Supporting Information

Bonding-Regulated Construction of Covalent Organic Framework-Supported Frustrated Lewis Pairs for 1,4-Hydrosilylation of *α,β*-Unsaturated Ketone

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1. Materials, Methods and Synthetic Procedures.

Materials. Norbornylene (NBE), 2,5-norbornadiene (NBDE), boron trifluoride diethyl etherate ($BF_3 \cdot Et_2O$), 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), aniline ($PhNH_2$), benzaldehyde (PhCHO), tris(pentafluorophenyl)boron (BCF), iodomethane (MeI), chalcone (**1a**), 2-cyclohexen-1-one (**1q**), D(+)-carvone (**1r**), chromone (**1s**), triethylsilane (Et_3SiH), phenylsilane ($PhSiH_3$), diphenylsilane (Ph_2SiH_2), triphenylsilane (Ph_3SiH), dimethylphenylsilane ($PhMe_2SiH$), lithium aluminum deuteride ($LiAlD_4$), chlorotriethylsilane (Et_3SiCl) and phenyltrichlorosilane ($PhSiCl_3$) were purchased from commercial resources and used without further purification. Tetrahydrofuran (THF) and diethyl ether (Et_2O) were purchased from commercial sources and dried with sodium through a Schlenk line. Unless additional mentioned, other reagents were purchased from commercial sources and used without further purification.

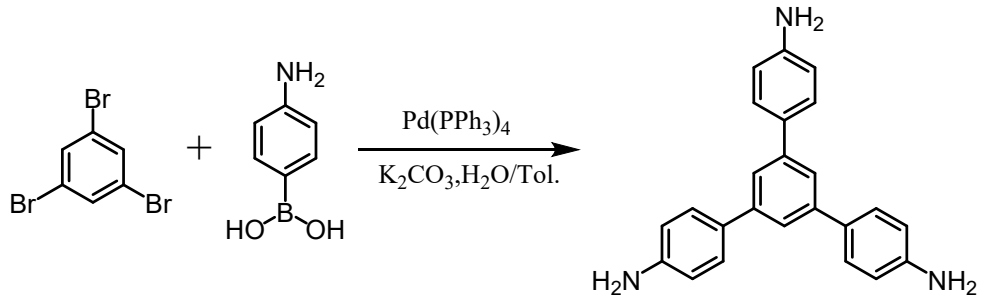
Methods. Fourier-transform infrared (FT-IR) spectroscopy measurements were recorded in a Perkin Elmer Spectrum 100 with a PIKE Technologies MIRacle Single Reflection Horizontal ATR Accesory with a spectral range of 4000-400 cm^{-1} using the KBr disk method. Powder X-ray diffraction (PXRD) patterns were measured on a MiniFlex600 (Rigaku) Bragg-Brentano geometry with a Cu-$K\alpha_1$-radiation (λ =1.540593 Å). Scanning electron microscopy (SEM) studies were performed on a HEM6000 (CIQTEK Co.，Ltd.) microscope operating at an accelerating voltage of 20 kV. The Brunauer-Emmet-Teller (BET) were measured using a BSD-PS1/2 (Beishide instrument-S&T, Beijing, CO., Ltd.) volumetric instrument with extra-high pure gases. Nuclear magnetic resonance (NMR) spectra of ^{1}H, ^{11}B and ^{13}C were recorded in solution using a JEOL JNM-ECS-400 with a 5 mm FG/RO Digital Auto Tune Switchable Probe at room temperature. The Solid-state ^{13}C cross-polarized magic angle spinning nuclear magnetic resonance (CP-MAS NMR) and ^{11}B solid NMR spectra were recorded on an AVANCE II 400 spectrometer (Bruker, SUI). The powder samples were placed in a pencil-type zirconia rotor of 4.0 mm o.d. The B content was detected by inductively coupled plasma optical emission spectroscopy (ICP-OES, AVIO 500). Low

resolution mass spectra (LRMS) were obtained using were obtained using EI or ESI TOF ionization techniques in a micrOTOF II of Bruker.

Density functional theory (DFT) calculations. All the DFT calculations were carried out using Gaussian 09[1]. Geometry optimization of all the minima and transition states involved was carried out at the B3LYP[2, 3] level with the 6-31G(d) basis of H, B, C, N, O, Si, and the def2-TZVP basis of I. Default convergence criteria were used. The vibrational frequency calculations were conducted at the same level of theory as geometry optimization to confirm whether each optimized structure is an energy minimum or a saddle point. For transition state, intrinsic reaction coordinate (IRC) analysis[4] was performed to verify that it connects the right reactants and products. The solvent effects were considered using the PCM model of Chloroform. The energy calculations were carried out at the M062x level with the 6-311G(d,p) basis and the zero-point energy (ZPE) was corrected by Shermo_2.6 software[5].

Synthetic Procedures

1,3,5-Tris(4-aminophenyl)benzene (TAPB)[6]



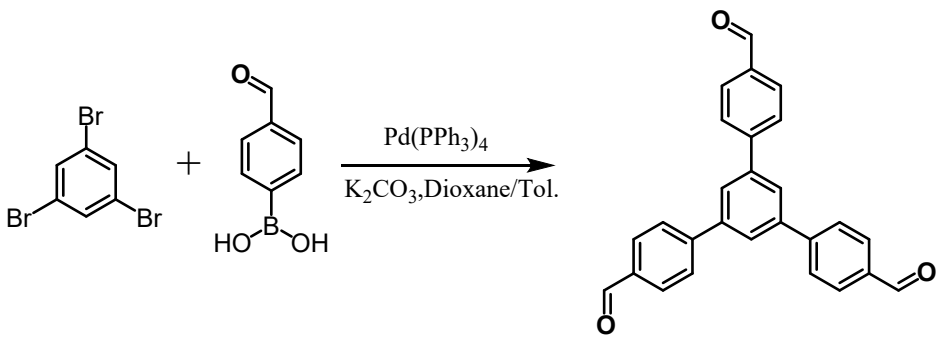
Scheme S1. Synthetic route of TAPB.

1,3,5-tribromobenzene (3.2 g, 10.0 mmol, 1.0 equiv.) and (4-aminophenyl)boronic acid (5.5 g, 40.0 mmol, 4.0 equiv.) were dissolved in 80 mL of toluene, and 24.0 mL of 2 M aqueous solution of K_2CO_3 were added to the solution. After degassing by Ar bubbling, tetrakis(triphenylphosphine)palladium (0.17 g, 0.15mmol, 0.015equiv.) were added. The reaction mixture was heated to 100 °C for 24 h. The crude product was purified by column chromatography (petroleum ether/ethyl acetate = 7/3) to yield 2.3 g of TAPB in 65 % as an off-white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (s, 3H), 7.51 (dd, 6H, J = 2.1, 8.7), 6.77 (dd, 6H, J = 2.2, 8.7), 3.82 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 146.79, 142.32, 131.69, 128.39, 122.80, 115.49.

1,3,5-Tris(4-formylphenyl)benzene (TFPB)[7]



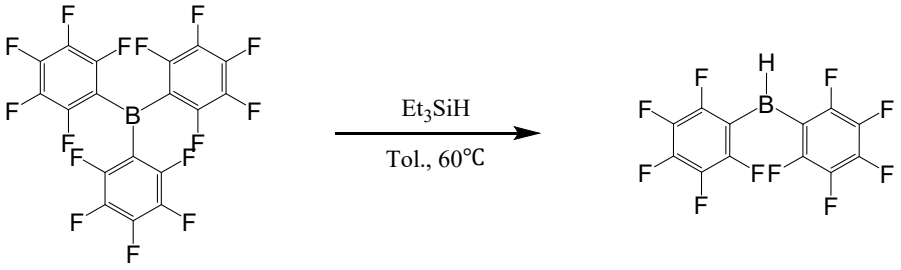
Scheme S2. Synthetic route of TFPB.

A mixture of 4-formylphenylboronic acid (5.0 g, 33.3 mmol, 4.0 equiv.), 1,3,5-tribromobenzene (2.6 g, 8.3 mmol, 1.0 equiv.), tetrakis(triphenylphosphine)palladium (0.49 g, 0.42 mmol, 0.05 equiv.), K_2CO_3 (11.5 g, 83.0 mmol, 10.0 equiv.), 1,4-dioxane (120 mL) and distilled water (12 mL) were stirred at 90 °C under Ar atmosphere for 24 h. After cooled at room temperature, the precipitate was collected by filtration and the residue was purified by flash column chromatography (petroleum ether/ethyl acetate = 10/1) to give TFPB as a white solid in 80 % yield (2.6 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.11 (s, 3H); 8.03 (d, 6H, J = 8.4 Hz), 7.91 (s, 3H), 7.88 (d, 6H, J = 8.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 191.74, 146.24, 141.54, 135.69, 130.41, 127.94, 126.44.

Bis(pentafluorophenyl)borane [$HB(C_6F_5)_2$][8]



Scheme S3. Synthetic route of $HB(C_6F_5)_2$.

Et_3SiH (1.2 g, 10.0 mmol) was added to a Schlenk flask of tris(pentafluorophenyl)borane (BCF) (5.1 g, 10.0 mmol) in toluene (50 mL). The flask was sealed, then heated to 60 °C and stirred for 5 days. The flask was cooled to room temperature, which was vacuum concentration and washed with cold toluene and pentane to yield the target product as a white crystalline powder in 68 % yield (2.4 g).

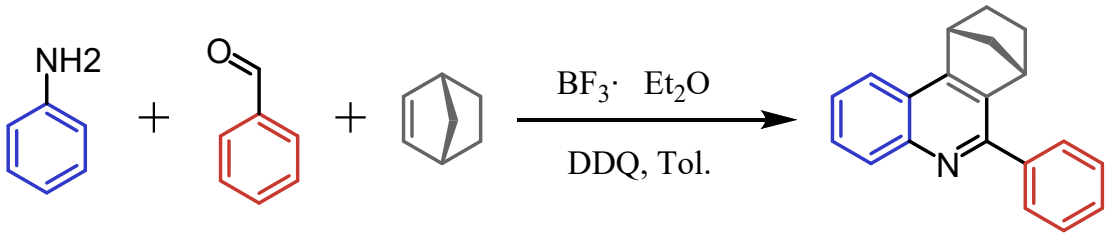
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.10 (br, s, B-H).

^{11}B NMR (128 MHz, $CDCl_3$) δ 18.4 ppm.

^{19}F NMR (377 MHz, $CDCl_3$) δ -132.16 (d, 2F, J = 14.4 Hz), -147.11 (t, 1F, J = 20.2 Hz), -158.78 (td, 2F, J = 7.6, 20.9 Hz).

1.1 Synthesis of Model Compounds.

6-Phenyl-7,8,9,10-tetrahydro-7,10-methanophenanthridine (CQ-NBE)



Scheme S4. Synthetic route of model compounds **CQ-NBE**.

A 10 mL high-pressure flask was charged with the $PhNH_2$ (0.93 g, 10.0 mmol, 1.0 equiv.), PhCHO (1.2 g, 11.0 mmol, 1.1 equiv.), norbornylene (NBE) (1.9 g, 20.0 mmol, 2.0 equiv.) and freshly distilled toluene (20.0 mL), and then 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) (4.8 g, 20.0 mmol, 2.1 equiv.) and $BF_3{\cdot}OEt_2$ (0.4 mL, 2.0 mmol, 0.2 equiv.) was added to the mixture. The flask was purged with Ar before it was tightly sealed, and the reaction mixture was heated to 110 °C for 48 h. The reaction mixture was cooled to room temperature, treated with a few drops of MeOH, and finally concentrated in vacuo. The crude residue was dry loaded onto silica and purified by silica gel flash chromatography (petroleum ether/ethyl acetate = 100/10~30) to give CQ-NBE as an off-white solid in 46 % yield (1.2 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, 1H, J = 8.4 Hz), 7.95 (d, 1H, J = 7.6 Hz), 7.88 (d, 2H, J = 7.2 Hz), 7.65 (t, 1H, J = 7.6 Hz), 7.58 - 7.42 (m, 4H), 4.04 (s, 1H), 3.82 (s, 1H), 2.22 – 2.09 (m, 2H), 1.90 (d, 1H, J = 9.2 Hz), 1.69 (d, 1H, J = 8.8 Hz), 1.49 – 1.24 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 154.96, 152.98, 147.22, 140.08, 138.40, 130.61, 129.56, 128.89, 128.59, 128.28, 125.86, 124.06, 122.44, 50.53, 43.21, 41.86, 27.36, 25.39.

HRMS (ESI) *m/z* calculated for $[M + H]^+$: 272.37, found: 272.24.

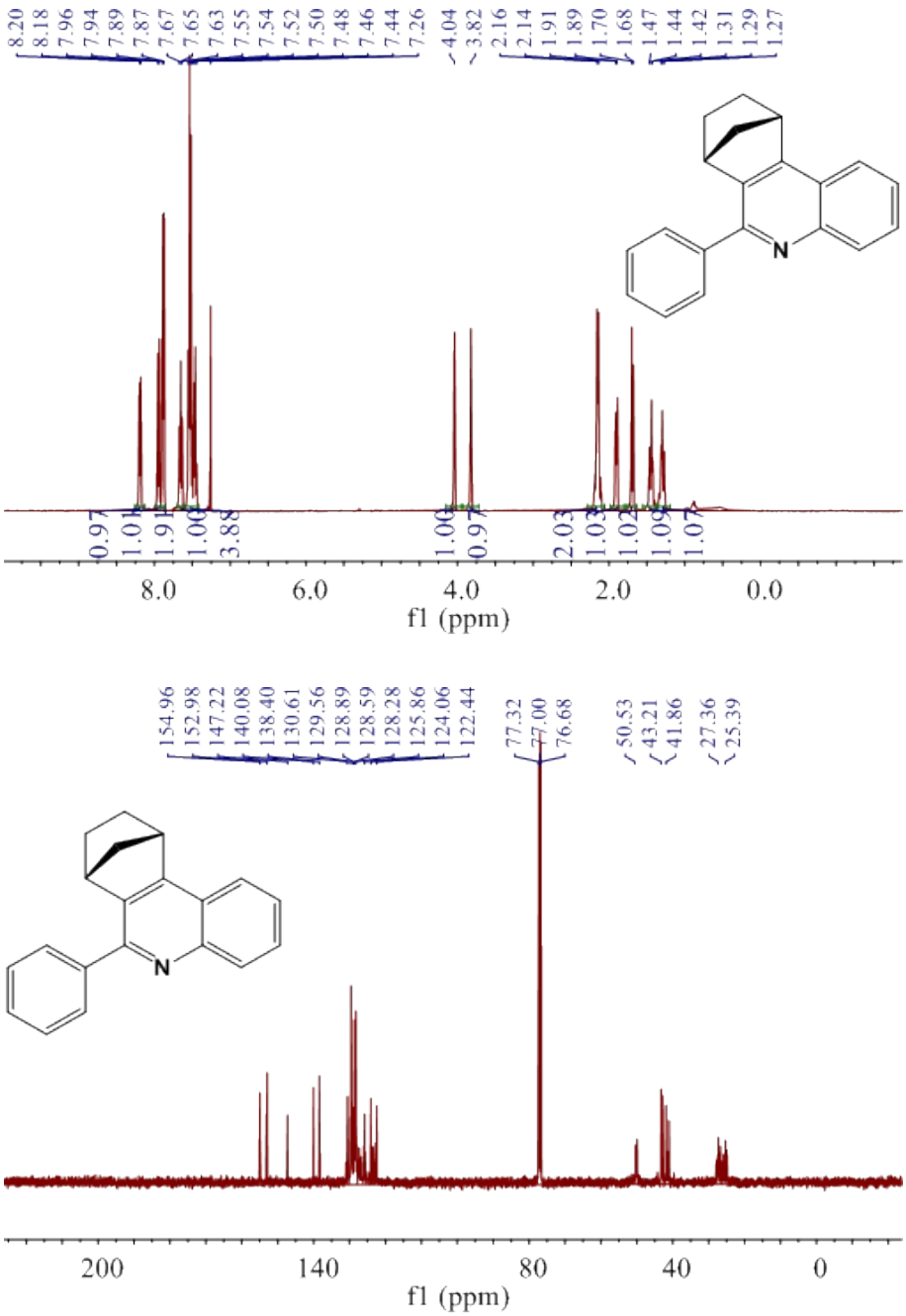
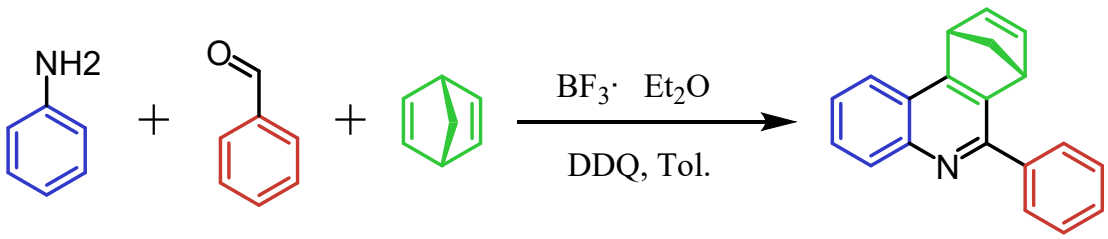


Figure S1. ^{1}H NMR and ^{13}C NMR of **CQ-NBE**.

6-Phenyl-7,10-dihydro-7,10-methanophenanthridine (CQ-NBDE)



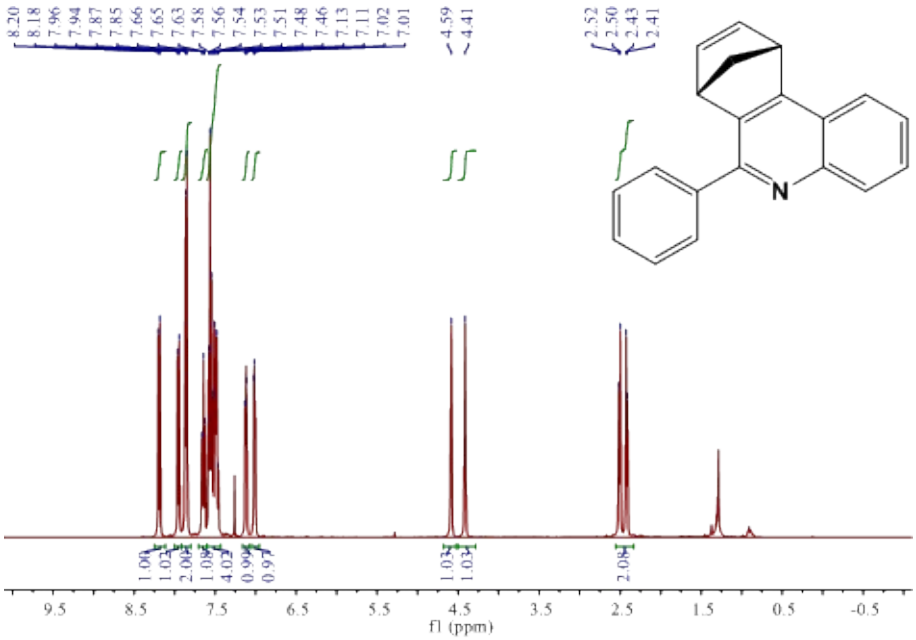
Scheme S5. Synthetic route of model compounds **CQ-NBDE**.

Similar to CQ-NBE synthesis process with the exception that NBE was changed to 2,5-Norbornadiene (NBDE) (1.9 g, 20.0 mmol, 2.0 equiv.). The crude product was purified by silica gel flash column chromatography, eluting with 5 % ethyl acetate in hexane to afford CQ-NBDE as a white solid in 30 % yield (0.8 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, 1H, J = 8.8 Hz), 7.95 (d, 1H, J = 8.4 Hz), 7.86 (d, 2H, J = 6.8 Hz), 7.65 (td, 1H, J_1 = 7.8 Hz, J_2 = 1.2 Hz), 7.58 - 7.44 (m, 4H), 7.15 - 7.09 (m, 1H), 7.04 – 6.98 (m, 1H), 4.59 (s, 1H), 4.41 (s, 1H), 2.46 (dd, 2H, J_1 = 35.6 Hz, J_2 = 6.8 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.67, 152.97, 146.57, 144.37, 143.34, 142.73, 139.98, 130.06, 128.84, 128.65, 128.47, 128.38, 125.65, 123.88, 122.98, 72.59, 50.37, 48.46.

HRMS (ESI) *m/z* calculated for $[M + H]^+$: 270.36, found: 270.21.



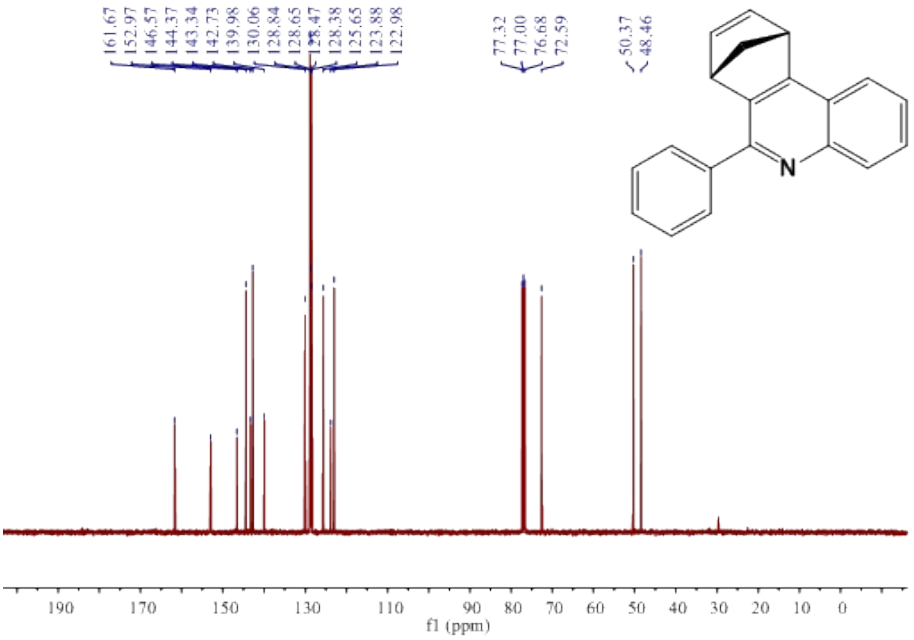
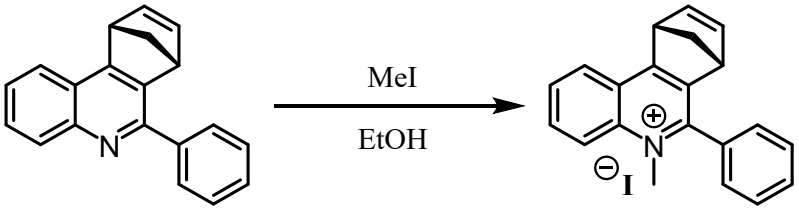


Figure S2. ^{1}H NMR and ^{13}C NMR of **CQ-NBDE**.

N-Methyl-6-Phenyl-7,10-dihydro-7,10-methanophenanthridinium iodide (CQ-NBDE-QA)



Scheme S6. Synthetic route of model compounds **CQ-NBDE-QA**.

A 10 mL high-pressure flask was charged with **CQ-NBDE** (100 mg, 0.37 mmol) and MeI (2 mL). The flask was sealed, then heated to 50 °C and stirred for 24 h. The flask was cooled to room temperature, filtered and the solid was washed with ether to give the target product as a yellow powder in 81 % yield (123 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, 1H, J = 9.2 Hz), 8.35 (d, 1H, J = 8.0 Hz), 8.20 (t, 1H, J = 8.0 Hz), 7.92 (t, 2H, J = 7.2 Hz), 7.75 - 7.61 (m, 3H), 7.43 – 7.35 (m, 1H), 7.04 (dt, 2H, J_1 = 19.6 Hz, J_2 = 4.0 Hz), 4.88 (s, 1H), 4.49 (s, 3H), 3.94 (s, 1H), 2.75 (d, 1H, J = 8.4 Hz), 2.62 (d, 1H, J = 8.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.53, 151.24, 147.09, 145.27, 141.79, 138.99, 136.60,

131.34, 130.75, 129.81, 129.69, 129.51, 129.28, 128.49, 126.14, 124.58, 120.44, 72.67, 53.90, 50.74, 50.44, 42.83.

HRMS (ESI) *m/z* calculated for $[M]^+$: 284.38, found: 284.23.

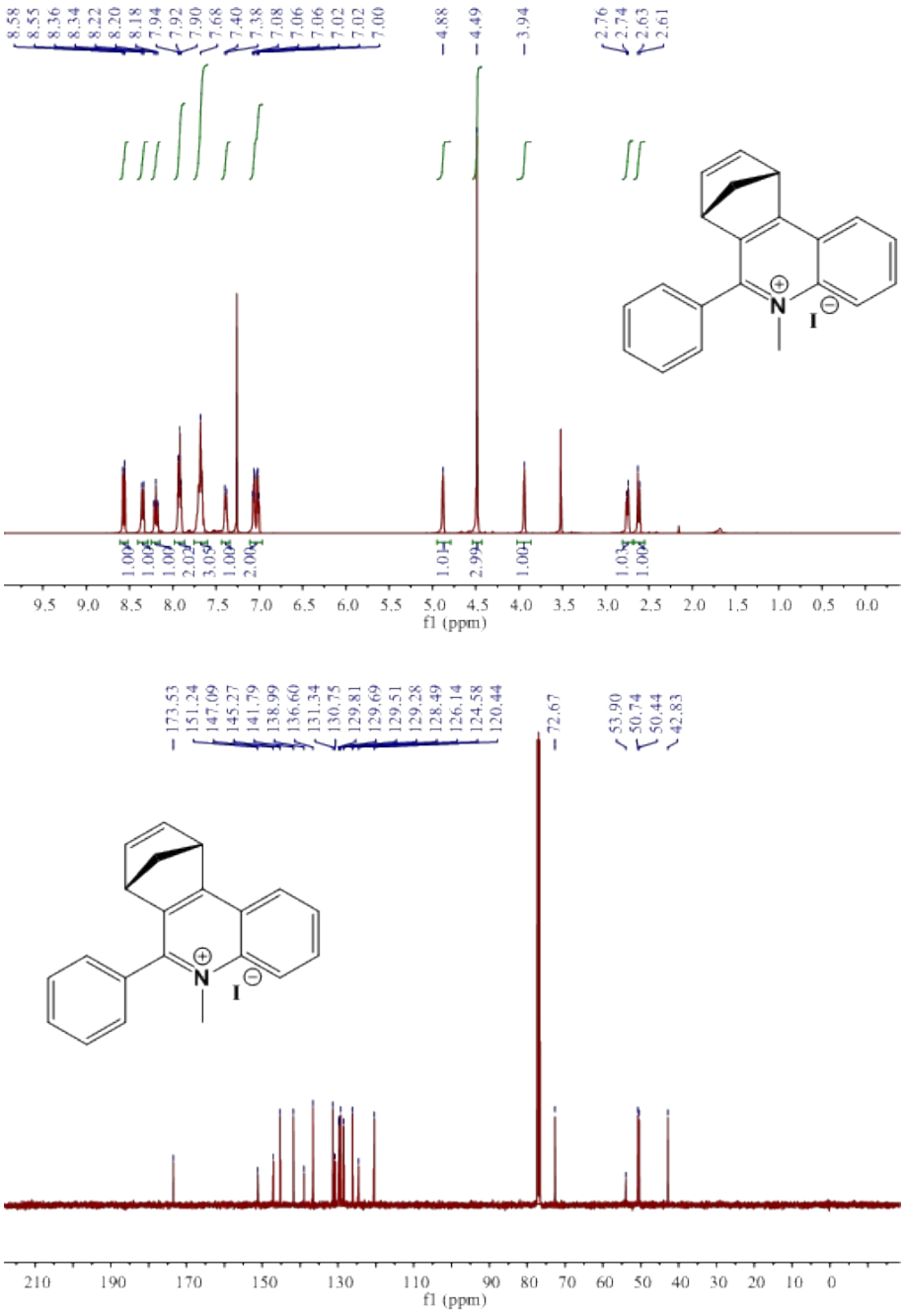
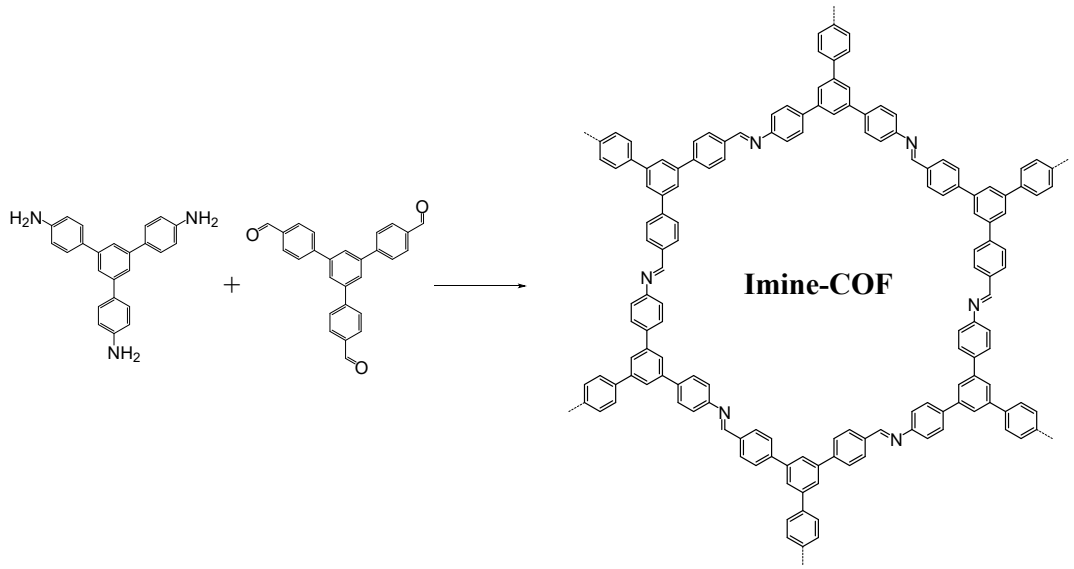


Figure S3. ^{1}H NMR and ^{13}C NMR of **CQ-NBDE-QA**.

1.2 Synthesis of COFs.

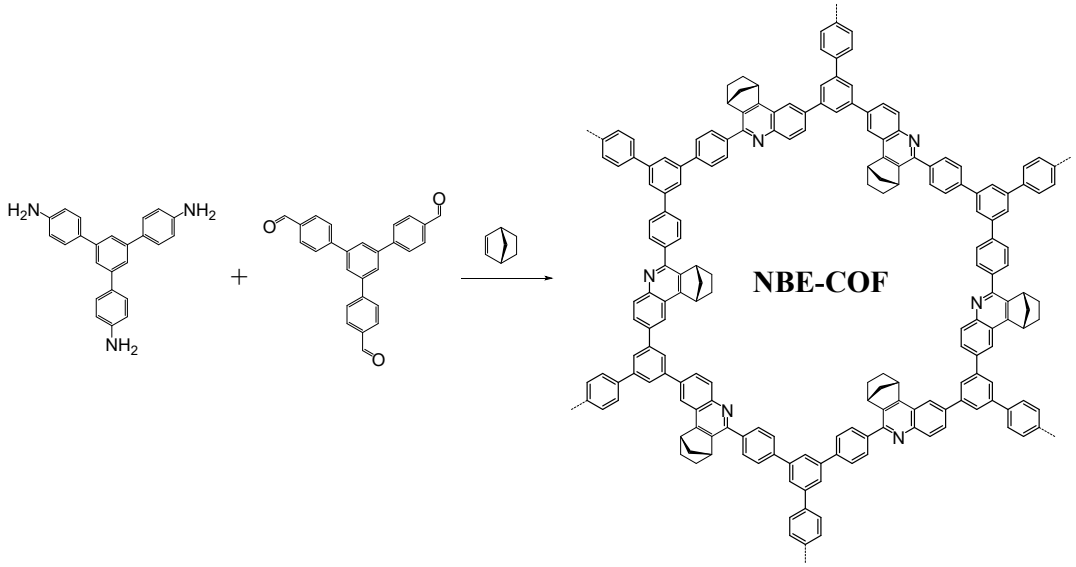
Imine-COF



Scheme S7. Synthetic route of **Imine-COF**.

To a flame-dried 10 mL high-pressure flask with vacuum valve, TAPB (52.7 mg, 0.15 mmol) and TFPB (58.6 mg, 0.15 mmol) were suspended in a mixture 1.5 mL mesitylene, 1.5 mL dioxane and 0.2 mL 6 M acetic acid by ultrasonication at room temperature for 30 min. The mixture was degassed through three freeze-pump-thaw cycles (vacuum < 50 mTorr). Then the flask was sealed and heated in an oven at 120 °C for 3 days at autogenous pressure. After cooling to room temperature, the flask was opened and the suspension was filtered and washed with THF. The crude solid was further extracted through a Soxhlet extractor using THF as extracting solution for 24 h and dried at 60 °C for 24 h under vacuum. A pale-yellow powder is obtained, yield: 98.4 mg.

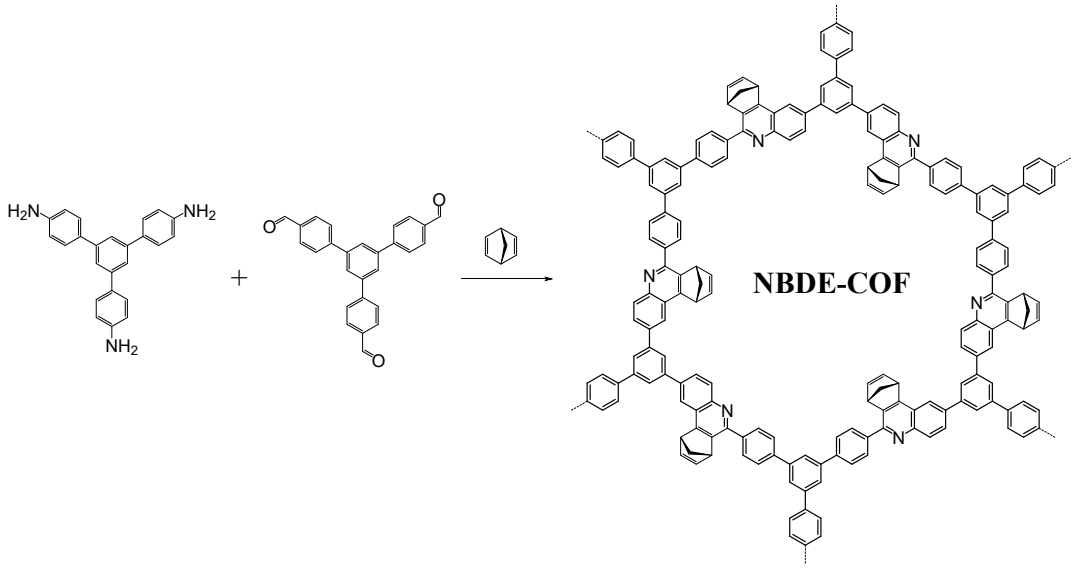
NBE-COF



Scheme S8. Synthetic route of **NBE-COF** connected by quinoline.

The synthesis process was similar to the literature.[9] To a flame-dried 10 mL high-pressure flask with vacuum valve, TAPB (52.7 mg, 0.15 mmol), TFPB (58.6 mg, 0.15 mmol), NBE (49 μL, 0.5 mmol), DDQ (5.0 mg), BF_3•OEt_2 (8 μL, 0.06 mmol) were suspended in a mixture 1.5 mL mesitylene, 1.5 mL dioxane, and 0.2 mL 6 M acetic acid by sonicating at room temperature for 30 min. The mixture was degassed through three freeze-pump-thaw cycles (vacuum < 50 mTorr). Then the flask was sealed and heated in an oven at 120 °C for 3 days at autogenous pressure. After cooling to room temperature, the flask was opened and the suspension was filtered and washed with THF. The crude solid was further extracted through a Soxhlet extractor using THF as extracting solution for 24 h and dried at 60 °C for 24 h under vacuum. A gray-brown powder is obtained, yield: 132.3 mg.

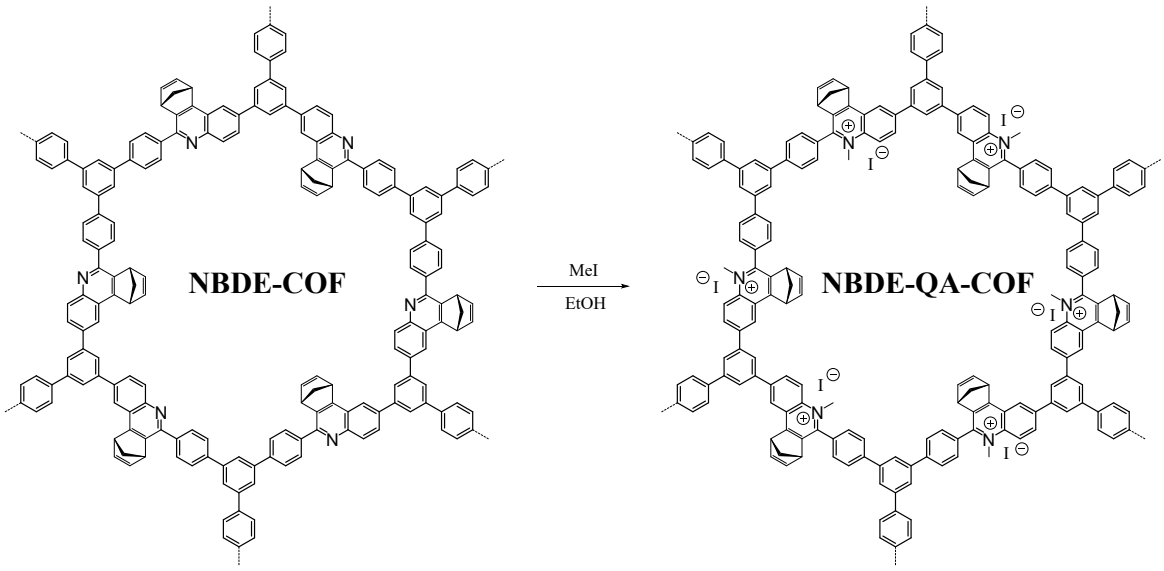
NBDE-COF



Scheme S9. Synthetic route of **NBDE-COF** connected by quinoline.

Synthesis process was similar to that of **NBE-COF** exception that NBE was changed to NBDE (42 μL, 0.5 mmol). A gray-brown powder is obtained, yield: 129.0 mg.

NBDE-QA-COF



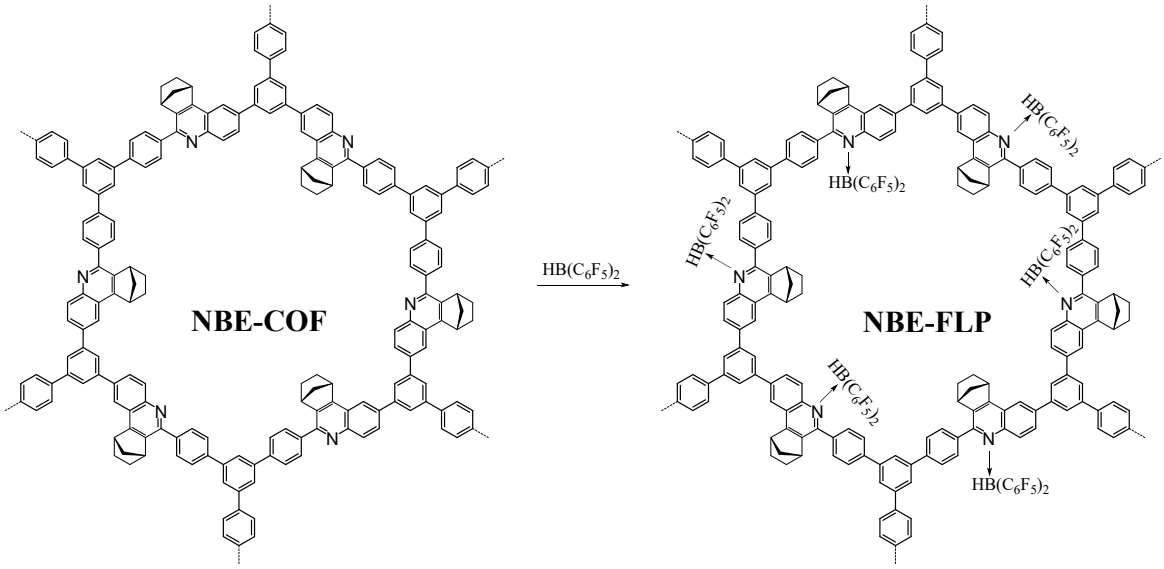
Scheme S10. The synthesis route of N-Methylquinolinium salts **NBDE-QA-COF**.

NBDE-COF (126.0 mg, 0.4 mmol/N atom) was suspended in EtOH (50 mL) and sonicated at room temperature for 12 h. Then MeI was added dropwise at 0 °C and

sonicated again for 12 h. The reaction was heated at 70 °C for 24 h and then cooled to room temperature. The reddish-brown precipitate was washed with ethanol, acetone and ether, and then collected by filtration. Finally, the powder was dried at 60 °C for 24 h under vacuum. Yield: 156.0 mg.

Post-modified Boronization of COFs

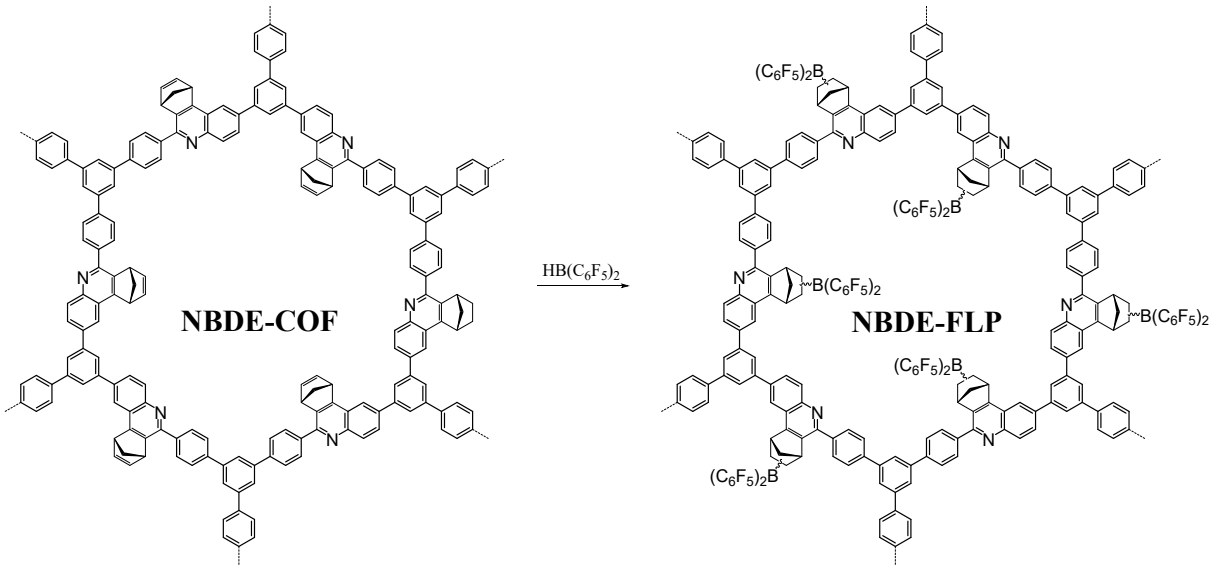
NBE-FLP



Scheme S11. The synthesis route of **NBE-FLP**.

Under Ar atmosphere, **NBE-COF** (32 mg, 0.1mmol/ N atoms) and HBCF (52 mg, 0.15mmol) were suspended in 5 mL anhydrous CH_2Cl_2. After stirring under room temperature for 48 h, the mixture was centrifuged to separate the solid sample, washed with anhydrous CH_2Cl_2 (3 × 5 mL), and then dried at 60 °C for 24 h under vacuum. **NBE-FLP** was obtained as orange powder (47 mg).

