

## Electronic Supporting Information

### **Cyclometallated Iron(II) Alkoxides in Iron-Catalyzed C–H Activations by Weak *O*-Carbonyl Chelation**

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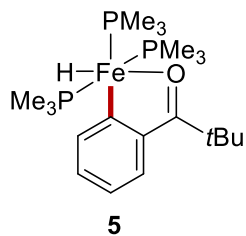
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## 1 General Remarks

All operations were conducted under an atmosphere of dry nitrogen using standard Schlenk and cannula techniques, or in a MBraun nitrogen filled glove box, unless otherwise stated. NMR-scale reactions were conducted using NMR tubes fitted with J. Young's tap valves. Nitrogen gas was passed through a drying column (CaCl<sub>2</sub>/Alumina/P<sub>2</sub>O<sub>5</sub>). [D]<sub>8</sub>-THF and C<sub>6</sub>D<sub>6</sub> were purchased from Deutero GmbH and were distilled from CaH<sub>2</sub>, degassed, and stored under nitrogen. Substrates were dried over calcium hydride, distilled, and degassed prior to use. Solution phase NMR spectra were collected on a Varian Inova 600 or Varian Inova 500 or Bruker Avance III HD 400 or Bruker Avance III 400 or Bruker Avance Neo 400 or Bruker Avance III HD 300 in the solvent indicated at ambient probe temperatures (290 K), unless otherwise stated. Chemical shifts were referenced to the residual proton signal in the deuterated solvent (<sup>1</sup>H), the <sup>13</sup>C shift of the solvent (<sup>13</sup>C), or to external 85% H<sub>3</sub>PO<sub>4</sub> aqueous solution (<sup>31</sup>P).<sup>1</sup> Chemical shifts are reported in ppm and coupling constants in Hz. All IR spectra were recorded on a Thermo Scientific Nicolet iS5 device equipped with an iD7 ATR detector. HESI-MS were recorded on a Thermo Scientific Exactive Plus equipped with an Orbitrap detector. LIFDI-MS measurements were performed on a Jeol AccuTOF GCv spectrometer. EPR spectra were measured on a Bruker ELEXSYS E500 spectrometer, equipped with the digital temperature control system ER 4131VT using nitrogen as coolant. All spectra were recorded in frozen matrices (temperature range 140 – 150K), at about 9.4 GHz microwave frequency, 4 G field modulation amplitude, 100 kHz field modulation frequency, and around 10 mW microwave power. The following compounds were synthesized according to literature procedures or slight modifications thereof: [Fe(PMe<sub>3</sub>)<sub>4</sub>]<sup>2</sup> and **2**.<sup>3</sup>

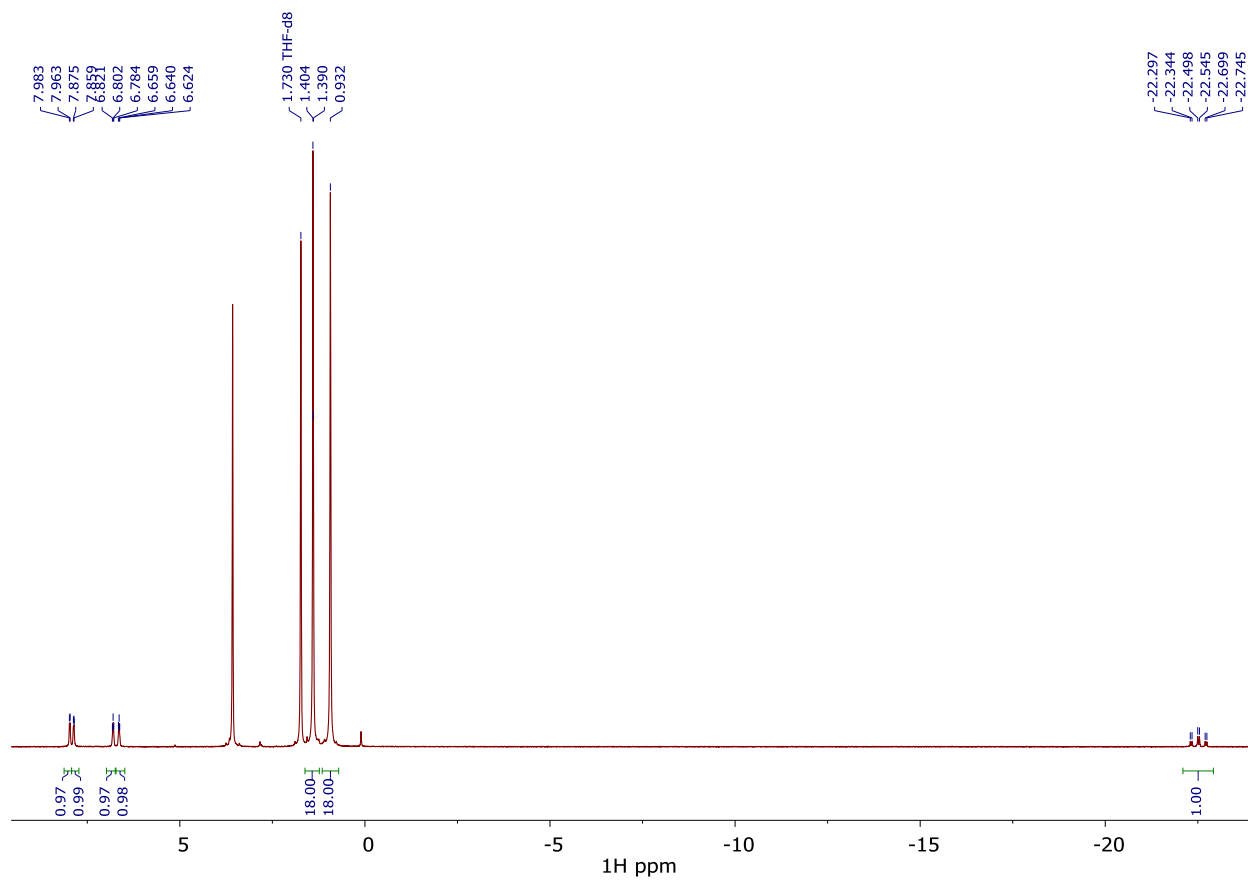
## 2 Synthesis, Isolation, and Characterization of Organometallic Complexes

