Supporting information for

Persistent Four-Coordinate Iron Centered Radical Stabilized by π-Donation

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Contents

General. Manipulation of air and moisture sensitive organometallic compounds was carried out under a dry argon atmosphere using standard Schlenk tube techniques associated with a high-vacuum line. Alternatively, the experiments were performed in a glove box filled with dry nitrogen. All solvents (pentane, *n*-octane, diethyl ether, hexamethyldisiloxane (HMDSO), mesitylene, C_6D_6, toluene-d_8) were distilled over Ph_2CO/Na prior to use. ^1H, ^{13}C, ^{29}Si, and ^{31}P NMR spectra were recorded on a JEOL Lambda 600 spectrometer at ambient temperature unless otherwise noted. ^1H, ^{13}C NMR chemical shifts (δ values) were given in ppm relative to the solvent signal (^1H, ^{13}C) or standard resonances (^{29}Si; external $SiMe_4$, ^{31}P; external H_3PO_4). Elemental analyses were performed by a Perkin Elmer 2400II/CHN analyzer. IR spectra were recorded on a JASCO FT/IR-550 spectrometer. UV-vis-NIR absorption spectra were recorded on a Shimadzu UV-3100PC UV-VIS-NIR scanning spectrophotometer. ESR spectra were recorded on a JEOL JES-FA 200 Electron Spin Resonance spectrometer. $Fe_2(CO)_9$[1], phosphinyl radical **1**[2] were synthesized by the method reported in the literature. Nor-AZADO was purchased from Wako Pure Chemical Industries and was used without further purification.

Synthesis of 2. In a glove box, $Fe_2(CO)_9$ (200 mg, 0.55 mmol) was suspended in pentane (5 mL), and phosphinyl radical **1** (207 mg, 0.55 mmol) was added to the suspension. The resulting mixture was stirred at room temperature for 16 h. The mixture gradually changed from a golden yellow suspension to a dark red solution. The solvent was evaporated and the residue was extracted with pentane (10 mL). A small amount of insoluble materials was removed by centrifugation, and the mother liquid was concentrated to ca. 5 mL under vacuum. This mixture was cooled to 238 K overnight, from which dark red crystals of **2** were obtained in 86 % (based on **1**) yield (244 mg). ^1H NMR (600 MHz, C_6D_6, r.t.) δ 0.38 (s, 72H, $SiMe_3$), 2.05 (br d, $J_{H\text{-}P}$ = 9.3 Hz, 8H, CH_2). ^1H NMR (toluene-d_8, r.t.) δ 0.35 (s, 72H, $SiMe_3$), 2.03 (br d, $J_{H\text{-}P}$ = 9.9 Hz, 8H, CH_2). ^1H NMR (600 MHz, toluene-d_8, 193 K) δ 0.31 (s, 18H, $SiMe_3$), 0.35 (s, 18H, $SiMe_3$), 0.37 (s, 18H, $SiMe_3$), 0.48 (s, 18H, $SiMe_3$), 1.69-1.87 (br, 8H, CH_2). $^{13}C\{^1H\}$ NMR (151 MHz, C_6D_6, r.t.) δ 3.15 (s, $SiMe_3$), 38.33 (s, CH_2), 54.33 (d, $J_{C\text{-}P}$ = 52 Hz, $C(SiMe_3)_2$), 223.79 (br s, Fe-CO). $^{29}Si\{^1H\}$ NMR (119 MHz, C_6D_6, r.t.) δ 2.85 (d, $J_{Si\text{-}P}$ = 12.8 Hz). $^{31}P\{^1H\}$ NMR (243 MHz, C_6D_6, r.t.) δ 425.9 (s). IR (ATR) ν_{CO} = 1916, 1932, 1963, 2014 cm^{-1}. IR (in *n*-octane, 293 K) ν_{CO} = 1921, 1940, 1968, 2017 cm^{-1}. UV-vis-NIR (*n*-octane, 293 K) λ_{max}/nm ($\varepsilon/M^{-1}cm^{-1}$) = 380 ($3.02\times10^4$), 502 ($6.26\times10^3$), 720 ($2.78\times10^3$). Anal. Calcd. for $C_{38}H_{80}O_6Si_8P_2Fe_2$: C, 44.25; H, 7.82. Found: C, 44.08; H, 7.76.

Synthesis of 4. In a glove box, complex **2** (20 mg, 0.019 mmol) was dissolved in toluene (0.5 mL), and nor-AZADO (5.4 mg, 0.0038 mmol) was added to the solution. The resulting mixture was allowed to stand at room temperature for 16 h. The color of the solution gradually changed from dark red to dark green. The solvent was evaporated and the residue was extracted with pentane (5 mL). A small amount of insoluble materials was removed by centrifugation, and the solvent was removed under vacuum. The remaining crude product was dissolved in pentane (3 mL), and the solution was cooled to 238 K overnight to afford **4** as pale green crystals in 74 % yield (18 mg). ^1H NMR (600

MHz, C_6D_6, r.t.) δ 0.36 (s, 18H, $SiMe_3$), 0.47 (s, 18H, $SiMe_3$), 1.14-1.17 (m, 2H, CH_2 of nor-AZADO), 1.25-1.28 (m, 2H, CH_2 of nor-AZADO), 2.00-2.03 (m, 1H, CH of nor-AZADO), 2.08 (d, $J_{H\text{-}P}$ = 9.9 Hz, 4H, CH_2), 2.11-2.19 (m, 5H, CH_2 and CH of nor-AZADO), 2.87 (s, 2H, NC*H* of nor-AZADO). $^{13}C\{^1H\}$ NMR (151 MHz, C_6D_6, r.t.) δ 2.46 (s, $SiMe_3$), 34.07, 35.37, 37.19 (d, $J_{C\text{-}P}$ = 79 Hz, $C(SiMe_3)_2$), 40.25, 43.27, 76.97 (s, *C*NH of nor-AZADO), 221.19 (d, $J_{C\text{-}P}$ = 20.9 Hz, Fe-CO). $^{29}Si\{^1H\}$ NMR (119 MHz, C_6D_6, r.t.) δ 1.38, 1.54 (s, $SiMe_3$). $^{31}P\{^1H\}$ NMR (243 MHz, C_6D_6, r.t.) δ 282.16 (s). IR (ATR) ν_{CO} = 1892, 1958 cm^{-1}. Anal. Calcd. for $C_{26}H_{52}O_3N_1Si_4P_1Fe_1$: C, 49.90; H, 8.37; N, 2.24. Found: C, 49.66; H, 8.14; N, 2.08.

Synthesis of 5. In a glove box, complex **2** (20 mg, 0.019 mmol) was dissolved in toluene (0.5 mL), and **1** (14.6 mg, 0.039 mmol) was added to the solution. The resulting mixture was allowed to stand at room temperature for 18 h. The color of the solution gradually changed from dark red to dark green. The solvent was evaporated and the residue was extracted with pentane (5 mL). A small amount of insoluble materials was removed by centrifugation, and the solvent was removed under vacuum. The remaining crude product was dissolved in hexamethyldisiloxane (5 mL), and the solution was cooled to 238 K overnight to afford **5** as pale green crystals in 92 % yield (21 mg). ^1H NMR (600 MHz, C_6D_6, r.t.) δ 0.29 (s, 36H, $C(Si\mathit{Me}_3)_2$), 0.81 (s, 9H, Fe-$Si\mathit{Me}_3$), 1.97 (br d, $J_{P\text{-}H}$ = 11.0 Hz, 4H, CH_2). $^{13}C\{^1H\}$ NMR (151 MHz, C_6D_6, r.t.) δ 2.69 (s, $C(Si\mathit{Me}_3)_2$), 8.15 (s, Fe-$Si\mathit{Me}_3$), 27.80 (s, CH_2), 55.75 (d, $J_{C\text{-}P}$ = 48.8 Hz, $C(SiMe_3)_2$), 218.77 (d, $J_{C\text{-}P}$ = 9.3 Hz, Fe-CO). $^{29}Si\{^1H\}$ NMR (119 MHz, C_6D_6, r.t.) δ 3.74 (d, $J_{Si\text{-}P}$ = 11.0 Hz, $C(\mathit{Si}Me_3)_2$), 29.05 (d, $J_{Si\text{-}P}$ = 7.3 Hz, Fe-$\mathit{Si}Me_3$). $^{31}P\{^1H\}$ NMR (243 MHz, C_6D_6, r.t.) δ 461.4 (s). IR (ATR) ν_{CO} = 1900, 1987, 2031 cm^{-1}. Anal. Calcd. for $C_{22}H_{49}O_3Si_5P_1Fe_1$: C, 44.87; H, 8.39. Found: C, 44.64; H, 8.22.

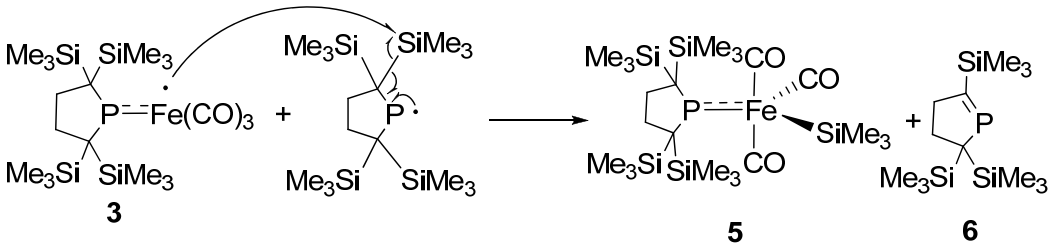
Synthesis of 8. In a glove box, complex **2** (60 mg, 0.058 mmol) was dissolved in C_6D_6 (1.5 mL), and $HSnPh_3$ (81.7 mg, 0.232 mmol) and 1,3,5-teimethoxybenzene (internal standard; 9.8 mg, 0.058 mmol) was added to the solution. The resulting mixture was allowed to stand at room temperature for 16 h. The color of the solution gradually changed from dark red to brown. Complete consumption of **2** was confirmed by ^1H and ^{31}P NMR spectra, then the solvent was evaporated. The residue was extracted with diethyl ether (5 mL), and the solution was cooled to 238 K overnight to afford the brown crystals. ^1H, ^{13}C, and ^{31}P NMR spectra of obtained brown crystals in C_6D_6 revealed that the crystals consist of complexes **8** and **9** in a ratio of 3 : 1 (8 mg). The mother liquid was again cooled to 238 K, then brown crystals of **8** was obtained as a single product in 26 % yield (26 mg). Spectral data for **8**: ^1H NMR (600 MHz, C_6D_6, r.t.) δ -9.24 (d, 1H, $J_{H\text{-}P}$ = 38.8 Hz, Fe-H, with a satellite signal due to the coupling with Sn, $J_{H\text{-}Sn}$ = 118.7 Hz), 0.17 (s, 18H, $SiMe_3$), 0.28 (s, 18H, $SiMe_3$), 1.66-1.85 (m, 4H, CH_2), 5.68 (d, 2H, $J_{H\text{-}P}$ = 321.7 Hz, HP), 7.16-7.20 (m, 3H, C_6H_5), 7.23-7.30 (m, 6H, C_6H_5), 7.93-8.04 (m, 6H, C_6H_5). $^{13}C\{^1H\}$ NMR (151 MHz, C_6D_6, r.t.) δ 1.91 (s, $SiMe_3$), 3.39 (s, $SiMe_3$), 22.57 (d, $J_{H\text{-}P}$ = 10.1 Hz, $C(SiMe_3)_2$), 37.0 (s, CH_2), 128.66 (s, *para* of C_6H_5), 128.73 (s, *ortho* of C_6H_5, with a satellite signal due to the coupling with Sn, $J_{H\text{-}Sn}$ = 47.7 Hz), 137.32 (s, *meta* of C_6H_5, with a satellite signal due to the coupling with Sn, $J_{H\text{-}Sn}$ = 37.6 Hz), 143.45 (s, *ipso* of C_6H_5, with a

satellite signal due to the coupling with Sn, $J_{H\text{-}Sn}$ = 381.5 Hz), 213.11 (br s, Fe-CO). $^{29}Si\{^1H\}$ NMR (119 MHz, C_6D_6, r.t.) δ 5.39 (d, $J_{Si\text{-}P}$ = 8.2 Hz), 8.20 (d, $J_{Si\text{-}P}$ = 2.7 Hz). $^{31}P\{^1H\}$ NMR (243 MHz, C_6D_6, r.t.) δ 29.3 (s, with a satellite signal due to the coupling with Sn, $J_{P\text{-}Sn}$ = 98.6 Hz). ^{31}P NMR (243 MHz, C_6D_6, r.t.) δ 29.3 (d, $J_{P\text{-}H}$ = 321.7 Hz). IR (ATR) ν_{CO} or $\nu_{Fe\text{-}H}$ = 2024, 1953, 1909 cm^{-1} (vibronic mixing prevents definitive assignments). Anal. Calcd. for $C_{37}H_{57}O_3Si_4P_1Sn_1Fe_1$: C, 51.21; H, 6.62. Found: C, 50.98; H, 6.48. Spectral data for **9** (complex **9** was obtained as the mixture with **8**. The actual ^1H, ^{13}C and ^{31}P NMR charts were given in Figures 12-1, 12-2 and 12-3. Spectral data of **9** were tentatively assigned by comparison with those of isolated **8**.): ^1H NMR (600 MHz, C_6D_6, r.t.) δ 0.21 (s, 36H, $SiMe_3$), 1.95 (br d, $J_{H\text{-}P}$ = 10.3 Hz, 4H, CH_2), 7.16-7.20 (m, 3H, C_6H_5), 7.23-7.28 (m, 6H, C_6H_5), 7.90-7.98 (m, 6H, C_6H_5). $^{13}C\{^1H\}$ NMR (151 MHz, C_6D_6, r.t.) δ 2.78 (s, $SiMe_3$), 22.68 (d, $J_{H\text{-}P}$ = 14.4 Hz, $C(SiMe_3)_2$), 38.09 (s, CH_2), 128.52, 128.61, 137.60, 144.27 (s, C_6H_5) (satellite signals due to the coupling with Sn should be observed along with these peaks, however, the intensity of these peaks were too weak to observe the satellite signals.), 217.79 (br s, Fe-CO). $^{31}P\{^1H\}$ NMR (243 MHz, C_6D_6, r.t.) δ 464.90 (s).

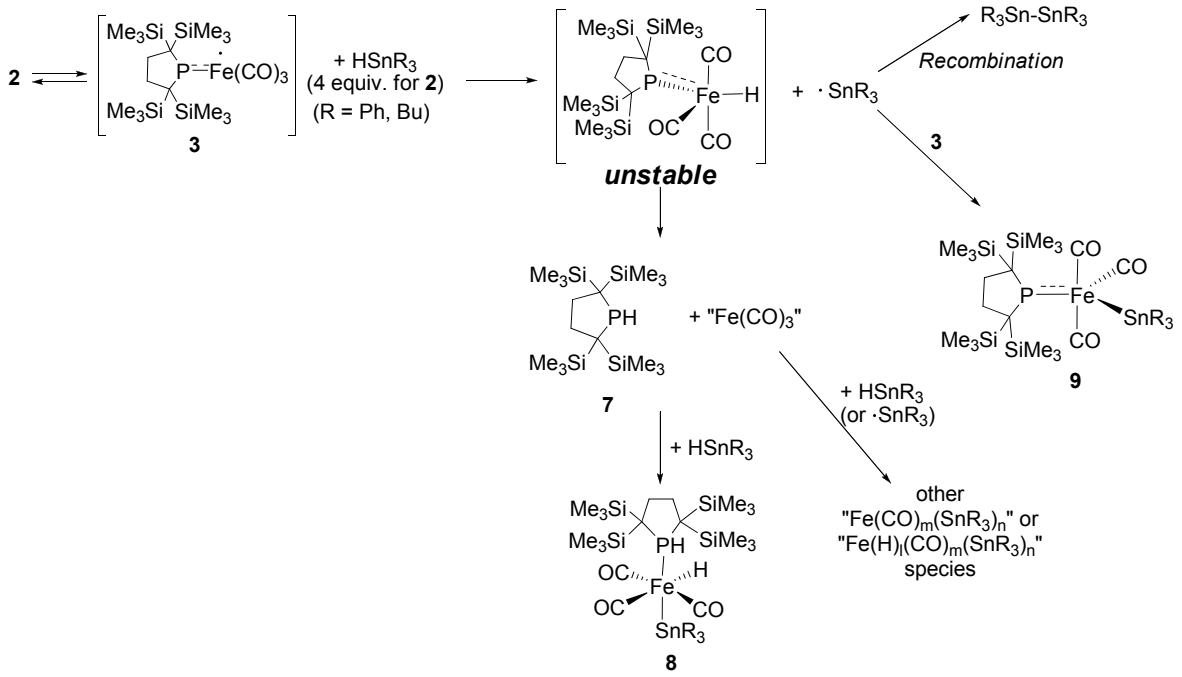
Reaction of 2 with $HSnBu_3$. In a glove box, complex **2** (20 mg, 0.019 mmol) was dissolved in C_6D_6 (0.5 mL), and $HSnBu_3$ (22.6 mg, 0.077 mmol) and 1,3,5-teimethoxybenzene (internal standard; 3.3 mg, 0.019 mmol) was added to the solution. The resulting mixture was allowed to stand at room temperature for 16 h. The color of the solution gradually changed from dark red to pale brown. The obtained crude product was analyzed by ^1H and ^{31}P NMR spectra. Actual charts were given in Figures 13-1 and 13-2.

Reaction of 2 with 9,10-dihydroanthracene. In a glove box, complex **2** (20 mg, 0.019 mmol) was dissolved in C_6D_6 (0.5 mL), and 9,10-dehydroanthracene (3.5 mg, 0.019 mmol) and 1,3,5-teimethoxybenzene (internal standard; 3.3 mg, 0.019 mmol) was added to the solution. The resulting mixture was allowed to stand at room temperature for 16 h. The ^1H and ^{31}P NMR spectra revealed that no reaction took place at this stage. Then, the mixture was allowed to stand at 333 K for 24 h, and no reaction took place which was confirmed by ^1H and ^{31}P NMR spectra. Then the mixture was allowed to stand at 353K for 24 h. The ^1H and ^{31}P NMR spectra revealed that partial decomposition including the formation of phosphaalkene **6** and free phosphine **7** occurred at this stage, however, formation of anthracene was not detected by ^1H NMR and GC-MS spectra. The actual NMR chart obtained after the reaction at 353K was attached in Figures 14-1 and 14-2.

In a similar manner, reaction of **2** (40 mg, 0.038 mmol) with 1,4-cyclohexadiene (3.1 mg, 0.038 mmol) was performed in the presence of anisole (4.1 mg, 0.038 mmol) as an internal standard. No reaction occurred at below 333K, and partial decomposition took place at 353K for 24 h without formation of benzene (confirmed by ^1H NMR and GC-MS).



Scheme S1. Possible reaction mechanism for the formation of **5** and **6** via homolytic substitution (S_H2).



Scheme S2. Possible reaction pathway for the formation of **7**, **8** and **9** in the reaction of **2** with $HSnR_3$ (R = Ph, Bu).

<Note>: In the ^1H NMR spectrum of the crude product obtained by the reaction of **3** (*in situ* generated from **2**) with $HSnPh_3$, some unidentified signals were observed in the 7-8 ppm region in the ^1H NMR spectrum (see Figure S12-1), suggesting that iron species consisting of carbonyl and $SnPh_3$ ligands {such as "$Fe(CO)_m(SnPh_3)_n$ (m+n = 5 or 6)" or "$Fe(H)_l(CO)_m(SnPh_3)_n$ (l+m+n = 5 or 6)" shown in Scheme S2} may be generated in the course of this reaction.

Figure S1-1. ^{1}H NMR spectrum of solution of **2** in C_6D_6 at 293K.

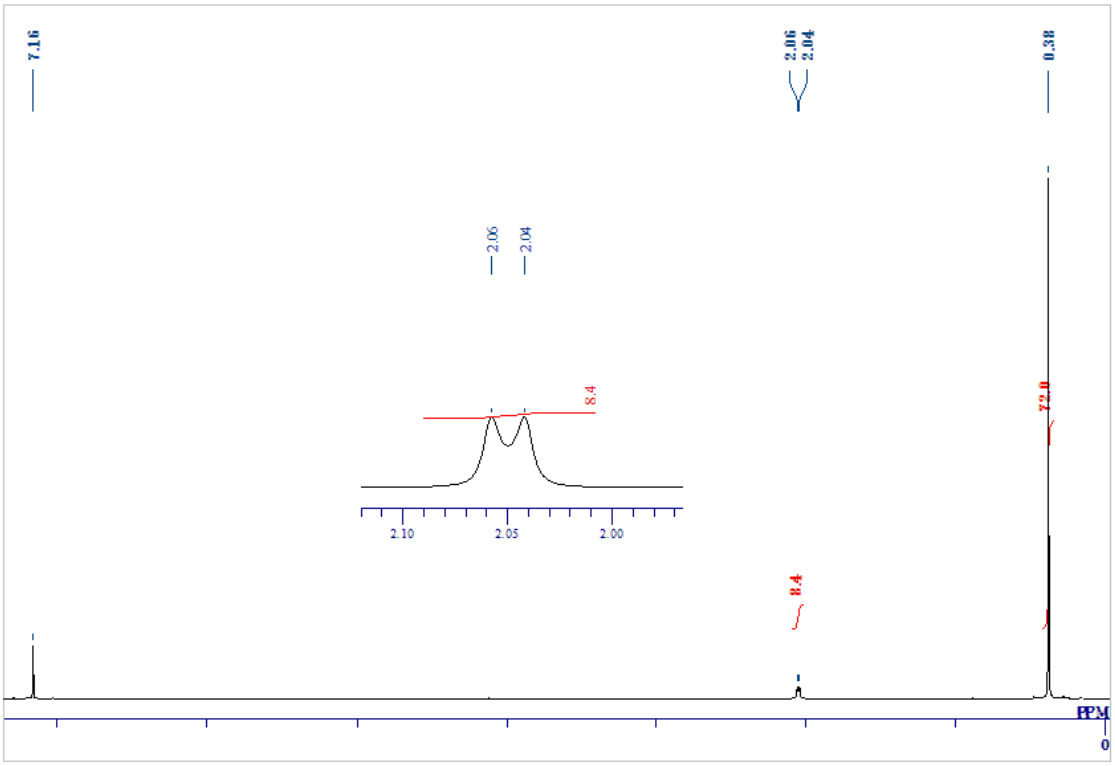


Figure S1-2. $^{13}C\{^{1}H\}$ NMR spectrum of solution of **2** in C_6D_6 at 293K.

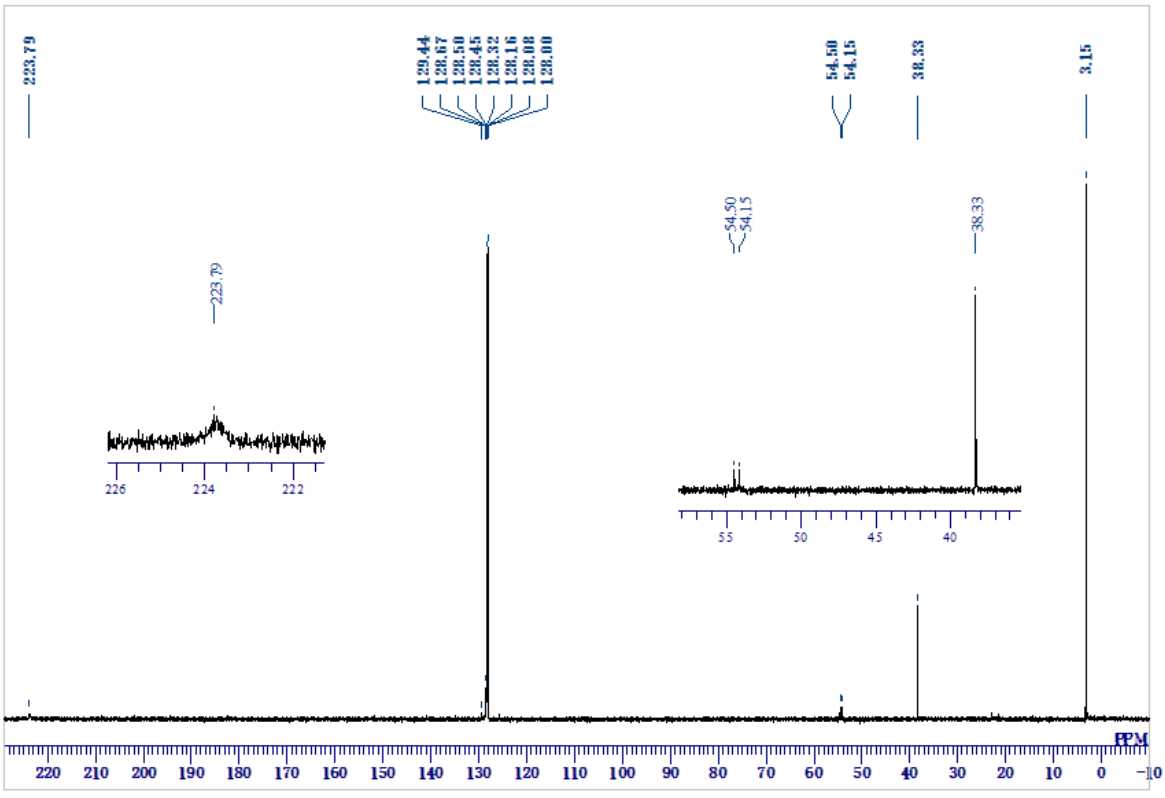


Figure S1-3. $^{29}Si\{^{1}H\}$ NMR spectrum of solution of **2** in C_6D_6 at 293K.

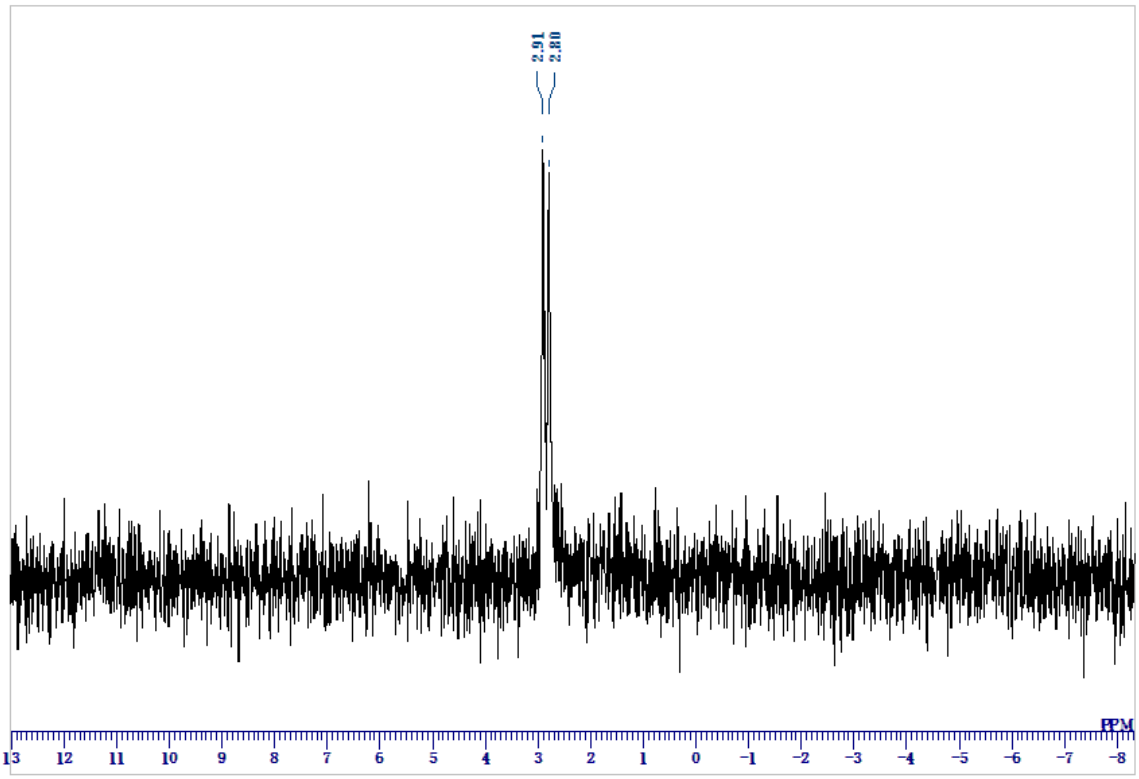


Figure S1-4. $^{31}P\{^{1}H\}$ NMR spectrum of solution of **2** in C_6D_6 at 293K.

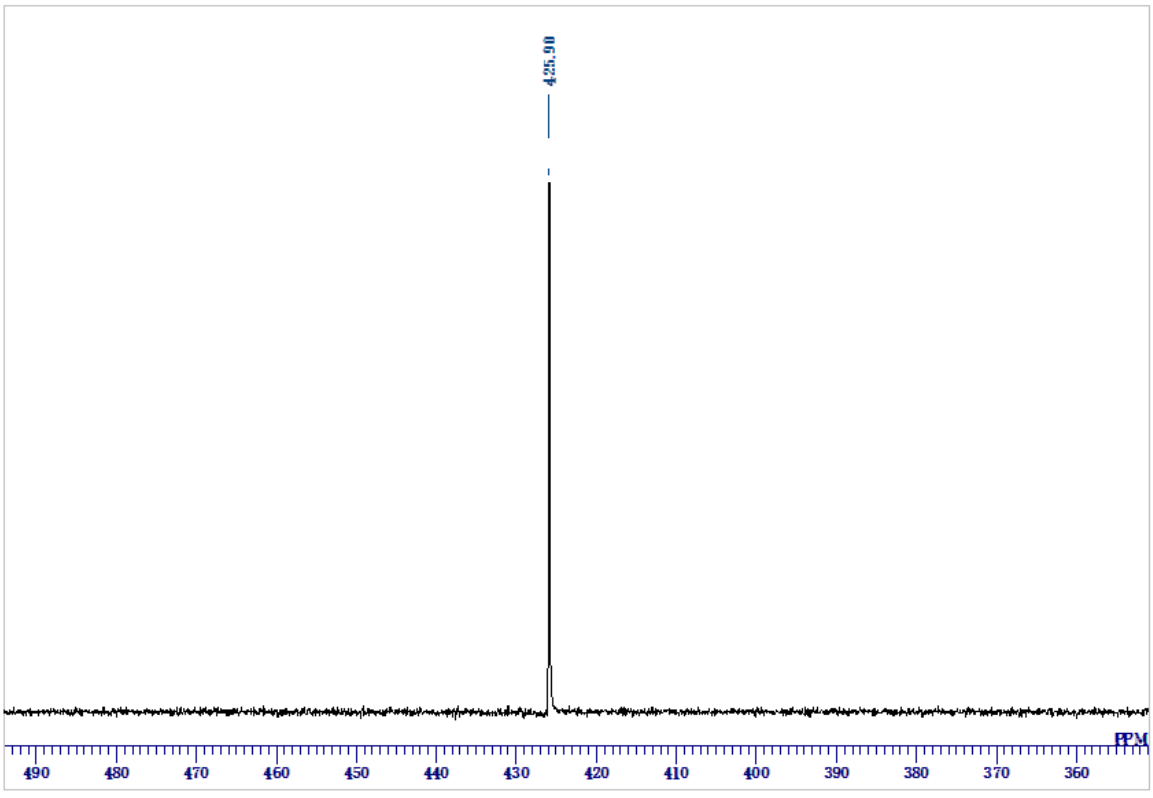


Figure S2-1. ^{1}H NMR spectrum of **4** in C_6D_6 at 293K.

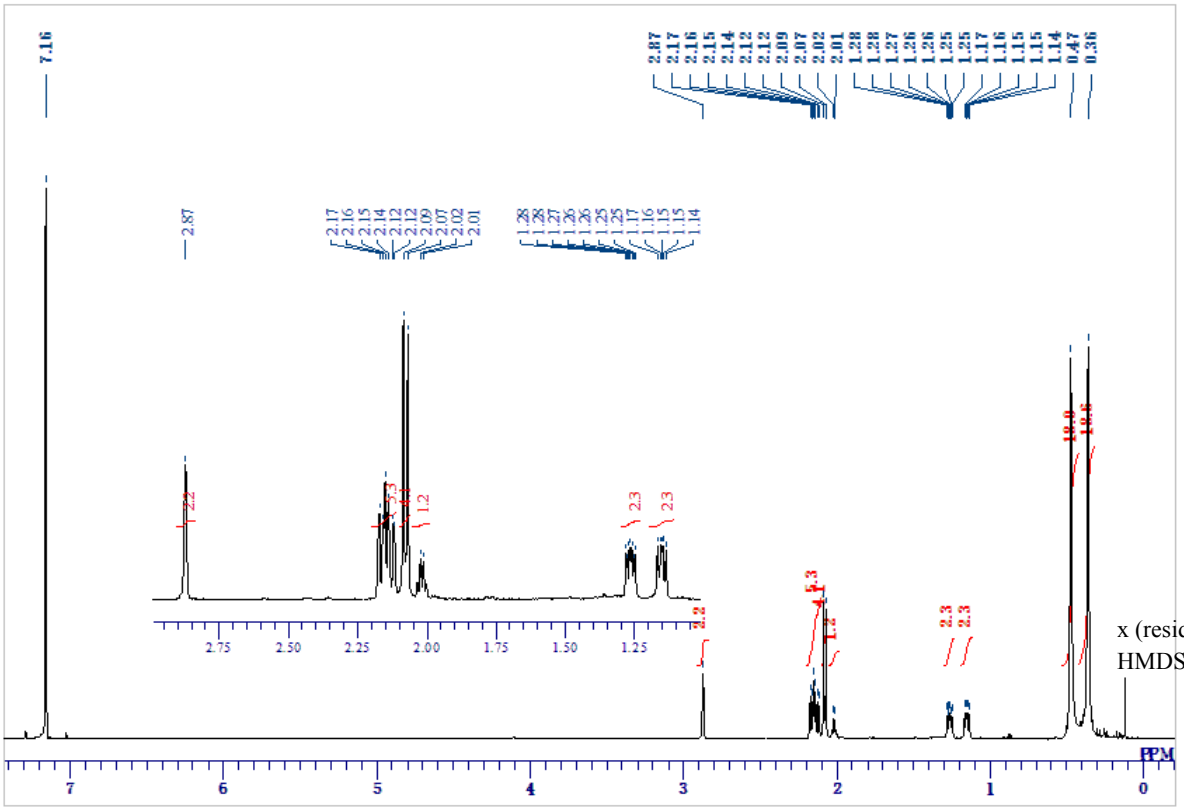


Figure S2-2. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in C_6D_6 at 293K.

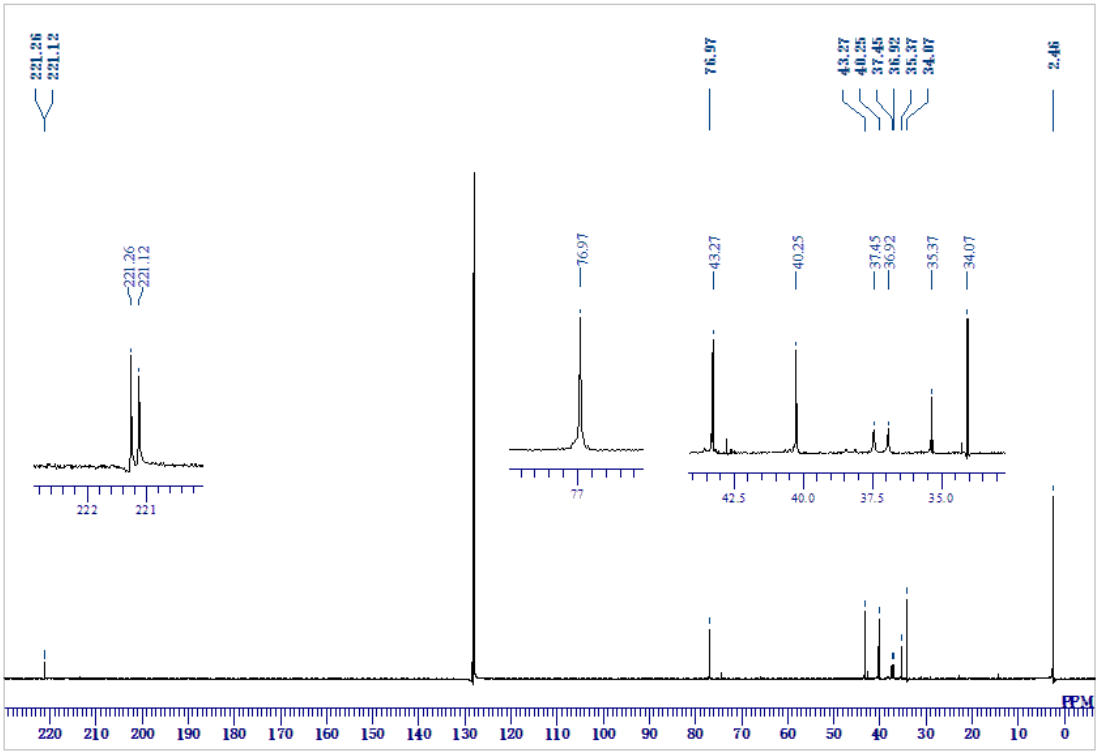


Figure S2-3. $^{29}Si\{^{1}H\}$ NMR spectrum of **4** in C_6D_6 at 293K.

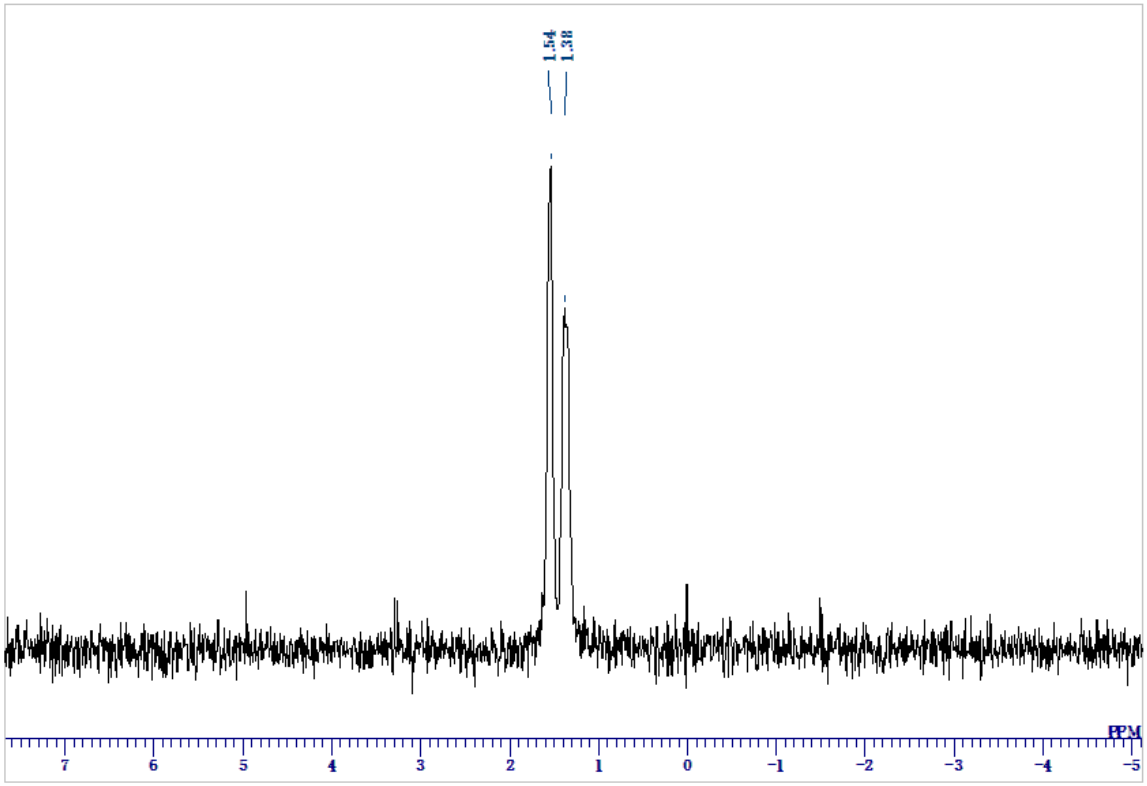


Figure S2-4. $^{31}P\{^{1}H\}$ NMR spectrum of **4** in C_6D_6 at 293K.

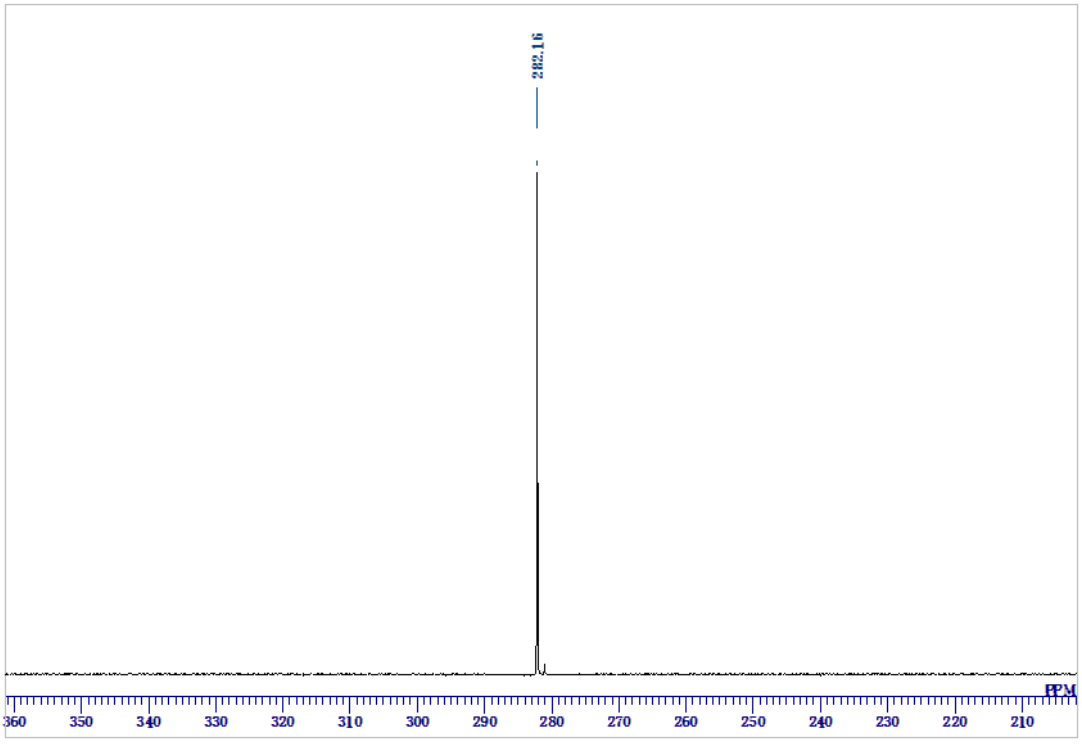


Figure S3-1. ^{1}H NMR spectrum of **5** in C_6D_6 at 293K.

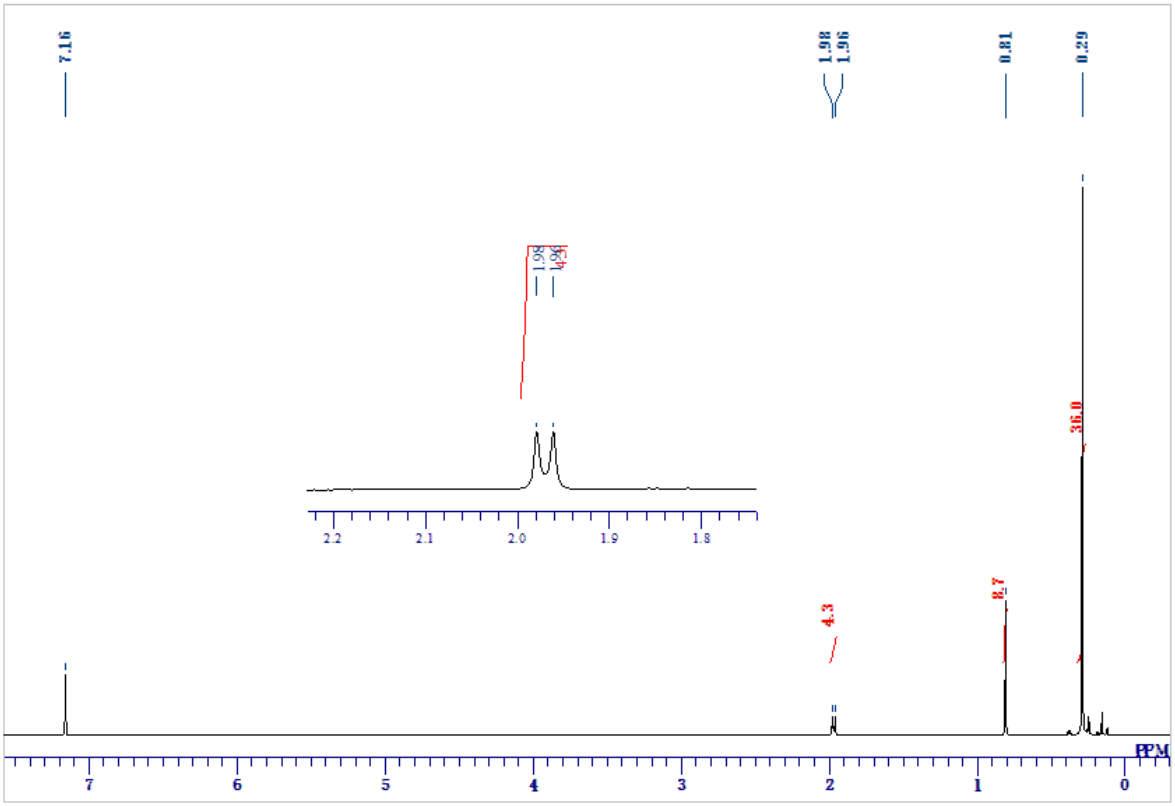


Figure S3-2. $^{13}C\{^{1}H\}$ NMR spectrum of **5** in C_6D_6 at 293K.

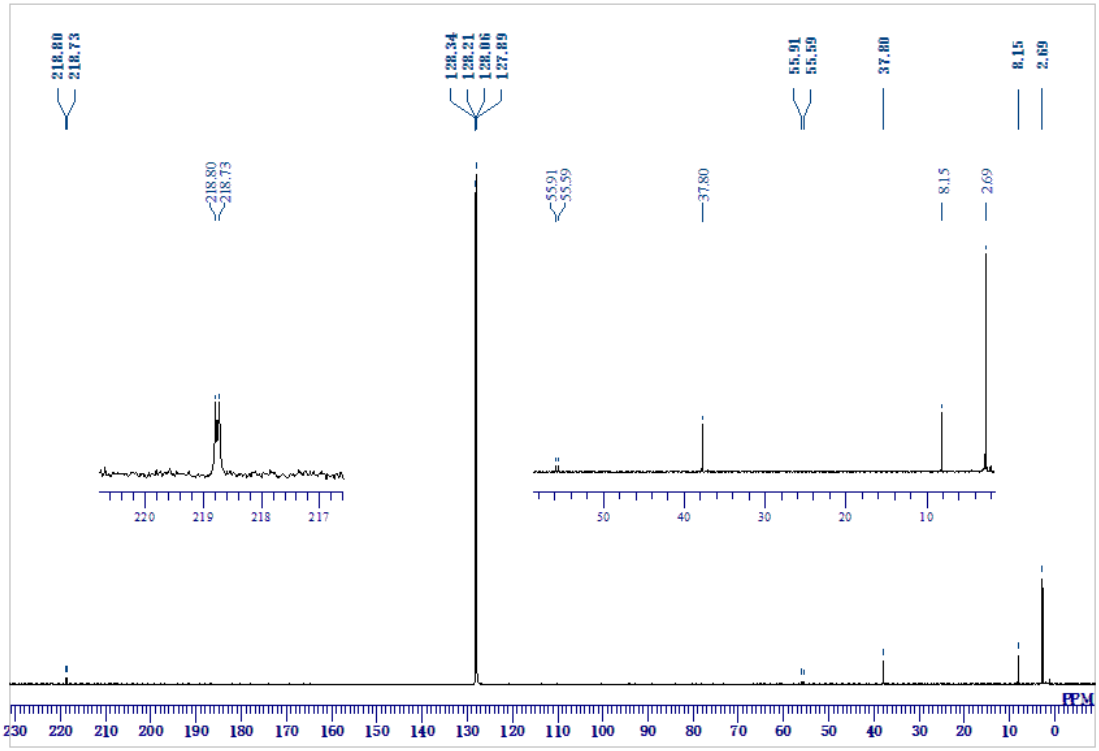


Figure S3-3. $^{29}Si\{^{1}H\}$ NMR spectrum of **5** in C_6D_6 at 293K.

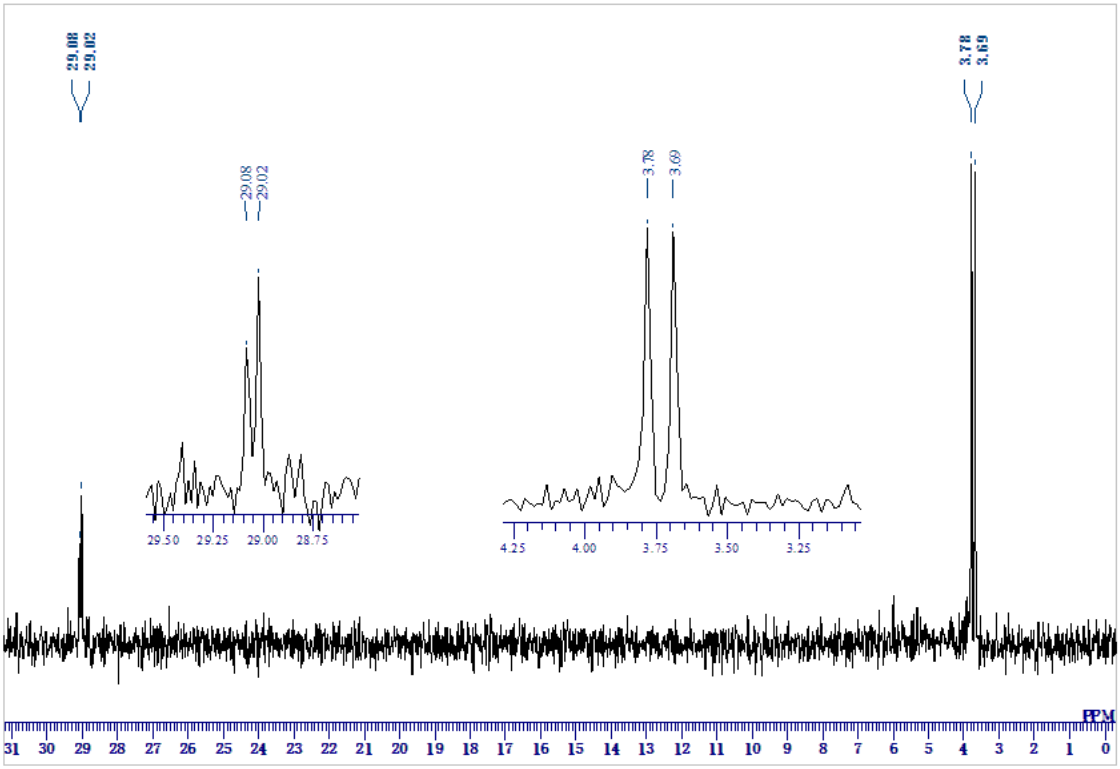


Figure S3-4. $^{31}P\{^{1}H\}$ NMR spectrum of **5** in C_6D_6 at 293K.