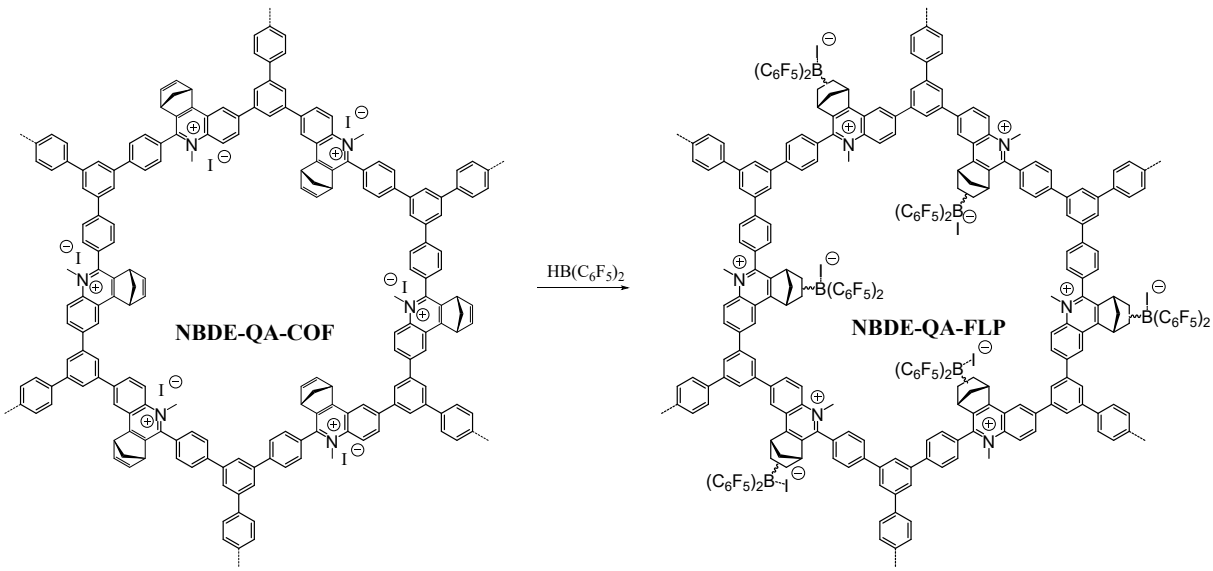
NBDE-FLP



Scheme S12. The synthesis route of **NBDE-FLP**.

Under Ar atmosphere, **NBDE-COF** (32 mg, 0.1mmol/ N atoms) and HBCF (104 mg, 0.30mmol) were suspended in 10 mL anhydrous CH_2Cl_2. After stirring under room temperature for 48 h, the mixture was centrifuged to separate the solid sample, which was then washed with anhydrous CH_2Cl_2 (3 × 10 mL) and dried at 60 °C for 24 h under vacuum. **NBDE-FLP** was obtained as orange powder (76 mg).

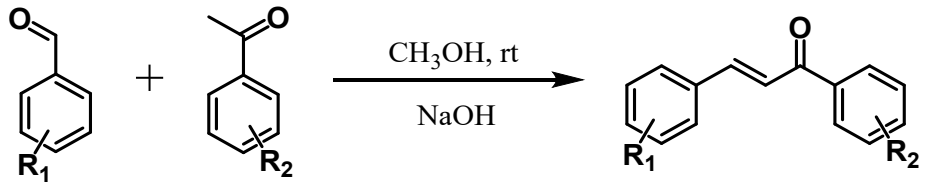
NBDE-QA-FLP



Scheme S13. The synthesis route of **NBDE-QA-FLP**.

Under Ar atmosphere, **NBDE-QA-COF** (46 mg, 0.1mmol/ N atoms) and HBCF (69 mg, 0.20mmol) were suspended in 5 mL anhydrous CH_2Cl_2. After stirring under room temperature for 48 h, the mixture was centrifuged to separate the solid sample, which was then washed with anhydrous CH_2Cl_2 (3 × 5 mL) and dried at 60 °C for 24 h under vacuum. **NBDE-QA-FLP** was obtained as reddish-brown powder (58 mg).

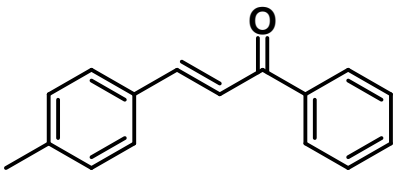
1.3 Synthesis of *α,β*-Unsaturated Ketone



Scheme S14. The synthesis route of *α,β*-Unsaturated Ketone.

General procedure A (**GPA**)

In an ice water bath, a solution of substituted acetophenone (20 mmol) in methanol (10 mL) was added dropwise to a stirred solution of NaOH (26 mmol) in methanol (20 mL). After 15 min, the resulting mixture was further treated with substituted benzaldehydes (20 mmol) and stirred at room temperature until the conversion was completed (monitored by TLC). Then, the mixture was poured into 100 mL H_2O and the solid was filtered, washed with cold ethanol and water, and recrystallized from ethanol to yield the desired *α,β*-unsaturated ketones.

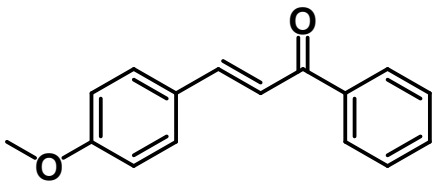


1-phenyl-3-*p*-tolyl-propenone (**1b**)[10]

The target compound was obtained as a white powder using **GPA**. All the spectral data were matched the data that previously reported in the literature.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 8.00 (m, 2H), 7.81 (d, 1H, J = 16.0 Hz), 7.60 - 7.48 (m, 6H), 7.23 (d, 2H, J = 8.0 Hz), 2.39 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 190.57, 144.88, 141.04, 138.28, 132.62, 132.07, 129.66, 128.54, 128.44, 128.41, 120.99, 21.49.

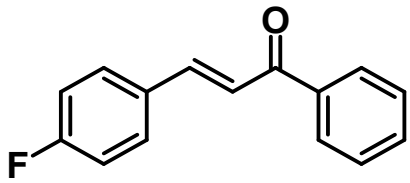


3-(4-Methoxy-phenyl)-1-phenyl-propenone (1c)[10]

The target compound was obtained as a yellowish powder using **GPA**. All the spectral data were in agreement with the data previously reported in the literature.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 8.00 (m, 2H), 7.79 (d, 1H, J = 15.6 Hz), 7.62 - 7.55 (m, 3H), 7.49 (t, 2H, J = 7.6 Hz), 7.42 (d, 1H, J = 15.6 Hz), 6.93 (d, 2H, J = 8.8 Hz), 3.84 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 190.50, 161.61, 144.64, 138.42, 132.51, 130.18, 128.50, 128.35, 127.52, 119.67, 114.35, 55.34.

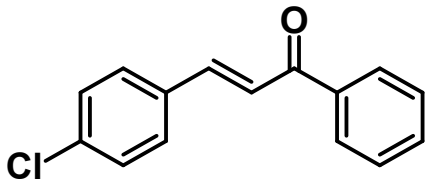


3-(4-Fluorophenyl)-1-phenyl-propenone (1d)[10]

The target compound was obtained as a white powder using **GPA**. All the spectral data were in agreement with the data previously reported in the literature.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 8.00 (m, 2H), 7.78 (d, 1H, J = 15.6 Hz), 7.65 - 7.44 (m, 6H), 7.11 (t, 2H, J = 8.8 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 190.24, 165.25, 162.75, 143.45, 138.05, 132.82, 131.09, 131.06, 130.35, 130.27, 128.61, 128.43, 121.70, 121.67, 116.19, 115.98.

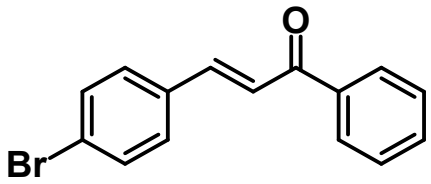


3-(4-Chlorophenyl)-1-phenyl-propenone (1e)[10]

The target compound was obtained as a white powder using **GPA**. All the spectral data were in agreement with the data previously reported in the literature.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 8.00 (m, 2H), 7.75 (d, 1H, J = 15.6 Hz), 7.61 - 7.48 (m, 6H), 7.38 (d, 2H, J = 7.6 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 190.13, 143.23, 137.94, 136.36, 133.30, 132.89, 129.54, 129.18, 128.62, 128.44, 122.35.

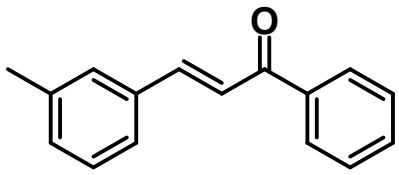


3-(4-Bromophenyl)-1-phenyl-propenone (1f)[11]

The target compound was obtained as a white powder using **GPA**. All the spectral data were in agreement with the data previously reported in the literature.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 8.00 (m, 2H), 7.74 (d, 1H, J = 16.0 Hz), 7.62 - 7.48 (m, 8H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 190.19, 143.34, 137.95, 133.75, 132.93, 132.18, 129.77, 128.65, 128.47, 124.78, 122.48.



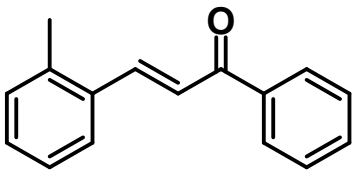
1-Phenyl-3-*m*-tolyl-propenone (1g)[10]

The target compound was obtained as a white powder using **GPA**. All the spectral data

were in agreement with the data previously reported in the literature.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 8.01 (m, 2H), 7.80 (d, 1H, J = 15.6 Hz), 7.62 - 7.43 (m, 6H), 7.31 (t, 1H, J = 8.0 Hz), 7.24 (d, 1H, J = 7.6 Hz), 2.40 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 190.53, 145.02, 138.57, 138.19, 134.76, 132.70, 131.38, 129.00, 128.80, 128.57, 128.46, 125.68, 121.79, 21.31.

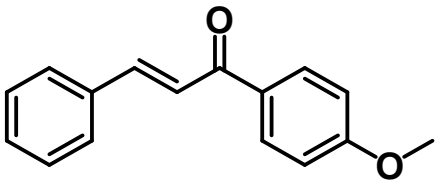


1-Phenyl-3-*o*-tolyl-propenone (1h)[12]

The target compound was obtained as a yellow oil using **GPA**. All the spectral data were in agreement with the data previously reported in the literature.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, 1H, J = 15.6 Hz), 8.16 (d, 2H, J = 7.2 Hz), 7.82 (d, 1H, J = 8.0 Hz), 7.70 (t, 1H, J = 7.2 Hz), 7.64 - 7.55 (m, 3H), 7.44 – 7.32 (m, 3H), 2.59 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 190.29, 142.30, 138.27, 138.11, 133.78, 132.71, 130.84, 130.20, 128.53, 128.42, 126.31, 126.26, 122.94, 19.78.

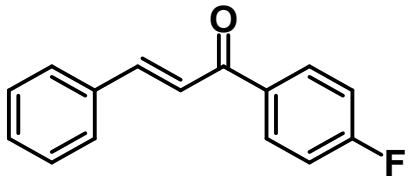


1-(4-Methoxy-phenyl)-3-phenyl-propenone (1i)[10]

The target compound was obtained as a white powder using **GPA**. All the spectral data were in agreement with the data previously reported in the literature.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 – 8.02 (m, 2H), 7.81 (d, 1H, J = 15.6 Hz), 7.67 - 7.62 (m, 2H), 7.55 (d, 1H, J = 15.6 Hz), 7.44 – 7.38 (m, 3H), 7.00 - 6.96 (m, 2H, J = 7.6 Hz), 3.88 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 188.60, 163.35, 143.87, 134.98, 130.99, 130.75, 130.27, 128.85, 128.30, 121.76, 113.77, 55.42.

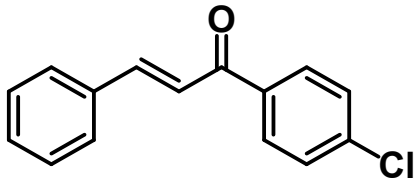


1-(4-Fluorophenyl)-3-phenyl-propenone (1j)[13]

The target compound was obtained as a white powder using **GPA**. All the spectral data were in agreement with the data previously reported in the literature.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 – 8.03 (m, 2H), 7.82 (d, 1H, J = 15.6 Hz), 7.70 - 7.62 (m, 2H), 7.51 (d, 1H, J = 16.0 Hz), 7.45 – 7.40 (m, 3H), 7.21 – 7.14 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 188.77, 166.82, 164.29, 145.01, 134.70, 134.48, 134.45, 131.10, 131.01, 130.63, 128.95, 128.44, 121.49, 115.82, 115.60.

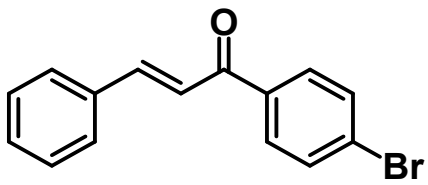


1-(4-Chlorophenyl)-3-phenyl-propenone (1k)[10]

The target compound was obtained as a white powder using **GPA**. All the spectral data were in agreement with the data previously reported in the literature.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.94 (m, 2H), 7.82 (d, 1H, J = 15.6 Hz), 7.67 - 7.62 (m, 2H), 7.51 - 7.45 (m, 3H), 7.44 – 7.40 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 189.10, 145.29, 139.16, 136.42, 134.62, 130.70, 129.86, 128.95, 128.89, 128.47, 121.39.

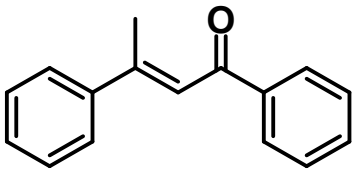


1-(4-Bromophenyl)-3-phenyl-propenone (1l)[13]

The target compound was obtained as a white powder using **GPA**. All the spectral data were in agreement with the data previously reported in the literature.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.87 (m, 2H), 7.82 (d, 1H, J = 15.6 Hz), 7.67 - 7.62 (m, 4H), 7.48 (d, 1H, J = 15.6 Hz), 7.45 – 7.41 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 189.31, 145.37, 136.85, 134.61, 131.89, 130.73, 129.99, 128.97, 128.48, 127.86, 121.38.

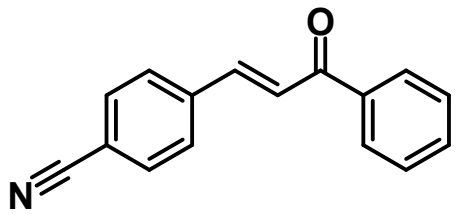


(E)-1,3-Diphenylbut-2-en-1-one (1m)[14]

Tetrachlorosilane (229 μL, 2.0 mmol) was added dropwise to a solution of acetophenone (2.0 mmol) in EtOH (2.0 mL) at 0 °C. The reaction was warmed to 25 °C and stirred for 3 h. The reaction was neutralized by dropwise addition of saturated aqueous $NaHCO_3$ solution (10 mL). The product was extracted with EtOAc (3 × 10 mL). The organic phases were combined and washed with brine (10 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure. The crude residue was purified by flash chromatography to give the (E)-1,3-Diphenylbut-2-en-1-one as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, 2H, J = 7.6 Hz), 7.62 – 7.54 (m, 3H), 7.51 - 7.40 (m, 5H), 7.19 (s, 1H), 2.62 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 191.79, 155.05, 142.71, 139.29, 132.49, 129.08, 128.56, 128.49, 128.22, 126.44, 122.04, 18.84.

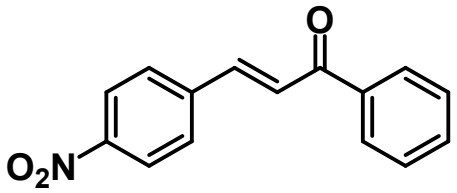


4-(3-oxo-3-phenylprop-1-en-1-yl)benzonitrile (1n)[15]

The target compound was obtained as a white powder using **GPA**. All the spectral data were in agreement with the data previously reported in the literature.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 8.00 (m, 2H), 7.77 (d, 1H, J = 16.0 Hz), 7.74 - 7.68 (m, 4H), 7.64 - 7.58 (m, 2H), 7.54 – 7.49 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 189.67, 142.01, 139.12, 137.53, 133.25, 132.63, 128.74, 128.65, 128.51, 124.98, 118.35, 113.41.

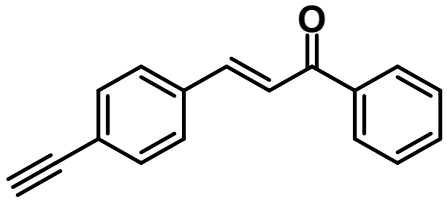


3-(4-Nitrophenyl)-1-phenyl-propenone (1o)[13]

The target compound was obtained as an orange powder using **GPA**. All the spectral data were in agreement with the data previously reported in the literature.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, 2H, J = 8.8 Hz), 8.05 – 8.01 (m, 2H), 7.84 - 7.77 (m, 3H), 7.67 – 7.60 (m, 2H), 7.53 (t, 2H, J = 16.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 189.58, 148.49, 141.45, 140.99, 137.47, 133.34, 128.90, 128.78, 128.55, 125.64, 124.17.

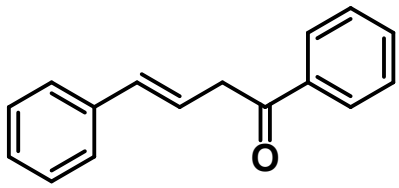


3-(4-Ethynylphenyl)-1-phenyl-propenone (1p)[16]

The target compound was obtained as a white powder using **GPA**. All the spectral data were in agreement with the data previously reported in the literature.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, 2H, J = 8.4 Hz), 7.78 (d, 1H, J = 16.0 Hz), 7.60 (d, 3H, J = 8.0 Hz), 7.57 – 7.49 (m, 5H), 3.21 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 190.15, 143.53, 137.99, 135.18, 132.88, 132.59, 128.62, 128.46, 128.22, 124.09, 122.85, 83.16, 79.39.



(E)-1,4-diphenylbut-3-en-1-one (**1t**)[17]

To a solution of acetophenone (2.00 g, 16.64 mmol) and phenyl acetylene (1.83 mL, 16.64 mmol) in DMSO (42 mL) was added *t*-BuOK (1.87 g, 16.64 mmol). The resulting solution was stirred at 100 °C for 0.5 h. The reaction mixture was cooled to room temperature, and the reaction was quenched with the addition of a saturated aqueous NH_4Cl solution (50 mL). The reaction mixture was extracted with EtOAc (50 mL×2). The combined organic solution was washed with brine (25 mL), dried over $MgSO_4$ and concentrated under reduced pressure to give crude product. The resulting residue was purified by flash chromatography to yield the target product as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 8.00 (m, 2H), 7.59 (tt, 1H, J_1 = 7.2 Hz, J_2 = 1.2 Hz), 7.52 - 7.47 (m, 2H), 7.42 – 7.38 (m,2H), 7.34 – 7.29 (m, 2H), 7.26 – 7.20 (m, 1H), 6.59 – 6.45 (m, 2H), 3.92 (d, 2H, J = 5.6 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.93, 136.92, 136.53, 133.51, 133.20, 128.64, 128.48, 128.29, 127.45, 126.24, 122.52, 42.66.

2. Structural Simulation

The structural crystal models with hcb topology of all the COFs were initially constructed in hexagonal unit cell with the Accelrys Materials Studio (ver. 8.0)[18] suite of programs. Geometry optimization of the structures with Dmol3 molecular dynamics module method led to satisfactory models whose theoretical pattern matched well the experimentally obtained patterns in terms of reflection position and relative intensity. The Pawley profile refinements were performed using a Pseudo-Voigt profile function. The observed diffraction patterns were subjected to a polynomial background subtraction and the refined parameters included the zero-point shift, the unit cell parameters, the FWHM parameters and the peak asymmetry (Berar-Baldizzoni function). For all the COFs, AA stacking were constructed, and their corresponding PXRD patterns were calculated.

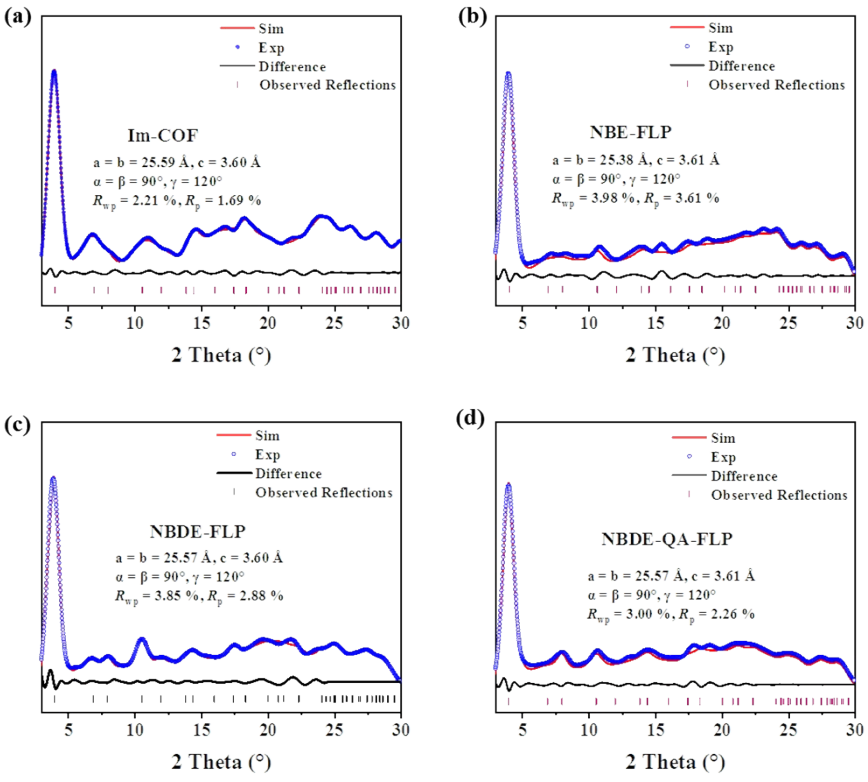


Figure S4. Experimental PXRD, corresponding Pawley-refined patterns, simulated observed reflections from the AA-stacking mode and their difference of (a) Imine-COF, (b) NBE-FLP, (c) NBDE-QA-FLP, and (d) NBDE-FLP.

3. Characterization

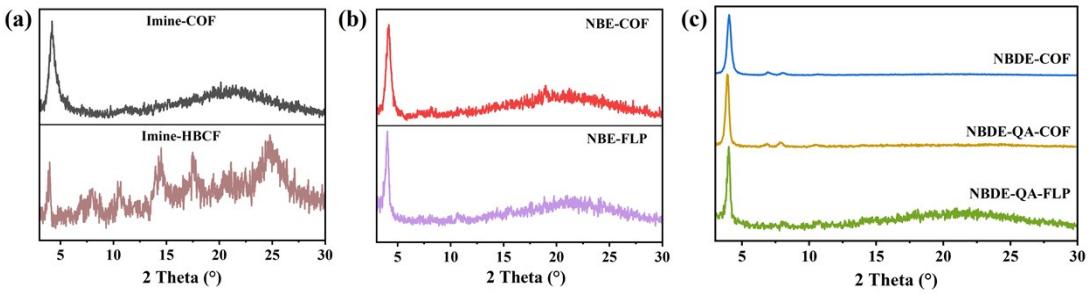


Figure S5. PXRD of (a) **Imine-COF** and **Imine-HBCF**, (b) **NBE-COF** and **NBE-FLP**, (c) **NBDE-COF**, **NBDE-QA-COF** and **NBDE-QA-FLP**.

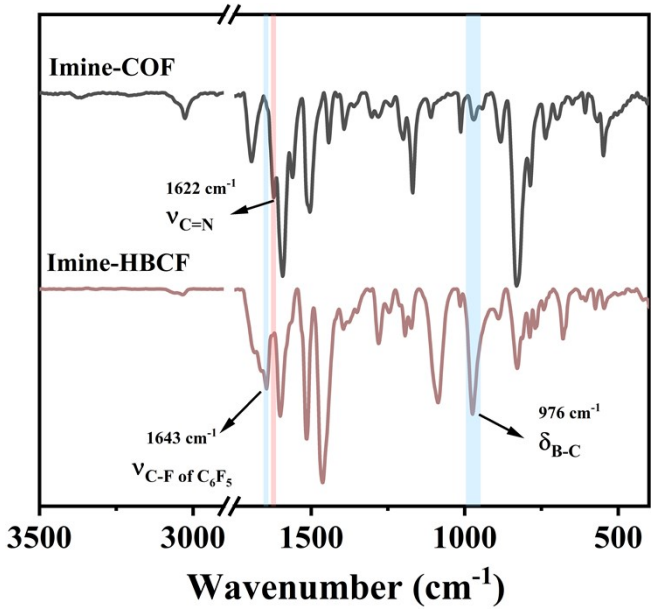


Figure S6. FT-IR of **Imine-COF** and **Imine-HBCF.**

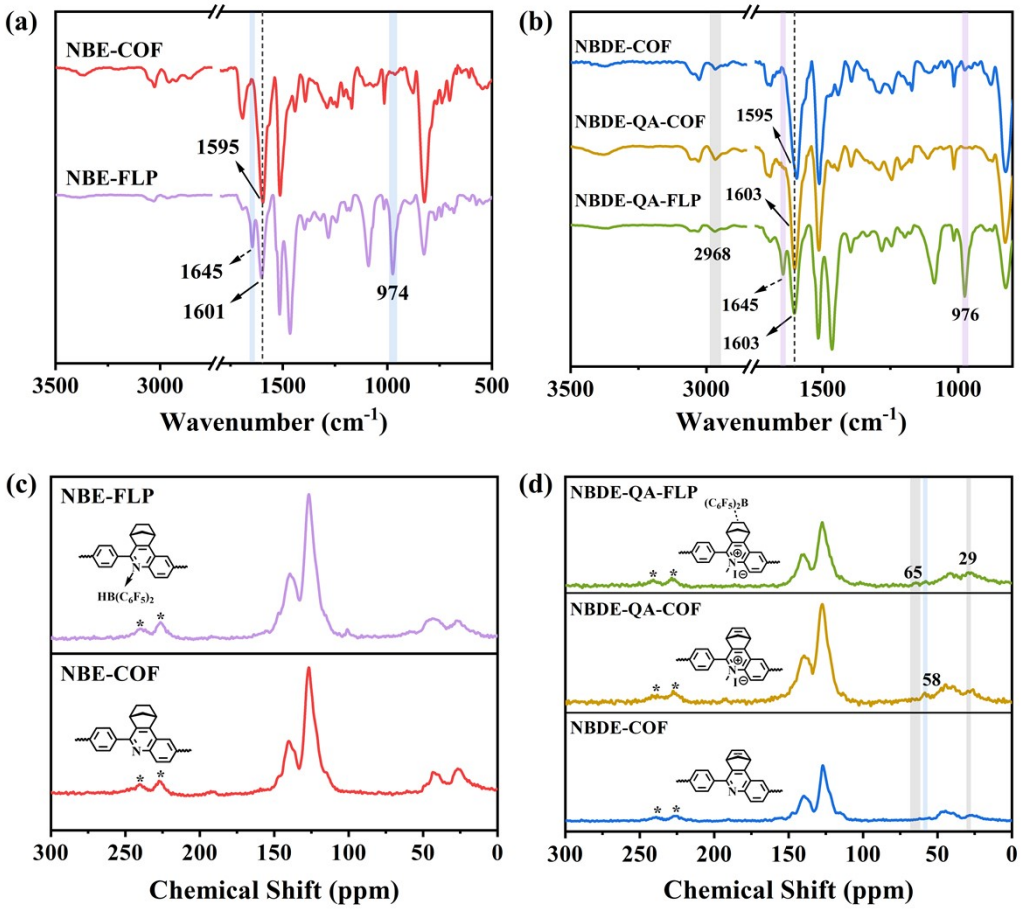


Figure S7. (a) FT-IR and (c) solid state ^{13}C CP-MAS NMR spectra of **NBE-COF** and **NBE-FLP**. (b) FT-IR and (d) solid state ^{13}C CP-MAS NMR spectra of **NBDE-COF**, **NBDE-QA-COF** and **NBDE-QA-FLP**.

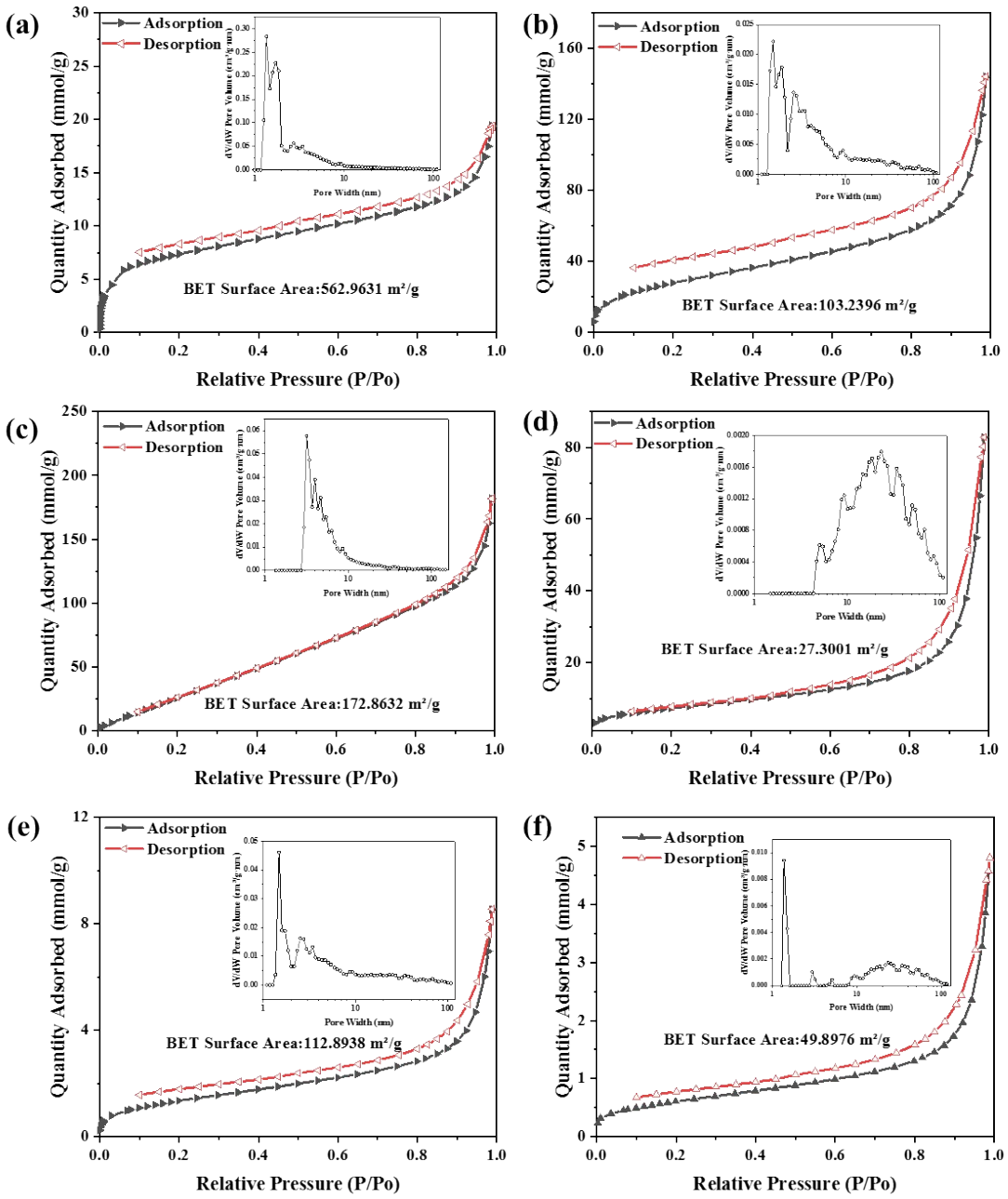


Figure S8. N_2 adsorption-desorption isotherms and the pore size distribution curves of (a) **NBDE-COF**, (b) **NBDE-FLP**, (c) **NBDE-QA-COF**, and (d) **NBDE-QA-FLP,** (e) **NBE-COF** and (f) **NBE-FLP**.

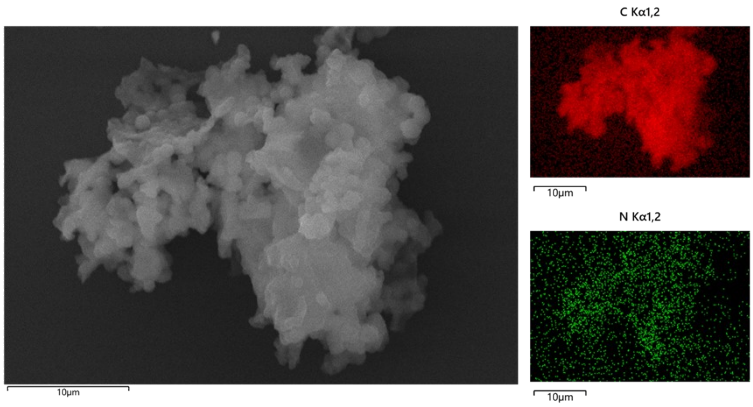


Figure S9. SEM images and EDS Mapping of **Imine-COF**.

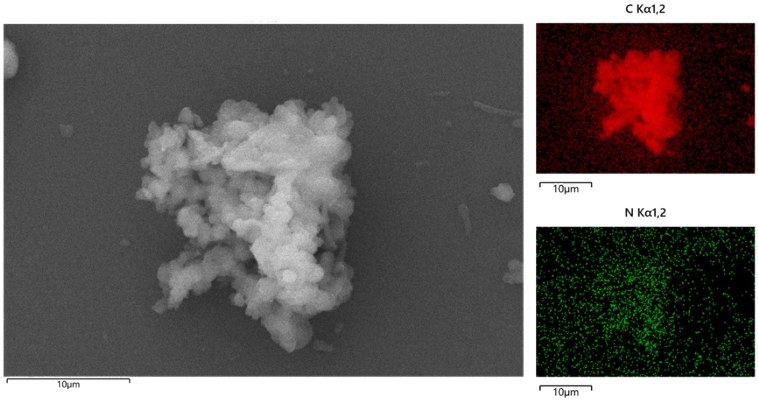


Figure S10. SEM images and EDS Mapping of **NBE-COF**.

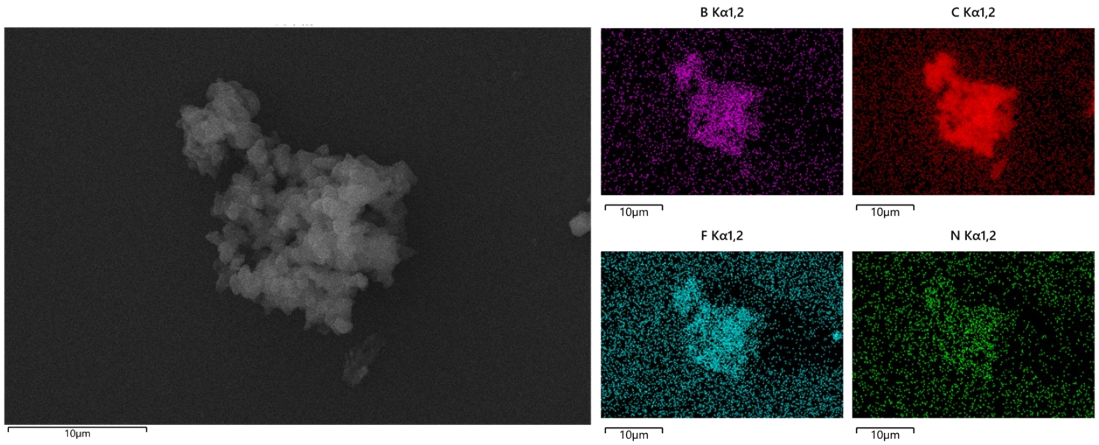


Figure S11. SEM images and EDS Mapping of **NBE-FLP**.

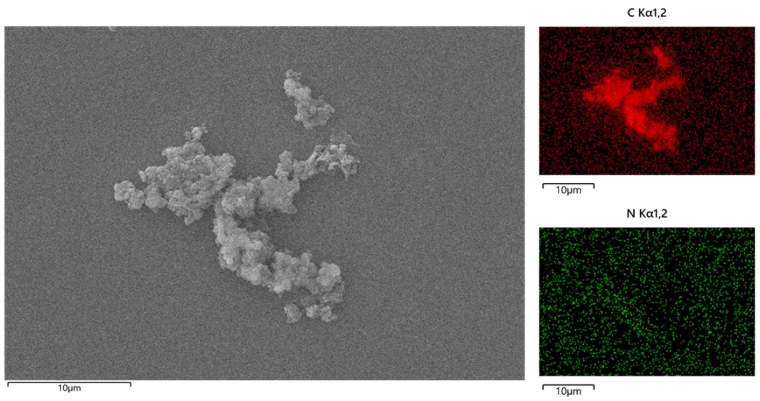


Figure S12. SEM images and EDS Mapping of **NBDE-COF**.

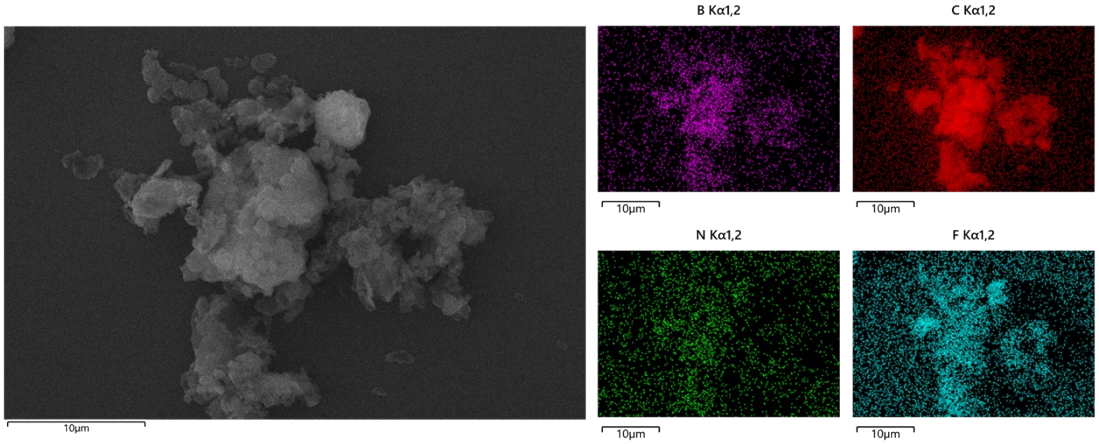


Figure S13. SEM images and EDS Mapping of **NBDE-FLP**.

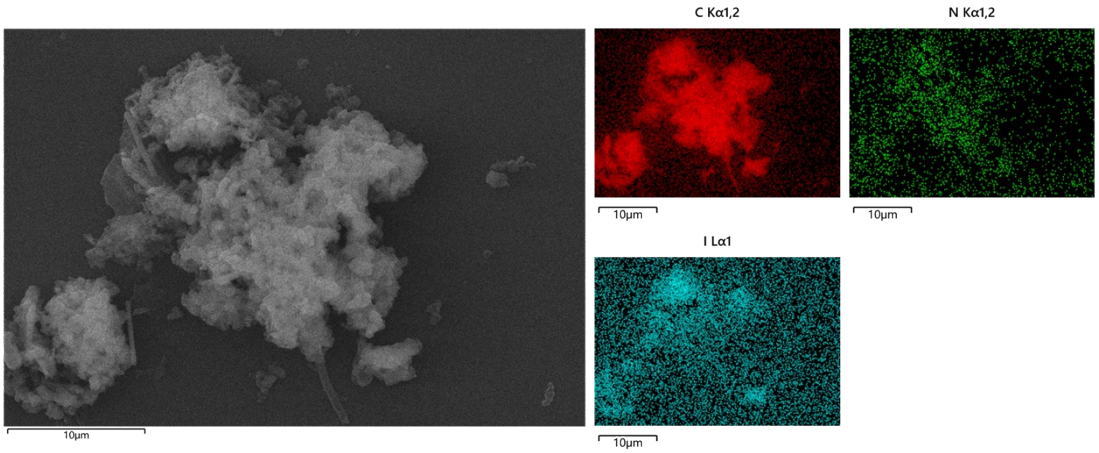


Figure S14. SEM images and EDS Mapping of **NBDE-QA-COF**.

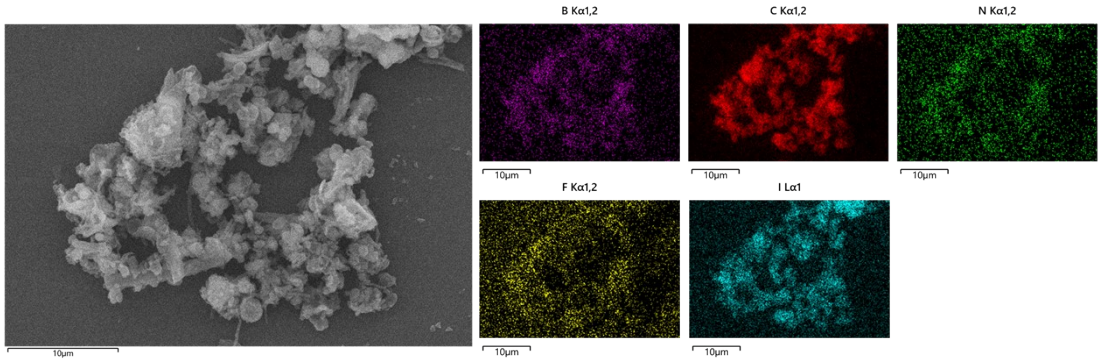


Figure S15. SEM images and EDS Mapping of **NBDE-QA-FLP**.

General Procedure for *in situ* ^{11}B NMR: In a glove box, dissolving a certain amount of HBCF in 0.5ml $CDCl_3$ with a nuclear magnetic tube, then 0.1mmol model compounds (CQ-NBE, CQ-NBDE or CQ-NBDE-QA) was added in air or Ar atmospheres, and the ^{11}B NMR spectrums were tested after shaking evenly.

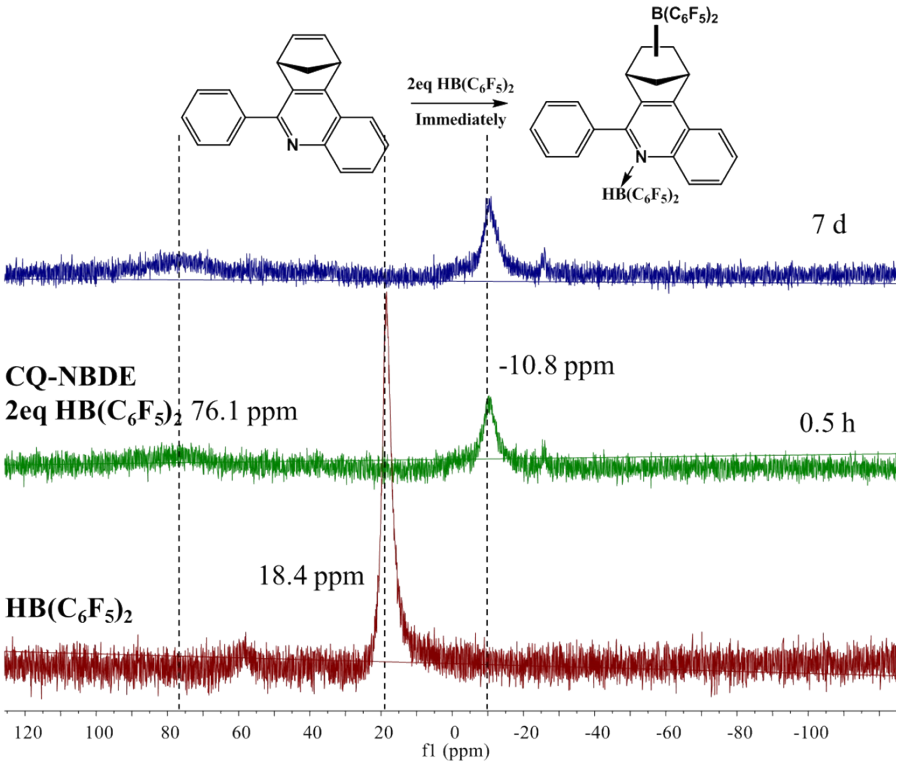


Figure S16. *In situ* ^{11}B NMR of **CQ-NBDE** with 2 equivalents $HB(C_6F_5)_2$ in Ar.