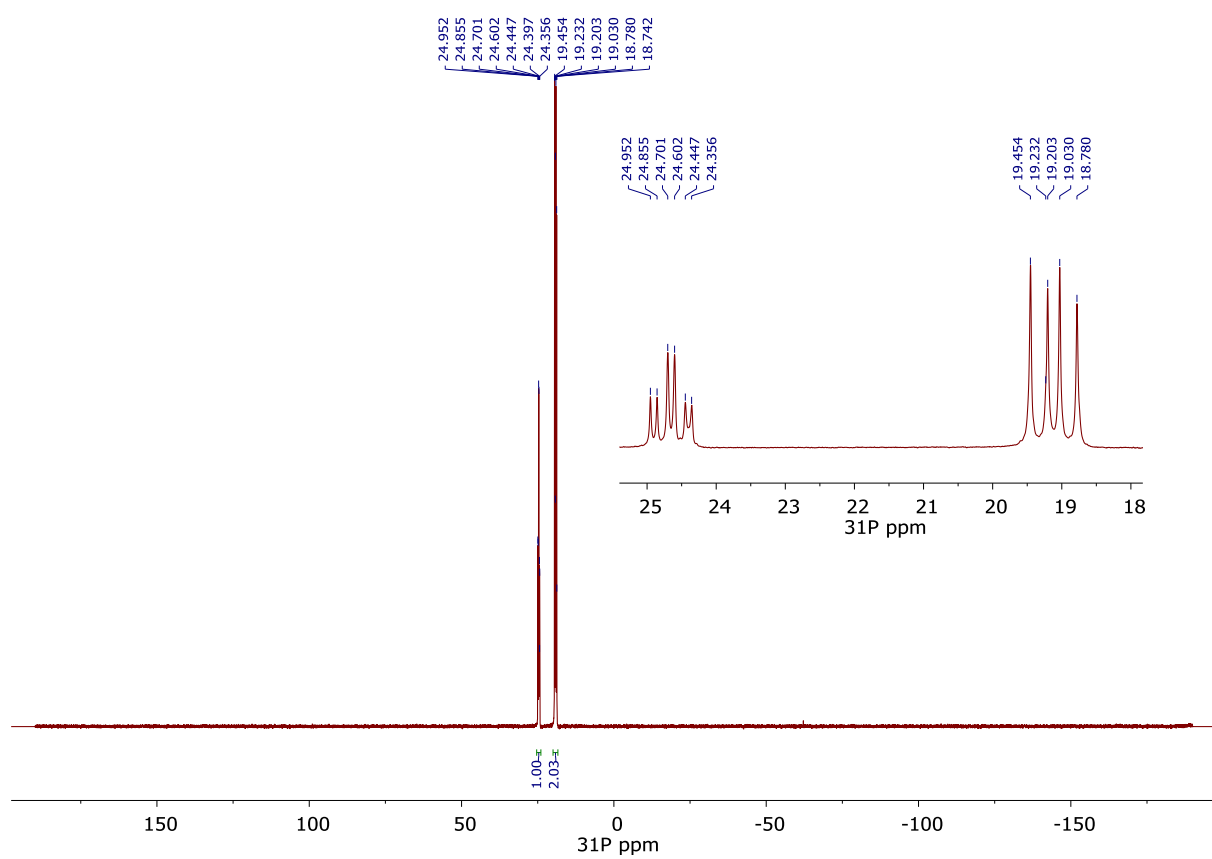
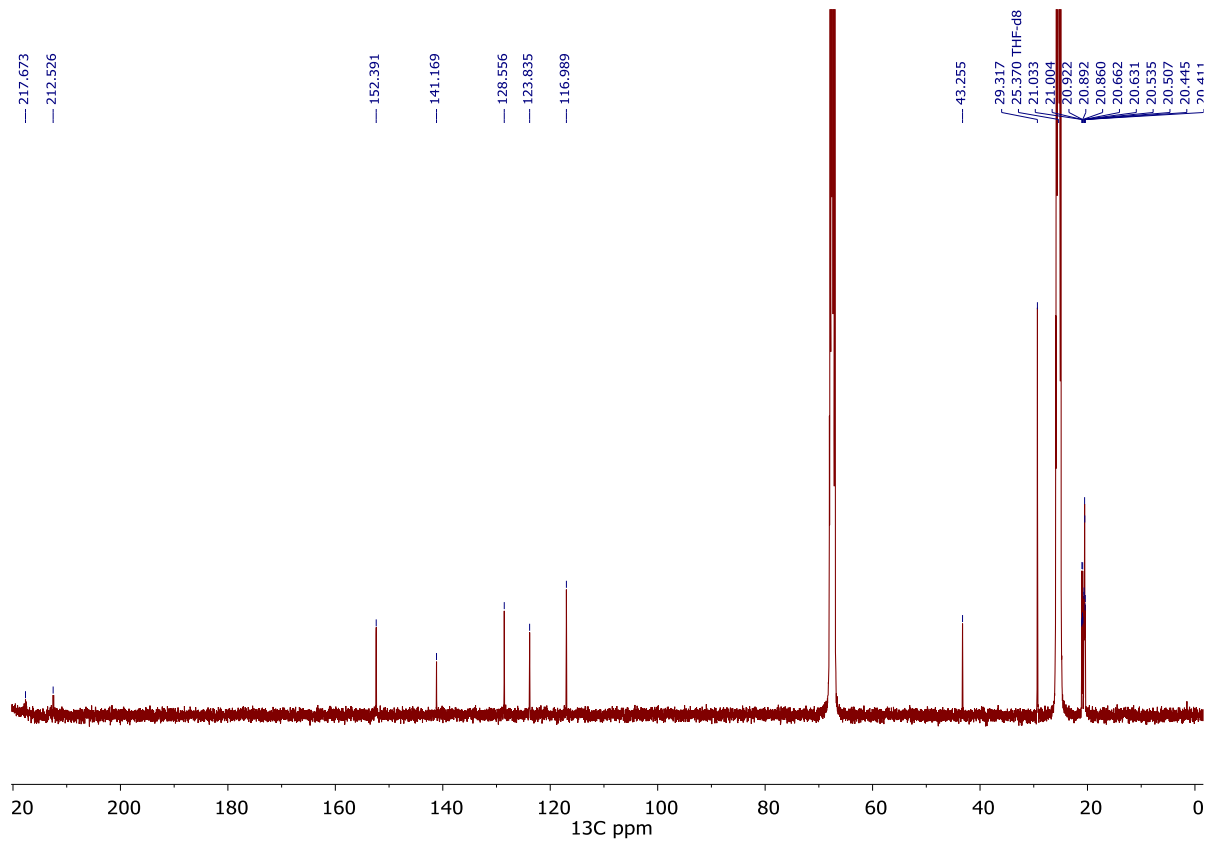
### 2.1 Iron Hydride Complex **5**