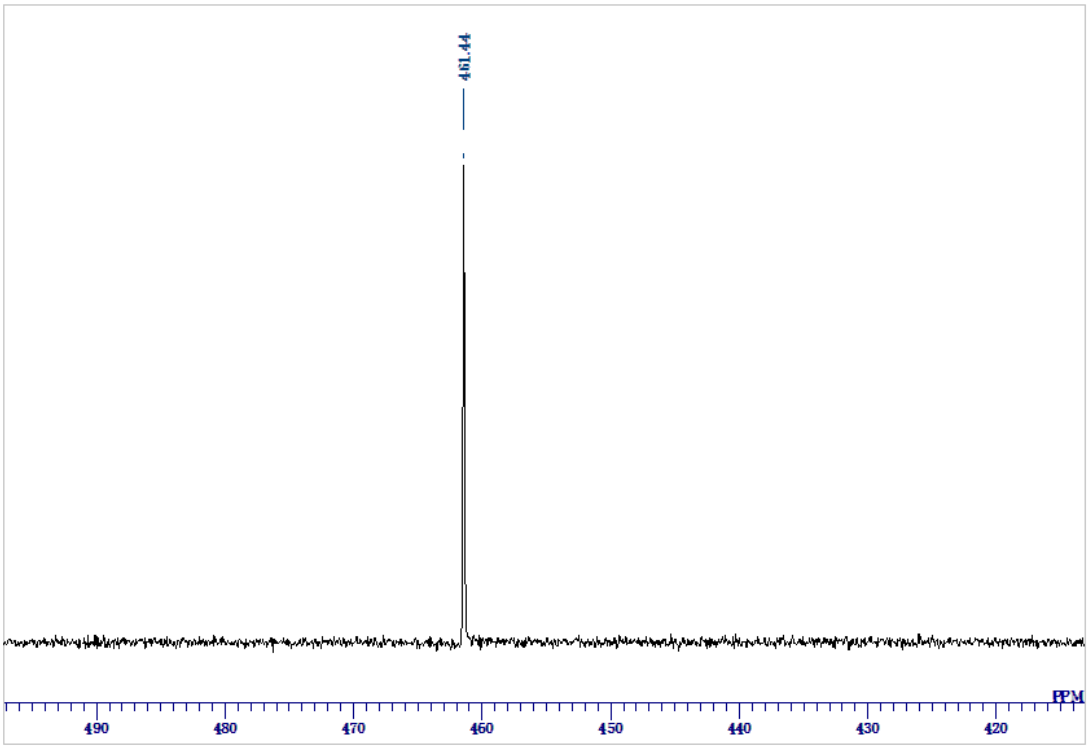


Figure S4-1. ^{1}H NMR spectrum of **8** in C_6D_6 at 293K.

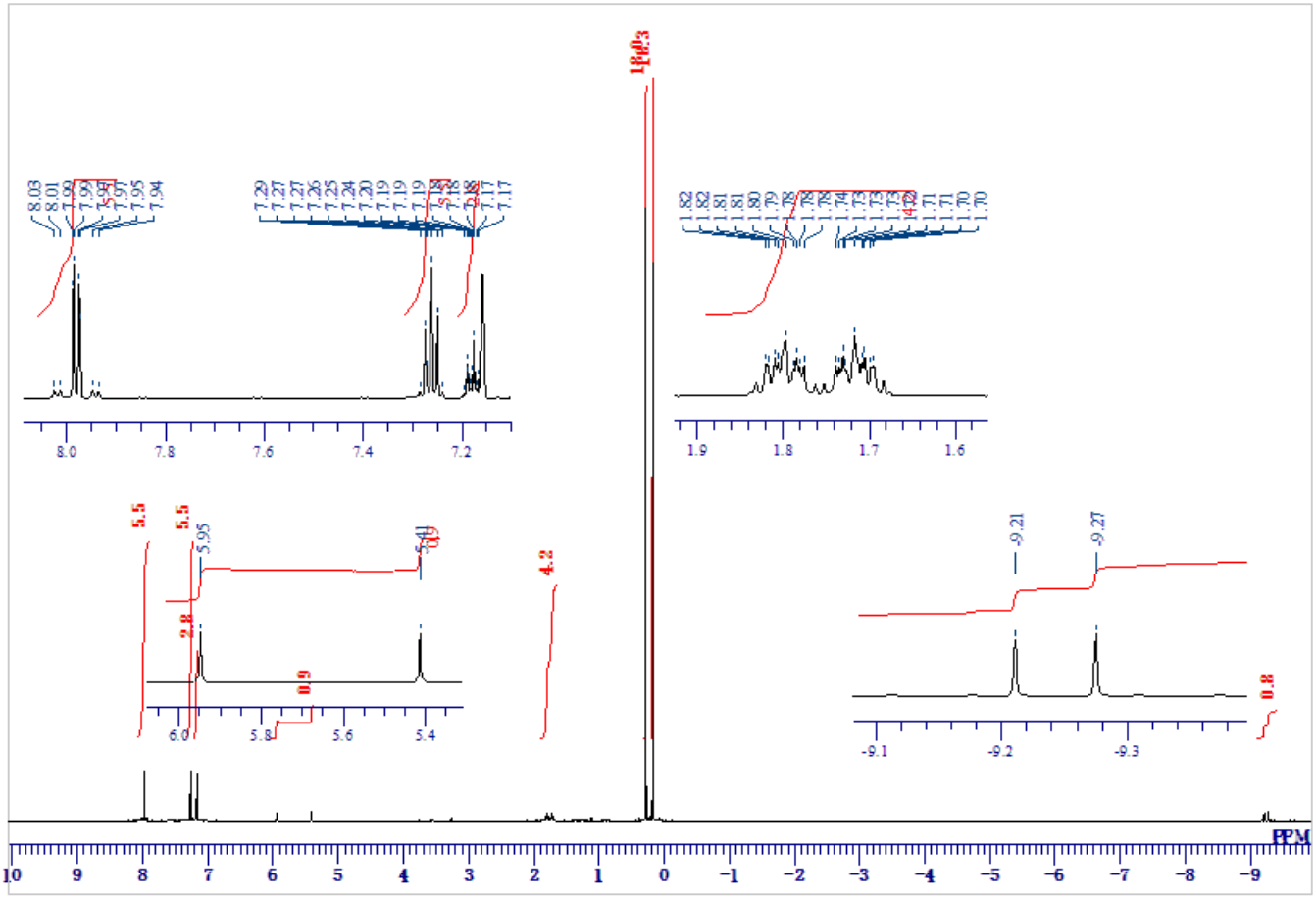


Figure S4-2. $^{13}C\{^{1}H\}$ NMR spectrum of **8** in C_6D_6 at 293K.

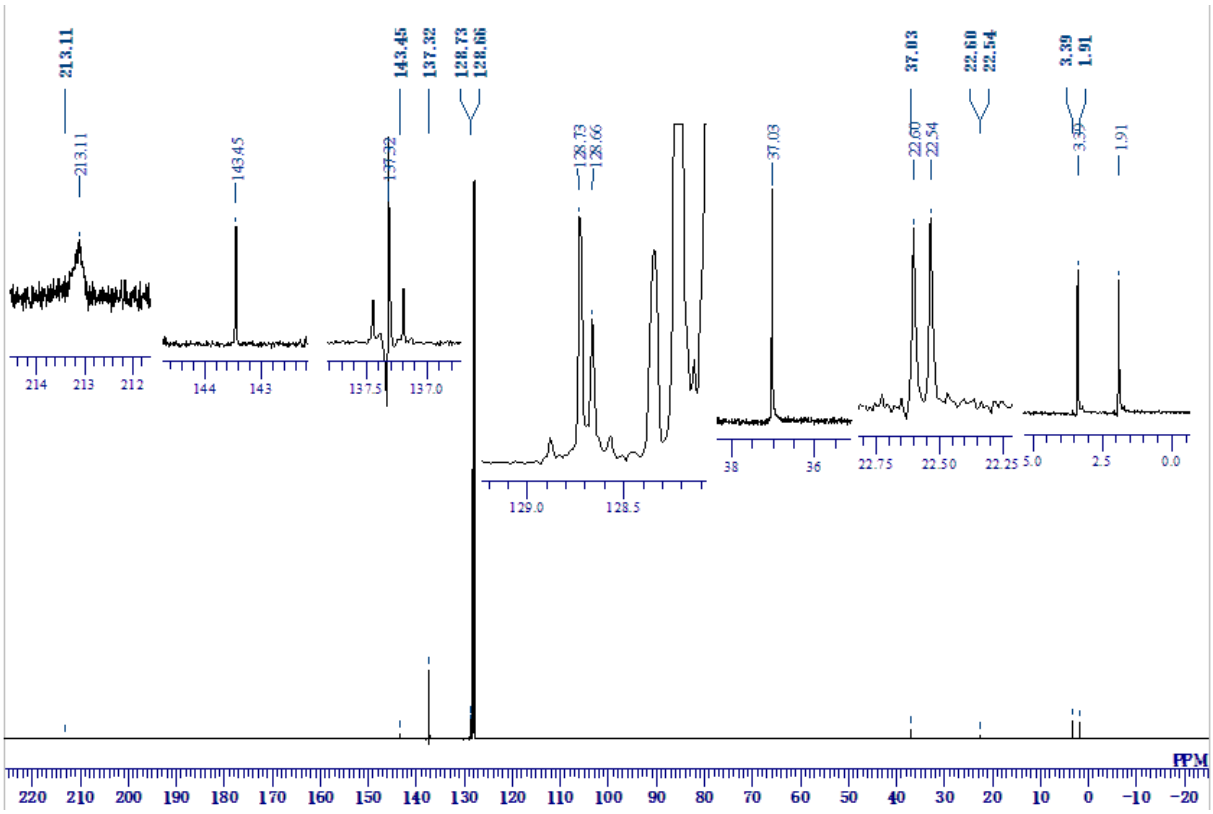


Figure S4-3. $^{29}Si\{^{1}H\}$ NMR spectrum of **8** in C_6D_6 at 293K.

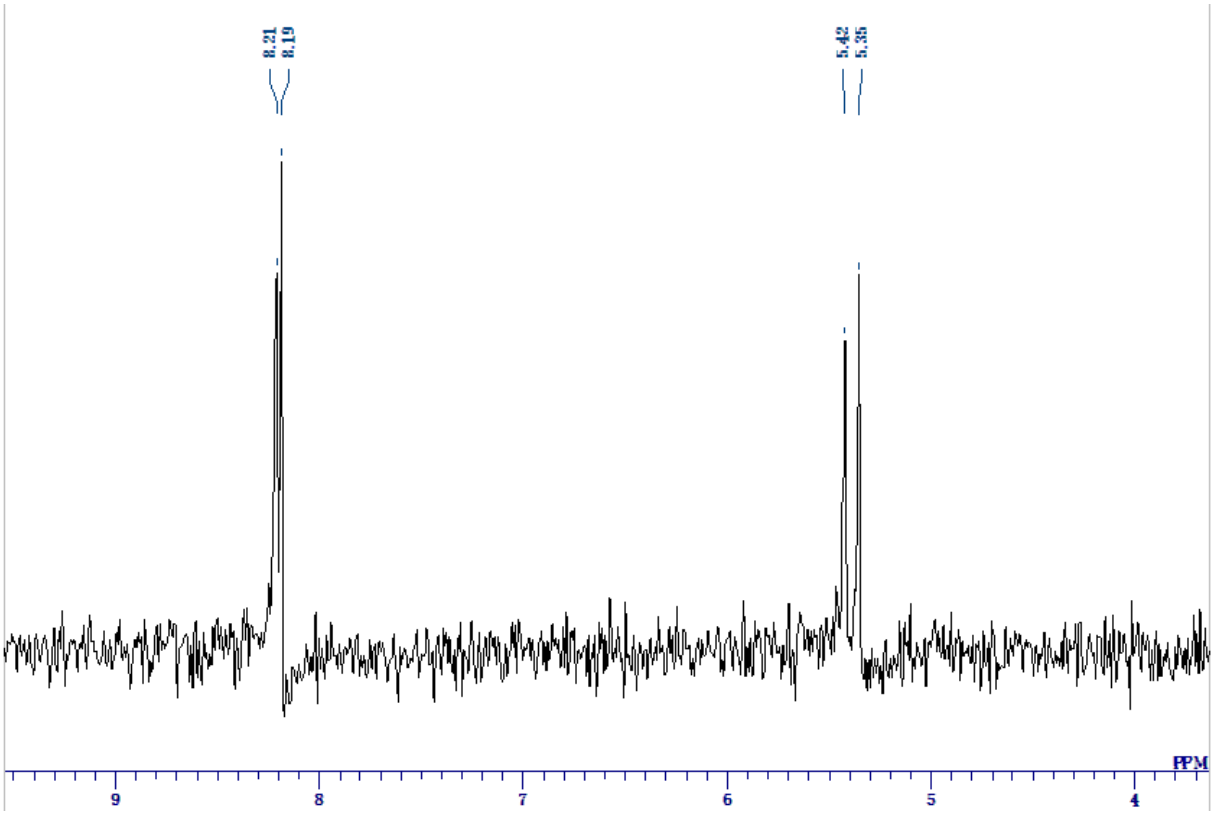


Figure S4-4. $^{31}P\{^{1}H\}$ NMR spectrum of **8** in C_6D_6 at 293K.

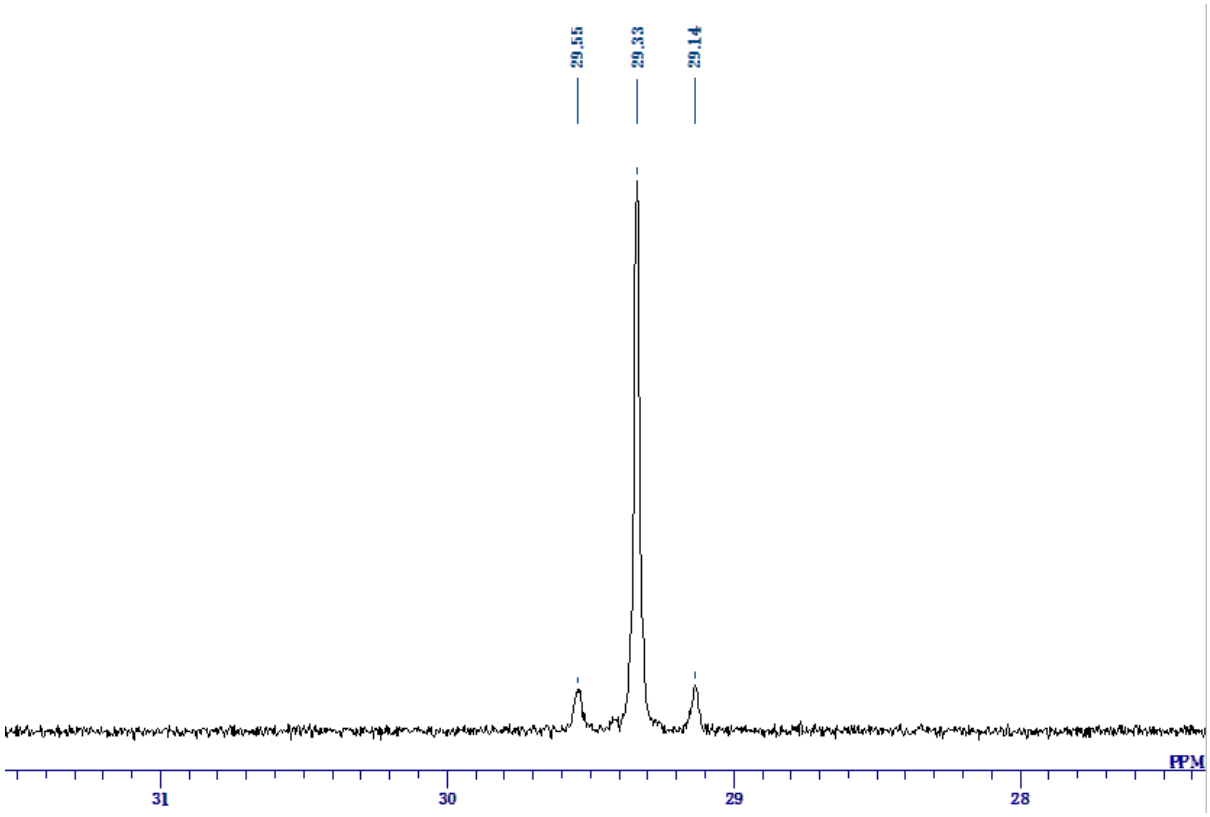
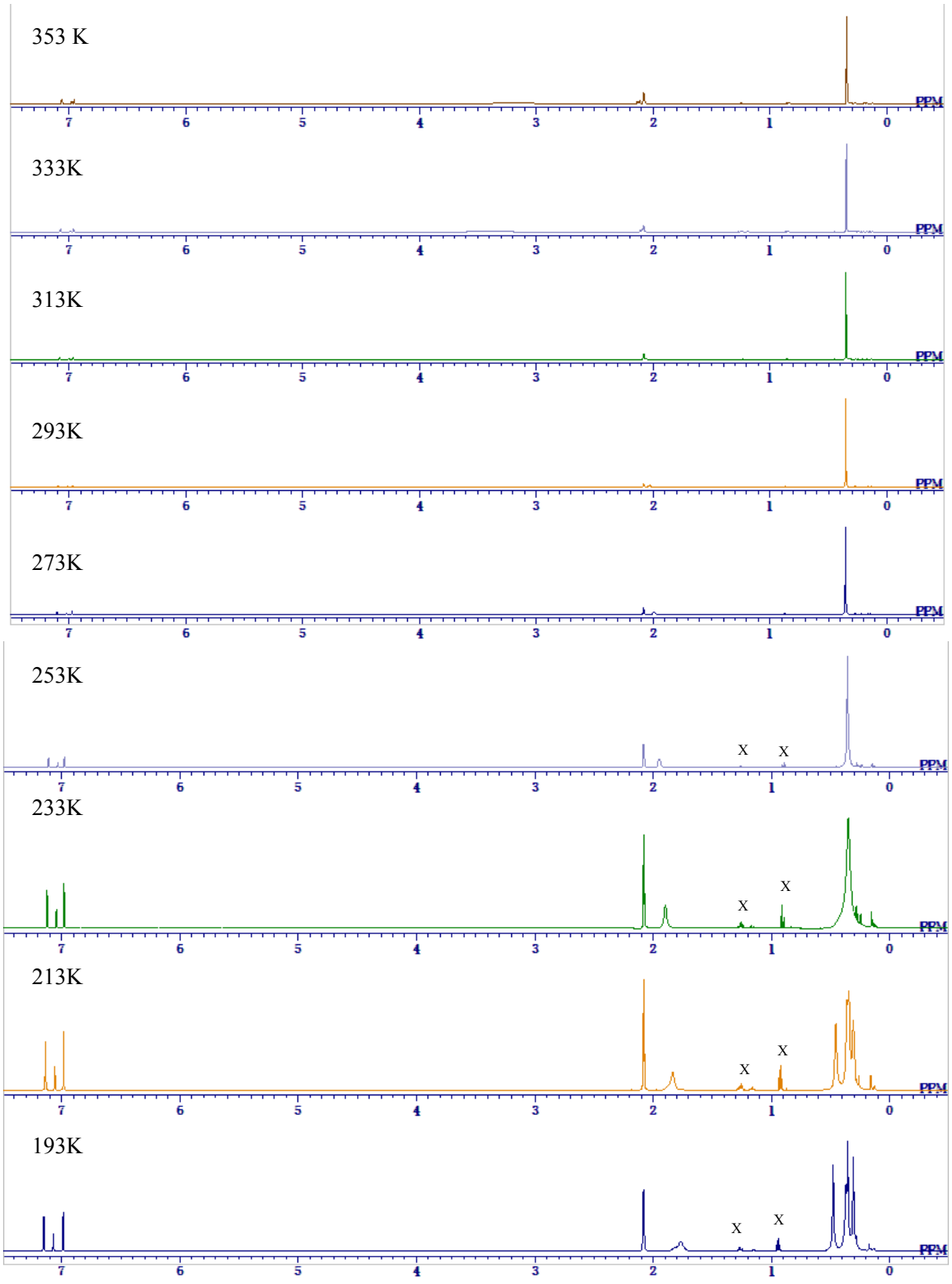
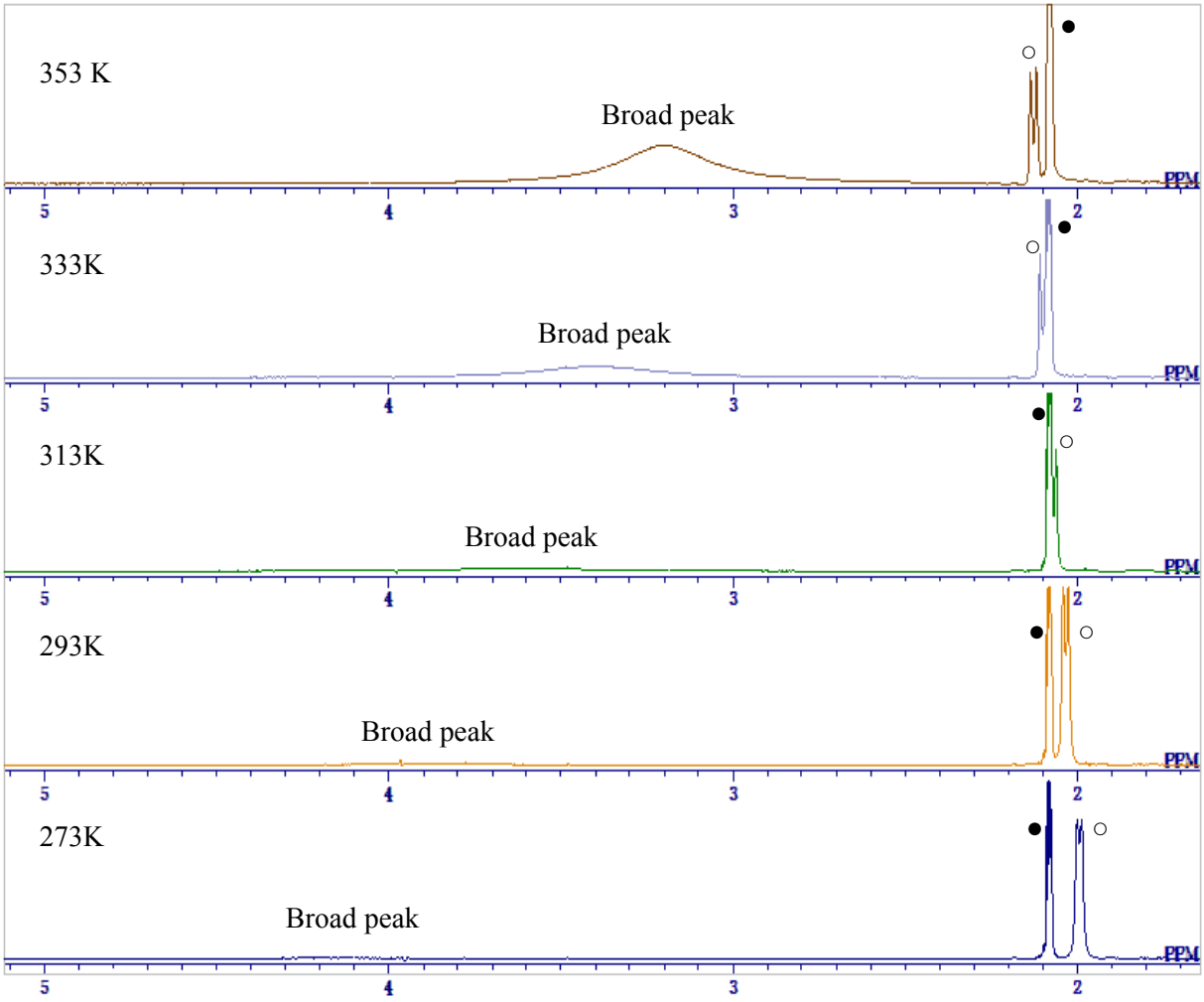


Figure S5-1. ^{1}H NMR spectra of solution of **2** in toluene-d$_8$ at various temperature (193 K~353 K).



^{1}H NMR (600 MHz, in toluene-d$_8$)
(x = residual pentane)

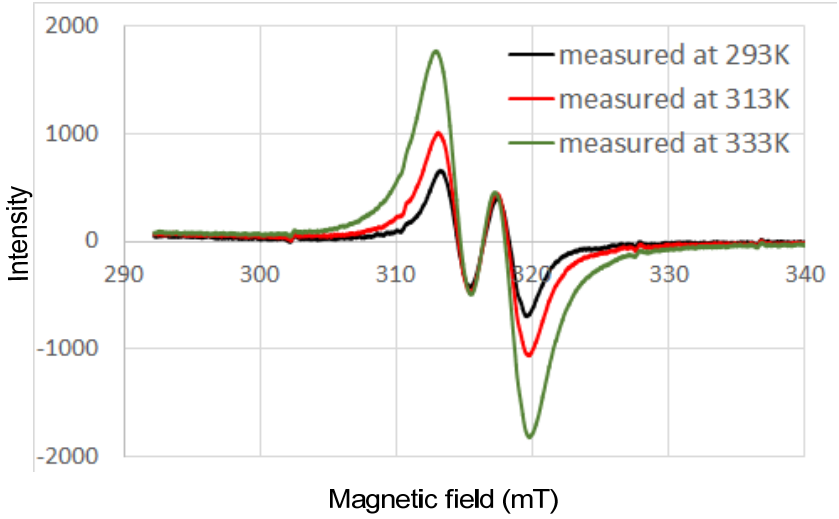
Figure S5-2. Enlarged view of ^{1}H NMR spectra of solution of **2** in toluene-d_8 at various temperature (273 K~353 K). The solid-circles and open-circles indicate signals of C_7D_7H and $–CH_2$- moiety of complex **2**.



ESR spectra

A toluene solution of **2** (ca. 0.12 mM) was prepared by dissolving **2** (1.4 mg, 1.36 x 10^{-3} mmol) in toluene (11 mL); the ESR spectrum was immediately recorded at 293 K. Measurements at 313 K and 333 K were carried out subsequently. The sample was allowed to stand in the instrument for 30 min at each temperature prior to the measurement.

Figure S6-1. ESR spectra of solution of **2** in toluene.



ESR spectrum of a flash-frozen toluene solution

A toluene solution of **2** (ca. 1.2 mM) was heated to 353 K, then this solution was flash-frozen. Then, the ESR spectrum was recorded at 77 K.

Figure S6-2. ESR spectrum of flash-frozen toluene solution measured at 77K.

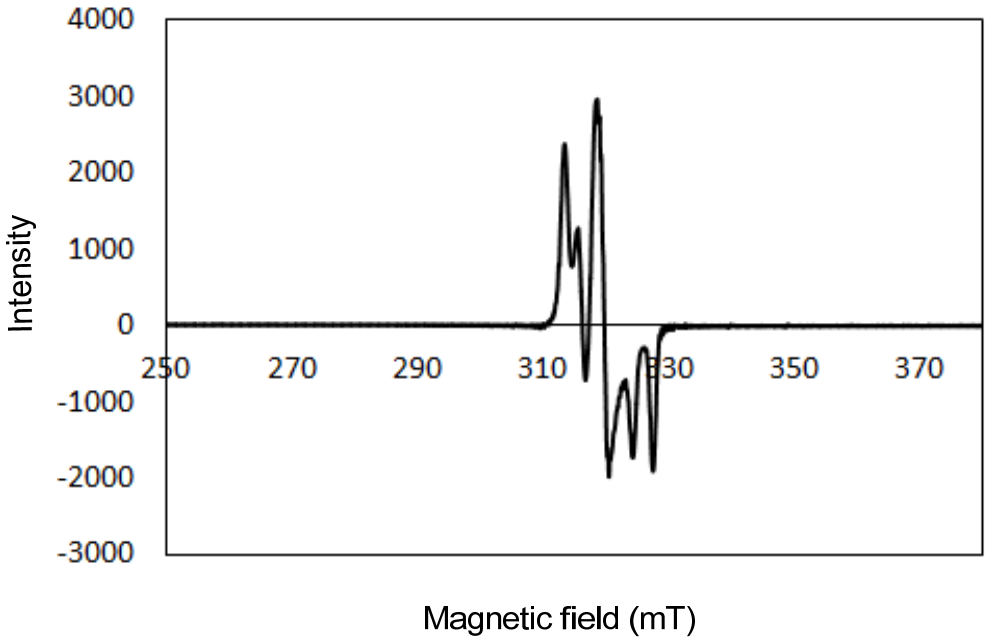
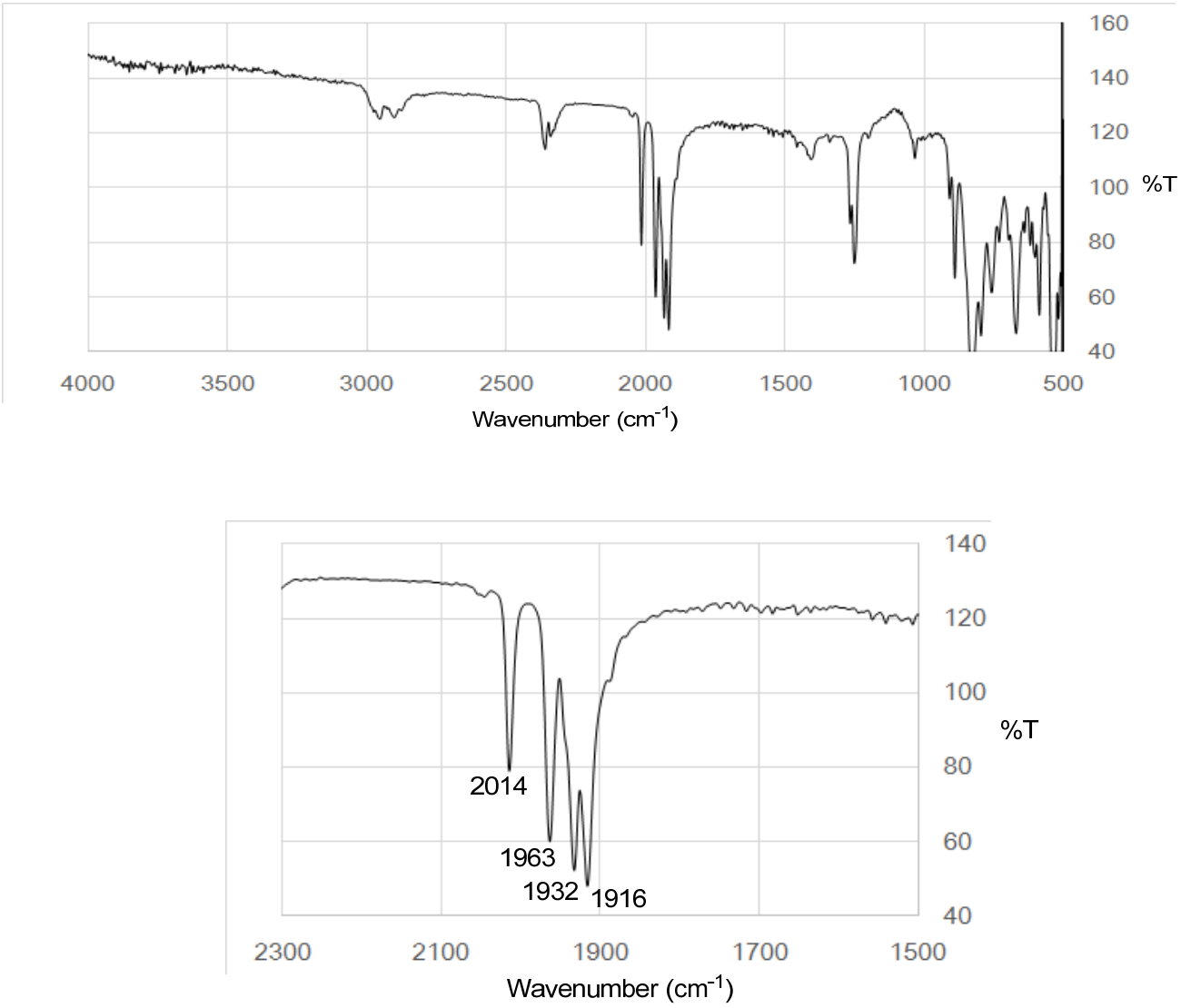


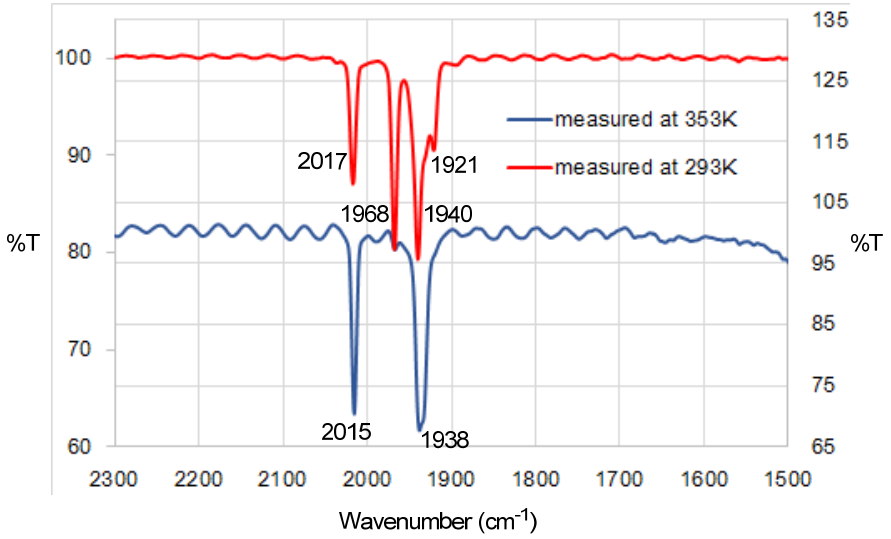
Figure S7-1. ATR-IR spectrum of **2** in the solid state.



IR spectra in *n*-octane

An *n*-octane solution of **2** (ca. 0.12 mM) was prepared by dissolving **2** (1.3 mg, 1.24 x 10^{-3} mmol) in *n*-octane (10 mL) at room temperature; the IR spectrum was recorded immediately at 293 K. Next, the solution was allowed to stand for 10 min at 353 K, then the IR spectrum was measured again.

Figure S7-2-1. IR spectra of solution of **2** in *n*-octane at 293 K and 353 K.



The time-course of IR spectra

An *n*-octane solution of **2** (ca. 0.12 mM) was prepared by dissolving **2** (1.3 mg, 1.24 x 10^{-3} mmol) in *n*-octane (10 mL). The IR spectrum was recorded at 353 K, then the temperature of the instrument was set to 293 K. The IR spectra were obtained periodically over 2 h.

Figure S7-2-2. The time-course of IR spectra of solution of **2** in *n*-octane after heating.

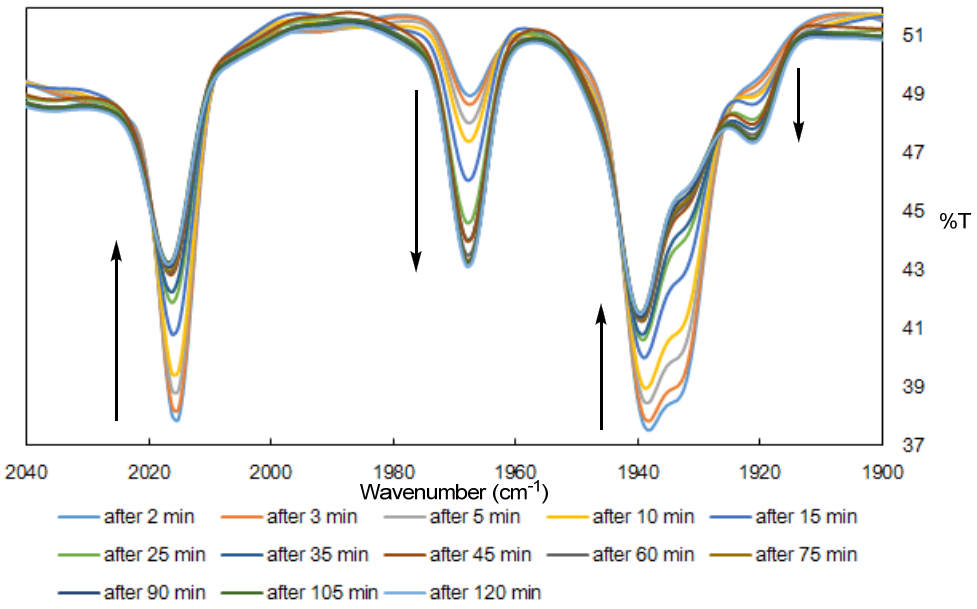


Figure S7-3. ATR-IR spectrum of **4** in the solid state.

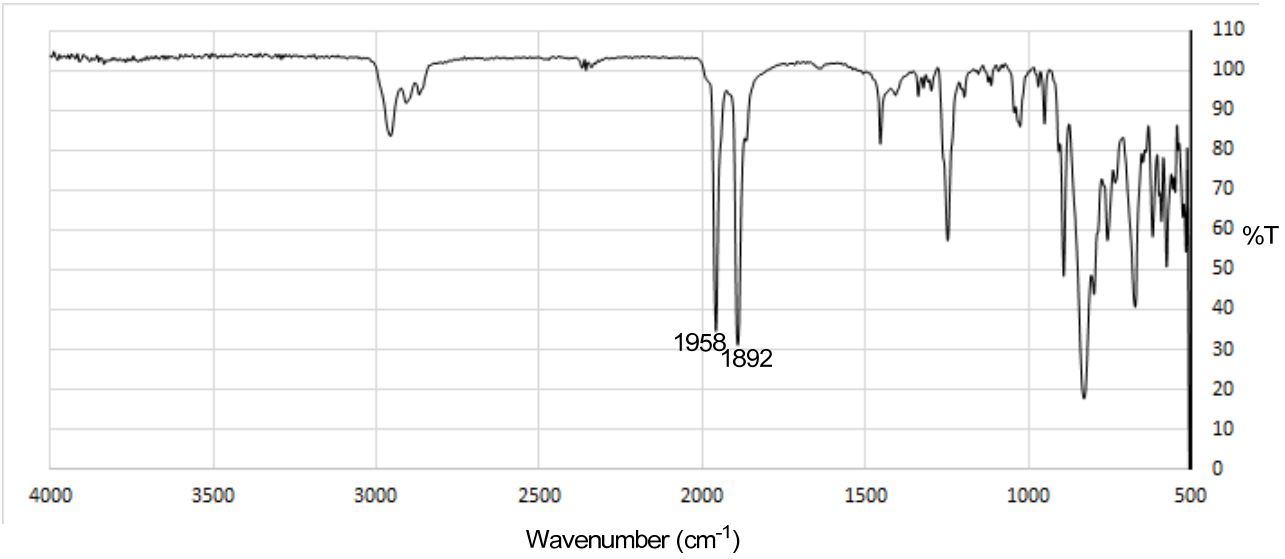


Figure S7-4. ATR-IR spectrum of **5** in the solid state.

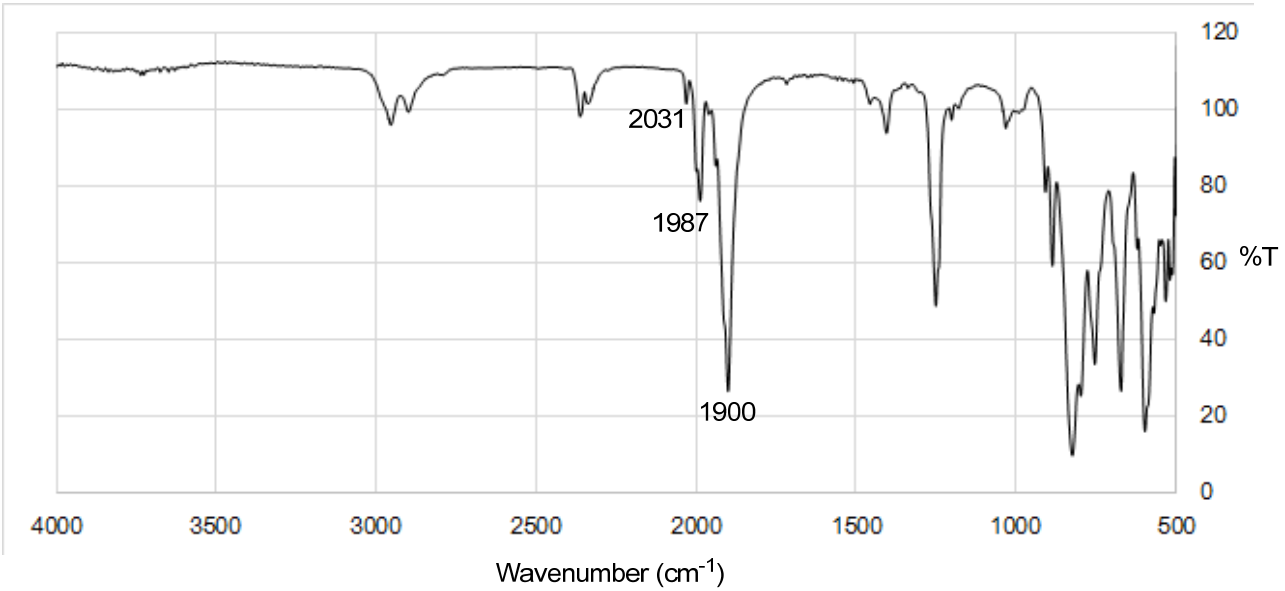
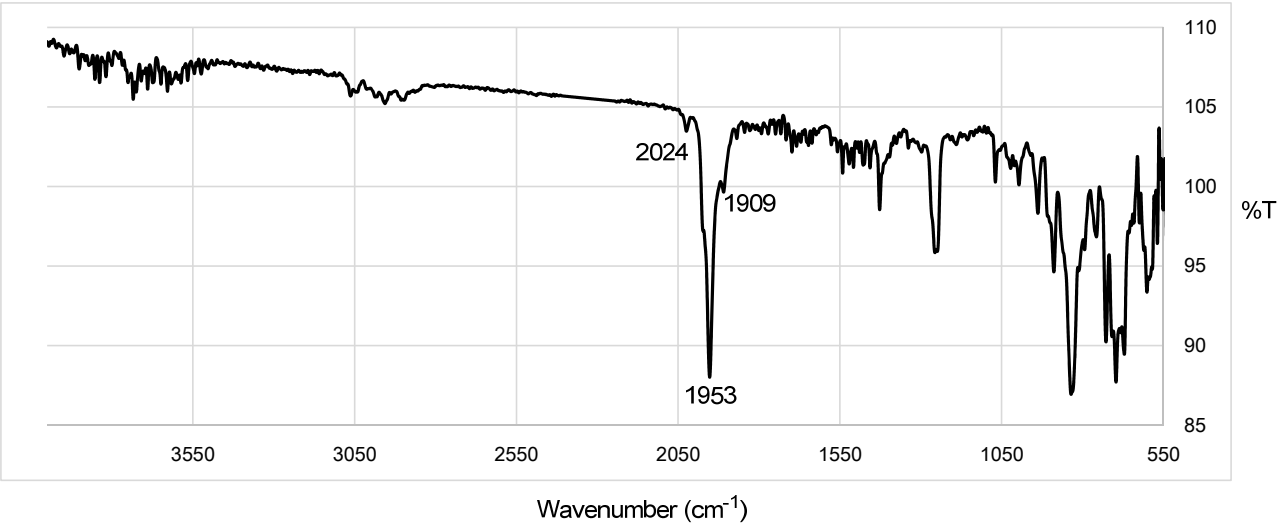


Figure S7-5. ATR-IR spectrum of **8** in the solid state.



UV-vis-NIR spectra

An *n*-octane solution of **2** (ca. 0.12 mM) was prepared by dissolving **2** (1.3 mg, 1.24 x 10^{-3} mmol) in *n*-octane (10 mL) at room temperature. The UV-vis-NIR spectrum was recorded immediately at 293 K after preparing the solution (Figure S7-1). Next, this solution was allowed to stand for 10 min at 353 K, then the UV-vis-NIR spectrum was re-measured (Figure S7-2). Next, the sample was cooled to 293 K, and UV-vis-NIR spectra were recorded at 293K after 30 min, 1 h, 2 h, 3 h, and 5 h (Figure S7-3).

Figure S8-1. UV-vis-NIR spectrum of solution of **2** in *n*-octane at 293 K [λ_{max}/nm (ε/$M^{-1}cm^{-1}$) = 380 (3.02×10^4), 502 (6.26×10^3), 720 (2.78×10^3)].

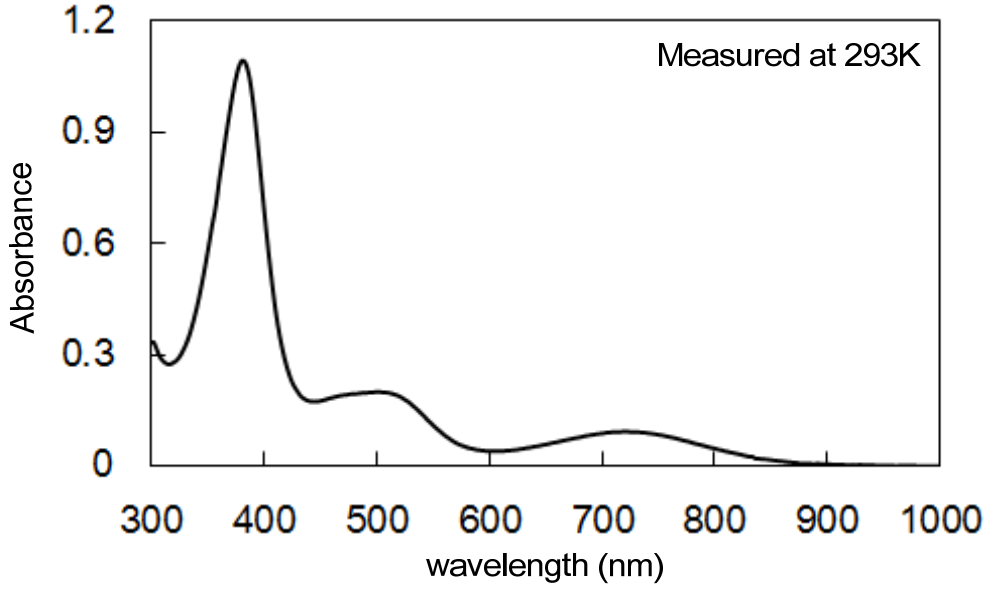


Figure S8-2. UV-vis-NIR spectrum of solution of **2** in *n*-octane at 353 K. [λ_{max}/nm (ε/$M^{-1}cm^{-1}$) = 362 (2.93×10^4), 496 (3.34×10^3), 818 (9.14×10^2)].