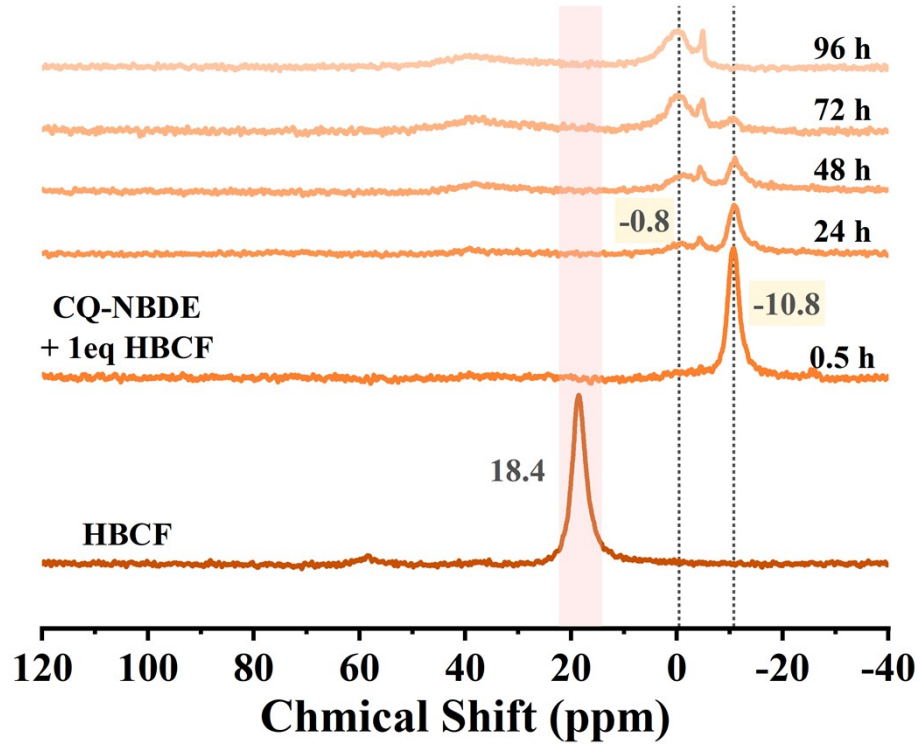
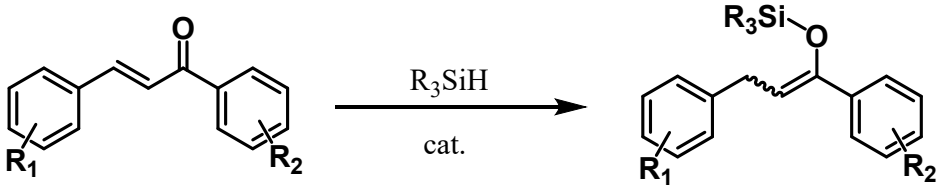


Figure S17. *In situ* ^{11}B NMR of **CQ-NBDE** with 1 equivalents $HB(C_6F_5)_2$ in air.

4. Experimental Details for Catalytic Reactions and Characterization of the Corresponding Products

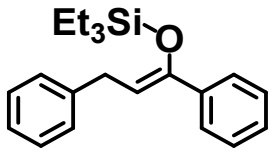
General procedure for the selective 1,4-hydrosilylation of *α,β*-unsaturated ketone.

General Procedure B (**GPB**)



Under ambient conditions, **chalcone 1** (0.5 mmol) and chloroform (1 mL) were added to a 10 mL glass bottle, followed by the catalyst **NBDE -FLP** (1 mol%) and the corresponding silane (0.55 mmol). The bottle was capped tightly and the reaction was stirred at room temperature for 24 h. After the reaction was completed, mesitylene (0.5 mmol, 69 μL) was added to the mixture as the internal standard. 100 μL of the reaction mixture was taken and 500 μL $CDCl_3$ was added for ^{1}H NMR experiment. The reaction mixture was filtered, the remaining solid was washed with chloroform (3×2 mL), the

organic phases were combined and the solvent was evaporated under vacuum. The crude product was purified by silica gel column chromatography (EA : PE = 1:100 ~ 1:10).



(*Z*)-((1,3-Diphenylprop-1-en-1-yl)oxy)triethylsilane ((*Z*)-**2a-1**)

The target compound was obtained as a colorless oil using **GPB** (Et_3SiH as the reductant). All the spectral data were in agreement with the data previously reported in the literature.[19]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, 2H, J = 8.0 Hz), 7.32 – 7.15 (m, 8H), 5.31 (t, 1H, J = 7.2 Hz), 3.58 (d, 2H, J = 7.2 Hz), 0.94 (t, 9H, J = 8.0 Hz), 0.63 (d, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.14, 141.55, 139.40, 128.40, 128.34, 127.96, 127.61, 125.79, 125.67, 109.72, 32.25, 6.72, 5.39.

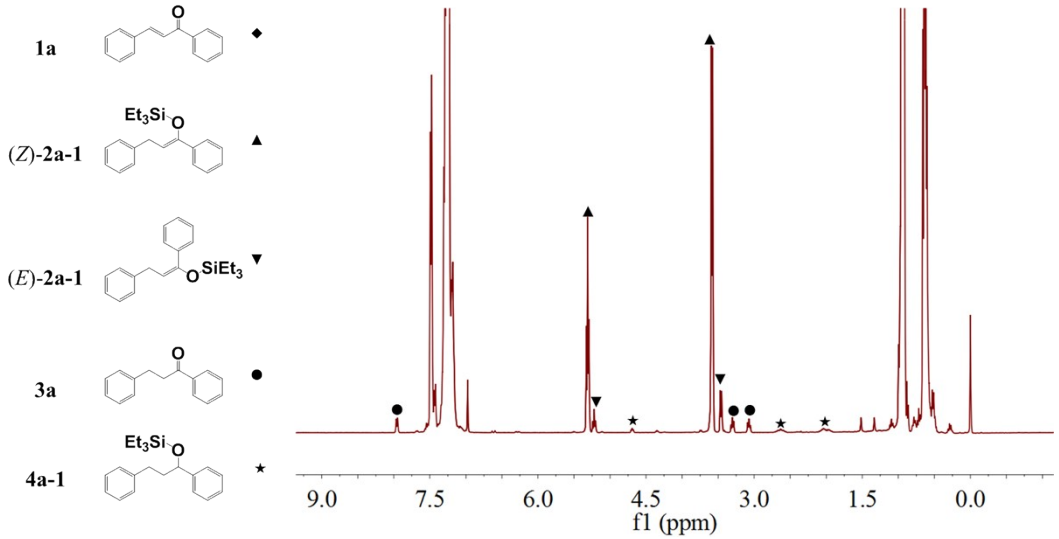
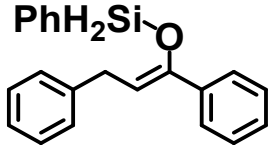


Figure S18. ^{1}H NMR of the mixture after the reaction was completed according to GPB, using Et_3SiH as reducing agent.



(*Z*)-((1,3-Diphenylprop-1-en-1-yl)oxy)phenylsilane ((*Z*)-**2a-2**)

The target compound cannot be obtained using **GPB** ($PhSiH_3$ as the reductant) due to the rapid desiliconization on silica gel, but the pure ketone compound **3a** was obtained. The presence of the (*Z*)-**2a-2** can be observed by ^1H NMR of the reaction mixture.

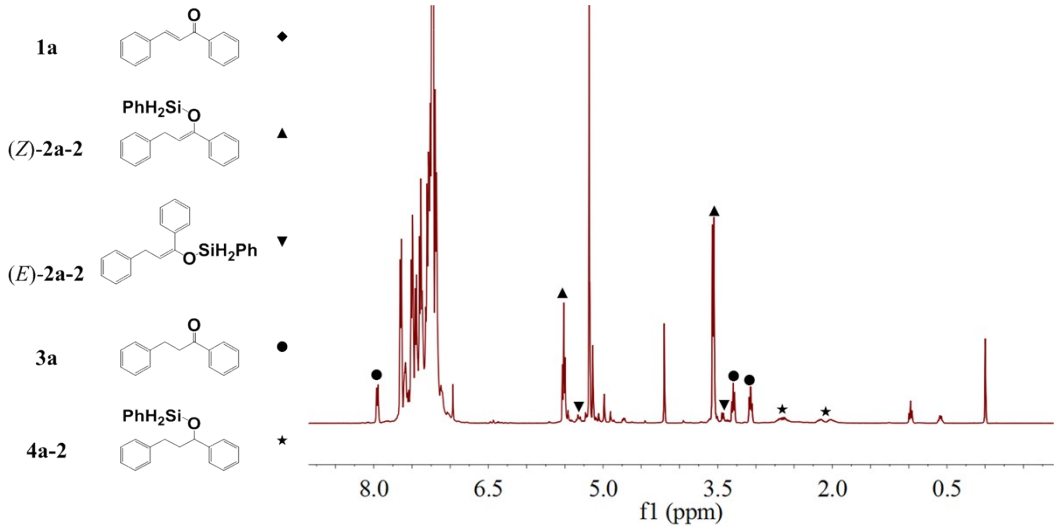
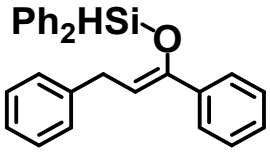


Figure S19. ^1H NMR of the mixture after the reaction was completed according to GPB, using $PhSiH_3$ as reducing agent.



(*Z*)-((1,3-Diphenylprop-1-en-1-yl)oxy)diphenylsilane ((*Z*)-**2a-3**)

The purity target compound cannot be obtained using **GPB** (Ph_2SiH_2 as the reductant) due to the desiliconization on silica gel. The presence of the product can be observed by ^1H NMR of the reaction mixture, which is consistent with previous literature reports.[20]

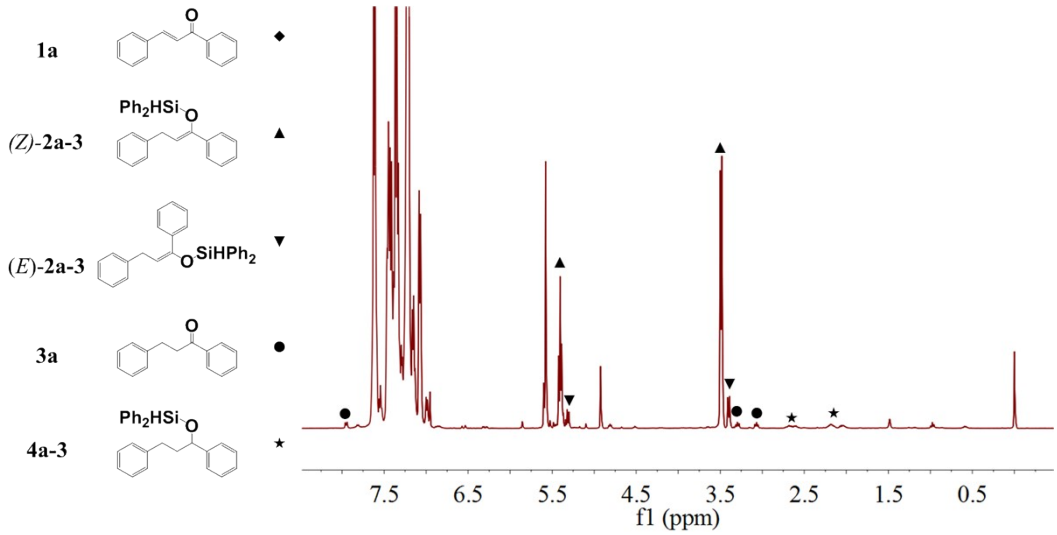
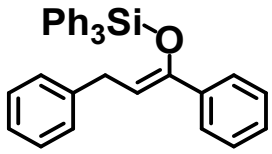


Figure S20. ^{1}H NMR of the mixture after the reaction was completed according to GPB, using Ph_2SiH_2 as reducing agent.



(*Z*)-((1,3-Diphenylprop-1-en-1-yl)oxy)triphenylsilane ((*Z*)-**2a-4**)

The target compound cannot be obtained using **GPB** (Ph_3SiH as the reductant) due to the large steric hindrance of triphenyl silane that the reaction cannot be carried out.

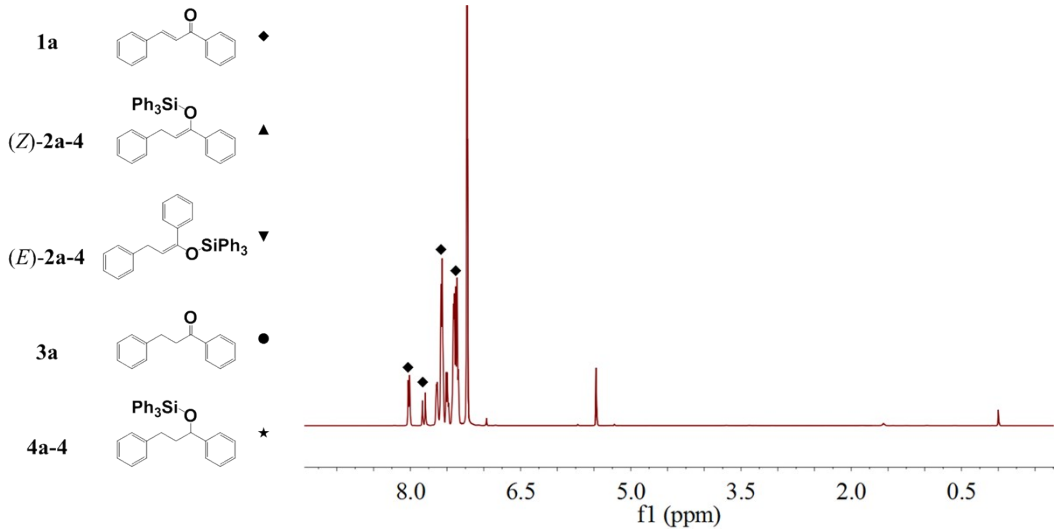
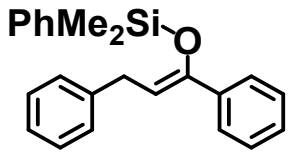


Figure S21. ^{1}H NMR of the mixture after the reaction was completed according to GPB, using Ph_3SiH as reducing agent.



(*Z*)-((1,3-Diphenylprop-1-en-1-yl)oxy)dimethylphenylsilane ((*Z*)-**2a-5**)

The target compound was obtained as a colorless oil using **GPB** ($PhMe_2SiH$ as the reductant). All the spectral data were in agreement with the data previously reported in the literature.[19]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, 2H, J = 4.8 Hz), 7.44 (d, 2H, J = 4.8 Hz), 7.37 (dt, 3H, J_1 = 20.8 Hz, J_2 = 4.8 Hz), 7.26 – 7.21 (m, 5H), 7.15 (dd, 3H, J_1 = 12.8 Hz, J_2 = 4.8 Hz), 5.37 (t, 1H, J = 4.8 Hz), 3.44 (d, 2H, J = 4.8 Hz),0.38 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.56, 141.35, 138.76, 137.14, 133.43, 129.80, 128.37, 128.29, 127.99, 127.79, 127.62, 125.76, 125.70, 110.23, 32.32, -0.89.

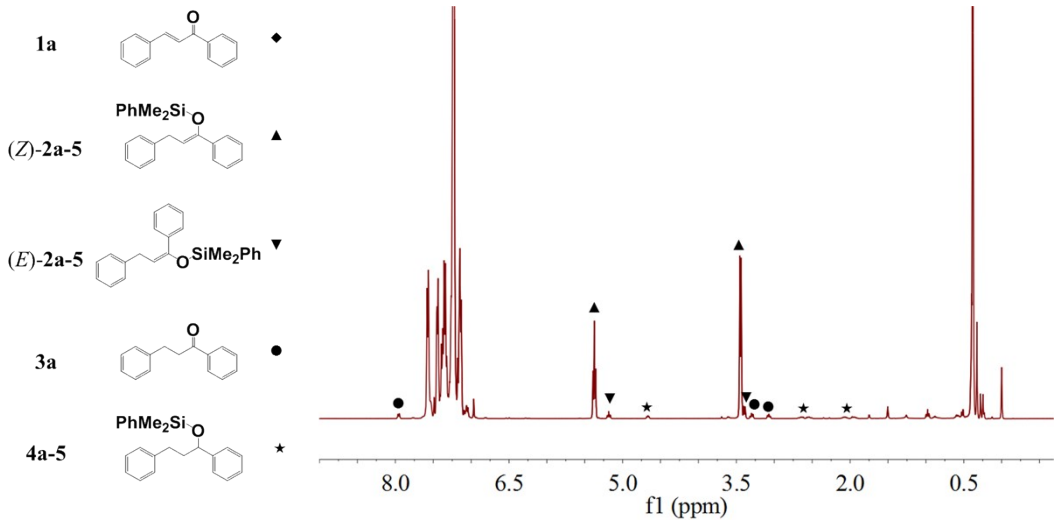
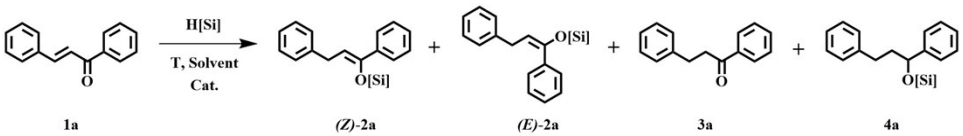


Figure S22. ^{1}H NMR of the mixture after the reaction was completed according to GPB, using $PhMe_2SiH$ as reducing agent.

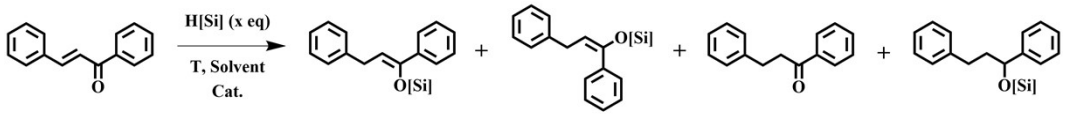
Table S1. Optimization of reduction of α,β-unsaturated carbonyl compounds.[a]



Entry	Silane	Sol.	Cat.	Conv. (%)[b]	Yield ratio of (*Z*)-**2a**:(*E*)-**2a**:**3a**:**4a**[b]
1	Et_3SiH	$CHCl_3$	-	0	-
2	Et_3SiH	$CHCl_3$	HBCF	58	81:6:12:1
3	Et_3SiH	$CHCl_3$	NBE-COF	0	-
4	Et_3SiH	$CHCl_3$	NBE-FLP	> 99	83:7:7:3
5	Et_3SiH	$CHCl_3$	NBDE-COF	0	-
6	Et_3SiH	$CHCl_3$	NBDE-FLP	> 99	87:8:4:1
7	Et_3SiH	$CHCl_3$	NBDE-QA-COF	0	-
8	Et_3SiH	$CHCl_3$	NBDE-QA-FLP	> 99	79:7:11:3
9	Et_3SiH	toluene	NBDE-FLP	6	29:N:71:N
10	Et_3SiH	C_6H_5Br	NBDE-FLP	5	67:23:N:N
11	Et_3SiH	CH_2Cl_2	NBDE-FLP	< 1	N:N:100:N
12	Et_3SiH	THF	NBDE-FLP	0	-
13	Et_3SiH	CH_3CN	NBDE-FLP	0	-
14	Et_3SiH	CH_3OH	NBDE-FLP	0	-
15	$PhSiH_3$	$CHCl_3$	NBDE-FLP	> 99	69:5:15:11
16	$PhMe_2SiH$	$CHCl_3$	NBDE-FLP	> 99	85:7:4:4
17	Ph_2SiH_2	$CHCl_3$	NBDE-FLP	> 99	79:10:2:9
18	Ph_3SiH	$CHCl_3$	NBDE-FLP	0	-
19	Et_3SiH[c]	$CHCl_3$	NBDE-FLP	> 99	87:8:5:N
20	Et_3SiH[d]	$CHCl_3$	NBDE-FLP	> 99	89:8:3:N
21	Et_3SiH	$CHCl_3$	NBDE-FLP[e]	25	80:6:14:N
22	Et_3SiH	$CHCl_3$	NBDE-FLP[f]	> 99	67:2:27:4
23	Et_3SiH	$CHCl_3$	CQ-NBDE+HBCF[g]	>99	83:13:0:4
24	Et_3SiH	$CHCl_3$	CQ-NBDE-FLP	85	81:16:2:1
25	Et_3SiH	$CHCl_3$	CQ-NBDE-QA+HBCF[g]	2	61:39:N:N
26	Et_3SiH	$CHCl_3$	CQ-NBDE-QA-FLP	24	75:17:8:N

[a] Reaction conditions: 1a (0.5 mmol), catalyst (1.0 mol%), silane (1.1 equiv.) and solvent (1.0 mL) in 25 ºC at 24 h. [b] Conversion and yields based on the ^1H NMR analysis (internal standard: mesitylene). [c] The amount of Et_3SiH is 2.0 equiv. [d] The amount of Et_3SiH is 3.0 equiv. [e] The amount of NBDE-FLP is 0.5 mol%. [f] The amount of NBDE-FLP is 3.0 mol%. [g] The model compound and HBCF were added to the reaction system without premixing.

Table S2. Effect of substrate concentration (conc.), reaction time (t) and temperature (T) on reduction of *α*,*β*-unsaturated carbonyl compounds.[a]



1a (Z)-2a (E)-2a 3a 4a

Entry	Conc./M	Silane	T/°C	t/h	Conv. (%)[b]	Yield ratio of (*Z*)-**2a**:(*E*)-**2a**:**3a**:**4a** [b]
1	**0.5**	**Et_3SiH**	**25**	**24**	**>99**	**87:8:4:1**
2	**1**	Et_3SiH	25	24	>99	86:8:4:2
3	**0.25**	Et_3SiH	25	24	>99	87:9:3:1
4	**0.1**	Et_3SiH	25	24	>99	84:11:1:4
5	0.5	Et_3SiH	25	**1**	45	74:5:19:2
6	0.5	Et_3SiH	25	**2**	53	79:5:15:1
7	0.5	Et_3SiH	25	**12**	>99	87:8:4.5:0.5
8	0.5	Et_3SiH	25	**18**	>99	87:8:4:1
9	0.5	Et_3SiH	**-20**	24	0	-
10	0.5	Et_3SiH	**0**	24	<1	100:N:N:N
11	0.5	Et_3SiH	**40**	24	>99	87:11:1:1
12	0.5	Et_3SiH	**60**	24	>99	85:14:0.5:0.5
13	0.5	$PhSiH_3$	**-20**	24	19	72:8:20:N
14	0.5	$PhSiH_3$	**0**	24	73	73:5:22:N
15	0.5	$PhSiH_3$	**25**	24	>99	69:5:15:11
16	0.5	$PhSiH_3$	**40**	24	>99	68:12:12:8
17	0.5	$PhSiH_3$	**60**	24	>99	66:16:11:7

[a] Reaction conditions: **1** (0.5 mmol), **NBDE-FLP** (1.0 mol%), silane (1.1 equiv.) and solvent (1.0 mL) at 25ºC.

[b] Conversion and yields based on the ^1H NMR analysis (internal standard: mesitylene).

The experimental procedure for the recycle test.

Under ambient conditions, 1a (5.0 mmol) and chloroform (10 mL) were added to a 25 mL glass bottle, the catalyst **NBE-FLP**, **NBDE-FLP** or **NBDE-QA-FLP** (1.0 mol%) and $PhSiH_3$ (5.5 mmol) was added, the cap was tightly capped, and the reaction was stirred at 40 °C for 24 h. Upon completion, the mixture was cooled to room temperature, the solid catalyst was separated from the reaction mixture and washed with chloroform three times before reuse. As for the liquid, it was evaporated under vacuum and separated by silica gel column to obtain the product and determine yield. To verify the

recyclability of **NBE-FLP, NBDE-FLP** and **NBDE-QA-FLP**, the above procedure was repeated another 4 times with the catalyst used in the former batch.

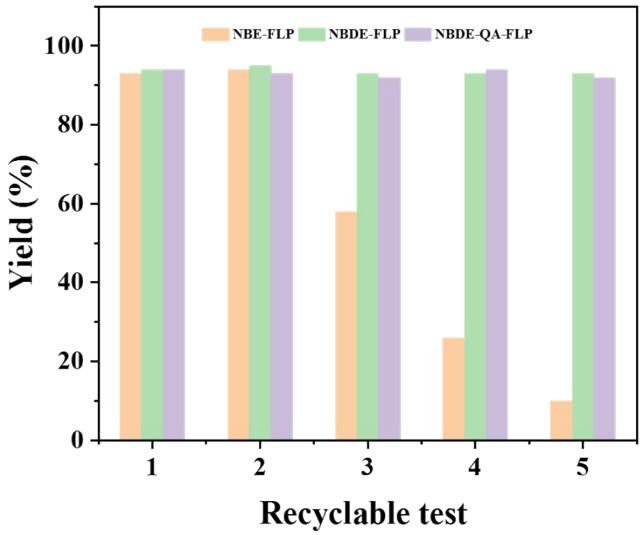


Figure S23. Catalysis performance of **NBE-FLP**, **NBDE-FLP** and **NBDE-QA-FLP** in a 5-run recycle test.

Table S3. B Contents of COF-FLPs before and after 5-run recycle test.

COF-FLPs	B Content (mg/g)		
	Theoretical value	Experimental value	
		Before	After
NBE-FLP	3.2	2.46	0.41
NBDE-FLP	3.2	3.24	2.16
NBDE-QA-FLP	2.6	2.22	1.50

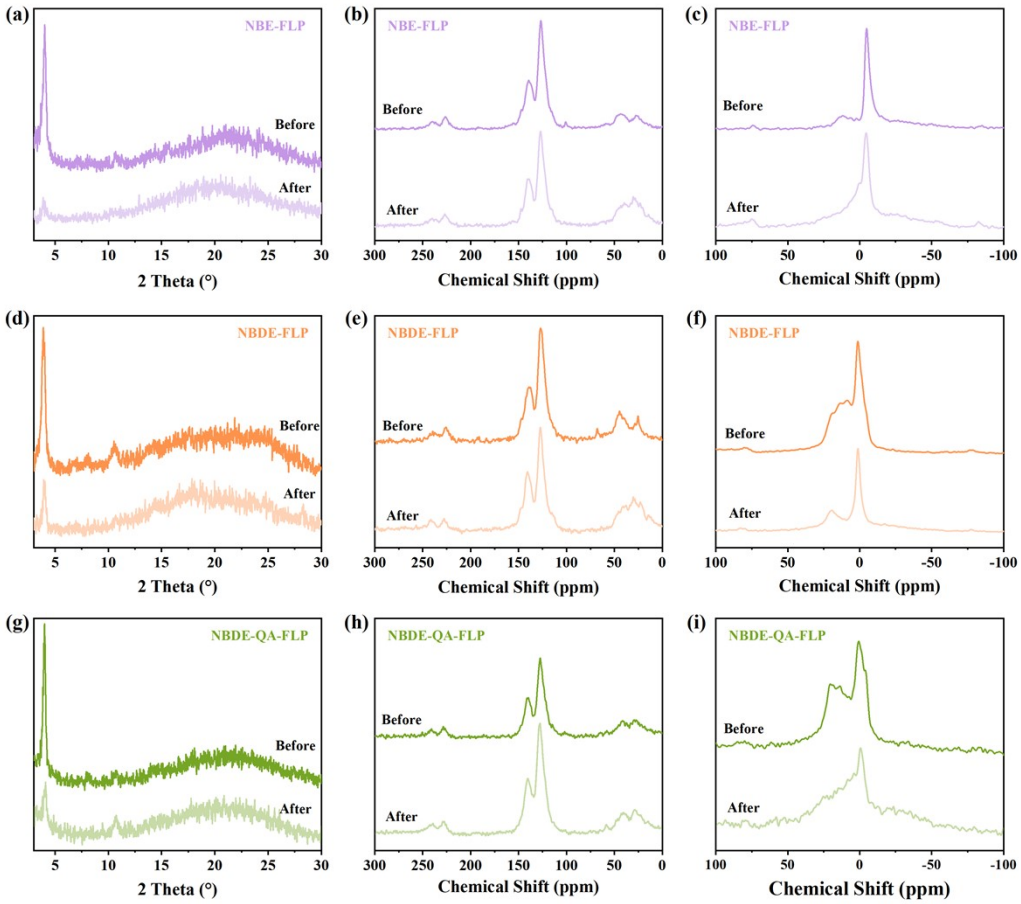
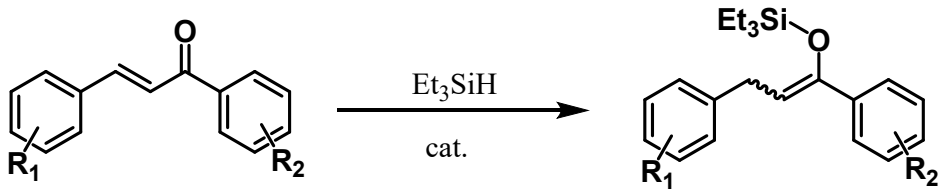


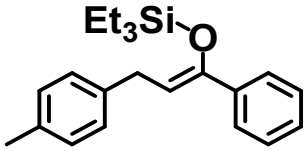
Figure S24. PXRD of (a) **NBE-FLP**, (d) **NBDE-FLP** and (g) **NBDE-QA-FLP** before and after 5-run recycle test. ^{13}C CP-MAS solid state NMR spectra of (b) **NBE-FLP**, (e) **NBDE-FLP** and (h) **NBDE-QA-FLP** before and after 5-run recycle test. Solid state ^{11}B NMR spectra of (c) **NBE-FLP**, (f) **NBDE-FLP** and (i) **NBDE-QA-FLP** before and after 5-run recycle test.

General Procedure C (**GPC**)



Under ambient conditions, corresponding *α,β*-unsaturated ketone (0.5 mmol) and chloroform (1 mL) were added to a 10 mL glass bottle, followed by the catalyst **NBDE-QA-FLP** (1.0 mol%) and Et_3SiH (0.55 mmol). The bottle was capped tightly and the reaction was stirred at room temperature for 24 h. The reaction mixture was filtered, the remaining solid was washed with chloroform (3×2 mL), the organic fractions were combined and the solvent was evaporated under vacuum. The crude product was purified by silica gel column chromatography (EA : PE = 1:100 ~ 1:10).

Characterization of the products 2a – 2t and 3a – 3t.



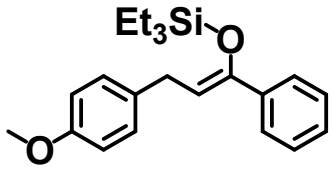
2b

The target compound was obtained as a colorless oil using **GPC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 75%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, 2H, J = 6.8 Hz), 7.32 – 7.22 (m, 3H), 7.13 (dd, 4H, J_1 = 22.8 Hz, J_2 = 8.0 Hz), 5.30 (t, 1H, J = 7.2 Hz), 3.55 (d, 2H, J = 7.2 Hz), 2.32 (s, 3H), 0.94 (t, 9H, J = 8.0 Hz), 0.64 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.96, 139.47, 138.47, 135.22, 129.03, 128.28, 127.94, 127.55, 125.67, 110.04, 31.82, 20.98, 6.71, 5.41.



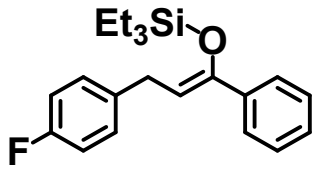
2c

The target compound was obtained as a colorless oil using **GPC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 73%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, 2H, J = 8.4 Hz), 7.33 – 7.23 (m, 3H), 7.19 (d, 2H, J = 8.4 Hz), 6.85 (d, 2H, J = 8.4 Hz), 5.30 (t, 1H, J = 7.2 Hz), 3.80 (s, 3H), 3.54 (d, 2H, J = 7.2 Hz), 0.96 (t, 9H, J = 8.0 Hz), 0.65 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.83, 149.92, 139.47, 133.62, 129.40, 127.80, 127.39, 125.57, 113.93, 110.06, 55.34, 31.34, 6.73, 5.42.



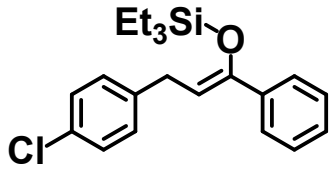
2d

The target compound was obtained as a colorless oil using **GPC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 76%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, 2H, J = 7.6 Hz), 7.36 – 7.19 (m, 5H), 6.98 (td, 2H, J_1 = 8.8 Hz, J_2 = 3.6 Hz), 5.28 (td, 1H, J_1 = 7.2 Hz, J_2 = 3.6 Hz), 3.56 (dd, 2H, J_1 = 7.2 Hz, J_2 = 3.6 Hz), 0.95 (td, 9H, J_1 = 8.0 Hz, J_2 = 3.6 Hz), 0.64 (qd, 6H, J_1 = 8.0 Hz, J_2 = 3.6 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.48, 160.06, 150.37, 139.30, 137.11, 129.88, 129.43, 128.16, 127.88, 125.70, 115.46, 115.25, 114.78, 114.57, 109.38, 108.83, 31.38, 6.73, 5.38.



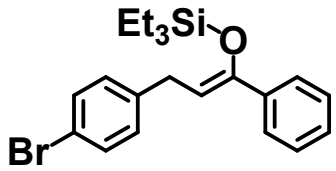
2e

The target compound was obtained as a colorless oil using **GPC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 71%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, 2H, J = 7.6 Hz), 7.34 – 7.24 (m, 4H), 7.19 (d, 2H, J = 8.0 Hz), 5.26 (t, 1H, J = 7.2 Hz), 3.55 (d, 2H, J = 7.2 Hz), 0.94 (t, 9H, J = 8.0 Hz), 0.63 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.60, 139.99, 139.22, 131.48, 129.69, 128.38, 128.01, 127.76, 125.70, 108.98, 31.52, 6.70, 5.37.



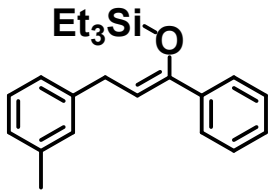
2f

The target compound was obtained as a colorless oil using **GPC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 70%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, 2H, J = 7.6 Hz), 7.41 (d, 2H, J = 8.0 Hz), 7.34 – 7.26 (m, 3H), 7.14 (d, 2H, J = 8.0 Hz), 5.26 (t, 1H, J = 7.2 Hz), 3.53 (d, 2H, J = 7.2 Hz), 0.94 (t, 9H, J = 8.0 Hz), 0.63 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.60, 139.98, 139.22, 131.47, 129.22, 128.44, 127.93, 127.61, 125.79, 108.89, 31.52, 6.71, 5.37.



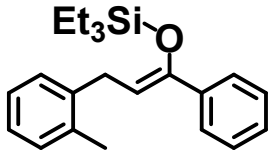
2g

The target compound was obtained as a colorless oil using **GPC, expect the reaction temperature was 40 ºC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 68%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, 2H, J = 7.2 Hz), 7.33 – 7.23 (m, 3H), 7.20 (t, 1H, J = 7.2 Hz), 7.12 – 7.05 (m, 2H), 7.02 (d, 1H, J = 6.8 Hz), 5.33 (t, 1H, J = 7.2 Hz), 3.57 (d, 2H, J = 7.2 Hz), 2.35 (s, 3H), 0.97 (t, 9H, J = 8.0 Hz), 0.66 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.04, 141.48, 139.48, 137.87, 129.15, 128.31, 127.98, 127.63, 126.61, 125.71, 125.49, 109.90, 32.23, 21.40, 6.71, 5.44.



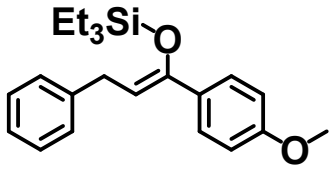
2h

The target compound was obtained as a colorless oil using **GPC, expect the reaction temperature was 40 ºC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 20%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, 2H, J = 8.0 Hz), 7.33 – 7.21 (m, 4H), 7.17 – 7.09 (m, 3H), 5.24 (t, 1H, J = 7.2 Hz), 3.55 (d, 2H, J = 7.2 Hz), 2.34 (s, 3H), 0.96 (t, 9H, J = 8.0 Hz), 0.65 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.05, 139.66, 139.45, 136.35, 130.27, 129.66, 128.13, 127.78, 126.27, 125.57, 108.92, 108.39, 30.20, 19.44, 6.75, 5.43.



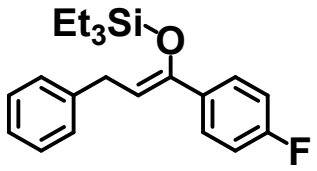
2i

The target compound was obtained as a colorless oil using **GPC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 72%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, 2H, J = 8.4 Hz), 7.33 – 7.23 (m, 4H), 7.22 – 7.14 (m, 1H), 6.84 (d, 2H, J = 8.4 Hz), 5.22 (t, 1H, J = 6.8 Hz), 3.82 (s, 3H), 3.58 (d, 2H, J = 6.8 Hz), 0.96 (t, 9H, J = 8.0 Hz), 0.65 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.19, 149.84, 141.76, 132.10, 128.38, 128.30, 126.94, 125.73, 113.27, 108.18, 55.16, 32.22, 6.74, 5.39.



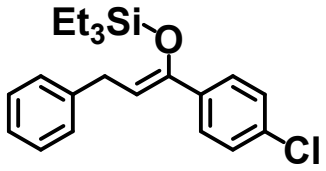
2j

The target compound was obtained as a colorless oil using **GPC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 65%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.42 (m, 2H), 7.33 – 7.25 (m, 4H), 7.20 (t, 1H, J = 6.8 Hz), 6.99 (t, 2H, J = 8.4 Hz), 5.25 (t, 1H, J = 7.2 Hz), 3.58 (d, 2H, J = 7.2 Hz), 0.95 (t, 9H, J = 8.0 Hz), 0.64 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.62, 161.17, 149.25, 141.45, 135.66, 135.63, 128.38, 127.41, 127.34, 125.85, 114.95, 114.74, 109.61, 109.55, 32.26, 6.68, 5.40.



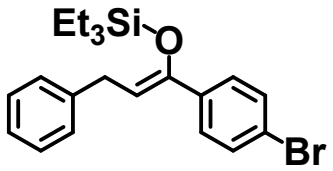
2k

The target compound was obtained as a colorless oil using **GPC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 67%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, 2H, J = 8.4 Hz), 7.34 – 7.24 (m, 6H), 7.21 (t, 1H, J = 7.0 Hz), 5.32 (t, 1H, J = 7.2 Hz), 3.59 (d, 2H, J = 7.2 Hz), 0.96 (t, 9H, J = 8.0 Hz), 0.65 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.08, 141.25, 137.90, 133.29, 128.37, 128.16, 126.89, 125.89, 110.27, 32.26, 6.70, 5.37.



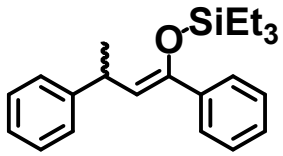
2l

The target compound was obtained as a colorless oil using **GPC, expect the reaction temperature was 40 ºC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 59%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, 2H, J = 8.4 Hz), 7.36 (d, 2H, J = 8.8 Hz), 7.33 – 7.24 (m, 4H), 7.20 (t, 1H, J = 7.0 Hz), 5.32 (t, 1H, J = 7.2 Hz), 3.58 (d, 2H, J = 7.2 Hz), 0.96 (t, 9H, J = 8.0 Hz), 0.65 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.14, 141.22, 138.39, 131.18, 128.57, 128.21, 127.11, 125.65, 121.48, 110.33, 32.29, 6.73, 5.40.



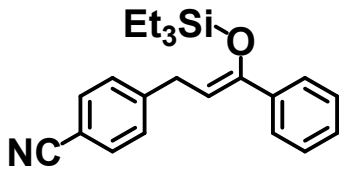
2m

The target compound was obtained as a colorless oil using **GPC, in which the reaction temperature was 60 ºC and the catalyst was 3.0 mol%.**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 6%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, 2H, J = 8.0 Hz), 7.36 – 7.26 (m, 7H), 7.18 (t, 1H, J = 7.2 Hz), 5.29 (dd, 1H, J_1 = 9.6 Hz, J_2 = 1.6 Hz), 4.10 – 3.98 (m, 1H), 1.41 (dd, 3H, J_1 = 6.8 Hz, J_2 = 1.2 Hz) 0.93 (t, 9H, J = 8.0 Hz), 0.60 (qd, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.68, 146.97, 139.65, 128.46, 128.16, 127.78, 127.07, 126.79, 125.80, 116.00, 35.95, 22.62, 6.72, 5.38.



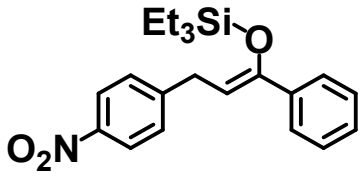
2n

The target compound was obtained as a colorless oil using **GPC, expect the reaction temperature was 60 ºC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 40%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, 2H, J = 6.8 Hz), 7.47 (d, 2H, J = 6.8 Hz), 7.39 – 7.27 (m, 5H), 5.23 (t, 1H, J = 7.2 Hz), 3.62 (d, 2H, J = 7.2 Hz), 0.93 (t, 9H, J = 8.0 Hz), 0.61 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.44, 147.27, 138.94, 132.17, 132.04, 129.19, 129.00, 128.09, 127.93, 125.81, 125.65, 119.10, 109.60, 107.58, 107.38, 32.24, 6.62, 5.32.



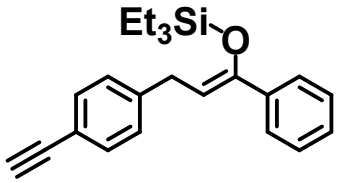
2o

The target compound was obtained as a pale yellow oil using **GPC, expect the reaction temperature was 60 ºC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 45%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, 2H, J = 8.8 Hz), 7.48 (d, 2H, J = 6.8 Hz), 7.41 (d, 2H, J = 8.8 Hz), 7.35 – 7.27 (m, 3H), 5.25 (t, 1H, J = 7.2 Hz), 3.67 (d, 2H, J = 7.2 Hz), 0.93 (t, 9H, J = 8.0 Hz), 0.61 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.63, 149.51, 146.29, 138.93, 128.95, 127.90, 125.89, 125.68, 123.48, 107.18, 32.04, 6.64, 5.35.



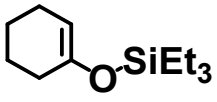
2p

The target compound was obtained as a colorless oil using **GPC, expect the reaction temperature was 40 ºC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 57%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, 2H, J = 8.0 Hz), 7.42 (d, 2H, J = 8.0 Hz), 7.34 – 7.27 (m, 3H), 7.22 (d, 2H, J = 7.6 Hz), 5.27 (t, 1H, J = 7.2 Hz), 3.58 (d, 2H, J = 7.2 Hz), 3.03 (s, 1H), 0.94 (t, 9H, J = 8.0 Hz), 0.62 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.69, 142.58, 139.28, 132.19, 128.30, 128.07, 127.83, 125.76, 119.49, 108.70, 83.84, 76.44, 32.12, 6.68, 5.39.



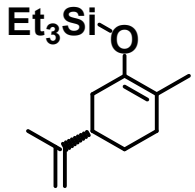
2q

The target compound was obtained as a colorless oil using **GPC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 85%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.88 – 4.85 (m, 1H), 2.05 – 1.95 (m, 4H), 1.69 – 1.61 (m, 2H), 1.54 – 1.46 (m, 2H), 0.97 (t, 9H, J = 8.0 Hz), 0.65 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.39, 104.22, 29.84, 23.82, 23.20, 22.35, 6.59, 5.05.



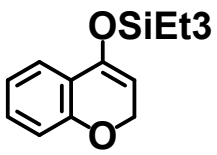
2r

The target compound was obtained as a colorless oil using **GPC, expect the reaction temperature was 40 ºC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 77%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.75 – 4.69 (m, 2H), 2.28 – 2.17 (m, 1H), 2.13 – 1.90 (m, 4H), 1.78 – 1.69 (m, obstructed, 1H), 1.74 (s, 3H), 1.59 (s, 3H), 1.44 – 1.31 (m, 1H), 0.99 (t, 9H, J = 8.0 Hz), 0.66 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.40, 142.37, 110.90, 108.63, 42.63, 35.52, 30.15, 28.34, 20.90, 15.82, 6.96, 5.62.



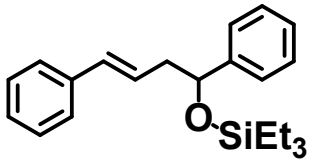
2s

The target compound was obtained as a colorless oil using **GPC, expect the reaction temperature was 60 ºC**. (Note: The chromatographic column is filled with neutral alumina!) All the spectral data were in agreement with the data previously reported in the literature.

Yield: 38%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (dd, 1H, J_1 = 7.6 Hz, J_2 = 1.6 Hz), 7.13 (td, 1H, J_1 = 7.6 Hz, J_2 = 1.6 Hz), 6.90 (td, 1H, J_1 = 7.6 Hz, J_2 = 0.8 Hz), 6.78 (d, 1H, J = 7.6 Hz), 4.89 (t, 1H, J = 7.6 Hz), 4.83 (d, 2H, J = 7.6 Hz), 1.02 (t, 9H, J = 8.0 Hz), 0.77 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.62, 145.97, 129.46, 122.41, 122.29, 120.85, 115.37, 97.50, 65.75, 6.65, 4.96.



2t

The target compound was obtained as a colorless oil using **GPC, expect the reaction temperature was 40 ºC**. All the spectral data were in agreement with the data previously reported in the literature.