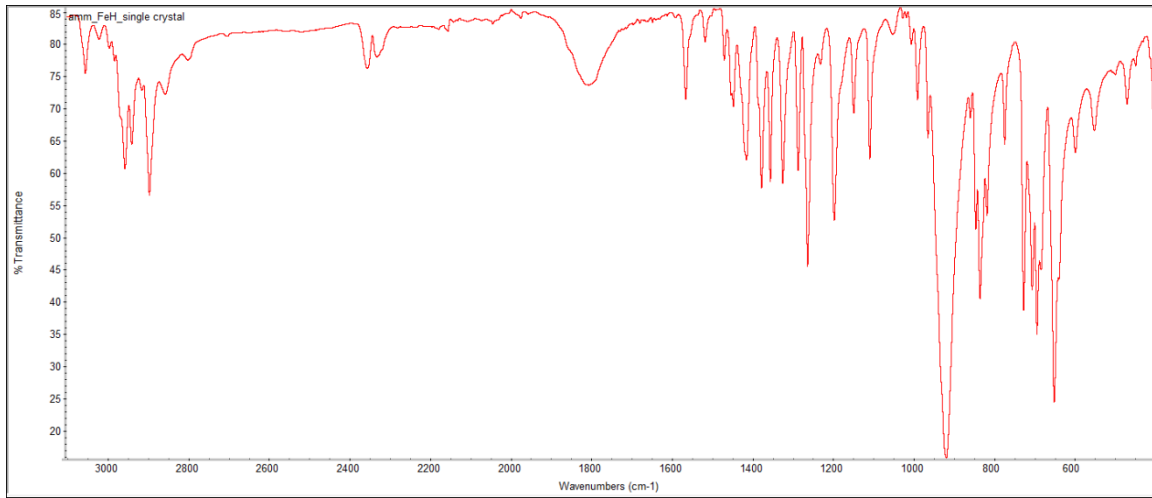
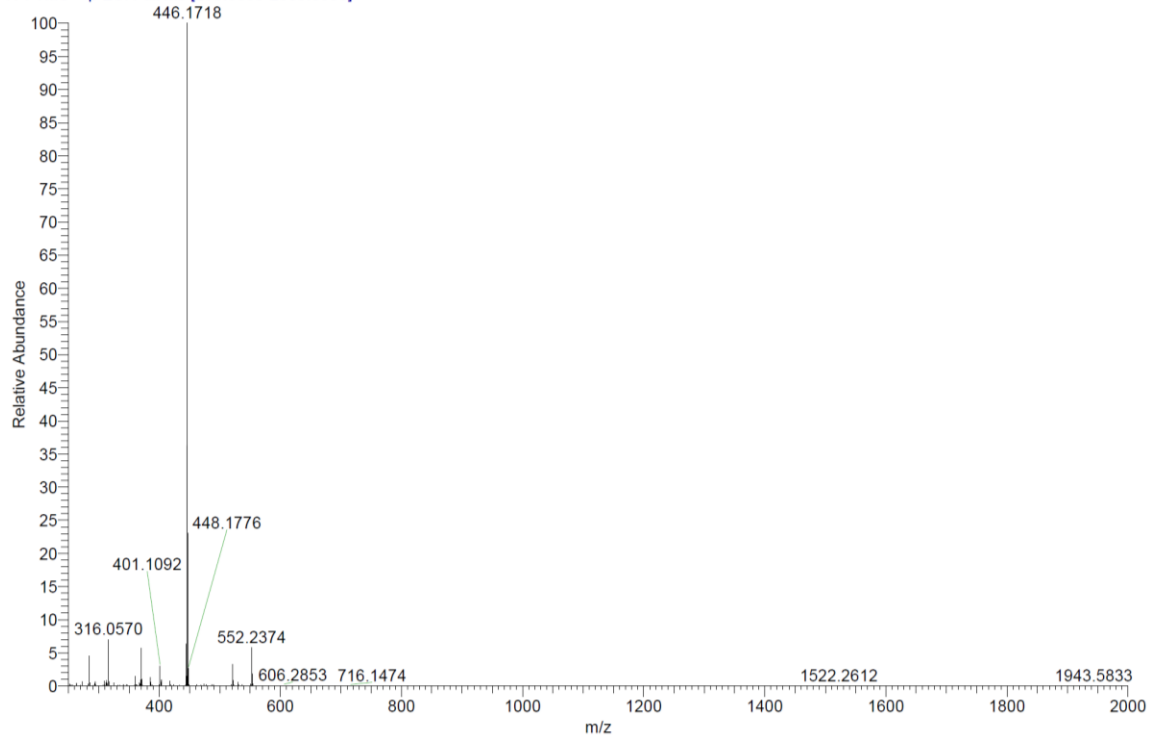
Complex **5** has been previously isolated from the reaction between **4** and **1** in toluene.<sup>4</sup> Here an improved methodology for obtaining **5** in good yield is reported: in a nitrogen filled glove box a vial was loaded with a PTFE coated stirring bar, **4** (200 mg, 0.56 mmol), **1** (200  $\mu$ L, 1.18 mmol), and benzene (150  $\mu$ L). The resulted dark yellow solution was stirred for 12 h during which time it gradually changed color to deep ink blue. The solution was diluted with benzene (300  $\mu$ L) and the reaction was stirred for an additional 2 h. The mixture was then dried under reduced pressure and extracted with ether. The dark ink blue ether extracts were stirred for an additional hour, condensed to 2 mL, and stored at -20 °C. After 12 hours dark crystals of **5** formed which were isolated by decanting the solution. The filtrate was condensed and a second crop of **5** obtained which was combined with the first crop to give **5** in the form of dichroic blue/yellow thin crystalline plates (130 mg, 52% yield).