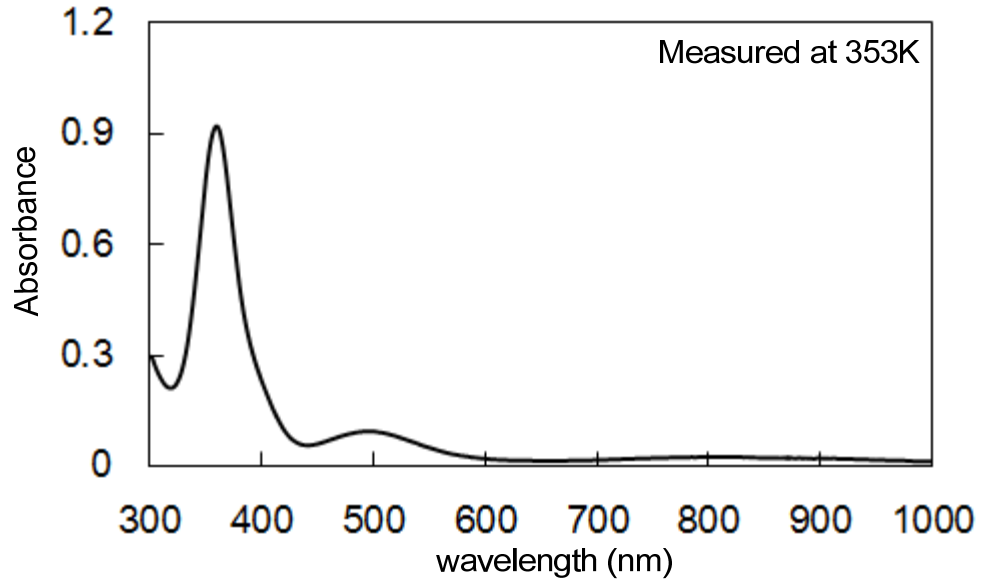
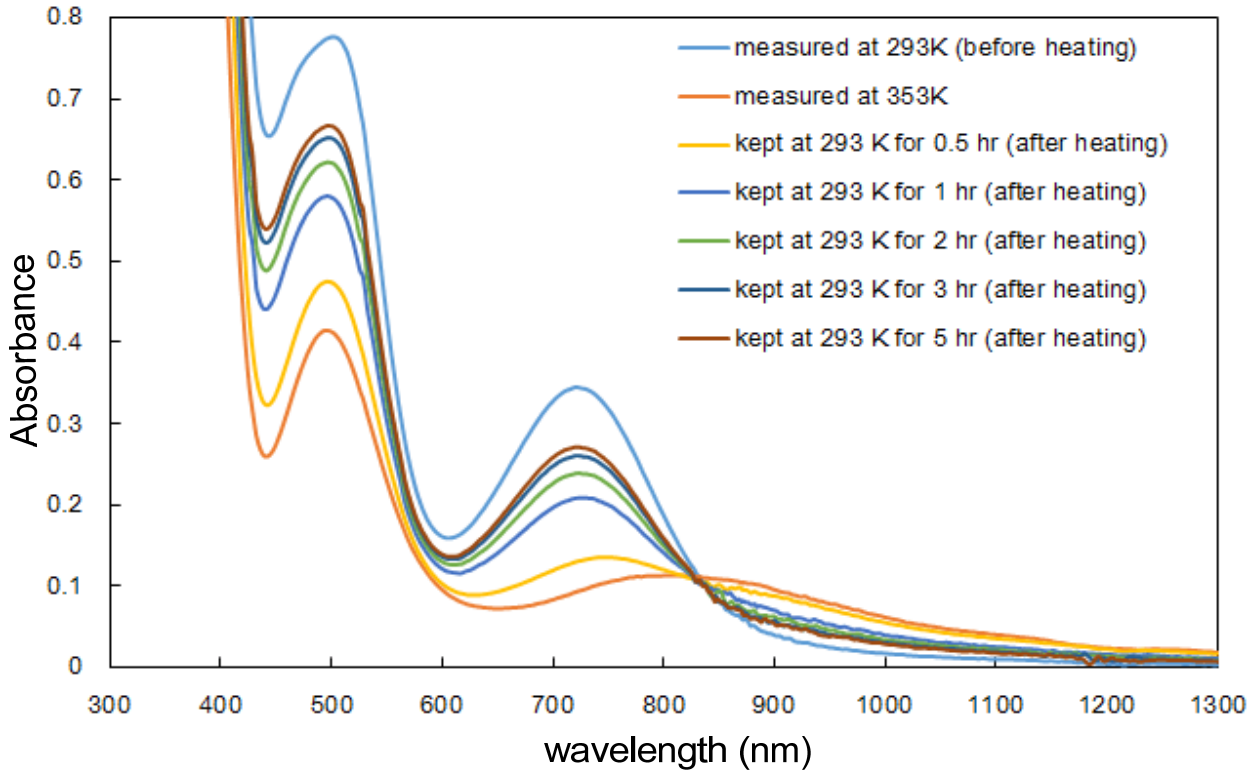


Figure S8-3. The time-course of UV-vis-NIR spectra of solution of **2** in *n*-octane before and after heating.



Thermodynamic analysis

The thermodynamic parameters were estimated using variable temperature ^{1}H NMR spectra. The equilibrium constant (K_{eq}) between **2** and **3** was estimated by two independent methods described below, and the K_{eq} values are summarized in Table S1-1 and S1-2. Plots of ln(K_{eq}) at various reciprocal temperatures are shown in Figure S5-1 and S5-2.

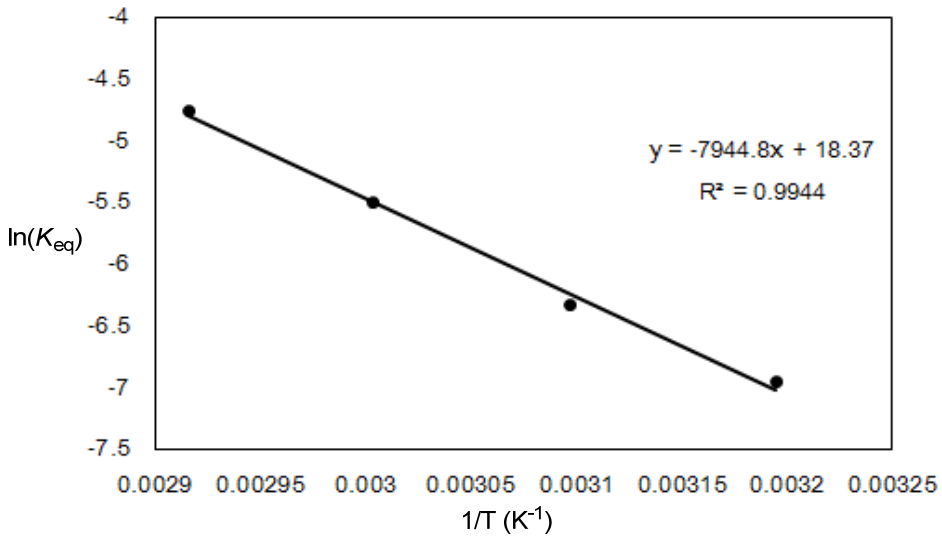
1) Estimation of K_{eq} using integral values

Complex **2** (10.0 mg, 9.7 x 10^{-3} mmol) was dissolved in C_6D_6 (16.5 mL); then mesitylene (2.7 μL, 1.95 x 10^{-2} mmol) was added as an internal standard. The initial concentration of **2** was ca. 0.588 mM. A portion of the solution (ca. 0.5 mL) was transferred into a J. Young NMR tube, and ^{1}H NMR spectra were measured at various temperatures. This solution was kept in the NMR instrument for 1 h at each temperature prior to the measurement, and ^{1}H NMR spectra were recorded at each temperature. The concentration of dinuclear complex **2** was calculated from the relative ratio of the integral value of the signals for the $SiMe_3$ group of **2** to that of the Me group of the internal standard (mesitylene), and the concentration of **3** was calculated from the following formula: [**3**]/2 = c_0 – [**2**] (c_0 = initial concentration of **2** = 0.588 mM). K_{eq} = [**3**]^2/[**2**].

Table S1-1. Equilibrium constants K_{eq} between **2** and **3** in C_6D_6 at various temperatures estimated by the values of integral.

Temp (K)	T^{-1} (K^{-1})	[**2**] (mmol L^{-1})	[**3**] (mmol L^{-1})	K_{eq} (mol L^{-1})	Ln(K_{eq})
343	0.002915	0.1068	0.9616	0.00866	-4.7494
333	0.003003	0.1705	0.8342	0.00408	-5.5013
323	0.003096	0.2515	0.6723	0.00180	-6.3215
313	0.003195	0.3132	0.5488	0.00096	-6.9467

Figure S9-1. A plot of ln(K_{eq}) vs 1/T for the equilibrium between **2** and **3**.



2) Estimation of K_{eq} by Evans method

Complex **2** (10.0 mg, 0.97 x 10^{-2} mmol) was dissolved in C_6D_6 (1.65 mL), then $SiMe_4$ (1.7 mg, 1.93 x 10^{-2} mmol) was added. The initial concentration of **2** was adjusted to ca. 5.88 mM. This solution was transferred into a J. Young NMR tube, and ^{1}H NMR spectra were measured at various temperatures. The solution was kept in the NMR instrument for 1 h at each temperature prior to measurement, and the ^{1}H NMR spectra were recorded at each temperature. The concentration of mononuclear complex **3** was estimated by the Evans method,[3] in which the number of unpaired electrons at the iron center was assumed to be 1, and the concentration of **2** was calculated from the following formula: [**2**] = c_0 – 0.5[**3**] (c_0 = initial concentration of **2** = 0.588 mM). K_{eq} = [**3**]^2/[**2**].

Table S1-2. Equilibrium constants K_{eq} between **2** and **3** in C_6D_6 at various temperatures estimated by using Evans method.

Temp (K)	T^{-1} (K^{-1})	[**2**] (mmol L^{-1})	[**3**] (mmol L^{-1})	K_{eq} (mol L^{-1})	Ln(K_{eq})
353	0.002833	2.1414	7.4696	0.02606	-3.6475
343	0.002915	2.7512	6.2501	0.01420	-4.2555
333	0.003003	3.5275	4.6975	0.00626	-5.0743
323	0.003096	4.2625	3.2275	0.00244	-6.0142
313	0.003195	4.7723	2.2078	0.00102	-6.8866

Figure S9-2. A plot of ln(K_{eq}) vs 1/T for the equilibrium between **2** and **3**.

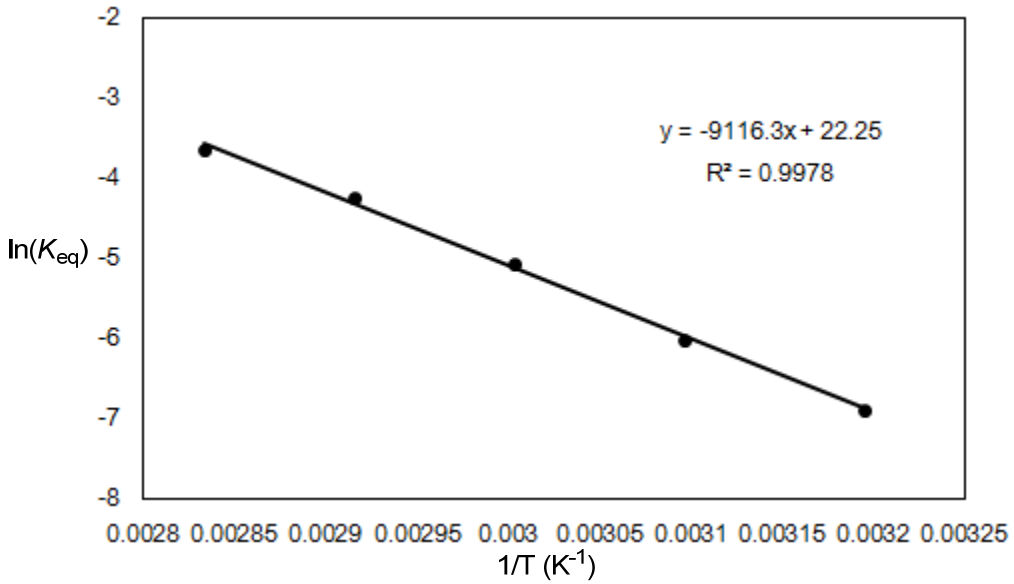
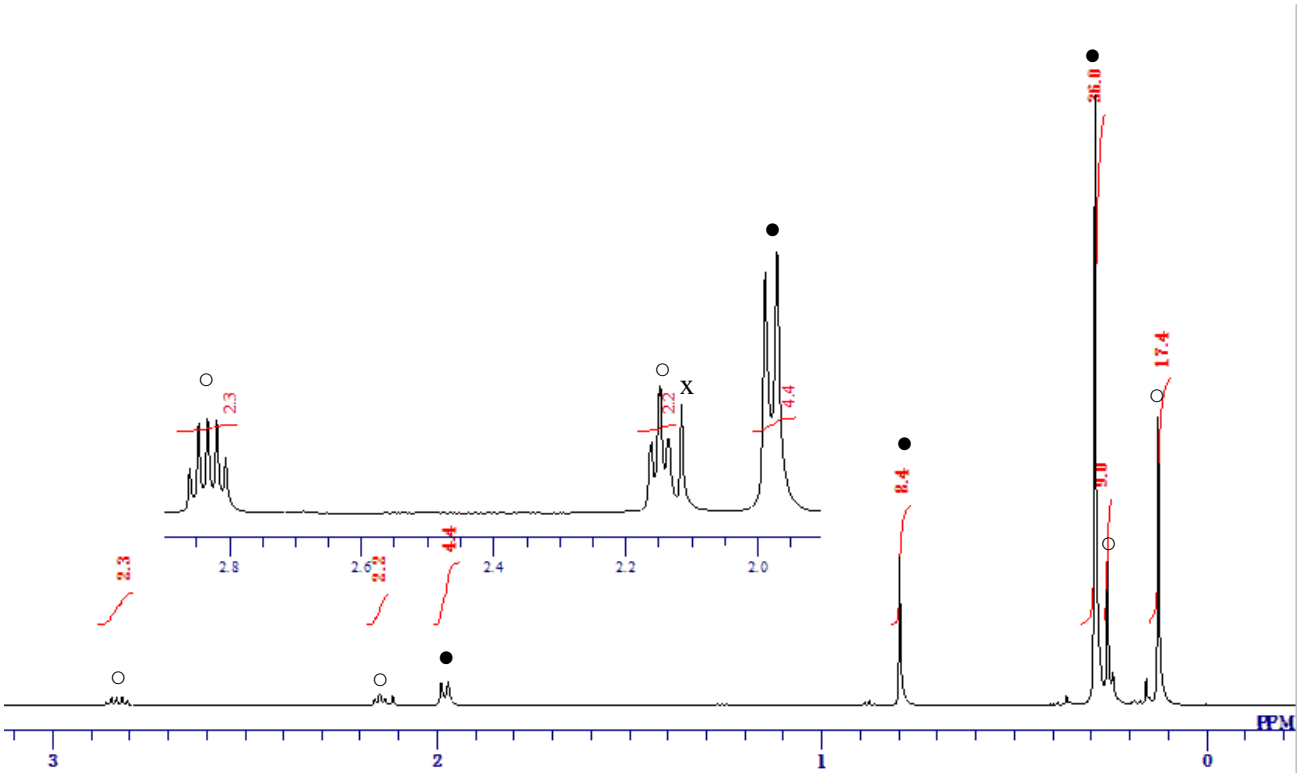


Figure S10-1. ^{1}H NMR spectrum (in C_6D_6 at room temperature) of the crude product obtained by the reaction of **2** with **1** in toluene at room temperature. The solid-circles and open-circles indicate signals of complex **5** and phosphaalkene **6**. Identification of **6** was achieved by comparison with the previously reported data.[2]



x = residual toluene

Figure S10-2. $^{31}P\{^{1}H\}$ NMR spectrum (in C_6D_6 at room temperature) of the crude product obtained by the reaction of **2** with **1** in toluene at room temperature. The solid-circles and open-circles indicate signals of **5** and **6**. Identification of **6** was achieved by comparison with the previously reported data.[2]

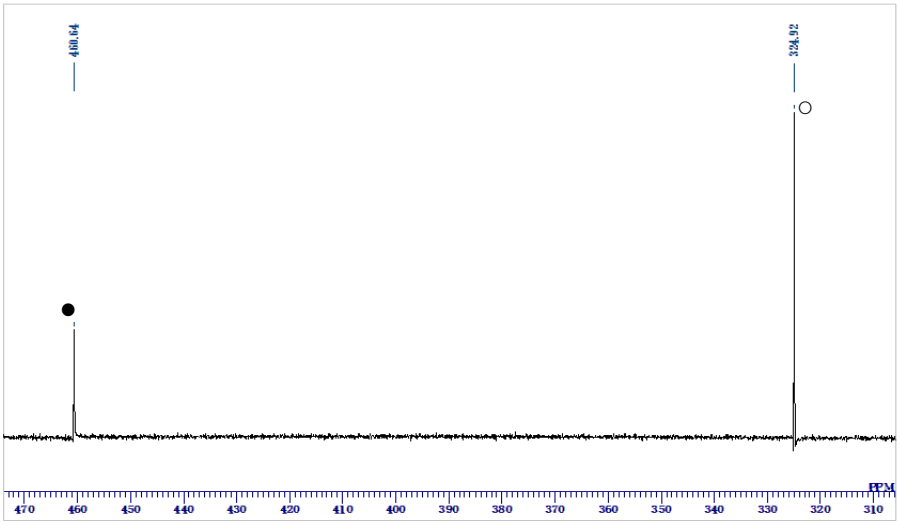


Figure S11-1. ^{1}H NMR spectrum (in C_6D_6 at room temperature) of the mixture of **8** and **9** formed by recrystallization of the crude product obtained from the reaction of **2** with $HSnPh_3$ in C_6D_6 at room temperature. The solid-circles and open-circles indicate signals of complex **8** and **9**.

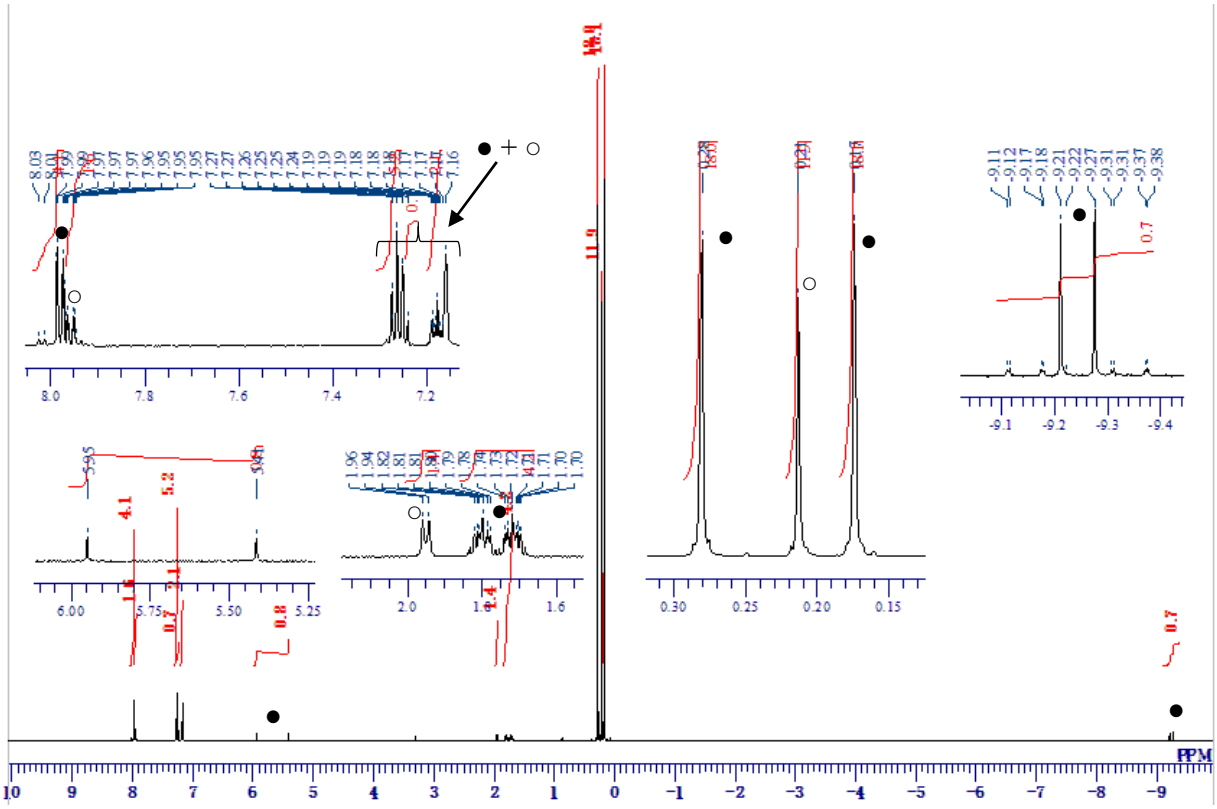


Figure S11-2. $^{13}C\{^{1}H\}$ NMR spectrum (in C_6D_6 at room temperature) of the mixture of **8** and **9** formed by recrystallization of the crude product obtained from the reaction of **2** with $HSnPh_3$ in C_6D_6 at room temperature. The solid-circles and open-circles indicate signals of complex **8** and **9**.

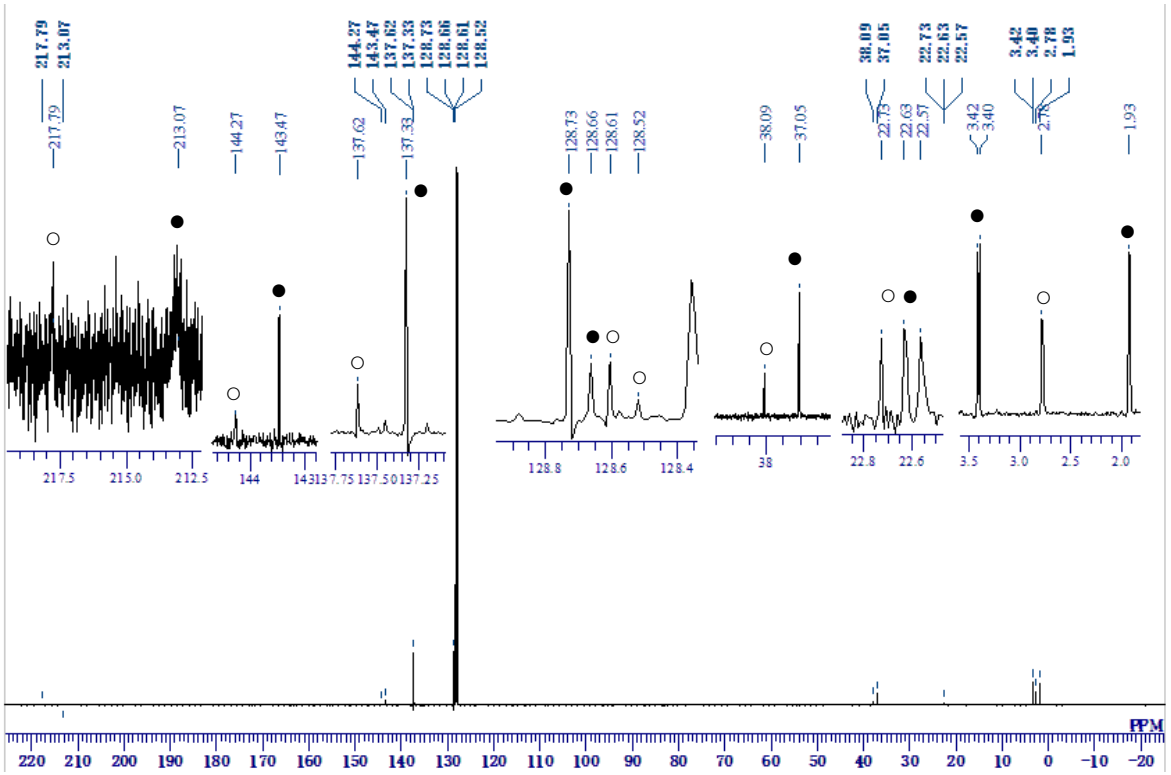


Figure S11-3. $^{31}P\{^{1}H\}$ NMR spectrum (in C_6D_6 at room temperature) of the mixture of **8** and **9** formed by recrystallization of the crude product obtained from the reaction of **2** with $HSnPh_3$ in C_6D_6 at room temperature. The solid-circles and open-circles indicate signals of complex **8** and **9**.

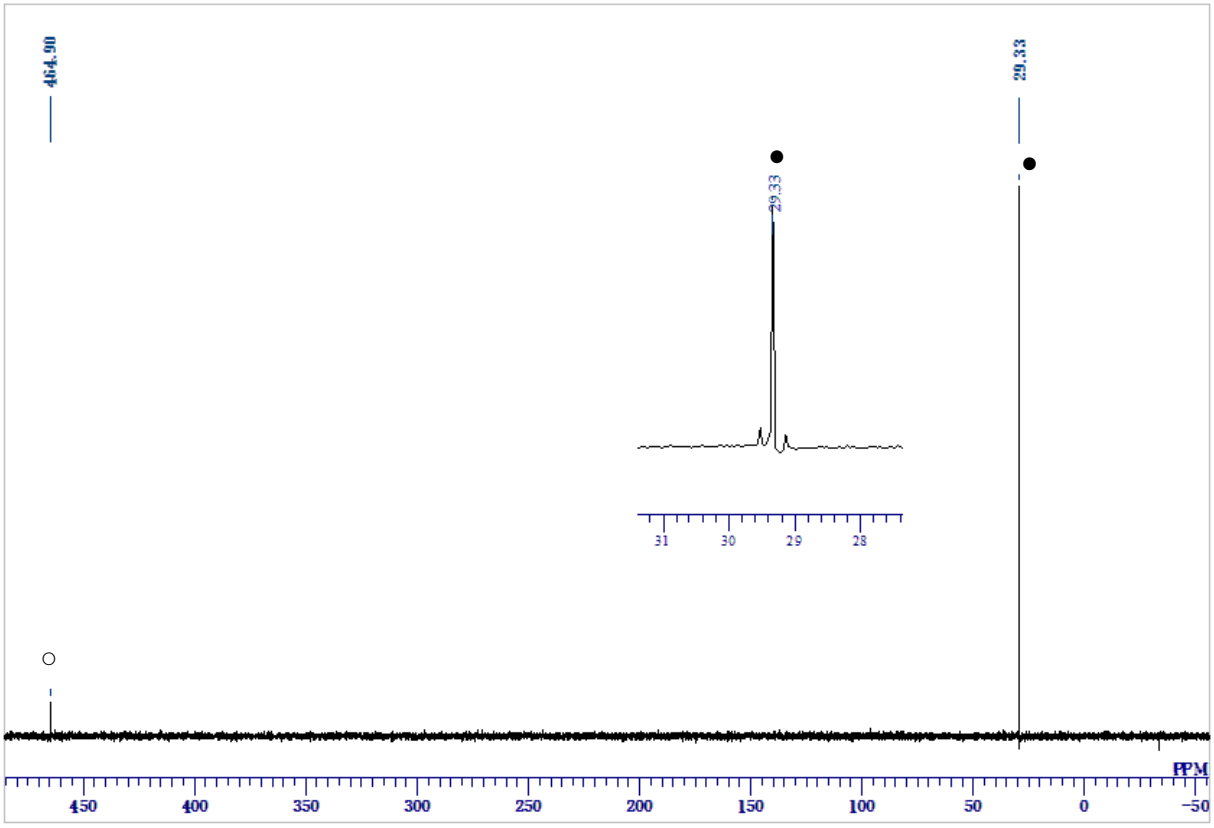


Figure S12-1. ^{1}H NMR spectrum (in C_6D_6 at room temperature) of the crude product obtained by the reaction of **2** with $HSnPh_3$ in C_6D_6 at room temperature. The solid-triangle, solid-circles, and open-circles indicate signals of free phosphine **7**, complex **8** and **9**. Identification of **7** was achieved by comparison with the previously reported data.[2] The solid-square indicates signals of internal standard (1,3,5-trimethoxybenzene).

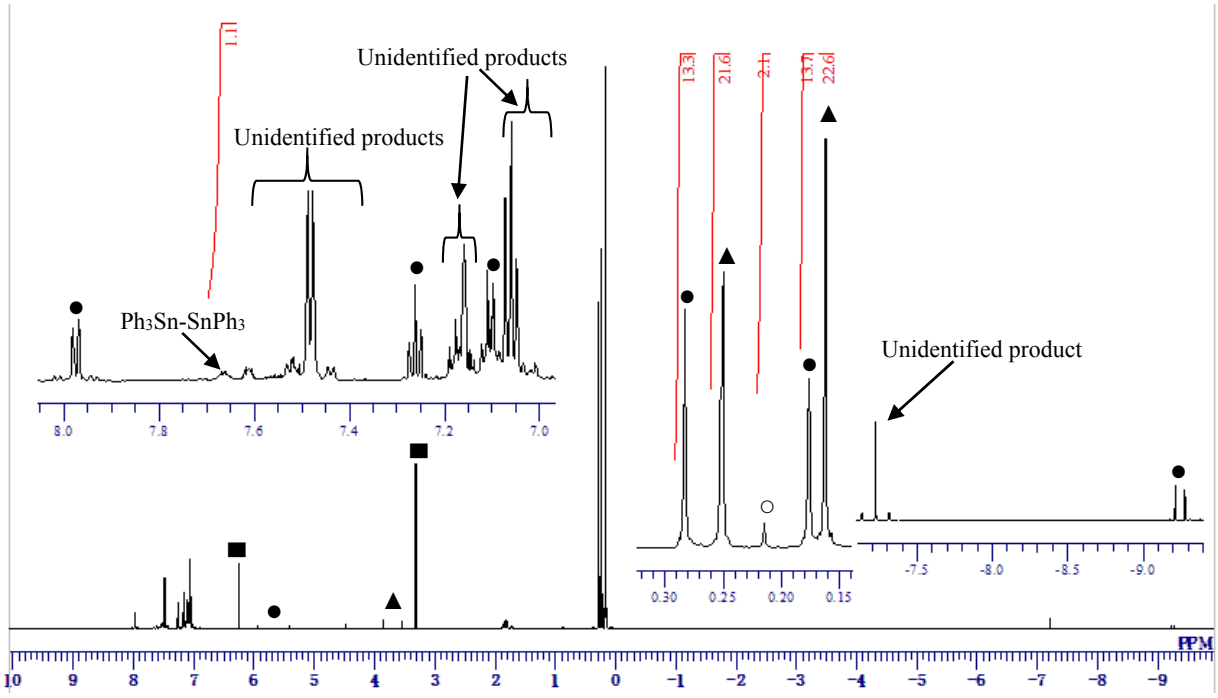


Figure S12-2. $^{31}P\{^{1}H\}$ NMR spectrum (in C_6D_6 at room temperature) of the crude product obtained by the reaction of **2** with $HSnPh_3$ in C_6D_6 at room temperature. The solid-triangles, solid-circles, and open-circles indicate signals of free phosphine **7**, complex **8** and **9**. Identification of **7** was achieved by comparison with the previously reported data.[2]

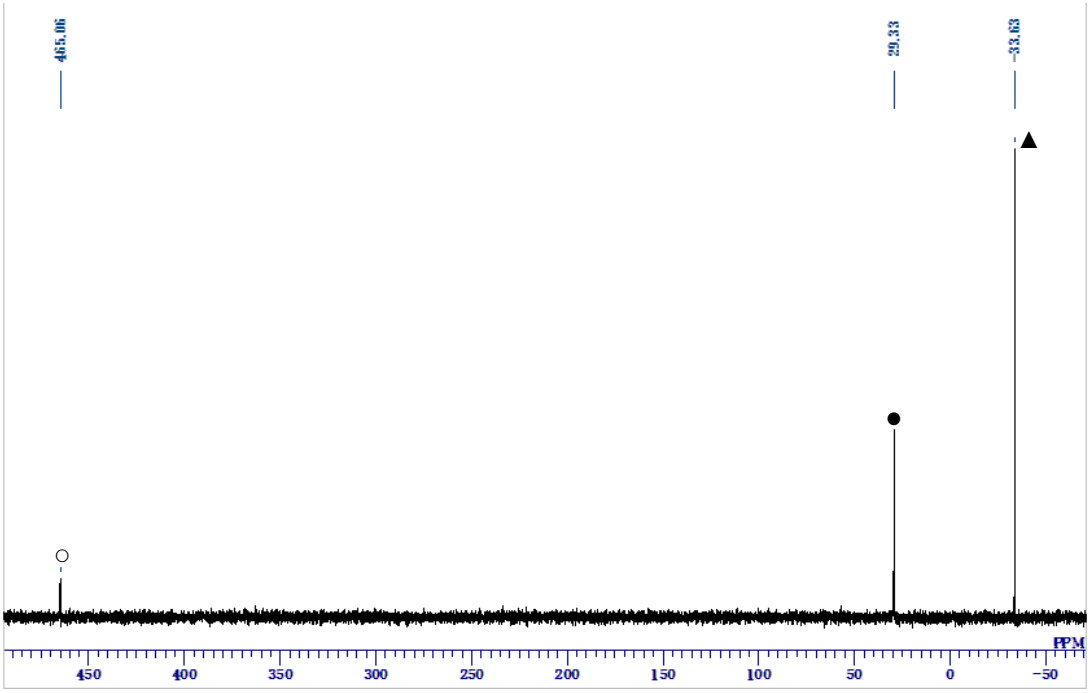


Figure S12-3. ^{31}P off-resonance NMR spectrum (in C_6D_6 at room temperature) of the crude product obtained by the reaction of **2** with $HSnPh_3$ in C_6D_6 at room temperature. The solid-triangles and solid-circles indicate signals of free phosphine **7** and complex **8**. Identification of **7** was achieved by comparison with the previously reported data.[2]

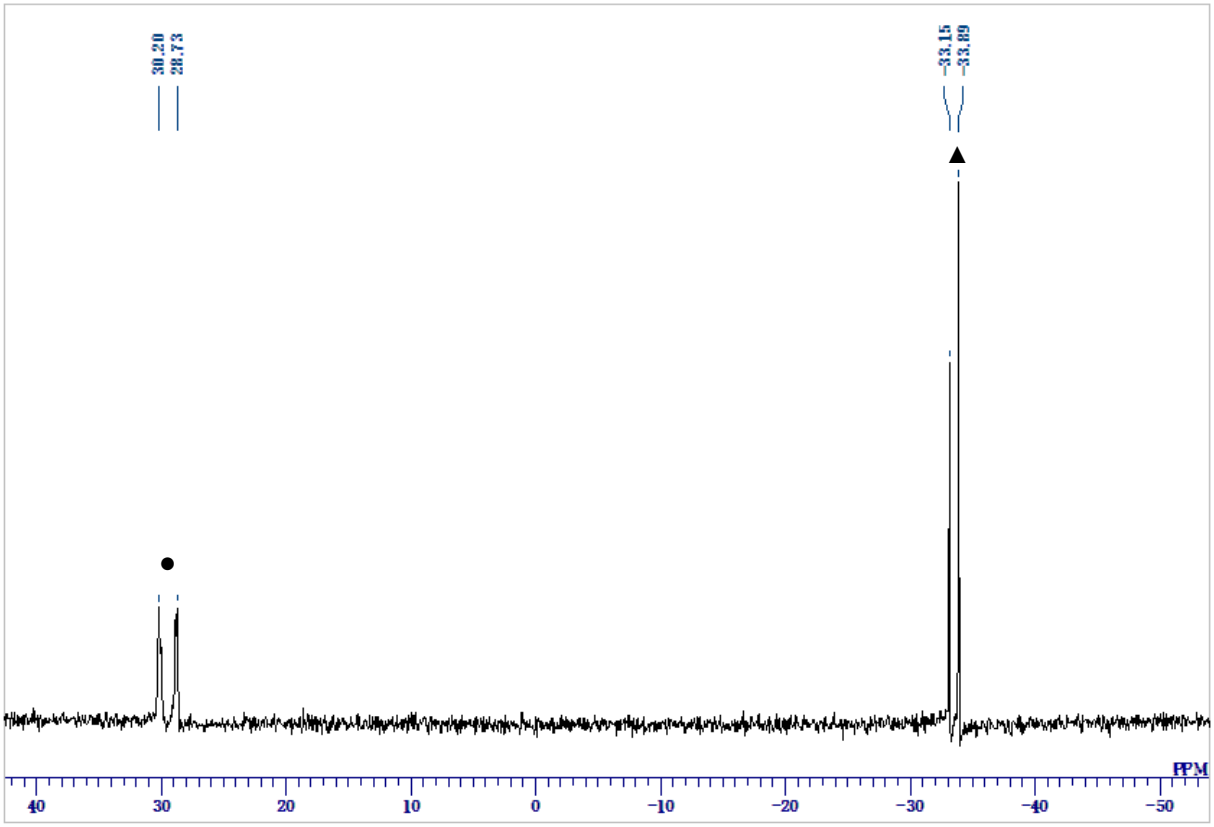


Figure S13-1. ^{1}H NMR spectrum (in C_6D_6 at room temperature) of the crude product obtained by the reaction of **2** with $HSnBu_3$ in C_6D_6 at room temperature. The solid-triangle and solid-circles indicate signals of free phosphine **7** and complex **8'**. Identification of **7** was achieved by comparison with the previously reported data.[2]

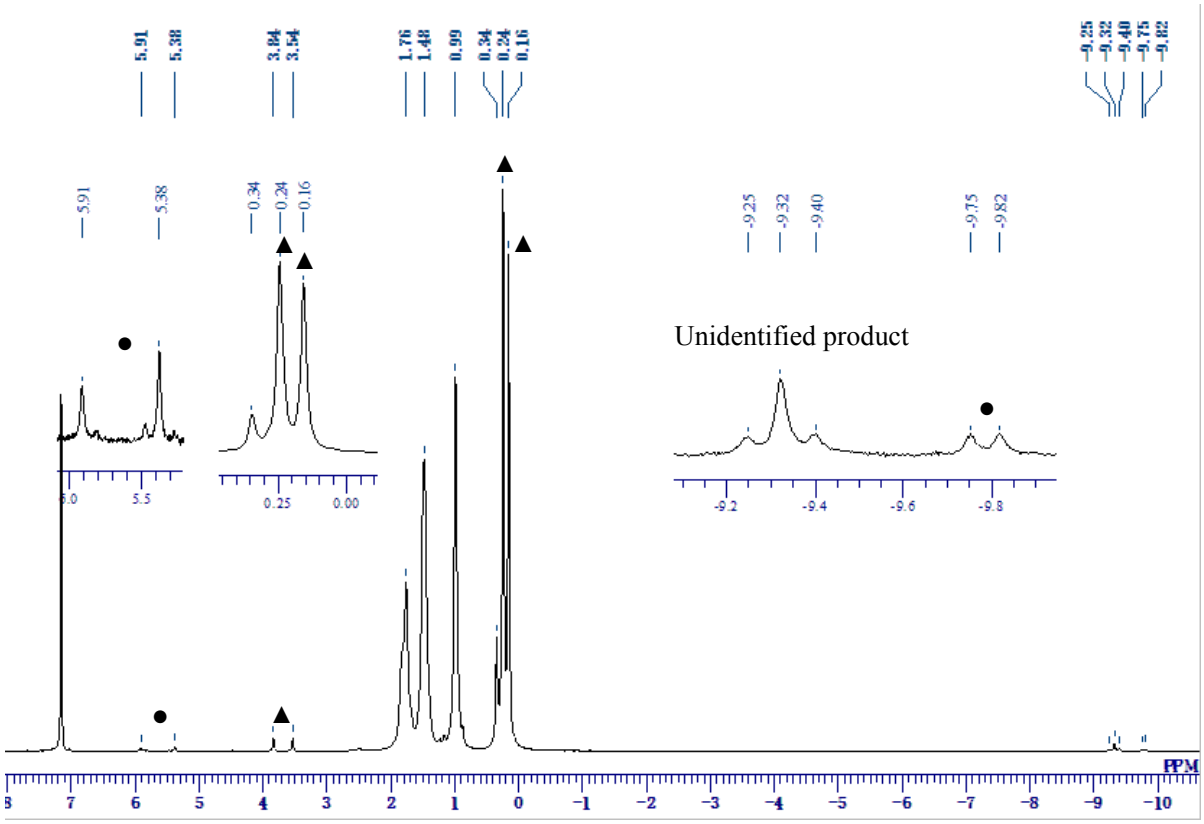


Figure S13-2. $^{31}P\{^{1}H\}$ NMR spectrum (in C_6D_6 at room temperature) of the crude product obtained by the reaction of **2** with $HSnBu_3$ in C_6D_6 at room temperature. The solid-triangle and solid-circles indicate signals of free phosphine **7** and complex **8'**. Identification of **7** was achieved by comparison with the previously reported data.[2]

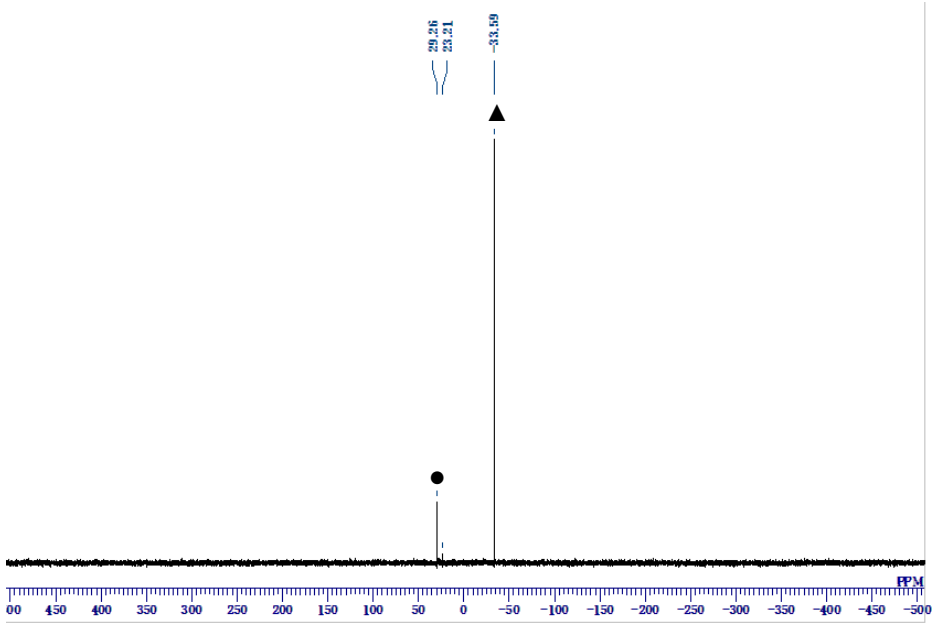


Figure S13-3. ^{31}P-off resonance NMR spectrum (in C_6D_6 at room temperature) of the crude product obtained by the reaction of **2** with $HSnBu_3$ in C_6D_6 at room temperature. The solid-triangle and solid-circles indicate signals of free phosphine **7** and complex **8'**. Identification of **7** was achieved by comparison with the previously reported data.[2]

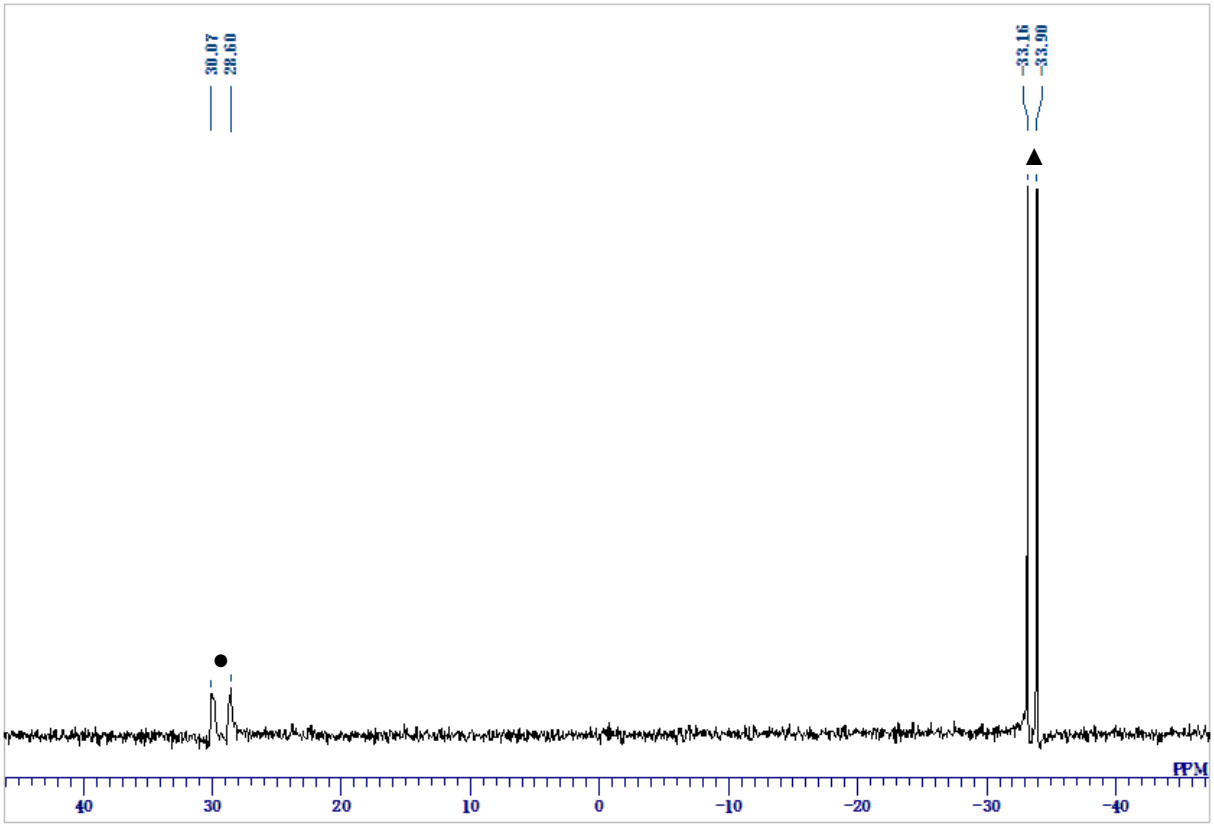


Figure S14-1. ^{1}H NMR spectrum (in C_6D_6 at room temperature) of the crude product obtained by the reaction of **2** with 9,10-dihydroanthracne in C_6D_6 at 353 K for 24 h. The solid-triangle indicates signal of free phosphine **7**, and the solid-square indicates signals of internal standard (1,3,5-trimethoxybenzene). The solid-circles indicate signal of phosphaalkene **6**. Identification of **6** was achieved by comparison with the previously reported data.[2]

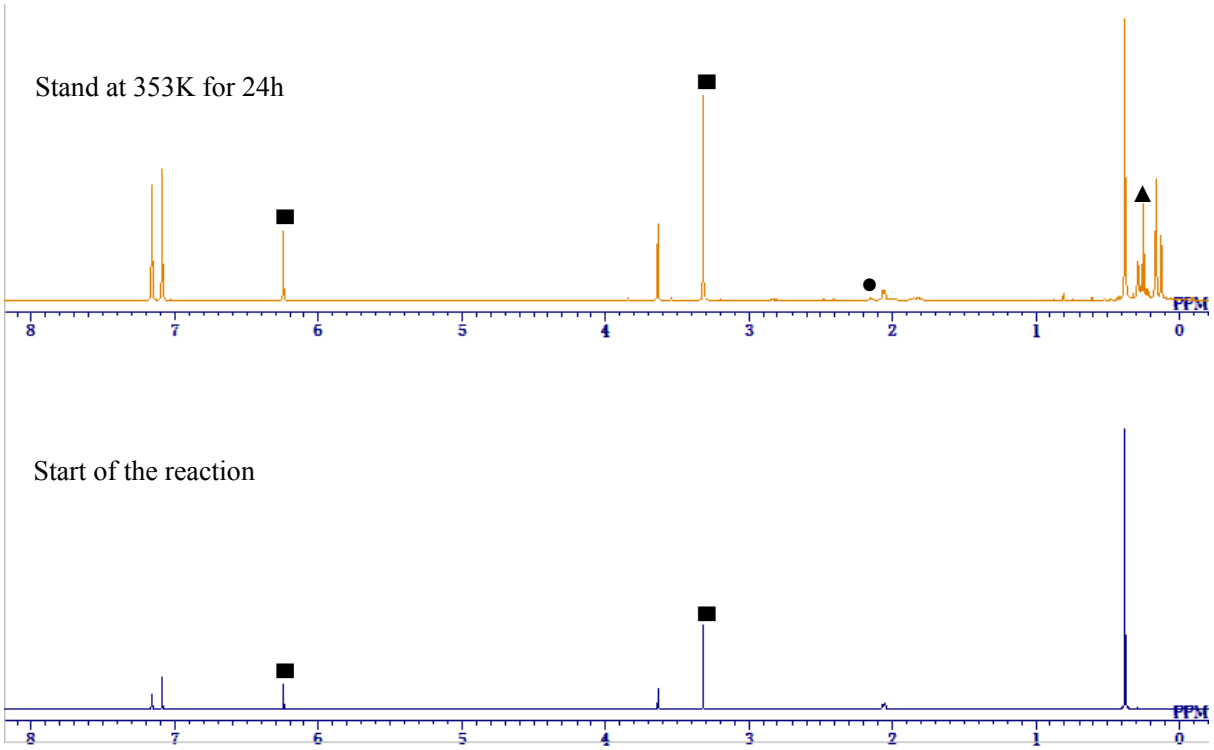
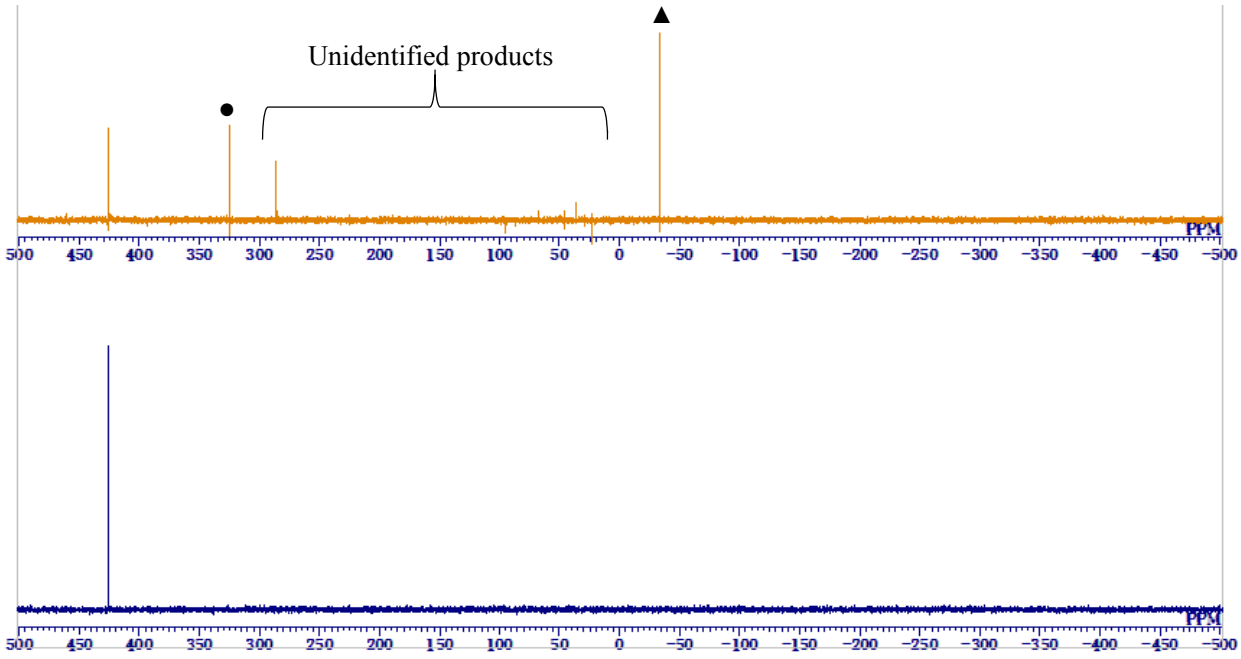


Figure S14-2. ^{31}P{^{1}H} NMR spectrum (in C_6D_6 at room temperature) of the crude product obtained by the reaction of **2** with 9,10-dihydroanthracne in C_6D_6 at 353 K for 24 h. The solid-triangle indicates signal of free phosphine **7**. The solid-circles indicate signal of phosphaalkene **6**. Identification of **6** was achieved by comparison with the previously reported data.[2]



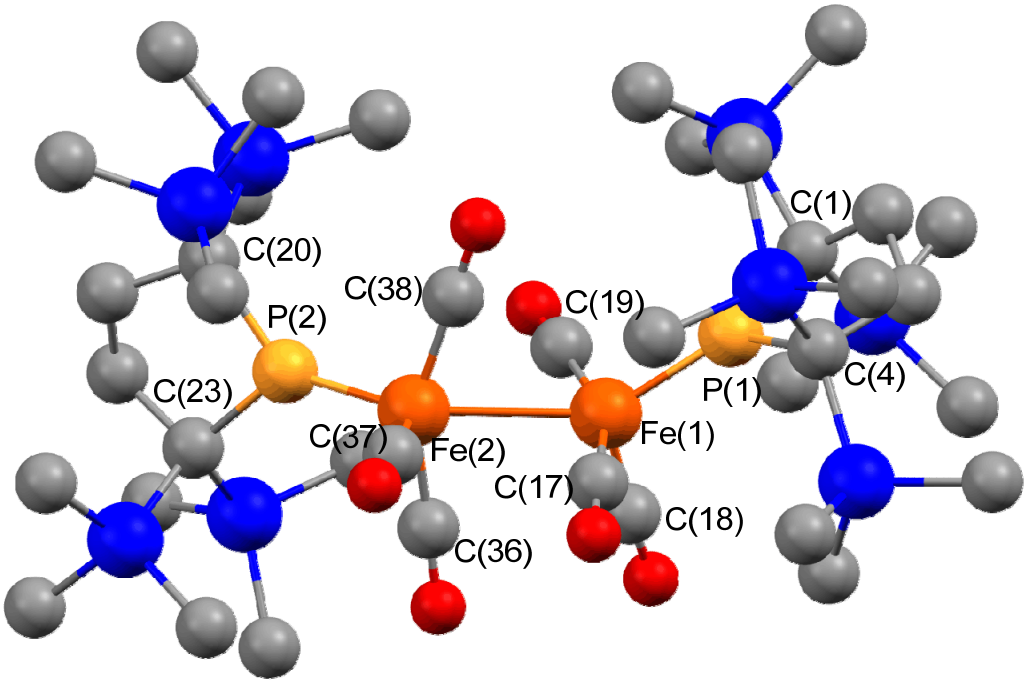
Theoretical calculations

All theoretical calculations were performed using the Gaussian 09 program package.[4] All calculations of the compounds were carried out at the PBE0, B3LYP, and CAM-B3LYP functionals[5] (Wachters-Hay basis[6,7] for Fe atoms and D95** basis[8] for H, and C, O, P, Si atoms). The Mayer bond order[9] is used as a natural extension of the Wiberg bond order. No imaginary frequencies were found in the optimized structures. The optimized structure of $\mathbf{2}_{\mathbf{opt}}$ and $\mathbf{3}_{\mathbf{opt}}$ obtained by the calculation at the PBE0 level are shown in Figures S15 and S18, and their MO diagrams are summarized in Figures S16 and S19. Atomic coordinates and their energies of $\mathbf{2}_{\mathbf{opt}}$ and $\mathbf{3}_{\mathbf{opt}}$ calculated by PBE0 level of theory are summarized in Tables S3 and S4. The transition energies and oscillator strengths of all electron transitions of $\mathbf{2}_{\mathbf{opt}}$ and $\mathbf{3}_{\mathbf{opt}}$ were calculated by using the time-dependent DFT method[10] (TD-DFT) at the PBE0, B3LYP or CAM-B3LYP level, and the results obtained by the calculation at the PBE0 level are summarized in Tables S5 and S6. Density distributions in (a) HOMO and (b) HOMO-1 of $\mathbf{2}_{\mathbf{opt}}$ as well as the density distributions in (a) αHOMO and (b) βHOMO of $\mathbf{3}_{\mathbf{opt}}$ are shown in Figures S17 and S21. The orbital interactions between the P ligand and the $Fe(CO)_3$ moiety in $\mathbf{3}_{\mathbf{opt}}$ are summarized in Figure S20. Electron density difference map at the PBE0 level are summarized in Figures S22 and S23. The results of TD-DFT calculated by B3LYP or CAM-B3LYP are summarized in Figure S24.