Yield: 33%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.16 (m, 10H), 6.38 (d, 1H, J = 15.6 Hz), 6.27 – 6.14 (m, 1H), 4.75 (t, 1H, J = 6.4 Hz), 2.70 – 2.49 (m, 2H), 0.88 (t, 9H, J = 16.0 Hz), 0.54 (q, 6H, J = 16.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.12, 137.70, 132.02, 128.41, 128.02, 127.03, 126.88, 125.97, 125.85, 75.10, 44.64, 6.76, 4.82.

5. Mechanistic Control Experiments with Deuterosilane

Preparation of Deuterated Triethylsilane (Et_3SiD)[21]

A dry Et_2O (3 mL) solution of chlorotriethylsilane (2.2 mL, 13.1 mmol, 1.0 equiv.) was added dropwise to a suspension of anhydrous Et_2O (10 mL) of $LiAlD_4$ (0.44 g, 10.5 mmol, 0.8 equiv.) at 0 °C. After dropwise addition, the solution was heated to reflux for 24 h. After cooling to room temperature, the system was carefully quenched with water (5 mL) and aqueous HCl solution (2 N, 10 mL) at 0 °C. The organic phase was separated, and the aqueous layer was extracted with Et_2O (3 × 10 mL). The combined organic phases were dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The residue was purified by vacuum distillation (360 mbar/100 °C) to give the colorless liquid Et_3SiD (0.61g, 40%).

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.97 (t, 9H, J = 8.0 Hz), 0.58 (q, 6H, J = 8.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$): δ 8.13, 2.37.

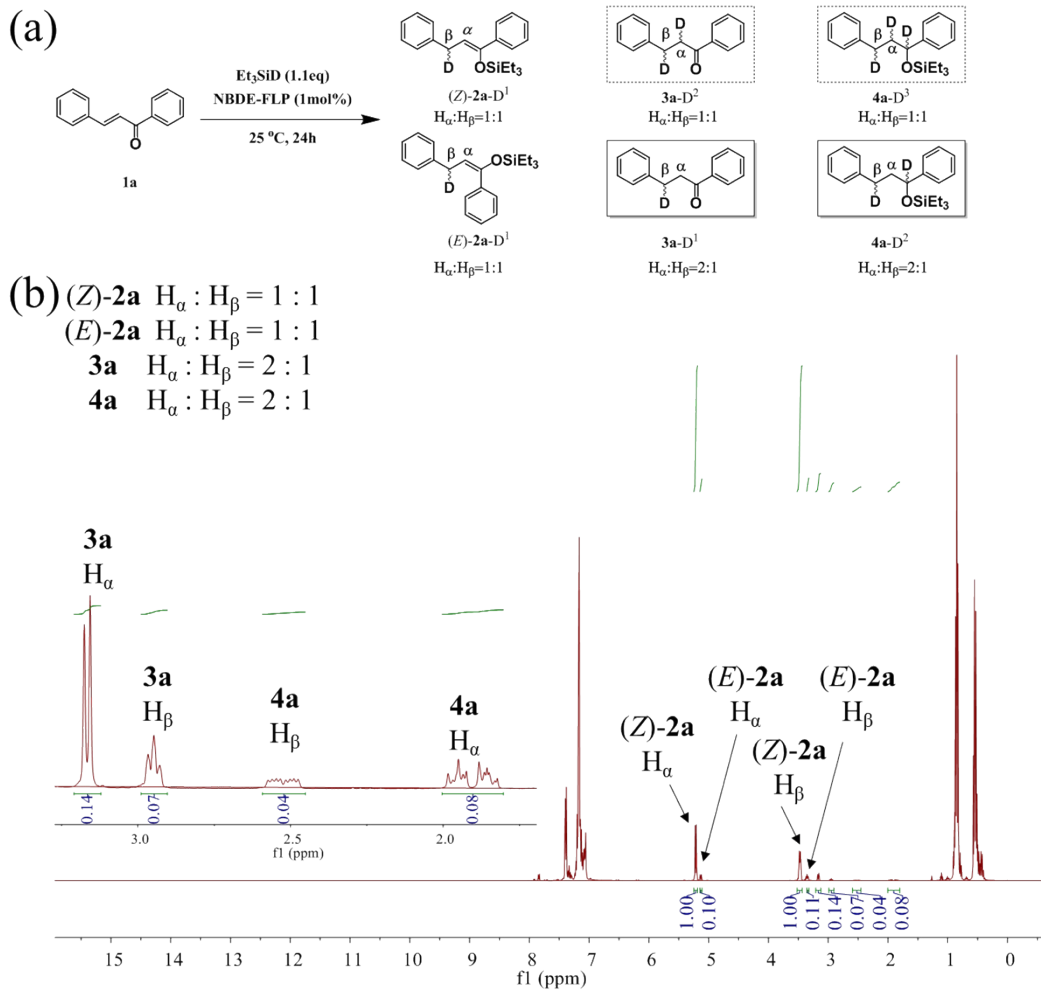


Figure S25. ^{1}H NMR of the mixture after the reaction was completed according to

GPB, using Et_3SiD as reducing agent.

Preparation of Deuterium-Labeled $PhSiH_3$[22]

Trichlorophenylsilane (2.5 mL, 15.61 mmol) was added slowly to a suspension of $LiAlD_4$ (1.2 g, 31.22 mmol) in dry Et_2O (100 mL) at 0 °C. After dropwise addition, the reaction mixture was refluxed for 24 h. The solvent was evacuated and $PhSiD_3$ was distilled into a cold trap to give $PhSiD_3$ as a colorless oil (1.1 g, 65%).

^1H NMR (400 MHz, $CDCl_3$): δ 7.66–7.60 (m, 2H) and 7.48–7.36 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 135.84, 129.80, 128.10.

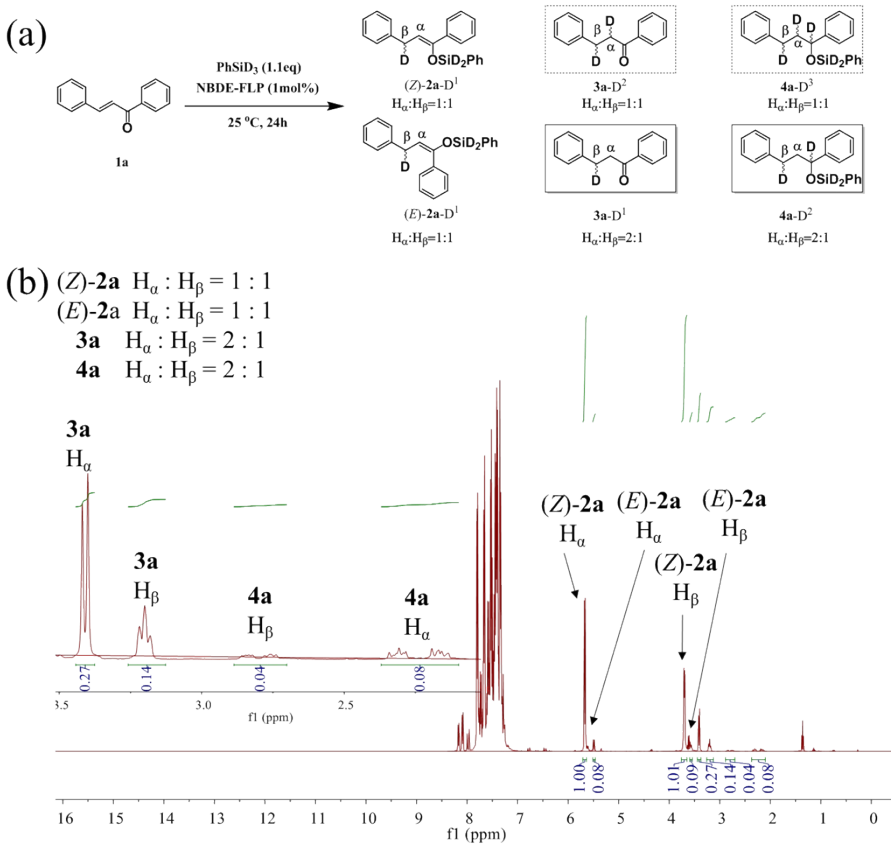


Figure S26. ^1H NMR of the mixture after the reaction was completed according to GPB, using $PhSiD_3$ as reducing agent.

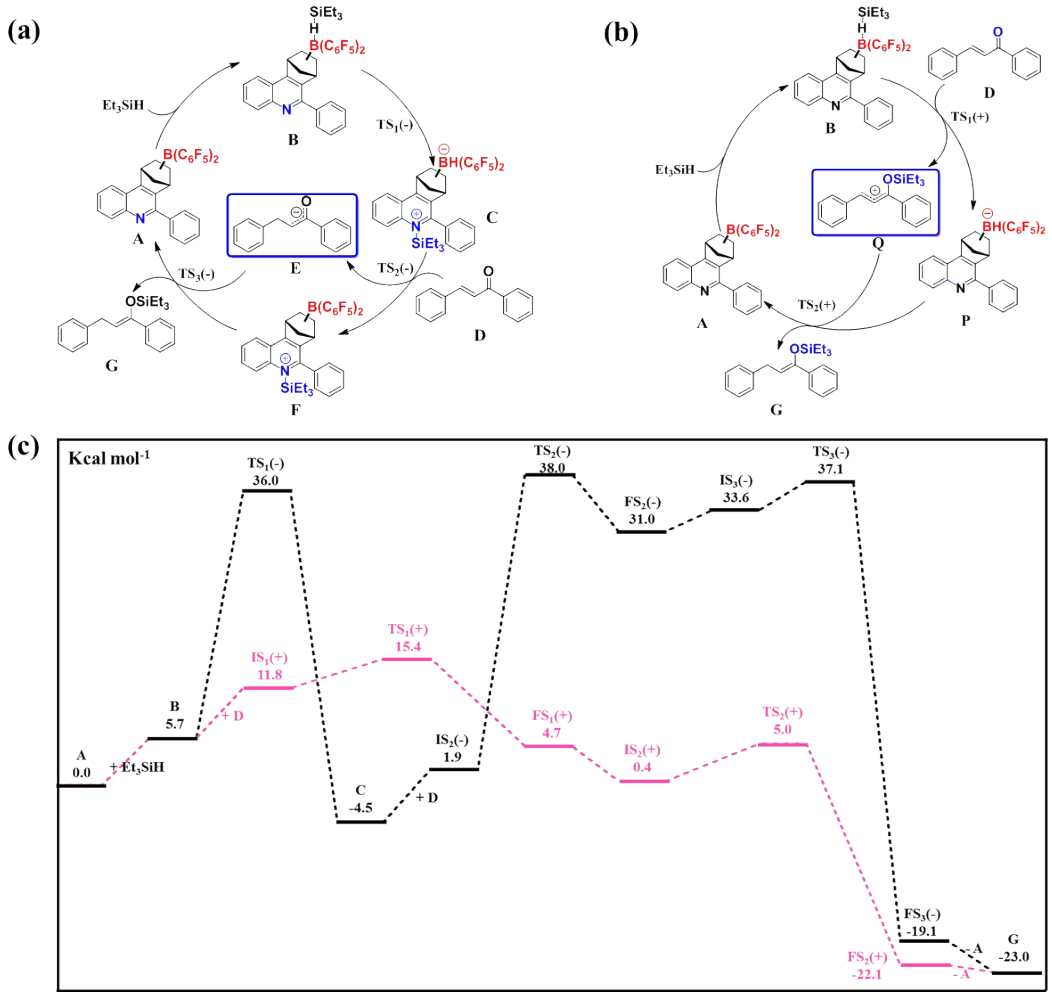


Figure S27. Possible mechanism of NBDE-FLP for the 1,4-hydrosilylation of *α,β*-unsaturated ketone *via* (a) enolate anion intermediate and (b) allylic cation intermediate. (c) energy profile of two possible mechanism.

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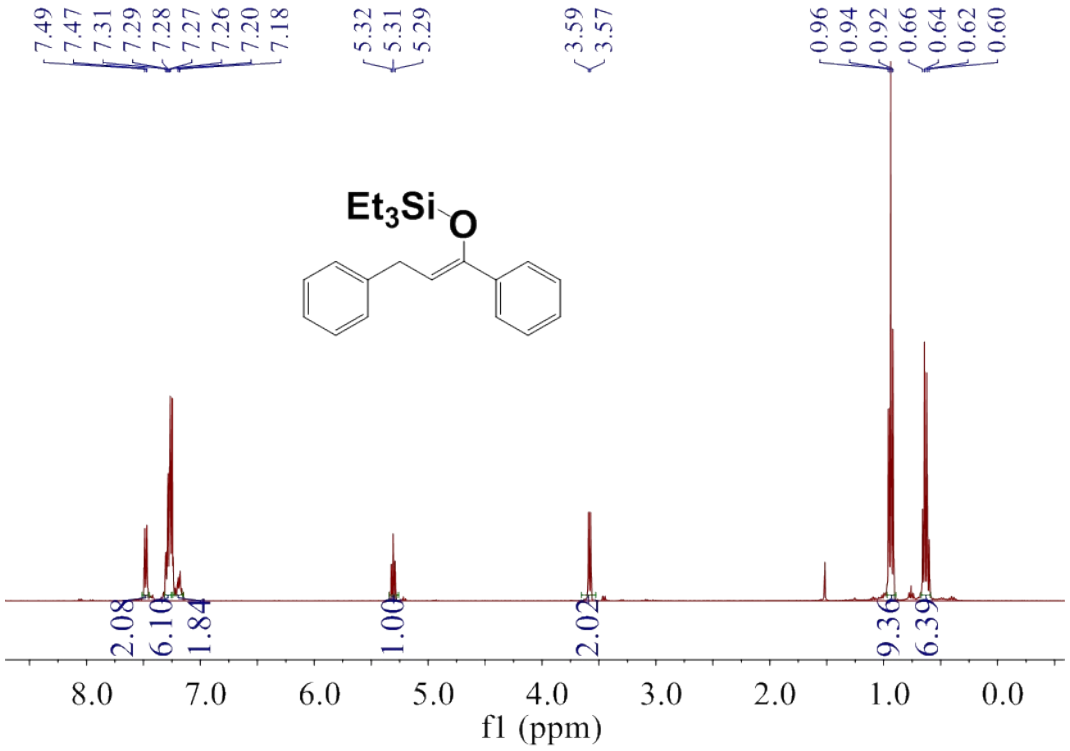
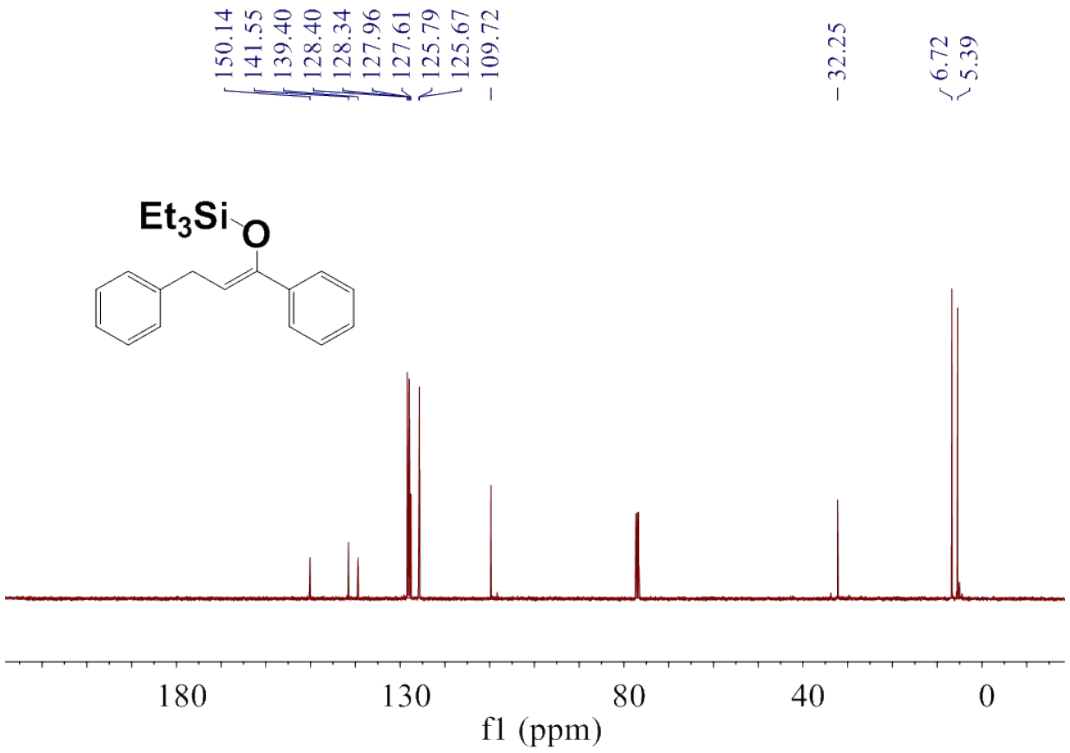
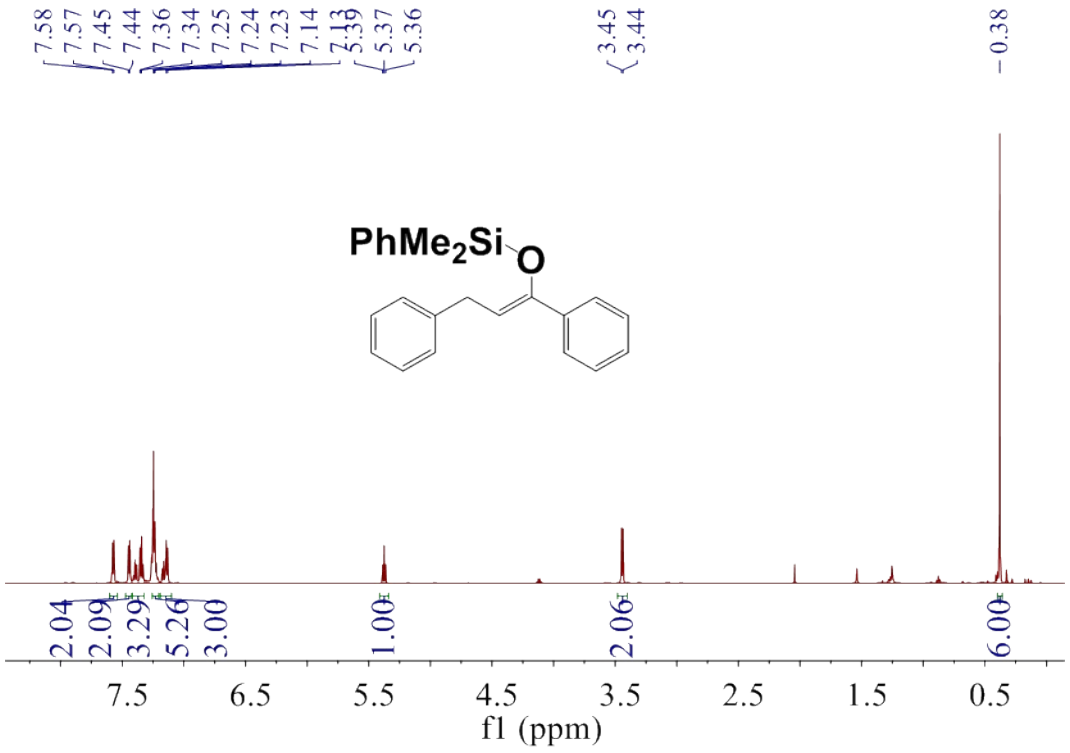
7. ^{1}H NMR and ^{13}C NMR spectra for the products