**<sup>1</sup>H NMR** (400 MHz, THF-*d*<sub>8</sub>, -40 °C)  $\delta$  = 7.97 (d, *J* = 7.3 Hz, 1H), 7.87 (d, *J* = 6.4 Hz, 1H), 6.80 (dd, *J* = 6.4, 6.4 Hz, 1H), 6.64 (dd, *J* = 7.3, 6.4 Hz, 1H), 1.40 (s, 9H), 1.39 (s, 9H), 0.93 (s, 18H), -22.52 (td, *J* = 80.3, 18.7 Hz, 1H). **<sup>13</sup>C{<sup>1</sup>H} NMR** (101 MHz, THF-*d*<sub>8</sub>, -40 °C)  $\delta$  = 217.7 (s, C<sub>q</sub>), 212.5 (m, C<sub>q</sub>), 152.4 (s, CH), 141.2 (s, CH), 128.6 (s, CH), 123.8 (s, CH), 117.0 (s), 43.3 (s, C<sub>q</sub>), 29.3 (s, CH<sub>3</sub>), 21.0 (dt, *J* = 14.4, 3.1 Hz, CH<sub>3</sub>), 20.5 (td, *J* = 11.2, 9.7, 3.3 Hz, CH<sub>3</sub>). **<sup>31</sup>P NMR** (162 MHz, THF-*d*<sub>8</sub>, -40 °C)  $\delta$  = 24.7 (td, *J* = 40.4, 15.2 Hz, 1P), 19.1 (dd, *J* = 68.6, 40.4 Hz, 2P). **IR** (ATR): 3061, 3027, 2361, 2337, 1812, 1523, 1475, 1236, 1011, 454 cm<sup>-1</sup>. **HRMS** (H-ESI) *m/z* calcd for C<sub>20</sub>H<sub>41</sub>FeOP<sub>3</sub> [M]<sup>+</sup>: 446.1720, found: 446.1718. **Anal.** Calcd for C<sub>20</sub>H<sub>41</sub>FeOP<sub>3</sub>: C, 53.82%; H, 9.26%. Found: C, 53.41%; H, 8.77%.