Table S2. Comparison between the DFT-optimized geometry and experimental structure of isolated complex **2**. Selected bond lengths and bond angles are shown.

	Calcd. by PBE0	Calcd. by B3LYP	Calcd. by CAM-B3LYP	Exptl.
Bond lengths (Å)				
Fe(1)-Fe(2)	2.715	2.824	2.748	2.7374(10)
Fe(1)-P(1)	2.095	2.129	2.091	2.0934(12)
Fe(2)-P(2)	2.096	2.128	2.091	2.1047(13)
Fe(1)-C(17)	1.781	1.799	1.788	1.796(4)
Fe(1)-C(18)	1.740	1.761	1.756	1.771(4)
Fe(1)-C(19)	1.777	1.796	1.785	1.794(4)
Fe(2)-C(36)	1.780	1.800	1.788	1.799(4)
Fe(2)-C(37)	1.740	1.761	1.755	1.766(4)
Fe(2)-C(38)	1.778	1.794	1.786	1.790(4)
Bond angles (deg)				
Fe(2)-Fe(1)-P(1)	139.55	138.76	138.75	142.66(4)
Fe(1)-P(1)-C(1)	129.42	130.06	129.54	130.01(14)
Fe(1)-P(1)-C(4)	132.36	131.30	131.98	131.20(11)
C(1)-P(1)-C(4)	96.71	97.02	96.97	97.32(18)
Fe(1)-Fe(2)-P(2)	138.69	140.71	140.77	132.61(4)
Fe(2)-P(2)-C(20)	131.61	131.57	132.90	132.13(15)
Fe(2)-P(2)-C(23)	129.97	129.79	128.09	129.04(12)
C(20)-P(2)-C(23)	96.76	97.00	97.04	97.55(19)

Figure S15. Optimized structure of $\mathbf{2}_{opt}$.



Tabale S3. Cartesian coordinates of $\mathbf{2}_{opt}$ in the closed shell singlet state.

Fe	-1.258627	0.792395	-0.547262
Fe	1.277433	0.878792	0.419366
P	-3.124233	-0.023942	-0.057054
P	3.133201	-0.023584	0.053274
Si	-4.702706	-1.113092	-2.603791
Si	-3.283158	-3.227160	-0.713892
Si	-4.950003	2.603942	0.613370
Si	-4.182997	0.461212	2.862503
Si	3.864462	-1.502013	2.855710
Si	3.503320	-3.180998	0.178361
Si	5.479537	2.190162	-0.173907
Si	4.238285	0.913769	-2.818435
O	-1.316052	3.237825	1.080658
O	-1.421825	2.340748	-2.990170
O	-0.039283	-1.449050	-1.998729
O	1.340410	3.062437	-1.544461
O	1.498368	2.805363	2.571375
O	0.011503	-1.090116	2.193986
C	-4.112393	-1.454063	-0.779644
C	-5.348265	-1.532136	0.155799
C	-5.769337	-0.130106	0.580846
C	-4.519843	0.715656	0.959650
C	-5.974853	0.283924	-2.766083
C	-5.664639	-2.617527	-3.253024
C	-3.286298	-0.726902	-3.785470
C	-4.655729	-4.515421	-0.461018
C	-2.342049	-3.775943	-2.261725
C	-2.121040	-3.425934	0.757647
C	-4.254759	3.289755	-1.008022
C	-4.431936	3.854562	1.938114
C	-6.842190	2.749456	0.514829
C	-5.726062	1.016907	3.822015
C	-3.930240	-1.350916	3.341441

C	-2.649066	1.339477	3.514779
C	-1.294556	2.236332	0.495441
C	-1.315844	1.735551	-2.008391
C	-0.519441	-0.589724	-1.383865
C	4.017016	-1.449421	0.901855
C	5.514826	-1.226841	0.551226
C	5.631562	-0.559804	-0.814841
C	4.615616	0.611498	-0.914147
C	5.550755	-2.043962	3.540102
C	2.600110	-2.710987	3.580472
C	3.447486	0.162269	3.650424
C	4.494735	-4.543230	1.056249
C	1.663110	-3.544691	0.312263
C	3.963795	-3.402500	-1.646570
C	6.289325	1.916995	1.520117
C	6.961856	2.637524	-1.275376
C	4.343307	3.680834	0.011664
C	2.679090	0.032008	-3.411744
C	4.035064	2.710730	-3.382030
C	5.699868	0.225208	-3.815775
C	1.322886	2.160689	-0.814976
C	1.367558	2.037967	1.714128
C	0.506853	-0.351215	1.446781
H	-6.185642	-2.048864	-0.330623
H	-5.105930	-2.119234	1.048923
H	-6.483924	-0.186857	1.411264
H	-6.308352	0.335539	-0.246892
H	-6.139963	0.445823	-3.839132
H	-5.658650	1.238532	-2.339584
H	-6.940994	0.008781	-2.328180
H	-6.059367	-2.348342	-4.240895
H	-6.524972	-2.853084	-2.616350
H	-5.069810	-3.526495	-3.372100
H	-2.934602	0.301182	-3.665142
H	-3.654362	-0.830502	-4.813840
H	-2.430288	-1.395680	-3.666910
H	-5.171050	-4.397095	0.497719
H	-4.182068	-5.505372	-0.454018
H	-5.408483	-4.517020	-1.254192
H	-2.073773	-4.828304	-2.101554
H	-1.414529	-3.222552	-2.419603
H	-2.932800	-3.728256	-3.180727
H	-1.408283	-2.605079	0.862397
H	-1.548418	-4.351501	0.621710
H	-2.676785	-3.518989	1.695875
H	-4.910782	4.106034	-1.335998
H	-4.189461	2.564738	-1.822400
H	-3.255653	3.710357	-0.863647
H	-4.871008	4.813467	1.632620
H	-3.350479	3.995885	1.986742
H	-4.802007	3.632535	2.942619
H	-7.094844	3.816901	0.522034
H	-7.350794	2.283613	1.365491
H	-7.257260	2.322880	-0.404415
H	-6.552682	0.310137	3.686650
H	-6.090692	2.013938	3.560112
H	-5.482771	1.025089	4.891699
H	-3.764385	-1.380388	4.425941
H	-3.039214	-1.768682	2.864353
H	-4.789196	-1.994385	3.126691
H	-2.653853	2.422732	3.385724
H	-1.746660	0.938408	3.042969
H	-2.577807	1.125578	4.588710
H	5.993526	-0.588767	1.298473
H	6.073757	-2.171385	0.558069
H	5.433951	-1.304440	-1.591228
H	6.660495	-0.216286	-0.980732
H	5.432364	-2.241375	4.612644
H	6.318567	-1.270521	3.433515
H	5.923694	-2.961143	3.073667
H	1.569495	-2.442401	3.337783

H	2.705287	-2.639878	4.671210
H	2.761378	-3.756776	3.305554
H	2.365103	0.304040	3.719347
H	3.856493	1.033241	3.133641
H	3.845863	0.158491	4.672888
H	5.572196	-4.435963	0.886963
H	4.196814	-5.504453	0.618727
H	4.327102	-4.606981	2.134349
H	1.484173	-4.558563	-0.067237
H	1.086103	-2.854459	-0.308966
H	1.277941	-3.492942	1.332385
H	3.564328	-4.373181	-1.966882
H	5.046620	-3.427401	-1.809899
H	3.527805	-2.641398	-2.299321
H	5.610043	1.545119	2.291147
H	6.659400	2.893783	1.857761
H	7.154569	1.247162	1.465213
H	7.708449	1.835173	-1.289048
H	7.448177	3.518035	-0.836660
H	6.711961	2.882400	-2.310180
H	4.953337	4.537551	0.324010
H	3.592781	3.512606	0.790068
H	3.823952	3.954714	-0.909078
H	1.774875	0.533473	-3.056704
H	2.609930	-1.014042	-3.102450
H	2.670028	0.060858	-4.508760
H	3.126443	3.176381	-2.995963
H	3.940323	2.673595	-4.475245
H	4.882030	3.361766	-3.152116
H	5.565959	0.524779	-4.862480
H	5.751398	-0.868258	-3.793866
H	6.665394	0.618782	-3.481608

Figure S16. MO diagrams for $\mathbf{2}_{opt}$ obtained from DFT calculations at the PBE0 level.

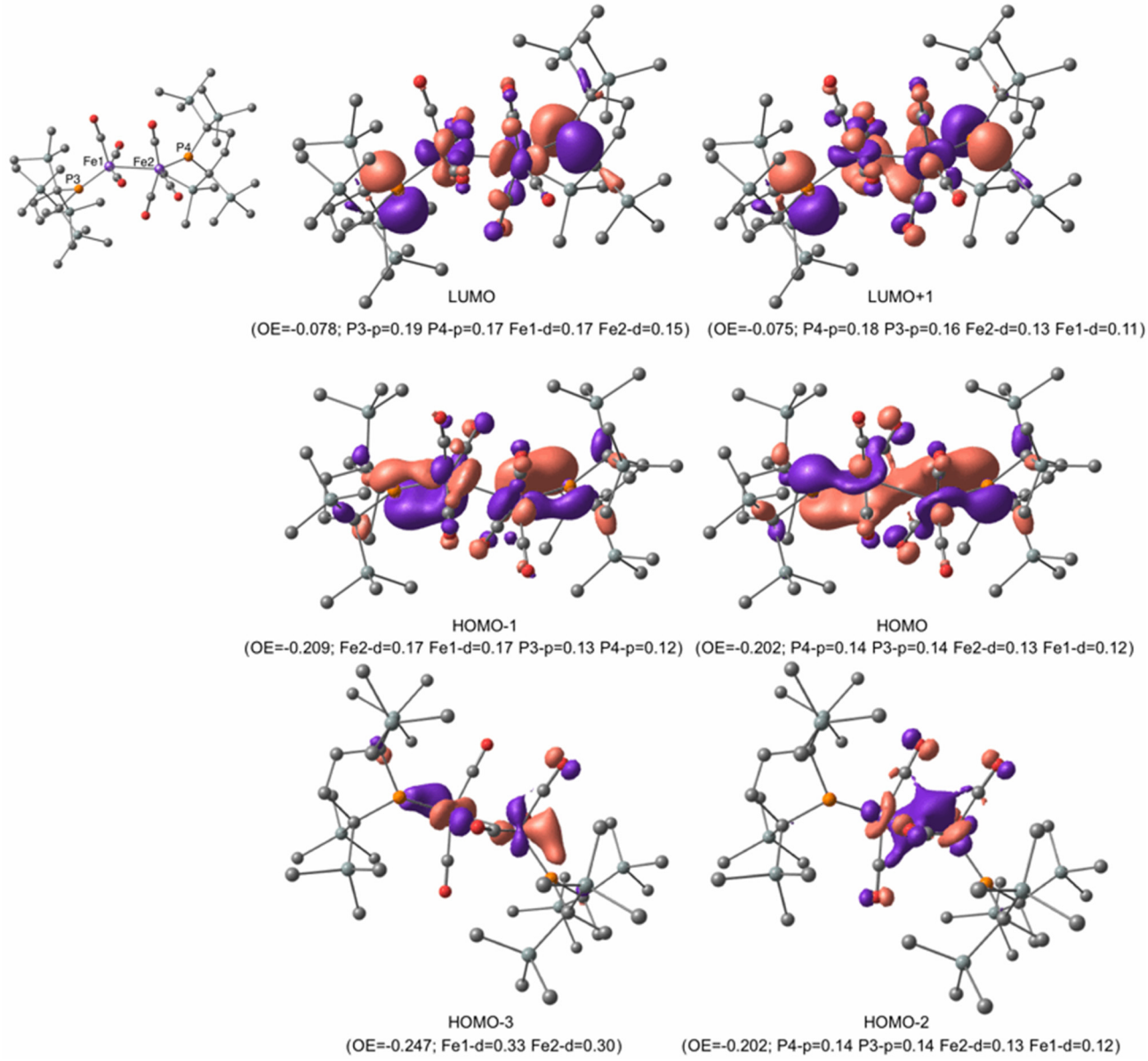
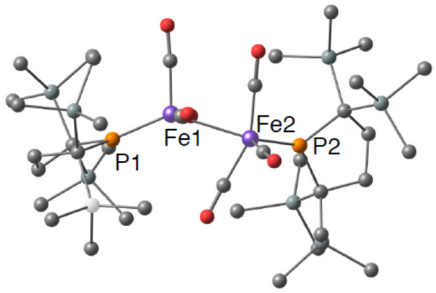
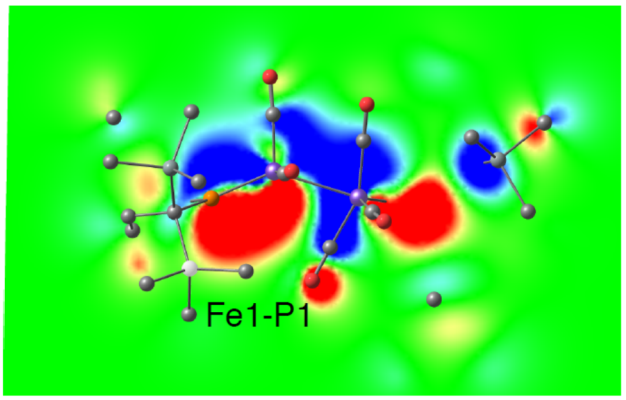
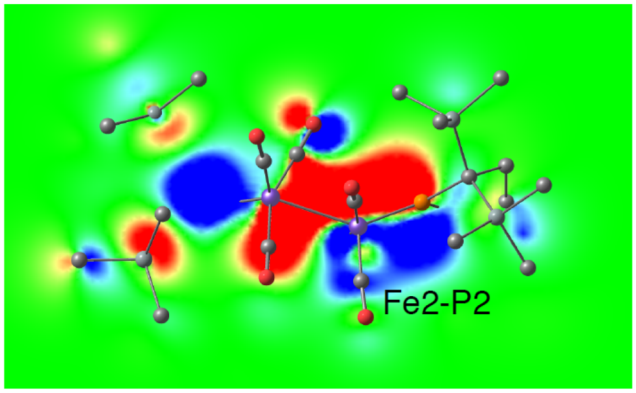


Figure S17. Density distributions in (a) HOMO and (b) HOMO-1 of $\mathbf{2}_{\mathbf{opt}}$. The two plot planes (left and right) indicate the π-bonding interaction in the Fe-P bonds.

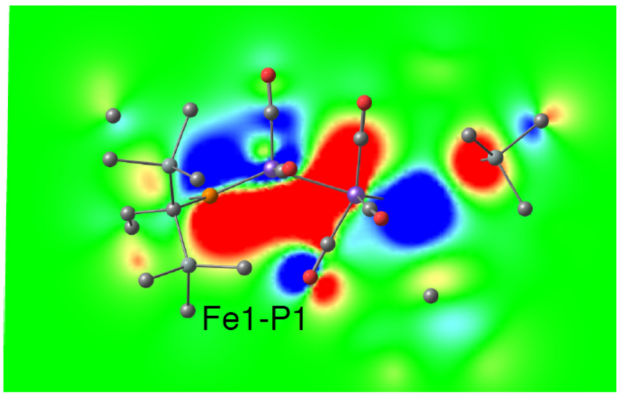


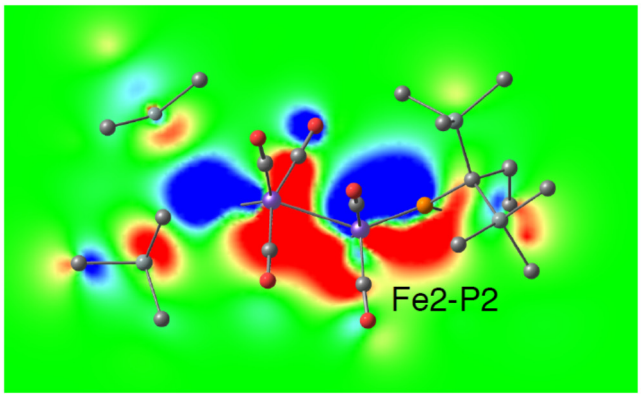
(a) HOMO





(b) HOMO-1





The plot planes are arranged in parallel with the Fe, P, and C(CO) atoms.

Figure S18. Optimized structure of $\mathbf{3}_{opt}$.

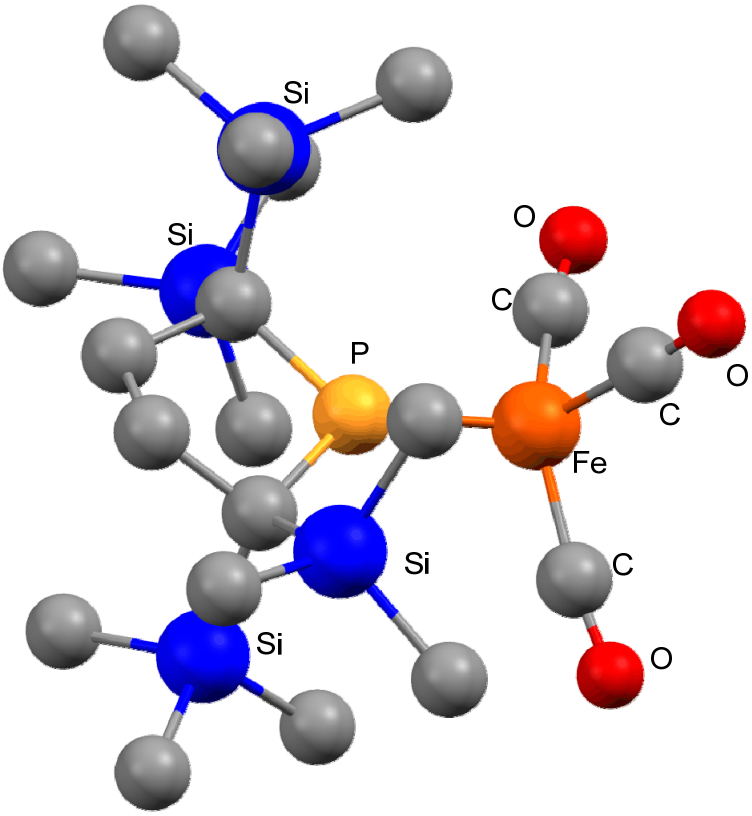


Table S4. Cartesian coordinates of $\mathbf{3}_{opt}$ in the doublet state.

Fe	0.016360	2.207397	-0.903133
P	0.000582	0.219536	-0.099467
Si	2.232402	-1.840889	-1.112871
Si	2.733619	-0.017642	1.484496
Si	-2.570703	-1.300321	-1.182608
Si	-2.453579	-0.286028	1.847931
O	2.716348	2.623756	-2.060478
O	-2.783231	2.840750	-1.643724
O	0.213187	4.417692	1.009671
C	1.697717	2.381501	-1.571189
C	-1.720901	2.504917	-1.331720
C	0.134169	3.570612	0.222746
C	1.397328	-0.926784	0.393123
C	0.693306	-1.963514	1.310104
C	-0.708774	-2.253718	0.772330
C	-1.408001	-0.930034	0.345659
C	2.452803	-0.750815	-2.634966
C	3.934594	-2.538367	-0.647879
C	1.289719	-3.395723	-1.659737
C	1.959852	1.177016	2.728561
C	4.025469	0.967276	0.515574
C	3.637450	-1.306035	2.542651
C	-3.127687	-3.110631	-1.072097
C	-4.155512	-0.273320	-1.292619
C	-1.687919	-1.059415	-2.837930
C	-3.887118	-1.489512	2.170641
C	-3.124788	1.461013	1.630734
C	-1.465112	-0.284022	3.459932
H	1.271775	-2.894196	1.383965
H	0.611820	-1.571304	2.331977
H	-1.298001	-2.796518	1.523223
H	-0.617301	-2.930698	-0.080870
H	3.171087	0.058014	-2.474373

H	1.510373	-0.301879	-2.965012
H	2.834541	-1.376129	-3.451560
H	3.866383	-3.280605	0.154727
H	4.669897	-1.782881	-0.357379
H	4.325089	-3.053506	-1.534694
H	1.892921	-3.870063	-2.444372
H	0.300481	-3.204155	-2.083671
H	1.184116	-4.126322	-0.849860
H	1.244043	1.866026	2.271789
H	2.770916	1.775784	3.161848
H	1.469848	0.651509	3.554366
H	4.911966	1.074399	1.153091
H	3.667613	1.974434	0.286289
H	4.347930	0.505324	-0.421549
H	2.944650	-1.908076	3.140195
H	4.285875	-0.767176	3.244970
H	4.267489	-1.984343	1.963109
H	-2.316415	-3.821668	-1.259862
H	-3.896125	-3.282777	-1.835629
H	-3.569442	-3.349407	-0.099008
H	-3.970830	0.788024	-1.469160
H	-4.805333	-0.370087	-0.418541
H	-4.713763	-0.653513	-2.157836
H	-1.497911	0.000193	-3.036128
H	-2.335279	-1.444988	-3.635709
H	-0.729293	-1.582348	-2.904937
H	-4.612477	-1.559567	1.355326
H	-4.425721	-1.143200	3.061456
H	-3.524288	-2.500992	2.386807
H	-2.309042	2.183698	1.525995
H	-3.691319	1.726702	2.531765
H	-3.791393	1.569605	0.772090
H	-0.618338	0.406079	3.423964
H	-1.101176	-1.277879	3.741935
H	-2.133813	0.057190	4.260185

Figure S19. MO diagrams for $\mathbf{3}_{opt}$ obtained from DFT calculations at the PBE0 level.

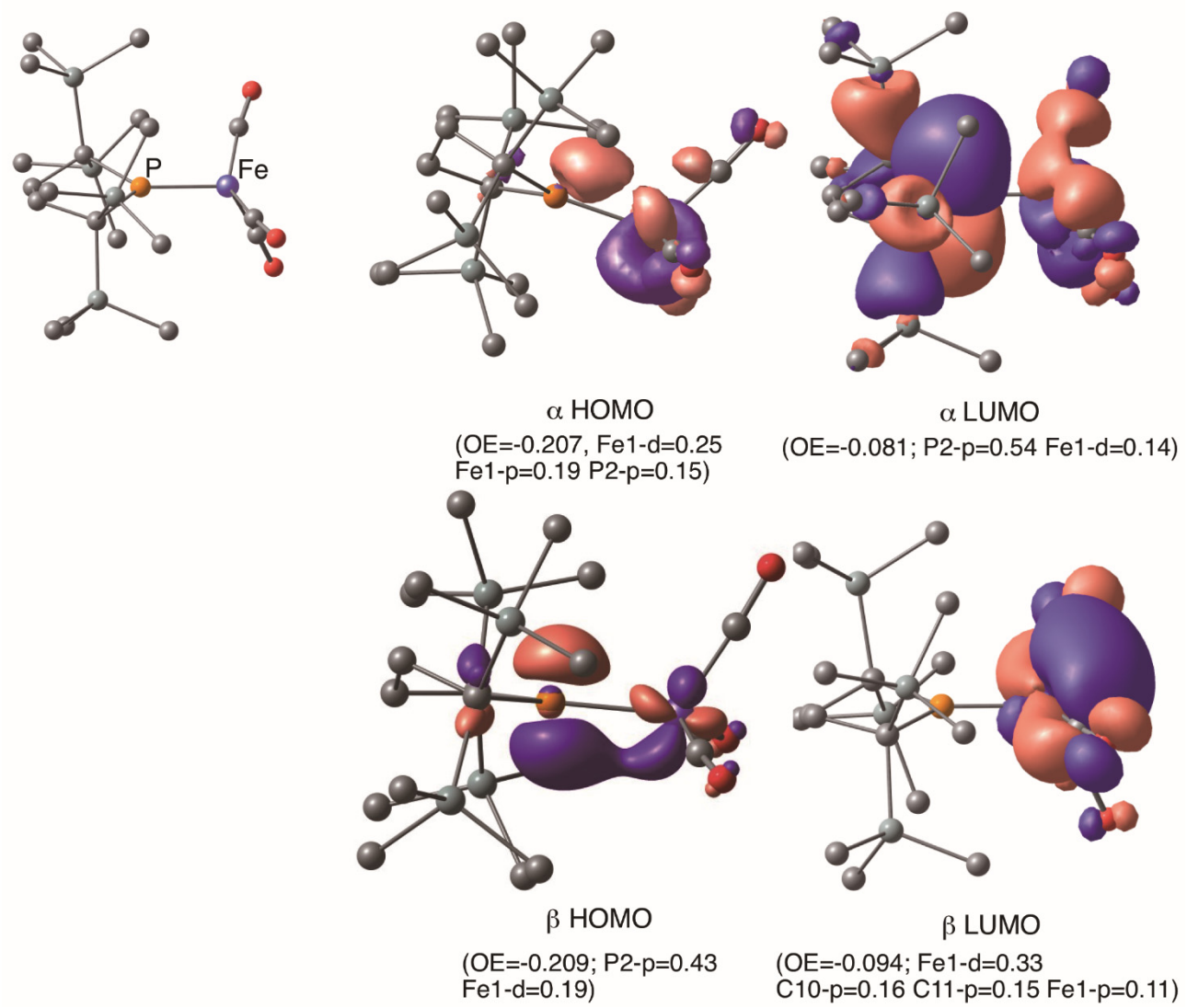


Figure S20. Orbital interactions between the P ligand and the $Fe(CO)_3$ moiety in $\mathbf{3}_{opt}$.

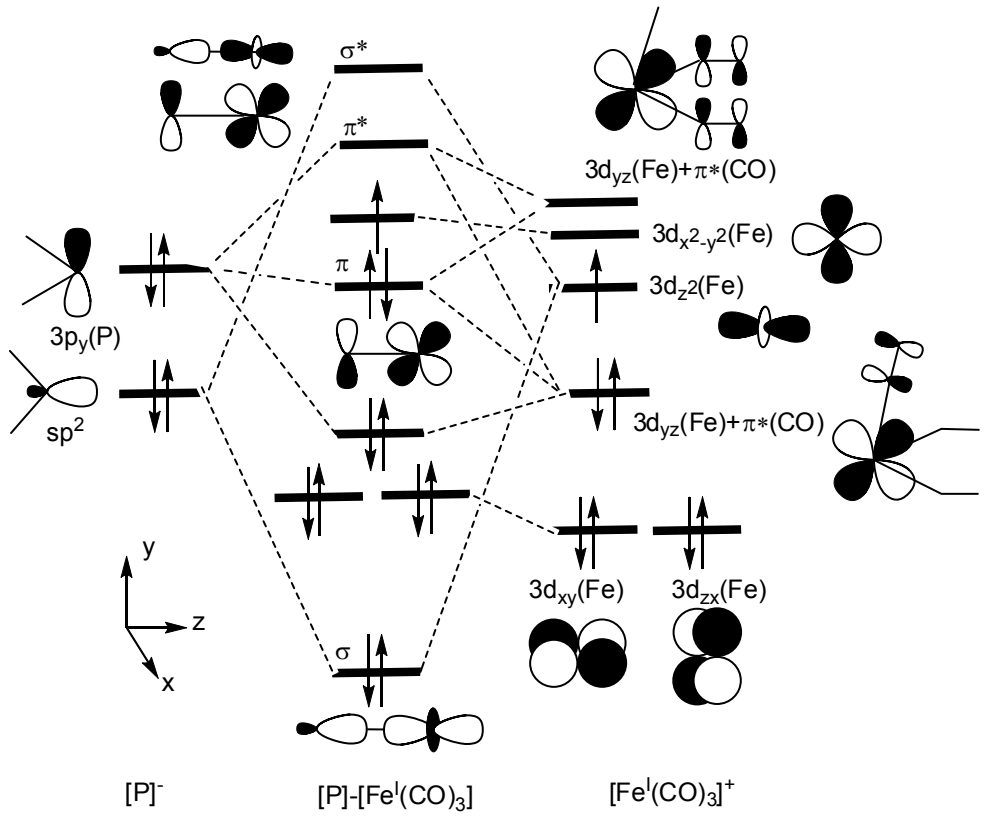
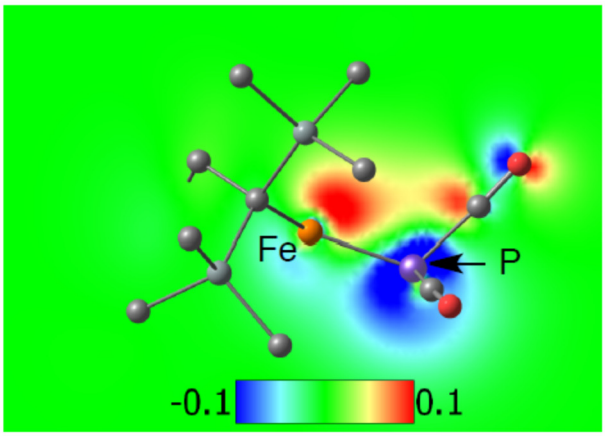


Figure S21. Density distributions in (a) αHOMO and (b) βHOMO of $\mathbf{3}_{opt}$. The plot plane for βHOMO indicates the π-bonding interaction between Fe and P atoms, whereas the plot plane for αHOMO indicates the non-bonding interaction between Fe and P atoms.

(a) αHOMO



(b) βHOMO

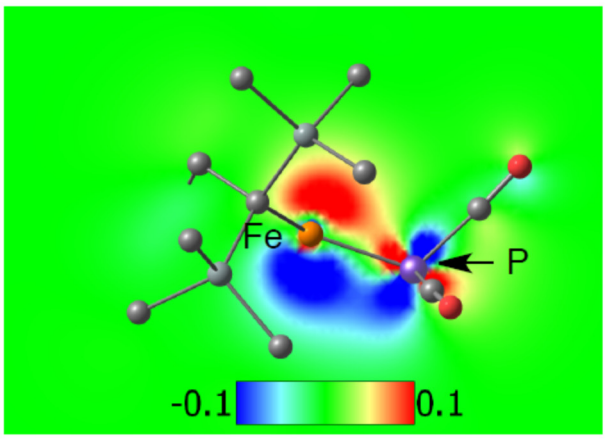


Figure S22. Calculated electron density difference map that details the nature of the transition in $\mathbf{2}_{opt}$ (red: electron density loss in transition, purple: electron density gain in transition).

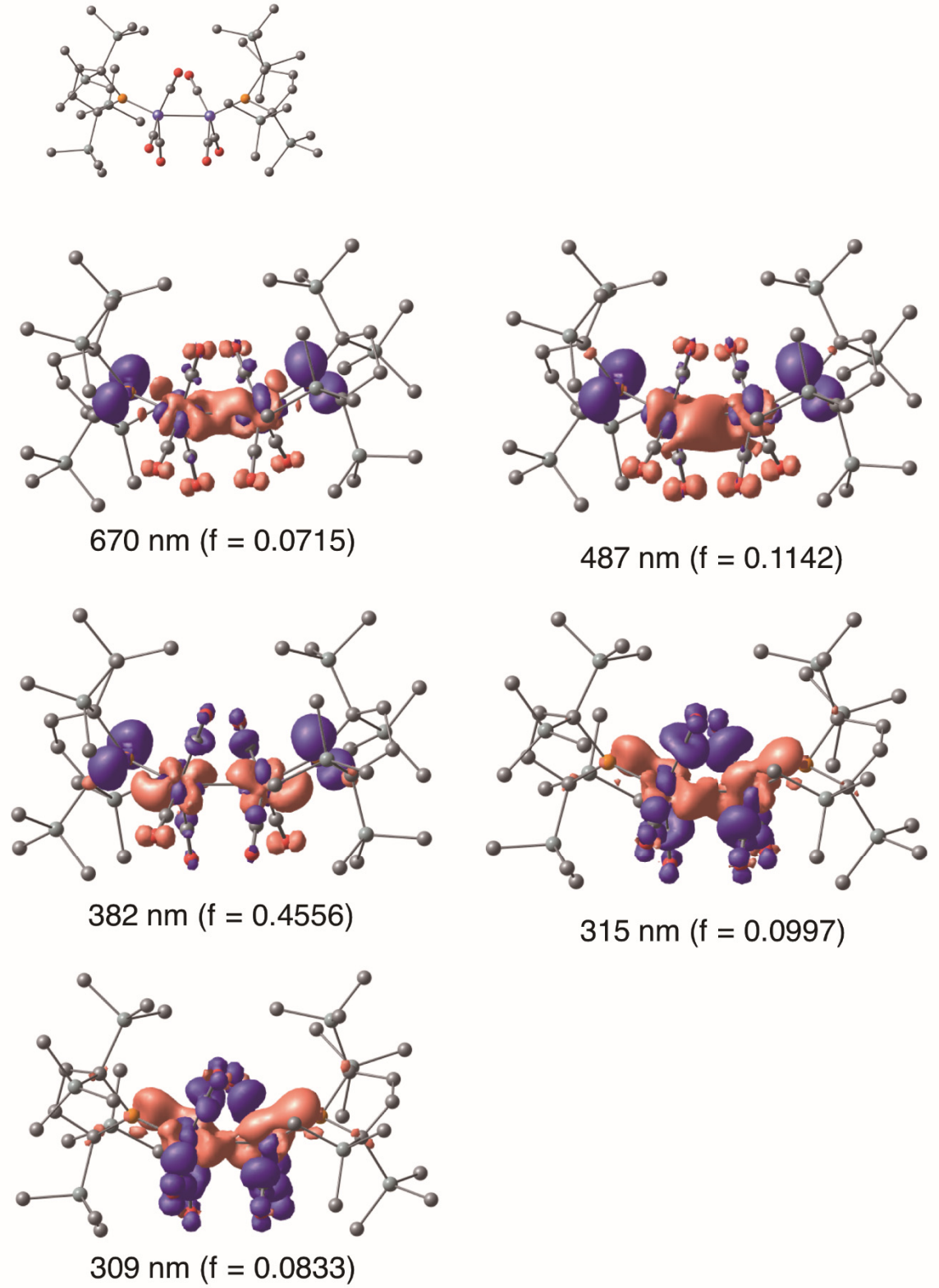


Figure S23. Calculated electron density difference map that details the nature of the transition in $\mathbf{3}_{opt}$ (red: electron density loss in transition, purple: electron density gain in transition).

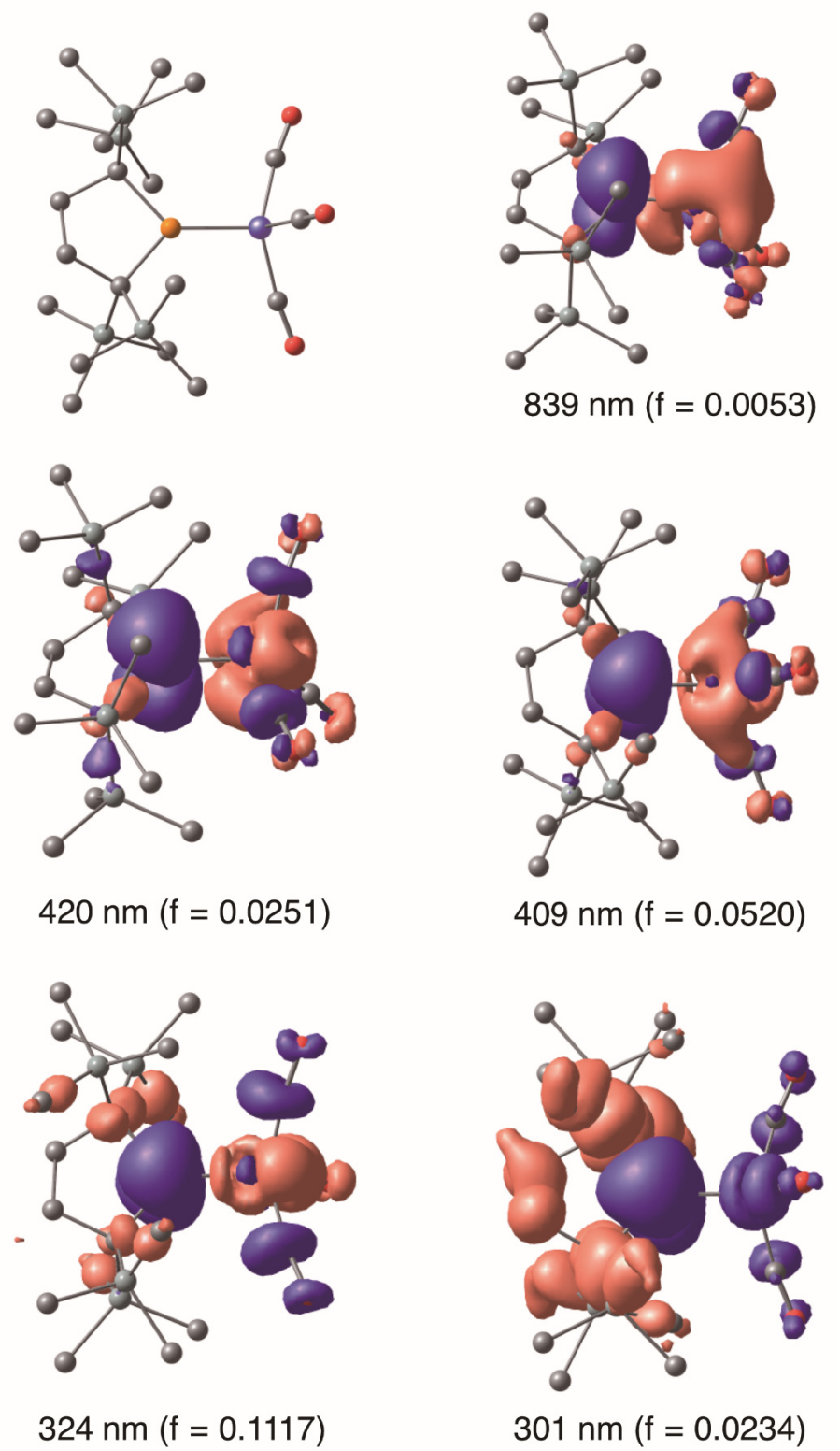


Table S5. Transition Energies, Wavelengths, and Oscillator Strengths of the Electronic Transitions of $\mathbf{2}_{\mathbf{opt}}$.

Excited State 1: Singlet-A 1.8495 eV 670.36 nm f=0.0715 <S**2>=0.000
269 -> 276 0.17716
270 -> 277 -0.10083
271 -> 276 0.10795
272 -> 277 0.20560
273 -> 276 0.35188
274 -> 277 -0.24540
275 -> 276 0.42736
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -7470.12262527
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 1.9342 eV 641.01 nm f=0.0036 <S**2>=0.000
269 -> 277 -0.17654
272 -> 276 -0.32306
273 -> 277 -0.29809
274 -> 276 0.39734
275 -> 277 -0.26362

Excited State 3: Singlet-A 2.3982 eV 516.98 nm f=0.0299 <S**2>=0.000
271 -> 276 0.13923
272 -> 277 -0.15330
273 -> 276 -0.26572
274 -> 277 0.37730
275 -> 276 0.44880

Excited State 4: Singlet-A 2.4348 eV 509.22 nm f=0.0003 <S**2>=0.000
270 -> 276 -0.21741
271 -> 277 0.21031
272 -> 276 -0.11767
273 -> 277 0.17162
274 -> 276 0.38281
275 -> 277 0.41376

Excited State 5: Singlet-A 2.5456 eV 487.06 nm f=0.1142 <S**2>=0.000
269 -> 276 -0.14827
270 -> 277 -0.12527
271 -> 276 0.17476
272 -> 277 -0.16238
273 -> 276 0.47876
274 -> 277 0.30359
275 -> 276 -0.16528

Excited State 6: Singlet-A 2.5667 eV 483.05 nm f=0.0063 <S**2>=0.000
269 -> 277 -0.14402
272 -> 276 -0.11196
273 -> 277 0.53839
275 -> 277 -0.35940

Excited State 7: Singlet-A 2.9050 eV 426.79 nm f=0.0001 <S**2>=0.000
270 -> 276 0.34883
271 -> 276 -0.16970
271 -> 277 -0.31978
272 -> 276 0.19508
273 -> 277 0.20860
274 -> 276 0.27086
274 -> 278 0.14172
275 -> 277 0.12368

Excited State 8: Singlet-A 2.9486 eV 420.48 nm f=0.0233 <S**2>=0.000
270 -> 276 0.20831
270 -> 277 -0.31997
271 -> 276 0.35969
271 -> 277 0.10266
273 -> 276 -0.19876
274 -> 277 -0.29510

275 -> 276 -0.11047

Excited State 9: Singlet-A 3.0919 eV 400.99 nm f=0.0005 <S**2>=0.000
271 -> 278 0.13676
273 -> 278 0.27497
274 -> 277 -0.13201
275 -> 276 -0.10385
275 -> 278 0.55362

Excited State 10: Singlet-A 3.2167 eV 385.44 nm f=0.0038 <S**2>=0.000
272 -> 278 -0.21536
273 -> 277 -0.12106
274 -> 276 -0.17064
274 -> 278 0.57185
275 -> 279 -0.10300

Excited State 11: Singlet-A 3.2422 eV 382.41 nm f=0.4556 <S**2>=0.000
265 -> 276 -0.12274
269 -> 276 0.26541
270 -> 277 -0.13013
271 -> 276 0.11530
272 -> 277 0.40401
273 -> 278 0.10593
274 -> 277 0.28292
274 -> 279 -0.10630
275 -> 276 -0.21054
275 -> 281 -0.11767

Excited State 12: Singlet-A 3.3195 eV 373.50 nm f=0.0040 <S**2>=0.000
263 -> 277 0.13333
264 -> 276 0.10894
265 -> 277 0.36711
266 -> 276 0.47435
272 -> 276 -0.15405

Excited State 13: Singlet-A 3.3476 eV 370.37 nm f=0.0267 <S**2>=0.000
263 -> 276 0.12898
264 -> 277 0.10310
265 -> 276 0.39087
266 -> 277 0.43224
269 -> 276 0.15069
271 -> 276 0.13182
275 -> 276 -0.10109

Excited State 14: Singlet-A 3.3772 eV 367.12 nm f=0.0230 <S**2>=0.000
266 -> 276 0.14955
269 -> 277 0.20028
270 -> 276 -0.12833
271 -> 277 0.15532
272 -> 276 0.38854
274 -> 276 0.25320
275 -> 277 -0.28565
275 -> 279 0.16509

Excited State 15: Singlet-A 3.6312 eV 341.44 nm f=0.0326 <S**2>=0.000
269 -> 278 -0.14023
270 -> 277 0.25252
271 -> 276 0.19668
271 -> 277 -0.20196
271 -> 278 0.32404
272 -> 277 0.12423
273 -> 278 0.21153
274 -> 279 0.13863
275 -> 278 -0.22206

Excited State 16: Singlet-A 3.6502 eV 339.66 nm f=0.0040 <S**2>=0.000
270 -> 276 0.17186
270 -> 277 0.20829
270 -> 278 0.32913
271 -> 277 0.29380
272 -> 278 0.19888

274 -> 278	0.17850				
275 -> 279	-0.19358				
Excited State 17:	Singlet-A	3.7743 eV	328.50 nm	f=0.0635	<S**2>=0.000
269 -> 276	0.37776				
269 -> 278	0.19021				
272 -> 277	-0.33966				
272 -> 279	0.11434				
273 -> 278	0.27994				
275 -> 278	-0.22387				
Excited State 18:	Singlet-A	3.7963 eV	326.59 nm	f=0.0018	<S**2>=0.000
269 -> 277	0.41509				
270 -> 276	0.15549				
270 -> 278	0.15312				
271 -> 277	0.16007				
272 -> 276	-0.22985				
272 -> 278	-0.29763				
274 -> 278	-0.13532				
Excited State 19:	Singlet-A	3.9119 eV	316.94 nm	f=0.0085	<S**2>=0.000
273 -> 280	0.17259				
274 -> 282	0.25820				
275 -> 280	0.56138				
Excited State 20:	Singlet-A	3.9315 eV	315.36 nm	f=0.0997	<S**2>=0.000
269 -> 276	0.11155				
271 -> 278	0.19439				
272 -> 277	-0.14621				
272 -> 280	-0.10782				
273 -> 278	-0.31736				
273 -> 282	0.12019				
274 -> 280	0.33656				
274 -> 284	-0.11656				
275 -> 281	-0.24173				
275 -> 282	0.16910				
Excited State 21:	Singlet-A	4.0122 eV	309.02 nm	f=0.0833	<S**2>=0.000
269 -> 276	-0.13528				
270 -> 277	-0.16541				
271 -> 278	-0.14896				
273 -> 278	0.25843				
273 -> 282	0.12646				
274 -> 280	0.39086				
275 -> 281	0.14121				
275 -> 282	0.27986				
Excited State 22:	Singlet-A	4.0299 eV	307.66 nm	f=0.0051	<S**2>=0.000
270 -> 276	0.20087				
272 -> 276	-0.13654				
274 -> 278	0.18653				
274 -> 281	0.16726				
275 -> 279	0.54601				
Excited State 23:	Singlet-A	4.0638 eV	305.10 nm	f=0.0029	<S**2>=0.000
269 -> 276	0.14283				
270 -> 277	-0.27065				
271 -> 276	-0.24580				
271 -> 277	0.11884				
271 -> 278	0.27808				
274 -> 279	0.38551				
275 -> 281	0.17067				
Excited State 24:	Singlet-A	4.1474 eV	298.95 nm	f=0.0001	<S**2>=0.000
269 -> 277	0.14800				
270 -> 276	-0.24838				
270 -> 277	-0.13796				
270 -> 278	0.26498				
271 -> 276	0.10839				
271 -> 277	-0.26276				
271 -> 278	-0.11842				