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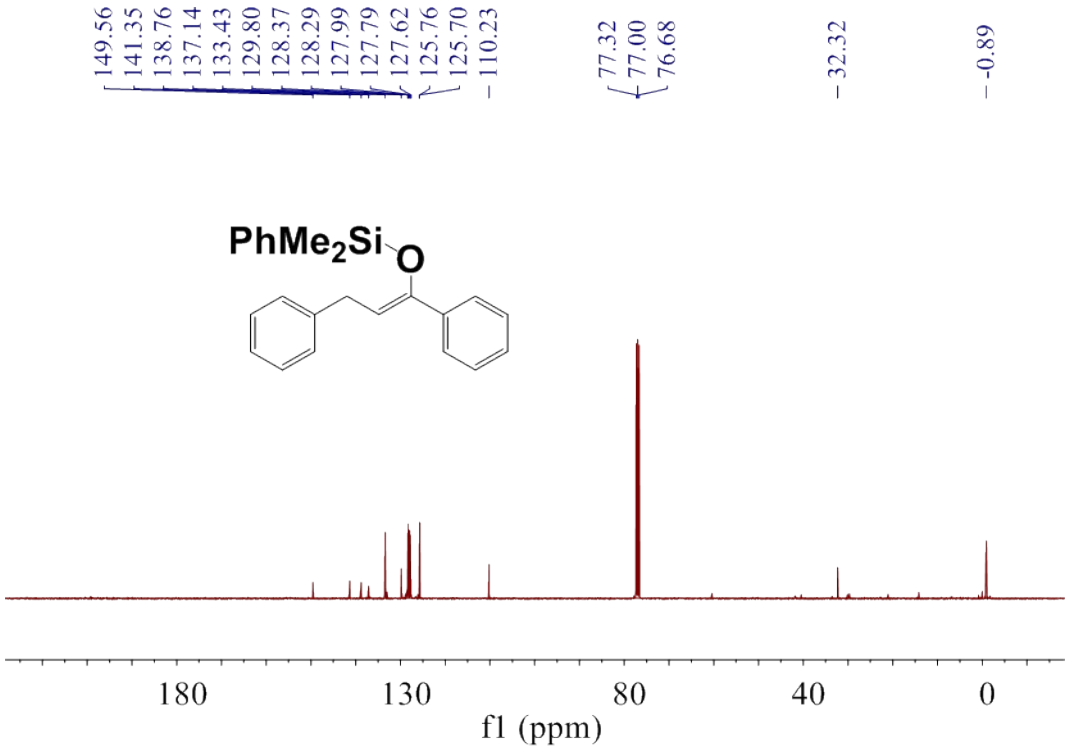
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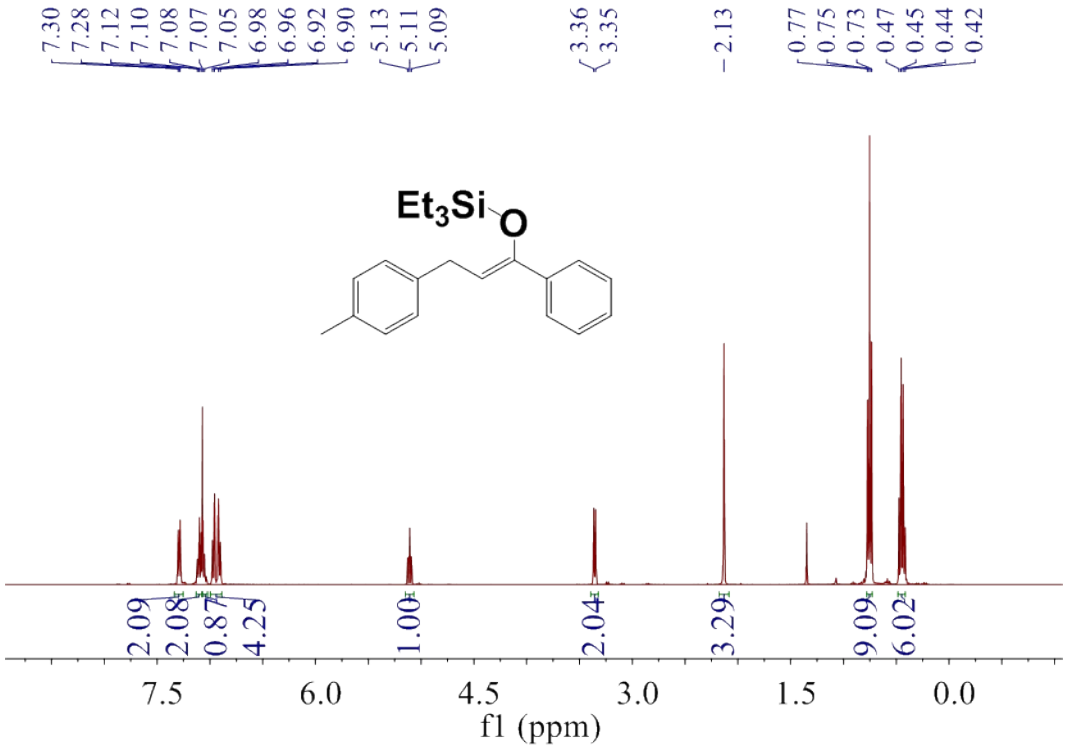
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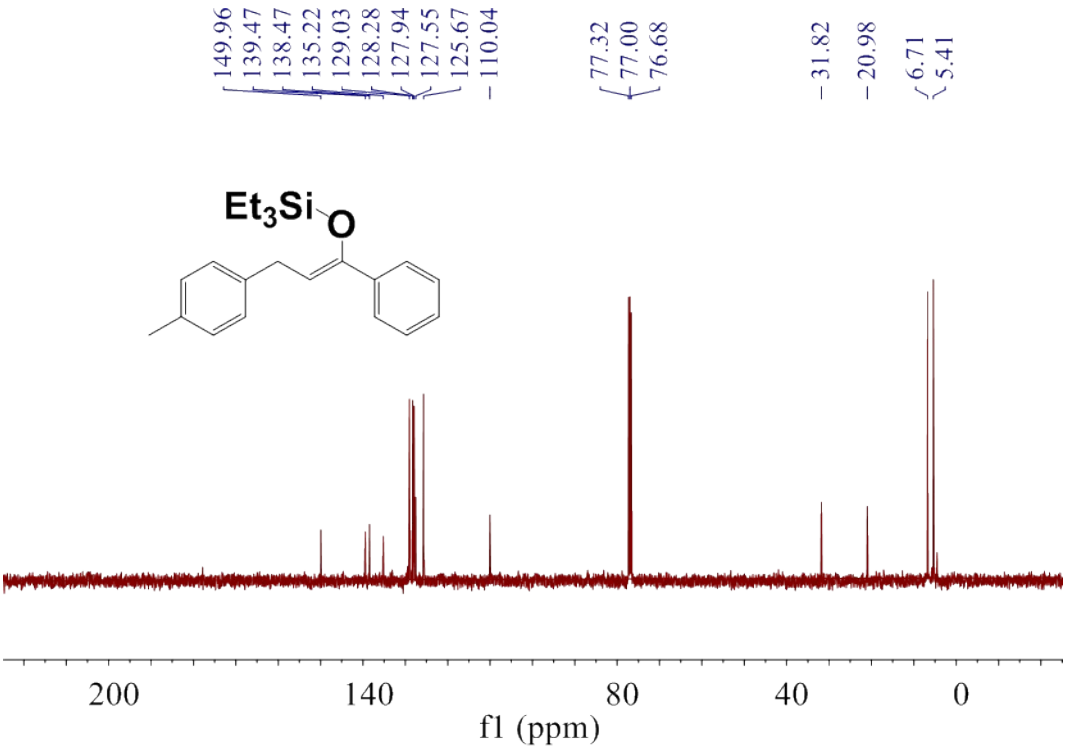
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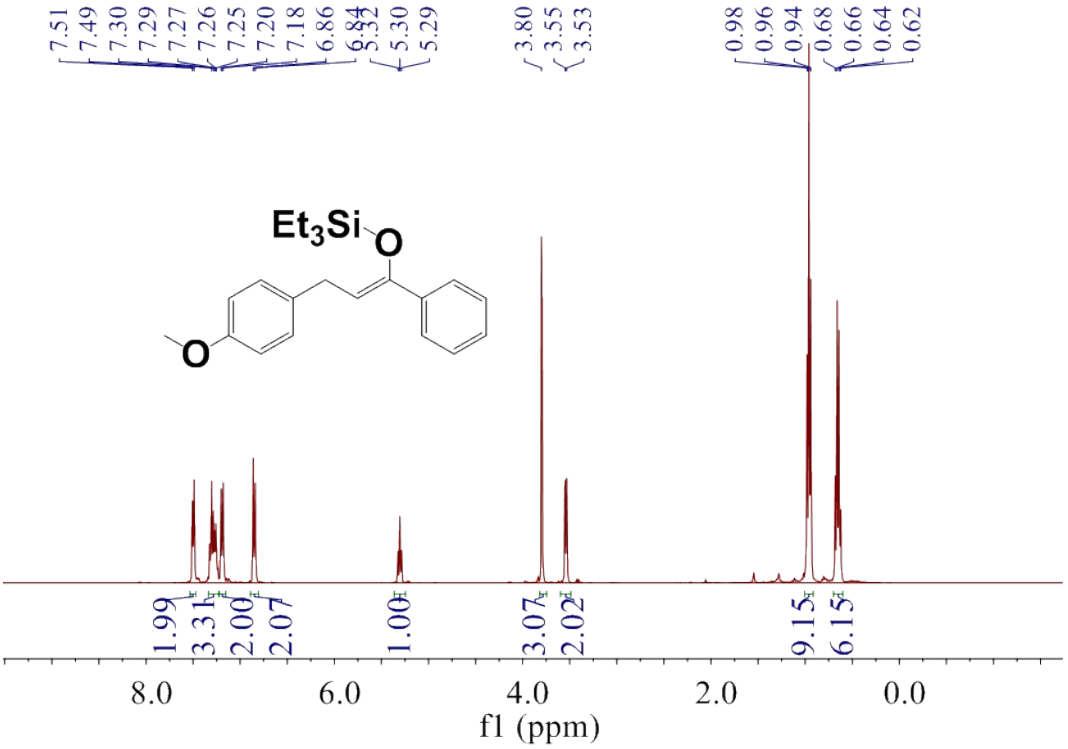
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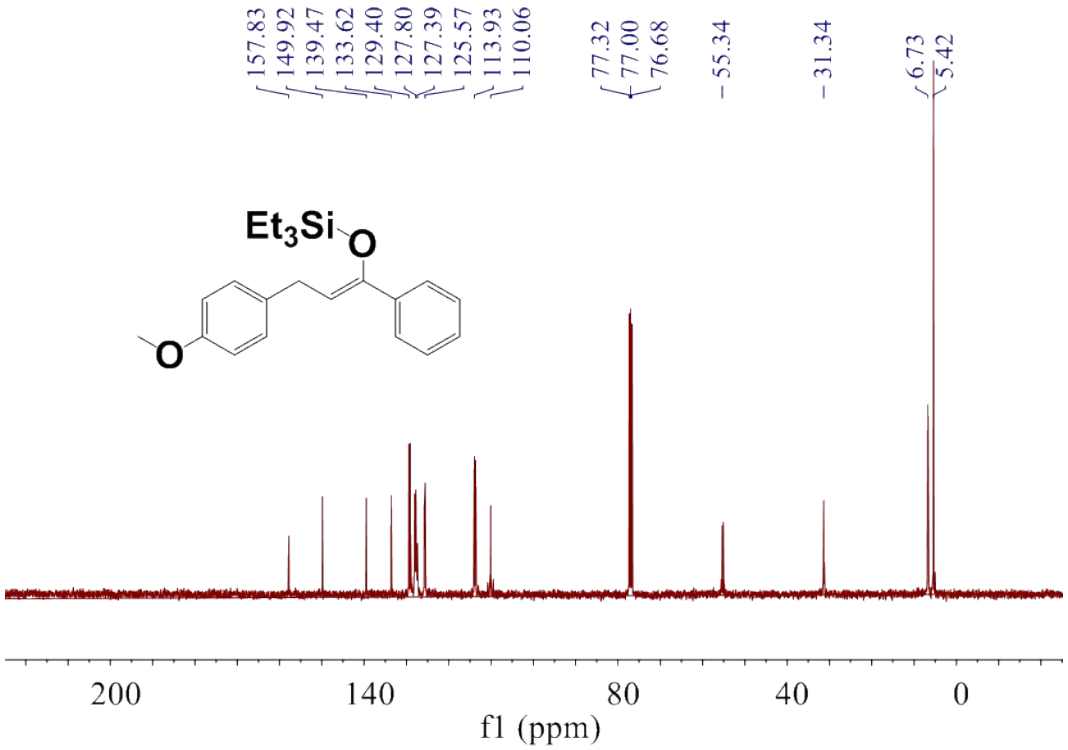
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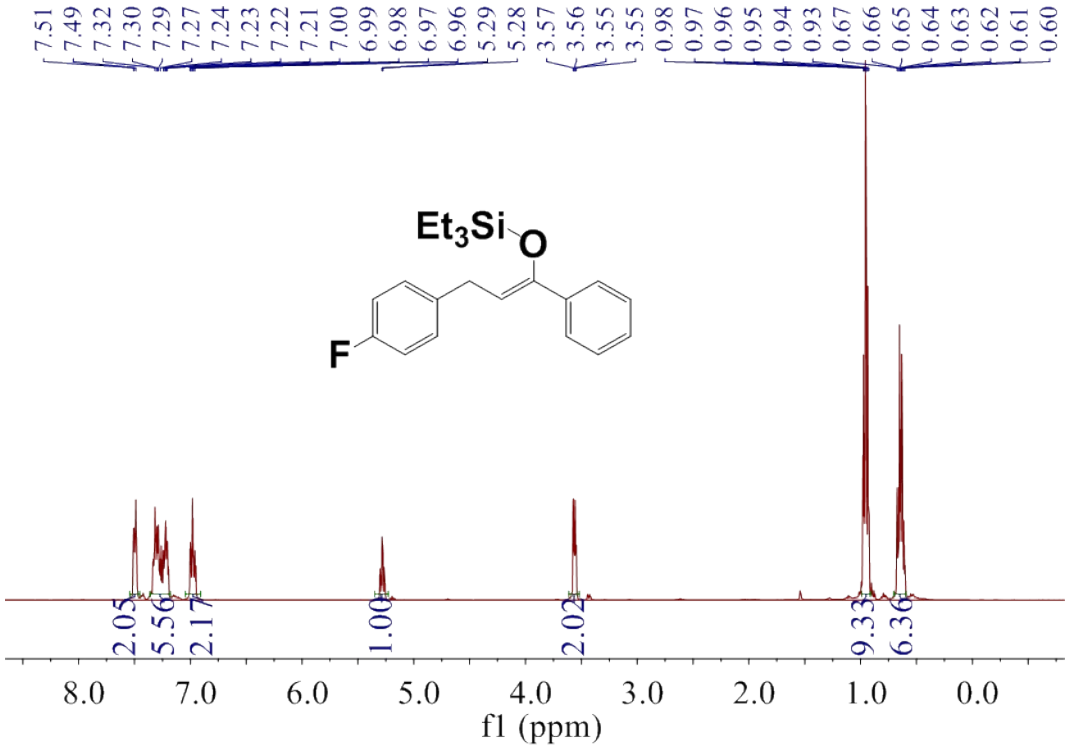
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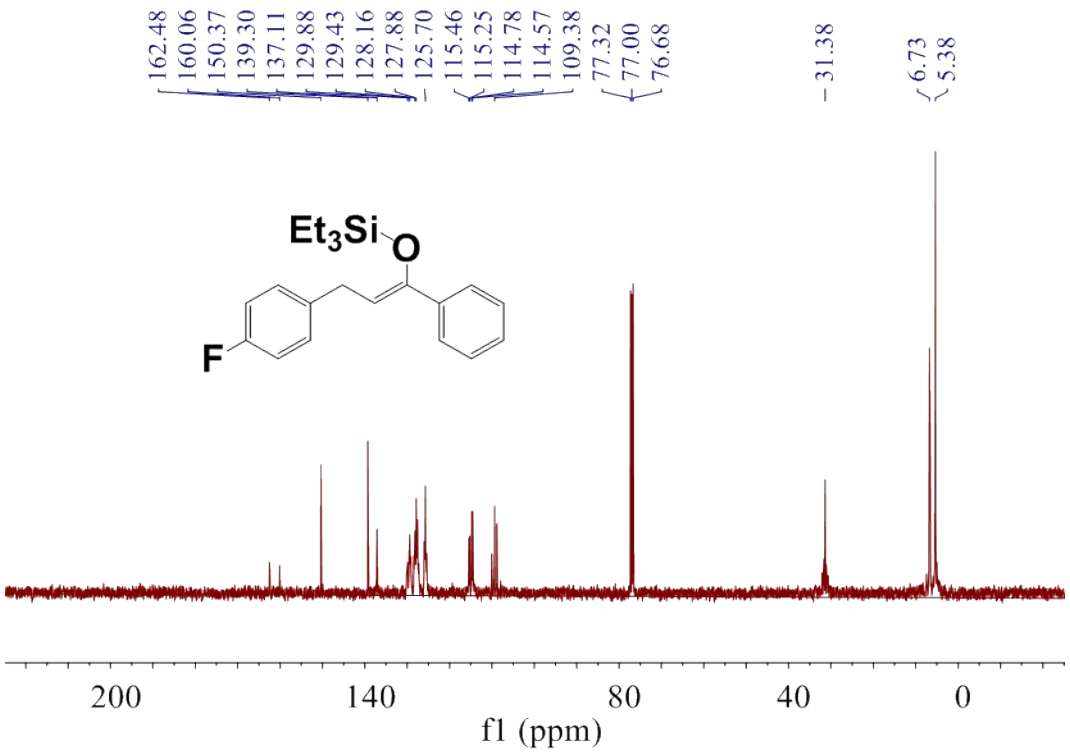
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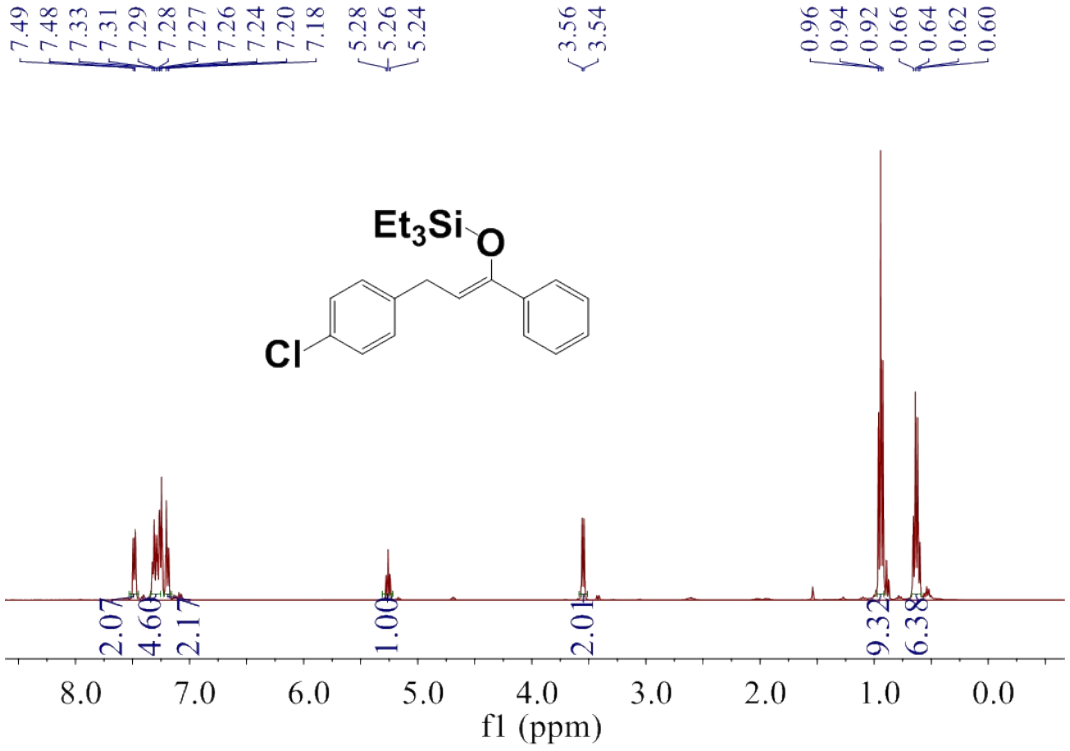
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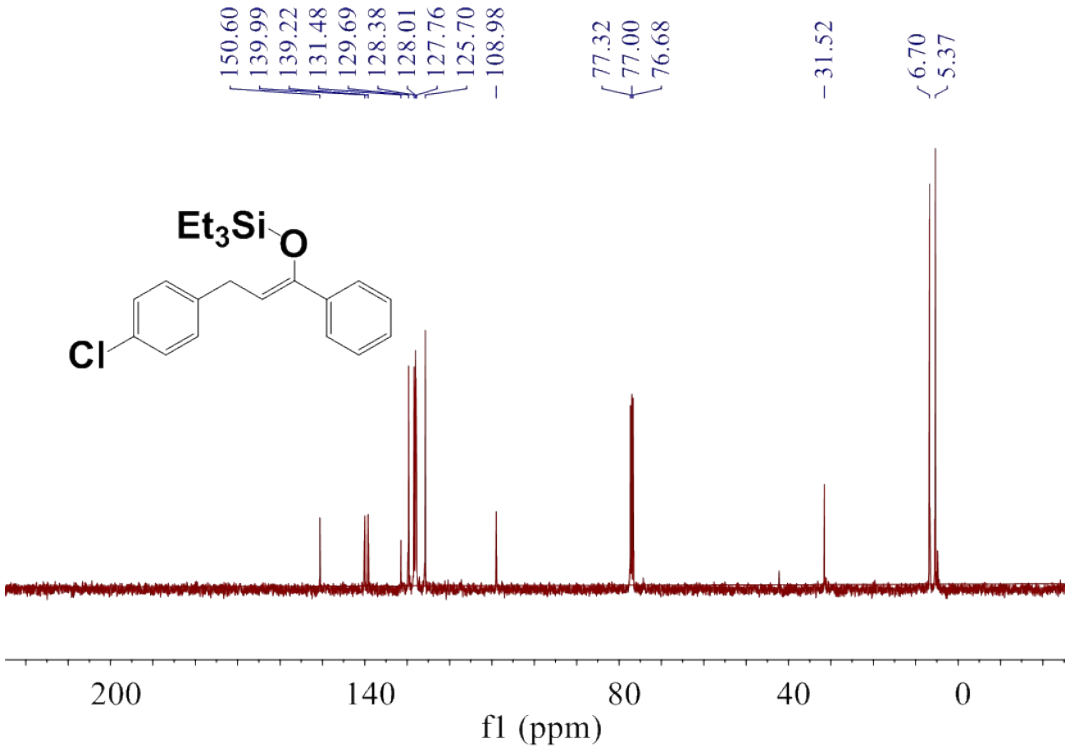
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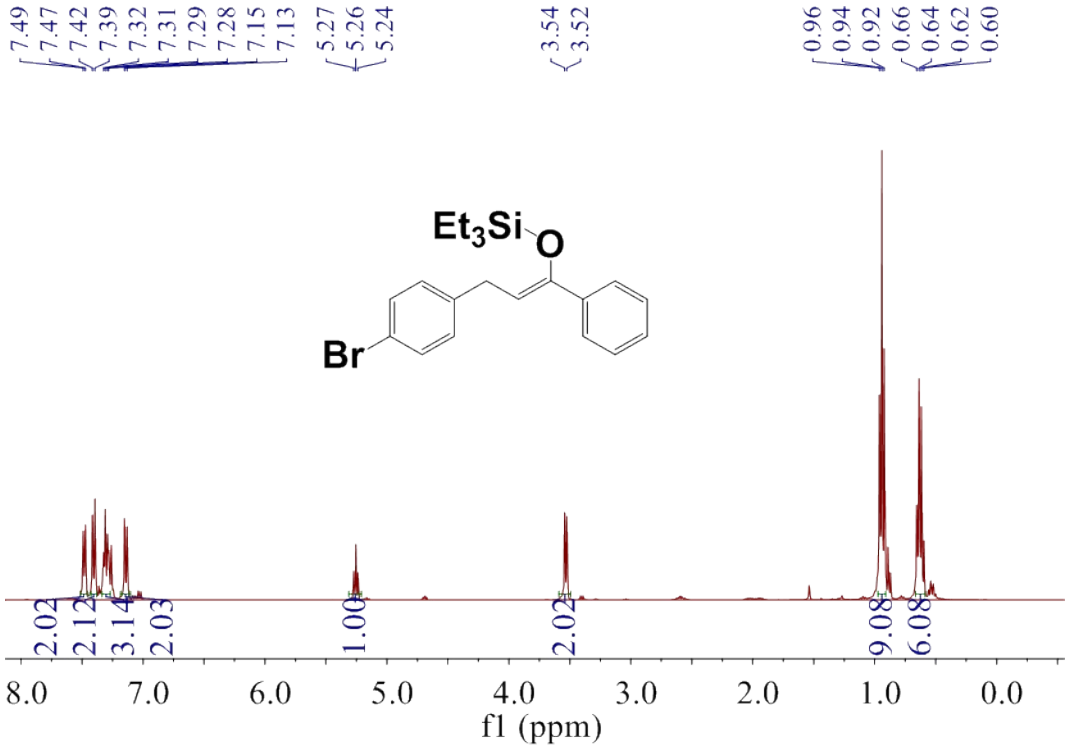
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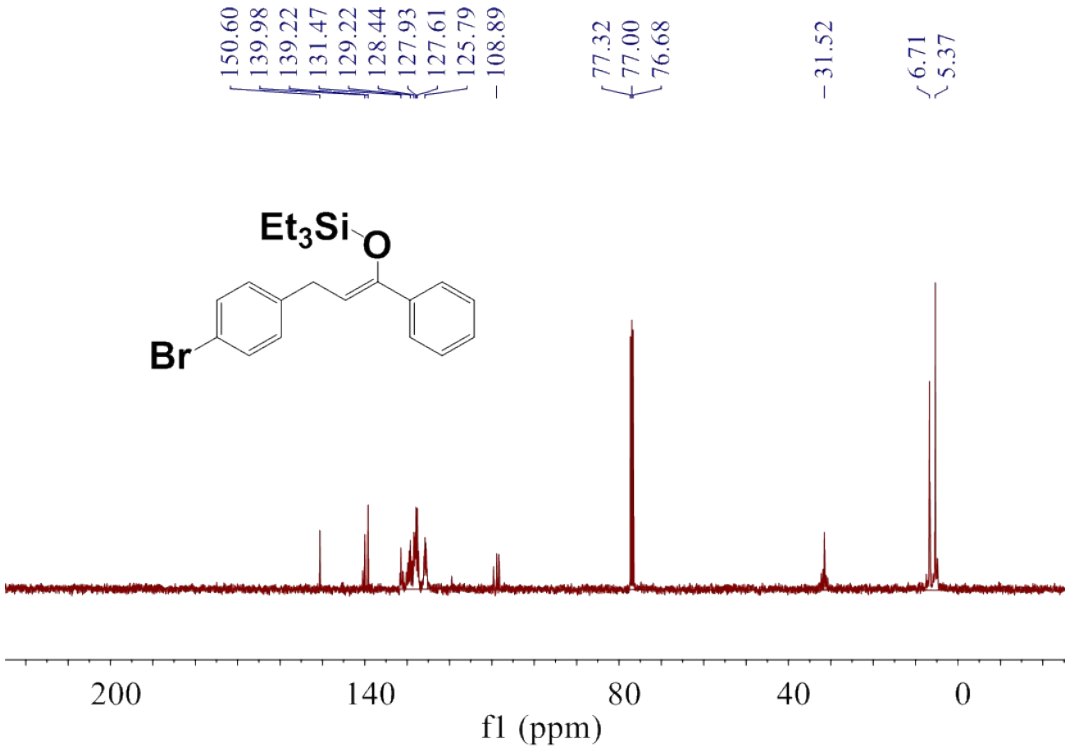
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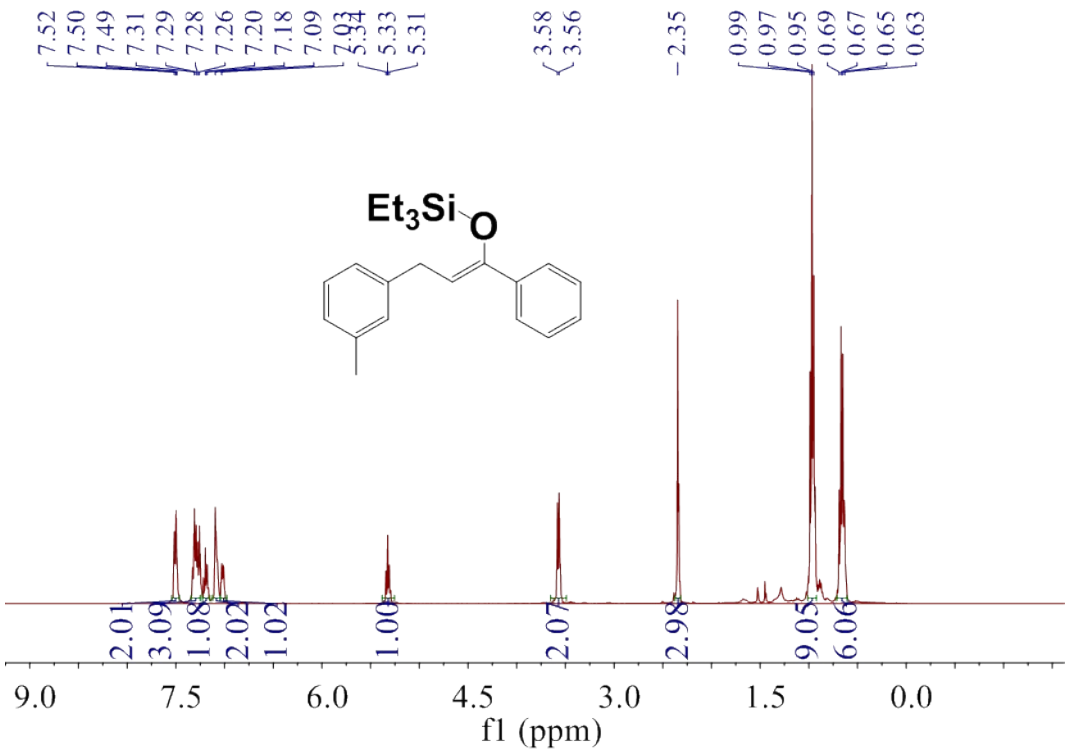
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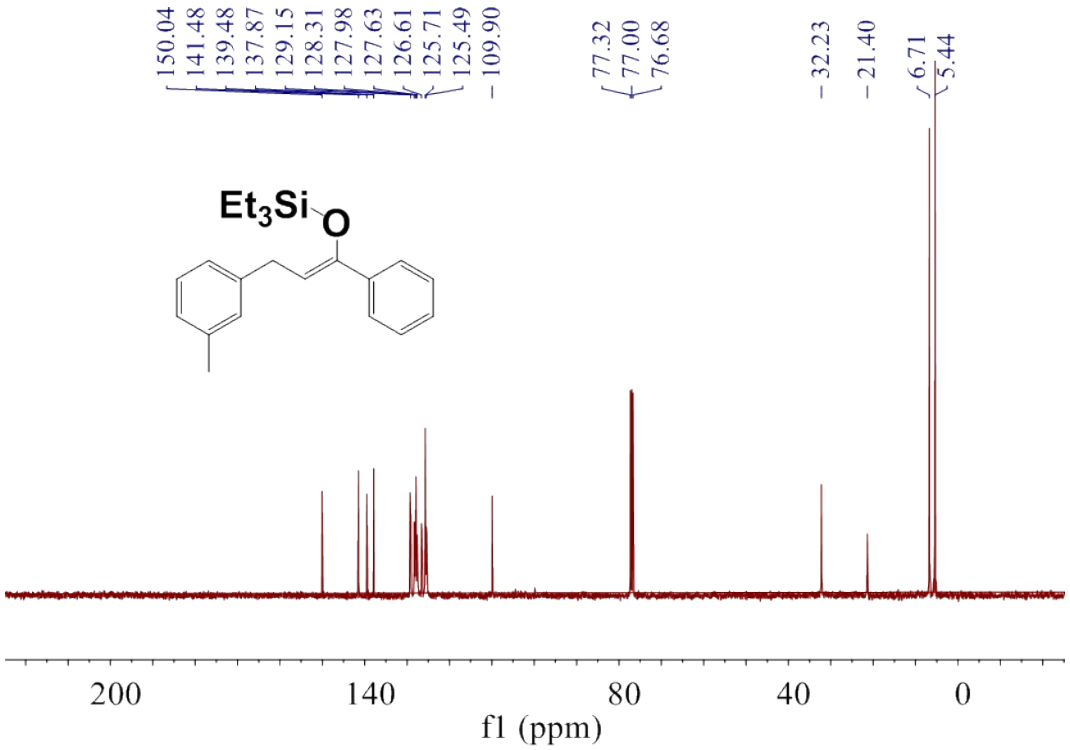
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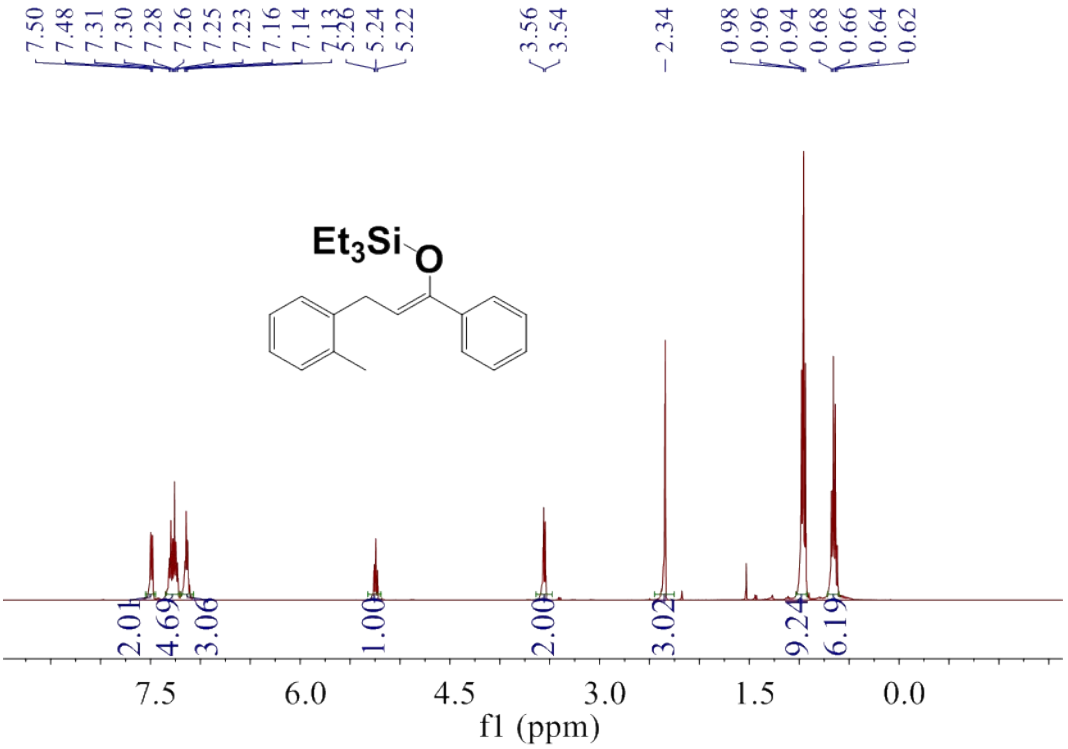
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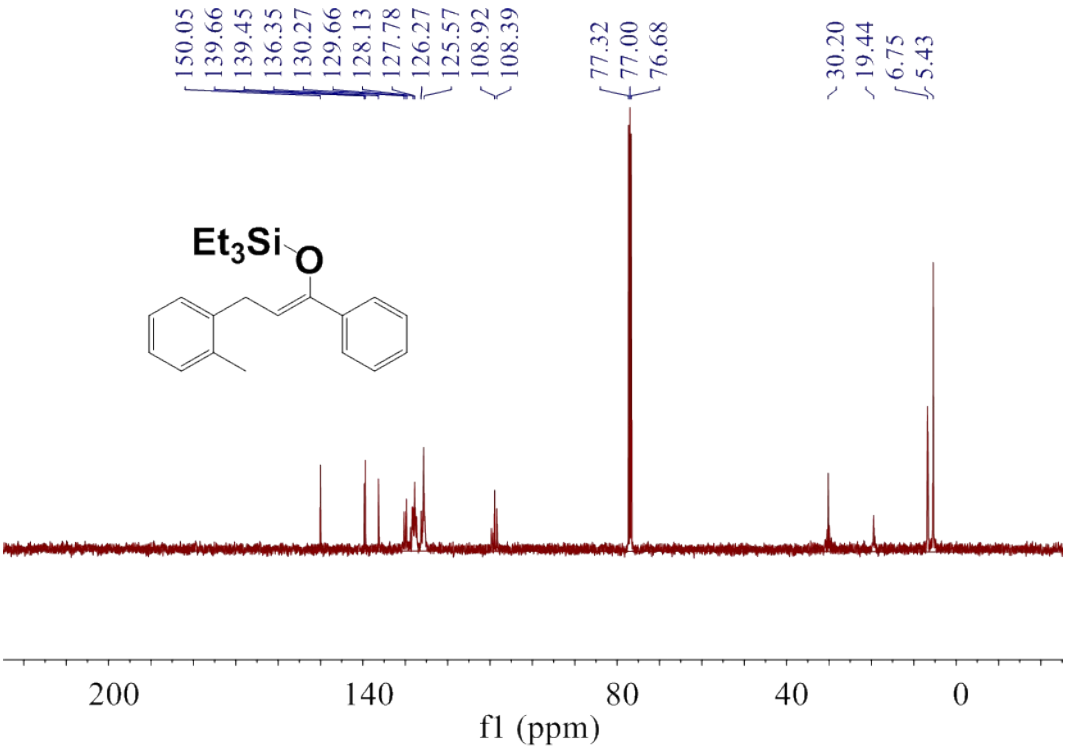
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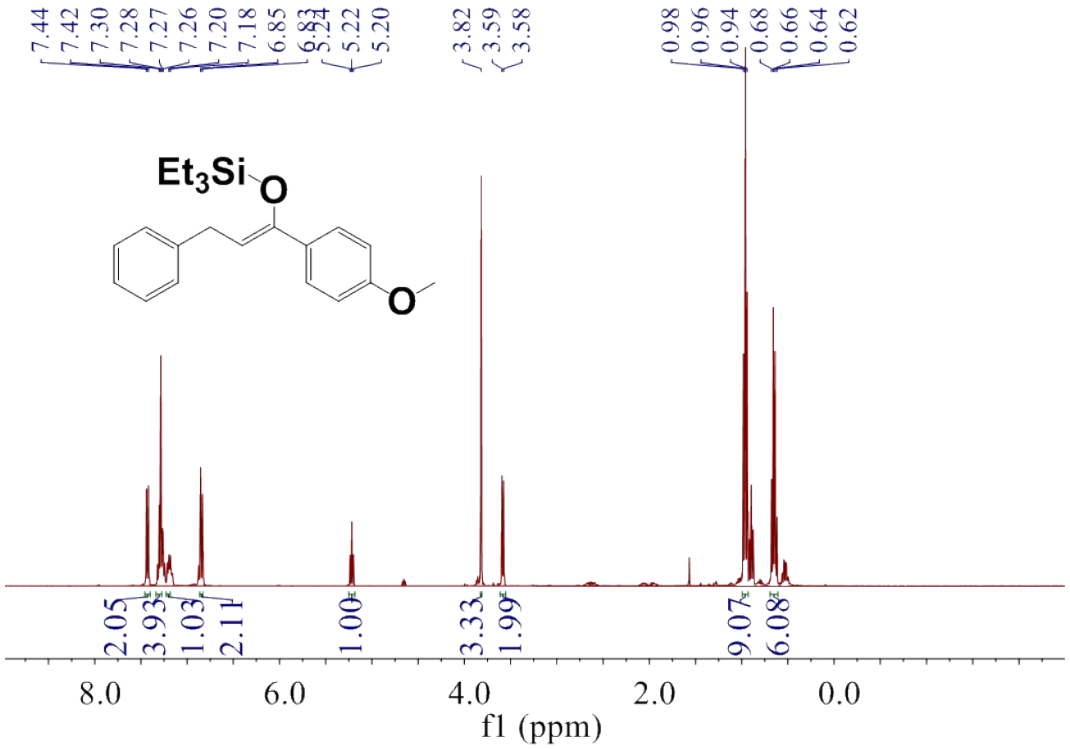
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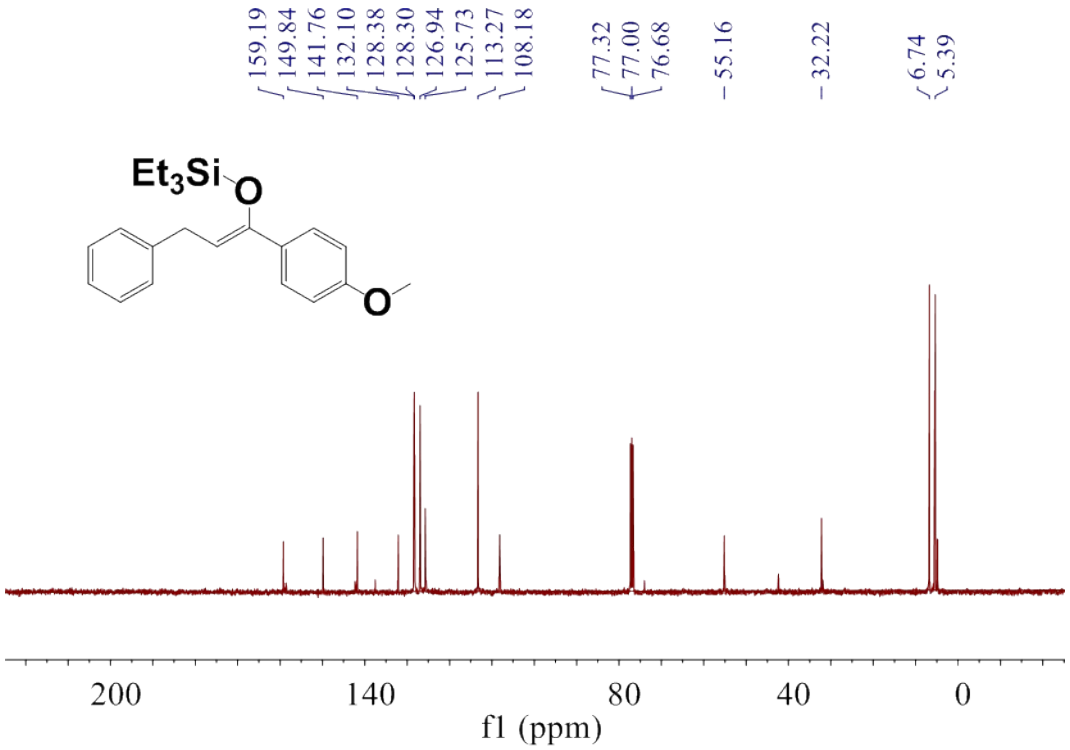
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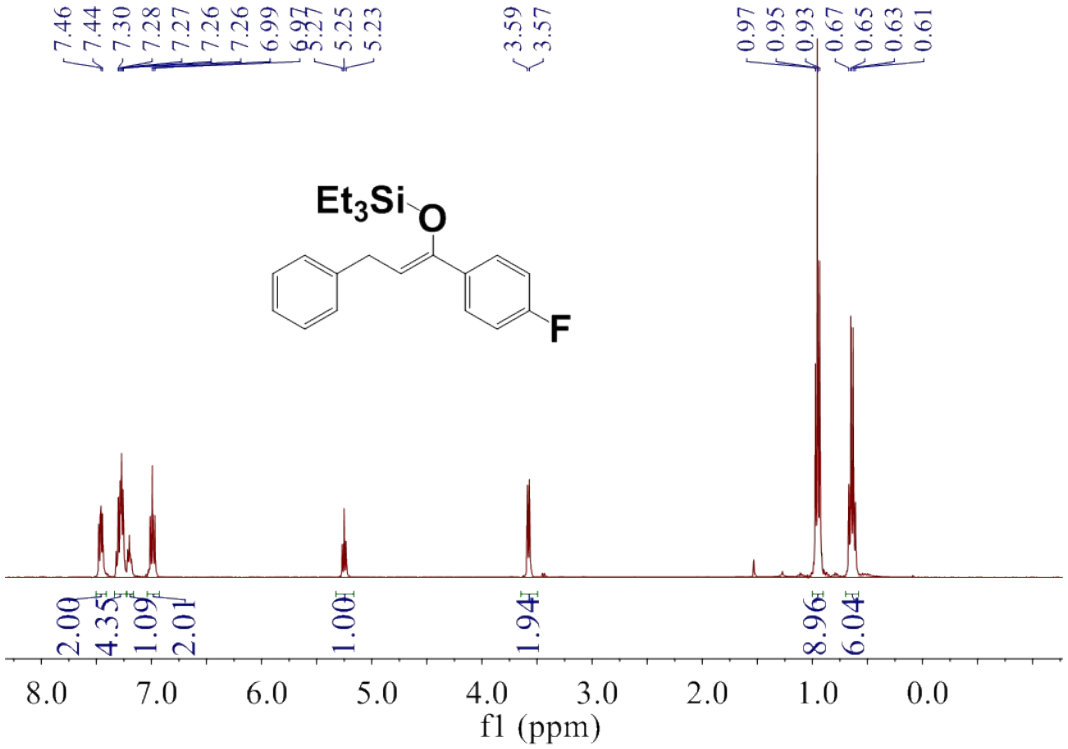
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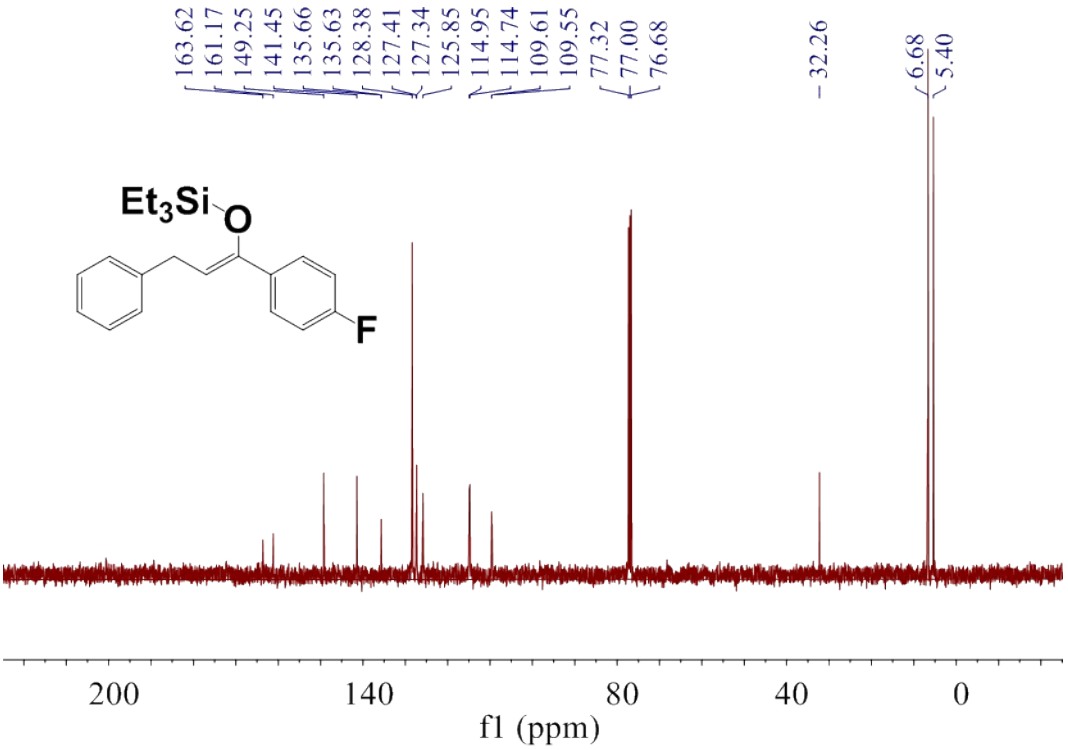
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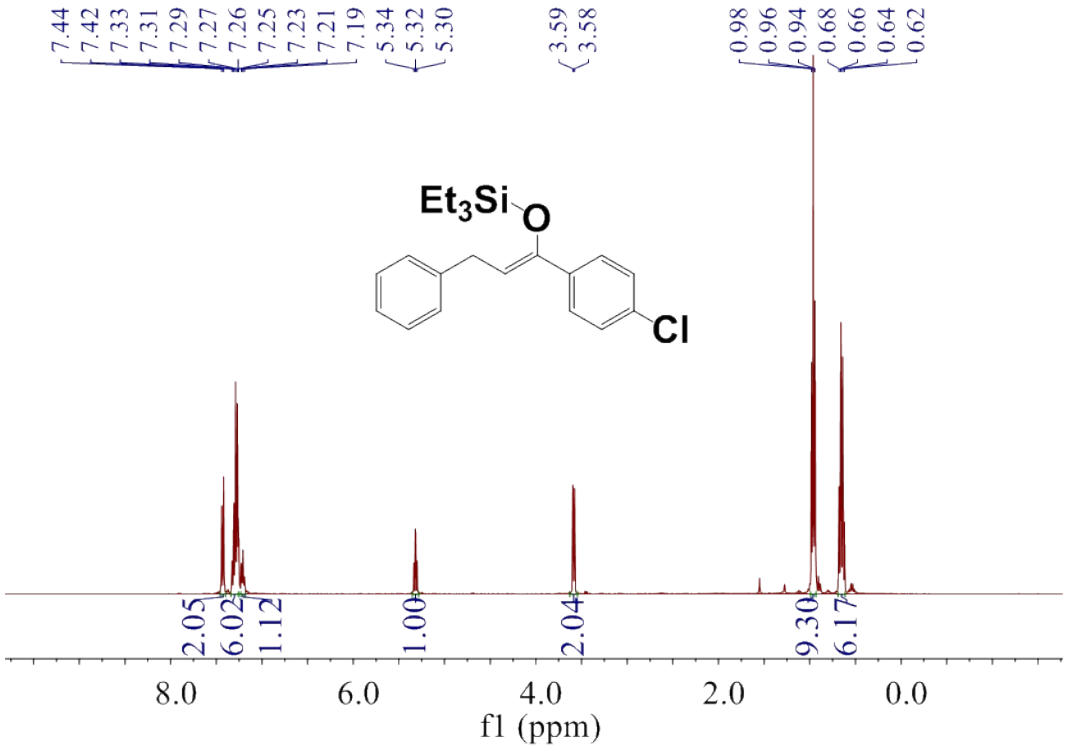
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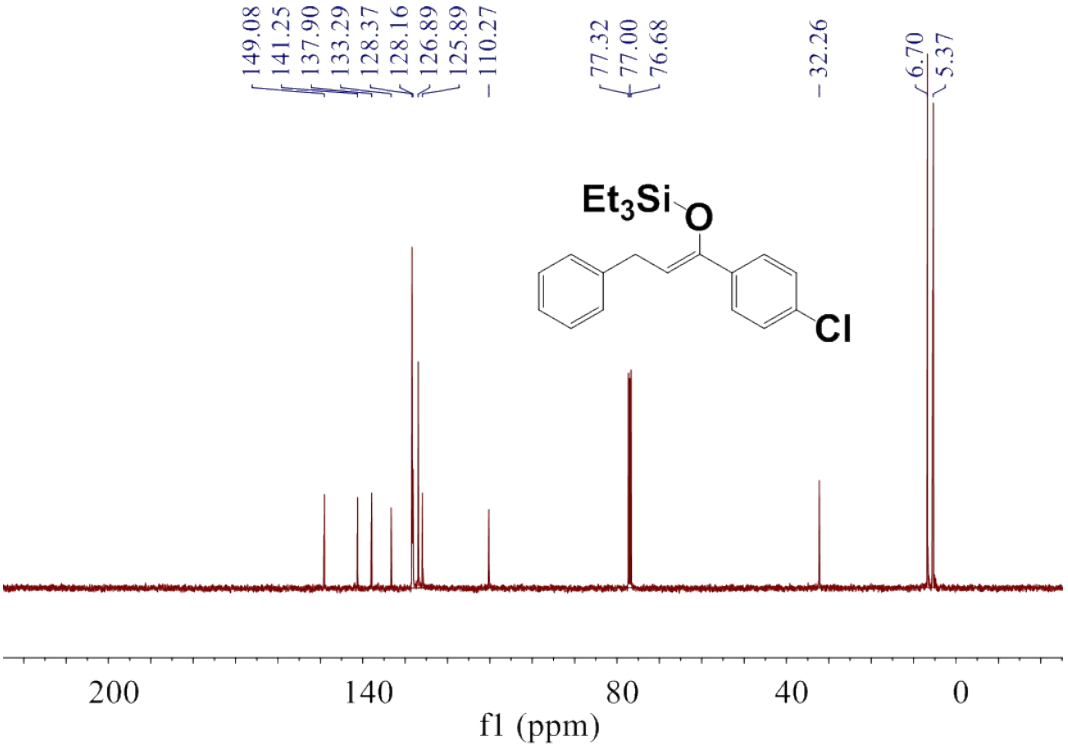
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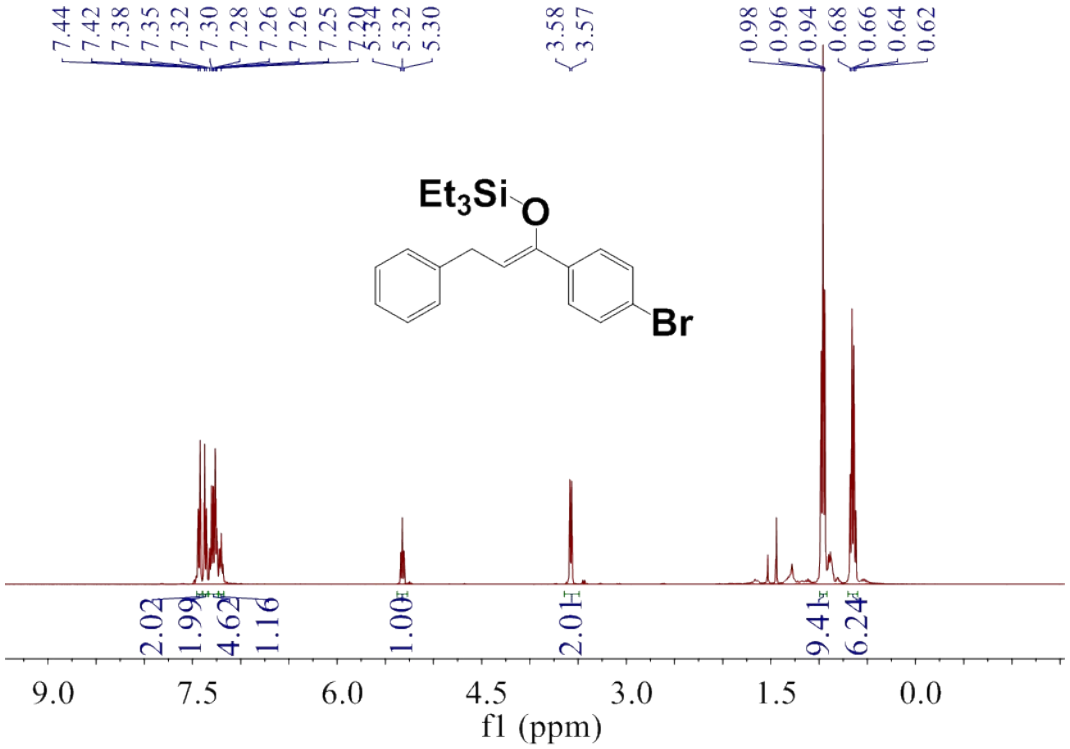
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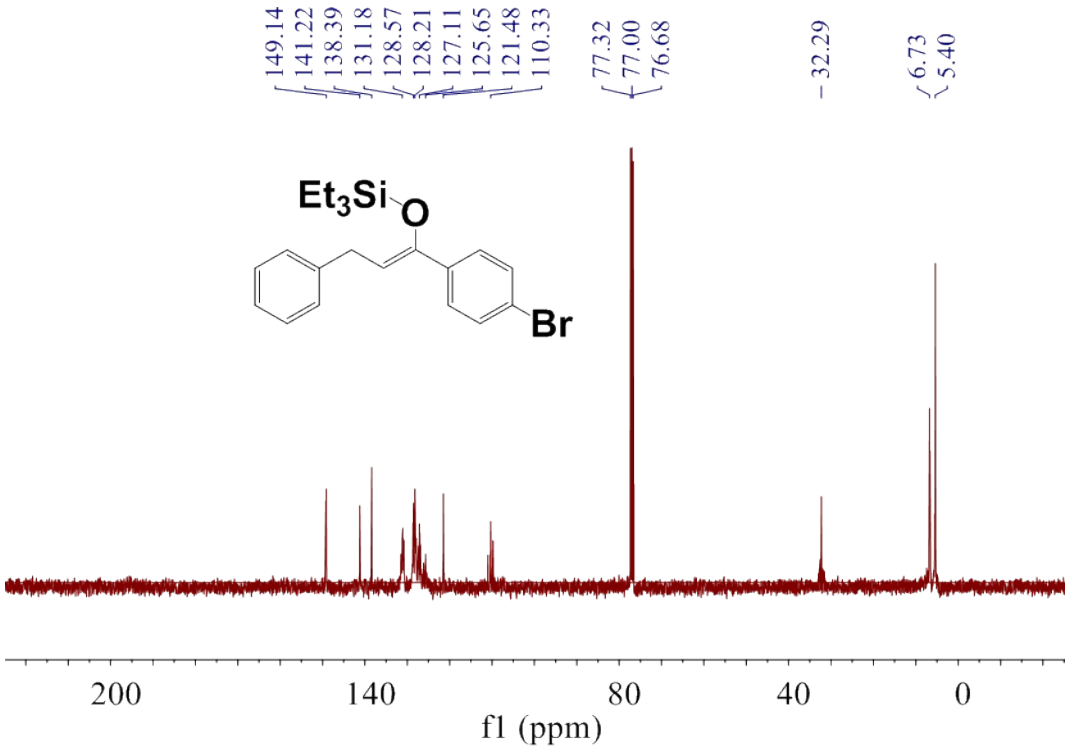
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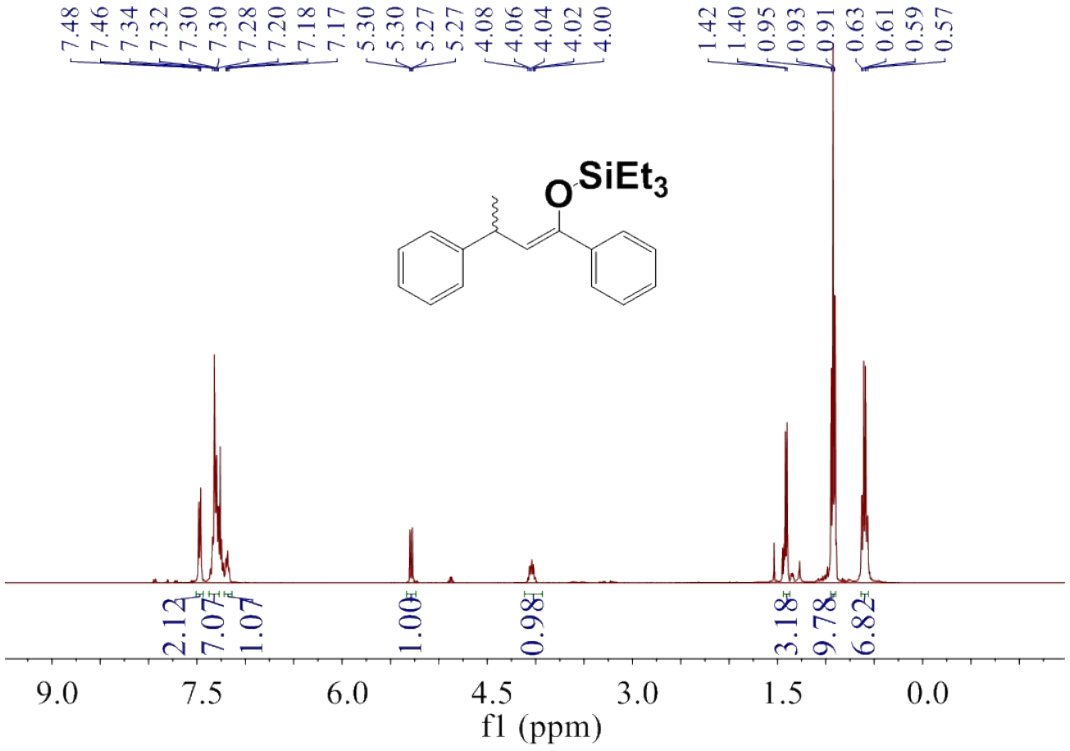
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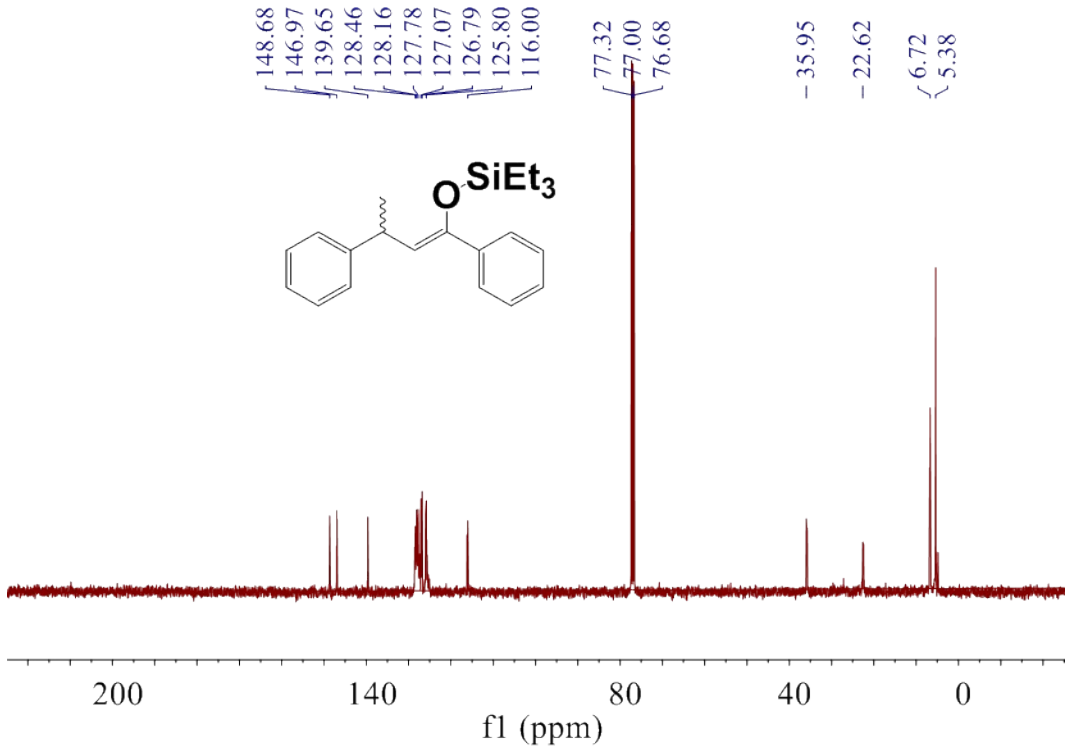
f1 (ppm)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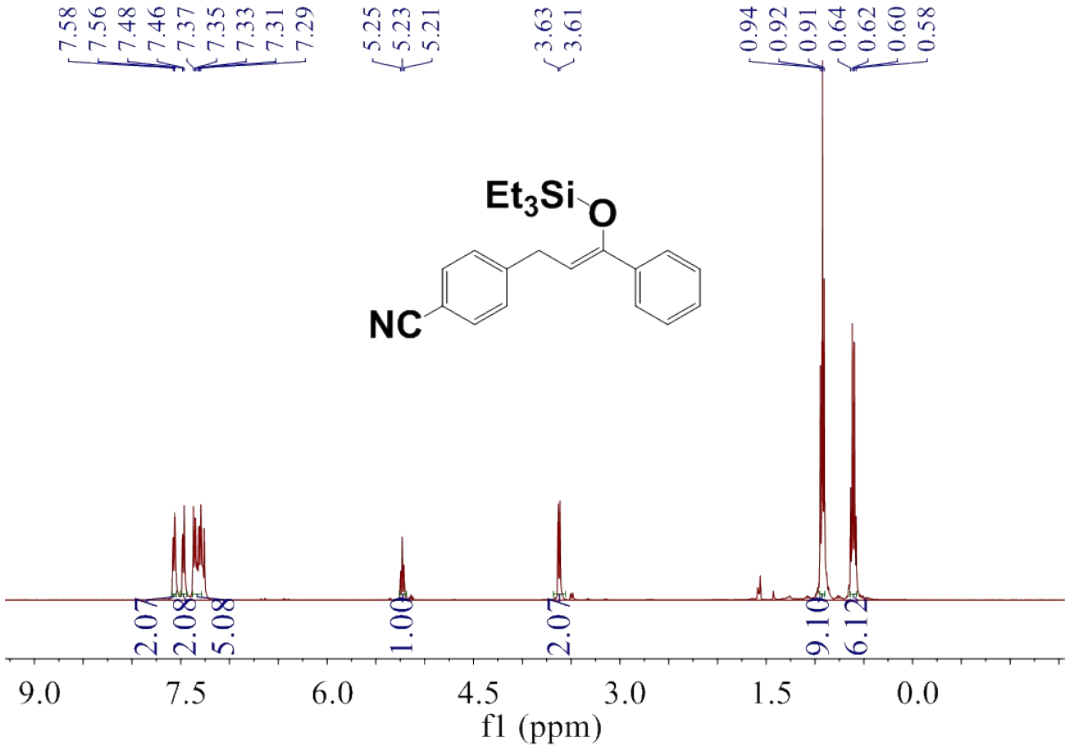
128.16
127.78
127.07
126.79
125.80
116.00
77.32
77.00
76.68
35.95
22.62
6.72
5.38
O SiEt3
200
140
80
40
0
f1 (ppm)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7.56
7.48
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7.35
7.33
7.31
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5.23
5.21
3.63
3.61
0.94
0.92
0.91
0.64
0.62
0.60
0.58
Et3Si
O
NC
2.07
2.08
5.08
1.00
2.07
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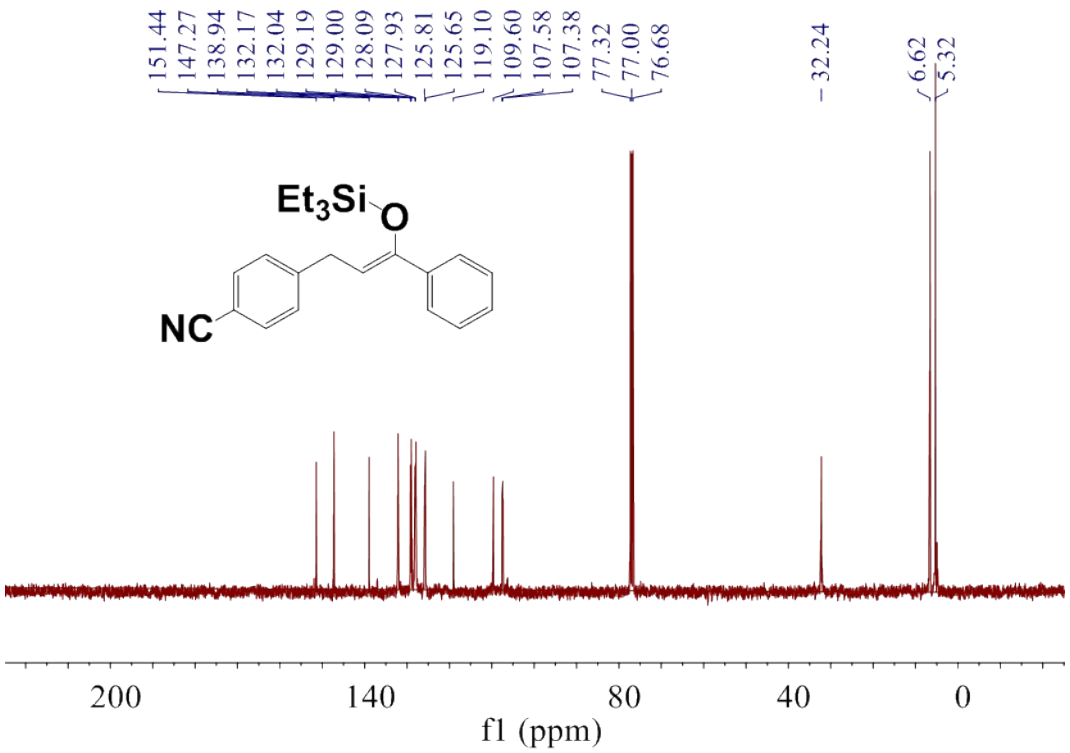
6.12
9.0
7.5
6.0
4.5
3.0
1.5
0.0
f1 (ppm)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138.94
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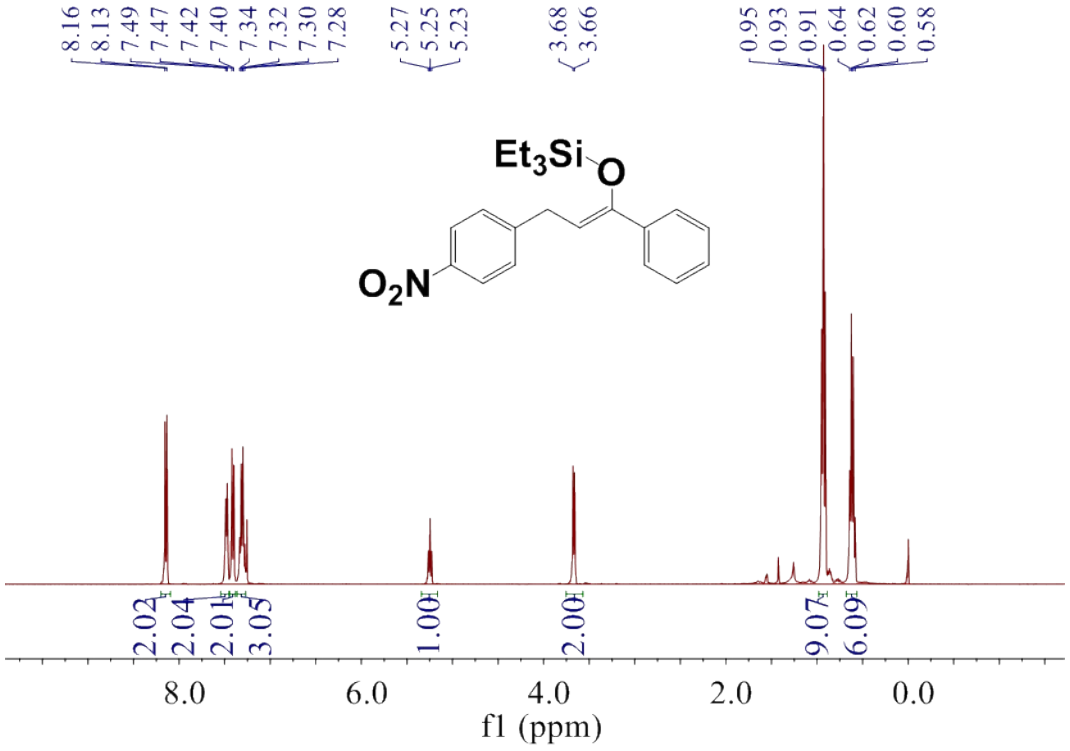
129.19
129.00
128.09
127.93
125.81
125.65
119.10
109.60
107.58
107.38
77.32
77.00
76.68
32.24
6.62
5.32
Et3Si
O
NC
200
140
80
40
0
f1 (ppm)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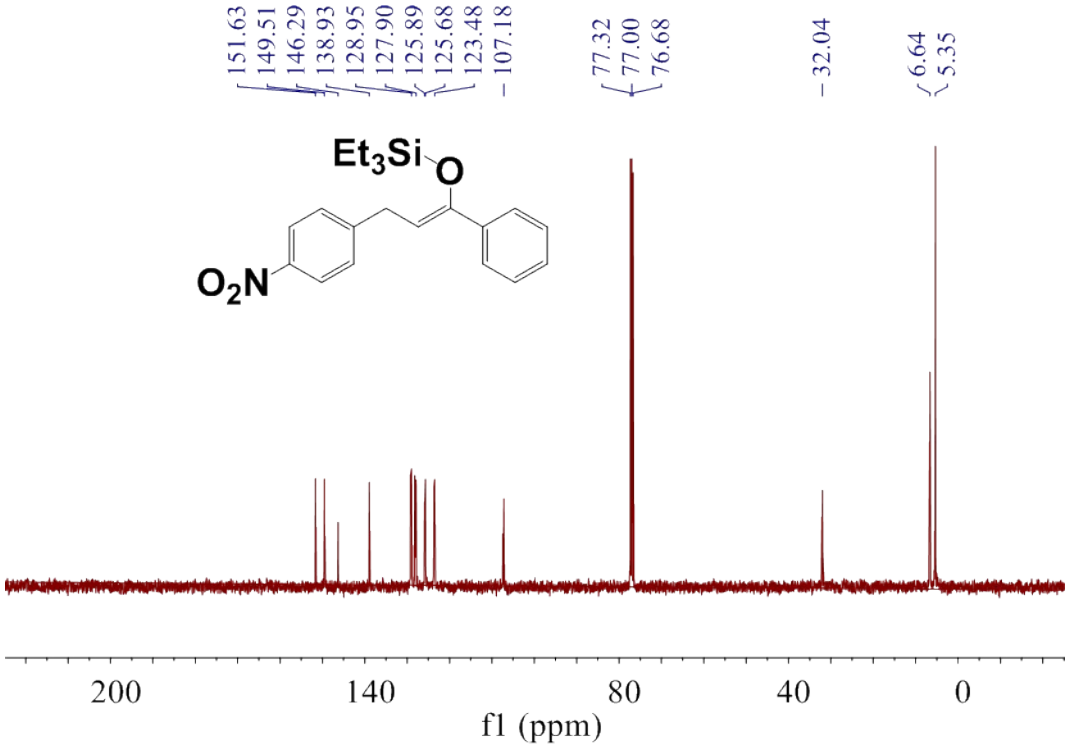
8.13
7.49
7.47
7.42
7.40
7.34
7.32
7.30
7.28
5.27
5.25
5.23
3.68
3.66
0.95
0.93
0.91
0.64
0.62
0.60
0.58
Et3Si
O
O2N
2.02
2.04
2.01
3.05
1.00
2.00
9.07
6.09
8.0
6.0
4.0
2.0
0.0
f1 (ppm)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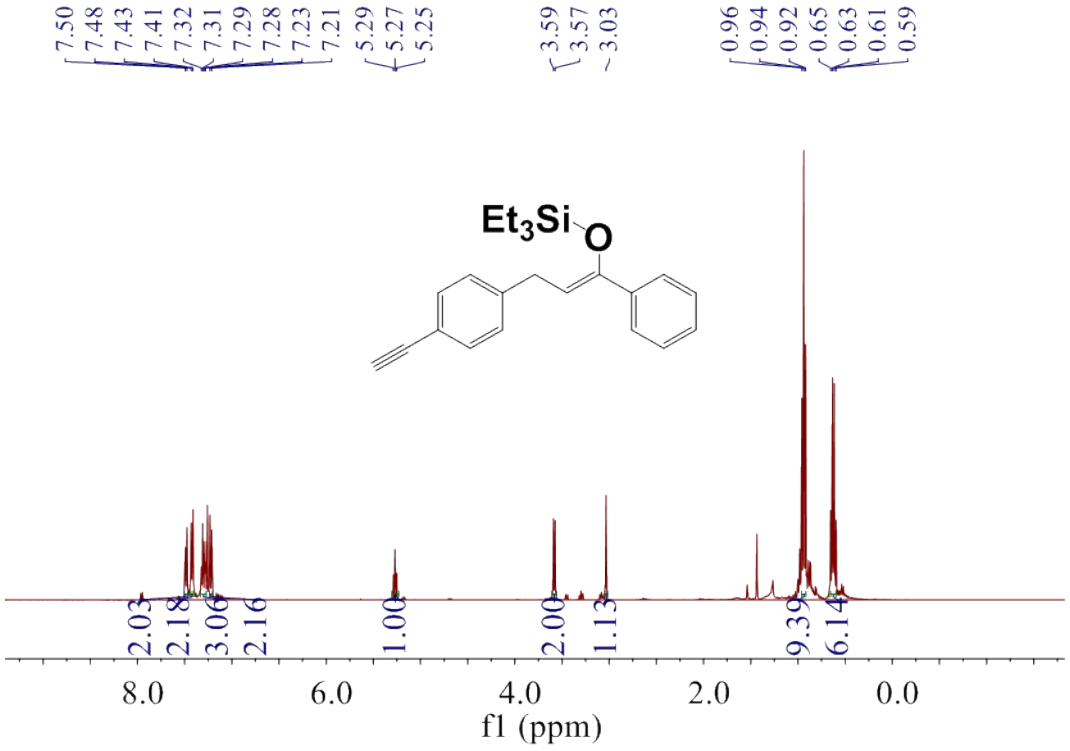
127.90
125.89
125.68
123.48
107.18
77.32
77.00
76.68
32.04
6.64
5.35
Et3Si
O
O2N
200
140
80
40
0
f1 (ppm)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7.31
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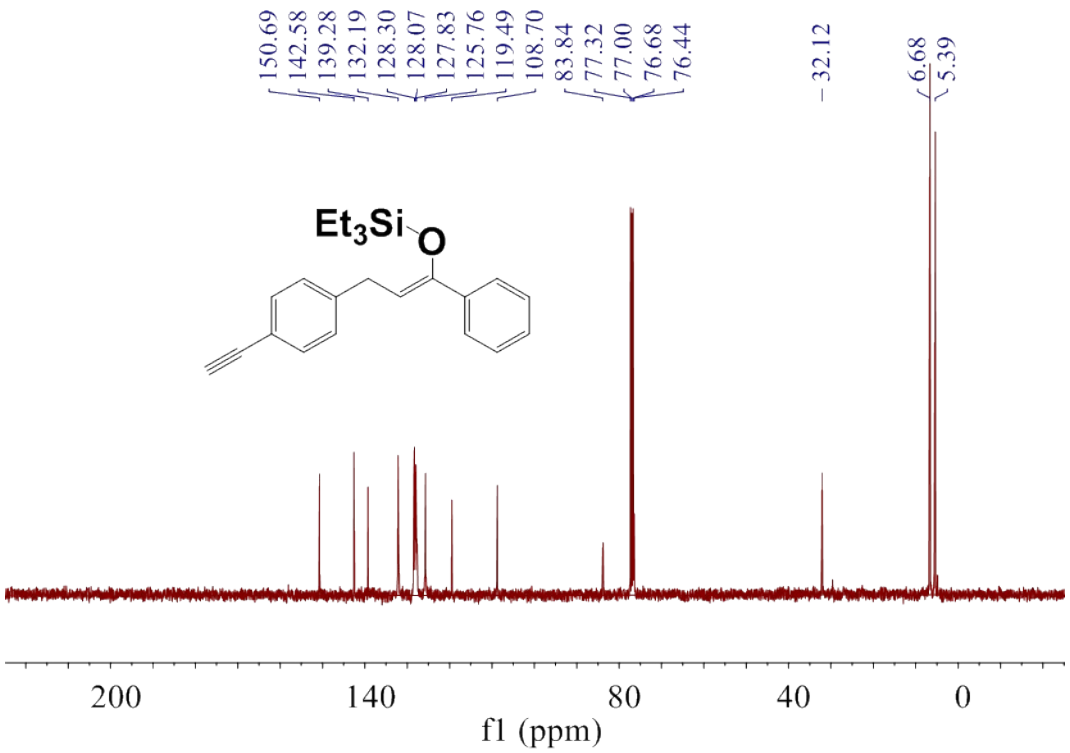
7.23
7.21
5.29
5.27
5.25
3.59
3.57
3.03
0.96
0.94
0.92
0.65
0.63
0.61
0.59
Et3Si
O
2.03
2.18
3.06
2.16
1.00
2.00
1.13
9.39
6.14
8.0
6.0
4.0
2.0
0.0
f1 (ppm)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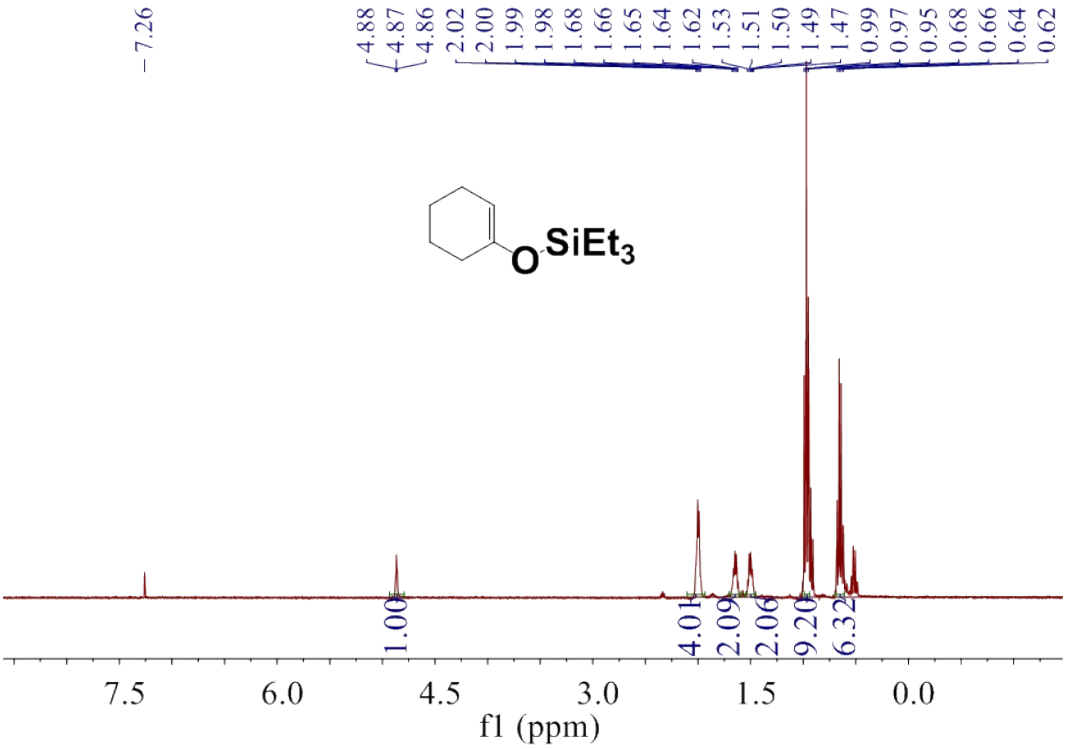
142.58
139.28
132.19
128.30
128.07
127.83
125.76
119.49
108.70
83.84
77.32
77.00
76.68
76.44
32.12
6.68
5.39
Et3Si
O
200
140
80
40
0
f1 (ppm)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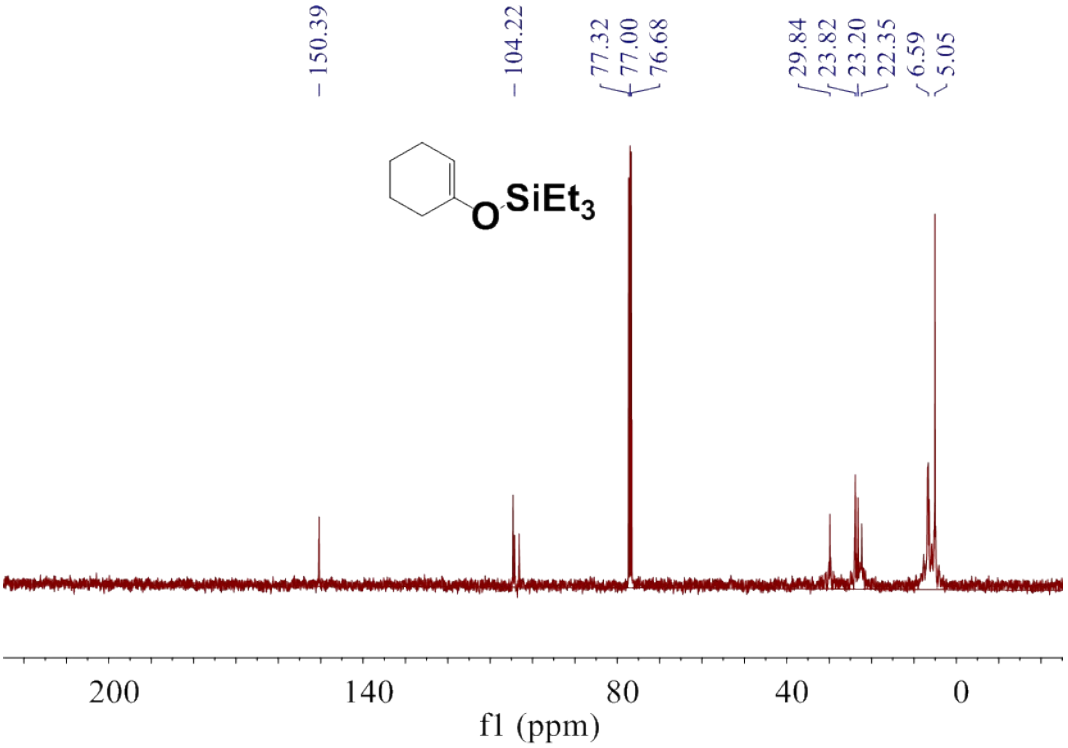
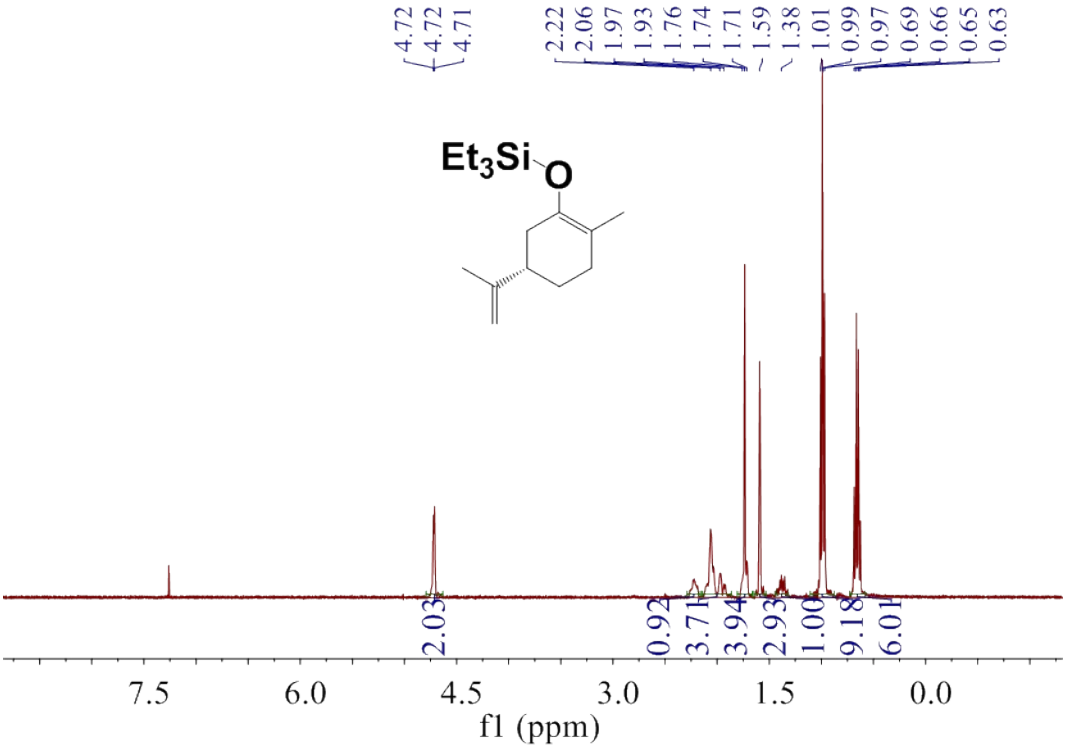
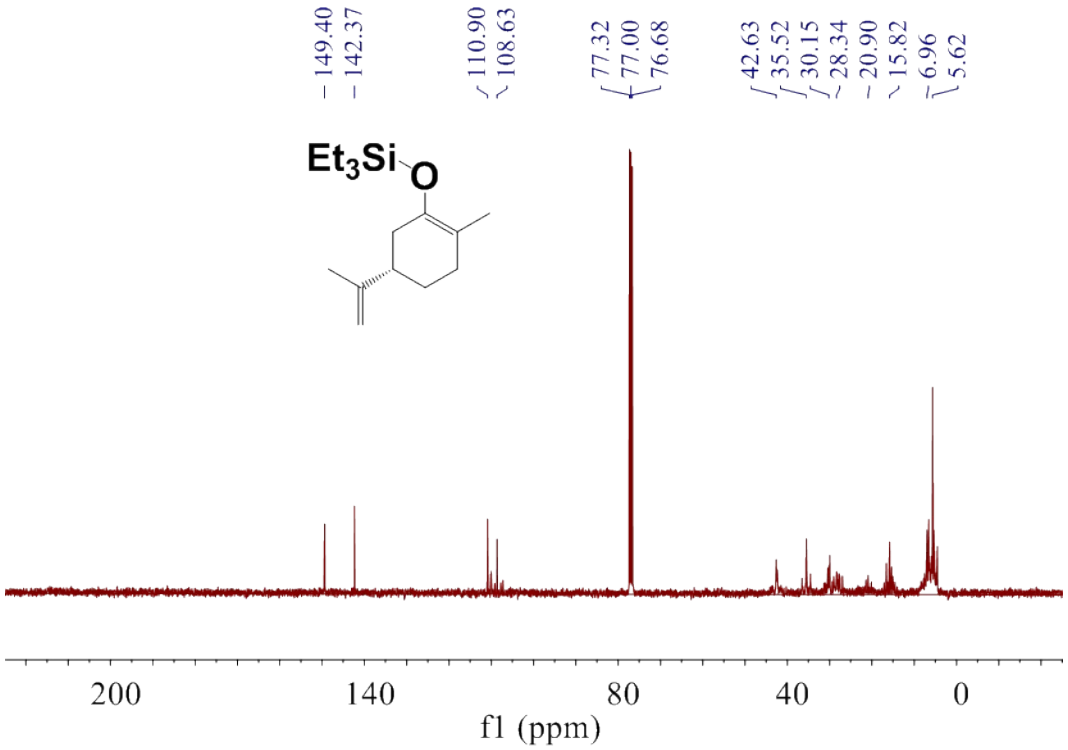
4.88
4.87
4.86
2.02
2.00
1.99
1.98
1.68
1.66
1.65
1.64
1.62
1.53
1.51
1.50
1.49
1.47
0.99
0.97
0.95
0.68
0.66
0.64
0.62
OSiEt3
1.00
4.01
2.09
2.06
9.20
6.32
7.5
6.0
4.5
3.0
1.5
0.0
f1 (ppm)


