUC 1H
CTEMP 20.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.62 Hz
RGAIN 26
PPM
200
150
100
50
0




```
DFILE  C:\WINDOWS\Desktc
COMNT
DATIM  Fri Feb 11 07:53:
OBNUC  1H
EXMOD  NON
OBFRQ        300.40 MHz
OBSET        130.00 KHz
OBFIN        1150.0 Hz
POINT         16384
FREQU        6013.2 Hz
SCANS             8
ACQTM         2.725 sec
PD            1.551 sec
PW1             5.8 us
IRNUC  1H
CTEMP          20.9 c
SLVNT  CDCL3
EXREF          0.00 ppm
BF             0.09 Hz
RGAIN            13
```




```
DFILE  C:\WINDOWS\Desktc
COMNT
DATIM  Fri Feb 11 19:02:
OBNUC  1H
EXMOD  NON
OBFRQ        300.40 MHz
OBSET        130.00 KHz
OBFIN        1150.0 Hz
POINT         16384
FREQU        6013.2 Hz
SCANS             8
ACQTM         2.725 sec
PD            1.551 sec
PW1             5.8 us
IRNUC  1H
CTEMP          20.3 c
SLVNT  CDCL3
EXREF          0.00 ppm
BF             0.09 Hz
RGAIN            10
```