271 -> 279	-0.11436				
272 -> 276	-0.13936				
272 -> 278	0.16913				
273 -> 280	0.20187				
274 -> 281	0.19945				
274 -> 282	0.10031				
Excited State 25:	Singlet-A	4.1600 eV	298.04 nm	f=0.0013	<S**2>=0.000
265 -> 277	0.15520				
266 -> 276	-0.19481				
266 -> 278	-0.25410				
269 -> 277	0.25247				
270 -> 278	-0.20478				
272 -> 276	-0.11710				
272 -> 278	0.27189				
273 -> 280	0.16075				
275 -> 280	-0.11864				
Excited State 26:	Singlet-A	4.2054 eV	294.82 nm	f=0.0035	<S**2>=0.000
265 -> 277	0.10049				
266 -> 278	-0.14427				
269 -> 277	-0.18832				
272 -> 276	0.11623				
272 -> 278	-0.29457				
273 -> 280	0.42939				
274 -> 282	0.11015				
275 -> 279	0.12108				
275 -> 280	-0.23948				
Excited State 27:	Singlet-A	4.2207 eV	293.75 nm	f=0.0118	<S**2>=0.000
269 -> 276	0.19005				
269 -> 278	-0.14005				
270 -> 277	0.16806				
271 -> 276	0.20059				
271 -> 278	-0.19173				
273 -> 281	0.11076				
274 -> 279	0.20273				
274 -> 284	-0.10977				
275 -> 278	0.18601				
275 -> 281	0.32145				
Excited State 28:	Singlet-A	4.2793 eV	289.73 nm	f=0.0013	<S**2>=0.000
265 -> 276	0.10401				
265 -> 277	-0.19960				
266 -> 276	0.23779				
266 -> 278	0.26285				
270 -> 278	-0.15947				
271 -> 280	0.10026				
273 -> 280	0.26482				
275 -> 279	-0.11902				
275 -> 284	-0.19898				
Excited State 29:	Singlet-A	4.2935 eV	288.77 nm	f=0.0013	<S**2>=0.000
263 -> 278	0.10276				
265 -> 276	0.34563				
265 -> 278	0.28127				
266 -> 277	-0.25893				
269 -> 278	0.13223				
275 -> 282	-0.13464				
Excited State 30:	Singlet-A	4.3159 eV	287.27 nm	f=0.0276	<S**2>=0.000
268 -> 276	0.51658				
268 -> 277	-0.39691				
Excited State 31:	Singlet-A	4.3376 eV	285.84 nm	f=0.0175	<S**2>=0.000
267 -> 276	0.32051				
267 -> 277	0.30019				
268 -> 276	-0.11686				
269 -> 276	0.12507				
269 -> 278	-0.25337				
271 -> 276	-0.11494				

272 -> 279	-0.13200				
274 -> 281	-0.10582				
275 -> 282	0.14784				
275 -> 284	0.13337				
Excited State 32:	Singlet-A	4.3526 eV	284.85 nm	f=0.0220	<S**2>=0.000
266 -> 277	0.10439				
267 -> 276	0.33049				
267 -> 277	0.22784				
268 -> 277	-0.13101				
269 -> 278	0.28043				
270 -> 277	0.10491				
272 -> 277	0.11140				
272 -> 279	0.14642				
274 -> 280	0.10503				
275 -> 281	0.10371				
275 -> 283	-0.12526				
Excited State 33:	Singlet-A	4.3650 eV	284.04 nm	f=0.0250	<S**2>=0.000
267 -> 276	-0.21939				
267 -> 277	-0.21769				
268 -> 276	0.10892				
273 -> 279	0.24693				
273 -> 280	0.16608				
274 -> 279	-0.11927				
274 -> 281	-0.23758				
274 -> 284	-0.11699				
275 -> 281	0.13830				
275 -> 284	0.30775				
Excited State 34:	Singlet-A	4.3799 eV	283.08 nm	f=0.0029	<S**2>=0.000
265 -> 276	-0.14182				
266 -> 277	0.10261				
271 -> 278	0.10505				
272 -> 280	-0.12249				
274 -> 279	-0.29764				
274 -> 281	0.17970				
274 -> 284	-0.25491				
275 -> 281	0.30499				
275 -> 284	-0.13136				
275 -> 287	-0.17094				
Excited State 35:	Singlet-A	4.4081 eV	281.27 nm	f=0.0044	<S**2>=0.000
273 -> 279	0.51461				
274 -> 281	0.34645				
275 -> 279	-0.12367				
Excited State 36:	Singlet-A	4.4820 eV	276.63 nm	f=0.0003	<S**2>=0.000
269 -> 278	0.16326				
272 -> 279	0.12603				
273 -> 281	0.12025				
273 -> 282	-0.13818				
273 -> 283	0.10773				
274 -> 279	0.11932				
274 -> 280	-0.24326				
275 -> 282	0.44463				
275 -> 283	0.12700				
Excited State 37:	Singlet-A	4.5007 eV	275.48 nm	f=0.0004	<S**2>=0.000
271 -> 280	-0.11651				
272 -> 282	-0.11503				
273 -> 280	-0.14682				
274 -> 282	0.44641				
274 -> 283	0.26250				
274 -> 286	0.10686				
275 -> 280	-0.13052				
275 -> 282	-0.10021				
275 -> 284	0.12378				
275 -> 289	0.14701				
Excited State 38:	Singlet-A	4.5575 eV	272.05 nm	f=0.0019	<S**2>=0.000

272 -> 280 -0.18066
273 -> 282 0.47555
274 -> 279 0.16315
274 -> 289 0.10214
275 -> 281 -0.13023
275 -> 282 -0.17397
275 -> 283 0.24242

Excited State 39: Singlet-A 4.5736 eV 271.09 nm f=0.0058 <S**2>=0.000
269 -> 278 -0.10826
270 -> 280 -0.16933
271 -> 282 -0.12781
273 -> 281 0.11127
273 -> 282 -0.15123
273 -> 283 0.12558
274 -> 280 0.20180
274 -> 284 0.14728
275 -> 281 0.11056
275 -> 283 0.38836
275 -> 286 0.14954

Excited State 40: Singlet-A 4.6099 eV 268.95 nm f=0.0030 <S**2>=0.000
269 -> 280 -0.11886
270 -> 278 -0.12732
272 -> 282 0.11495
273 -> 279 -0.25863
274 -> 281 0.33012
275 -> 279 -0.16687
275 -> 284 0.39021

Excited State 41: Singlet-A 4.6800 eV 264.92 nm f=0.0009 <S**2>=0.000
271 -> 278 0.10957
273 -> 281 0.21661
273 -> 282 0.19789
274 -> 279 -0.22026
274 -> 280 -0.11767
274 -> 284 0.30925
275 -> 281 0.15633
275 -> 287 0.18004
275 -> 288 -0.14974

Excited State 42: Singlet-A 4.7036 eV 263.60 nm f=0.0043 <S**2>=0.000
263 -> 276 0.11450
265 -> 277 -0.10065
265 -> 278 -0.15681
266 -> 277 -0.14146
272 -> 280 -0.19162
273 -> 281 0.40854
273 -> 283 0.14034
273 -> 290 -0.12545
275 -> 283 -0.12294

Excited State 43: Singlet-A 4.7126 eV 263.09 nm f=0.0019 <S**2>=0.000
264 -> 276 -0.13441
265 -> 277 0.35222
266 -> 276 -0.19577
266 -> 278 0.28212
269 -> 277 0.10649
274 -> 290 0.10996
275 -> 287 -0.12788
275 -> 288 -0.11115

Excited State 44: Singlet-A 4.7297 eV 262.14 nm f=0.0003 <S**2>=0.000
265 -> 277 -0.10388
266 -> 278 -0.13658
270 -> 282 0.10902
271 -> 280 0.18414
274 -> 281 -0.14031
274 -> 282 -0.19483
274 -> 283 0.40519
274 -> 286 0.13311

275 -> 280	0.11218				
275 -> 289	0.12398				
Excited State 45:	Singlet-A	4.7506 eV	260.99 nm	f=0.0048	<S**2>=0.000
262 -> 276	-0.11574				
263 -> 276	0.29002				
264 -> 276	-0.23589				
264 -> 277	0.25969				
265 -> 278	-0.15943				
266 -> 277	-0.24159				
273 -> 281	-0.27223				
Excited State 46:	Singlet-A	4.7595 eV	260.50 nm	f=0.0038	<S**2>=0.000
261 -> 276	-0.11934				
262 -> 277	-0.10645				
263 -> 276	0.23872				
263 -> 277	0.36727				
264 -> 276	0.34155				
266 -> 276	-0.22674				
266 -> 278	0.15633				
268 -> 277	0.10354				
Excited State 47:	Singlet-A	4.7728 eV	259.77 nm	f=0.0011	<S**2>=0.000
264 -> 277	0.10067				
265 -> 276	-0.12144				
265 -> 278	0.12091				
267 -> 276	0.12502				
268 -> 276	0.36187				
268 -> 277	0.47615				
273 -> 281	0.10520				
Excited State 48:	Singlet-A	4.7799 eV	259.39 nm	f=0.0006	<S**2>=0.000
263 -> 276	-0.14427				
264 -> 276	0.14390				
264 -> 277	-0.18997				
265 -> 276	0.23789				
265 -> 278	-0.18742				
267 -> 277	0.18742				
268 -> 276	0.17972				
268 -> 277	0.17215				
272 -> 280	-0.18045				
273 -> 281	-0.12732				
275 -> 288	-0.10344				
Excited State 49:	Singlet-A	4.7879 eV	258.96 nm	f=0.0037	<S**2>=0.000
245 -> 277	0.10428				
253 -> 276	0.12061				
253 -> 277	0.12330				
263 -> 276	-0.15470				
263 -> 277	-0.11360				
265 -> 276	0.13161				
265 -> 277	0.16465				
265 -> 278	-0.11819				
268 -> 277	0.16960				
274 -> 282	-0.11128				
274 -> 283	0.21471				
274 -> 287	-0.10819				
274 -> 290	-0.12064				
Excited State 50:	Singlet-A	4.7917 eV	258.75 nm	f=0.0009	<S**2>=0.000
267 -> 276	-0.41474				
267 -> 277	0.48664				
Excited State 51:	Singlet-A	4.8124 eV	257.63 nm	f=0.0168	<S**2>=0.000
245 -> 276	0.10745				
254 -> 277	-0.11235				
265 -> 278	-0.10605				
272 -> 279	-0.10930				
272 -> 280	0.20563				
273 -> 278	0.10673				
273 -> 281	0.22844				

273 -> 290	0.14766				
274 -> 280	0.13912				
274 -> 284	-0.14644				
274 -> 288	-0.15692				
275 -> 282	-0.10793				
275 -> 290	0.19491				
Excited State 52:	Singlet-A	4.8634 eV	254.93 nm	f=0.0023	<S**2>=0.000
269 -> 280	0.24551				
269 -> 282	0.10193				
270 -> 279	0.11407				
270 -> 282	0.10139				
271 -> 280	0.12176				
272 -> 280	-0.17163				
272 -> 281	0.11230				
272 -> 282	-0.23486				
272 -> 283	0.12012				
273 -> 282	-0.10730				
273 -> 283	-0.18745				
274 -> 289	-0.14238				
275 -> 290	0.11029				
Excited State 53:	Singlet-A	4.8663 eV	254.78 nm	f=0.0020	<S**2>=0.000
269 -> 280	0.24704				
269 -> 282	-0.10596				
271 -> 279	0.12165				
271 -> 281	-0.10817				
272 -> 280	0.18064				
272 -> 282	-0.22522				
272 -> 283	0.10922				
273 -> 282	0.12513				
273 -> 283	0.20610				
274 -> 289	0.16015				
275 -> 290	-0.14223				
Excited State 54:	Singlet-A	4.9241 eV	251.79 nm	f=0.0048	<S**2>=0.000
241 -> 276	0.10695				
245 -> 276	0.16966				
246 -> 277	0.14335				
253 -> 276	0.17782				
253 -> 277	0.12370				
254 -> 277	-0.16569				
257 -> 276	0.10196				
265 -> 278	0.14594				
266 -> 277	0.11923				
269 -> 282	0.10203				
272 -> 280	-0.19689				
273 -> 283	0.19854				
275 -> 283	-0.16182				
275 -> 286	-0.10146				
275 -> 287	-0.11423				
Excited State 55:	Singlet-A	4.9469 eV	250.63 nm	f=0.0081	<S**2>=0.000
254 -> 276	0.12302				
273 -> 284	0.33642				
274 -> 282	0.12533				
274 -> 290	-0.11942				
275 -> 284	-0.12798				
275 -> 287	0.23094				
275 -> 288	0.27781				
275 -> 289	0.13328				
Excited State 56:	Singlet-A	4.9999 eV	247.98 nm	f=0.0039	<S**2>=0.000
254 -> 276	-0.11407				
262 -> 276	0.12003				
271 -> 280	0.31527				
271 -> 282	-0.18278				
272 -> 279	-0.12195				
273 -> 289	-0.10125				
274 -> 282	0.16864				
274 -> 290	0.12451				

275 -> 283	-0.11541				
275 -> 289	0.10172				
275 -> 290	0.10866				
Excited State 57:	Singlet-A	5.0037 eV	247.78 nm	f=0.0058	<S**2>=0.000
269 -> 279	-0.18408				
272 -> 281	0.22507				
273 -> 284	0.33797				
273 -> 288	0.10068				
274 -> 287	0.16486				
274 -> 288	-0.12012				
275 -> 284	-0.13422				
275 -> 287	-0.18072				
275 -> 288	-0.21515				
Excited State 58:	Singlet-A	5.0127 eV	247.34 nm	f=0.0136	<S**2>=0.000
261 -> 276	0.28880				
261 -> 277	-0.13541				
262 -> 276	-0.21286				
262 -> 277	0.23598				
264 -> 276	0.15674				
270 -> 280	0.16066				
270 -> 282	0.11766				
271 -> 280	0.13272				
272 -> 279	0.16500				
274 -> 282	0.11649				
Excited State 59:	Singlet-A	5.0278 eV	246.60 nm	f=0.0126	<S**2>=0.000
261 -> 276	0.19687				
261 -> 277	0.32251				
262 -> 276	0.41555				
262 -> 277	0.16125				
263 -> 276	0.12840				
272 -> 279	0.17381				
Excited State 60:	Singlet-A	5.0335 eV	246.32 nm	f=0.0016	<S**2>=0.000
261 -> 276	0.30970				
262 -> 277	0.23100				
264 -> 276	0.11149				
270 -> 280	-0.26998				
270 -> 282	-0.13997				
271 -> 282	-0.16983				
272 -> 279	-0.14299				
274 -> 280	-0.10326				
275 -> 290	0.11245				
Excited State 61:	Singlet-A	5.0468 eV	245.67 nm	f=0.0035	<S**2>=0.000
261 -> 276	-0.11505				
269 -> 278	-0.10857				
269 -> 281	-0.14598				
270 -> 279	-0.19845				
270 -> 284	-0.11376				
271 -> 281	-0.13630				
272 -> 279	0.31351				
273 -> 288	0.10606				
274 -> 284	0.19718				
275 -> 287	-0.11371				
275 -> 290	0.20631				
Excited State 62:	Singlet-A	5.0954 eV	243.32 nm	f=0.0246	<S**2>=0.000
273 -> 282	0.13082				
273 -> 283	0.28598				
273 -> 287	-0.15846				
273 -> 288	0.13118				
273 -> 290	-0.10486				
274 -> 284	-0.22571				
274 -> 289	-0.17004				
275 -> 286	0.13680				
275 -> 287	0.23372				
275 -> 288	-0.23230				
275 -> 290	0.13722				

Excited State 63:	Singlet-A	5.1200 eV	242.16 nm	f=0.0098	<S**2>=0.000
269 -> 279	0.23390				
270 -> 278	0.10383				
270 -> 281	0.14288				
271 -> 279	0.24284				
271 -> 280	-0.10255				
272 -> 281	-0.22163				
273 -> 284	0.28378				
273 -> 289	-0.11282				
274 -> 288	0.10279				
275 -> 287	-0.12263				
275 -> 288	-0.16560				
275 -> 289	0.16309				
Excited State 64:	Singlet-A	5.1744 eV	239.61 nm	f=0.0021	<S**2>=0.000
269 -> 279	0.12322				
271 -> 280	0.15558				
272 -> 281	-0.21275				
273 -> 287	0.23984				
273 -> 288	0.25297				
273 -> 289	0.24197				
274 -> 288	-0.12183				
274 -> 290	-0.13759				
275 -> 287	-0.11536				
275 -> 288	-0.11342				
Excited State 65:	Singlet-A	5.1816 eV	239.28 nm	f=0.0032	<S**2>=0.000
257 -> 276	-0.15042				
257 -> 277	0.13512				
258 -> 276	0.23758				
258 -> 277	-0.17059				
259 -> 276	0.25862				
259 -> 277	-0.21679				
260 -> 276	-0.22583				
260 -> 277	0.12397				
273 -> 288	-0.10487				
274 -> 288	-0.21266				
Excited State 66:	Singlet-A	5.1907 eV	238.86 nm	f=0.0037	<S**2>=0.000
259 -> 277	0.11457				
260 -> 276	0.15114				
269 -> 279	0.10896				
271 -> 284	-0.10011				
272 -> 281	-0.25960				
272 -> 282	-0.18278				
274 -> 286	0.10288				
274 -> 287	0.32972				
274 -> 288	-0.16613				
275 -> 289	-0.13480				
Excited State 67:	Singlet-A	5.1935 eV	238.73 nm	f=0.0052	<S**2>=0.000
258 -> 276	0.12233				
259 -> 276	0.19006				
259 -> 277	-0.17061				
260 -> 276	-0.20276				
271 -> 279	-0.13422				
272 -> 279	0.10622				
273 -> 283	-0.18361				
273 -> 286	-0.11384				
273 -> 290	-0.18362				
274 -> 287	0.13459				
274 -> 288	0.25401				
275 -> 289	0.10830				
Excited State 68:	Singlet-A	5.2015 eV	238.36 nm	f=0.0003	<S**2>=0.000
255 -> 276	0.14928				
255 -> 277	0.11519				
257 -> 276	-0.18257				
257 -> 277	-0.11164				
259 -> 276	0.26414				

259 -> 277	0.12149				
260 -> 276	0.29020				
260 -> 277	0.31047				
261 -> 276	0.11172				
261 -> 277	0.12677				
274 -> 287	-0.11747				
Excited State 69:	Singlet-A	5.2107 eV	237.94 nm	f=0.0011	<S**2>=0.000
259 -> 276	0.12752				
260 -> 276	0.14000				
260 -> 277	0.14595				
270 -> 279	0.11250				
270 -> 281	0.15656				
271 -> 279	0.22771				
272 -> 282	0.14756				
273 -> 284	-0.13604				
273 -> 290	-0.10326				
274 -> 282	0.10812				
274 -> 287	0.19372				
275 -> 284	-0.10559				
275 -> 291	0.14256				
Excited State 70:	Singlet-A	5.2270 eV	237.20 nm	f=0.0005	<S**2>=0.000
269 -> 278	0.13331				
270 -> 279	-0.15755				
270 -> 280	0.20198				
271 -> 281	-0.11431				
271 -> 283	-0.11532				
272 -> 279	-0.18859				
272 -> 280	-0.10350				
273 -> 282	-0.19640				
273 -> 286	-0.10664				
273 -> 287	-0.15983				
273 -> 288	0.15854				
273 -> 290	-0.12669				
274 -> 289	0.18105				
275 -> 287	0.19022				
275 -> 288	-0.14198				
Excited State 71:	Singlet-A	5.2481 eV	236.25 nm	f=0.0027	<S**2>=0.000
273 -> 284	-0.13011				
274 -> 283	-0.12430				
274 -> 286	0.10453				
274 -> 287	0.17167				
274 -> 288	-0.16115				
275 -> 285	0.36713				
275 -> 289	0.41999				
Excited State 72:	Singlet-A	5.2594 eV	235.74 nm	f=0.0018	<S**2>=0.000
261 -> 277	-0.16045				
262 -> 276	0.10607				
263 -> 276	-0.36788				
263 -> 277	0.20938				
264 -> 276	0.15882				
264 -> 277	0.43420				
265 -> 276	0.11583				
266 -> 277	-0.11026				
Excited State 73:	Singlet-A	5.2609 eV	235.67 nm	f=0.0001	<S**2>=0.000
261 -> 276	0.12199				
262 -> 277	-0.14322				
263 -> 276	-0.18369				
263 -> 277	0.42651				
264 -> 276	-0.34802				
264 -> 277	-0.22264				
265 -> 277	-0.15697				
Excited State 74:	Singlet-A	5.2834 eV	234.67 nm	f=0.0030	<S**2>=0.000
258 -> 276	0.34969				
258 -> 277	-0.28332				
259 -> 276	-0.22368				

259 -> 277	0.13037				
274 -> 287	0.11050				
275 -> 285	-0.29752				
275 -> 289	0.10850				
Excited State 75:	Singlet-A	5.2866 eV	234.52 nm	f=0.0009	<S**2>=0.000
257 -> 276	0.10112				
258 -> 276	0.31619				
258 -> 277	-0.15296				
259 -> 277	0.15903				
260 -> 276	0.12605				
274 -> 287	-0.10693				
275 -> 285	0.35419				
275 -> 286	-0.11676				
275 -> 289	-0.15310				
275 -> 290	-0.10299				
Excited State 76:	Singlet-A	5.2934 eV	234.22 nm	f=0.0012	<S**2>=0.000
256 -> 276	-0.20856				
256 -> 277	-0.14523				
257 -> 276	-0.22086				
257 -> 277	-0.19259				
258 -> 277	-0.13695				
259 -> 276	-0.16419				
259 -> 277	-0.10038				
260 -> 276	-0.15481				
260 -> 277	-0.12665				
262 -> 276	-0.15139				
262 -> 277	-0.12646				
264 -> 277	0.11236				
275 -> 285	0.25419				
275 -> 289	-0.13195				
Excited State 77:	Singlet-A	5.3099 eV	233.49 nm	f=0.0008	<S**2>=0.000
255 -> 277	-0.12995				
257 -> 276	0.17324				
270 -> 280	0.11890				
273 -> 283	0.10986				
273 -> 287	0.13841				
274 -> 288	0.13025				
275 -> 285	0.18227				
275 -> 286	0.30324				
275 -> 288	0.10171				
275 -> 289	-0.13745				
275 -> 290	0.23580				
Excited State 78:	Singlet-A	5.3136 eV	233.33 nm	f=0.0042	<S**2>=0.000
254 -> 276	-0.19768				
254 -> 277	0.14531				
255 -> 276	0.30765				
255 -> 277	-0.20985				
256 -> 276	-0.18182				
256 -> 277	0.12590				
257 -> 276	0.26307				
257 -> 277	-0.20435				
273 -> 290	0.10511				
Excited State 79:	Singlet-A	5.3289 eV	232.67 nm	f=0.0011	<S**2>=0.000
253 -> 276	0.10977				
255 -> 276	0.34590				
255 -> 277	0.25098				
256 -> 276	0.32462				
256 -> 277	0.27773				
275 -> 286	0.13160				
Excited State 80:	Singlet-A	5.3535 eV	231.60 nm	f=0.0119	<S**2>=0.000
270 -> 279	-0.11652				
273 -> 290	0.30581				
274 -> 285	0.18477				
274 -> 287	0.12209				
274 -> 288	0.14899				

274 -> 290	-0.12786				
275 -> 283	-0.11926				
275 -> 286	0.31174				
275 -> 290	-0.18624				
Excited State 81:	Singlet-A	5.3606 eV	231.29 nm	f=0.0014	<S**2>=0.000
266 -> 279	-0.10926				
270 -> 279	0.16128				
271 -> 281	0.11099				
272 -> 280	0.10098				
273 -> 283	-0.10642				
273 -> 288	0.13414				
273 -> 290	-0.10173				
274 -> 285	0.20423				
274 -> 287	-0.17679				
274 -> 288	-0.18627				
274 -> 289	0.17920				
275 -> 283	-0.15810				
275 -> 286	0.23045				
275 -> 290	-0.18791				
Excited State 82:	Singlet-A	5.3783 eV	230.53 nm	f=0.0075	<S**2>=0.000
261 -> 276	-0.16716				
262 -> 277	0.17490				
273 -> 287	0.17027				
273 -> 288	0.15512				
273 -> 290	0.13376				
274 -> 286	0.16827				
274 -> 289	0.13545				
274 -> 290	0.37135				
275 -> 287	0.16598				
275 -> 291	-0.14036				
Excited State 83:	Singlet-A	5.3830 eV	230.33 nm	f=0.0019	<S**2>=0.000
261 -> 276	-0.30703				
261 -> 277	0.24255				
262 -> 276	-0.19107				
262 -> 277	0.39778				
263 -> 277	0.14767				
274 -> 290	-0.14426				
Excited State 84:	Singlet-A	5.3893 eV	230.06 nm	f=0.0010	<S**2>=0.000
253 -> 276	-0.10175				
256 -> 276	0.22324				
256 -> 277	0.17014				
257 -> 276	0.12628				
261 -> 276	0.12029				
261 -> 277	0.40487				
262 -> 276	-0.27922				
262 -> 277	-0.17199				
264 -> 277	0.12946				
Excited State 85:	Singlet-A	5.4256 eV	228.52 nm	f=0.0121	<S**2>=0.000
249 -> 276	0.11500				
249 -> 277	-0.15190				
250 -> 276	0.26644				
251 -> 276	-0.16626				
251 -> 277	0.23521				
252 -> 276	0.12676				
254 -> 276	-0.25686				
257 -> 276	-0.19801				
257 -> 277	0.14721				
260 -> 276	0.11206				
273 -> 289	0.12403				
274 -> 289	0.16251				
Excited State 86:	Singlet-A	5.4315 eV	228.27 nm	f=0.0130	<S**2>=0.000
250 -> 276	-0.15300				
251 -> 276	0.10871				
251 -> 277	-0.10286				
270 -> 279	0.11900				

273 -> 289 0.12266
273 -> 290 0.15148
274 -> 285 -0.11647
274 -> 289 0.39783
274 -> 290 -0.14237
275 -> 286 -0.11130
275 -> 288 -0.13230
275 -> 290 0.17636

Excited State 87: Singlet-A 5.4382 eV 227.99 nm f=0.0166 <S**2>=0.000
250 -> 276 -0.18714
250 -> 277 0.26573
251 -> 276 0.18955
252 -> 276 0.45393
252 -> 277 -0.25844

Excited State 88: Singlet-A 5.4432 eV 227.78 nm f=0.0193 <S**2>=0.000
250 -> 276 0.21625
250 -> 277 0.14472
251 -> 276 0.29118
251 -> 277 0.13374
252 -> 276 -0.12580
252 -> 277 0.22409
253 -> 276 0.11617
254 -> 277 -0.13781
273 -> 287 -0.11735
273 -> 289 0.24378

Excited State 89: Singlet-A 5.4484 eV 227.56 nm f=0.0023 <S**2>=0.000
249 -> 276 0.17469
250 -> 276 -0.13941
250 -> 277 -0.14084
251 -> 276 -0.19326
252 -> 277 -0.10594
254 -> 277 0.14992
256 -> 276 -0.12115
261 -> 277 0.11879
273 -> 287 -0.15978
273 -> 289 0.28567
274 -> 291 0.11681

Excited State 90: Singlet-A 5.4637 eV 226.92 nm f=0.0299 <S**2>=0.000
249 -> 276 0.36392
249 -> 277 0.24320
251 -> 276 0.16761
251 -> 277 0.18549
253 -> 276 0.23060
253 -> 277 0.20055
273 -> 287 0.11579

Excited State 91: Singlet-A 5.4692 eV 226.70 nm f=0.0207 <S**2>=0.000
270 -> 279 0.14125
271 -> 278 0.10714
271 -> 281 0.12915
272 -> 284 0.12470
273 -> 288 0.17598
273 -> 289 -0.16820
273 -> 290 0.19346
274 -> 291 0.30948
275 -> 292 0.26924

Excited State 92: Singlet-A 5.5047 eV 225.23 nm f=0.0011 <S**2>=0.000
272 -> 284 -0.17194
272 -> 289 0.10081
274 -> 285 0.46888
274 -> 291 0.12931
275 -> 286 -0.22151
275 -> 291 -0.13880

Excited State 93: Singlet-A 5.5130 eV 224.89 nm f=0.0312 <S**2>=0.000
266 -> 279 -0.10013

269 -> 279 -0.14087
272 -> 283 -0.12508
272 -> 284 -0.18004
272 -> 287 0.10840
272 -> 288 -0.11898
272 -> 289 0.13106
273 -> 287 -0.11018
273 -> 289 0.14910
274 -> 283 -0.15175
274 -> 286 0.11770
275 -> 291 0.27567

Excited State 94: Singlet-A 5.5234 eV 224.47 nm f=0.0891 <S**2>=0.000
265 -> 281 -0.12561
266 -> 279 0.16496
266 -> 280 -0.16810
269 -> 278 -0.12655
272 -> 284 0.10366
272 -> 289 -0.10455
273 -> 287 0.13661
273 -> 288 -0.16375
273 -> 289 0.10468
273 -> 290 -0.13017
274 -> 284 -0.10304
274 -> 285 0.23550
274 -> 286 0.11012
275 -> 286 -0.13558
275 -> 288 -0.11202
275 -> 291 0.16834

Excited State 95: Singlet-A 5.5362 eV 223.95 nm f=0.0426 <S**2>=0.000
271 -> 283 0.12230
272 -> 284 0.17921
273 -> 287 -0.14383
273 -> 288 0.12725
273 -> 290 0.11106
273 -> 292 -0.16441
274 -> 285 0.29606
274 -> 287 0.10291
274 -> 291 -0.23682
275 -> 286 -0.13750
275 -> 290 0.13646

Excited State 96: Singlet-A 5.5622 eV 222.90 nm f=0.0030 <S**2>=0.000
265 -> 279 -0.18360
266 -> 281 0.13408
269 -> 280 0.11288
269 -> 284 -0.11141
269 -> 289 -0.12763
272 -> 281 -0.19873
272 -> 282 0.15965
272 -> 283 0.33932
272 -> 286 0.10808
272 -> 290 -0.10079
273 -> 291 0.13949
274 -> 292 0.11613
275 -> 291 0.15262

Excited State 97: Singlet-A 5.5731 eV 222.47 nm f=0.0000 <S**2>=0.000
257 -> 276 0.12467
258 -> 276 -0.14799
258 -> 277 -0.19761
259 -> 276 -0.35523
259 -> 277 -0.27235
260 -> 277 0.41208

Excited State 98: Singlet-A 5.5802 eV 222.18 nm f=0.0009 <S**2>=0.000
249 -> 277 -0.10558
257 -> 277 -0.10991
259 -> 276 -0.10225
259 -> 277 0.40893

260 -> 276 -0.38905
260 -> 277 0.28893

Excited State 99: Singlet-A 5.5831 eV 222.07 nm f=0.0005 <S**2>=0.000
269 -> 279 0.10388
269 -> 284 0.10308
273 -> 285 0.13846
273 -> 291 0.16392
274 -> 283 -0.18910
274 -> 286 0.49412
274 -> 290 -0.14182
275 -> 285 -0.13025

Excited State 100: Singlet-A 5.6153 eV 220.80 nm f=0.0058 <S**2>=0.000
257 -> 277 -0.17773
258 -> 276 0.15842
258 -> 277 0.19369
269 -> 279 0.11738
269 -> 284 0.13728
271 -> 279 -0.15208
272 -> 287 -0.10330
273 -> 291 0.22142
274 -> 286 -0.17008
274 -> 290 0.12849
275 -> 291 0.14908

Table S6. Transition Energies, Wavelengths, and Oscillator Strengths of the Electronic Transitions of $\mathbf{3}_{\mathbf{opt}}$.

Excited State 1: 2.310-A 0.8409 eV 1474.39 nm f=0.0012 <S**2>=1.084
135B ->138B -0.19341
136B ->138B 0.65822
136B ->139B 0.29841
136B ->140B 0.15795
136B ->144B 0.14877
137B ->138B -0.52334
137B ->139B -0.18819
137B ->140B -0.11012
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -3735.04705016
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.304-A 1.0107 eV 1226.73 nm f=0.0031 <S**2>=1.077
135B ->138B 0.82148
135B ->139B 0.23357
135B ->140B 0.21630
135B ->144B 0.15750
135B ->146B 0.10672
135B ->147B 0.12312
136B ->138B 0.30466
136B ->139B 0.10165

Excited State 3: 2.877-A 1.4777 eV 839.04 nm f=0.0053 <S**2>=1.820
137A ->139A -0.18898
138A ->139A 0.78592
137B ->139B -0.56220
137B ->146B 0.10009
138A <-139A 0.12942
137B <-139B -0.14385

Excited State 4: 2.596-A 1.7589 eV 704.92 nm f=0.0018 <S**2>=1.435
137A ->139A -0.10377
138A ->139A -0.20185
134B ->138B -0.39745
135B ->138B -0.15461

135B ->139B -0.13125
136B ->139B 0.48818
136B ->144B 0.10028
136B ->146B -0.12955
137B ->138B 0.60336
137B ->139B -0.15758

Excited State 5: 2.447-A 1.8418 eV 673.17 nm f=0.0010 <S**2>=1.247
138A ->139A -0.14528
132B ->138B 0.10951
134B ->138B 0.81636
134B ->139B 0.14142
134B ->140B 0.14868
134B ->144B 0.12004
134B ->146B 0.10275
135B ->139B -0.11455
136B ->139B 0.28196
137B ->138B 0.22008
137B ->139B -0.11276

Excited State 6: 2.609-A 2.0147 eV 615.41 nm f=0.0042 <S**2>=1.452
137A ->139A 0.22649
138A ->139A 0.24383
134B ->138B 0.12971
135B ->138B -0.19315
136B ->138B 0.55354
136B ->139B -0.37492
136B ->146B 0.16802
137B ->138B 0.51736
137B ->139B 0.18578

Excited State 7: 3.176-A 2.1324 eV 581.44 nm f=0.0009 <S**2>=2.272
136A ->139A -0.30769
135B ->138B -0.25005
135B ->139B 0.79069
135B ->146B -0.22819
136B ->139B 0.21772

Excited State 8: 2.406-A 2.4568 eV 504.66 nm f=0.0013 <S**2>=1.197
137A ->139A 0.83528
137A ->140A -0.10069
137A ->145A 0.10417
138A ->139A 0.24949
135B ->139B -0.13206
136B ->138B -0.17804
136B ->139B 0.33282

Excited State 9: 3.092-A 2.6460 eV 468.57 nm f=0.0021 <S**2>=2.140
132A ->139A -0.13372
134A ->139A 0.13259
132B ->139B 0.10644
134B ->138B -0.13964
134B ->139B 0.85759
134B ->144B 0.12821
134B ->146B -0.27875

Excited State 10: 2.792-A 2.8578 eV 433.85 nm f=0.0071 <S**2>=1.699
136A ->139A -0.22104
137A ->139A 0.12817
137A ->140A 0.13599
138A ->140A 0.69342
138A ->145A -0.14163
134B ->141B 0.18683
135B ->143B -0.13046
136B ->139B -0.18336
136B ->140B -0.25853
137B ->139B -0.35284
137B ->140B 0.11441

Excited State 11: 2.615-A 2.9462 eV 420.83 nm f=0.0251 <S**2>=1.459
132A ->139A -0.16174

133A ->139A	-0.17145				
136A ->139A	0.66777				
136A ->143A	0.10924				
137A ->139A	-0.19403				
138A ->139A	0.23653				
138A ->140A	0.33793				
135B ->139B	0.17891				
136B ->139B	0.13924				
136B ->140B	-0.13020				
137B ->139B	0.29083				
Excited State 12:	2.500-A	3.0322 eV	408.89 nm	f=0.0520	<S**2>=1.312
131A ->139A	0.21161				
132A ->139A	0.13170				
133A ->139A	0.27695				
136A ->139A	0.54305				
137A ->139A	0.22368				
138A ->139A	-0.30651				
138A ->140A	-0.13649				
135B ->139B	0.27854				
136B ->140B	0.10726				
137B ->139B	-0.43883				
Excited State 13:	3.353-A	3.2276 eV	384.13 nm	f=0.0066	<S**2>=2.561
132A ->141A	0.12211				
134A ->141A	-0.12073				
137A ->139A	-0.11491				
137A ->140A	-0.47496				
137A ->142A	-0.13303				
138A ->140A	0.52062				
134B ->141B	-0.14776				
136B ->140B	0.32698				
136B ->144B	-0.11033				
137B ->139B	0.10413				
137B ->140B	-0.39532				
Excited State 14:	2.772-A	3.4475 eV	359.63 nm	f=0.0033	<S**2>=1.671
132A ->139A	0.14115				
134A ->139A	-0.14919				
138A ->141A	0.91029				
136B ->141B	0.10702				
137B ->141B	-0.16243				
Excited State 15:	3.322-A	3.6037 eV	344.05 nm	f=0.0013	<S**2>=2.508
131A ->139A	0.14876				
132A ->139A	-0.17892				
132A ->140A	0.11879				
133A ->139A	0.14288				
134A ->139A	0.22533				
134A ->140A	-0.10350				
137A ->141A	-0.40257				
138A ->141A	-0.11104				
134B ->139B	-0.10309				
134B ->140B	-0.17308				
135B ->141B	-0.14152				
136B ->141B	0.55592				
137B ->141B	-0.42764				
137B ->143B	0.10422				
Excited State 16:	3.417-A	3.6165 eV	342.83 nm	f=0.0015	<S**2>=2.669
134A ->140A	0.10338				
136A ->139A	-0.13640				
136A ->140A	-0.51663				
137A ->143A	-0.11501				
138A ->141A	-0.11123				
138A ->142A	0.23573				
138A ->143A	-0.20660				
135B ->138B	-0.21223				
135B ->140B	0.55357				
135B ->146B	0.15437				
135B ->147B	0.15208				

135B ->148B -0.10252
136B ->140B 0.15756
137B ->140B 0.12395

Excited State 17: 2.782-A 3.6495 eV 339.73 nm f=0.0016 <S**2>=1.686
128A ->139A -0.10010
131A ->139A 0.27564
132A ->139A -0.41146
133A ->139A 0.23063
134A ->139A 0.49953
135A ->139A -0.11548
137A ->141A 0.15363
138A ->141A 0.30030
134B ->139B -0.16556
135B ->140B 0.22478
136B ->140B 0.11579
136B ->141B -0.17617
137B ->141B 0.18807

Excited State 18: 3.136-A 3.6914 eV 335.87 nm f=0.0040 <S**2>=2.209
132A ->139A -0.14641
134A ->139A 0.12833
134A ->141A -0.13960
136A ->141A 0.19866
137A ->139A 0.10807
137A ->140A 0.20205
137A ->142A -0.13347
138A ->140A 0.11961
138A ->142A 0.52365
138A ->143A 0.37702
134B ->141B -0.25630
134B ->143B 0.11889
135B ->141B -0.23212
135B ->143B 0.20667
136B ->140B -0.19610
136B ->146B -0.14767
137B ->146B 0.13755

Excited State 19: 2.463-A 3.8213 eV 324.46 nm f=0.1117 <S**2>=1.266
131A ->139A 0.22401
132A ->139A 0.30063
133A ->139A 0.60196
134A ->139A -0.16010
137A ->140A 0.34417
138A ->139A 0.14724
135B ->141B -0.10270
136B ->139B 0.21486
137B ->139B 0.32787

Excited State 20: 3.283-A 3.8935 eV 318.44 nm f=0.0017 <S**2>=2.445
133A ->139A 0.10952
134A ->141A 0.11911
136A ->141A -0.30969
138A ->142A 0.46022
134B ->145B 0.11016
135B ->141B 0.62637
135B ->143B -0.10144
135B ->146B 0.11041
136B ->140B -0.10779
136B ->141B 0.20261
137B ->140B -0.24230

Excited State 21: 2.893-A 3.9701 eV 312.29 nm f=0.0057 <S**2>=1.843
136A ->140A -0.29945
137A ->141A -0.10144
137A ->143A -0.15160
138A ->142A -0.34873
138A ->143A 0.74639
138A ->146A -0.11113
135B ->140B 0.12420
135B ->141B 0.15448

136B ->141B	0.11397				
Excited State 22:	2.695-A	3.9857 eV	311.07 nm	f=0.0021	<S**2>=1.566
121A ->139A	0.10537				
133A ->139A	0.10210				
137A ->139A	-0.14690				
137A ->140A	-0.49303				
137A ->142A	0.31655				
137A ->143A	0.17416				
137A ->145A	0.11586				
138A ->142A	0.13869				
138A ->143A	0.20509				
135B ->141B	0.10905				
135B ->143B	0.15220				
135B ->145B	-0.12804				
136B ->139B	0.16233				
136B ->140B	-0.15174				
137B ->140B	0.53270				
Excited State 23:	3.116-A	4.0754 eV	304.22 nm	f=0.0148	<S**2>=2.177
135A ->139A	-0.15224				
137A ->140A	0.28464				
137A ->142A	-0.22290				
137A ->143A	-0.13912				
138A ->140A	0.13638				
138A ->144A	-0.11731				
138A ->145A	0.37814				
135B ->140B	-0.11458				
135B ->141B	0.25841				
135B ->143B	-0.11734				
136B ->138B	0.10015				
136B ->140B	0.28584				
136B ->141B	0.11462				
136B ->142B	0.11935				
136B ->144B	-0.27609				
137B ->140B	0.38299				
137B ->144B	0.20867				
137B ->146B	0.12624				
Excited State 24:	2.963-A	4.1151 eV	301.29 nm	f=0.0234	<S**2>=1.944
133A ->139A	0.10447				
135A ->139A	0.94235				
137B ->140B	0.12651				
Excited State 25:	3.129-A	4.1369 eV	299.70 nm	f=0.0101	<S**2>=2.197
131A ->141A	0.10233				
132A ->141A	-0.19165				
134A ->141A	0.16218				
135A ->139A	0.16118				
136A ->142A	-0.16976				
136A ->143A	0.17819				
137A ->140A	0.11353				
137A ->142A	0.15220				
137A ->145A	0.13467				
138A ->142A	0.42364				
138A ->143A	0.20563				
138A ->145A	0.26166				
134B ->141B	0.33277				
135B ->141B	-0.17109				
135B ->143B	-0.14409				
135B ->145B	0.17967				
136B ->138B	-0.12827				
136B ->140B	0.25467				
136B ->141B	-0.11295				
136B ->146B	0.13233				
137B ->140B	-0.10328				
137B ->146B	-0.10376				
Excited State 26:	2.767-A	4.2253 eV	293.43 nm	f=0.0001	<S**2>=1.664
136A ->140A	0.32189				
136A ->142A	-0.13845				

136A ->143A -0.12894
137A ->141A -0.30329
137A ->143A -0.10889
138A ->145A -0.12385
133B ->138B 0.65635
134B ->138B 0.12036
134B ->140B -0.19078
135B ->140B 0.22893
135B ->146B -0.12388
136B ->141B -0.11551
136B ->143B 0.11927
136B ->145B -0.10831
137B ->143B -0.15251

Excited State 27: 2.711-A 4.2325 eV 292.93 nm f=0.0000 <S**2>=1.588
136A ->140A -0.30917
136A ->142A 0.11726
136A ->143A 0.13852
137A ->141A 0.24204
137A ->143A 0.11676
133B ->138B 0.73925
134B ->140B 0.12289
135B ->140B -0.25001
135B ->141B -0.10932
135B ->146B 0.12890

Excited State 28: 2.687-A 4.2458 eV 292.01 nm f=0.0078 <S**2>=1.555
136A ->139A 0.13382
136A ->140A 0.24175
136A ->142A -0.10694
137A ->141A 0.54342
137A ->142A 0.11560
137A ->143A -0.21857
134B ->140B 0.32044
135B ->140B 0.28111
135B ->142B 0.11709
135B ->144B -0.19086
135B ->146B -0.14901
136B ->141B 0.33499
137B ->141B -0.27541

Excited State 29: 3.044-A 4.3060 eV 287.94 nm f=0.0017 <S**2>=2.066
136A ->140A 0.22173
136A ->142A 0.12784
137A ->141A -0.14681
137A ->142A -0.11860
137A ->143A 0.19216
138A ->143A 0.12846
138A ->146A -0.10428
134B ->140B 0.16550
135B ->138B -0.10712
135B ->140B 0.31439
135B ->143B 0.16134
135B ->145B -0.10138
136B ->140B 0.21917
136B ->143B -0.30299
136B ->144B 0.13089
136B ->145B 0.29827
137B ->141B 0.25985
137B ->143B 0.32569
137B ->145B -0.27940

Excited State 30: 3.229-A 4.3530 eV 284.82 nm f=0.0122 <S**2>=2.357
136A ->142A 0.19385
136A ->143A -0.29790
137A ->140A 0.14431
137A ->141A 0.14081
138A ->145A -0.29099
134B ->141B 0.41174
135B ->140B -0.19609
135B ->141B 0.10423

135B ->143B 0.38445
135B ->145B -0.19289
136B ->140B 0.27922
136B ->143B 0.18703
136B ->145B -0.12930
137B ->140B 0.16404
137B ->141B -0.14960

Excited State 31: 3.049-A 4.3808 eV 283.01 nm f=0.0015 <S**2>=2.074
133A ->139A -0.11406
136A ->141A -0.13229
136A ->143A -0.20237
137A ->140A 0.21484
137A ->142A 0.14755
138A ->140A 0.11489
138A ->144A -0.14151
138A ->145A 0.45484
123B ->138B 0.10489
124B ->138B 0.12308
128B ->138B 0.12901
129B ->138B 0.19127
134B ->141B -0.20192
135B ->141B 0.17320
135B ->145B -0.14573
136B ->138B -0.13309
136B ->141B 0.10969
136B ->142B -0.10074
136B ->143B 0.11492
136B ->144B 0.17097
136B ->146B 0.26067
137B ->144B -0.21181
137B ->146B -0.23016

Excited State 32: 2.997-A 4.4269 eV 280.07 nm f=0.0060 <S**2>=1.995
132A ->141A 0.14607
136A ->141A -0.22869
136A ->143A 0.19817
138A ->145A -0.24335
124B ->138B 0.12420
128B ->138B 0.11929
129B ->138B 0.17502
134B ->141B -0.27104
135B ->140B -0.20486
135B ->141B -0.15038
135B ->143B -0.19906
135B ->145B 0.15146
136B ->138B -0.12476
136B ->139B -0.12251
136B ->140B 0.28696
136B ->144B 0.26908
137B ->140B 0.37822
137B ->142B 0.10149
137B ->144B -0.18162

Excited State 33: 3.032-A 4.4657 eV 277.64 nm f=0.0018 <S**2>=2.049
123A ->139A 0.12933
128A ->139A 0.11528
131A ->139A -0.19424
132A ->139A 0.45487
132A ->140A -0.14159
134A ->139A 0.68948
134A ->140A 0.14154
136A ->139A 0.11630
136A ->140A -0.13861
137A ->141A -0.11734
137A ->143A 0.10032
136B ->141B -0.10278

Excited State 34: 2.867-A 4.5253 eV 273.98 nm f=0.0003 <S**2>=1.805
132A ->139A -0.22352
134A ->139A -0.16931

134A ->140A 0.12012
136A ->140A -0.10121
136A ->142A -0.12371
137A ->141A -0.22347
137A ->143A 0.15756
132B ->138B 0.60705
134B ->138B -0.16639
134B ->140B 0.32230
134B ->146B 0.10127
135B ->138B 0.12662
135B ->141B 0.10201
135B ->144B -0.16153
135B ->146B -0.14260
136B ->141B -0.15221
137B ->141B -0.22346

Excited State 35: 2.782-A 4.5733 eV 271.10 nm f=0.0043 <S**2>=1.684
136A ->141A 0.21189
137A ->142A 0.16191
137A ->143A -0.11437
138A ->145A -0.20971
132B ->138B 0.56497
134B ->140B -0.14557
136B ->141B 0.34176
137B ->141B 0.49876

Excited State 36: 2.922-A 4.6041 eV 269.29 nm f=0.0060 <S**2>=1.885
132A ->139A 0.11489
132A ->140A 0.19111
133A ->139A 0.10174
134A ->140A -0.15377
134A ->141A 0.11650
136A ->141A -0.25649
137A ->140A -0.18683
137A ->141A 0.12397
137A ->143A -0.22325
137A ->145A -0.14755
138A ->144A -0.11801
138A ->145A 0.33844
132B ->138B 0.36137
134B ->140B -0.30042
134B ->143B -0.11957
135B ->141B -0.15602
135B ->143B 0.12912
136B ->141B -0.18829
136B ->146B -0.12642
137B ->143B 0.23415
137B ->144B -0.13842
137B ->146B 0.14608

Excited State 37: 2.933-A 4.6392 eV 267.25 nm f=0.0050 <S**2>=1.901
136A ->141A 0.57839
137A ->142A 0.19265
137A ->143A 0.19628
137A ->145A -0.28303
138A ->145A 0.18627
135B ->141B 0.19157
135B ->143B -0.13549
136B ->139B -0.19517
136B ->140B 0.16245
136B ->143B -0.12613
136B ->144B 0.12944
136B ->146B -0.23732
137B ->144B -0.13333
137B ->146B 0.17137

Excited State 38: 3.039-A 4.6652 eV 265.76 nm f=0.0028 <S**2>=2.058
131A ->140A -0.15173
132A ->140A 0.13048
132A ->141A 0.12732
133A ->139A -0.17845

133A ->140A -0.14803
134A ->140A -0.15395
134A ->141A -0.11709
136A ->141A 0.11180
137A ->140A 0.13040
137A ->141A 0.12421
137A ->142A 0.12722
137A ->145A 0.10860
138A ->145A -0.18994
134B ->140B -0.21099
134B ->141B -0.20546
135B ->141B 0.25809
135B ->146B -0.12728
136B ->141B -0.32465
136B ->143B -0.23409
137B ->141B -0.30910
137B ->143B 0.36595
137B ->145B -0.11989
137B ->146B -0.13980

Excited State 39: 3.016-A 4.7077 eV 263.37 nm f=0.0052 <S**2>=2.024
134A ->142A -0.10821
136A ->140A 0.28918
136A ->141A 0.18881
136A ->142A 0.37923
136A ->143A 0.21325
137A ->142A 0.14183
138A ->146A -0.37358
129B ->138B 0.11233
132B ->138B 0.22000
135B ->141B 0.15328
135B ->144B 0.16770
135B ->146B 0.28240
135B ->147B 0.11091
136B ->141B -0.11341
136B ->143B 0.10486
137B ->141B -0.23449
137B ->143B -0.21249
137B ->144B 0.11631
137B ->145B 0.10739