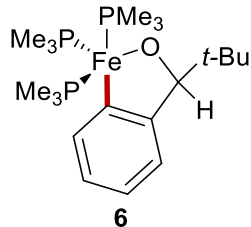




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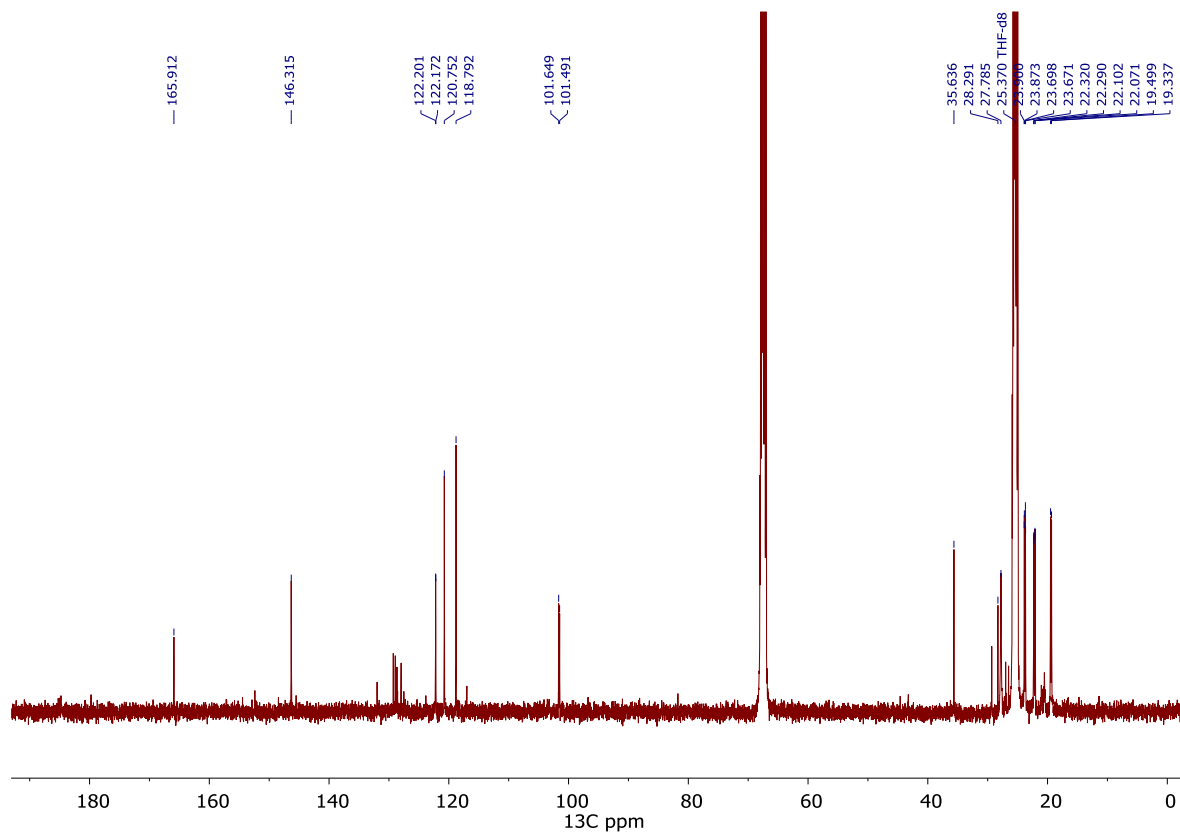
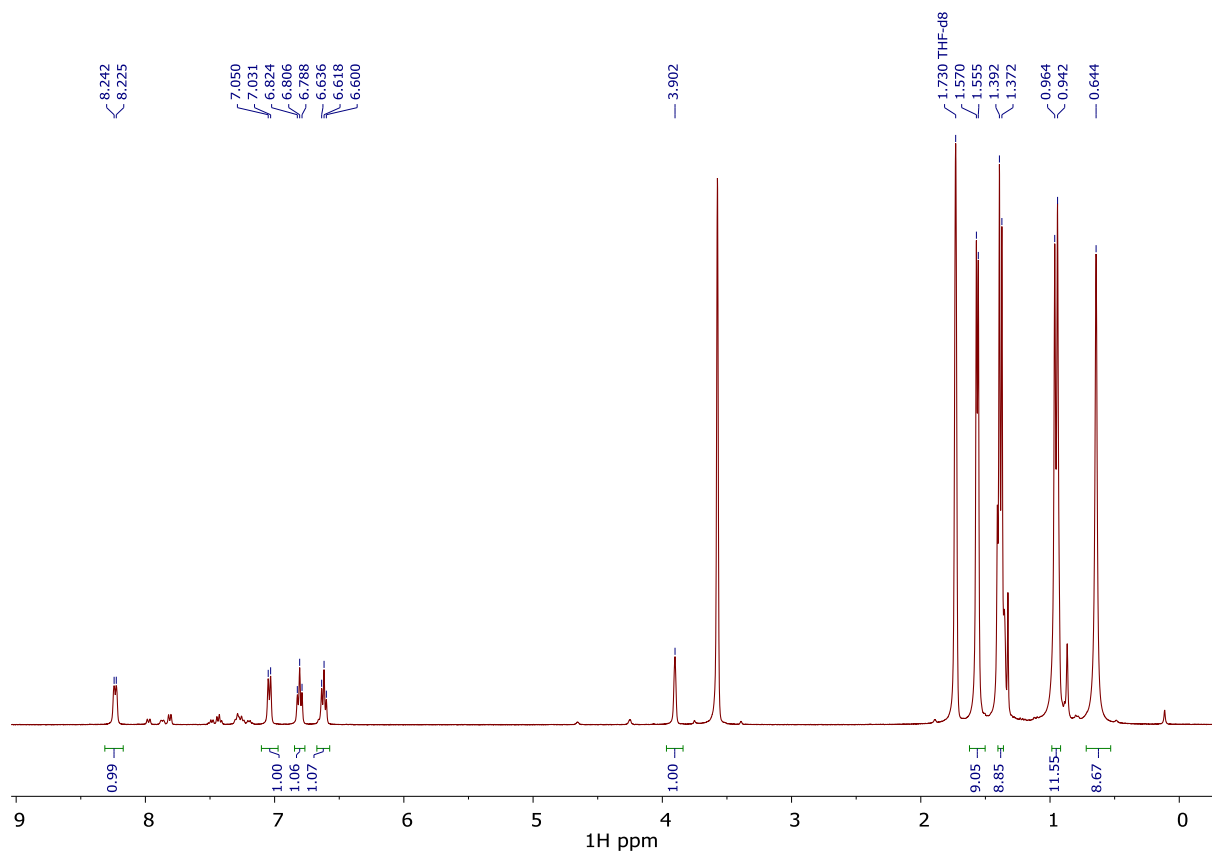
## 2.2 Iron Alkoxide Complex **6**