150.39
104.22
77.32
77.00
76.68
29.84
23.82
23.20
22.35
6.59
5.05
OSiEt3
200
140
80
40
0
f1 (ppm)


4.72
4.72
4.71
2.22
2.06
1.97
1.93
1.76
1.74
1.71
1.59
1.38
1.01
0.99
0.97
0.69
0.66
0.65
0.63
Et3Si
O
2.03
0.92
3.71
3.94
2.93
1.00
9.18
6.01
7.5
6.0
4.5
3.0
1.5
0.0
f1 (ppm)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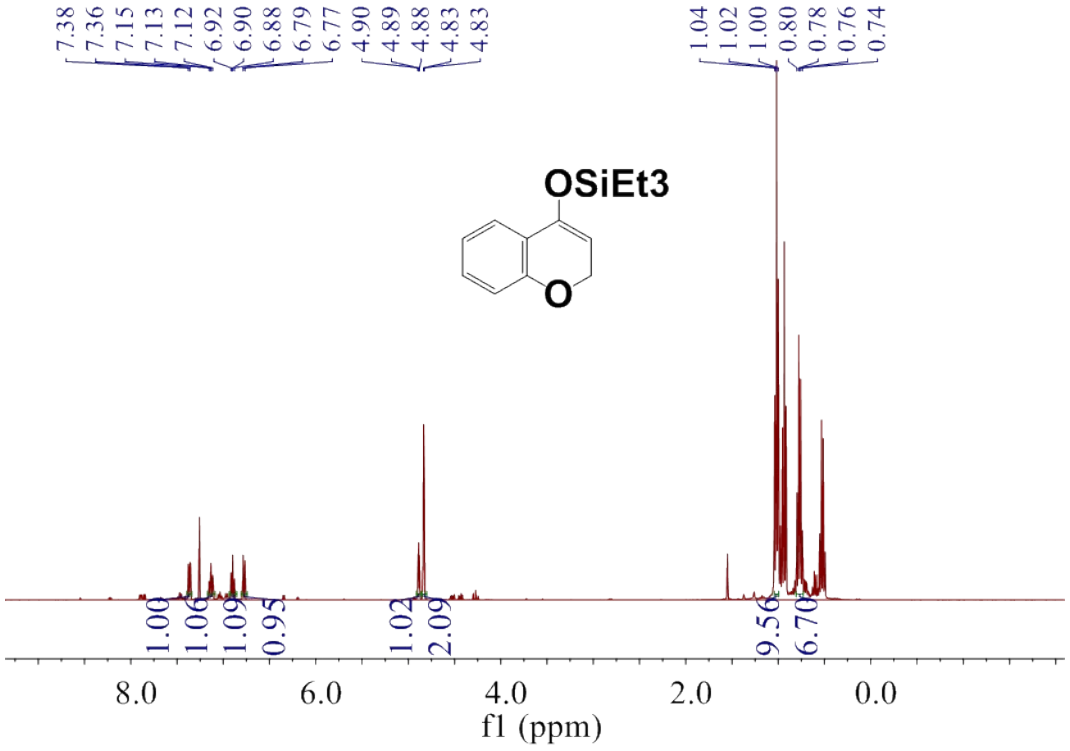
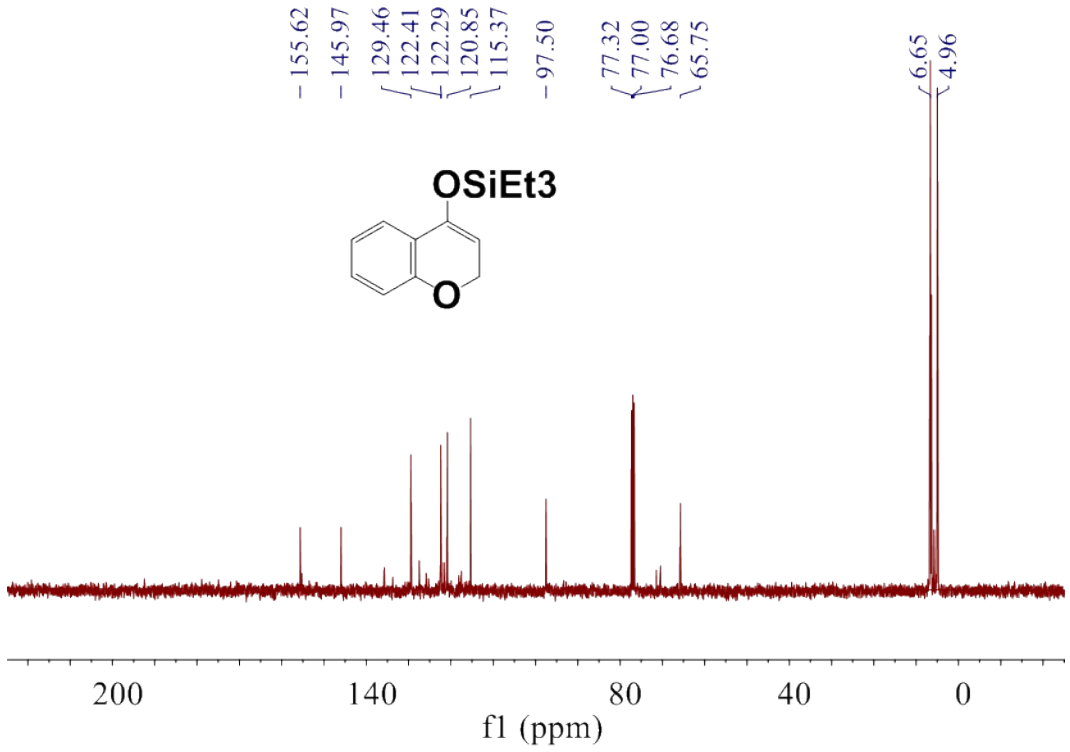
142.37
110.90
108.63
77.32
77.00
76.68
42.63
35.52
30.15
28.34
20.90
15.82
6.96
5.62
Et3Si
O
200
140
80
40
0
f1 (ppm)


7.38
7.36
7.15
7.13
7.12
6.92
6.90
6.88
6.79
6.77
4.90
4.89
4.88
4.83
4.83
1.04
1.02
1.00
0.80
0.78
0.76
0.74
OSiEt3
O
1.00
1.06
1.09
0.95
1.02
2.09
9.56
6.70
8.0
6.0
4.0
2.0
0.0
f1 (ppm)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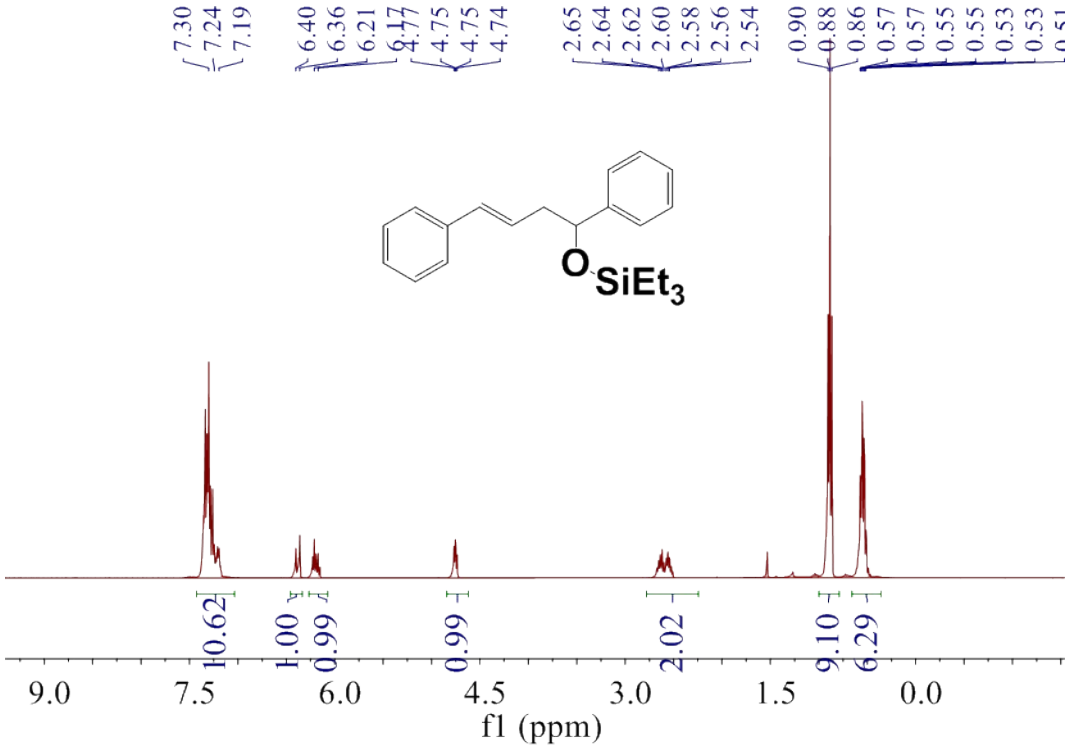
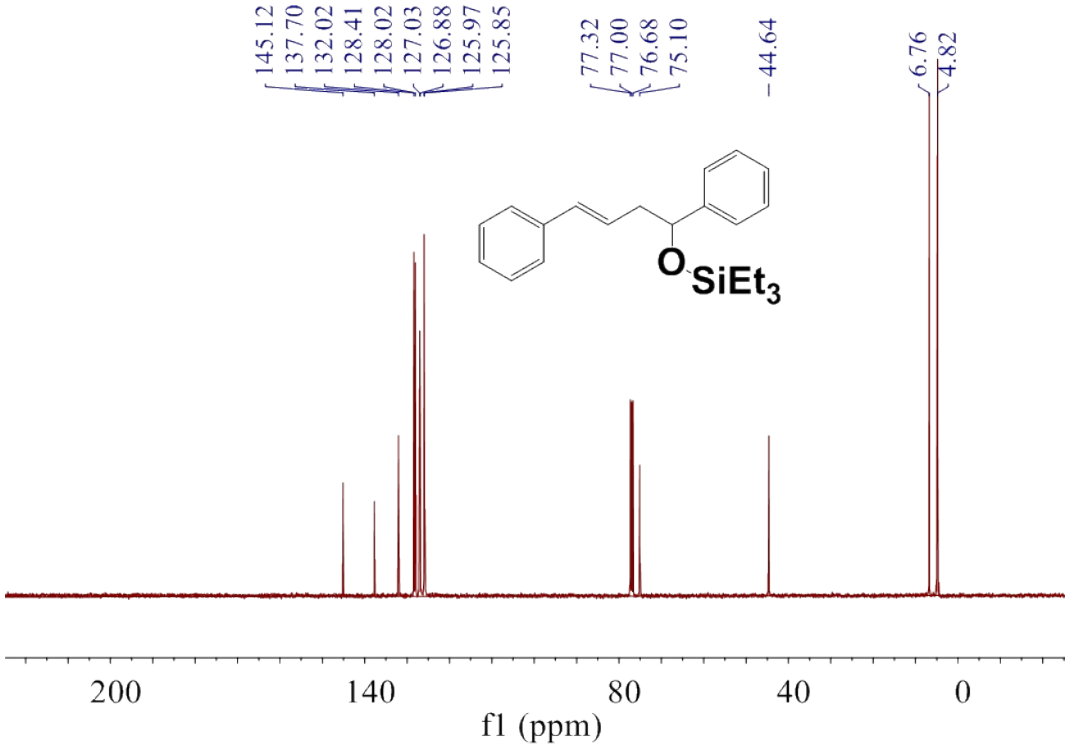
122.29
120.85
115.37
97.50
77.32
77.00
76.68
65.75
6.65
4.96
OSiEt3
O
200
140
80
40
0
f1 (ppm)


7.30
7.24
7.19
6.40
6.36
6.21
6.17
4.77
4.75
4.75
4.74
2.65
2.64
2.62
2.60
2.58
2.56
2.54
0.90
0.88
0.86
0.57
0.57
0.55
0.55
0.53
0.53
O
SiEt3
10.62
1.00
0.99
0.99
2.02
9.10
6.29
9.0
7.5
6.0
4.5
3.0
1.5
0.0
f1 (ppm)


145.12
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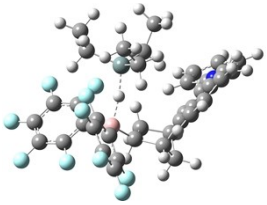
128.41
128.02
127.03
126.88
125.97
125.85
77.32
77.00
76.68
75.10
44.64
6.76
4.82
O
SiEt3
200
140
80
40
0
f1 (ppm)

8. Geometry optimization coordinates

A

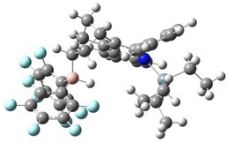
C	-4.31795400	-0.12790000	0.11010500	H	-1.83804400	-1.21923000	2.76612300
C	-4.08313500	-2.10150500	-1.11160600	H	-0.40916700	-0.14536900	2.73246800
C	-2.70744100	-2.27562400	-0.73585300	H	-0.32986800	0.01032700	-1.00290700
C	-2.19493200	-1.30667400	0.15314700	H	-0.20865900	-2.03965500	0.82441600
C	-2.97996600	-0.24311200	0.57498900	H	-2.63720500	1.25553200	2.19156200
H	-5.72072700	-2.92028600	-2.24745300	B	1.39924100	0.24394000	0.10753200
C	-4.67945000	-3.06315900	-1.97459300	C	2.33827000	-1.01939600	0.29519600
C	-1.98099300	-3.38752100	-1.24063500	C	2.50420700	-1.68459500	1.50787200
C	-2.58963300	-4.29436600	-2.07940700	C	3.06054200	-1.52404700	-0.78557700
C	-3.95030500	-4.13105100	-2.44646400	C	3.33560200	-2.78985000	1.65497500
H	-0.93966100	-3.51434000	-0.95781700	C	3.89194600	-2.63544800	-0.68596000
H	-2.02869300	-5.14187800	-2.46335400	C	4.03108900	-3.26839800	0.54663300
H	-4.41599900	-4.85723000	-3.10711600	C	2.09613100	1.61881500	-0.21488500
C	-5.22435600	0.98561700	0.50640100	C	3.28016100	2.01148900	0.42747100
C	-6.59743800	0.73447400	0.67087600	C	1.59902800	2.52453400	-1.16309300
C	-4.75662300	2.29633800	0.69427900	C	3.92513400	3.21490700	0.16383500
C	-7.47136000	1.75752600	1.03155800	C	2.22862200	3.72550200	-1.46975200
H	-6.96448500	-0.27398300	0.51156500	C	3.39666100	4.07383200	-0.79610400
C	-5.63393700	3.32321200	1.04707300	F	1.85653000	-1.23598800	2.60318400
H	-3.70852600	2.52595100	0.53282500	F	3.47456900	-3.39212200	2.84249900
C	-6.99273300	3.05693700	1.22349700	F	4.82885600	-4.33337800	0.66645500
H	-8.52830600	1.54158900	1.16368800	F	4.55477200	-3.09615000	-1.75395400
H	-5.25432600	4.33319800	1.17679900	F	2.94013700	-0.93259800	-1.99212400
H	-7.67458300	3.85552800	1.50306500	F	0.48308600	2.23528100	-1.85634700
N	-4.84462300	-1.05658600	-0.68866100	F	3.82586200	1.22793100	1.37406800
C	-2.11064300	0.58867400	1.50811200	F	5.04139300	3.55290700	0.81959400
C	-0.82930200	-1.14379300	0.79341300	F	4.00566100	5.22805100	-1.06817600
C	-1.02891400	1.29832800	0.63162600	F	1.72560000	4.54514700	-2.39989700
C	-0.16559100	0.09994200	0.08821200	H	-1.45925400	1.89660200	-0.17476400
C	-1.25283500	-0.52900400	2.15064700	H	-0.43366200	1.96979600	1.26021800



B

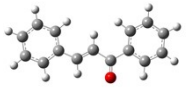
C	4.03807800	-0.39612800	-0.70044700	C	2.11016100	-2.43957700	-0.52762000
C	3.37887100	-2.46699800	0.14794300	C	1.87564500	-1.30682500	-1.33766000

C	2.82910600	-0.30206600	-1.43974200	C	-3.77174100	-2.37111300	0.70720500
H	4.66110000	-3.60471000	1.45346500	C	-3.45543100	-2.79919600	-1.62572900
C	3.70049000	-3.60047500	0.94711200	C	-4.06283900	-3.12988300	-0.41960900
C	1.22694300	-3.54580600	-0.39571400	F	-3.79764500	1.06441800	-1.70585700
C	1.57640300	-4.62953400	0.37852300	F	-4.99026900	3.43121500	-1.47068600
C	2.82154700	-4.65405300	1.05860400	F	-3.78379800	5.47482300	-0.10925200
H	0.27418100	-3.52769400	-0.91720600	F	-1.31480700	5.06989900	1.01510300
H	0.89821800	-5.47323300	0.47142300	F	-0.08810200	2.72630400	0.77714900
H	3.08123800	-5.51615100	1.66689700	F	-2.08731400	-1.44740500	-2.91303800
C	5.10030100	0.64621400	-0.74695100	F	-2.70156500	-0.58302300	1.72603300
C	4.79508100	2.01294700	-0.85290600	F	-4.35359700	-2.65219700	1.88171500
C	6.45002700	0.26591700	-0.65436100	F	-4.91811900	-4.15443800	-0.34816600
C	5.81026000	2.97064100	-0.87626900	F	-3.75154000	-3.49373800	-2.73314800
H	3.75948900	2.33561400	-0.88628800	H	1.32108700	1.77799200	-0.81209800
C	7.46340700	1.22129300	-0.68663800	H	0.76722700	2.27551600	-2.40853300
H	6.68832300	-0.78808100	-0.55743600	Si	0.10173000	0.05472200	2.22213900
C	7.14777200	2.57850300	-0.79983300	C	-1.01574000	1.15034000	3.30831600
H	5.55357700	4.02416300	-0.94796600	C	1.90103800	0.63553400	2.16939900
H	8.50201200	0.90732900	-0.62391400	C	-0.01840300	-1.80953100	2.58550600
H	7.93816600	3.32385400	-0.82342400	C	-0.37006000	2.39376400	3.94722600
N	4.29462900	-1.46549500	0.05602800	C	-0.82544000	-2.22328200	3.82999300
C	2.29498600	0.68688200	-2.46642400	C	2.71542000	0.26201300	3.42566700
C	0.74743500	-0.96497200	-2.28914100	H	-1.41675900	0.49922200	4.09577500
C	1.07132400	1.41063000	-1.80883400	H	-1.88785100	1.45263800	2.71880500
C	-0.04767900	0.30874300	-1.79744100	H	-0.03487700	3.10770400	3.18973600
C	1.58601500	-0.30598200	-3.42136100	H	-1.09357900	2.91070500	4.58915100
H	2.28140900	-1.00025600	-3.90399700	H	0.49233300	2.13809800	4.57197800
H	0.96866200	0.18169900	-4.18447300	H	-0.42592200	-2.31349400	1.70184300
H	0.11460000	-1.79945900	-2.58163300	H	1.01076100	-2.18106400	2.67168000
H	3.03134900	1.35730300	-2.91058700	H	-0.77316200	-3.30843500	3.97898600
B	-1.17105000	0.30103200	-0.64184400	H	-0.44591400	-1.75115600	4.74351900
C	-1.89157100	1.74397300	-0.43854400	H	-1.88170500	-1.95512600	3.72801400
C	-3.14632800	2.01261000	-1.00035300	H	2.38127100	0.19695200	1.28965200
C	-1.31449900	2.83814800	0.21006700	H	1.91962700	1.72133000	2.02168400
C	-3.79031700	3.24417900	-0.90367700	H	2.29570300	0.69980200	4.33848600
C	-1.92630600	4.07995500	0.34915600	H	2.76412900	-0.82279800	3.56988600
C	-3.17881700	4.28739300	-0.21739500	H	3.74613600	0.62303500	3.33336200
C	-2.19694000	-0.95876000	-0.57068800	H	-0.41336700	0.17345400	0.70150400
C	-2.88583000	-1.30432200	0.59505400	H	-0.70316300	0.53717600	-2.65492100
C	-2.56317800	-1.73074900	-1.68159400				



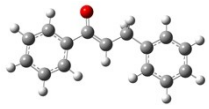
C

C	2.74034300	0.15832300	-1.18825700
C	2.26304200	-2.06404300	-0.43465000
C	1.02439200	-2.08583600	-1.14814600
C	0.66825600	-0.91841000	-1.85511200
C	1.56311600	0.15206200	-1.93672600
H	3.71200300	-3.31019500	0.59370700
C	2.73239400	-3.27023800	0.13445800
C	0.25622200	-3.27917800	-1.18250300
C	0.71714000	-4.42793900	-0.58167900
C	1.97621200	-4.42325000	0.05667300
H	-0.69185900	-3.27104300	-1.70861400
H	0.13166500	-5.34094200	-0.61895200
H	2.36689100	-5.34252700	0.48252700
C	3.76948300	1.20449800	-1.39465400
C	3.44420800	2.57132900	-1.41227500
C	5.09044900	0.81387100	-1.67792800
C	4.42774700	3.52501600	-1.66680000
H	2.42960700	2.88891500	-1.19734100
C	6.06912400	1.77101600	-1.94362800
H	5.33991400	-0.24167500	-1.71936400
C	5.74202300	3.12858500	-1.93012100
H	4.16731000	4.57921000	-1.65931300
H	7.08335900	1.45518100	-2.16977800
H	6.50472100	3.87460800	-2.13346300
N	3.01932500	-0.89013500	-0.33943000
C	0.94349400	1.15933600	-2.89041200
C	-0.52114300	-0.57149700	-2.70031900
C	-0.25902000	1.79020200	-2.11456100
C	-1.27987300	0.60777700	-1.95901700
C	0.19711000	0.19545700	-3.84513900
H	0.87138200	-0.42883300	-4.44301700
H	-0.50754100	0.70857100	-4.50751100
H	-1.17062600	-1.39850100	-2.98351800
H	1.63329900	1.87234900	-3.34325200
B	-1.72176800	0.32344400	-0.40130700
C	-2.46519000	1.65938300	0.21492600
C	-3.76209300	2.03716800	-0.13952800
C	-1.84579200	2.52620500	1.11720000
C	-4.41372100	3.16247500	0.35892600
C	-2.45297100	3.66606200	1.64267200
C	-3.75125000	3.98572100	1.26314600
C	-2.67405800	-1.00318600	-0.15318100
C	-2.70493000	-1.60211000	1.11125300
C	-3.49995000	-1.62764000	-1.08947100
C	-3.46182900	-2.72730600	1.42880200
C	-4.27197500	-2.75853300	-0.82369600
C	-4.25586900	-3.31376700	0.44961000
F	-4.46293600	1.29082800	-1.02821200
F	-5.66837800	3.46576400	-0.02452100
F	-4.35530900	5.08045500	1.75640100
F	-1.79784700	4.46210100	2.50994900
F	-0.57248300	2.30256700	1.52872300
F	-3.58751000	-1.15858400	-2.36006000
F	-1.96716200	-1.08940100	2.12364000
F	-3.43575000	-3.25296500	2.66867500
F	-4.99399300	-4.40152400	0.73005800
F	-5.03864800	-3.31177600	-1.78324900
H	0.05483200	2.19970700	-1.14896400
H	-0.67683200	2.61609500	-2.70189200
Si	3.98120200	-0.59990600	1.30089300
C	2.94532200	-1.45184800	2.65117100
C	4.04748100	1.23778400	1.73627100
C	5.72033000	-1.32049200	1.05573800
C	3.29747700	-1.01232100	4.08936500
C	6.43775400	-1.76390500	2.34625700
C	2.70695300	1.95251700	1.98584200
H	3.03514200	-2.53981200	2.58803800
H	1.88773500	-1.23087800	2.45453500
H	3.14361600	0.05946800	4.24639700
H	2.66018600	-1.54003700	4.80800800
H	4.33699000	-1.24041800	4.34721900
H	5.66971100	-2.16543900	0.35689200
H	6.32157300	-0.55550600	0.54792100
H	7.44300100	-2.13733900	2.11995000
H	6.55074800	-0.93731000	3.05659400
H	5.89612500	-2.56838800	2.85581400
H	4.63175200	1.23734900	2.67046300
H	4.65581900	1.79554100	1.02005500
H	2.07135100	1.97038200	1.09627500
H	2.12586500	1.46944700	2.77761200
H	2.87477800	2.99217600	2.28934700
H	-0.70885400	0.13747600	0.24638900
H	-2.14923700	0.81787600	-2.59237600