Excited State 40: 2.849-A 4.7211 eV 262.62 nm f=0.0071 <S**2>=1.779
124A ->139A 0.14219
131A ->139A 0.35657
132A ->139A 0.16524
133A ->139A -0.18964
133A ->140A 0.13356
136A ->142A -0.11435
137A ->142A -0.19095
138A ->146A 0.10333
121B ->138B 0.12414
123B ->138B 0.17195
124B ->138B 0.21750
126B ->138B 0.12643
127B ->138B 0.13491
128B ->138B 0.28190
129B ->138B 0.41150
130B ->138B -0.14622
131B ->138B 0.15481
134B ->141B 0.12554
136B ->140B -0.19469
136B ->144B -0.18135
136B ->146B -0.14918
137B ->142B -0.11342
137B ->144B 0.16237
137B ->146B 0.16468

Excited State 41: 2.899-A 4.7276 eV 262.26 nm f=0.0044 <S**2>=1.851
124A ->139A 0.20744
131A ->139A 0.51767
132A ->139A 0.22098

133A ->139A	-0.41634				
137A ->143A	0.17445				
123B ->138B	-0.10479				
124B ->138B	-0.11312				
128B ->138B	-0.16398				
129B ->138B	-0.24160				
136B ->140B	0.16039				
136B ->144B	0.14625				
137B ->139B	0.11584				
137B ->142B	0.10951				
137B ->143B	-0.12996				
137B ->144B	-0.22067				
137B ->146B	0.12886				
Excited State 42:	2.767-A	4.7610 eV	260.42 nm	f=0.0047	<S**2>=1.664
131A ->139A	-0.17698				
133A ->139A	0.11102				
137A ->141A	0.26622				
137A ->142A	-0.37399				
137A ->143A	0.51497				
138A ->146A	-0.20377				
132B ->138B	0.13104				
134B ->138B	0.10890				
134B ->140B	-0.34649				
134B ->146B	-0.18953				
134B ->147B	-0.10650				
135B ->140B	0.13686				
135B ->144B	-0.12189				
136B ->143B	0.11372				
137B ->141B	-0.11849				
137B ->143B	-0.21066				
Excited State 43:	2.558-A	4.8167 eV	257.40 nm	f=0.0004	<S**2>=1.386
138A ->146A	0.31200				
128B ->138B	-0.10938				
129B ->138B	-0.13816				
131B ->138B	0.81974				
132B ->138B	0.16885				
135B ->146B	0.10265				
136B ->145B	0.10027				
137B ->143B	-0.10054				
137B ->145B	-0.11839				
Excited State 44:	2.893-A	4.8315 eV	256.62 nm	f=0.0011	<S**2>=1.842
138A ->146A	0.53515				
131B ->138B	-0.46860				
134B ->146B	-0.17984				
135B ->144B	0.14905				
135B ->146B	0.21645				
136B ->145B	0.22615				
137B ->141B	-0.16267				
137B ->143B	-0.24314				
137B ->145B	-0.23984				
Excited State 45:	2.776-A	4.8598 eV	255.12 nm	f=0.0039	<S**2>=1.677
121A ->139A	-0.27738				
122A ->139A	-0.32302				
123A ->139A	0.17536				
125A ->139A	0.37453				
126A ->139A	-0.22460				
127A ->139A	-0.36614				
130A ->139A	0.14316				
131A ->140A	-0.17705				
132A ->140A	-0.15859				
133A ->139A	-0.15884				
133A ->140A	-0.32277				
137A ->142A	-0.12856				
137A ->145A	-0.10444				
136B ->139B	0.13114				
136B ->140B	-0.12090				
136B ->144B	-0.10307				

136B ->146B 0.21567

Excited State 46: 2.854-A 4.9094 eV 252.55 nm f=0.0077 <S**2>=1.786
122A ->139A -0.11361
125A ->139A 0.14180
127A ->139A -0.14476
131A ->139A 0.10008
132A ->140A 0.25261
133A ->140A 0.22450
134A ->140A -0.14823
136A ->141A -0.12420
136A ->142A -0.13439
137A ->142A 0.18468
137A ->143A 0.21175
138A ->146A -0.19431
134B ->140B 0.17193
135B ->139B -0.15444
135B ->144B 0.36389
135B ->146B -0.25871
136B ->140B 0.11980
136B ->144B 0.14266
137B ->143B -0.12037
137B ->144B 0.34340

Excited State 47: 2.675-A 4.9269 eV 251.65 nm f=0.0041 <S**2>=1.539
125A ->139A 0.11077
127A ->139A -0.13350
131A ->139A 0.18854
131A ->140A 0.33381
133A ->140A 0.53095
136A ->141A 0.12837
136A ->143A 0.27584
138A ->146A 0.20882
128B ->138B -0.10832
129B ->138B -0.12039
134B ->140B -0.17051
134B ->143B 0.11004
135B ->141B 0.10596
135B ->144B -0.19998
136B ->140B 0.11896
136B ->146B 0.15815
137B ->146B -0.19581

Excited State 48: 2.565-A 4.9565 eV 250.15 nm f=0.0087 <S**2>=1.395
132A ->140A -0.15457
132A ->141A 0.14125
134A ->140A 0.12753
136A ->141A -0.29587
136A ->142A 0.20759
136A ->143A -0.12183
137A ->142A 0.44237
137A ->143A 0.30844
138A ->146A 0.17687
134B ->140B -0.15313
135B ->141B -0.17122
135B ->144B -0.20820
135B ->145B 0.11698
135B ->146B 0.10921
136B ->144B -0.11488
136B ->146B -0.12042
137B ->142B -0.16945
137B ->144B 0.27683
137B ->146B 0.14132

Excited State 49: 2.781-A 4.9800 eV 248.96 nm f=0.0091 <S**2>=1.684
133B ->139B 0.97296

Excited State 50: 2.470-A 5.0063 eV 247.66 nm f=0.0004 <S**2>=1.276
126B ->138B 0.15335
128B ->138B -0.15602
129B ->138B 0.32961

130B ->138B 0.91370

Excited State 51: 2.711-A 5.0407 eV 245.97 nm f=0.0011 <S**2>=1.587
132A ->139A -0.10905
132A ->140A -0.23276
134A ->140A 0.20871
136A ->142A 0.19882
136A ->143A 0.12457
138A ->144A -0.20476
138A ->146A 0.21714
127B ->138B -0.10896
128B ->138B 0.56826
129B ->138B -0.24801
130B ->138B 0.19400
134B ->140B -0.14861
135B ->144B 0.18718
135B ->146B -0.27996

Excited State 52: 2.669-A 5.0457 eV 245.72 nm f=0.0002 <S**2>=1.531
132A ->139A 0.13161
132A ->140A 0.24856
134A ->140A -0.22151
138A ->144A 0.19367
138A ->146A -0.13370
127B ->138B -0.10428
128B ->138B 0.60107
129B ->138B -0.29166
130B ->138B 0.19542
134B ->140B 0.12095
135B ->139B 0.10487
135B ->144B -0.22804
135B ->146B 0.25799
136B ->144B -0.14334

Excited State 53: 2.730-A 5.0684 eV 244.62 nm f=0.0064 <S**2>=1.613
131A ->140A 0.11024
132A ->139A -0.11611
132A ->140A -0.20034
134A ->140A 0.20734
136A ->142A -0.11459
137A ->143A -0.13312
138A ->144A 0.73117
138A ->145A 0.21976
134B ->140B -0.11574
135B ->144B 0.13165
136B ->145B 0.13044
137B ->144B -0.14973
137B ->145B -0.26876

Excited State 54: 2.668-A 5.0804 eV 244.04 nm f=0.0017 <S**2>=1.529
130A ->139A 0.18270
132A ->140A 0.16603
132A ->141A -0.12856
133A ->141A -0.19300
134A ->140A -0.15268
136A ->142A 0.40242
136A ->143A 0.16619
137A ->143A 0.10467
137A ->145A 0.17856
138A ->144A 0.27147
138A ->146A 0.31886
128B ->138B -0.10624
135B ->146B -0.19297
136B ->143B -0.12406
136B ->144B -0.17803
136B ->145B -0.11815
136B ->146B -0.15349
137B ->142B 0.14122
137B ->144B -0.23595
137B ->145B 0.23053
137B ->146B -0.12797

Excited State 55:	2.876-A	5.0884 eV	243.66 nm	f=0.0041	<S**2>=1.818
130A ->139A	0.48725				
136A ->143A	-0.15402				
137A ->142A	0.14930				
137A ->145A	0.26520				
138A ->144A	-0.41159				
138A ->145A	-0.14585				
138A ->146A	-0.19023				
136B ->144B	-0.18649				
136B ->145B	0.10502				
136B ->146B	-0.12283				
137B ->142B	0.28524				
137B ->144B	-0.27567				
137B ->145B	-0.18224				
Excited State 56:	2.475-A	5.0949 eV	243.35 nm	f=0.0001	<S**2>=1.281
125B ->138B	-0.10458				
127B ->138B	0.93319				
129B ->138B	-0.26964				
130B ->138B	0.11050				
Excited State 57:	2.903-A	5.1086 eV	242.70 nm	f=0.0018	<S**2>=1.857
121A ->139A	0.15065				
125A ->139A	-0.16905				
128A ->139A	0.16485				
130A ->139A	0.77976				
137A ->142A	-0.14022				
137A ->145A	-0.10540				
138A ->144A	0.12095				
136B ->144B	0.19580				
136B ->146B	0.11585				
137B ->142B	-0.18984				
137B ->144B	0.19594				
137B ->145B	0.16069				
Excited State 58:	2.952-A	5.1448 eV	240.99 nm	f=0.0013	<S**2>=1.928
120A ->139A	0.10655				
125A ->139A	0.16787				
128A ->139A	0.63691				
129A ->139A	0.16295				
130A ->139A	-0.16072				
131A ->139A	0.10324				
132A ->139A	-0.20430				
136A ->143A	-0.10578				
136A ->145A	-0.10495				
135B ->143B	0.12340				
135B ->146B	0.10169				
136B ->143B	-0.30714				
136B ->145B	0.11342				
137B ->143B	-0.13307				
137B ->145B	0.34833				
137B ->149B	0.10201				
Excited State 59:	2.682-A	5.1796 eV	239.37 nm	f=0.0082	<S**2>=1.548
128A ->139A	0.13031				
137A ->143A	0.10979				
137A ->145A	0.19816				
125B ->138B	-0.31233				
126B ->138B	0.51813				
127B ->138B	-0.12379				
129B ->138B	-0.25401				
129B ->139B	0.12623				
135B ->143B	-0.14943				
135B ->144B	0.18705				
136B ->143B	0.26610				
136B ->145B	-0.20275				
137B ->142B	-0.17527				
137B ->143B	0.26707				
137B ->144B	-0.14604				

Excited State 60: 2.726-A 5.1883 eV 238.97 nm f=0.0047 <S**2>=1.608

128A ->139A	0.21558
137A ->143A	0.11529
125B ->138B	0.43728
126B ->138B	-0.40140
128B ->138B	0.13159
129B ->138B	0.17975
135B ->143B	-0.11226
135B ->144B	0.19539
135B ->145B	0.10113
136B ->143B	0.36949
136B ->144B	-0.10217
136B ->145B	-0.20608
137B ->143B	0.33744
137B ->144B	-0.15139

Excited State 61: 2.650-A 5.1924 eV 238.78 nm f=0.0012 <S**2>=1.505

137A ->145A	0.25737
123B ->139B	0.12168
124B ->139B	0.14270
125B ->138B	0.69285
126B ->138B	0.13137
128B ->139B	0.14330
129B ->139B	0.21450
135B ->145B	-0.10446
136B ->143B	-0.13313
136B ->144B	0.13729
137B ->142B	-0.28571
137B ->143B	-0.10480

Excited State 62: 2.754-A 5.2024 eV 238.32 nm f=0.0167 <S**2>=1.646

128A ->139A	0.33988
129A ->139A	0.23110
136A ->142A	0.14669
136A ->143A	0.15290
137A ->145A	-0.17425
137A ->146A	-0.14731
125B ->138B	0.27403
126B ->138B	0.48227
128B ->138B	-0.12985
135B ->144B	-0.19347
136B ->143B	0.12457
137B ->142B	0.24431
137B ->144B	0.15126
137B ->145B	-0.25663

Excited State 63: 2.783-A 5.2080 eV 238.06 nm f=0.0088 <S**2>=1.686

128A ->139A	-0.30864
129A ->139A	-0.18318
132A ->141A	0.10137
136A ->142A	-0.16946
137A ->145A	-0.17387
123B ->139B	-0.11444
124B ->139B	-0.12498
125B ->138B	0.33268
126B ->138B	0.41216
128B ->139B	-0.11599
129B ->139B	-0.19703
134B ->144B	0.10986
135B ->143B	0.11219
135B ->144B	0.23061
136B ->144B	-0.12877
137B ->142B	0.17680
137B ->144B	-0.12757
137B ->145B	0.26018

Excited State 64: 2.824-A 5.2260 eV 237.25 nm f=0.0078 <S**2>=1.743

129A ->139A	-0.11276
131A ->141A	0.10280
133A ->141A	0.12579
137A ->146A	0.12382

124B ->139B 0.10034
129B ->139B 0.13309
136B ->144B 0.12468
136B ->145B -0.13360
137B ->142B 0.69932
137B ->143B 0.18689
137B ->144B 0.42171
137B ->147B -0.12755

Excited State 65: 2.889-A 5.2349 eV 236.84 nm f=0.0027 <S**2>=1.836
126A ->139A -0.14944
127A ->139A 0.20878
128A ->139A -0.34819
129A ->139A 0.85115
131A ->139A 0.10586

Excited State 66: 3.009-A 5.2861 eV 234.55 nm f=0.0068 <S**2>=2.013
127A ->139A 0.11249
129A ->139A -0.18605
132A ->142A 0.11537
132A ->143A 0.11113
136A ->142A -0.11271
137A ->145A -0.19104
137A ->146A 0.18444
132B ->139B -0.37401
134B ->138B -0.11619
134B ->139B 0.18551
134B ->142B -0.10767
134B ->144B 0.18701
134B ->145B 0.17201
134B ->146B 0.41311
134B ->147B 0.13120
135B ->145B 0.17760
135B ->146B 0.14213
137B ->143B -0.16077
137B ->145B -0.21121
137B ->146B -0.24404

Excited State 67: 2.784-A 5.3025 eV 233.82 nm f=0.0026 <S**2>=1.688
127A ->139A 0.12261
128A ->139A 0.10313
131A ->141A -0.13943
132A ->141A -0.20626
133A ->141A -0.29434
136A ->143A -0.11908
132B ->139B 0.66290
134B ->139B -0.15032
134B ->141B -0.10297
134B ->143B -0.11293
134B ->144B 0.32383
134B ->145B 0.10811
135B ->145B 0.12660
137B ->146B -0.17713

Excited State 68: 3.002-A 5.3074 eV 233.61 nm f=0.0068 <S**2>=2.003
127A ->139A -0.13714
131A ->141A -0.19140
132A ->142A 0.11030
133A ->141A -0.29449
136A ->141A -0.11494
136A ->142A -0.17420
137A ->145A 0.15570
134B ->141B 0.13317
134B ->142B -0.13908
134B ->143B 0.31000
134B ->144B 0.23251
134B ->145B -0.31661
134B ->146B 0.24007
134B ->147B 0.10992
135B ->143B -0.10400
135B ->145B -0.25156

136B ->144B 0.11154
136B ->145B -0.12805
136B ->146B 0.11175
137B ->145B -0.10009
137B ->146B 0.35883

Excited State 69: 2.915-A 5.3274 eV 232.73 nm f=0.0150 <S**2>=1.874
124A ->139A -0.12128
125A ->139A 0.30614
126A ->139A -0.33334
127A ->139A 0.76148
129A ->139A -0.24978
131A ->139A 0.10566
134B ->143B 0.12073
134B ->145B -0.11394

Excited State 70: 3.042-A 5.3658 eV 231.06 nm f=0.0031 <S**2>=2.064
125A ->139A 0.17169
126A ->139A 0.40760
131A ->141A 0.11428
132A ->141A 0.14590
132A ->142A 0.12083
132A ->143A -0.11920
133A ->141A 0.23219
134A ->142A -0.13226
136A ->141A -0.14880
137A ->145A -0.11374
132B ->139B 0.34266
134B ->141B 0.10396
134B ->143B 0.43734
134B ->144B -0.13413
134B ->145B -0.20037
135B ->143B 0.10675
135B ->144B 0.10603
136B ->146B -0.17667
137B ->146B -0.16504

Excited State 71: 2.943-A 5.3690 eV 230.92 nm f=0.0002 <S**2>=1.915
125A ->139A 0.55331
126A ->139A 0.62835
127A ->139A 0.12454
128A ->139A -0.22146
132B ->139B -0.13031
134B ->143B -0.24607
135B ->145B -0.12753

Excited State 72: 2.948-A 5.3748 eV 230.68 nm f=0.0049 <S**2>=1.922
126A ->139A 0.26028
131A ->141A -0.12531
133A ->141A -0.20830
133A ->143A 0.10038
134A ->143A 0.10959
137A ->146A -0.17731
123B ->139B 0.13081
124B ->139B 0.12077
128B ->139B 0.14208
129B ->139B 0.22110
132B ->139B -0.32342
134B ->143B 0.18333
134B ->146B -0.17896
135B ->143B 0.17753
135B ->145B 0.33937
136B ->143B 0.19536
136B ->144B -0.12422
136B ->145B 0.30137
137B ->143B 0.17078
137B ->145B 0.18907

Excited State 73: 2.776-A 5.4192 eV 228.79 nm f=0.0041 <S**2>=1.676
124A ->139A -0.10412
125A ->139A -0.16218

131A ->141A -0.14672
132A ->140A -0.10015
132A ->141A 0.10827
132A ->142A -0.15130
133A ->140A -0.16592
133A ->141A -0.15409
133A ->142A -0.16949
134A ->141A -0.13280
134A ->142A 0.13163
136A ->142A -0.25046
136A ->143A 0.30613
137A ->145A -0.16653
124B ->139B 0.11136
128B ->139B 0.11813
129B ->139B 0.17063
134B ->141B 0.15504
134B ->143B -0.11865
134B ->146B -0.16416
135B ->143B 0.14211
135B ->145B -0.29471
135B ->146B 0.13874
136B ->143B -0.17245
136B ->145B -0.30606
137B ->146B -0.24083

Excited State 74: 2.732-A 5.4389 eV 227.96 nm f=0.0012 <S**2>=1.616
132A ->141A 0.20580
134A ->141A -0.15952
134A ->143A -0.10737
136A ->143A 0.16369
123B ->138B 0.21971
124B ->138B 0.37971
126B ->138B -0.17818
128B ->138B -0.13598
128B ->139B 0.11651
129B ->138B -0.22737
129B ->139B 0.18315
132B ->139B 0.15948
134B ->143B -0.18012
134B ->145B 0.16527
134B ->146B 0.20200
135B ->146B -0.21659
136B ->144B -0.13617
136B ->145B 0.11091
136B ->146B 0.25502
137B ->146B 0.30481

Excited State 75: 2.794-A 5.4611 eV 227.03 nm f=0.0022 <S**2>=1.702
124A ->139A -0.14758
132A ->141A 0.11177
136A ->143A 0.17852
136A ->145A -0.12737
123B ->138B -0.23887
124B ->138B -0.37007
126B ->138B 0.14416
129B ->138B 0.21328
134B ->143B -0.17771
134B ->146B 0.19694
135B ->145B -0.22281
136B ->142B -0.11208
136B ->143B 0.32632
136B ->145B 0.41613
137B ->145B 0.22425
137B ->149B 0.12549

Excited State 76: 2.736-A 5.4921 eV 225.75 nm f=0.0013 <S**2>=1.621
123A ->139A -0.13285
124A ->139A 0.53506
131A ->139A -0.20705
123B ->138B -0.24054
123B ->139B 0.14589

124B ->138B -0.36299
126B ->138B 0.11696
128B ->139B 0.12702
129B ->138B 0.15803
129B ->139B 0.21187
131B ->139B -0.28738
135B ->143B 0.15190
135B ->145B 0.16418
135B ->146B -0.10615
136B ->143B -0.12342
136B ->145B -0.11648
136B ->146B 0.16412

Excited State 77: 2.904-A 5.5056 eV 225.20 nm f=0.0022 <S**2>=1.858
123A ->139A -0.10955
124A ->139A 0.50603
125A ->139A 0.16932
126A ->139A -0.14627
131A ->139A -0.15145
133A ->142A -0.12812
123B ->138B 0.16530
124B ->138B 0.22829
131B ->139B -0.22934
135B ->145B -0.22993
135B ->146B 0.15859
136B ->143B 0.18923
136B ->145B 0.18887
136B ->146B -0.29888
137B ->143B 0.10441
137B ->145B 0.14960
137B ->146B -0.29783

Excited State 78: 2.907-A 5.5909 eV 221.76 nm f=0.0058 <S**2>=1.863
121A ->139A 0.21802
122A ->139A 0.37469
123A ->139A -0.13304
125A ->139A 0.35488
126A ->139A -0.25177
127A ->139A -0.18257
133A ->142A -0.13768
136A ->146A -0.18118
137A ->145A 0.13208
124B ->138B 0.13316
131B ->139B 0.30389
134B ->143B -0.10027
134B ->144B -0.12330
135B ->143B 0.30578
135B ->145B 0.26676
136B ->144B 0.11723

Excited State 79: 2.779-A 5.6205 eV 220.59 nm f=0.0002 <S**2>=1.681
134A ->145A -0.19931
136A ->140A 0.12961
136A ->144A -0.24377
136A ->145A 0.83735
137A ->146A 0.13687
135B ->144B 0.13055
135B ->146B -0.11341
136B ->145B 0.17900

Excited State 80: 2.606-A 5.6276 eV 220.31 nm f=0.0007 <S**2>=1.447
121A ->139A 0.10326
122A ->139A 0.17183
125A ->139A 0.11805
131A ->143A -0.11736
133A ->143A -0.17470
122B ->138B 0.25448
123B ->138B 0.66154
124B ->138B -0.48813
134B ->144B 0.19476

Excited State 81:	2.900-A	5.6352 eV	220.02 nm	f=0.0029	<S**2>=1.852
122A ->139A	0.10987				
131A ->143A	-0.20548				
132A ->142A	0.15785				
133A ->141A	0.18626				
133A ->142A	0.17019				
133A ->143A	-0.32901				
137A ->146A	-0.23233				
123B ->138B	-0.30944				
124B ->138B	0.21030				
132B ->139B	-0.12391				
134B ->139B	-0.12933				
134B ->142B	-0.14630				
134B ->144B	0.51379				
134B ->146B	-0.18628				
137B ->145B	0.10566				
Excited State 82:	2.887-A	5.6543 eV	219.27 nm	f=0.0067	<S**2>=1.834
122A ->139A	0.18480				
124A ->139A	0.29883				
131A ->143A	0.12238				
133A ->142A	0.17598				
133A ->143A	0.18840				
136A ->146A	0.18724				
137A ->145A	-0.20115				
131B ->139B	0.61132				
134B ->143B	0.10964				
134B ->145B	0.15289				
135B ->143B	-0.22979				
135B ->145B	-0.19830				
136B ->144B	-0.17508				
136B ->146B	0.10566				
Excited State 83:	2.653-A	5.6735 eV	218.53 nm	f=0.0114	<S**2>=1.509
121A ->139A	0.14447				
122A ->139A	0.29241				
124A ->139A	-0.16249				
125A ->139A	0.14068				
131A ->142A	-0.11443				
131A ->143A	-0.14222				
132A ->141A	-0.17742				
132A ->142A	-0.26883				
133A ->142A	-0.28505				
133A ->143A	-0.15051				
134A ->141A	0.16597				
134A ->142A	0.13594				
136A ->143A	-0.10266				
137A ->144A	0.10923				
137A ->145A	-0.21751				
123B ->138B	-0.16641				
129B ->139B	0.10332				
131B ->139B	-0.26627				
134B ->143B	0.26255				
134B ->145B	0.10785				
135B ->143B	-0.23142				
135B ->145B	-0.10484				
136B ->146B	0.19960				
Excited State 84:	2.772-A	5.7039 eV	217.37 nm	f=0.0003	<S**2>=1.671
121A ->139A	-0.13165				
122A ->139A	-0.34469				
123A ->139A	0.15827				
124A ->139A	0.32670				
125A ->139A	-0.14678				
131A ->142A	-0.11786				
131A ->143A	-0.19621				
132A ->141A	-0.11782				
132A ->142A	-0.25167				
133A ->142A	-0.28983				
133A ->143A	-0.24446				
134A ->141A	0.12260				

134A ->142A 0.12939
134A ->143A -0.13597
131B ->139B 0.44876
134B ->143B 0.10254
137B ->146B 0.12107

Excited State 85: 3.124-A 5.7503 eV 215.62 nm f=0.0005 <S**2>=2.190
135A ->140A 0.94000
137B ->149B -0.12136

Excited State 86: 3.046-A 5.7745 eV 214.71 nm f=0.0010 <S**2>=2.070
122A ->139A -0.16741
123A ->139A -0.34312
133A ->143A -0.10065
135A ->140A -0.17295
138A ->147A -0.22752
138A ->150A 0.13115
122B ->138B -0.21199
123B ->138B 0.11796
136B ->142B -0.45809
137B ->145B 0.11277
137B ->147B 0.47570
137B ->149B -0.26676
137B ->150B -0.10843

Excited State 87: 2.455-A 5.7887 eV 214.18 nm f=0.0003 <S**2>=1.256
123A ->139A -0.18192
137A ->146A 0.12936
122B ->138B 0.90045
123B ->138B -0.21885
124B ->138B 0.16206
136B ->142B -0.12546

Excited State 88: 2.987-A 5.7997 eV 213.78 nm f=0.0010 <S**2>=1.980
122A ->139A 0.29732
123A ->139A 0.68740
124A ->139A 0.14246
138A ->147A -0.13321
122B ->138B 0.12638
136B ->142B -0.42302
137B ->147B 0.26462
137B ->149B 0.14714

Excited State 89: 2.847-A 5.8268 eV 212.78 nm f=0.0094 <S**2>=1.776
131A ->142A 0.19166
132A ->142A -0.18160
132A ->143A -0.20340
133A ->141A -0.14493
133A ->142A 0.18496
133A ->143A -0.18434
134A ->142A 0.20471
134A ->143A 0.11477
137A ->146A 0.73149
122B ->138B -0.12600
136B ->145B 0.11858

Excited State 90: 2.863-A 5.8281 eV 212.74 nm f=0.0001 <S**2>=1.799
126B ->139B 0.14521
129B ->139B 0.22092
130B ->139B 0.93983

Excited State 91: 2.969-A 5.8335 eV 212.54 nm f=0.0009 <S**2>=1.954
122A ->139A -0.13274
123A ->139A -0.26268
131A ->143A 0.17402
132A ->142A -0.17188
133A ->141A 0.16291
133A ->142A -0.10600
133A ->143A 0.24478
134A ->142A 0.10799
135A ->140A 0.13910

138A ->148A	0.10229				
138A ->149A	0.21979				
138A ->150A	-0.25348				
130B ->139B	-0.16120				
134B ->142B	-0.10097				
134B ->144B	0.24858				
136B ->142B	-0.33314				
136B ->145B	-0.17953				
137B ->145B	-0.12583				
137B ->148B	-0.11195				
137B ->149B	0.38035				
137B ->150B	0.14660				
Excited State 92:	2.969-A	5.8764 eV	210.99 nm	f=0.0005	<S**2>=1.954
123A ->139A	0.11994				
131A ->143A	0.10363				
132A ->142A	-0.17726				
133A ->141A	0.14350				
133A ->143A	0.18110				
134A ->142A	0.12926				
138A ->147A	-0.39742				
134B ->144B	0.18024				
135B ->142B	0.26841				
136B ->142B	0.49516				
136B ->143B	0.11878				
136B ->144B	0.16540				
137B ->147B	0.37952				
137B ->148B	-0.11899				
137B ->149B	-0.12749				
Excited State 93:	2.861-A	5.8800 eV	210.86 nm	f=0.0001	<S**2>=1.797
125B ->139B	0.14100				
127B ->139B	-0.17605				
128B ->139B	0.84779				
129B ->139B	-0.40860				
130B ->139B	0.11578				
Excited State 94:	2.886-A	5.9017 eV	210.08 nm	f=0.0022	<S**2>=1.833
122A ->139A	-0.10767				
123A ->139A	-0.16586				
131A ->143A	-0.18375				
132A ->141A	-0.12060				
132A ->142A	0.17619				
133A ->141A	-0.16773				
133A ->142A	0.13856				
133A ->143A	-0.27135				
134A ->142A	-0.11086				
138A ->147A	-0.42062				
138A ->148A	0.12463				
138A ->149A	0.11163				
138A ->150A	-0.10864				
134B ->144B	-0.23780				
136B ->142B	0.19486				
137B ->145B	-0.13136				
137B ->148B	-0.20083				
137B ->149B	0.44570				
137B ->150B	0.15887				
Excited State 95:	2.780-A	5.9307 eV	209.05 nm	f=0.0069	<S**2>=1.682
132A ->143A	0.12060				
133A ->142A	0.10878				
134A ->143A	-0.12777				
138A ->147A	0.44333				
127B ->139B	0.53837				
129B ->139B	-0.17362				
135B ->142B	0.42385				
135B ->144B	0.12319				
137B ->147B	0.23725				
137B ->148B	-0.10303				
137B ->149B	0.12151				

Excited State 96: 2.761-A 5.9345 eV 208.92 nm f=0.0044 <S**2>=1.656
132A ->143A -0.16936
133A ->142A -0.10670
134A ->143A 0.15974
138A ->147A -0.37111
125B ->139B -0.10874
127B ->139B 0.73636
129B ->139B -0.19286
135B ->142B -0.11630
137B ->147B -0.22139
137B ->148B 0.10286

Excited State 97: 2.912-A 5.9404 eV 208.71 nm f=0.0027 <S**2>=1.870
132A ->143A -0.25341
134A ->142A -0.11729
134A ->143A 0.20335
138A ->147A -0.10006
127B ->139B -0.19708
135B ->140B -0.11553
135B ->142B 0.73276
135B ->144B 0.23015
137B ->147B -0.25944
137B ->148B 0.13128

Excited State 98: 2.685-A 5.9940 eV 206.85 nm f=0.0019 <S**2>=1.553
122A ->139A 0.13331
131A ->142A 0.21209
132A ->142A -0.13240
132A ->143A 0.28608
133A ->142A 0.25520
134A ->142A 0.20184
134A ->143A -0.24698
136A ->146A 0.11690
137A ->144A 0.34615
137A ->145A 0.16879
138A ->147A -0.32688
134B ->145B -0.21297
135B ->142B 0.16391
135B ->143B 0.11299
136B ->142B -0.14645
136B ->146B -0.16418
137B ->147B -0.32723
137B ->148B 0.10547

Excited State 99: 2.853-A 6.0177 eV 206.03 nm f=0.0146 <S**2>=1.785
132A ->143A -0.18062
134A ->143A 0.14953
134A ->146A -0.14018
136A ->146A 0.26640
137A ->144A 0.68184
138A ->147A 0.13187
126B ->139B -0.10119
134B ->141B -0.12084
134B ->143B -0.28187
134B ->145B -0.27772
137B ->147B 0.13492

Excited State 100: 2.852-A 6.0258 eV 205.75 nm f=0.0075 <S**2>=1.783
124B ->139B 0.10399
125B ->139B -0.16400
126B ->139B 0.87172
128B ->139B -0.10961
129B ->139B -0.36891

Figure S24-1. The calculated absorption spectra based on B3LYP level of theory. The upper chart indicates the actual spectrum of **2** (black line) and calculated spectrum of $\mathbf{2}_{opt}$ (red solid bars), whereas the lower chart includes the actual spectrum of **3** (black line) and calculated spectrum of $\mathbf{3}_{opt}$ (red solid bars).

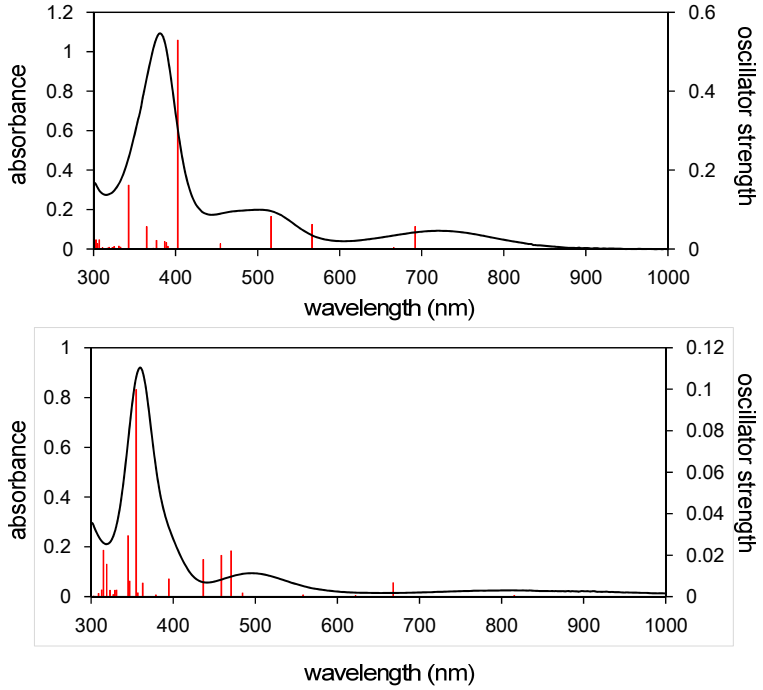
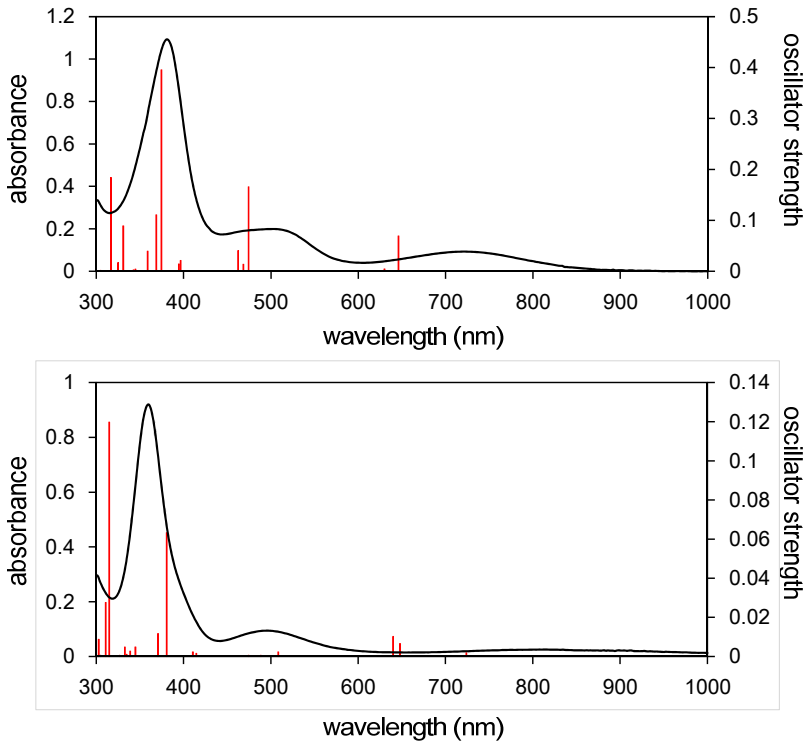


Figure S24-2. The calculated absorption spectra based on CAM-B3LYP level of theory. The upper chart indicates the actual spectrum of **2** (black line) and calculated spectrum of $\mathbf{2}_{opt}$ (red solid bars), whereas the lower chart includes the actual spectrum of **3** (black line) and calculated spectrum of $\mathbf{3}_{opt}$ (red solid bars).



X-ray data collection and reduction

X-ray crystallography was performed on a Rigaku Saturn CCD area detector with graphite monochromated Mo-Kα radiation (λ=0.71075 Å). The data were collected at 123(2) K using ω scan in the θ range of $1.55 \leq \theta \leq 30.60$ deg (**2**), $1.88 \leq \theta \leq 30.66$ deg (**4**), $2.08 \leq \theta \leq 30.47$ deg (**5**) and $3.03 \leq \theta \leq 27.48$ deg (**8**). The data obtained were processed using Crystal-Clear (Rigaku) on a Pentium computer, and were corrected for Lorentz and polarization effects. The structures were solved by direct methods[11], and expanded using Fourier techniques[12]. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement on F^2 was based on 12,402 observed reflections and 505 variable parameters for **2**, 7,658 observed reflections and 325 variable parameters for **4**, 7,170 observed reflections and 289 variable parameters for **5**, and 9,661 observed reflections and 422 variable parameters for **8**. Neutral atom scattering factors were taken from Cromer and Waber[13]. All calculations were performed using SHELXL-97[14]. Details of final refinement as well as the bond lengths and angle are summarized in Tables S7, S8, S9 and S10, and the numbering scheme employed is also shown in Figures S25, 26, 27 and 28, which were drawn with ORTEP at 50% probability ellipsoids.

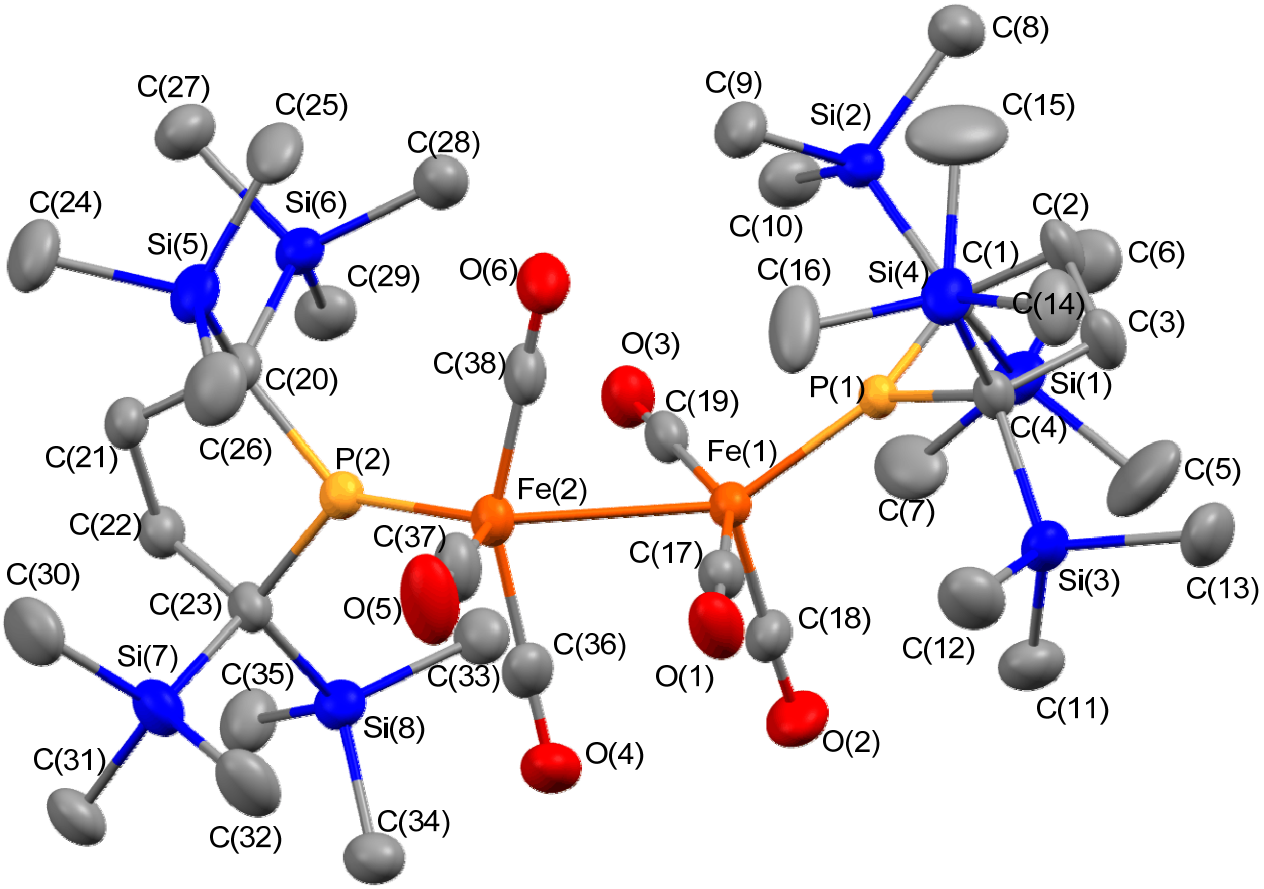


Figure S25. ORTEP drawing of **2** (50% probability of the thermal ellipsoids)

Table S7-1. Crystal data and structure refinement for **2**

Empirical Formula	$C_{38}H_{80}Fe_2O_6P_2Si_8$
Formula Weight	1031.37
Crystal Color, Habit	red, platelet
Crystal Dimensions	0.050 X 0.020 X 0.020 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 15.6926(12) Å b = 17.5019(12) Å c = 21.2042(17) Å β = 110.6328(14) ° V = 5450.2(7) Å^3
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.257 g/cm^3
F_{000}	2200.00
μ(MoKα)	8.037 cm^{-1}
Diffractometer	Saturn724
Radiation	MoKα (λ = 0.71075 Å) multi-layer mirror monochromated
Voltage, Current	50kV, 40mA
Temperature	123 K
Detector Aperture	72.8 x 72.8 mm
Data Images	720 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	-105.0 - 75.0°
Exposure Rate	80.0 sec./°
Detector Swing Angle	-14.85°
Detector Position	40.15 mm
Pixel Size	0.070 mm
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 52592 Unique: 12402 (R_{int} = 0.1118)
Corrections	Lorentz-polarization
Structure Solution	Direct Methods (SIR2008)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w (Fo^2 - Fc^2)^2
Least Squares Weights	$\omega = 1/ [\sigma^2(Fo^2) + (0.0722 \cdot P)^2 + 10.6473 \cdot P]$ where P = (Max(Fo^2,0) + 2Fc^2)/3
$2\theta_{max}$ cutoff	55.0°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	12402
No. Variables	505
Reflection/Parameter Ratio	24.56
Residuals: R1 (I>2.00σ(I))	0.0716
Residuals: R (All reflections)	0.0829
Residuals: wR2 (All reflections)	0.1846
Goodness of Fit Indicator	1.092
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	1.20 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.81 e$^-$/Å^3

Table S7-2. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Fe1	0.63753(4)	0.00563(3)	0.74022(3)	2.167(11)
Fe2	0.70293(4)	0.09218(3)	0.65975(3)	2.356(11)
P1	0.61672(6)	0.00639(5)	0.83246(4)	1.804(15)
P2	0.82505(6)	0.08855(5)	0.63974(5)	2.153(16)
Si1	0.68699(8)	-0.15121(6)	0.90833(6)	3.08(2)
Si2	0.80445(7)	-0.00180(6)	0.95545(5)	2.266(17)
Si3	0.39861(7)	0.00480(7)	0.78925(6)	2.74(2)
Si4	0.51607(8)	0.14115(6)	0.87359(6)	2.94(2)
Si5	0.91258(8)	0.25357(6)	0.68062(6)	2.93(2)
Si6	1.01251(7)	0.10723(6)	0.75867(6)	2.517(18)
Si7	0.78921(9)	0.09290(7)	0.48235(6)	2.99(2)
Si8	0.82148(8)	-0.06597(6)	0.55925(6)	2.601(19)
O1	0.4778(2)	0.0917(2)	0.65338(16)	3.97(6)
O2	0.5748(2)	-0.13849(18)	0.67055(18)	4.22(7)
O3	0.8298(2)	-0.04213(18)	0.78622(15)	3.36(5)
O4	0.5927(2)	-0.0219(2)	0.56309(16)	4.00(6)
O5	0.5784(2)	0.2070(2)	0.5779(2)	4.99(8)
O6	0.7448(2)	0.19350(17)	0.77764(17)	3.55(6)
C1	0.6822(2)	-0.0411(2)	0.91341(18)	2.07(5)
C2	0.6277(3)	-0.0221(3)	0.9604(2)	3.13(8)
C3	0.5273(3)	-0.0132(3)	0.9190(2)	3.06(7)
C4	0.5155(2)	0.0331(2)	0.85400(18)	2.16(6)
C5	0.5747(4)	-0.1980(3)	0.8922(4)	5.93(15)
C6	0.7594(4)	-0.1872(3)	0.9946(3)	4.30(10)
C7	0.7306(4)	-0.1901(3)	0.8438(3)	4.54(11)
C8	0.8317(3)	0.0043(3)	1.0487(2)	3.36(8)
C9	0.8975(3)	-0.0616(3)	0.9446(3)	3.53(8)
C10	0.8164(3)	0.0966(2)	0.9267(2)	3.49(8)
C11	0.4048(3)	-0.0822(3)	0.7410(3)	3.95(9)
C12	0.3372(3)	0.0810(3)	0.7281(3)	4.29(10)
C13	0.3218(3)	-0.0195(3)	0.8377(3)	4.35(10)
C14	0.4087(3)	0.1700(3)	0.8855(3)	4.06(10)
C15	0.6026(4)	0.1664(4)	0.9577(3)	6.41(17)
C16	0.5371(4)	0.2006(3)	0.8084(3)	4.90(12)
C17	0.5410(3)	0.0600(2)	0.6888(2)	2.81(7)
C18	0.5997(3)	-0.0814(2)	0.6968(2)	2.97(7)
C19	0.7554(3)	-0.0210(2)	0.76866(19)	2.55(6)
C20	0.9321(3)	0.1446(2)	0.6735(2)	2.43(6)
C21	0.9810(3)	0.1307(2)	0.6214(2)	2.65(6)
C22	0.9520(3)	0.0534(2)	0.5868(2)	2.64(6)
C23	0.8479(3)	0.0432(2)	0.56804(19)	2.40(6)
C24	0.9983(4)	0.3055(3)	0.6535(3)	4.18(10)
C25	0.9271(4)	0.2894(3)	0.7671(3)	3.88(9)
C26	0.7972(3)	0.2878(3)	0.6263(3)	4.24(10)
C27	1.1214(3)	0.1638(3)	0.7852(3)	3.71(8)
C28	0.9650(3)	0.1110(3)	0.8276(2)	3.36(8)
C29	1.0467(3)	0.0060(2)	0.7529(2)	3.33(8)
C30	0.8352(4)	0.1895(3)	0.4748(3)	4.54(10)
C31	0.8175(4)	0.0373(3)	0.4164(2)	3.74(8)
C32	0.6632(3)	0.1049(3)	0.4590(3)	4.24(10)
C33	0.8191(3)	-0.1112(2)	0.6380(2)	3.10(7)
C34	0.7135(3)	-0.0939(3)	0.4897(2)	3.53(8)
C35	0.9165(3)	-0.1150(3)	0.5399(3)	3.75(9)
C36	0.6392(3)	0.0202(3)	0.6017(2)	3.14(7)
C37	0.6261(3)	0.1618(3)	0.6113(3)	3.61(8)
C38	0.7317(3)	0.1508(2)	0.7335(2)	2.87(7)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S7-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe1	0.0290(3)	0.0258(3)	0.0295(3)	-0.00177(19)	0.0127(2)	0.0001(2)
Fe2	0.0304(3)	0.0278(3)	0.0339(3)	0.0025(2)	0.0145(2)	0.0051(2)