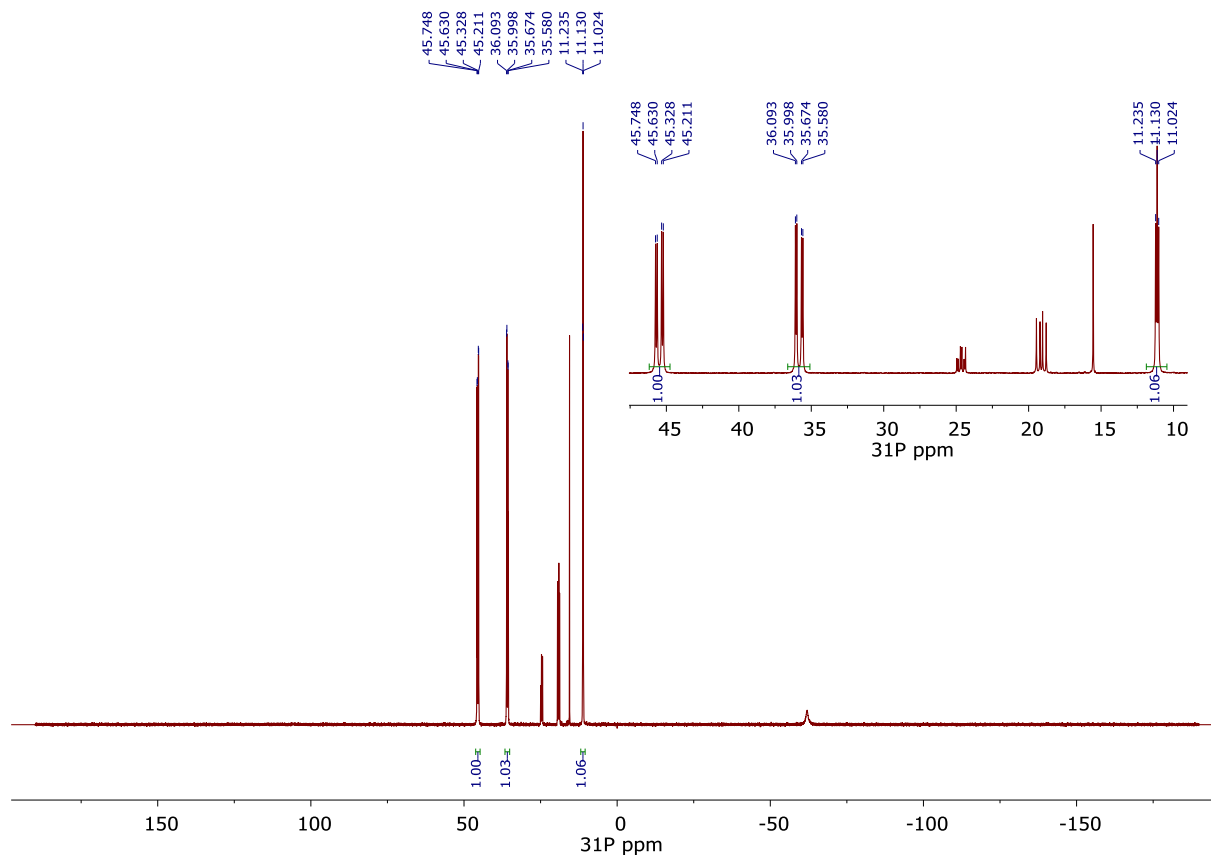


In a nitrogen filled glove box a vial was loaded with a PTFE coated stirring bar, **4** (220 mg, 0.61 mmol), and **1** (220  $\mu$ L, 1.32 mmol). The resulted dark yellow solution was slowly stirred for 3 hours during which time a gradual color change occurred from dark yellow to green, cyan-green, and blue at which time the viscous solution solidified to give a dark paste. The residue was subsequently dissolved in pentane (6 mL) and filtered through a PTFE Millipore filter (0.22 micron). The dark solution was immediately stored at - 30  $^{\circ}$ C for 24 hours during which time **6** precipitated as a solid which was isolated by decanting the supernatant solution, washed with cold pentane (- 30  $^{\circ}$ C, 1 mL), and dried under reduced pressure to yield **6** in the form of a green/cyan microcrystalline solid (151.3 mg, 56% yield). Crystals of **6** suitable for an X-ray crystallographic study were obtained by slowly cooling a pentane solution of **6** at - 30  $^{\circ}$ C. It must be noted that a minor contamination with **5** in the spectra of **6** is sometimes observed due to the instability of **6** and its fast rearrangement to **5** in solution. The above reaction was repeated in a vial sealed with an airtight septum. Subsequently, a headspace sample was collected from the vial with an airtight micro syringe and submitted for a gas chromatographic analysis. No hydrogen gas was detected with only nitrogen and a trace amount of oxygen observed.

**$^1\text{H}$  NMR** (400 MHz, THF- $d_8$ )  $\delta$  = 8.23 (d,  $J$  = 6.8 Hz, 1H), 7.04 (d,  $J$  = 7.3 Hz, 1H), 6.81 (dd,  $J$  = 7.3, 6.8 Hz, 1H), 6.62 (dd,  $J$  = 7.3, 7.3 Hz, 1H), 3.90 (s, 1H), 1.56 (d,  $J$  = 5.9 Hz, 9H), 1.38 (d,  $J$  = 7.6 Hz, 9H), 0.95 (d,  $J$  = 8.8 Hz, 9H), 0.64 (s, 9H).  **$^{13}\text{C}\{^1\text{H}\}$  NMR** (101 MHz, THF- $d_8$ )  $\delta$  = 165.9 (s), 146.3 (s), 122.2 (d,  $J$  = 3.0 Hz), 120.8 (s), 118.8 (s), 101.6 (d,  $J$  = 15.9 Hz), 35.6 (s,  $\text{C}_q$ ), 28.3 (s,  $\text{CH}_3$ ), 27.8 (s, CH), 23.8 (dd,  $J$  = 20.3, 2.7 Hz,  $\text{CH}_3$ ), 22.2 (dd,  $J$  = 21.9, 3.1 Hz,  $\text{CH}_3$ ), 19.4 (d,  $J$  = 16.4 Hz,  $\text{CH}_3$ ).  **$^{31}\text{P}$  NMR** (162 MHz, THF- $d_8$ )  $\delta$  = 45.5 (dd,  $J$  = 68.0, 19.0 Hz, 1P), 35.8 (dd,  $J$  = 67.8, 15.3 Hz, 1P), 11.2 (t,  $J$  = 17.1 Hz, 1P). **IR** (ATR): 3028, 2361, 2338, 1566, 1477, 1200, 1173, 784, 491, 445  $\text{cm}^{-1}$ . **HRMS** (H-ESI)  $m/z$  calcd for  $\text{C}_{20}\text{H}_{41}\text{FeOP}_3$   $[\text{M}]^+$ : 446.1720, found: 446.1720. **Anal.** Calcd for  $\text{C}_{20}\text{H}_{41}\text{FeOP}_3$ : C, 53.82%; H, 9.26%. Found: C, 53.60%; H, 8.72%.