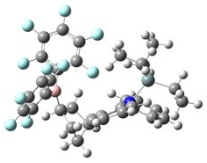
D

C	3.86690100	1.79662800	-0.00001300	H	-0.04038400	0.91087100	-0.00002100
C	2.60998600	1.19069100	-0.00002600	O	1.17209100	-2.17554300	0.00001800
C	2.49278000	-0.20931600	-0.00001500	C	-2.61085200	-0.23046000	-0.00000200
C	3.66629800	-0.98355900	0.00001200	C	-2.85167200	1.15876600	0.00001400
C	4.91962400	-0.37992200	0.00002600	C	-3.71993700	-1.09829400	-0.00001000
C	5.02344500	1.01485700	0.00001300	C	-4.15126500	1.65433100	0.00002000
H	3.94128800	2.88041800	-0.00002200	H	-2.01773200	1.85425000	0.00002100
H	1.73039400	1.82455700	-0.00004500	C	-5.02197700	-0.60168200	-0.00000300
H	3.56695500	-2.06363200	0.00002100	H	-3.55007900	-2.17206200	-0.00002200
H	5.81649900	-0.99316900	0.00004600	C	-5.24199300	0.77702800	0.00001200
H	6.00100600	1.48922900	0.00002400	H	-4.31782200	2.72792100	0.00003200
C	1.18080400	-0.94157600	-0.00002600	H	-5.86294900	-1.28933700	-0.00001000
C	-0.08406000	-0.17163200	-0.00001900	H	-6.25542000	1.16844000	0.00001700
C	-1.27122700	-0.81428300	-0.00001100	H	-1.22961200	-1.90260400	-0.00001100



E

C	-3.81307900	1.85222800	0.00934100	O	-1.28328600	-2.26891200	0.00518800
C	-2.57337200	1.21189600	0.01161200	C	2.63007600	-0.31237400	0.00077200
C	-2.47249700	-0.19259800	0.00186900	C	2.72864700	1.08538700	-0.00440200
C	-3.67440800	-0.92091100	-0.01008100	C	3.83318600	-1.04224700	0.00314700
C	-4.91771400	-0.28741900	-0.01269900	C	3.97288600	1.72742200	-0.00714400
C	-4.99738800	1.10720700	-0.00298800	H	1.82768800	1.68923600	-0.00645700
H	-3.85578500	2.93997300	0.01733300	C	5.07574900	-0.41167800	0.00048600
H	-1.67419500	1.82121300	0.02168500	H	3.78510300	-2.13015800	0.00713300
H	-3.58547400	-2.00271000	-0.01703900	C	5.15274700	0.98533900	-0.00472100
H	-5.82902200	-0.88334700	-0.02213900	H	4.01380700	2.81460000	-0.01121300
H	-5.96329700	1.60753200	-0.00470000	H	5.98519400	-1.00861500	0.00241900
C	-1.17254800	-0.98833400	0.00350200	H	6.11900300	1.48399100	-0.00686100
C	0.02814000	-0.30374100	0.00243900	H	1.34575400	-1.77000200	0.86761900
C	1.31585200	-1.07931000	0.00355400	H	1.34460200	-1.77400600	-0.857355000
H	0.05525800	0.77838400	-0.00005100				



F

C	-2.48708000	-0.75012700	1.07102400	C	-1.34026700	-0.86067500	1.86727700
C	-1.50953200	-2.24529200	-0.52136400	H	-2.62542500	-3.14956000	-2.14275300
C	-0.30411000	-2.34883800	0.24678600	C	-1.68417700	-3.12501800	-1.61239400
C	-0.23677000	-1.58868800	1.43195300	C	0.71269000	-3.25306900	-0.16059600

C	0.53214700	-4.06253400	-1.25783200	C	5.13391800	-1.86163400	0.68730600
C	-0.68680100	-4.01100200	-1.96846300	C	5.27330500	-1.90353100	-0.69821900
H	1.62147200	-3.31713500	0.42779100	F	3.93920100	2.71972800	0.87832000
H	1.30569600	-4.76141800	-1.55866800	F	3.46053400	5.07146400	-0.36991200
H	-0.85483300	-4.69126800	-2.79754800	F	1.04413900	5.52477600	-1.55576100
C	-3.71616700	-0.12342900	1.60822900	F	-0.90392800	3.59567400	-1.46702800
C	-3.69774600	1.14378200	2.21629400	F	-0.44089700	1.27478500	-0.18171900
C	-4.91124800	-0.86427200	1.60405300	F	4.02427800	-1.11168700	2.58831700
C	-4.85984100	1.67129300	2.77363000	F	2.55420800	0.21779500	-1.74179300
H	-2.78536600	1.73105500	2.21923700	F	4.50948300	-1.24507900	-2.83509200
C	-6.06941200	-0.33649900	2.17427400	F	6.24014900	-2.63344500	-1.24931700
H	-4.92056300	-1.86586200	1.18617600	F	5.97942000	-2.54589200	1.46356000
C	-6.04784000	0.93407400	2.75251900	H	-0.31826900	1.59767100	2.25109000
H	-4.83938100	2.65911700	3.22374400	H	0.29588500	1.37216600	3.88533800
H	-6.98376500	-0.92207500	2.17454900	Si	-3.54274500	-0.50721200	-1.60252800
H	-6.95049400	1.34620400	3.19360400	C	-3.82937300	1.31253800	-1.15371100
N	-2.51408800	-1.33496500	-0.17084700	C	-5.19769700	-1.38701100	-1.85208000
C	-0.97506600	-0.28156400	3.22488000	C	-2.49442200	-0.54179400	-3.18113900
C	0.83935200	-1.43613500	2.48116100	C	-4.26258000	2.15556400	-2.37463400
C	0.06490500	0.85321300	2.95022200	C	-1.12342200	0.15857200	-3.15945600
C	1.31708000	0.07755300	2.41781900	C	-5.23321100	-2.88126300	-2.21501300
C	-0.04800900	-1.40489000	3.75231900	H	-2.91429500	1.74070600	-0.72935400
H	-0.57387900	-2.34798000	3.93025300	H	-4.59922800	1.38978200	-0.38204900
H	0.50979200	-1.12155500	4.65018600	H	-5.16441900	1.75753800	-2.85387500
H	1.65280600	-2.15896900	2.45568000	H	-4.49037600	3.17950800	-2.05819200
H	-1.80946500	0.01245800	3.86021700	H	-3.47800100	2.21652400	-3.13474800
B	2.06508300	0.53523700	1.10481900	H	-2.39210500	-1.55151000	-3.58737400
C	1.76168700	1.92093300	0.40575400	H	-3.14852700	-0.01793400	-3.89513800
C	2.73328400	2.91931700	0.31449100	H	-0.69071100	0.17817800	-4.16594800
C	0.54142500	2.20853900	-0.20006400	H	-1.19933500	1.19409300	-2.81278700
C	2.50694700	4.13621000	-0.32259300	H	-0.40932600	-0.35469100	-2.50713000
C	0.27966300	3.39647600	-0.86868200	H	-5.81776800	-1.20215300	-0.96736600
C	1.27288300	4.37176400	-0.92629900	H	-5.67382800	-0.81154700	-2.66098900
C	3.20594000	-0.35036900	0.47992100	H	-4.67956800	-3.09084000	-3.13761900
C	3.39183400	-0.42689600	-0.91095700	H	-4.81444400	-3.50697200	-1.41877500
C	4.10756100	-1.10770600	1.24473100	H	-6.26454300	-3.21278400	-2.37859600
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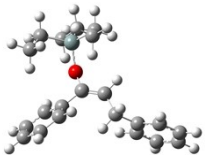
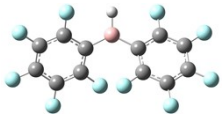


G

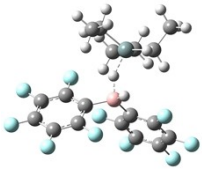
C	2.17655300	0.46652800	-0.93732500	C	-0.17849500	0.26040800	0.06872500
C	0.96755200	-0.26520600	-0.40570700	C	-0.52592300	1.70503500	0.13493900
H	1.06100400	-1.34828100	-0.35537700	C	-0.28147200	2.57913200	-0.93723900

C	-1.13852300	2.21902100	1.29216800	H	-3.49031400	0.33329700	-2.21320500
C	-0.61444700	3.93207600	-0.84508000	C	-2.91386700	-2.26719800	2.79815400
H	0.14389800	2.19304000	-1.85829800	H	-3.85111300	-1.69960600	2.75550200
C	-1.46669200	3.57011300	1.38443300	H	-3.03920700	-3.04696900	3.55954300
H	-1.35029000	1.54831400	2.11871700	H	-2.13216400	-1.58426400	3.14829100
C	-1.20308700	4.43349300	0.31681400	C	-1.50153300	-1.83204200	-2.82369100
H	-0.42376900	4.59067500	-1.68824100	H	-2.47785300	-1.48749000	-3.18156100
H	-1.93047400	3.95080700	2.29066000	H	-0.84897500	-0.95598900	-2.74523800
H	-1.46325200	5.48611900	0.38775300	H	-1.08362200	-2.48618100	-3.59918900
O	-1.11652400	-0.56065600	0.66057400	H	2.23325600	0.36670700	-2.03097400
Si	-2.27964000	-1.62437300	0.02956200	C	3.47678500	-0.05158700	-0.33964400
C	-3.90704200	-0.71502100	-0.32572800	C	3.69271500	-0.00166000	1.04565600
H	-4.58806600	-1.46026600	-0.76552500	C	4.48595000	-0.58128600	-1.15257400
H	-4.35094400	-0.45674500	0.64629900	C	4.88664600	-0.46229000	1.60073700
C	-2.55300000	-2.86904200	1.42822400	H	2.91482600	0.40027700	1.69061900
H	-3.34014900	-3.56886100	1.11070400	C	5.68340800	-1.04570400	-0.60125100
H	-1.63935900	-3.47337600	1.52070500	H	4.33409300	-0.62908700	-2.22885100
C	-1.62205700	-2.57027200	-1.47816500	C	5.88780100	-0.98708300	0.77795800
H	-2.28764400	-3.43859400	-1.60005200	H	5.03672200	-0.41220700	2.67626300
H	-0.64657100	-2.99353200	-1.19997700	H	6.45416400	-1.45330300	-1.25051600
C	-3.87788700	0.54448000	-1.21088200	H	6.81784400	-1.34727700	1.20971600
H	-4.88459300	0.96368600	-1.33243300	H	2.08667800	1.53955300	-0.73359000
H	-3.24725700	1.32465800	-0.77333000				



H

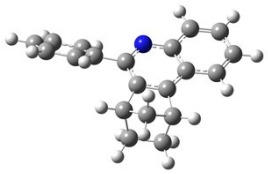
C	2.90404500	-1.18680400	0.69894500	C	-3.99050700	-0.48359100	-0.18150700
C	1.63365200	-0.62984300	0.62084600	F	0.63165400	-1.33534900	1.16602300
C	1.38623000	0.62704400	0.04375800	F	3.09788600	-2.38172500	1.26952400
C	2.51820700	1.30391800	-0.44348600	F	5.21280800	-1.01010900	0.24280200
C	3.80005100	0.76876100	-0.39765000	F	4.84605800	1.43990300	-0.89393600
C	3.99046100	-0.48363100	0.18141800	F	2.38495400	2.51277800	-1.00801400
B	-0.00000700	1.32651800	-0.00005600	F	-0.63158400	-1.33552500	-1.16575200
C	-1.38623300	0.62688900	-0.04369700	F	-3.09797200	-2.38175200	-1.26958900
C	-2.51817200	1.30390400	0.44343600	F	-5.21286700	-1.00999300	-0.24290200
C	-1.63367100	-0.62995900	-0.62073300	F	-4.84601800	1.43994100	0.89392300
C	-3.80001600	0.76880800	0.39759500	F	-2.38485600	2.51277700	1.00800800
C	-2.90411400	-1.18679200	-0.69896900	H	-0.00013900	2.51666600	-0.00023900



I

B	0.02754700	0.16208100	-0.82693300	C	-1.21582800	-0.72279700	-0.33904400

C	-1.27580900	-1.36544800	0.90179100	C	-1.76561100	2.60443700	1.60737900
C	-2.32466700	-0.93124400	-1.16725100	C	-1.63935900	3.11861200	-1.50037800
C	-2.33762400	-2.17156200	1.29978200	C	0.87267100	3.83405600	0.32738200
C	-3.40625400	-1.73305900	-0.80967200	C	-1.06558600	2.18454800	2.91313700
C	-3.40939300	-2.36026800	0.43192400	C	1.80192100	3.94362700	-0.89540900
C	1.51619400	-0.32433200	-0.46744500	C	-2.48487600	4.40810100	-1.44860800
C	2.17431100	-1.16388400	-1.36947400	H	-2.56926900	1.89685900	1.36300000
C	2.24575700	0.00638600	0.67367900	H	-2.26270900	3.57644700	1.74472200
C	3.46551200	-1.64378800	-1.16902100	H	-0.28564800	2.89853400	3.19990100
C	3.54219100	-0.44274700	0.91111300	H	-1.78517900	2.13499600	3.73835100
C	4.15536400	-1.27770700	-0.01737300	H	-0.59678400	1.20097500	2.81837000
F	-0.27798200	-1.20054100	1.79575200	H	0.53185400	4.83455400	0.63299400
F	-2.34120500	-2.76211600	2.50353100	H	1.42248900	3.42784000	1.18478700
F	-4.44045900	-3.13056400	0.79503900	H	2.66921400	4.57439400	-0.66958500
F	-4.44169100	-1.90249800	-1.64499100	H	2.18027800	2.96241700	-1.20275400
F	-2.39485300	-0.34073200	-2.37689000	H	1.28951500	4.38579100	-1.75679800
F	1.70962700	0.81764600	1.61502700	H	-0.92937000	3.16889100	-2.33533100
F	1.54611300	-1.55025400	-2.49918500	H	-2.28019200	2.25276600	-1.70799200
F	4.04741800	-2.45019900	-2.06939800	H	-3.24444100	4.36467600	-0.66010900
F	5.39974300	-1.72413100	0.19520400	H	-1.86703400	5.29510700	-1.26608000
F	4.20008300	-0.08298900	2.02387700	H	-3.00794700	4.56499600	-2.39857400
H	-0.07826500	0.56222900	-1.94753000	H	-0.07144300	1.32881200	-0.07470100
Si	-0.67195800	2.77993700	0.08108800				



J

C	-0.65087100	-0.45970100	-0.11292000	C	-4.11632400	-1.65969400	0.84159900
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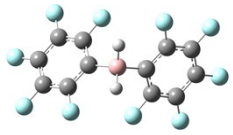
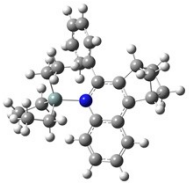
C	2.15769000	-0.36315000	-0.17431500	C	-4.35166100	0.02905800	-0.86831800
C	1.40271100	0.82837400	-0.24953200	H	-2.52345600	0.87208000	-1.61967200
C	0.01580700	0.79121500	-0.21715000	C	-4.93262300	-0.88588400	0.01183900
H	1.50125000	-3.72216300	0.08161500	H	-4.56039500	-2.37794300	1.52581700
C	2.09171700	-2.81384400	0.00665100	H	-4.97697800	0.62099500	-1.53136300
C	3.57670300	-0.43094000	-0.19174200	H	-6.01271000	-1.00033300	0.04673200
C	4.21738800	-1.64769200	-0.11295400	N	0.03381000	-1.60044700	-0.04034500
C	3.46796600	-2.84785000	-0.01392900	C	-0.45073500	2.24084900	-0.16024900
H	4.15100400	0.48813700	-0.26859800	C	1.50826300	2.81481400	1.19653200
H	5.30284500	-1.69289000	-0.12760400	C	0.64029600	2.90840200	-1.03533000
H	3.98882500	-3.79966100	0.04557400	C	1.81873900	2.28563200	-0.24437700
C	-2.13553800	-0.58370000	-0.07222500	C	-0.05150900	2.77843400	1.25567100
C	-2.73089900	-1.51481700	0.79462200	H	-0.43291900	2.13883500	2.05661500
C	-2.96479300	0.18080600	-0.90848600	H	-0.46650800	3.78117700	1.40450000

H	2.82855000	2.50348000	-0.59740800	H	0.60852000	2.58856800	-2.08194900
H	1.88725300	3.83656500	1.30605000	H	0.62257600	4.00320400	-0.98661000
H	-1.48842700	2.43568900	-0.42642800	H	1.98011700	2.20033800	1.96868700



K

C	2.72454300	-1.36247000	-0.65847400	C	-3.65759600	0.33245700	-0.71442600
C	1.60136800	-1.21724100	0.15132500	F	0.72852700	-2.25367200	0.15136800
C	1.33916900	-0.09255300	0.93661200	F	2.91956500	-2.47989900	-1.38819000
C	2.30241400	0.91231500	0.83648500	F	4.75212100	-0.44568000	-1.49029800
C	3.44398100	0.81430200	0.04044100	F	4.34236000	1.81927100	-0.00953800
C	3.65758000	-0.33251900	-0.71444200	F	2.17554500	2.06450500	1.53431400
B	0.00000900	0.00007900	1.87688300	F	-0.72861600	2.25376200	0.15129800
H	0.05811300	0.99416000	2.57693500	F	-2.91968100	2.47985200	-1.38823900
C	-1.33915000	0.09263300	0.93660300	F	-4.75215200	0.44555200	-1.49027000
C	-2.30235200	-0.91227700	0.83651400	F	-4.34227000	-1.81934600	-0.00945800
C	-1.60140500	1.21728700	0.15128600	F	-2.17541500	-2.06444700	1.53436400
C	-3.44393600	-0.81433400	0.04048400	H	-0.05810500	-0.99394600	2.57701600
C	-2.72460100	1.36245000	-0.65849700				



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C	1.69864800	-1.92730100	-0.05821900	H	-1.59092400	3.62663400	-2.87956700
C	2.42318300	-0.79496600	0.36759900	H	-0.30594600	5.13073900	0.94262400
C	1.84536000	0.47204700	0.32222200	H	-1.38651700	5.50731400	-1.26443200
H	-1.39537600	-2.66756500	-1.33686400	N	-0.28385400	-0.47597800	-0.24255500
C	-0.38716900	-2.80927700	-0.97075000	C	2.97069700	1.46781100	0.57340500
C	2.28387300	-3.21174000	-0.20977500	C	3.88278600	-0.61356500	0.69855800
C	1.55358400	-4.25635600	-0.72744900	C	3.89828000	1.41367900	-0.68493000
C	0.21806800	-4.04028200	-1.13105100	C	4.52771700	-0.00999300	-0.60147400
H	3.32404400	-3.34725300	0.06664200	C	3.80692500	0.65121500	1.59105600
H	2.00584500	-5.23470700	-0.85253600	H	3.28967300	0.48066300	2.54028000
H	-0.34133300	-4.84856800	-1.59160600	H	4.79022100	1.09050400	1.78486400
C	-0.05735800	1.97471300	-0.31837300	H	4.32856800	-0.62328400	-1.48427600
C	-0.66149600	2.19781200	-1.56873300	H	4.40146300	-1.48613000	1.09653100
C	0.08393500	3.05066900	0.57495700	H	2.67680000	2.47265600	0.86739600
C	-1.13518700	3.46506000	-1.90738100	H	3.34267400	1.58210900	-1.61134700
H	-0.72917700	1.38512500	-2.28486400	H	4.66330700	2.19224100	-0.60957300
C	-0.40252000	4.31117900	0.23706700	Si	-2.17881700	-0.43969300	0.16131400

C	-3.09876800	-0.33449300	-1.49218000	H	-2.52288100	-2.90434800	0.51379900
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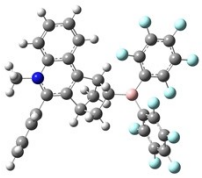
C	-2.51315200	-2.02381600	1.16150400	H	-3.97381000	-2.93472200	2.49483900
C	-4.54202600	-0.87817200	-1.46583000	H	-3.85801800	-1.18699300	2.69957800
C	-3.83757400	-1.98994800	1.95682700	H	-4.70553200	-1.86020400	1.30239600
C	-1.86995200	1.03357100	2.66876600	H	-2.44495000	1.97192400	0.78629600
H	-2.52540500	-0.85712600	-2.26862900	H	-3.65727800	0.91472800	1.45379400
H	-3.11054500	0.72016700	-1.79466900	H	-2.08515700	0.13049800	3.24922400
H	-5.16244100	-0.35964100	-0.72649100	H	-0.78146100	1.10442200	2.57284200
H	-5.01963800	-0.74337800	-2.44260700	H	-2.20158000	1.89224300	3.26285000
H	-4.56958200	-1.94806700	-1.23238300	H	5.61232600	0.03787300	-0.46621200



M

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C	-2.71827200	2.27503600	0.01916400	H	-1.63794900	0.16723000	-2.96195100
C	-2.12684900	1.12042100	-0.53386100	H	-0.17086500	-0.74555900	-2.50132700
C	-2.84592800	-0.06877900	-0.62109200	H	-0.21247000	0.37671400	1.04843000
H	-5.75163000	3.27834300	1.30932800	H	-0.15059600	1.69255800	-1.36197300
C	-4.72451800	3.31866900	0.97472700	H	-2.36845200	-2.00945500	-1.59166200
C	-2.03752500	3.51255700	0.16598400	B	1.53973900	-0.14007100	0.00576800
C	-2.67818800	4.60731900	0.69701200	C	2.40883100	1.15415800	-0.19125100
C	-4.02625100	4.50295900	1.10245300	C	3.64152800	1.12333300	-0.86594500
H	-0.99791500	3.57508100	-0.12927000	C	2.03747400	2.41082500	0.30889600
H	-2.15111200	5.54890300	0.80966700	C	4.43968200	2.24864100	-1.04208900
H	-4.52742500	5.36613300	1.52888000	C	2.81462400	3.55299800	0.16868100
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C	-5.19773600	-2.10892500	1.01148700	C	2.30725000	-1.49617700	0.27942000
C	-5.19844200	-2.07013200	-1.41615500	C	2.35687100	-2.54877400	-0.63125900
C	-5.81530700	-3.35873700	0.98779500	C	3.00079400	-1.68362600	1.47444800
H	-4.94647100	-1.64475300	1.96122300	C	3.04798300	-3.72953400	-0.38466700
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C	-6.13134100	-3.96229900	-0.23172500	F	4.08473700	-0.01793400	-1.41487700
H	-6.04643200	-3.86108400	1.92221000	F	5.59344400	2.16887800	-1.71068200
H	-6.07220200	-3.78128700	-2.38091200	F	4.77911700	4.55495300	-0.67218700
H	-6.61418000	-4.93483400	-0.24676100	F	2.41203800	4.72135700	0.67911200
N	-4.77158900	0.97234500	0.29503800	F	0.88132400	2.55141200	0.99021000
C	-1.90158100	-1.12114100	-1.16911300	F	2.98658300	-0.70536000	2.40276500
C	-0.73325100	0.82942700	-1.04472600	F	1.72498100	-2.42396200	-1.82010200
C	-0.85404600	-1.41761700	-0.05013800	F	3.07685300	-4.71149300	-1.29255100

F	4.38330200	-5.00886000	1.08655900	C	-6.21831000	0.96199100	0.61562200
F	4.33321100	-2.99802200	2.93430200	H	-6.70826700	1.76525700	0.06381400
H	-1.32716600	-1.69840500	0.89461000	H	-6.64418600	0.01159500	0.31281100
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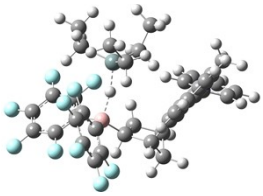

N

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C	1.85920200	-1.21883500	-1.27090100	C	-3.89433400	3.24122500	-0.88648000
C	2.78853900	-0.18203700	-1.33955900	C	-2.06340600	4.03959300	0.44042300
H	4.58394600	-3.59425800	1.58304600	C	-3.30201900	4.26253600	-0.15142400
C	3.65761400	-3.52819100	1.02947300	C	-2.28644300	-0.96500500	-0.67081600
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C	1.56708900	-4.57458200	0.34443100	C	-2.58080700	-1.71093700	-1.82026000
C	2.78013700	-4.59413700	1.06715800	C	-3.94256000	-2.40041000	0.47079000
H	0.31937500	-3.44481500	-0.97943200	C	-3.47879400	-2.77546700	-1.84786900
H	0.89825700	-5.42780600	0.38750500	C	-4.16347100	-3.13083300	-0.69086200
H	3.03744400	-5.46623300	1.65989400	F	-3.87676100	1.08701200	-1.75664800
C	4.99233200	0.85867100	-0.76933700	F	-5.07862900	3.44530000	-1.47650000
C	4.67784000	2.16516300	-0.36511200	F	-3.91163200	5.44338000	-0.02054300
C	6.22990800	0.60145400	-1.38290200	F	-1.47254000	5.00554500	1.15652800
C	5.59952200	3.19520600	-0.55269900	F	-0.23513300	2.66950500	0.87269900
H	3.72179100	2.37137700	0.10647300	F	-2.01914200	-1.40431000	-3.01057500
C	7.14100400	1.63805600	-1.57817900	F	-2.93011800	-0.64281300	1.59815500
H	6.47142000	-0.40311900	-1.71858400	F	-4.59691900	-2.70776900	1.59780100
C	6.82948000	2.93426400	-1.16005000	F	-5.02273300	-4.15236600	-0.69785000
H	5.35387300	4.20114600	-0.22618600	F	-3.70129300	-3.44394000	-2.98657800
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C	2.25581100	0.81475100	-2.35053700	C	-1.32517100	1.05606300	3.34631900
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C	1.00083400	1.48369100	-1.69667300	C	-0.32910800	-1.90156600	2.59433800
C	-0.08872600	0.35724500	-1.74076300	C	-0.70354300	2.29393700	4.01947400
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H	0.98560800	0.29190900	-4.10563500	H	-1.75193600	0.39710500	4.11359700
H	0.14630600	-1.73499500	-2.56059900	H	-2.17664400	1.36157500	2.72888400
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B	-1.27307000	0.30157300	-0.64490900	H	-1.44843000	2.79631200	4.64757400

H	0.14157100	2.03334500	4.66544100	H	2.42417200	-0.99658400	3.72319100
H	-0.70769800	-2.37349900	1.68007600	H	3.43548600	0.44641000	3.58771200
H	0.68931500	-2.29188700	2.71917900	H	-0.58348500	0.13096700	0.74794800
H	-1.17052100	-3.42470500	3.91073200	H	-0.71169800	0.57918200	-2.62247500
H	-0.85325100	-1.89370100	4.73100800	C	5.43353900	-1.34377500	1.03871000
H	-2.24396900	-2.04647000	3.64611200	H	5.13200600	-1.56370500	2.06310500
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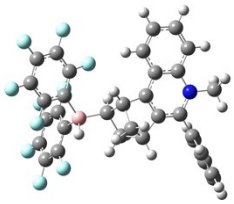
H	1.94263700	0.50137000	4.52400300				



O

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C	1.99683800	-1.32436100	-0.53919600	H	0.05572600	-1.87526500	-1.44157500
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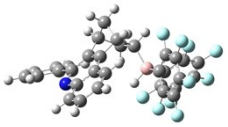
H	5.15789700	-3.35820100	2.12849400	B	-1.52550300	0.44346700	-0.83280900
C	4.16429800	-3.36640100	1.70198600	C	-2.56472300	-0.83385700	-0.73271400
C	1.54899600	-3.45403900	0.67361700	C	-3.74220100	-0.82203000	-1.48934200
C	1.99856700	-4.45863700	1.49930800	C	-2.42128900	-1.97370300	0.05712600
C	3.31305400	-4.40983100	2.00961400	C	-4.68455800	-1.84767300	-1.48983700
H	0.53239700	-3.45878800	0.30081600	C	-3.32766700	-3.03207800	0.08647200
H	1.34491300	-5.28321500	1.76464600	C	-4.47595200	-2.96759300	-0.69213100
H	3.66520200	-5.20040000	2.66517100	C	-2.09473500	1.68820800	0.08440500
C	5.01756900	0.97431400	-0.45370900	C	-2.28451800	2.97784000	-0.41642000
C	5.31628200	1.85196100	0.60103800	C	-2.40974700	1.54876900	1.43779600
C	5.50141100	1.25084800	-1.74108300	C	-2.75971100	4.04451700	0.34587300
C	6.09340800	2.98601800	0.36778600	C	-2.88965800	2.58073800	2.24008600
H	4.93123500	1.65300500	1.59728500	C	-3.06864700	3.84380100	1.68610100
C	6.28502700	2.38285500	-1.96650400	F	-4.02471900	0.23366600	-2.28623400
H	5.27056600	0.57568800	-2.55977300	F	-5.79377500	-1.76831200	-2.24856000
C	6.58062500	3.25180400	-0.91414900	F	-5.36902600	-3.97145300	-0.67746400
H	6.31378500	3.66354200	1.18734800	F	-3.10569500	-4.10874500	0.86553400
H	6.66113500	2.58559400	-2.96485900	F	-1.33245700	-2.12779900	0.85826600
H	7.18610800	4.13561100	-1.09266000	F	-2.24472100	0.34954200	2.04934600
N	4.56090700	-1.25305500	0.54138900	F	-1.98925200	3.26713200	-1.70561100
C	2.09421900	0.73982600	-1.63528700	F	-2.91929700	5.26628700	-0.19786100
C	0.70889600	-1.02588300	-1.24766300	F	-3.52553600	4.85853700	2.43963500
C	0.99400500	1.34482300	-0.70308400	F	-3.17658400	2.37471800	3.53972900
C	0.04322400	0.13969000	-0.39400200	H	1.42946700	1.79700100	0.19493700
C	1.24423700	-0.24552200	-2.47453200	H	0.46769400	2.13480600	-1.24890500

C	5.96265800	-1.31723000	1.00694900	H	6.00481600	-1.22618500	2.09478300
H	6.39845300	-2.26884800	0.69824600	H	-1.53336500	0.79894000	-1.99344800
H	6.52641500	-0.50687700	0.55736900				



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C	-1.78044600	-2.44657400	0.10318300	H	-3.24542900	1.21954600	2.41991600
C	-1.73434700	-1.33797900	0.97676000	B	0.84091500	0.32574800	0.14196700
C	-2.75923200	-0.39953900	0.97177300	C	1.54530600	1.79568100	-0.13720400
H	-3.97418200	-3.72377500	-2.20749800	C	2.67548800	2.24616500	0.54886200
C	-3.08344400	-3.66647000	-1.58856000	C	1.03746500	2.71586900	-1.05716700
C	-0.79253200	-3.46579600	0.03056400	C	3.27592900	3.48624500	0.34424900
C	-0.95317200	-4.53729200	-0.81930100	C	1.59866400	3.96994600	-1.29604400
C	-2.11037400	-4.63876600	-1.63398200	C	2.73161300	4.35857400	-0.59141100
H	0.09493300	-3.38292000	0.65066800	C	1.99433000	-0.85672900	0.04244100
H	-0.19094000	-5.31021600	-0.87107100	C	2.40544500	-1.31398300	-1.21470700
H	-2.22317100	-5.49044600	-2.29998900	C	2.63883900	-1.49084600	1.10617400
C	-4.96455400	0.43539100	-0.01472600	C	3.34535000	-2.32233100	-1.41573200
C	-4.75905700	1.81427900	0.15529400	C	3.58025500	-2.50954400	0.95837500
C	-6.26415900	-0.01510900	-0.30412300	C	3.94031900	-2.92929100	-0.31580100
C	-5.82232800	2.71304300	0.05121100	F	3.25602500	1.46013100	1.49008000
H	-3.75835400	2.19141000	0.33801800	F	4.37026100	3.85328600	1.04134300
C	-7.32678300	0.88083300	-0.40023200	F	3.28931300	5.56452600	-0.80573200
H	-6.42299200	-1.07800300	-0.45351200	F	1.05643600	4.81137400	-2.19940700
C	-7.11108400	2.25044600	-0.22034600	F	-0.07347400	2.43069800	-1.77685900
H	-5.63925700	3.77731100	0.17488900	F	2.36785600	-1.14405800	2.39011100
H	-8.32598200	0.51076500	-0.61616900	F	1.88636700	-0.76945500	-2.33938400
H	-7.93916900	2.95026900	-0.29737300	F	3.68729700	-2.71577100	-2.65909700
N	-3.93941300	-1.60871100	-0.73041200	F	4.85035200	-3.90678200	-0.48244500
C	-2.41345600	0.61588100	2.05184700	F	4.15445100	-3.08287800	2.03564300
C	-0.73890400	-0.91549300	2.03506000	H	-1.36682200	1.83122700	0.52669400
C	-1.18244700	1.42941200	1.52895800	H	-0.98830500	2.28059800	2.19387500
C	-0.00047500	0.39338500	1.55010700	H	0.06324300	0.11361600	-0.76587800
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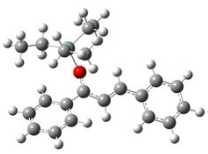
H	-2.41220900	-1.05984200	3.50832800				



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C	1.40789900	-0.81132800	2.91292800	C	3.13747700	3.79355300	-0.21086000
C	4.52325900	-1.49071800	-0.84530300	H	1.77264100	4.82565400	1.10490600
C	0.08691900	-3.84349000	-0.86233800	H	0.09009200	3.02453100	1.07866200
H	3.01368300	-0.12690100	1.61053900	H	2.60304000	0.72918800	-1.57807000
H	3.19692400	-1.77746100	2.15023200	H	4.28641700	2.53960400	-1.54093200
H	0.66124900	-0.06428800	2.61960700	H	3.87460200	4.59071200	-0.19892700
H	0.87222900	-1.73200000	3.16859500	C	0.24107500	0.66700900	-0.28430500
H	1.88937300	-0.44644000	3.82679200	C	-1.14905400	0.96053000	-0.20827200
H	3.16220700	-3.11646400	-1.28022400	C	-2.10392400	-0.02557300	-0.20796600
H	2.74536400	-1.63816000	-2.10306400	H	-1.42693100	2.00652700	-0.18115300
H	5.21011900	-1.74033600	-1.66148900	O	0.61325600	-0.56894400	-0.45938700
H	4.53883400	-0.40249900	-0.72445000	C	-3.53285900	0.13790000	-0.16271500
H	4.93291300	-1.92630900	0.07240400	C	-4.16921500	1.40237100	-0.12530200
H	1.32914000	-4.01352800	0.91322500	C	-4.33467000	-1.02781400	-0.15498300
H	-0.08746800	-3.01238800	1.14255400	C	-5.55240100	1.48808200	-0.07960800
H	-0.55913100	-3.11855300	-1.37083900	H	-3.57883500	2.31256400	-0.13458000
H	0.85798900	-4.15241900	-1.57685200	C	-5.72020200	-0.93620400	-0.10860200
H	-0.52148600	-4.72611400	-0.63570000	H	-3.85420800	-2.00177200	-0.18618000
C	1.95149600	3.93047400	0.51794300	C	-6.33021300	0.32128800	-0.07073200
C	0.99777100	2.91927100	0.49398100	H	-6.03372100	2.46053400	-0.05172700
C	1.23574400	1.73914600	-0.24214600	H	-6.32525600	-1.83716200	-0.10294700
C	2.43712300	1.61011100	-0.96877600	H	-7.41302200	0.39617900	-0.03527300
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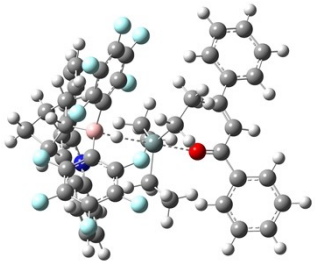

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C	-1.72003000	2.23002100	-2.15226300	H	0.79194300	4.48198500	0.19705000
C	-0.94640300	3.29310800	-1.70234600	C	2.75893800	6.46475300	-2.48599100
H	1.26210200	1.55223700	-5.54216200	H	1.80148000	5.16732300	-3.91976900
C	0.34134100	1.21621500	-5.07437500	C	2.89880800	6.79255000	-1.13406000
C	-2.04456300	0.38889500	-3.83148700	H	2.29521400	6.31179800	0.88038700
C	-1.59101100	-0.24955600	-4.96446600	H	3.31434600	7.01640400	-3.24002800
C	-0.38690000	0.16721400	-5.58884500	H	3.56340900	7.59756600	-0.83206900
H	-2.96767600	0.07252300	-3.35400200	N	0.65802900	2.93569400	-3.44609500
H	-2.15630600	-1.07576300	-5.38679700	C	-1.74019900	3.94770800	-0.57957000
H	-0.04291800	-0.34605200	-6.48284100	C	-2.98961400	2.20717100	-1.33018600
C	1.16822400	4.71273300	-1.91858300	C	-1.74306300	2.95283600	0.63081100

C	-2.70631200	1.79849400	0.17086400
C	-3.16973100	3.74139100	-1.14176000
H	-3.33738300	4.28024000	-2.08069300
H	-3.96339600	3.99415800	-0.42943000
H	-3.82459600	1.67837300	-1.78405500
H	-1.45215000	4.96964000	-0.32907300
B	-2.42050700	0.25706400	0.66503200
C	-2.39313100	0.24594600	2.31509500
C	-3.51776700	-0.00864600	3.10866700
C	-1.25806500	0.58210800	3.05523400
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C	-1.19671100	0.61701400	4.44501300
C	-2.34067800	0.33363200	5.18105300
C	-3.49378500	-0.85605800	0.07354000
C	-3.20848200	-2.22242200	0.09622800
C	-4.77513400	-0.58472200	-0.42602700
C	-4.02562600	-3.22663900	-0.41457500
C	-5.63726000	-1.54951000	-0.94543400
C	-5.26043000	-2.88688700	-0.94949500
F	-4.71236600	-0.29355400	2.54333500
F	-4.63386900	-0.23802500	5.19532700
F	-2.31566000	0.36639700	6.52084200
F	-0.04872600	0.92530300	5.07261300
F	-0.09931800	0.89896300	2.41872100
F	-5.28927300	0.66700600	-0.40889300
F	-2.05403200	-2.65883400	0.65716500
F	-3.63059000	-4.51113500	-0.38007900
F	-6.07584400	-3.82681400	-1.44661600
F	-6.84427600	-1.19760500	-1.41914000
H	-0.73332200	2.60982400	0.86529600
H	-2.12729300	3.45094200	1.52852600
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C	0.53132300	-2.02555000	1.63848400
C	1.40758200	0.64088300	-0.15139100
C	-0.00383700	-1.86238100	-1.58946300
C	1.61643200	-1.75531100	2.69220500
C	-0.09185200	-3.39869600	-1.61917500
C	2.42032300	0.80913700	-1.29865700
H	0.56914400	-3.07803100	1.33004000
H	-0.45457100	-1.88866800	2.08812300
H	2.61436500	-1.99892400	2.32254800
H	1.61373400	-0.71247300	3.02235600
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H	-0.96446600	-1.42517100	-1.88219000
H	0.71356600	-1.51841100	-2.34608400
H	-0.29492500	-3.74504000	-2.63990600
H	0.84401700	-3.86105000	-1.29397400
H	-0.89341000	-3.77104900	-0.97857800
H	0.60852100	1.37652700	-0.27590000
H	1.87789700	0.87615500	0.81115800
H	3.30385000	0.18282000	-1.16040200
H	1.98137700	0.56378600	-2.26991700
H	2.74952000	1.85239000	-1.35343200
H	-1.22200500	-0.18122400	0.30342400
H	-3.66707300	2.01012900	0.65938100
C	5.26041800	-5.80998400	-1.68621800
C	5.03158700	-4.70954400	-0.86182200
C	4.09162600	-3.73110800	-1.22955600
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C	3.64980500	-4.95620600	-3.27852200
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H	5.97348200	-6.57109500	-1.38339100
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H	2.68570300	-3.10691600	-2.73462000
H	3.12292500	-5.04409000	-4.22418700
H	4.76586900	-6.78296500	-3.54566900
C	3.80474200	-2.55122100	-0.36255400
C	4.92229100	-1.98864400	0.40058500
C	4.81007900	-0.85302900	1.13111500
H	5.87759800	-2.49198100	0.30702900
O	2.65709700	-2.06138200	-0.35194200
C	5.85480900	-0.17267300	1.88526600
C	7.18885800	-0.62787200	1.94402400
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C	8.13933200	0.06418700	2.68522600
H	7.48302900	-1.52416600	1.40687900
C	6.46643200	1.68906300	3.33578100
H	4.48877500	1.35904500	2.55568700
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H	9.16284600	-0.29751100	2.72075300
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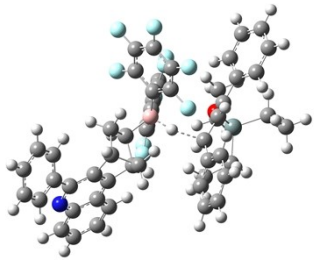
H	3.83242900	-0.37981200	1.16422400



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C	6.18310400	-1.64941300	1.46401100	H	-8.59966300	-1.14094300	0.46700700
C	3.61864800	-3.41491200	1.57580200	C	-7.93820000	2.51263900	-0.63155600
C	5.93779900	-2.17488700	-2.10897500	H	-5.89932400	1.89898200	-0.91027700
C	2.48895100	-4.17758700	0.85723400	C	-9.22758700	2.12724600	-0.26081700
C	7.18485900	-2.77954600	1.77688600	H	-10.46599900	0.49819800	0.42546500
H	4.13424300	-3.29137300	-1.64889000	H	-7.74591400	3.53104000	-0.95881300
H	5.56982800	-3.94092900	-0.90288900	H	-10.04211900	2.84623700	-0.28643900
H	6.86591400	-1.83931600	-1.63238000	N	-6.37142100	-1.99478000	-0.47422200
H	6.21514600	-2.77183200	-2.98522400	C	-4.00108100	0.83498900	0.68987700
H	5.41292000	-1.28882300	-2.47832600	C	-2.41725200	-0.78626100	0.66722000
H	4.32261300	-4.14027900	2.00940800	C	-3.03439300	1.28613300	-0.45259500
H	3.21584300	-2.86044800	2.43518200	C	-1.92882400	0.16544900	-0.49742400
H	1.95491700	-4.83560900	1.55298900	C	-2.97383000	0.23952200	1.68402100
H	1.74702600	-3.50826400	0.40695100	H	-3.44061400	-0.22724800	2.55831700
H	2.88072300	-4.80566500	0.04982400	H	-2.22195400	0.96473700	2.01403800
H	6.68304000	-0.86589300	0.88083000	H	-2.03076600	-0.37737100	-1.44428400
H	5.86730500	-1.16793800	2.39991100	H	-1.65854400	-1.47447300	1.03169200
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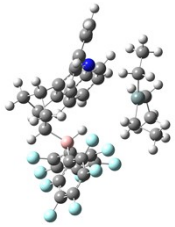
H	7.55656600	-3.25584500	0.86230900	B	-0.33365500	0.65600100	-0.39321700
H	8.05505200	-2.39225100	2.31921600	C	0.67034700	-0.13084700	-1.42952800
C	-6.02155400	-0.74676900	-0.15756900	C	1.73427400	0.43086000	-2.14792000
C	-5.42814800	-2.97477900	-0.49076400	C	0.57210500	-1.51751600	-1.59713500
C	-4.04422800	-2.74463100	-0.17579700	C	2.57012300	-0.28997900	-2.99734700
C	-3.71691700	-1.42675200	0.21725400	C	1.37932400	-2.28063500	-2.43259100
C	-4.69095400	-0.43621700	0.22524900	C	2.38980900	-1.65627400	-3.15220900
H	-6.88771800	-4.44642800	-1.07731600	C	-0.18581500	2.28415500	-0.42893700
C	-5.83804900	-4.29098600	-0.84548200	C	-0.01349800	3.09473900	0.68926800
C	-3.12811600	-3.82982100	-0.24562400	C	-0.36667900	2.99346700	-1.62036500
C	-3.56065600	-5.08857700	-0.59947900	C	0.02555900	4.48870000	0.64831800
C	-4.92773300	-5.32180400	-0.89755000	C	-0.33762500	4.37933700	-1.71743200
H	-2.07948400	-3.65213900	-0.03266200	C	-0.13540200	5.13853000	-0.56773600
H	-2.85213100	-5.91071500	-0.65488300	F	2.05824500	1.73766900	-2.02521700
H	-5.25291500	-6.32149700	-1.17331900	F	3.60932800	0.31517000	-3.60679400
C	-7.11477100	0.26530700	-0.18778700	F	3.21514700	-2.37362700	-3.92917900
C	-8.42057900	-0.11357500	0.16758800	F	1.23864700	-3.61591800	-2.49925900