P1	0.0231(4)	0.0215(4)	0.0254(4)	0.0008(3)	0.0103(3)	0.0019(3)
P2	0.0291(5)	0.0229(4)	0.0312(5)	0.0015(3)	0.0123(4)	0.0020(4)
Si1	0.0421(6)	0.0233(5)	0.0453(7)	-0.0032(4)	0.0077(5)	0.0070(5)
Si2	0.0276(5)	0.0278(5)	0.0302(5)	-0.0006(4)	0.0096(4)	-0.0028(4)
Si3	0.0247(5)	0.0415(6)	0.0372(6)	-0.0018(4)	0.0102(4)	0.0024(5)
Si4	0.0372(6)	0.0302(5)	0.0509(7)	0.0032(4)	0.0241(5)	-0.0056(5)
Si5	0.0428(6)	0.0208(5)	0.0526(7)	-0.0015(4)	0.0227(5)	0.0022(5)
Si6	0.0304(5)	0.0291(5)	0.0354(6)	-0.0033(4)	0.0107(4)	-0.0011(4)
Si7	0.0468(7)	0.0367(6)	0.0323(6)	0.0080(5)	0.0168(5)	0.0070(5)
Si8	0.0356(6)	0.0252(5)	0.0376(6)	0.0013(4)	0.0124(5)	-0.0008(4)
O1	0.0349(17)	0.073(2)	0.0440(18)	0.0125(15)	0.0154(14)	0.0156(16)
O2	0.064(2)	0.0397(18)	0.060(2)	-0.0163(15)	0.0253(18)	-0.0153(15)
O3	0.0367(16)	0.0479(18)	0.0461(17)	0.0065(13)	0.0184(13)	0.0083(14)
O4	0.0463(19)	0.064(2)	0.0380(17)	-0.0115(16)	0.0106(14)	-0.0070(15)
O5	0.055(2)	0.068(2)	0.076(3)	0.0325(18)	0.0345(19)	0.041(2)
O6	0.0549(19)	0.0364(16)	0.0519(19)	-0.0043(14)	0.0292(16)	-0.0041(14)
C1	0.0281(17)	0.0248(16)	0.0271(17)	0.0012(13)	0.0116(14)	0.0040(13)
C2	0.037(2)	0.058(3)	0.029(2)	0.0092(19)	0.0182(17)	0.0124(18)
C3	0.032(2)	0.054(3)	0.033(2)	0.0093(18)	0.0147(17)	0.0159(18)
C4	0.0250(17)	0.0314(18)	0.0271(17)	0.0038(14)	0.0110(14)	0.0049(14)
C5	0.059(3)	0.044(3)	0.103(5)	-0.021(2)	0.005(3)	0.021(3)
C6	0.064(3)	0.032(2)	0.058(3)	0.005(2)	0.009(2)	0.013(2)
C7	0.083(4)	0.025(2)	0.061(3)	0.005(2)	0.022(3)	-0.002(2)
C8	0.039(2)	0.049(3)	0.037(2)	-0.0026(18)	0.0105(18)	-0.0015(19)
C9	0.030(2)	0.051(3)	0.051(3)	0.0044(18)	0.0115(19)	-0.008(2)
C10	0.052(3)	0.037(2)	0.049(3)	-0.0118(19)	0.023(2)	-0.0042(19)
C11	0.040(2)	0.055(3)	0.049(3)	-0.006(2)	0.008(2)	-0.010(2)
C12	0.042(3)	0.068(3)	0.047(3)	0.009(2)	0.008(2)	0.007(2)
C13	0.037(2)	0.070(3)	0.063(3)	-0.013(2)	0.023(2)	-0.002(3)
C14	0.057(3)	0.039(2)	0.074(3)	0.014(2)	0.042(3)	0.007(2)
C15	0.072(4)	0.069(4)	0.089(5)	0.018(3)	0.012(3)	-0.047(3)
C16	0.091(4)	0.025(2)	0.101(4)	0.002(2)	0.071(4)	0.002(2)
C17	0.035(2)	0.042(2)	0.034(2)	-0.0046(17)	0.0154(17)	-0.0006(17)
C18	0.036(2)	0.039(2)	0.041(2)	-0.0084(17)	0.0180(18)	-0.0023(18)
C19	0.041(2)	0.0284(18)	0.0312(19)	-0.0005(16)	0.0174(17)	0.0043(15)
C20	0.036(2)	0.0223(17)	0.036(2)	-0.0024(14)	0.0151(16)	0.0018(14)
C21	0.035(2)	0.0327(19)	0.037(2)	-0.0040(15)	0.0177(17)	0.0010(16)
C22	0.035(2)	0.033(2)	0.036(2)	0.0005(16)	0.0177(17)	-0.0006(16)
C23	0.039(2)	0.0265(17)	0.0297(18)	-0.0001(15)	0.0167(16)	0.0020(14)
C24	0.060(3)	0.031(2)	0.079(4)	-0.007(2)	0.038(3)	0.005(2)
C25	0.063(3)	0.028(2)	0.066(3)	-0.0113(19)	0.035(3)	-0.013(2)
C26	0.056(3)	0.030(2)	0.077(4)	0.010(2)	0.026(3)	0.014(2)
C27	0.037(2)	0.049(3)	0.054(3)	-0.0066(19)	0.014(2)	-0.006(2)
C28	0.040(2)	0.048(2)	0.038(2)	-0.0031(19)	0.0110(18)	0.0030(19)
C29	0.041(2)	0.037(2)	0.042(2)	0.0039(17)	0.0060(19)	0.0054(18)
C30	0.084(4)	0.045(3)	0.045(3)	0.003(3)	0.025(3)	0.016(2)
C31	0.058(3)	0.055(3)	0.031(2)	0.006(2)	0.018(2)	0.0016(19)
C32	0.051(3)	0.069(3)	0.040(3)	0.022(2)	0.015(2)	0.015(2)
C33	0.045(2)	0.0295(19)	0.044(2)	0.0029(17)	0.0161(19)	0.0031(17)
C34	0.049(3)	0.041(2)	0.040(2)	-0.0027(19)	0.011(2)	-0.0043(18)
C35	0.048(3)	0.034(2)	0.067(3)	0.0005(19)	0.029(2)	-0.001(2)
C36	0.028(2)	0.049(2)	0.041(2)	0.0002(18)	0.0118(17)	0.0034(19)
C37	0.045(2)	0.047(3)	0.053(3)	0.006(2)	0.028(2)	0.012(2)
C38	0.039(2)	0.032(2)	0.046(2)	0.0016(16)	0.0250(19)	0.0077(18)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S7-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Fe1	Fe2	2.7374(10)	Fe1	P1	2.0934(12)
Fe1	C17	1.796(4)	Fe1	C18	1.771(4)
Fe1	C19	1.794(4)	Fe2	P2	2.1047(13)
Fe2	C36	1.799(4)	Fe2	C37	1.766(4)
Fe2	C38	1.790(4)	P1	C1	1.858(3)
P1	C4	1.861(4)	P2	C20	1.857(4)

P2	C23	1.859(5)	Si1	C1	1.933(4)
Si1	C5	1.862(6)	Si1	C6	1.889(5)
Si1	C7	1.860(7)	Si2	C1	1.935(4)
Si2	C8	1.872(5)	Si2	C9	1.875(5)
Si2	C10	1.859(5)	Si3	C4	1.928(3)
Si3	C11	1.856(5)	Si3	C12	1.873(5)
Si3	C13	1.887(7)	Si4	C4	1.936(4)
Si4	C14	1.859(6)	Si4	C15	1.874(6)
Si4	C16	1.850(7)	Si5	C20	1.946(4)
Si5	C24	1.874(6)	Si5	C25	1.873(6)
Si5	C26	1.869(5)	Si6	C20	1.918(4)
Si6	C27	1.881(5)	Si6	C28	1.862(6)
Si6	C29	1.868(4)	Si7	C23	1.931(4)
Si7	C30	1.867(6)	Si7	C31	1.880(6)
Si7	C32	1.873(5)	Si8	C23	1.949(4)
Si8	C33	1.860(5)	Si8	C34	1.877(4)
Si8	C35	1.886(6)	O1	C17	1.154(5)
O2	C18	1.143(5)	O3	C19	1.154(5)
O4	C36	1.151(5)	O5	C37	1.147(6)
O6	C38	1.158(5)	C1	C2	1.561(7)
C2	C3	1.518(5)	C3	C4	1.552(6)
C20	C21	1.571(7)	C21	C22	1.531(5)
C22	C23	1.549(6)			

Table S7-5. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Fe2	Fe1	P1	142.66(4)	Fe2	Fe1	C17	75.51(16)
Fe2	Fe1	C18	106.41(17)	Fe2	Fe1	C19	77.57(14)
P1	Fe1	C17	100.83(16)	P1	Fe1	C18	110.93(17)
P1	Fe1	C19	99.76(14)	C17	Fe1	C18	94.81(18)
C17	Fe1	C19	153.0(2)	C18	Fe1	C19	93.89(18)
Fe1	Fe2	P2	132.61(4)	Fe1	Fe2	C36	78.40(16)
Fe1	Fe2	C37	114.53(19)	Fe1	Fe2	C38	78.87(15)
P2	Fe2	C36	99.60(16)	P2	Fe2	C37	112.76(19)
P2	Fe2	C38	103.10(15)	C36	Fe2	C37	89.1(2)
C36	Fe2	C38	155.2(2)	C37	Fe2	C38	91.3(2)
Fe1	P1	C1	130.01(14)	Fe1	P1	C4	131.20(11)
C1	P1	C4	97.32(18)	Fe2	P2	C20	132.13(15)
Fe2	P2	C23	129.04(12)	C20	P2	C23	97.55(19)
C1	Si1	C5	113.3(2)	C1	Si1	C6	107.49(18)
C1	Si1	C7	115.9(2)	C5	Si1	C6	103.8(3)
C5	Si1	C7	105.8(3)	C6	Si1	C7	109.7(2)
C1	Si2	C8	109.1(2)	C1	Si2	C9	115.68(18)
C1	Si2	C10	112.13(18)	C8	Si2	C9	105.3(2)
C8	Si2	C10	106.4(2)	C9	Si2	C10	107.7(2)
C4	Si3	C11	112.43(19)	C4	Si3	C12	116.0(2)
C4	Si3	C13	107.5(2)	C11	Si3	C12	108.4(2)
C11	Si3	C13	106.4(3)	C12	Si3	C13	105.4(3)
C4	Si4	C14	111.0(2)	C4	Si4	C15	112.4(2)
C4	Si4	C16	112.2(2)	C14	Si4	C15	101.2(3)
C14	Si4	C16	111.0(3)	C15	Si4	C16	108.5(3)
C20	Si5	C24	107.6(2)	C20	Si5	C25	115.86(19)
C20	Si5	C26	114.24(18)	C24	Si5	C25	106.5(2)
C24	Si5	C26	107.5(2)	C25	Si5	C26	104.7(3)
C20	Si6	C27	109.3(2)	C20	Si6	C28	114.5(2)
C20	Si6	C29	111.75(18)	C27	Si6	C28	108.6(2)
C27	Si6	C29	105.5(2)	C28	Si6	C29	106.8(2)
C23	Si7	C30	114.71(19)	C23	Si7	C31	107.9(2)
C23	Si7	C32	114.1(2)	C30	Si7	C31	101.9(3)
C30	Si7	C32	106.3(3)	C31	Si7	C32	111.4(2)
C23	Si8	C33	113.70(19)	C23	Si8	C34	115.68(18)
C23	Si8	C35	107.9(2)	C33	Si8	C34	107.2(2)
C33	Si8	C35	105.6(2)	C34	Si8	C35	105.9(2)
P1	C1	Si1	114.49(18)	P1	C1	Si2	113.7(2)
P1	C1	C2	104.2(2)	Si1	C1	Si2	109.17(17)
Si1	C1	C2	106.8(3)	Si2	C1	C2	107.9(2)
C1	C2	C3	110.0(3)	C2	C3	C4	110.0(4)
P1	C4	Si3	116.2(2)	P1	C4	Si4	111.0(2)
P1	C4	C3	104.0(3)	Si3	C4	Si4	109.57(17)

Si3	C4	C3	106.5(3)	Si4	C4	C3	109.2(3)
Fe1	C17	O1	176.3(4)	Fe1	C18	O2	177.8(5)
Fe1	C19	O3	176.4(3)	P2	C20	Si5	113.7(2)
P2	C20	Si6	112.9(2)	P2	C20	C21	104.4(2)
Si5	C20	Si6	109.26(18)	Si5	C20	C21	109.6(3)
Si6	C20	C21	106.7(2)	C20	C21	C22	109.7(3)
C21	C22	C23	109.5(3)	P2	C23	Si7	114.3(2)
P2	C23	Si8	113.6(2)	P2	C23	C22	103.3(2)
Si7	C23	Si8	109.68(17)	Si7	C23	C22	107.4(3)
Si8	C23	C22	107.9(3)	Fe2	C36	O4	174.5(4)
Fe2	C37	O5	176.9(5)	Fe2	C38	O6	173.9(3)

Table S7-6. Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Fe2	Fe1	P1	C1	-103.17(7)	Fe2	Fe1	P1	C4	93.84(8)
P1	Fe1	Fe2	P2	103.37(6)	P1	Fe1	Fe2	C36	-164.20(6)
P1	Fe1	Fe2	C37	-80.58(6)	P1	Fe1	Fe2	C38	5.74(6)
C17	Fe1	Fe2	P2	-167.71(14)	C17	Fe1	Fe2	C36	-75.28(14)
C17	Fe1	Fe2	C37	8.34(14)	C17	Fe1	Fe2	C38	94.66(14)
C18	Fe1	Fe2	P2	-76.90(14)	C18	Fe1	Fe2	C36	15.54(14)
C18	Fe1	Fe2	C37	99.15(14)	C18	Fe1	Fe2	C38	-174.53(14)
C19	Fe1	Fe2	P2	13.53(13)	C19	Fe1	Fe2	C36	105.96(13)
C19	Fe1	Fe2	C37	-170.42(13)	C19	Fe1	Fe2	C38	-84.10(13)
C17	Fe1	P1	C1	176.58(14)	C17	Fe1	P1	C4	13.59(15)
C18	Fe1	P1	C1	77.11(15)	C18	Fe1	P1	C4	-85.88(15)
C19	Fe1	P1	C1	-20.91(14)	C19	Fe1	P1	C4	176.10(14)
Fe1	Fe2	P2	C20	-98.96(7)	Fe1	Fe2	P2	C23	97.01(7)
C36	Fe2	P2	C20	178.02(15)	C36	Fe2	P2	C23	13.99(16)
C37	Fe2	P2	C20	84.93(18)	C37	Fe2	P2	C23	-79.09(18)
C38	Fe2	P2	C20	-12.14(15)	C38	Fe2	P2	C23	-176.16(14)
Fe1	P1	C1	Si1	-60.1(3)	Fe1	P1	C1	Si2	66.3(2)
Fe1	P1	C1	C2	-176.46(8)	Fe1	P1	C4	Si3	37.6(3)
Fe1	P1	C4	Si4	-88.40(18)	Fe1	P1	C4	C3	154.28(10)
C1	P1	C4	Si3	-129.3(2)	C1	P1	C4	Si4	104.65(18)
C1	P1	C4	C3	-12.7(2)	C4	P1	C1	Si1	107.0(2)
C4	P1	C1	Si2	-126.5(2)	C4	P1	C1	C2	-9.3(2)
Fe2	P2	C20	Si5	-43.3(3)	Fe2	P2	C20	Si6	81.9(2)
Fe2	P2	C20	C21	-162.67(9)	Fe2	P2	C23	Si7	69.4(2)
Fe2	P2	C23	Si8	-57.5(2)	Fe2	P2	C23	C22	-174.21(9)
C20	P2	C23	Si7	-98.7(2)	C20	P2	C23	Si8	134.35(19)
C20	P2	C23	C22	17.7(2)	C23	P2	C20	Si5	124.2(2)
C23	P2	C20	Si6	-110.6(2)	C23	P2	C20	C21	4.9(2)
C5	Si1	C1	P1	-67.7(4)	C5	Si1	C1	Si2	163.5(3)
C5	Si1	C1	C2	47.1(3)	C6	Si1	C1	P1	178.1(3)
C6	Si1	C1	Si2	49.4(3)	C6	Si1	C1	C2	-67.0(3)
C7	Si1	C1	P1	55.0(3)	C7	Si1	C1	Si2	-73.8(3)
C7	Si1	C1	C2	169.8(2)	C8	Si2	C1	P1	140.2(2)
C8	Si2	C1	Si1	-90.6(2)	C8	Si2	C1	C2	25.1(3)
C9	Si2	C1	P1	-101.4(3)	C9	Si2	C1	Si1	27.8(3)
C9	Si2	C1	C2	143.5(2)	C10	Si2	C1	P1	22.6(3)
C10	Si2	C1	Si1	151.8(2)	C10	Si2	C1	C2	-92.5(3)
C11	Si3	C4	P1	29.2(3)	C11	Si3	C4	Si4	155.9(2)
C11	Si3	C4	C3	-86.1(3)	C12	Si3	C4	P1	-96.5(3)
C12	Si3	C4	Si4	30.2(3)	C12	Si3	C4	C3	148.3(3)
C13	Si3	C4	P1	145.9(2)	C13	Si3	C4	Si4	-87.4(3)
C13	Si3	C4	C3	30.7(3)	C14	Si4	C4	P1	173.5(2)
C14	Si4	C4	Si3	43.9(3)	C14	Si4	C4	C3	-72.4(3)
C15	Si4	C4	P1	-73.9(3)	C15	Si4	C4	Si3	156.5(3)
C15	Si4	C4	C3	40.2(4)	C16	Si4	C4	P1	48.7(3)
C16	Si4	C4	Si3	-80.8(3)	C16	Si4	C4	C3	162.8(2)
C24	Si5	C20	P2	-139.8(2)	C24	Si5	C20	Si6	93.1(3)
C24	Si5	C20	C21	-23.4(3)	C25	Si5	C20	P2	101.2(3)
C25	Si5	C20	Si6	-25.9(3)	C25	Si5	C20	C21	-142.4(2)
C26	Si5	C20	P2	-20.6(4)	C26	Si5	C20	Si6	-147.7(3)
C26	Si5	C20	C21	95.8(3)	C27	Si6	C20	P2	176.3(2)
C27	Si6	C20	Si5	-56.1(3)	C27	Si6	C20	C21	62.3(3)
C28	Si6	C20	P2	-61.6(3)	C28	Si6	C20	Si5	65.9(3)
C28	Si6	C20	C21	-175.7(2)	C29	Si6	C20	P2	60.0(3)

C29	Si6	C20	Si5	-172.5(2)	C29	Si6	C20	C21	-54.1(3)
C30	Si7	C23	P2	69.0(3)	C30	Si7	C23	Si8	-162.1(3)
C30	Si7	C23	C22	-45.0(3)	C31	Si7	C23	P2	-178.3(2)
C31	Si7	C23	Si8	-49.4(3)	C31	Si7	C23	C22	67.7(3)
C32	Si7	C23	P2	-54.0(3)	C32	Si7	C23	Si8	75.0(3)
C32	Si7	C23	C22	-168.0(2)	C33	Si8	C23	P2	-20.8(3)
C33	Si8	C23	Si7	-150.1(2)	C33	Si8	C23	C22	93.2(3)
C34	Si8	C23	P2	104.0(3)	C34	Si8	C23	Si7	-25.3(3)
C34	Si8	C23	C22	-142.1(2)	C35	Si8	C23	P2	-137.6(2)
C35	Si8	C23	Si7	93.1(2)	C35	Si8	C23	C22	-23.7(3)
P1	C1	C2	C3	30.0(4)	Si1	C1	C2	C3	-91.5(3)
Si2	C1	C2	C3	151.2(2)	C1	C2	C3	C4	-42.4(5)
C2	C3	C4	P1	32.5(4)	C2	C3	C4	Si3	155.8(3)
C2	C3	C4	Si4	-86.0(4)	P2	C20	C21	C22	-27.2(3)
Si5	C20	C21	C22	-149.30(19)	Si6	C20	C21	C22	92.5(2)
C20	C21	C22	C23	43.2(4)	C21	C22	C23	P2	-36.6(4)
C21	C22	C23	Si7	84.6(3)	C21	C22	C23	Si8	-157.2(3)

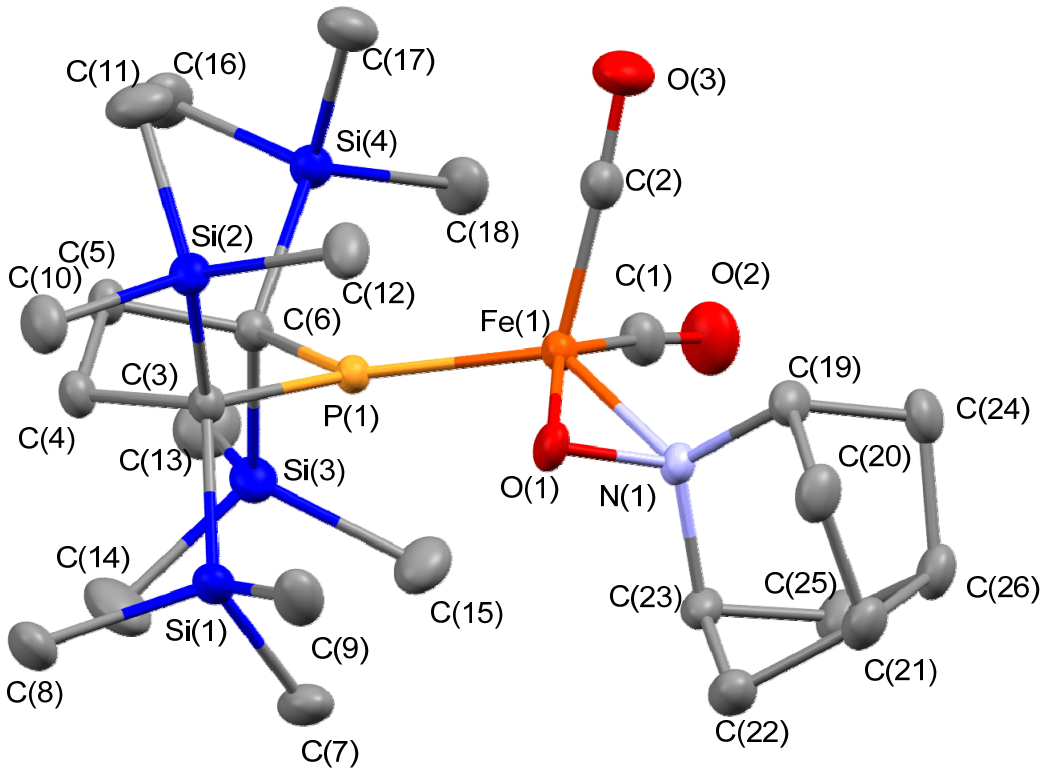


Figure S26. ORTEP drawing of **4** (50% probability of the thermal ellipsoids)

Table S8-1. Crystal data and structure refinement for **4**

Empirical Formula	$C_{26}H_{52}FeNO_3PSi_4$
Formula Weight	625.86
Crystal Color, Habit	palegreen, platelet
Crystal Dimensions	0.100 X 0.080 X 0.050 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 9.4542(8) Å b = 11.3877(10) Å c = 16.3807(15) Å α = 75.408(5) ° β = 87.846(7) ° γ = 79.154(6) ° V = 1676.1(3) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.240 g/cm^3
F_{000}	672.00
μ(MoKα)	6.662 cm^{-1}
Diffractometer	Saturn724
Radiation	MoKα (λ = 0.71075 Å) multi-layer mirror monochromated
Voltage, Current	50kV, 40mA
Temperature	123 K
Detector Aperture	72.8 x 72.8 mm
Data Images	1080 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	-105.0 - 75.0°
Exposure Rate	32.0 sec./°
Detector Swing Angle	-14.70°
Detector Position	40.10 mm
Pixel Size	0.070 mm
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 24288 Unique: 7658 (R_{int} = 0.0235)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.851 - 0.967)
Structure Solution	Direct Methods (SIR2008)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w (Fo^2 - Fc^2)^2
Least Squares Weights	$\omega = 1/ [\sigma^2(Fo^2) + (0.0455 \cdot P)^2 + 0.9471 \cdot P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	55.0°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	7658
No. Variables	325
Reflection/Parameter Ratio	23.56
Residuals: R1 (I>2.00σ(I))	0.0318
Residuals: R (All reflections)	0.0328
Residuals: wR2 (All reflections)	0.0855
Goodness of Fit Indicator	1.069
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.46 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.45 e$^-$/Å^3

Table S8-2. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Fe1	0.29167(2)	-0.001720(17)	0.292965(12)	1.258(5)
P1	0.20257(4)	0.18630(3)	0.23918(2)	1.163(6)
Si1	0.36415(4)	0.27691(4)	0.07178(3)	1.547(7)
Si2	0.07636(4)	0.17867(4)	0.06396(2)	1.431(7)
Si3	0.20217(5)	0.40374(4)	0.32197(3)	1.683(7)
Si4	-0.05414(4)	0.25412(4)	0.36025(2)	1.517(7)
O1	0.40689(11)	-0.03521(10)	0.19880(6)	1.561(17)
O2	0.30749(16)	-0.01942(13)	0.47266(8)	3.08(2)
O3	0.07799(13)	-0.16114(12)	0.31119(9)	2.87(2)
N1	0.47381(12)	-0.10214(11)	0.27445(7)	1.282(17)
C1	0.29260(17)	-0.00579(14)	0.40099(10)	1.94(2)
C2	0.16602(17)	-0.10172(14)	0.30349(10)	1.92(2)
C3	0.18013(14)	0.26033(12)	0.12445(8)	1.23(2)
C4	0.09146(16)	0.39269(13)	0.11973(9)	1.49(2)
C5	-0.00158(15)	0.39199(13)	0.19848(9)	1.49(2)
C6	0.08590(15)	0.31063(12)	0.27849(9)	1.29(2)
C7	0.50149(17)	0.28705(17)	0.14797(11)	2.30(3)
C8	0.33835(18)	0.42468(15)	-0.01431(10)	2.27(3)
C9	0.44820(19)	0.14934(16)	0.02336(10)	2.28(3)
C10	0.07256(19)	0.25885(15)	-0.05165(10)	2.12(3)
C11	-0.11714(17)	0.19451(18)	0.09453(12)	2.49(3)
C12	0.14916(19)	0.01096(14)	0.07665(10)	2.10(3)
C13	0.0996(2)	0.49375(18)	0.39356(13)	2.97(3)
C14	0.2624(3)	0.52835(18)	0.23730(13)	3.24(4)
C15	0.36279(19)	0.30283(17)	0.38228(12)	2.57(3)
C16	-0.20532(18)	0.38722(16)	0.36026(12)	2.51(3)
C17	-0.14235(18)	0.13730(16)	0.33055(11)	2.30(3)
C18	0.01604(19)	0.18980(17)	0.47072(10)	2.46(3)
C19	0.48657(16)	-0.23851(13)	0.28429(9)	1.59(2)
C20	0.60589(17)	-0.28277(15)	0.22754(10)	2.01(3)
C21	0.73649(17)	-0.25202(15)	0.26566(10)	2.02(3)
C22	0.72857(17)	-0.11198(15)	0.23060(10)	2.09(3)
C23	0.61294(15)	-0.06291(13)	0.28748(9)	1.59(2)
C24	0.55011(18)	-0.30574(14)	0.37134(10)	1.97(2)
C25	0.67368(17)	-0.13552(15)	0.37431(10)	1.95(2)
C26	0.69900(17)	-0.26774(15)	0.36295(10)	1.97(2)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S8-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe1	0.01673(11)	0.01323(10)	0.01645(11)	-0.00078(7)	-0.00029(7)	-0.00254(8)
P1	0.01487(16)	0.01270(16)	0.01569(16)	-0.00112(12)	-0.00006(12)	-0.00285(12)
Si1	0.01815(19)	0.01960(19)	0.01925(19)	-0.00364(15)	0.00332(14)	-0.00196(15)
Si2	0.01924(19)	0.01772(19)	0.01783(18)	-0.00287(14)	-0.00168(14)	-0.00534(15)
Si3	0.0245(2)	0.01868(19)	0.0231(2)	-0.00532(16)	-0.00122(16)	-0.00817(16)
Si4	0.01850(19)	0.01891(19)	0.01882(19)	-0.00132(15)	0.00288(14)	-0.00411(15)
O1	0.0195(5)	0.0210(5)	0.0151(5)	0.0030(4)	-0.0037(4)	-0.0021(4)
O2	0.0513(8)	0.0422(7)	0.0205(6)	-0.0005(6)	0.0011(5)	-0.0081(5)
O3	0.0280(6)	0.0309(6)	0.0518(8)	-0.0131(5)	0.0024(6)	-0.0078(6)
N1	0.0167(5)	0.0147(5)	0.0160(5)	-0.0005(4)	-0.0032(4)	-0.0029(4)
C1	0.0270(8)	0.0205(7)	0.0240(7)	-0.0002(6)	0.0024(6)	-0.0048(6)
C2	0.0226(7)	0.0199(7)	0.0272(8)	0.0003(6)	-0.0005(6)	-0.0033(6)
C3	0.0165(6)	0.0139(6)	0.0153(6)	-0.0015(5)	0.0002(5)	-0.0029(5)
C4	0.0222(7)	0.0146(6)	0.0178(6)	-0.0010(5)	-0.0003(5)	-0.0022(5)
C5	0.0194(7)	0.0155(6)	0.0194(7)	0.0007(5)	-0.0006(5)	-0.0030(5)
C6	0.0175(6)	0.0139(6)	0.0175(6)	-0.0012(5)	0.0004(5)	-0.0047(5)
C7	0.0207(7)	0.0369(9)	0.0296(8)	-0.0106(6)	0.0014(6)	-0.0040(7)
C8	0.0292(8)	0.0261(8)	0.0273(8)	-0.0082(6)	0.0045(6)	0.0017(6)
C9	0.0305(8)	0.0277(8)	0.0245(8)	0.0001(6)	0.0091(6)	-0.0044(6)
C10	0.0351(9)	0.0251(8)	0.0193(7)	-0.0037(6)	-0.0047(6)	-0.0042(6)
C11	0.0213(7)	0.0440(10)	0.0362(9)	-0.0101(7)	0.0014(6)	-0.0197(8)
C12	0.0338(8)	0.0192(7)	0.0283(8)	-0.0038(6)	-0.0093(6)	-0.0078(6)

C13	0.0408(10)	0.0361(10)	0.0435(10)	-0.0040(8)	0.0008(8)	-0.0263(8)
C14	0.0570(12)	0.0343(10)	0.0386(10)	-0.0276(9)	-0.0012(9)	-0.0075(8)
C15	0.0297(8)	0.0334(9)	0.0380(9)	-0.0037(7)	-0.0102(7)	-0.0150(7)
C16	0.0256(8)	0.0295(8)	0.0370(9)	0.0026(7)	0.0078(7)	-0.0089(7)
C17	0.0265(8)	0.0294(8)	0.0345(9)	-0.0112(6)	0.0089(7)	-0.0103(7)
C18	0.0314(9)	0.0381(9)	0.0199(7)	-0.0033(7)	0.0023(6)	-0.0024(7)
C19	0.0211(7)	0.0141(6)	0.0255(7)	-0.0014(5)	-0.0016(6)	-0.0067(5)
C20	0.0287(8)	0.0220(7)	0.0245(7)	0.0043(6)	-0.0015(6)	-0.0101(6)
C21	0.0207(7)	0.0254(8)	0.0275(8)	0.0040(6)	-0.0008(6)	-0.0066(6)
C22	0.0196(7)	0.0282(8)	0.0282(8)	-0.0021(6)	0.0014(6)	-0.0027(6)
C23	0.0177(7)	0.0179(7)	0.0246(7)	-0.0033(5)	-0.0043(5)	-0.0044(6)
C24	0.0303(8)	0.0160(7)	0.0249(7)	0.0004(6)	-0.0003(6)	-0.0015(6)
C25	0.0249(7)	0.0242(7)	0.0246(7)	0.0002(6)	-0.0089(6)	-0.0072(6)
C26	0.0244(7)	0.0225(7)	0.0241(7)	0.0041(6)	-0.0059(6)	-0.0038(6)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S8-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Fe1	P1	2.1205(4)	Fe1	O1	1.9300(11)
Fe1	N1	1.9389(11)	Fe1	C1	1.7587(17)
Fe1	C2	1.7699(18)	P1	C3	1.8580(13)
P1	C6	1.8585(15)	Si1	C3	1.9327(14)
Si1	C7	1.8729(19)	Si1	C8	1.8856(15)
Si1	C9	1.8627(19)	Si2	C3	1.9209(16)
Si2	C10	1.8822(15)	Si2	C11	1.8661(17)
Si2	C12	1.8656(16)	Si3	C6	1.9282(17)
Si3	C13	1.874(2)	Si3	C14	1.875(2)
Si3	C15	1.8672(17)	Si4	C6	1.9271(15)
Si4	C16	1.8775(17)	Si4	C17	1.864(2)
Si4	C18	1.8684(16)	O1	N1	1.3851(14)
O2	C1	1.155(2)	O3	C2	1.152(2)
N1	C19	1.502(2)	N1	C23	1.505(2)
C3	C4	1.5656(19)	C4	C5	1.533(2)
C5	C6	1.5625(18)	C19	C20	1.528(2)
C19	C24	1.524(2)	C20	C21	1.539(3)
C21	C22	1.541(2)	C21	C26	1.592(2)
C22	C23	1.527(2)	C23	C25	1.525(2)
C24	C26	1.540(2)	C25	C26	1.537(3)

Table S8-5. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
P1	Fe1	O1	98.58(3)	P1	Fe1	N1	131.31(4)
P1	Fe1	C1	101.54(5)	P1	Fe1	C2	113.69(5)
O1	Fe1	N1	41.95(4)	O1	Fe1	C1	145.35(6)
O1	Fe1	C2	103.06(7)	N1	Fe1	C1	104.91(6)
N1	Fe1	C2	104.29(6)	C1	Fe1	C2	94.29(8)
Fe1	P1	C3	125.47(5)	Fe1	P1	C6	134.73(4)
C3	P1	C6	97.90(6)	C3	Si1	C7	112.10(7)
C3	Si1	C8	108.15(6)	C3	Si1	C9	115.42(8)
C7	Si1	C8	107.62(8)	C7	Si1	C9	105.71(8)
C8	Si1	C9	107.51(7)	C3	Si2	C10	109.17(7)
C3	Si2	C11	111.35(8)	C3	Si2	C12	115.13(7)
C10	Si2	C11	104.42(8)	C10	Si2	C12	108.62(8)
C11	Si2	C12	107.58(9)	C6	Si3	C13	112.68(8)
C6	Si3	C14	112.65(9)	C6	Si3	C15	112.17(8)
C13	Si3	C14	102.11(9)	C13	Si3	C15	107.35(9)
C14	Si3	C15	109.29(9)	C6	Si4	C16	108.57(7)
C6	Si4	C17	112.13(7)	C6	Si4	C18	115.00(7)
C16	Si4	C17	104.29(8)	C16	Si4	C18	107.90(8)
C17	Si4	C18	108.34(8)	Fe1	O1	N1	69.37(6)
Fe1	N1	O1	68.68(6)	Fe1	N1	C19	120.69(9)
Fe1	N1	C23	119.89(10)	O1	N1	C19	111.16(12)
O1	N1	C23	112.14(10)	C19	N1	C23	114.32(10)

Fe1	C1	O2	171.85(14)	Fe1	C2	O3	175.90(14)
P1	C3	Si1	111.08(7)	P1	C3	Si2	114.41(7)
P1	C3	C4	104.54(9)	Si1	C3	Si2	109.59(7)
Si1	C3	C4	108.35(9)	Si2	C3	C4	108.58(9)
C3	C4	C5	110.21(10)	C4	C5	C6	109.91(11)
P1	C6	Si3	110.30(7)	P1	C6	Si4	114.38(7)
P1	C6	C5	103.64(10)	Si3	C6	Si4	110.79(8)
Si3	C6	C5	111.29(10)	Si4	C6	C5	106.17(9)
N1	C19	C20	109.70(12)	N1	C19	C24	108.32(13)
C20	C19	C24	100.99(11)	C19	C20	C21	100.17(14)
C20	C21	C22	105.77(12)	C20	C21	C26	104.37(13)
C22	C21	C26	104.36(14)	C21	C22	C23	100.19(12)
N1	C23	C22	109.60(13)	N1	C23	C25	108.37(11)
C22	C23	C25	100.73(11)	C19	C24	C26	100.28(12)
C23	C25	C26	100.47(14)	C21	C26	C24	104.30(14)
C21	C26	C25	104.17(12)	C24	C26	C25	105.88(13)

Table S8-6. Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
P1	Fe1	O1	N1	146.18(4)	O1	Fe1	P1	C3	24.26(4)
O1	Fe1	P1	C6	-175.10(4)	P1	Fe1	N1	O1	-47.12(8)
P1	Fe1	N1	C19	-149.77(5)	P1	Fe1	N1	C23	56.90(9)
N1	Fe1	P1	C3	53.95(6)	N1	Fe1	P1	C6	-145.41(6)
C1	Fe1	P1	C3	175.89(6)	C1	Fe1	P1	C6	-23.47(6)
C2	Fe1	P1	C3	-84.15(7)	C2	Fe1	P1	C6	76.49(7)
O1	Fe1	N1	O1	-0.00(5)	O1	Fe1	N1	C19	-102.65(11)
O1	Fe1	N1	C23	104.02(10)	N1	Fe1	O1	N1	-0.00(6)
C1	Fe1	O1	N1	21.13(13)	C2	Fe1	O1	N1	-96.95(6)
C1	Fe1	N1	O1	-167.75(7)	C1	Fe1	N1	C19	89.60(9)
C1	Fe1	N1	C23	-63.74(9)	C2	Fe1	N1	O1	93.75(7)
C2	Fe1	N1	C19	-8.90(10)	C2	Fe1	N1	C23	-162.23(8)
Fe1	P1	C3	Si1	-70.83(9)	Fe1	P1	C3	Si2	53.89(8)
Fe1	P1	C3	C4	172.52(4)	Fe1	P1	C6	Si3	91.75(8)
Fe1	P1	C6	Si4	-33.92(12)	Fe1	P1	C6	C5	-149.04(4)
C3	P1	C6	Si3	-104.07(7)	C3	P1	C6	Si4	130.26(8)
C3	P1	C6	C5	15.14(9)	C6	P1	C3	Si1	122.93(8)
C6	P1	C3	Si2	-112.36(8)	C6	P1	C3	C4	6.27(9)
C7	Si1	C3	P1	-26.85(10)	C7	Si1	C3	Si2	-154.24(7)
C7	Si1	C3	C4	87.44(9)	C8	Si1	C3	P1	-145.32(8)
C8	Si1	C3	Si2	87.29(8)	C8	Si1	C3	C4	-31.03(10)
C9	Si1	C3	P1	94.26(9)	C9	Si1	C3	Si2	-33.13(8)
C9	Si1	C3	C4	-151.45(8)	C10	Si2	C3	P1	-176.65(7)
C10	Si2	C3	Si1	-51.15(8)	C10	Si2	C3	C4	67.03(9)
C11	Si2	C3	P1	68.58(9)	C11	Si2	C3	Si1	-165.92(7)
C11	Si2	C3	C4	-47.74(9)	C12	Si2	C3	P1	-54.20(9)
C12	Si2	C3	Si1	71.29(8)	C12	Si2	C3	C4	-170.53(7)
C13	Si3	C6	P1	-161.09(7)	C13	Si3	C6	Si4	-33.42(9)
C13	Si3	C6	C5	84.46(10)	C14	Si3	C6	P1	84.02(9)
C14	Si3	C6	Si4	-148.30(8)	C14	Si3	C6	C5	-30.43(11)
C15	Si3	C6	P1	-39.81(10)	C15	Si3	C6	Si4	87.87(9)
C15	Si3	C6	C5	-154.25(9)	C16	Si4	C6	P1	-157.32(9)
C16	Si4	C6	Si3	77.26(9)	C16	Si4	C6	C5	-43.69(11)
C17	Si4	C6	P1	-42.63(10)	C17	Si4	C6	Si3	-168.05(6)
C17	Si4	C6	C5	71.00(9)	C18	Si4	C6	P1	81.72(11)
C18	Si4	C6	Si3	-43.69(10)	C18	Si4	C6	C5	-164.65(9)
Fe1	O1	N1	Fe1	0.000(11)	Fe1	O1	N1	C19	115.88(8)
Fe1	O1	N1	C23	-114.76(9)	Fe1	N1	C19	C20	152.05(7)
Fe1	N1	C19	C24	-98.57(10)	Fe1	N1	C23	C22	-151.82(7)
Fe1	N1	C23	C25	99.12(9)	O1	N1	C19	C20	74.97(12)
O1	N1	C19	C24	-175.65(9)	O1	N1	C23	C22	-74.46(12)
O1	N1	C23	C25	176.48(9)	C19	N1	C23	C22	53.24(13)
C19	N1	C23	C25	-55.82(14)	C23	N1	C19	C20	-53.23(14)
C23	N1	C19	C24	56.15(13)	P1	C3	C4	C5	-27.19(13)
Si1	C3	C4	C5	-145.71(9)	Si2	C3	C4	C5	95.33(10)
C3	C4	C5	C6	41.11(16)	C4	C5	C6	P1	-33.54(14)
C4	C5	C6	Si3	84.99(13)	C4	C5	C6	Si4	-154.38(11)
N1	C19	C20	C21	62.04(12)	N1	C19	C24	C26	-63.15(13)
C20	C19	C24	C26	52.07(14)	C24	C19	C20	C21	-52.14(13)

C19	C20	C21	C22	-78.51(12)	C19	C20	C21	C26	31.27(12)
C20	C21	C22	C23	78.60(14)	C20	C21	C26	C24	-0.14(14)
C20	C21	C26	C25	-110.96(12)	C22	C21	C26	C24	110.67(12)
C22	C21	C26	C25	-0.15(14)	C26	C21	C22	C23	-31.18(14)
C21	C22	C23	N1	-62.01(13)	C21	C22	C23	C25	52.07(14)
N1	C23	C25	C26	62.65(13)	C22	C23	C25	C26	-52.35(13)
C19	C24	C26	C21	-31.15(13)	C19	C24	C26	C25	78.43(13)
C23	C25	C26	C21	31.50(13)	C23	C25	C26	C24	-78.17(12)

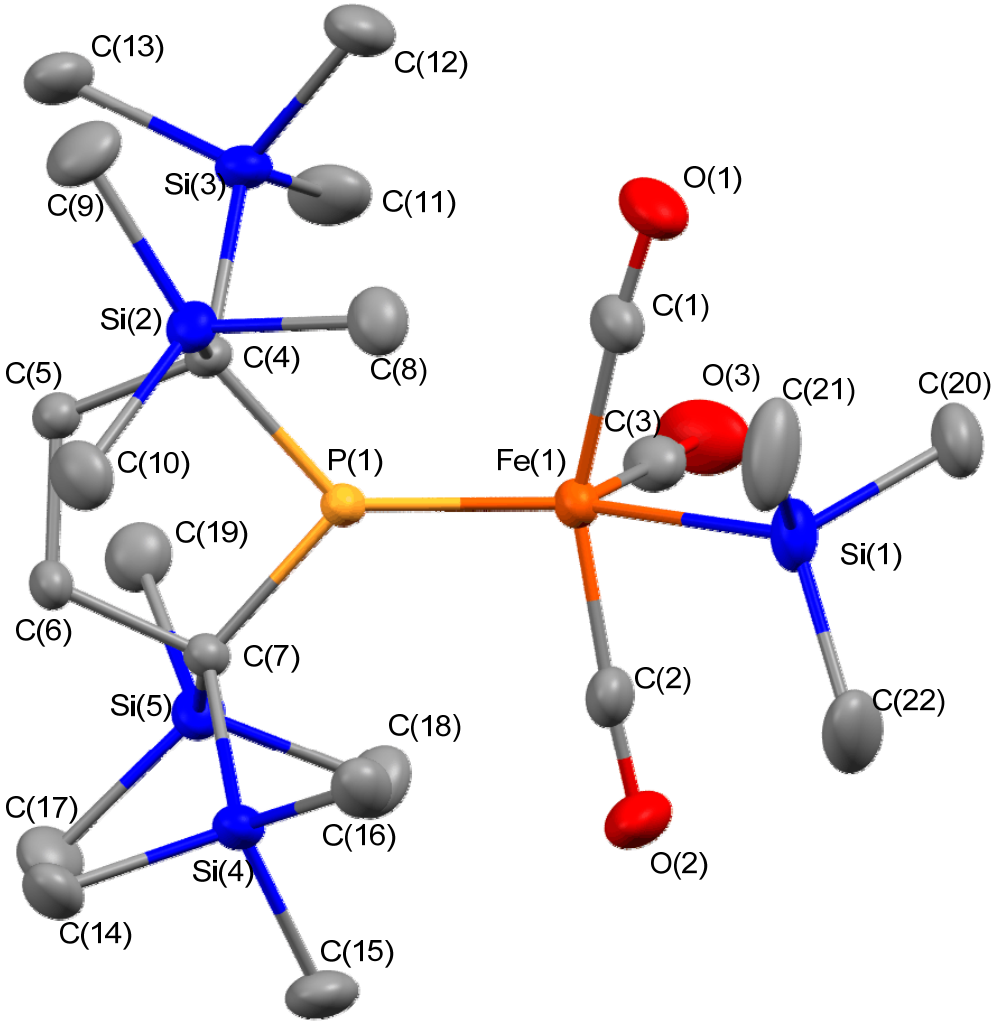


Figure S27. ORTEP drawing of **5** (50% probability of the thermal ellipsoids)

Table S9-1. Crystal data and structure refinement for **5**

Empirical Formula	$C_{22}H_{49}FeO_3PSi_5$
Formula Weight	588.88
Crystal Color, Habit	palegreen, platelet
Crystal Dimensions	0.050 X 0.020 X 0.015 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 11.1846(9) Å b = 11.2283(10) Å c = 14.972(2) Å α = 83.758(15) ° β = 76.946(13) ° γ = 60.902(8) ° V = 1600.5(3) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.222 g/cm^3
F_{000}	632.00
μ(MoKα)	7.279 cm^{-1}
Diffractometer	Saturn724
Radiation	MoKα (λ = 0.71075 Å) multi-layer mirror monochromated
Voltage, Current	50kV, 40mA
Temperature	123 K
Detector Aperture	72.8 x 72.8 mm
Data Images	720 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	-105.0 - 75.0°
Exposure Rate	48.0 sec./°
Detector Swing Angle	-14.83°
Detector Position	40.15 mm
Pixel Size	0.070 mm
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 15690 Unique: 7170 (R_{int} = 0.0405)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.888 - 0.989)
Structure Solution	Direct Methods (SIR2008)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w (Fo^2 - Fc^2)^2
Least Squares Weights	$\omega = 1/ [\sigma^2(Fo^2) + (0.0434 \cdot P)^2 + 1.0913 \cdot P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	54.9°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	7170
No. Variables	289
Reflection/Parameter Ratio	24.81
Residuals: R1 (I>2.00σ(I))	0.0444
Residuals: R (All reflections)	0.0561
Residuals: wR2 (All reflections)	0.1048
Goodness of Fit Indicator	1.072
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.47 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.42 e$^-$/Å^3

Table S9-2. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Fe1	0.32634(3)	0.06317(3)	0.82748(2)	1.669(7)
P1	0.18346(6)	0.21841(6)	0.75550(4)	1.401(10)
Si1	0.52825(8)	-0.16076(7)	0.79686(5)	2.437(13)
Si2	0.04508(7)	0.14433(7)	0.62541(4)	1.769(11)
Si3	-0.10598(7)	0.21646(7)	0.83390(5)	1.919(12)
Si4	0.34403(7)	0.34095(7)	0.60729(5)	1.895(12)
Si5	0.15623(7)	0.50191(7)	0.79220(5)	1.944(12)
O1	0.2205(2)	-0.1325(2)	0.85931(15)	3.38(4)
O2	0.5546(2)	0.1310(2)	0.78977(16)	3.62(4)
O3	0.2874(3)	0.0995(3)	1.02420(14)	4.26(5)
C1	0.2586(3)	-0.0527(3)	0.84385(17)	2.30(4)
C2	0.4639(3)	0.1054(3)	0.80123(18)	2.37(4)
C3	0.3038(3)	0.0839(3)	0.94691(19)	2.50(4)
C4	0.0168(2)	0.2467(2)	0.73049(15)	1.49(3)
C5	-0.0598(2)	0.4029(2)	0.70883(16)	1.69(4)
C6	0.0474(2)	0.4466(2)	0.65889(16)	1.72(4)
C7	0.1813(2)	0.3760(2)	0.70272(15)	1.52(3)
C8	0.1854(3)	-0.0355(3)	0.62773(18)	2.53(5)
C9	-0.1220(3)	0.1500(3)	0.6162(2)	3.04(5)
C10	0.0933(3)	0.2176(3)	0.51323(17)	2.68(5)
C11	-0.0844(3)	0.2569(3)	0.94472(19)	3.34(5)
C12	-0.0905(3)	0.0422(3)	0.8431(2)	3.08(5)
C13	-0.2908(3)	0.3388(3)	0.8241(2)	2.81(5)
C14	0.2840(3)	0.4562(3)	0.50836(18)	2.74(5)
C15	0.4777(3)	0.3763(3)	0.6367(2)	3.09(5)
C16	0.4421(3)	0.1608(3)	0.56517(18)	2.53(5)
C17	0.1471(3)	0.6595(3)	0.7299(2)	2.97(5)
C18	0.2928(3)	0.4353(3)	0.8634(2)	3.05(5)
C19	-0.0134(3)	0.5604(3)	0.87518(18)	2.67(5)
C20	0.5496(3)	-0.2597(3)	0.9066(2)	3.05(5)
C21	0.5145(4)	-0.2633(3)	0.7126(2)	4.47(8)
C22	0.7003(3)	-0.1652(3)	0.7461(2)	3.91(6)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S9-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe1	0.02140(17)	0.01956(17)	0.02341(18)	-0.00974(14)	-0.00766(13)	0.00287(13)
P1	0.0170(3)	0.0162(3)	0.0210(3)	-0.0086(2)	-0.0047(2)	0.0014(2)
Si1	0.0309(4)	0.0240(4)	0.0286(4)	-0.0041(3)	-0.0113(3)	0.0011(3)
Si2	0.0223(3)	0.0231(3)	0.0242(3)	-0.0112(3)	-0.0075(3)	-0.0014(3)
Si3	0.0218(3)	0.0267(3)	0.0269(3)	-0.0149(3)	-0.0020(3)	0.0011(3)
Si4	0.0199(3)	0.0230(3)	0.0282(4)	-0.0113(3)	-0.0021(3)	0.0035(3)
Si5	0.0250(3)	0.0189(3)	0.0318(4)	-0.0106(3)	-0.0079(3)	-0.0021(3)
O1	0.0549(13)	0.0372(11)	0.0523(13)	-0.0325(11)	-0.0206(10)	0.0127(9)
O2	0.0278(10)	0.0418(12)	0.0727(16)	-0.0198(9)	-0.0149(10)	0.0078(11)
O3	0.0758(17)	0.0801(17)	0.0274(11)	-0.0532(15)	-0.0109(11)	-0.0018(11)
C1	0.0337(13)	0.0279(13)	0.0292(13)	-0.0161(11)	-0.0123(11)	0.0057(10)
C2	0.0236(12)	0.0255(13)	0.0356(14)	-0.0072(10)	-0.0093(11)	0.0050(11)
C3	0.0338(14)	0.0359(14)	0.0326(14)	-0.0212(12)	-0.0099(11)	0.0014(11)
C4	0.0164(10)	0.0193(11)	0.0228(11)	-0.0100(9)	-0.0043(9)	0.0004(9)
C5	0.0191(11)	0.0211(11)	0.0249(12)	-0.0101(9)	-0.0052(9)	0.0009(9)
C6	0.0215(11)	0.0188(11)	0.0256(12)	-0.0094(9)	-0.0085(9)	0.0047(9)
C7	0.0179(10)	0.0175(10)	0.0218(11)	-0.0088(9)	-0.0029(9)	0.0012(9)
C8	0.0381(14)	0.0266(13)	0.0322(14)	-0.0133(12)	-0.0118(12)	-0.0038(11)
C9	0.0315(14)	0.0495(17)	0.0420(16)	-0.0217(13)	-0.0100(12)	-0.0113(13)
C10	0.0443(16)	0.0369(15)	0.0234(13)	-0.0198(13)	-0.0105(11)	0.0003(11)
C11	0.0443(17)	0.061(2)	0.0279(14)	-0.0335(16)	0.0013(12)	-0.0019(13)
C12	0.0366(15)	0.0325(14)	0.0511(18)	-0.0225(13)	-0.0028(13)	0.0064(13)
C13	0.0236(12)	0.0380(15)	0.0433(16)	-0.0165(12)	0.0021(11)	-0.0025(12)
C14	0.0333(14)	0.0336(14)	0.0334(14)	-0.0168(12)	-0.0015(11)	0.0090(11)
C15	0.0277(14)	0.0432(16)	0.0514(18)	-0.0234(13)	-0.0025(13)	0.0023(14)
C16	0.0265(13)	0.0297(13)	0.0312(14)	-0.0096(11)	0.0012(11)	0.0001(11)