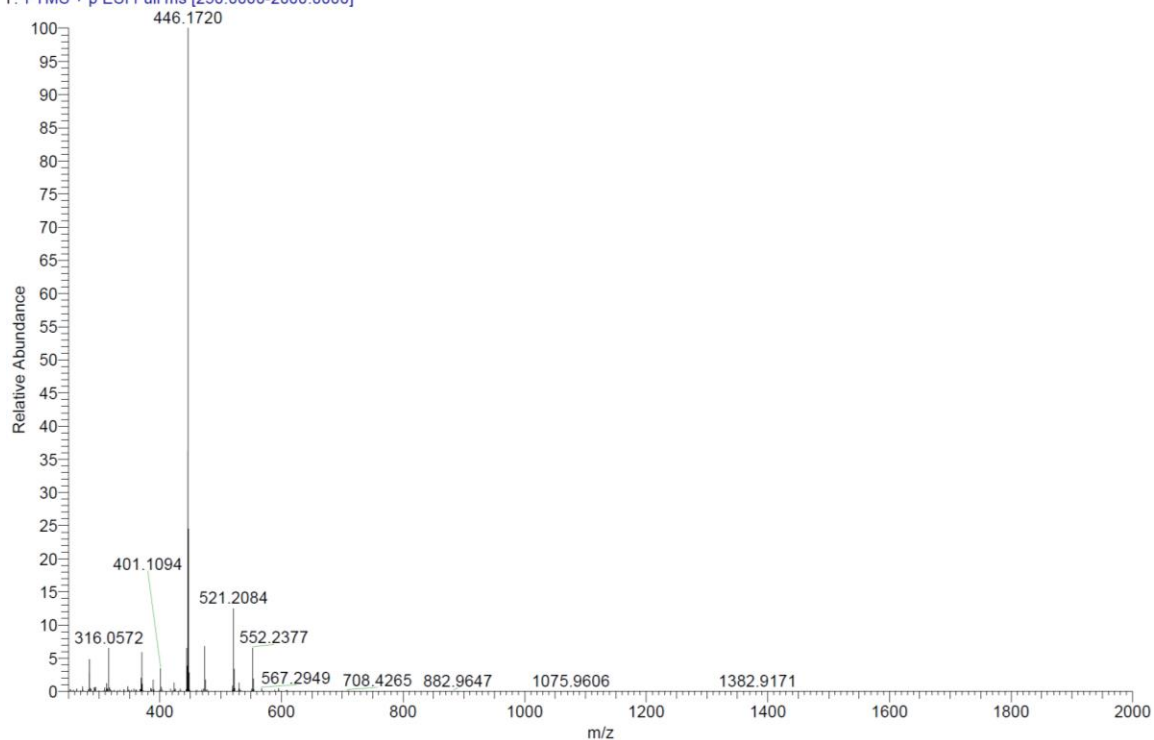


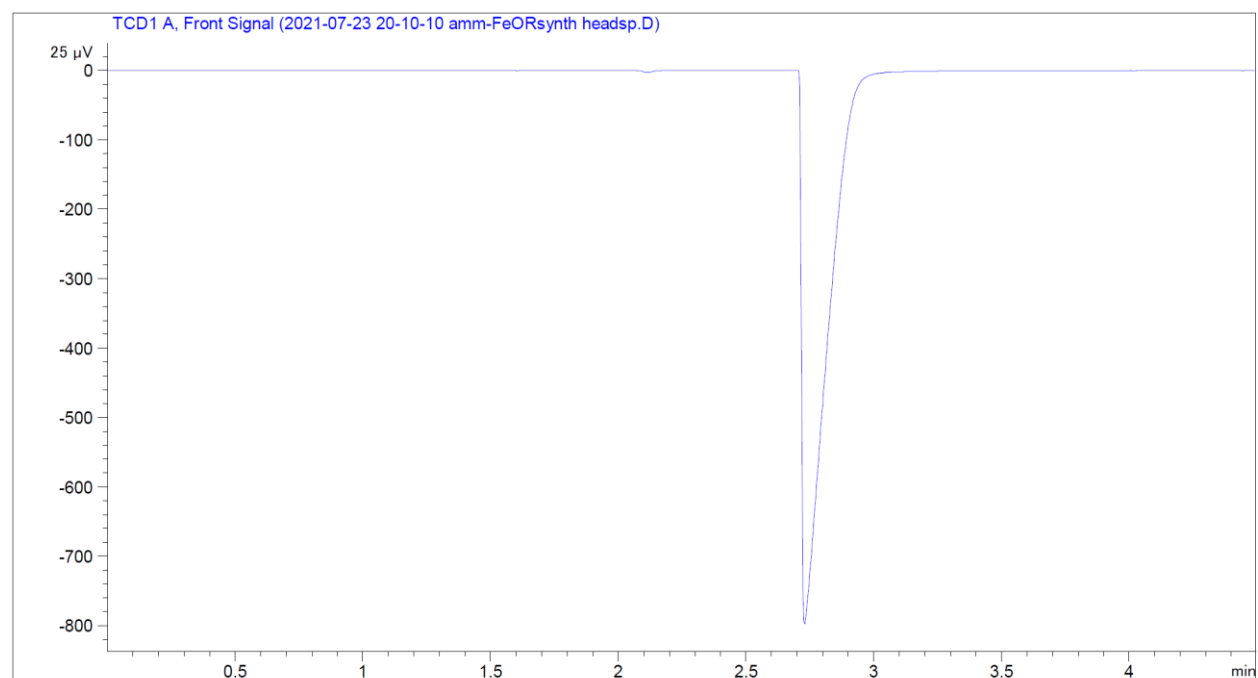
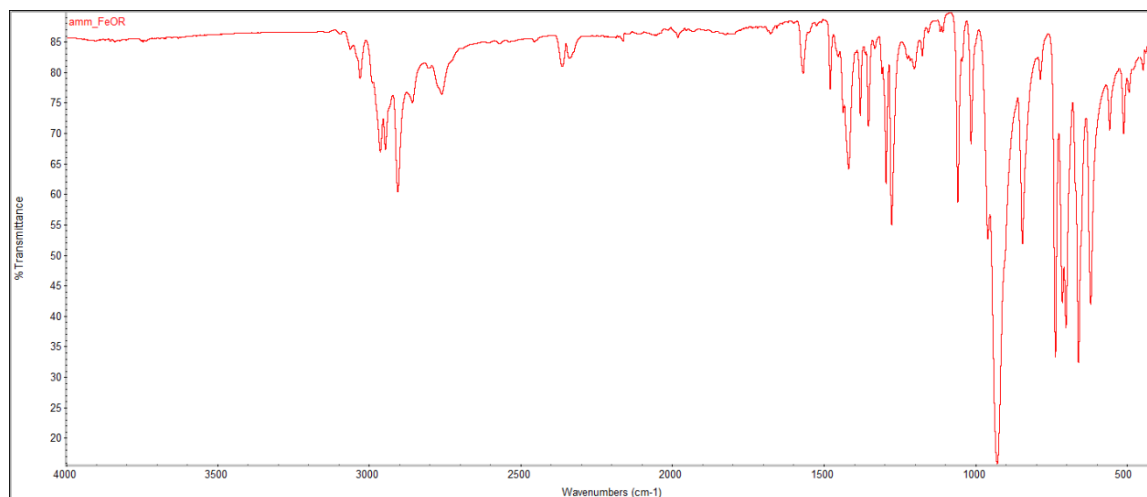