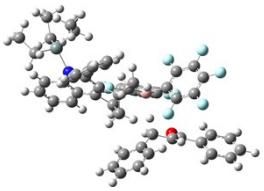
F	-0.32319200	-2.22722500	-0.86279900	H	7.31972700	4.03559500	0.14768100
F	-0.59197000	2.31444900	-2.76856300	C	3.53031200	0.30867900	0.90023100
F	0.11129100	2.54536700	1.92622400	C	2.44396300	0.54814500	1.72293900
F	0.20680300	5.20353000	1.77319800	C	1.37625000	-0.35817500	1.89591100
F	-0.10422800	6.47818800	-0.63497600	H	2.41577500	1.50180800	2.23322900
F	-0.50928200	4.99409900	-2.90034300	O	3.65052100	-0.83219900	0.21235300
H	-3.54926400	1.39637000	-1.41349400	C	0.57003300	-0.46312300	3.10783100
H	-2.62416500	2.26527600	-0.19343300	C	0.50694500	0.55073500	4.08665900
H	0.14124500	0.27080000	0.76021100	C	-0.10905200	-1.67650100	3.34715500
C	5.94143100	3.15678500	1.55513400	C	-0.21619300	0.35314900	5.25738700
C	4.95765800	2.19299300	1.75885500	H	1.01295400	1.49515000	3.92788600
C	4.58619300	1.32391200	0.71559800	C	-0.82458300	-1.87422100	4.52358500
C	5.21589600	1.45051500	-0.53679300	H	-0.06100800	-2.46792900	2.60418800
C	6.18656600	2.42839600	-0.73884400	C	-0.88269000	-0.85709300	5.48038400
C	6.55655100	3.27913200	0.30608000	H	-0.26080600	1.14273100	6.00146600
H	6.23181200	3.80971500	2.37285200	H	-1.33595700	-2.81656300	4.69477300
H	4.50260600	2.09036100	2.73893200	H	-1.44406400	-1.00594300	6.39825100
H	4.90813400	0.81580900	-1.35949900	H	1.41620400	-1.26012200	1.29343100
H	6.65074700	2.53020100	-1.71530100				



$TS_1(-)$

C	3.10414600	-0.09372700	-1.50794800	H	5.77224400	-0.42070300	-1.48874600
C	2.51941000	-2.25313100	-0.83770000	C	6.13453800	2.96542200	-1.41101500
C	1.22705600	-2.18263500	-1.45948300	H	4.49892800	4.37180300	-1.38153000
C	0.94508800	-0.98998900	-2.16066200	H	7.53705800	1.32524300	-1.44230800
C	1.89044800	0.02816600	-2.22825700	H	6.90405000	3.73232900	-1.38893300
H	3.89552500	-3.51996900	0.24021600	N	3.40118100	-1.21455000	-0.83634900
C	2.90026900	-3.46485300	-0.19258500	C	1.30664500	1.09997800	-3.14033800
C	0.35713700	-3.30455100	-1.38190100	C	-0.25269400	-0.54075300	-2.96212300
C	0.75191400	-4.45580000	-0.73781900	C	0.14518000	1.79595100	-2.36115300
C	2.03781000	-4.53858100	-0.14546300	C	-0.93645500	0.66685000	-2.19963300
H	-0.62286700	-3.24328200	-1.84413700	C	0.48787600	0.20405400	-4.10507400
H	0.08199700	-5.30944700	-0.68834900	H	1.11451500	-0.44988400	-4.72294700
H	2.34436300	-5.45999500	0.34241200	H	-0.18952500	0.77605800	-4.74943000
C	4.13958800	0.97718300	-1.48077200	H	-0.95287800	-1.32328900	-3.25568600
C	3.79587000	2.33957100	-1.45080700	H	2.03165300	1.77978800	-3.59240400
C	5.50218600	0.62977000	-1.46724700	B	-1.38366400	0.44488300	-0.63181200
C	4.78533800	3.32400200	-1.41232200	C	-2.20275200	1.78234800	-0.10302800
H	2.75121600	2.63234700	-1.43570500	C	-3.55756300	2.01379000	-0.35831600
C	6.48906300	1.61332900	-1.43833900	C	-1.58706000	2.81065500	0.61372200

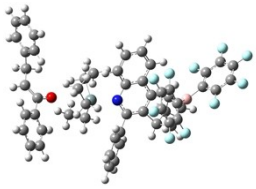
C	-4.25757800	3.13941200	0.07135400	C	4.21749000	0.49543800	2.35757700
C	-2.23900800	3.95704300	1.06405500	C	2.38304200	-2.04076200	3.11199000
C	-3.59167600	4.12311100	0.79336300	C	0.99677600	1.27475800	4.57042100
C	-2.25169100	-0.92443400	-0.31474100	C	1.09762900	-2.52462400	3.80898500
C	-2.15082500	-1.55115700	0.92882700	C	5.39980600	-0.47179500	2.18892200
C	-3.10389000	-1.58668900	-1.20199200	H	0.22326500	0.47950300	2.68252300
C	-2.79379200	-2.73588800	1.27580100	H	1.30061200	1.85384800	2.48190900
C	-3.77499300	-2.77279000	-0.90659300	H	1.89034700	1.76143900	4.97473200
C	-3.61918800	-3.35633900	0.34595600	H	0.15843500	1.96659000	4.69712600
F	-4.27916300	1.11559900	-1.07063600	H	0.78454700	0.38620800	5.17309400
F	-5.56609900	3.28843400	-0.20740800	H	2.48891000	-2.52802800	2.12714000
F	-4.24317500	5.21990200	1.21590600	H	3.28351200	-2.34681600	3.66486100
F	-1.57463800	4.90437200	1.75485700	H	1.12180800	-3.61518800	3.90052500
F	-0.26039800	2.75158100	0.91020800	H	1.00354500	-2.11144400	4.81807800
F	-3.31718100	-1.09655400	-2.44644800	H	0.20084700	-2.25858800	3.24393700
F	-1.37193900	-1.01538400	1.91140400	H	4.07610800	1.10141600	1.45020700
F	-2.62082600	-3.28416200	2.49456900	H	4.40829600	1.23267000	3.15602600
F	-4.25600200	-4.49925900	0.65175100	H	5.56424300	-1.07969200	3.08455700
F	-4.57848200	-3.35608300	-1.81563300	H	5.23235900	-1.13366800	1.33513200
H	0.48014100	2.19272700	-1.39826600	H	6.31629900	0.09523700	1.99834800
H	-0.23128500	2.64109200	-2.95078300	H	-0.37165800	0.35466000	0.04054000
Si	2.55729700	-0.22451400	2.77310600	H	-1.80458200	0.93303500	-2.81678800
C	1.14269300	0.93910400	3.05893300				



$TS_2(-)$

Si	6.45661700	0.43822900	-0.78934100	H	6.59685600	1.62233800	-3.75919400
C	6.28610600	-0.90111900	-2.12833400	H	7.87389400	0.77806200	1.22090600
C	8.03928400	0.30475700	0.24445300	H	8.21177500	-0.75724200	0.45764600
C	6.23296400	2.12790300	-1.64371900	H	9.52601200	0.43808100	-1.37417600
C	7.33761600	-2.02562000	-2.14177400	H	9.18558300	1.98541600	-0.58861000
C	6.98707900	2.28603700	-2.98169200	H	10.17151800	0.77239200	0.23336000
C	9.29685700	0.91012700	-0.41215000	C	4.19813500	-0.83166400	0.47306400
H	6.35055700	-0.35304500	-3.07607400	C	4.43363200	1.50622400	0.92715900
H	5.27839700	-1.32729000	-2.11684600	C	3.02835900	1.64967600	1.16127000
H	7.29965900	-2.63836200	-1.23773800	C	2.23064500	0.49645900	0.99895700
H	7.17506500	-2.68899500	-2.99891700	C	2.82916000	-0.73886700	0.73154600
H	8.35328800	-1.62423100	-2.23031400	H	6.35974600	2.46764100	1.19272200
H	5.16029900	2.28923100	-1.81541400	C	5.28565000	2.58290600	1.26248700
H	6.54670900	2.93357500	-0.97382500	C	2.52097900	2.89096500	1.63079100
H	6.87941900	3.31223200	-3.35076200	C	3.37126500	3.93603700	1.90776100
H	8.05962300	2.08756600	-2.88186900	C	4.76340500	3.76615700	1.74592700

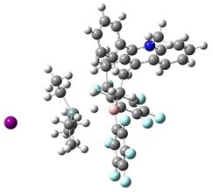
H	1.45294400	2.99445900	1.77690200
H	2.97948300	4.87869700	2.27580300
H	5.43917200	4.57061500	2.01974300
C	4.87011800	-2.15146600	0.41411900
C	5.95682400	-2.39099700	1.27404200
C	4.37090800	-3.20940000	-0.36550400
C	6.53255800	-3.65998400	1.34855700
H	6.31861800	-1.59380700	1.91567000
C	4.95961200	-4.47000600	-0.30016700
H	3.53488500	-3.03943100	-1.03660800
C	6.03794100	-4.70011700	0.55991000
H	7.35918100	-3.83581800	2.03053400
H	4.57310200	-5.27549200	-0.91724500
H	6.48559800	-5.68785100	0.61779700
N	4.96473000	0.31031200	0.42996000
C	1.72864400	-1.78112800	0.81754200
C	0.75533800	0.24585300	1.17529100
C	0.81635800	-1.60351800	-0.43499900
C	0.22528600	-0.16068300	-0.27122200
C	0.82121100	-1.13020200	1.88754300
H	1.28249200	-1.07417200	2.87862200
H	-0.15600600	-1.60791900	1.96803600
H	0.73398300	0.48588500	-0.99682500
H	0.18729700	1.02761400	1.67272900
H	2.05550000	-2.80490000	0.99922900
B	-1.34235800	0.09530600	-0.61479900
C	-1.83391700	1.57872500	-0.95140200
C	-3.13875300	1.86254900	-1.40238400
C	-1.04354100	2.72916600	-0.79205400
C	-3.61572100	3.14209900	-1.65879700
C	-1.47878200	4.02603600	-1.04308200
C	-2.78015600	4.23821100	-1.47965300
C	-2.11795500	-1.12725300	-1.30212300
C	-2.49170600	-2.29250600	-0.62871900
C	-2.41437500	-1.13067000	-2.67013400
C	-3.13947100	-3.36573400	-1.23588000
C	-3.05109100	-2.18095500	-3.32039300
C	-3.42535800	-3.30810900	-2.59410500
F	-4.02322300	0.87702800	-1.61012100
F	-4.87180300	3.32849000	-2.08379200
F	-3.21870800	5.47782100	-1.72684500
F	-0.64928600	5.06931700	-0.86835500
F	0.24375700	2.64079300	-0.37213500
F	-2.06156500	-0.07574600	-3.43634700
F	-2.19273700	-2.44718400	0.68252100
F	-3.47156200	-4.45501400	-0.52550800
F	-4.03857500	-4.33137300	-3.20242900
F	-3.30027700	-2.12352200	-4.63842800
H	1.35956600	-1.71942000	-1.37882000
H	0.04829900	-2.37803800	-0.40353300
H	-2.28067100	0.03406400	0.95322100
C	-8.52075800	-1.70048400	1.40136400
C	-7.24587300	-1.18016300	1.63310000
C	-6.78351500	-0.06018800	0.92359300
C	-7.64342300	0.52927500	-0.01720200
C	-8.91282300	0.00611400	-0.25978200
C	-9.35882800	-1.11283400	0.45009300
H	-8.86314500	-2.56222100	1.96998800
H	-6.61382100	-1.63470000	2.39068200
H	-7.28300200	1.40374200	-0.55037700
H	-9.55842400	0.47169900	-1.00128800
H	-10.35094400	-1.51902100	0.26842400
C	-5.41860800	0.56956400	1.12252700
C	-4.37954600	-0.23760600	1.62197200
C	-3.04749500	0.31520100	1.83852900
H	-4.55912700	-1.28705500	1.82694100
O	-5.30264500	1.79157300	0.81206000
C	-2.35794700	-0.05069800	3.13798600
C	-1.73480100	0.95162500	3.89723900
C	-2.35013700	-1.35981400	3.64737300
C	-1.12646300	0.66372800	5.12215300
H	-1.74375900	1.97594700	3.53028300
C	-1.74327000	-1.65261700	4.86899900
H	-2.82482100	-2.15592200	3.08292300
C	-1.12729100	-0.64231100	5.61401400
H	-0.66089700	1.46276700	5.69424700
H	-1.75449000	-2.67353300	5.24328100
H	-0.66069000	-0.87081600	6.56875700
H	-3.09167700	1.40323000	1.72697500



TS_3(-)

C	0.09356400	-1.42705900	-1.55114400	C	8.12376800	1.20095900	0.89587800
C	0.01818700	0.85806500	-0.89379500	C	8.30126000	2.28806100	0.04504900
C	1.33530300	1.10532700	-1.40549200	C	4.00121400	-0.59386100	1.12778000
C	1.98234500	0.02563900	-2.03935600	C	3.39826600	0.43735200	1.85144300
C	1.38043100	-1.22527000	-2.08183400	C	3.99444000	-1.84890400	1.73920000
H	-1.54538300	1.69619900	0.34866200	C	2.77356300	0.24014900	3.07848600
C	-0.59935500	1.88148500	-0.13679400	C	3.39601200	-2.08582900	2.97235000
C	1.93149900	2.38310000	-1.23532100	C	2.77559600	-1.03350600	3.64178200
C	1.27759100	3.37259300	-0.53970900	F	5.30186100	2.11470600	-1.94878300
C	0.01580200	3.10423700	0.03428200	F	7.49063500	3.62815800	-1.72594000
H	2.92481800	2.55439500	-1.63462600	F	9.39151300	3.04792600	0.14597000
H	1.73934700	4.34530200	-0.40385300	F	9.05493700	0.90860700	1.80978200
H	-0.47640200	3.86485100	0.63248200	F	6.86789200	-0.62474700	1.61273900
C	-0.42110300	-2.81248400	-1.39096700	F	4.62800600	-2.88213400	1.14935800
C	-0.45367900	-3.72072400	-2.46354300	F	3.39666000	1.68595000	1.34293400
C	-0.79136600	-3.25806700	-0.11209800	F	2.18597100	1.25608100	3.72082300
C	-0.87354300	-5.03292400	-2.26373900	F	2.19039000	-1.24428700	4.82248100
H	-0.19076500	-3.38746500	-3.46275100	F	3.42241700	-3.30482900	3.52352900
C	-1.20304100	-4.57667900	0.08681400	H	3.10569100	-2.57865700	-0.62962500
H	-0.73222500	-2.57948300	0.73187100	H	4.21853700	-3.14014200	-1.87105500
C	-1.24961600	-5.46490200	-0.98801000	Si	-2.66777700	-0.35862300	-1.08022200
H	-0.91313600	-5.71815400	-3.10527400	C	-3.10842100	-1.72851800	-2.32626400
H	-1.48242900	-4.90694000	1.08280800	C	-3.14694400	1.30209200	-1.84263800
H	-1.57419800	-6.48985700	-0.83444400	C	-3.04821900	-0.64694800	0.75913900
N	-0.62484200	-0.36628800	-1.08228100	C	-4.35855000	-1.46173000	-3.19191500
C	2.41005700	-2.17814500	-2.67370000	C	-3.66690800	0.52377900	1.54481100
C	3.36184400	-0.11389700	-2.64296900	C	-2.47372700	1.69952900	-3.16730700
C	3.53457500	-2.33031900	-1.60017900	H	-3.23479600	-2.67009900	-1.78014400
C	4.28148300	-0.94994600	-1.62748300	H	-2.25392200	-1.88313000	-2.99196900
C	3.07626700	-1.22209600	-3.68828300	H	-4.18782300	-0.64116000	-3.89762500
H	2.39593200	-0.89062000	-4.47912600	H	-4.59164200	-2.35576700	-3.78435300
H	3.98801800	-1.62842500	-4.13661600	H	-5.21826700	-1.19807600	-2.57125700
H	3.82759300	0.79875700	-3.00182600	H	-3.75609100	-1.48286600	0.77542000
H	2.03533600	-3.12543000	-3.05380100	H	-2.13695300	-0.99207400	1.26263100
B	4.71467500	-0.28702100	-0.25314500	H	-3.96803500	0.18774500	2.54438600
C	5.97405200	0.66997900	-0.17384000	H	-2.96640600	1.35497800	1.69060800
C	6.20950800	1.76558700	-1.01142400	H	-4.55331700	0.89467000	1.02783800
C	6.97361500	0.42707000	0.78043000	H	-4.22509300	1.14061200	-1.98225600
C	7.33337400	2.57775500	-0.91326800	H	-3.07617200	2.12386800	-1.12431400

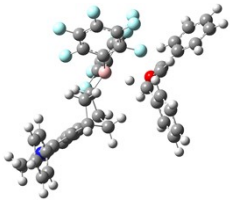
H	-1.41598400	1.95113900	-3.03188000	C	-7.75490900	0.78234400	0.00579200
H	-2.52862800	0.89957600	-3.91408500	C	-7.66517400	2.05673200	-0.78570500
H	-2.96391300	2.57995500	-3.59946500	H	-8.65179800	0.62159000	0.59841700
H	-8.45997200	2.12404600	-1.54889600	O	-5.71722700	-0.15666600	-0.79393400
H	5.21389000	-1.07806200	-2.19421300	C	-7.71093100	3.34671100	0.02616600
C	-7.88357200	-2.65844800	2.69304500	C	-7.03034900	3.46049600	1.24808000
C	-7.71227500	-1.47491900	1.97359300	C	-8.41516200	4.46765100	-0.43667400
C	-7.00178800	-1.45363000	0.75977000	C	-7.04268700	4.65226000	1.97407600
C	-6.45032900	-2.66562400	0.30957500	H	-6.50225700	2.58976100	1.62886300
C	-6.62449400	-3.85356900	1.02144300	C	-8.43557000	5.66340300	0.28633500
C	-7.34346400	-3.85806100	2.21974800	H	-8.95775800	4.39961000	-1.37821900
H	-8.43185900	-2.64267400	3.63271700	C	-7.74667600	5.76211900	1.49675800
H	-8.11666600	-0.54622900	2.36614300	H	-6.50594800	4.71492800	2.91839200
H	-5.88847500	-2.65482300	-0.61909100	H	-8.99470400	6.51550300	-0.09394800
H	-6.19768200	-4.77953900	0.64079700	H	-7.76307400	6.68907800	2.06478600
H	-7.47475300	-4.78009300	2.78105200	H	-6.71854500	2.02012700	-1.34309500
C	-6.78833600	-0.19719200	-0.05834200				



$TS_1'(-)$

C	4.58392200	2.15656100	-0.08069300	H	3.19271500	5.78100300	2.47882300
C	5.80682300	0.09258300	-0.37137200	H	4.33803000	7.41472300	0.99512200
C	4.61828500	-0.59027000	-0.78529100	N	5.74581300	1.43867200	-0.01390000
C	3.42751700	0.16064800	-0.84799200	C	1.99483600	1.99596400	-0.65840600
C	3.42190200	1.50997200	-0.49988200	C	2.01346600	-0.20694800	-1.21897800
H	7.95136400	-0.13349600	-0.04937300	C	1.16957800	1.32837800	0.48815300
C	7.02884800	-0.61973700	-0.33452300	C	1.22949800	-0.20405200	0.16197600
C	4.68925000	-1.96654100	-1.12754700	C	1.55853600	1.12612200	-1.86393500
C	5.88613400	-2.64201900	-1.07130100	H	2.09751400	1.36502000	-2.78630200
C	7.05731800	-1.95736100	-0.67856600	H	0.48455400	1.15444900	-2.05705700
H	3.78063700	-2.47441800	-1.43277400	H	1.87692100	-0.69310700	0.90095300
H	5.93610200	-3.69406100	-1.33182800	H	1.90428800	-1.11204000	-1.81216700
H	8.00351100	-2.48829200	-0.64725200	H	1.86682700	3.07517100	-0.74157700
C	4.56352700	3.60970400	0.24130700	B	-0.13365600	-1.10296600	0.24504400
C	5.20926600	4.53533800	-0.59540300	C	-0.17559600	-2.29811200	-0.84961500
C	3.82860200	4.06810100	1.34525600	C	-0.56274800	-2.13563600	-2.18002200
C	5.12457700	5.90012200	-0.32267200	C	0.30531200	-3.57320800	-0.53693900
H	5.76358900	4.18835200	-1.46288200	C	-0.53005600	-3.15440500	-3.12916400
C	3.75631400	5.43473200	1.61784600	C	0.36712800	-4.62000400	-1.45330100
H	3.32495300	3.35736500	1.99370100	C	-0.05978000	-4.41063400	-2.76087600
C	4.40155900	6.35126400	0.78475900	C	-0.66487500	-1.53003700	1.71867900
H	5.61971800	6.61020100	-0.97812500	C	-0.12136800	-1.09489200	2.93388700

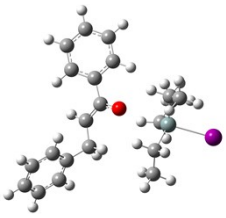
C	-1.72544800	-2.43710800	1.86779900	C	-2.71625300	1.59629500	1.38127700
C	-0.56805600	-1.52289500	4.18343400	C	-4.03750800	-0.55010000	-0.48621200
C	-2.20709700	-2.88790300	3.09211000	C	-2.44716500	1.83182000	-1.75034000
C	-1.61900100	-2.42751400	4.26629600	C	-3.48424800	0.91268000	2.52738500
F	-0.99939100	-0.92920100	-2.61338800	C	-1.75050000	3.18583200	-1.53177000
F	-0.93000000	-2.93126900	-4.38789700	C	-4.09226600	-1.40498700	-1.76316700
F	-0.00822000	-5.40275100	-3.65600300	H	-3.21952800	2.54193700	1.13260500
F	0.83732900	-5.82109400	-1.08825400	H	-1.70926400	1.87692100	1.71505700
F	0.75388900	-3.84014500	0.70890400	H	-3.01387700	-0.02469300	2.83866800
F	-2.35682200	-2.92568700	0.77913000	H	-3.52641500	1.56825600	3.40488300
F	0.90759900	-0.22087200	2.96965900	H	-4.51581300	0.68847900	2.23772600
F	0.01310200	-1.06874800	5.30260600	H	-2.00254000	1.29666700	-2.59657200
F	-2.05759000	-2.85021100	5.45455800	H	-3.49573800	2.02039600	-2.02911800
F	-3.22145600	-3.75986800	3.14942900	H	-1.79034900	3.78729800	-2.44724500
H	1.56143200	1.56494400	1.47885400	H	-2.24014000	3.76558000	-0.74279600
H	0.14574700	1.70835200	0.44601900	H	-0.69533800	3.07729600	-1.25903200
C	6.98154200	2.06281200	0.51098300	H	-4.11078500	-1.19098200	0.39867300
H	7.37213400	1.44677200	1.32199500	H	-4.91648600	0.11389300	-0.45117200
H	7.72564700	2.14915400	-0.28395600	H	-3.96427600	-0.80296700	-2.66892100
H	6.74888900	3.04955700	0.89624600	H	-3.31752000	-2.17704200	-1.75701900
Si	-2.61558900	0.66670000	-0.26858500	H	-5.06105100	-1.91174700	-1.84037000
H	-1.23780100	-0.19659800	-0.18949700	I	-6.48732800	3.27187200	-0.96131700



$TS_2'(-)$

C	-5.09365500	-0.73781200	0.18776800	H	-7.10994100	-0.65202400	2.01948400
C	-4.56002300	-3.02381100	-0.37262300	C	-6.95978500	2.53308600	-0.19326900
C	-3.17637900	-2.80960600	-0.06671600	H	-5.30108900	1.58407000	-1.18906700
C	-2.79657800	-1.52203300	0.36895200	C	-7.92081400	2.42535400	0.81381200
C	-3.75819800	-0.51832400	0.51125200	H	-8.71327500	1.19324700	2.39873000
H	-6.02489500	-4.51316500	-0.99274400	H	-6.91459500	3.42368400	-0.81285400
C	-4.98600900	-4.31281600	-0.77057700	H	-8.62490900	3.23493500	0.98209800
C	-2.26976500	-3.89839100	-0.17245900	N	-5.46703800	-1.97230900	-0.26821700
C	-2.70700800	-5.14186200	-0.56416400	C	-3.04927600	0.70167800	1.06230500
C	-4.07205500	-5.34384700	-0.86035100	C	-1.47334600	-0.92023000	0.77948400
H	-1.22414800	-3.72626500	0.04641200	C	-2.14226300	1.27830000	-0.06351900
H	-2.00754400	-5.96754900	-0.64351600	C	-1.12465400	0.12587800	-0.37088200
H	-4.41720500	-6.32827600	-1.16101500	C	-1.97090500	0.00369600	1.92431700
C	-6.10526900	0.33823500	0.38050400	H	-2.38088900	-0.55166400	2.77445800
C	-7.07223800	0.23540200	1.39393800	H	-1.20308400	0.69180200	2.27980100
C	-6.04896600	1.49790700	-0.40658100	H	-1.41307200	-0.32929100	-1.32495300
C	-7.97328900	1.27742900	1.60840600	H	-0.68316800	-1.62780900	1.01838300

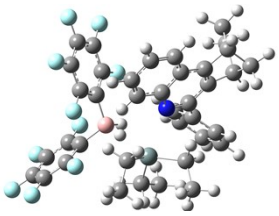
H	-3.68861300	1.43542700	1.55409000	H	1.16369200	0.46255400	0.85524900
B	0.43771400	0.55733300	-0.60490700	C	7.59717200	-0.15165900	1.89105500
C	1.46874100	-0.46371400	-1.27100900	C	6.20260600	-0.15323000	1.95540500
C	2.80443700	-0.11040800	-1.53829500	C	5.44968000	-1.11614700	1.26417900
C	1.18430500	-1.80925600	-1.54791800	C	6.13881500	-2.08434700	0.51655800
C	3.76335300	-1.00079800	-2.01167200	C	7.53088800	-2.07995700	0.44173200
C	2.11190800	-2.73229200	-2.00427400	C	8.26779000	-1.11231000	1.13016600
C	3.42602800	-2.33008200	-2.21316700	H	8.16084000	0.59785700	2.44153900
C	0.59777100	2.09784300	-1.10552300	H	5.70088400	0.58865400	2.56903900
C	1.40808500	3.09361400	-0.55987500	H	5.55541300	-2.83584400	-0.00510400
C	-0.12106300	2.50523700	-2.23443300	H	8.04347100	-2.83300400	-0.15241300
C	1.47554600	4.39578600	-1.05061000	H	9.35375500	-1.10960700	1.07837500
C	-0.08316500	3.79087300	-2.76553800	C	3.93472700	-1.19443100	1.30374700
C	0.72340300	4.75018400	-2.16426800	C	3.21391300	-0.02882000	1.67347700
F	3.23298900	1.15806500	-1.38091900	C	1.78520400	-0.06032300	1.83871400
F	5.02195100	-0.59026400	-2.23471000	H	3.74160200	0.89546800	1.87949400
F	4.34914900	-3.21261000	-2.61859500	O	3.40640900	-2.30257800	1.01652900
F	1.75590200	-4.00837300	-2.23322000	C	1.23587400	0.58310700	3.09362600
F	-0.07344000	-2.29513700	-1.38490500	C	1.13991000	1.96931300	3.28517000
F	-0.91787700	1.61937300	-2.88169600	C	0.84886300	-0.25832900	4.15113400
F	2.20445200	2.82669700	0.49660000	C	0.67232400	2.49396300	4.49330800
F	2.27145500	5.30537200	-0.46585100	H	1.43332100	2.64161700	2.48862700
F	0.77639800	5.99696000	-2.65286900	C	0.38446800	0.26385400	5.35840300
F	-0.80928900	4.10811000	-3.85063200	H	0.92378500	-1.33596700	4.02495100
H	-2.70329500	1.58243300	-0.95157300	C	0.29176600	1.64674900	5.53533900
H	-1.64173800	2.16913400	0.32895900	H	0.60644200	3.57223600	4.61774800
C	-6.85574600	-2.21525500	-0.71693700	H	0.09432200	-0.41036000	6.16057300
H	-6.83530600	-2.64002200	-1.72135100	H	-0.07158800	2.05775800	6.47358600
H	-7.35866500	-2.90295500	-0.03321200	H	1.43460200	-1.09133600	1.74014800
H	-7.39366700	-1.27373900	-0.74146700				



TS_3'(-)

C	-3.65528800	4.48386900	-0.18077400	H	-0.05072800	3.11910500	0.11986500
C	-3.42192900	3.10800100	-0.14306500	H	-0.44242800	5.57356100	0.03067200
C	-2.11735900	2.58860400	-0.05351100	H	-2.76685300	6.45578500	-0.14941800
C	-1.05854000	3.50920700	0.02379400	C	-1.81209400	1.10273700	0.00343300
C	-1.28442200	4.88588500	-0.02038400	C	-2.69751500	0.25142600	-0.62522500
C	-2.58636500	5.38366000	-0.12433300	C	-2.54522600	-1.24571600	-0.61440200
H	-4.67628500	4.85537900	-0.24147800	H	-3.54235600	0.65863700	-1.17454000
H	-4.26401200	2.42192400	-0.15809700	O	-0.72537600	0.76154400	0.62228000

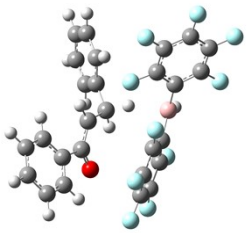
C	-3.81403700	-2.00268400	-0.25015300	C	2.02839800	1.38708900	-2.26738800
C	-4.51789000	-1.69904300	0.92711500	C	1.09102200	-2.95427600	0.19448800
C	-4.31653600	-3.02422300	-1.06774300	H	1.17169200	1.68192500	1.41941200
C	-5.67307700	-2.39768700	1.27823400	H	2.76110300	2.10210900	0.76097400
H	-4.15025100	-0.89615800	1.56149200	H	3.87568000	0.72777800	2.59666500
C	-5.47786600	-3.72497600	-0.72585600	H	2.86231500	2.01185000	3.27238700
H	-3.78946600	-3.27279500	-1.98719900	H	2.28112500	0.34457100	3.26182700
C	-6.16137500	-3.41561600	0.45099700	H	1.71979500	-0.76216300	-2.19287400
H	-6.19707400	-2.14745500	2.19816200	H	0.36169800	0.18171800	-1.56938500
H	-5.84810200	-4.50991700	-1.38175400	H	1.67246100	1.48190800	-3.30086700
H	-7.06504500	-3.95679200	0.72073800	H	1.72159800	2.29380800	-1.73365000
H	-2.18979400	-1.64296500	-1.58263100	H	3.12456500	1.36862100	-2.29582800
H	-1.75805200	-1.48912400	0.11202200	H	1.89107900	-1.91711400	1.92956400
Si	2.00394500	-0.18097700	0.18513500	H	0.29985700	-1.33498900	1.41877300
C	2.20404000	1.32871400	1.30617000	H	0.43301000	-2.76695900	-0.66175700
C	1.27028300	-1.69198500	1.05242900	H	2.04981000	-3.31802100	-0.19407000
C	1.45506600	0.12478600	-1.60239700	H	0.64193600	-3.76729500	0.77878400
C	2.84339000	1.08646100	2.68269400	I	4.51140400	-0.93511300	-0.19986100



$TS_1''(-)$

C	2.68161500	-0.96232600	-0.27136500	C	1.69879000	-3.86693100	-3.28458800
C	2.17533200	0.68343100	1.32815900	H	0.44615700	-2.32069000	-4.11717600
C	3.52720000	1.17083200	1.35529200	H	3.03467100	-5.19113200	-2.22453900
C	4.45388400	0.49456500	0.53799900	H	1.47717400	-4.58493000	-4.06932500
C	4.02927500	-0.53769900	-0.28329300	N	1.78853700	-0.40256600	0.56611100
H	0.17625400	1.07694600	2.04055100	C	5.21884500	-0.92054900	-1.15231900
C	1.20868100	1.38311600	2.09425000	C	5.92290100	1.42488700	-1.19476200
C	3.86083300	2.29015300	2.16383800	C	6.36770200	-0.68255200	-0.13933900
C	2.89651700	2.93009200	2.90720200	C	5.91057000	0.75407000	0.22272100
C	1.55823500	2.47539200	2.85841300	C	5.44863400	0.27409200	-2.13672100
H	4.88847100	2.64030700	2.17415600	H	4.54156500	0.52492800	-2.69342900
H	3.15479100	3.79018100	3.51764400	H	6.22381700	0.01166800	-2.86403800
H	0.78917300	3.00226700	3.41585300	H	6.48493000	1.28858100	0.98097500
C	2.27131800	-2.00816900	-1.25634600	H	6.94153800	1.74493000	-1.43657900
C	1.40057300	-1.67217000	-2.30283800	H	5.17258900	-1.89586000	-1.63451100
C	2.86779700	-3.28061800	-1.25011100	B	-1.51332100	-0.06549100	-0.45895200
C	1.11848900	-2.59791900	-3.31011700	C	-1.16052900	1.51681400	-0.56726200
H	0.96228300	-0.68262900	-2.34071100	C	-1.49509800	2.43564000	0.42874000
C	2.57381400	-4.20759400	-2.24971900	C	-0.55757800	2.08356400	-1.69205500
H	3.56568400	-3.54502500	-0.46024400	C	-1.24505400	3.80144700	0.35041300

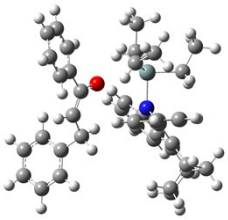
C	-0.29266000	3.44616500	-1.82281100	C	-0.66969700	-0.99300700	3.24091200
C	-0.64275300	4.31349400	-0.79435100	C	1.60815500	-2.75632500	2.15614900
C	-3.12219500	-0.32033800	-0.40445900	C	-1.18322500	-3.13010300	0.94971900
C	-3.83191900	-0.36016200	-1.61036000	C	-1.57277300	-1.92590600	4.08015700
C	-3.91886700	-0.46061800	0.73067700	C	-0.73062000	-3.99469900	-0.23457700
C	-5.21052900	-0.53484300	-1.69581300	C	1.38412800	-3.88338200	3.18679500
C	-5.30020400	-0.64483800	0.69680400	H	-1.24220900	-0.09891100	2.99171900
C	-5.95368800	-0.67875800	-0.52882700	H	0.19063200	-0.67182900	3.84040200
F	-2.06657100	1.99611600	1.57798300	H	-1.07582500	-2.85692200	4.36922600
F	-1.57196300	4.62477900	1.36144300	H	-1.86949100	-1.41530600	5.00439600
F	-0.39210000	5.62688400	-0.89909800	H	-2.48815200	-2.18213300	3.54044900
F	0.29167500	3.93038600	-2.93226300	H	-1.36579800	-3.78047400	1.82045800
F	-0.18778800	1.31334900	-2.74114500	H	-2.13930100	-2.65080100	0.72403700
F	-3.36085400	-0.45040500	1.96472900	H	-1.47755300	-4.76881600	-0.44908200
F	-3.17794700	-0.21341300	-2.78334500	H	-0.60143300	-3.39663400	-1.13974800
F	-5.82974900	-0.56319500	-2.88869700	H	0.21907200	-4.50145300	-0.03399400
F	-7.28301700	-0.85053300	-0.58654900	H	2.06575200	-3.18353100	1.26034700
F	-6.00324100	-0.78609800	1.83423000	H	2.32607100	-2.03474300	2.56090400
H	6.34207900	-1.37019200	0.71219200	H	1.02666200	-3.49903200	4.14729900
H	7.36064100	-0.70947400	-0.60093100	H	0.66662600	-4.63363200	2.83681400
H	5.27768500	2.30679000	-1.23667600	H	2.32904600	-4.40598400	3.38096500
H	-1.03754400	-0.68831700	-1.36463700	H	-0.91814900	-0.52568700	0.59273500
Si	0.00410900	-1.83195500	1.66311600				



$TS_2''(-)$

B	1.38532000	-0.99662700	-1.22404300	F	-3.97702000	-2.91364200	-0.75882400
C	0.00658400	-1.67748100	-1.04940100	F	-2.88814400	-2.40086400	-3.20826500
C	-0.59812000	-2.00272800	0.17784200	F	-0.35571200	-1.56603300	-3.40911700
C	-0.82197800	-1.85569600	-2.17770600	F	3.94681700	-2.14095400	-1.51799500
C	-1.91556500	-2.42819000	0.28781800	F	1.28956100	0.46437200	1.43389200
C	-2.13418000	-2.28067900	-2.10405400	F	3.33854200	0.59336600	3.15079600
C	-2.69758100	-2.53051600	-0.85562200	F	5.71557000	-0.62411800	2.56666900
C	2.51225100	-0.86335200	-0.11770800	F	5.99868400	-1.99083200	0.21302100
C	2.42175500	-0.18619200	1.10119500	H	0.43615000	0.69212500	-1.04153300
C	3.75680200	-1.45182400	-0.37326300	C	-4.26084700	2.19888200	3.10136100
C	3.47748100	-0.08933900	2.00287400	C	-3.38786000	2.13692400	2.01365300
C	4.83326400	-1.39057000	0.50616000	C	-3.50884500	1.12897900	1.04227400
C	4.69066500	-0.70271000	1.70673700	C	-4.54838600	0.19576100	1.19024000
F	0.10576200	-1.94019500	1.32476600	C	-5.41622600	0.24768000	2.28094000
F	-2.44971400	-2.71439000	1.48761300	C	-5.27790700	1.25111100	3.24381700

H	-4.15134600	2.99437700	3.83532500	C	0.17945700	3.59890100	-2.55322500
H	-2.61745300	2.89508300	1.90680200	C	2.07501500	4.44492500	-0.69954700
H	-4.65564300	-0.57178100	0.43066800	H	1.58616200	2.64771600	0.38224900
H	-6.20578200	-0.49440700	2.37955400	C	0.86935500	4.79616700	-2.75794900
H	-5.95739300	1.29810100	4.09154000	H	-0.56158200	3.27247100	-3.27955100
C	-2.60530000	1.00557300	-0.17360600	C	1.82114500	5.22549600	-1.83068200
C	-1.31964400	1.55885900	-0.08724900	H	2.81651600	4.76690100	0.02817800
C	-0.35357000	1.52303300	-1.19815100	H	0.66327400	5.39231500	-3.64396400
H	-0.99521800	2.01564100	0.84226500	H	2.36077700	6.15604600	-1.98816100
O	-3.08449500	0.39442600	-1.18017100	H	-0.86357500	1.21028300	-2.11588400
C	0.42161200	2.80743400	-1.42152900	H	1.75484800	-0.80233700	-2.34096000
C	1.38404300	3.24868500	-0.49987900				



TS3′′(-)

H	6.17558700	-1.29792700	-1.87527700	H	7.42130400	-5.06299500	0.60197300
C	3.58507500	4.14043100	1.71616200	H	5.86836300	-5.16194400	2.54618900
C	3.47090100	2.87254500	1.14491000	H	4.43018500	-1.28474000	-1.61627800
C	4.48607400	2.33993200	0.33262900	C	-3.23075500	0.36602000	-0.11412300
C	5.61290900	3.14605000	0.09001800	C	-2.61333500	-1.78790500	-0.92352300
C	5.73004900	4.41771700	0.65304900	C	-3.47349400	-2.44081400	0.01900800
C	4.71759000	4.92280200	1.47422800	C	-4.15607500	-1.61919900	0.93849200
H	2.78759700	4.52188800	2.35117100	C	-4.08129200	-0.23534500	0.82495800
H	2.58929900	2.26342000	1.31821800	H	-1.48465800	-2.09054900	-2.73825900
H	6.39555800	2.77747400	-0.56706900	C	-2.04854700	-2.57039800	-1.95439000
H	6.60991400	5.02167000	0.44078700	C	-3.65647000	-3.84663700	-0.04533200
H	4.80661500	5.91468300	1.91107300	C	-3.05525800	-4.58650900	-1.03764100
C	4.30755600	0.95406000	-0.25347500	C	-2.26938000	-3.93328600	-2.01024400
C	5.44414000	0.22449600	-0.52788200	H	-4.30032000	-4.32290400	0.68675900
C	5.39648900	-1.16477800	-1.10855200	H	-3.20559200	-5.65999500	-1.09153300
H	6.41932400	0.61526000	-0.24958500	H	-1.84061400	-4.50420200	-2.82814400
O	3.08615200	0.55097100	-0.43147500	C	-3.34367000	1.82650900	-0.36011200
C	5.54393400	-2.28994900	-0.09044900	C	-3.19239000	2.77277000	0.66618100
C	4.68094500	-2.35485400	1.01681000	C	-3.75050200	2.25571500	-1.63453300
C	6.52527600	-3.28078500	-0.21974500	C	-3.41699800	4.12500500	0.41291900
C	4.79141600	-3.38174200	1.95333800	H	-2.87095400	2.45399100	1.65259100
H	3.92239400	-1.58420400	1.12457800	C	-3.99230200	3.60735800	-1.87825000
C	6.64644100	-4.30881500	0.72173300	H	-3.89040200	1.52552700	-2.42629100
H	7.20630100	-3.24629500	-1.06856000	C	-3.82057400	4.54456700	-0.85769500
C	5.77803100	-4.36486200	1.81213000	H	-3.27728900	4.85091800	1.20840900
H	4.10974300	-3.41604200	2.80067900	H	-4.31313400	3.92690500	-2.86540500

H	-4.00250500	5.59793500	-1.04976900	C	0.89005800	2.55627100	-2.05188800
N	-2.39221300	-0.40287800	-0.87918700	C	1.20380200	-1.99009800	-2.05059600
C	-5.12803100	0.33415900	1.77348700	C	-0.32354700	0.60724400	1.81075300
C	-6.57650600	-1.58293700	1.30567800	H	-0.80550800	2.65538000	-0.69961900
C	-5.02618400	-0.70777700	2.91625700	H	-1.24760500	2.27309300	-2.34437100
C	-5.20159100	-1.93113300	1.98066500	H	1.08688300	2.23257800	-3.07988000
C	-6.52252100	-0.03039100	1.16594200	H	0.91991000	3.65248700	-2.04618400
H	-6.61978400	0.30926800	0.13115900	H	1.70752300	2.18133300	-1.42507900
H	-7.31482800	0.44886400	1.74928700	H	-0.10758500	-0.81277500	-3.37762500
H	-5.15751000	-2.92350200	2.43048800	H	1.24300400	0.04151000	-2.68304700
H	-7.38822300	-1.89825400	1.96840100	H	1.74717300	-2.39851400	-2.91138300
H	-5.01741900	1.38191300	2.04499500	H	1.93978400	-1.75822300	-1.27635900
H	-4.06044700	-0.69306400	3.43111900	H	0.53950600	-2.77549400	-1.67786200
H	-5.83313300	-0.61718300	3.65036500	H	0.11222400	-1.24232900	0.75462300
H	-6.70780800	-2.09723400	0.34980400	H	1.27748800	0.04453800	0.44922400
Si	-0.50420100	0.23212600	-1.11226500	H	-0.22838900	1.69143600	1.68131700
C	-0.49892200	2.07040700	-1.57204100	H	-1.37599200	0.38596000	2.02432500
C	0.20080500	-0.15986500	0.58762000	H	0.24865300	0.33821800	2.70671500
C	0.46692800	-0.69852100	-2.44963700				