C17	0.0430(16)	0.0226(13)	0.0515(18)	-0.0185(12)	-0.0101(13)	-0.0002(12)
C18	0.0378(15)	0.0363(15)	0.0462(17)	-0.0156(13)	-0.0177(13)	-0.0086(13)
C19	0.0358(14)	0.0320(14)	0.0325(14)	-0.0138(12)	-0.0061(11)	-0.0097(11)
C20	0.0429(16)	0.0294(14)	0.0425(16)	-0.0129(13)	-0.0208(13)	0.0092(12)
C21	0.055(2)	0.0368(17)	0.053(2)	0.0084(15)	-0.0282(17)	-0.0169(15)
C22	0.0308(15)	0.0418(17)	0.0472(18)	0.0011(13)	-0.0004(13)	0.0032(14)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S9-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Fe1	P1	2.1009(7)	Fe1	Si1	2.4274(7)
Fe1	C1	1.769(4)	Fe1	C2	1.773(3)
Fe1	C3	1.773(3)	P1	C4	1.852(3)
P1	C7	1.849(3)	Si1	C20	1.874(3)
Si1	C21	1.875(4)	Si1	C22	1.881(4)
Si2	C4	1.927(3)	Si2	C8	1.862(2)
Si2	C9	1.874(4)	Si2	C10	1.874(3)
Si3	C4	1.943(2)	Si3	C11	1.862(4)
Si3	C12	1.870(4)	Si3	C13	1.874(3)
Si4	C7	1.939(2)	Si4	C14	1.872(3)
Si4	C15	1.871(4)	Si4	C16	1.870(3)
Si5	C7	1.931(3)	Si5	C17	1.876(3)
Si5	C18	1.865(3)	Si5	C19	1.864(3)
O1	C1	1.150(4)	O2	C2	1.155(4)
O3	C3	1.149(4)	C4	C5	1.566(3)
C5	C6	1.525(4)	C6	C7	1.574(3)

Table S9-5. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
P1	Fe1	Si1	138.27(3)	P1	Fe1	C1	100.19(9)
P1	Fe1	C2	99.83(8)	P1	Fe1	C3	118.64(8)
Si1	Fe1	C1	74.51(7)	Si1	Fe1	C2	78.93(8)
Si1	Fe1	C3	103.05(8)	C1	Fe1	C2	153.44(10)
C1	Fe1	C3	93.04(15)	C2	Fe1	C3	92.51(15)
Fe1	P1	C4	131.74(8)	Fe1	P1	C7	130.30(9)
C4	P1	C7	97.88(11)	Fe1	Si1	C20	109.07(8)
Fe1	Si1	C21	113.63(10)	Fe1	Si1	C22	116.47(11)
C20	Si1	C21	107.54(16)	C20	Si1	C22	106.88(15)
C21	Si1	C22	102.65(17)	C4	Si2	C8	112.29(12)
C4	Si2	C9	110.55(12)	C4	Si2	C10	113.68(14)
C8	Si2	C9	110.38(15)	C8	Si2	C10	106.55(11)
C9	Si2	C10	102.95(15)	C4	Si3	C11	111.47(16)
C4	Si3	C12	116.15(12)	C4	Si3	C13	108.04(11)
C11	Si3	C12	108.10(16)	C11	Si3	C13	105.89(13)
C12	Si3	C13	106.62(16)	C7	Si4	C14	108.12(11)
C7	Si4	C15	116.51(13)	C7	Si4	C16	113.08(13)
C14	Si4	C15	104.89(16)	C14	Si4	C16	108.35(13)
C15	Si4	C16	105.36(13)	C7	Si5	C17	107.86(13)
C7	Si5	C18	115.37(11)	C7	Si5	C19	112.28(14)
C17	Si5	C18	109.85(17)	C17	Si5	C19	105.33(12)
C18	Si5	C19	105.68(13)	Fe1	C1	O1	175.0(3)
Fe1	C2	O2	175.7(3)	Fe1	C3	O3	178.8(2)
P1	C4	Si2	112.28(10)	P1	C4	Si3	114.62(12)
P1	C4	C5	103.6(2)	Si2	C4	Si3	110.33(15)
Si2	C4	C5	109.48(16)	Si3	C4	C5	106.08(13)
C4	C5	C6	109.33(17)	C5	C6	C7	110.38(19)
P1	C7	Si4	113.02(10)	P1	C7	Si5	112.58(12)
P1	C7	C6	104.64(19)	Si4	C7	Si5	110.51(15)
Si4	C7	C6	108.99(15)	Si5	C7	C6	106.69(13)

Table S9-6. Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
P1	Fe1	Si1	C20	-156.52(4)	P1	Fe1	Si1	C21	-36.56(7)
P1	Fe1	Si1	C22	82.45(7)	Si1	Fe1	P1	C4	87.10(6)
Si1	Fe1	P1	C7	-96.92(6)	C1	Fe1	P1	C4	8.99(9)
C1	Fe1	P1	C7	-175.03(8)	C2	Fe1	P1	C4	171.45(9)
C2	Fe1	P1	C7	-12.57(10)	C3	Fe1	P1	C4	-90.19(14)
C3	Fe1	P1	C7	85.79(14)	C1	Fe1	Si1	C20	-68.52(10)
C1	Fe1	Si1	C21	51.44(10)	C1	Fe1	Si1	C22	170.45(10)
C2	Fe1	Si1	C20	111.07(10)	C2	Fe1	Si1	C21	-128.97(10)
C2	Fe1	Si1	C22	-9.96(10)	C3	Fe1	Si1	C20	21.04(13)
C3	Fe1	Si1	C21	141.00(13)	C3	Fe1	Si1	C22	-99.99(13)
Fe1	P1	C4	Si2	-82.86(13)	Fe1	P1	C4	Si3	44.06(16)
Fe1	P1	C4	C5	159.14(6)	Fe1	P1	C7	Si4	60.96(17)
Fe1	P1	C7	Si5	-65.12(12)	Fe1	P1	C7	C6	179.41(5)
C4	P1	C7	Si4	-122.06(14)	C4	P1	C7	Si5	111.85(12)
C4	P1	C7	C6	-3.62(12)	C7	P1	C4	Si2	100.23(13)
C7	P1	C4	Si3	-132.85(12)	C7	P1	C4	C5	-17.77(12)
C8	Si2	C4	P1	45.54(18)	C8	Si2	C4	Si3	-83.65(15)
C8	Si2	C4	C5	159.98(15)	C9	Si2	C4	P1	169.29(13)
C9	Si2	C4	Si3	40.11(15)	C9	Si2	C4	C5	-76.27(18)
C10	Si2	C4	P1	-75.51(15)	C10	Si2	C4	Si3	155.30(12)
C10	Si2	C4	C5	38.92(18)	C11	Si3	C4	P1	30.77(16)
C11	Si3	C4	Si2	158.69(12)	C11	Si3	C4	C5	-82.84(17)
C12	Si3	C4	P1	-93.63(18)	C12	Si3	C4	Si2	34.29(17)
C12	Si3	C4	C5	152.76(16)	C13	Si3	C4	P1	146.71(15)
C13	Si3	C4	Si2	-85.38(15)	C13	Si3	C4	C5	33.1(2)
C14	Si4	C7	P1	136.40(16)	C14	Si4	C7	Si5	-96.42(16)
C14	Si4	C7	C6	20.5(2)	C15	Si4	C7	P1	-105.86(17)
C15	Si4	C7	Si5	21.32(15)	C15	Si4	C7	C6	138.26(15)
C16	Si4	C7	P1	16.43(19)	C16	Si4	C7	Si5	143.61(13)
C16	Si4	C7	C6	-99.45(16)	C17	Si5	C7	P1	-177.18(13)
C17	Si5	C7	Si4	55.39(15)	C17	Si5	C7	C6	-62.95(17)
C18	Si5	C7	P1	59.61(18)	C18	Si5	C7	Si4	-67.81(16)
C18	Si5	C7	C6	173.84(14)	C19	Si5	C7	P1	-61.56(14)
C19	Si5	C7	Si4	171.01(11)	C19	Si5	C7	C6	52.67(16)
P1	C4	C5	C6	35.4(2)	Si2	C4	C5	C6	-84.5(2)
Si3	C4	C5	C6	156.47(15)	C4	C5	C6	C7	-41.0(3)
C5	C6	C7	P1	25.5(2)	C5	C6	C7	Si4	146.64(17)
C5	C6	C7	Si5	-94.0(2)					

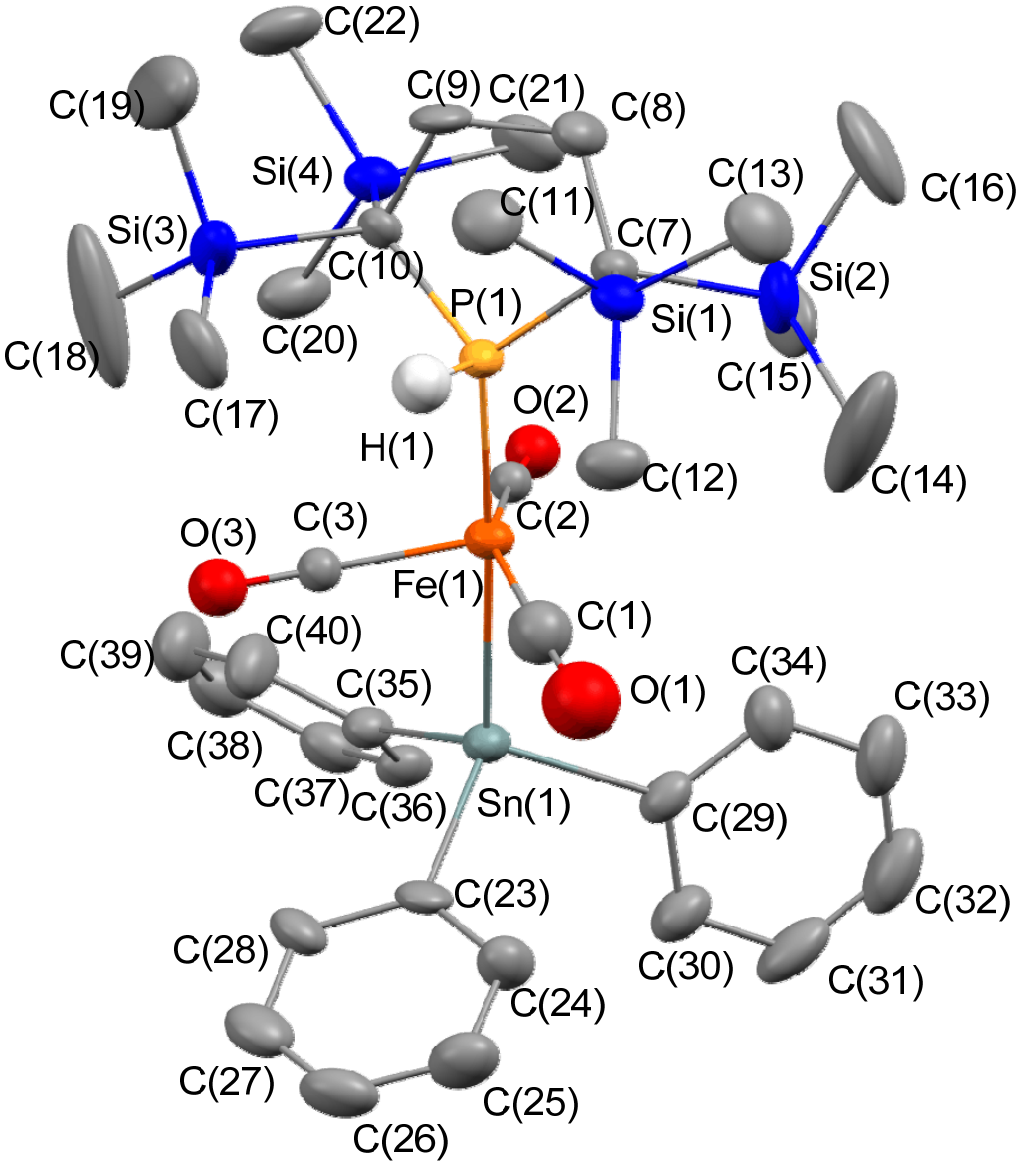


Figure S28. ORTEP drawing of **8** (50% probability of the thermal ellipsoids). (Three CO ligands on the iron were found to be disordered. The site occupancy factor for C1, C2, C3, O1, O2 and O3 was defined as 0.6, and the site occupancy factor for C4, C5, C6, O4, O5 and O6 was defined as 0.4. Only three CO ligands {C(1)-O(1), C(2)-O(2) and C(3)-O(3)} were shown in this figure for clarity.)

Table S10-1. Crystal data and structure refinement for **8**

Empirical Formula	$C_{37}H_{56}FeO_3PSi_4Sn$
Formula Weight	866.70
Crystal Color, Habit	colorless, block
Crystal Dimensions	0.120 X 0.120 X 0.100 mm
Crystal System	orthorhombic
Lattice Type	Primitive
Lattice Parameters	a = 11.387(3) Å b = 14.883(4) Å c = 24.983(6) Å V = 4234.0(17) Å^3
Space Group	$P2_12_12_1$ (#19)
Z value	4
D_{calc}	1.360 g/cm^3
F_{000}	1796.00
μ(MoKα)	11.149 cm^{-1}
Diffractometer	Saturn70
Radiation	MoKα (λ = 0.71075 Å) multi-layer mirror monochromated
Voltage, Current	50kV, 16mA
Temperature	-149.8°C
Detector Aperture	70.0 x 70.0 mm
Data Images	720 exposures
ω oscillation Range (χ=45.0, ϕ=270.0)	-110.0 - 70.0°
Exposure Rate	2.0 sec./°
Detector Swing Angle	-19.55°
Detector Position	45.06 mm
Pixel Size	0.137 mm
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 34784 Unique: 9661 (R_{int} = 0.0733) Friedel pairs: 4309
Corrections	Lorentz-polarization Absorption (trans. factors: 0.715 - 0.894)
Structure Solution	Direct Methods (SHELXS97)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w (Fo^2 - Fc^2)^2
Least Squares Weights	w = 1/ [σ^2(Fo^2) + (0.0618 · P)^2 + 0.0000 · P] where P = (Max(Fo^2,0) + 2Fc^2)/3
$2\theta_{max}$ cutoff	55.0°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	9661
No. Variables	422
Reflection/Parameter Ratio	22.89
Residuals: R1 (I>2.00σ(I))	0.0592
Residuals: R (All reflections)	0.0741
Residuals: wR2 (All reflections)	0.1351
Goodness of Fit Indicator	1.089
Flack Parameter (Friedel pairs = 4309)	0.02(2)
Max Shift/Error in Final Cycle	0.002
Maximum peak in Final Diff. Map	1.28 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.88 e$^-$/Å^3

Table S10-2. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Sn1	0.14482(3)	0.00222(3)	0.858978(13)	1.966(9)	1
Fe1	0.19779(7)	0.02449(5)	0.95825(3)	1.937(14)	1
P1	0.25188(12)	0.03918(10)	1.04406(5)	1.89(2)	1
Si1	0.20130(15)	0.20091(11)	1.11643(6)	2.28(3)	1
Si2	-0.00983(16)	0.06955(14)	1.09559(9)	3.68(4)	1
Si3	0.51013(15)	-0.02436(13)	1.06563(8)	3.41(4)	1
Si4	0.31121(16)	-0.16966(11)	1.07326(6)	2.39(3)	1
O1	0.1490(9)	0.2086(7)	0.9305(4)	5.9(2)	0.600000
O2	0.0997(7)	-0.1575(6)	0.9591(3)	2.85(16)	0.600000
O3	0.4473(6)	0.0180(5)	0.9193(3)	3.31(14)	0.600000
O4	0.0230(9)	0.1729(7)	0.9515(4)	2.86(19)	0.400000
O5	0.0597(11)	-0.1378(8)	0.9629(5)	3.0(3)	0.400000
O6	0.4006(12)	0.1154(9)	0.9176(5)	4.6(3)	0.400000
C1	0.1733(11)	0.1342(9)	0.9429(5)	4.1(2)	0.600000
C2	0.1434(9)	-0.0866(6)	0.9601(4)	1.75(15)	0.600000
C3	0.3510(7)	0.0137(6)	0.9321(3)	1.94(14)	0.600000
C4	0.0876(12)	0.1138(9)	0.9572(5)	1.6(2)	0.400000
C5	0.1009(16)	-0.0657(12)	0.9631(7)	2.9(3)	0.400000
C6	0.3100(15)	0.0840(11)	0.9339(6)	3.1(3)	0.400000
C7	0.1587(5)	0.0771(4)	1.1011(2)	1.95(9)	1
C8	0.1981(5)	0.0155(4)	1.1475(2)	2.76(11)	1
C9	0.3231(5)	-0.0139(4)	1.14020(19)	2.61(11)	1
C10	0.3458(5)	-0.0431(3)	1.0800(2)	1.78(9)	1
C11	0.3495(7)	0.2120(5)	1.1468(3)	3.96(14)	1
C12	0.1989(7)	0.2729(4)	1.0559(3)	3.37(13)	1
C13	0.1014(7)	0.2519(5)	1.1678(3)	4.15(15)	1
C14	-0.0798(7)	0.1646(7)	1.0598(6)	9.5(4)	1
C15	-0.0681(6)	-0.0336(6)	1.0627(3)	5.1(2)	1
C16	-0.0700(8)	0.0615(6)	1.1653(4)	6.6(3)	1
C17	0.5497(6)	0.0906(5)	1.0448(3)	4.45(16)	1
C18	0.5782(9)	-0.0980(7)	1.0163(6)	11.7(5)	1
C19	0.5909(7)	-0.0339(8)	1.1326(4)	7.5(3)	1
C20	0.3407(7)	-0.2193(4)	1.0053(3)	3.67(14)	1
C21	0.1556(6)	-0.1994(5)	1.0916(3)	3.77(14)	1
C22	0.4072(7)	-0.2315(5)	1.1227(3)	4.04(16)	1
C23	0.2140(6)	0.1053(4)	0.8077(2)	2.43(11)	1
C24	0.1540(7)	0.1860(4)	0.8006(3)	3.12(12)	1
C25	0.2014(7)	0.2553(5)	0.7690(3)	3.82(15)	1
C26	0.3097(7)	0.2423(5)	0.7446(3)	3.80(14)	1
C27	0.3683(7)	0.1638(5)	0.7509(2)	3.77(14)	1
C28	0.3230(6)	0.0935(5)	0.7824(2)	2.83(12)	1
C29	-0.0418(5)	0.0014(4)	0.8437(2)	2.35(9)	1
C30	-0.0820(5)	0.0021(5)	0.7910(2)	3.16(11)	1
C31	-0.2009(6)	-0.0018(6)	0.7794(3)	4.09(14)	1
C32	-0.2820(6)	-0.0081(5)	0.8199(4)	4.67(16)	1
C33	-0.2448(5)	-0.0083(6)	0.8722(3)	4.24(15)	1
C34	-0.1266(5)	-0.0043(5)	0.8843(3)	3.10(11)	1
C35	0.2109(5)	-0.1243(4)	0.8306(2)	2.29(10)	1
C36	0.1430(6)	-0.1828(4)	0.8014(2)	2.34(10)	1
C37	0.1825(6)	-0.2670(4)	0.7870(2)	3.02(12)	1
C38	0.2905(7)	-0.2966(5)	0.8013(3)	3.60(13)	1
C39	0.3618(7)	-0.2392(5)	0.8315(3)	4.38(16)	1
C40	0.3249(6)	-0.1546(5)	0.8456(3)	3.71(14)	1

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S10-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sn1	0.02882(19)	0.02694(19)	0.01892(16)	0.00196(19)	-0.00182(14)	-0.00054(17)
Fe1	0.0290(4)	0.0245(4)	0.0200(4)	-0.0029(3)	-0.0022(3)	-0.0003(3)
P1	0.0255(7)	0.0284(7)	0.0178(6)	0.0040(6)	-0.0007(6)	-0.0007(6)
Si1	0.0371(9)	0.0264(8)	0.0233(8)	0.0003(8)	0.0010(7)	-0.0027(7)
Si2	0.0234(9)	0.0451(11)	0.0712(14)	0.0024(8)	0.0123(9)	0.0039(11)

Si3	0.0254(8)	0.0463(12)	0.0576(12)	0.0012(8)	0.0062(8)	0.0234(9)
Si4	0.0407(9)	0.0246(8)	0.0254(8)	0.0004(8)	-0.0008(7)	0.0016(7)
C7	0.030(3)	0.023(3)	0.021(3)	0.002(2)	0.002(2)	0.002(2)
C8	0.044(3)	0.037(4)	0.023(3)	0.008(3)	0.003(2)	-0.001(3)
C9	0.049(3)	0.036(3)	0.014(2)	0.003(3)	-0.007(2)	0.006(3)
C10	0.023(3)	0.023(3)	0.022(2)	-0.003(2)	0.003(2)	0.004(2)
C11	0.062(5)	0.043(4)	0.046(4)	-0.001(4)	-0.006(4)	-0.011(3)
C12	0.063(4)	0.029(3)	0.036(4)	-0.004(3)	-0.008(3)	0.003(3)
C13	0.067(5)	0.038(4)	0.052(4)	0.001(4)	0.011(4)	-0.016(3)
C14	0.042(5)	0.070(7)	0.250(16)	0.006(5)	-0.023(7)	0.051(9)
C15	0.024(3)	0.100(7)	0.068(5)	-0.020(4)	0.002(3)	-0.000(5)
C16	0.076(6)	0.074(6)	0.099(7)	-0.021(5)	0.062(6)	-0.035(5)
C17	0.045(4)	0.053(4)	0.071(5)	-0.014(4)	0.027(4)	-0.005(4)
C18	0.078(7)	0.069(7)	0.295(19)	-0.030(6)	0.114(10)	-0.069(9)
C19	0.039(4)	0.149(11)	0.097(7)	-0.014(5)	-0.011(5)	0.047(7)
C20	0.071(5)	0.034(3)	0.034(3)	0.015(4)	-0.010(4)	-0.004(3)
C21	0.059(5)	0.043(4)	0.041(4)	-0.023(4)	0.006(4)	0.006(3)
C22	0.082(6)	0.030(4)	0.042(4)	0.009(4)	-0.020(4)	0.008(3)
C23	0.040(3)	0.040(3)	0.012(3)	-0.003(3)	-0.003(3)	0.003(2)
C24	0.044(4)	0.035(3)	0.040(4)	0.005(3)	0.004(4)	0.005(3)
C25	0.057(5)	0.038(4)	0.051(4)	-0.005(4)	-0.009(4)	0.012(3)
C26	0.072(5)	0.041(4)	0.032(4)	-0.016(4)	-0.002(4)	0.007(3)
C27	0.057(4)	0.062(5)	0.025(3)	-0.011(4)	0.001(3)	-0.005(3)
C28	0.040(4)	0.047(4)	0.021(3)	-0.006(3)	0.006(3)	-0.001(3)
C29	0.030(3)	0.024(3)	0.036(3)	0.001(3)	-0.012(2)	-0.003(3)
C30	0.041(3)	0.037(3)	0.043(3)	0.006(4)	-0.015(3)	-0.002(4)
C31	0.055(4)	0.038(3)	0.063(4)	0.006(4)	-0.036(4)	-0.004(4)
C32	0.036(4)	0.041(4)	0.101(6)	0.002(4)	-0.021(4)	-0.009(5)
C33	0.033(3)	0.044(4)	0.084(5)	0.008(3)	0.001(3)	-0.008(5)
C34	0.034(3)	0.034(3)	0.050(3)	0.002(3)	0.006(3)	-0.006(3)
C35	0.035(3)	0.031(3)	0.021(3)	0.005(3)	-0.001(3)	-0.000(2)
C36	0.040(3)	0.022(3)	0.026(3)	0.003(3)	-0.002(3)	0.003(2)
C37	0.052(4)	0.034(3)	0.029(3)	-0.002(3)	0.008(3)	-0.001(3)
C38	0.061(5)	0.036(4)	0.039(4)	0.011(4)	0.013(4)	0.001(3)
C39	0.052(4)	0.059(5)	0.055(5)	0.022(4)	0.004(4)	-0.007(4)
C40	0.043(4)	0.054(4)	0.044(4)	0.018(3)	-0.003(3)	-0.016(3)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S10-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Sn1	Fe1	2.5739(10)	Sn1	C23	2.147(6)
Sn1	C29	2.160(5)	Sn1	C35	2.148(6)
Fe1	P1	2.2412(16)	Fe1	C1	1.700(13)
Fe1	C2	1.766(10)	Fe1	C3	1.870(8)
Fe1	C4	1.828(13)	Fe1	C5	1.741(18)
Fe1	C6	1.670(17)	P1	C7	1.864(5)
P1	C10	1.856(5)	Si1	C7	1.944(5)
Si1	C11	1.858(8)	Si1	C12	1.853(6)
Si1	C13	1.876(8)	Si2	C7	1.927(6)
Si2	C14	1.854(11)	Si2	C15	1.864(8)
Si2	C16	1.875(9)	Si3	C10	1.925(5)
Si3	C17	1.844(8)	Si3	C18	1.822(12)
Si3	C19	1.915(9)	Si4	C10	1.932(5)
Si4	C20	1.881(6)	Si4	C21	1.883(7)
Si4	C22	1.888(7)	O1	O4	1.618(14)
O1	C1	1.184(17)	O1	C4	1.711(16)
O2	O5	0.550(15)	O2	C2	1.167(13)
O2	C5	1.37(2)	O3	O6	1.545(15)
O3	C3	1.143(11)	O3	C6	1.882(18)
O4	C1	1.819(16)	O4	C4	1.155(16)
O5	C2	1.222(16)	O5	C5	1.17(2)
O6	C3	1.655(16)	O6	C6	1.20(2)
C1	C4	1.082(18)	C1	C6	1.74(2)
C2	C5	0.58(2)	C3	C6	1.147(19)

C7	C8	1.546(8)	C8	C9	1.500(8)
C9	C10	1.588(7)	C23	C24	1.393(9)
C23	C28	1.404(9)	C24	C25	1.406(10)
C25	C26	1.390(11)	C26	C27	1.354(11)
C27	C28	1.406(10)	C29	C30	1.393(8)
C29	C34	1.403(8)	C30	C31	1.385(9)
C31	C32	1.373(11)	C32	C33	1.374(12)
C33	C34	1.381(8)	C35	C36	1.375(8)
C35	C40	1.425(9)	C36	C37	1.379(8)
C37	C38	1.354(10)	C38	C39	1.398(10)
C39	C40	1.374(11)	P1	H1	1.52(6)

Table S10-5. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Fe1	Sn1	C23	113.37(15)	Fe1	Sn1	C29	113.72(14)
Fe1	Sn1	C35	110.41(15)	C23	Sn1	C29	105.0(2)
C23	Sn1	C35	107.5(2)	C29	Sn1	C35	106.3(2)
Sn1	Fe1	P1	177.04(5)	Sn1	Fe1	C1	82.4(4)
Sn1	Fe1	C2	79.8(3)	Sn1	Fe1	C3	82.6(2)
Sn1	Fe1	C4	85.4(4)	Sn1	Fe1	C5	79.6(6)
Sn1	Fe1	C6	84.0(6)	P1	Fe1	C1	99.6(4)
P1	Fe1	C2	99.4(3)	P1	Fe1	C3	95.0(3)
P1	Fe1	C4	97.5(4)	P1	Fe1	C5	100.5(6)
P1	Fe1	C6	95.0(6)	C1	Fe1	C2	147.9(5)
C1	Fe1	C3	99.0(5)	C1	Fe1	C4	35.5(6)
C1	Fe1	C5	130.7(7)	C1	Fe1	C6	62.2(7)
C2	Fe1	C3	104.8(4)	C2	Fe1	C4	116.1(5)
C2	Fe1	C5	19.0(7)	C2	Fe1	C6	140.8(7)
C3	Fe1	C4	134.2(5)	C3	Fe1	C5	123.3(7)
C3	Fe1	C6	37.3(6)	C4	Fe1	C5	97.3(7)
C4	Fe1	C6	97.7(7)	C5	Fe1	C6	156.8(8)
Fe1	P1	C7	127.18(18)	Fe1	P1	C10	123.78(17)
C7	P1	C10	99.1(2)	C7	Si1	C11	113.0(3)
C7	Si1	C12	112.5(3)	C7	Si1	C13	111.5(3)
C11	Si1	C12	107.2(3)	C11	Si1	C13	103.6(3)
C12	Si1	C13	108.4(3)	C7	Si2	C14	114.7(3)
C7	Si2	C15	115.7(3)	C7	Si2	C16	107.5(3)
C14	Si2	C15	105.3(4)	C14	Si2	C16	109.9(5)
C15	Si2	C16	103.1(4)	C10	Si3	C17	115.1(3)
C10	Si3	C18	116.9(4)	C10	Si3	C19	107.1(3)
C17	Si3	C18	105.2(4)	C17	Si3	C19	101.5(4)
C18	Si3	C19	110.0(5)	C10	Si4	C20	115.1(3)
C10	Si4	C21	113.6(3)	C10	Si4	C22	107.5(3)
C20	Si4	C21	107.2(3)	C20	Si4	C22	107.2(3)
C21	Si4	C22	105.7(3)	O4	O1	C1	79.3(9)
O4	O1	C4	40.5(6)	C1	O1	C4	38.8(8)
O5	O2	C2	82.4(17)	O5	O2	C5	57.6(17)
C2	O2	C5	24.8(9)	O6	O3	C3	74.3(8)
O6	O3	C6	39.6(7)	C3	O3	C6	34.8(7)
O1	O4	C1	39.8(6)	O1	O4	C4	74.1(9)
C1	O4	C4	34.3(8)	O2	O5	C2	71.1(16)
O2	O5	C5	99(2)	C2	O5	C5	27.9(11)
O3	O6	C3	41.7(5)	O3	O6	C6	85.5(11)
C3	O6	C6	43.9(9)	Fe1	C1	O1	175.3(11)
Fe1	C1	O4	115.6(8)	Fe1	C1	C4	78.7(10)
Fe1	C1	C6	58.1(7)	O1	C1	O4	60.9(8)
O1	C1	C4	97.9(13)	O1	C1	C6	125.2(12)
O4	C1	C4	37.0(9)	O4	C1	C6	173.0(10)
C4	C1	C6	136.8(14)	Fe1	C2	O2	174.6(9)
Fe1	C2	O5	149.2(10)	Fe1	C2	C5	78(2)
O2	C2	O5	26.5(8)	O2	C2	C5	98(2)
O5	C2	C5	71(2)	Fe1	C3	O3	170.8(8)
Fe1	C3	O6	108.4(6)	Fe1	C3	C6	61.8(9)
O3	C3	O6	64.0(7)	O3	C3	C6	110.6(11)
O6	C3	C6	46.6(10)	Fe1	C4	O1	109.0(8)
Fe1	C4	O4	172.9(12)	Fe1	C4	C1	65.8(9)
O1	C4	O4	65.4(9)	O1	C4	C1	43.3(9)
O4	C4	C1	108.7(14)	Fe1	C5	O2	140.4(13)
Fe1	C5	O5	163.7(16)	Fe1	C5	C2	83(2)
O2	C5	O5	23.4(8)	O2	C5	C2	57.6(18)

O5	C5	C2	81(2)	Fe1	C6	O3	115.4(9)
Fe1	C6	O6	170.1(15)	Fe1	C6	C1	59.8(7)
Fe1	C6	C3	80.9(10)	O3	C6	O6	54.9(9)
O3	C6	C1	172.6(11)	O3	C6	C3	34.7(7)
O6	C6	C1	130.1(14)	O6	C6	C3	89.5(14)
C1	C6	C3	139.5(14)	P1	C7	Si1	107.2(3)
P1	C7	Si2	119.6(3)	P1	C7	C8	103.2(4)
Si1	C7	Si2	108.5(3)	Si1	C7	C8	110.0(4)
Si2	C7	C8	108.0(4)	C7	C8	C9	110.9(4)
C8	C9	C10	110.5(4)	P1	C10	Si3	112.0(3)
P1	C10	Si4	118.9(3)	P1	C10	C9	100.6(3)
Si3	C10	Si4	108.8(3)	Si3	C10	C9	107.1(3)
Si4	C10	C9	108.4(3)	Sn1	C23	C24	120.8(5)
Sn1	C23	C28	120.3(4)	C24	C23	C28	118.8(6)
C23	C24	C25	121.1(7)	C24	C25	C26	119.0(7)
C25	C26	C27	120.4(7)	C26	C27	C28	121.7(7)
C23	C28	C27	118.9(6)	Sn1	C29	C30	119.4(4)
Sn1	C29	C34	123.3(4)	C30	C29	C34	117.2(5)
C29	C30	C31	121.3(6)	C30	C31	C32	120.3(7)
C31	C32	C33	119.6(6)	C32	C33	C34	120.5(7)
C29	C34	C33	121.0(6)	Sn1	C35	C36	122.2(5)
Sn1	C35	C40	120.7(4)	C36	C35	C40	116.8(6)
C35	C36	C37	122.1(6)	C36	C37	C38	121.5(6)
C37	C38	C39	118.1(6)	C38	C39	C40	121.4(7)
C35	C40	C39	120.1(6)	Fe1	P1	H1	107(2)
C7	P1	H1	96(2)	C10	P1	H1	97(2)

Table S10-6. Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Fe1	Sn1	C23	C24	-84.4(4)	Fe1	Sn1	C23	C28	93.2(4)
C23	Sn1	Fe1	C1	38.93(19)	C23	Sn1	Fe1	C2	-167.86(18)
C23	Sn1	Fe1	C3	-61.23(19)	C23	Sn1	Fe1	C4	74.52(19)
C23	Sn1	Fe1	C5	172.82(18)	C23	Sn1	Fe1	C6	-23.73(19)
Fe1	Sn1	C29	C30	171.4(3)	Fe1	Sn1	C29	C34	-11.9(5)
C29	Sn1	Fe1	C1	-80.95(19)	C29	Sn1	Fe1	C2	72.26(19)
C29	Sn1	Fe1	C3	178.89(19)	C29	Sn1	Fe1	C4	-45.36(19)
C29	Sn1	Fe1	C5	52.94(19)	C29	Sn1	Fe1	C6	-143.61(19)
Fe1	Sn1	C35	C36	132.8(3)	Fe1	Sn1	C35	C40	-41.4(4)
C35	Sn1	Fe1	C1	159.61(17)	C35	Sn1	Fe1	C2	-47.18(17)
C35	Sn1	Fe1	C3	59.45(17)	C35	Sn1	Fe1	C4	-164.80(17)
C35	Sn1	Fe1	C5	-66.50(17)	C35	Sn1	Fe1	C6	96.95(17)
C23	Sn1	C29	C30	46.9(5)	C23	Sn1	C29	C34	-136.4(4)
C29	Sn1	C23	C24	40.3(4)	C29	Sn1	C23	C28	-142.1(4)
C23	Sn1	C35	C36	-103.1(4)	C23	Sn1	C35	C40	82.7(4)
C35	Sn1	C23	C24	153.3(4)	C35	Sn1	C23	C28	-29.2(4)
C29	Sn1	C35	C36	9.0(4)	C29	Sn1	C35	C40	-165.2(3)
C35	Sn1	C29	C30	-66.9(4)	C35	Sn1	C29	C34	109.8(4)
Sn1	Fe1	C1	O4	89.5(7)	Sn1	Fe1	C1	C4	92.7(6)
Sn1	Fe1	C1	C6	-87.2(2)	Sn1	Fe1	C2	O5	-83.6(14)
Sn1	Fe1	C2	C5	-87.7(9)	Sn1	Fe1	C3	O6	91.7(4)
Sn1	Fe1	C3	C6	89.9(3)	Sn1	Fe1	C4	O1	-81.0(6)
Sn1	Fe1	C4	C1	-83.4(6)	Sn1	Fe1	C5	O2	84.4(19)
Sn1	Fe1	C5	C2	88.8(17)	Sn1	Fe1	C6	O3	-89.1(8)
Sn1	Fe1	C6	C1	84.5(3)	Sn1	Fe1	C6	C3	-85.5(7)
P1	Fe1	C1	O4	-92.7(7)	P1	Fe1	C1	C4	-89.5(6)
P1	Fe1	C1	C6	90.6(2)	C1	Fe1	P1	C7	66.6(4)
C1	Fe1	P1	C10	-155.2(4)	P1	Fe1	C2	O5	99.3(14)
P1	Fe1	C2	C5	95.1(9)	C2	Fe1	P1	C7	-87.5(4)
C2	Fe1	P1	C10	50.8(4)	P1	Fe1	C3	O6	-89.9(4)
P1	Fe1	C3	C6	-91.7(3)	C3	Fe1	P1	C7	166.6(3)
C3	Fe1	P1	C10	-55.2(3)	P1	Fe1	C4	O1	98.5(6)
P1	Fe1	C4	C1	96.0(6)	C4	Fe1	P1	C7	30.7(4)
C4	Fe1	P1	C10	169.0(4)	P1	Fe1	C5	O2	-92.6(19)
P1	Fe1	C5	C2	-88.2(17)	C5	Fe1	P1	C7	-68.2(6)
C5	Fe1	P1	C10	70.1(6)	P1	Fe1	C6	O3	88.1(8)
P1	Fe1	C6	C1	-98.3(3)	P1	Fe1	C6	C3	91.6(7)
C6	Fe1	P1	C7	129.2(6)	C6	Fe1	P1	C10	-92.6(6)

C1	Fe1	C2	O5	-26(2)	C1	Fe1	C2	C5	-30.5(16)
C2	Fe1	C1	O4	32.8(14)	C2	Fe1	C1	C4	36.0(14)
C2	Fe1	C1	C6	-143.9(8)	C1	Fe1	C3	O6	10.6(6)
C1	Fe1	C3	C6	8.9(6)	C3	Fe1	C1	O4	170.6(6)
C3	Fe1	C1	C4	173.9(6)	C3	Fe1	C1	C6	-6.1(4)
C1	Fe1	C4	O1	2.5(7)	C1	Fe1	C4	C1	0.0(7)
C4	Fe1	C1	O4	-3.2(7)	C4	Fe1	C1	C4	0.0(7)
C4	Fe1	C1	C6	-179.9(11)	C1	Fe1	C5	O2	154.8(15)
C1	Fe1	C5	C2	159.2(14)	C5	Fe1	C1	O4	20.2(13)
C5	Fe1	C1	C4	23.5(12)	C5	Fe1	C1	C6	-156.5(8)
C1	Fe1	C6	O3	-173.7(12)	C1	Fe1	C6	C1	0.0(5)
C1	Fe1	C6	C3	-170.1(11)	C6	Fe1	C1	O4	176.7(11)
C6	Fe1	C1	C4	179.9(10)	C6	Fe1	C1	C6	0.0(6)
C2	Fe1	C3	O6	169.0(4)	C2	Fe1	C3	C6	167.2(4)
C3	Fe1	C2	O5	-163.0(13)	C3	Fe1	C2	C5	-167.1(9)
C2	Fe1	C4	O1	-157.2(6)	C2	Fe1	C4	C1	-159.6(5)
C4	Fe1	C2	O5	-4.0(16)	C4	Fe1	C2	C5	-8.1(11)
C2	Fe1	C6	O3	-23.3(15)	C2	Fe1	C6	C1	150.3(7)
C2	Fe1	C6	C3	-19.8(15)	C6	Fe1	C2	O5	-150.8(14)
C6	Fe1	C2	C5	-154.9(11)	C3	Fe1	C4	O1	-6.0(11)
C3	Fe1	C4	C1	-8.5(10)	C4	Fe1	C3	O6	15.6(8)
C4	Fe1	C3	C6	13.8(8)	C3	Fe1	C5	O2	11(2)
C3	Fe1	C5	C2	15(2)	C5	Fe1	C3	O6	164.0(7)
C5	Fe1	C3	C6	162.2(7)	C3	Fe1	C6	O3	-3.6(4)
C3	Fe1	C6	C1	170.1(11)	C3	Fe1	C6	C3	0.0(4)
C6	Fe1	C3	O6	1.8(9)	C6	Fe1	C3	C6	0.0(9)
C4	Fe1	C5	O2	168.3(18)	C4	Fe1	C5	C2	172.7(17)
C5	Fe1	C4	O1	-159.8(8)	C5	Fe1	C4	C1	-162.3(8)
C4	Fe1	C6	O3	-173.6(8)	C4	Fe1	C6	C1	0.1(6)
C4	Fe1	C6	C3	-170.0(8)	C6	Fe1	C4	O1	2.4(9)
C6	Fe1	C4	C1	-0.1(8)	C5	Fe1	C6	O3	-44(2)
C5	Fe1	C6	C1	129.8(19)	C5	Fe1	C6	C3	-40(2)
C6	Fe1	C5	O2	38(3)	C6	Fe1	C5	C2	43(3)
Fe1	P1	C7	Si1	-103.0(2)	Fe1	P1	C7	Si2	21.0(4)
Fe1	P1	C7	C8	140.87(18)	Fe1	P1	C10	Si3	82.2(3)
Fe1	P1	C10	Si4	-46.3(4)	Fe1	P1	C10	C9	-164.30(14)
C7	P1	C10	Si3	-130.3(3)	C7	P1	C10	Si4	101.3(3)
C7	P1	C10	C9	-16.8(3)	C10	P1	C7	Si1	111.1(3)
C10	P1	C7	Si2	-124.9(3)	C10	P1	C7	C8	-5.1(3)
C11	Si1	C7	P1	-70.5(4)	C11	Si1	C7	Si2	159.0(3)
C11	Si1	C7	C8	41.1(4)	C12	Si1	C7	P1	51.1(4)
C12	Si1	C7	Si2	-79.4(4)	C12	Si1	C7	C8	162.7(3)
C13	Si1	C7	P1	173.2(3)	C13	Si1	C7	Si2	42.7(4)
C13	Si1	C7	C8	-75.2(4)	C14	Si2	C7	P1	-82.7(5)
C14	Si2	C7	Si1	40.6(5)	C14	Si2	C7	C8	159.8(5)
C15	Si2	C7	P1	40.2(5)	C15	Si2	C7	Si1	163.5(3)
C15	Si2	C7	C8	-77.3(4)	C16	Si2	C7	P1	154.7(4)
C16	Si2	C7	Si1	-81.9(4)	C16	Si2	C7	C8	37.3(4)
C17	Si3	C10	P1	24.1(4)	C17	Si3	C10	Si4	157.7(3)
C17	Si3	C10	C9	-85.3(4)	C18	Si3	C10	P1	-100.1(5)
C18	Si3	C10	Si4	33.4(5)	C18	Si3	C10	C9	150.4(5)
C19	Si3	C10	P1	136.0(4)	C19	Si3	C10	Si4	-90.4(4)
C19	Si3	C10	C9	26.6(5)	C20	Si4	C10	P1	69.4(4)
C20	Si4	C10	Si3	-60.5(4)	C20	Si4	C10	C9	-176.7(3)
C21	Si4	C10	P1	-54.7(4)	C21	Si4	C10	Si3	175.4(3)
C21	Si4	C10	C9	59.2(4)	C22	Si4	C10	P1	-171.3(3)
C22	Si4	C10	Si3	58.8(3)	C22	Si4	C10	C9	-57.4(4)
O4	O1	C1	O4	-0.0(4)	O4	O1	C1	C4	-1.0(8)
O4	O1	C1	C6	176.1(11)	C1	O1	O4	C1	0.0(6)
C1	O1	O4	C4	1.0(8)	O4	O1	C4	Fe1	175.2(12)
O4	O1	C4	O4	0.0(6)	O4	O1	C4	C1	178.5(13)
C4	O1	O4	C1	-1.0(8)	C4	O1	O4	C4	0.0(7)
C1	O1	C4	Fe1	-3.3(11)	C1	O1	C4	O4	-178.5(15)
C1	O1	C4	C1	0.0(10)	C4	O1	C1	O4	1.0(10)
C4	O1	C1	C4	0.0(7)	C4	O1	C1	C6	177.1(19)
O5	O2	C2	O5	-0.0(13)	O5	O2	C2	C5	-2.3(19)
C2	O2	O5	C2	-0.0(5)	C2	O2	O5	C5	1.1(9)
O5	O2	C5	Fe1	-178(3)	O5	O2	C5	O5	0.0(16)
O5	O2	C5	C2	177(3)	C5	O2	O5	C2	-1.1(12)
C5	O2	O5	C5	0.0(9)	C2	O2	C5	Fe1	5.2(13)
C2	O2	C5	O5	-177(3)	C2	O2	C5	C2	0.0(11)

C5	O2	C2	O5	2(2)	C5	O2	C2	C5	0.0(18)
O6	O3	C3	O6	0.0(5)	O6	O3	C3	C6	-2.7(8)
C3	O3	O6	C3	0.0(4)	C3	O3	O6	C6	2.4(7)
O6	O3	C6	Fe1	-177.9(16)	O6	O3	C6	O6	0.0(8)
O6	O3	C6	C3	175.9(16)	C6	O3	O6	C3	-2.4(9)
C6	O3	O6	C6	0.0(8)	C3	O3	C6	Fe1	6.2(8)
C3	O3	C6	O6	-175.9(15)	C3	O3	C6	C3	-0.0(7)
C6	O3	C3	O6	2.7(10)	C6	O3	C3	C6	-0.0(9)
O1	O4	C1	Fe1	-176.4(13)	O1	O4	C1	O1	0.0(5)
O1	O4	C1	C4	178.4(14)	O1	O4	C4	O1	0.0(4)
O1	O4	C4	C1	-1.1(9)	C1	O4	C4	O1	1.1(11)
C1	O4	C4	C1	-0.0(7)	C4	O4	C1	Fe1	5.2(13)
C4	O4	C1	O1	-178.4(17)	C4	O4	C1	C4	-0.0(12)
O2	O5	C2	Fe1	173.3(18)	O2	O5	C2	O2	-0.0(9)
O2	O5	C2	C5	177.6(19)	O2	O5	C5	O2	-0.0(9)
O2	O5	C5	C2	-2(2)	C2	O5	C5	O2	2(2)
C2	O5	C5	C2	-0.0(10)	C5	O5	C2	Fe1	-4(2)
C5	O5	C2	O2	-178(3)	C5	O5	C2	C5	0.0(19)
O3	O6	C3	Fe1	174.3(8)	O3	O6	C3	O3	0.0(4)
O3	O6	C3	C6	176.5(10)	O3	O6	C6	O3	0.0(3)
O3	O6	C6	C1	-173.1(14)	O3	O6	C6	C3	-2.3(9)
C3	O6	C6	O3	2.3(9)	C3	O6	C6	C1	-171(2)
C3	O6	C6	C3	-0.0(4)	C6	O6	C3	Fe1	-2.1(13)
C6	O6	C3	O3	-176.5(14)	C6	O6	C3	C6	-0.0(11)
Fe1	C1	C4	Fe1	0.00(3)	Fe1	C1	C4	O1	-176.6(10)
Fe1	C1	C4	O4	-175.2(11)	Fe1	C1	C6	Fe1	0.00(3)
Fe1	C1	C6	O6	-179.2(18)	Fe1	C1	C6	C3	15.2(17)
O1	C1	C4	Fe1	176.6(11)	O1	C1	C4	O1	0.0(5)
O1	C1	C4	O4	1.4(15)	O1	C1	C6	Fe1	-175.9(14)
O1	C1	C6	O6	5(2)	O1	C1	C6	C3	-160.7(17)
O4	C1	C4	Fe1	175.2(12)	O4	C1	C4	O1	-1.4(15)
O4	C1	C4	O4	-0.0(5)	C4	C1	C6	Fe1	-0.1(18)
C4	C1	C6	O6	-179.3(17)	C4	C1	C6	C3	15(3)
C6	C1	C4	Fe1	0.1(16)	C6	C1	C4	O1	-177(2)
C6	C1	C4	O4	-175.1(14)	Fe1	C2	C5	Fe1	-0.00(2)
Fe1	C2	C5	O2	176.7(7)	Fe1	C2	C5	O5	177.8(10)
O2	C2	C5	Fe1	-176.7(8)	O2	C2	C5	O2	0.0(4)
O2	C2	C5	O5	1.1(10)	O5	C2	C5	Fe1	-177.8(12)
O5	C2	C5	O2	-1.1(11)	O5	C2	C5	O5	0.0(6)
Fe1	C3	C6	Fe1	-0.00(3)	Fe1	C3	C6	O3	174.3(7)
Fe1	C3	C6	O6	177.7(12)	Fe1	C3	C6	C1	-13.2(14)
O3	C3	C6	Fe1	-174.3(8)	O3	C3	C6	O3	0.0(4)
O3	C3	C6	O6	3.4(13)	O3	C3	C6	C1	172.4(15)
O6	C3	C6	Fe1	-177.7(13)	O6	C3	C6	O3	-3.4(14)
O6	C3	C6	O6	-0.0(6)	O6	C3	C6	C1	169(3)
P1	C7	C8	C9	28.0(5)	Si1	C7	C8	C9	-86.2(4)
Si2	C7	C8	C9	155.6(3)	C7	C8	C9	C10	-44.2(6)
C8	C9	C10	P1	36.1(5)	C8	C9	C10	Si3	153.3(4)
C8	C9	C10	Si4	-89.4(5)	Sn1	C23	C24	C25	177.1(4)
Sn1	C23	C28	C27	-177.3(3)	C24	C23	C28	C27	0.4(8)
C28	C23	C24	C25	-0.5(9)	C23	C24	C25	C26	0.1(10)
C24	C25	C26	C27	0.4(10)	C25	C26	C27	C28	-0.6(10)
C26	C27	C28	C23	0.2(9)	Sn1	C29	C30	C31	177.5(4)
Sn1	C29	C34	C33	-177.3(4)	C30	C29	C34	C33	-0.5(9)
C34	C29	C30	C31	0.6(10)	C29	C30	C31	C32	-1.2(12)
C30	C31	C32	C33	1.7(12)	C31	C32	C33	C34	-1.6(12)
C32	C33	C34	C29	1.0(11)	Sn1	C35	C36	C37	-174.6(3)
Sn1	C35	C40	C39	173.8(4)	C36	C35	C40	C39	-0.7(9)
C40	C35	C36	C37	-0.2(8)	C35	C36	C37	C38	0.5(9)
C36	C37	C38	C39	0.1(9)	C37	C38	C39	C40	-1.1(10)
C38	C39	C40	C35	1.4(10)					

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