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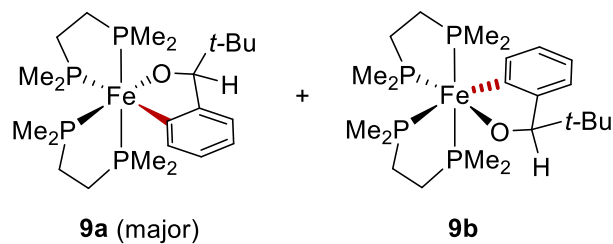
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### 2.3 Complex 9

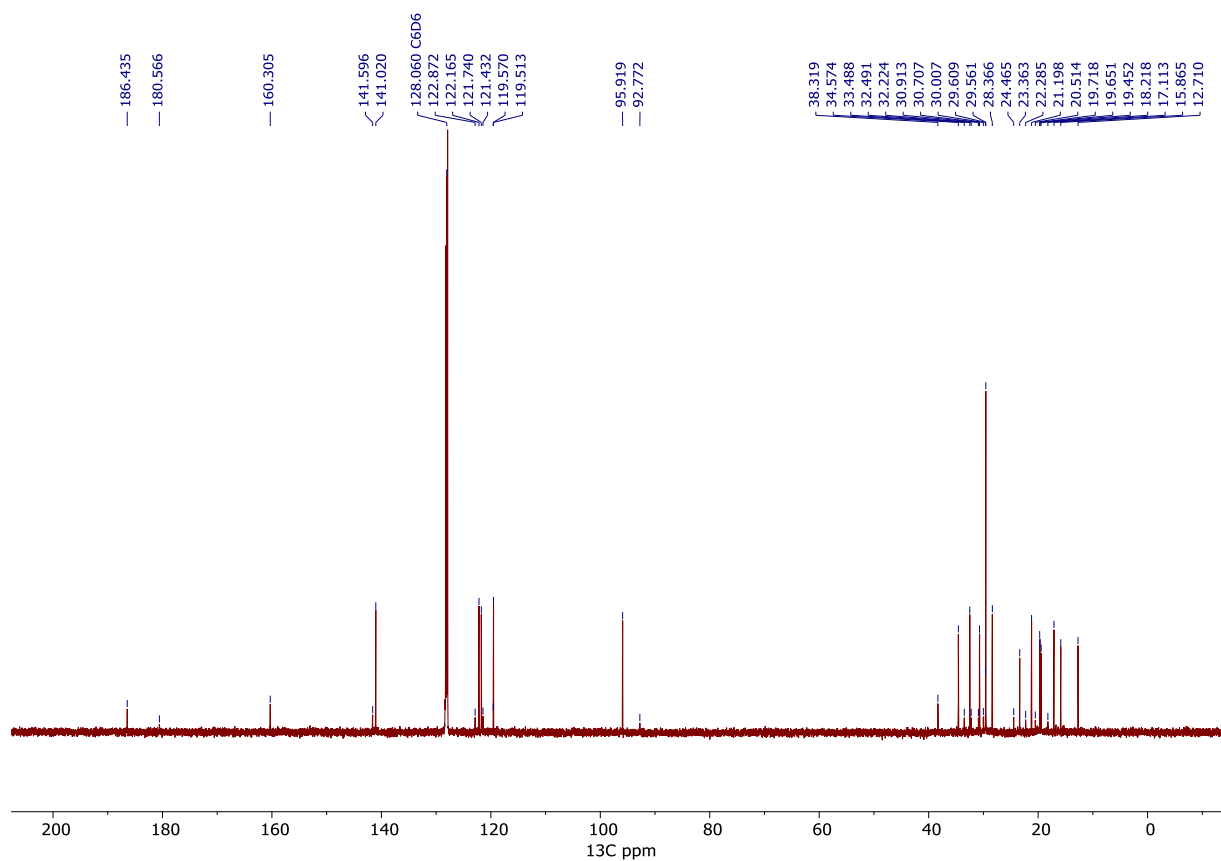
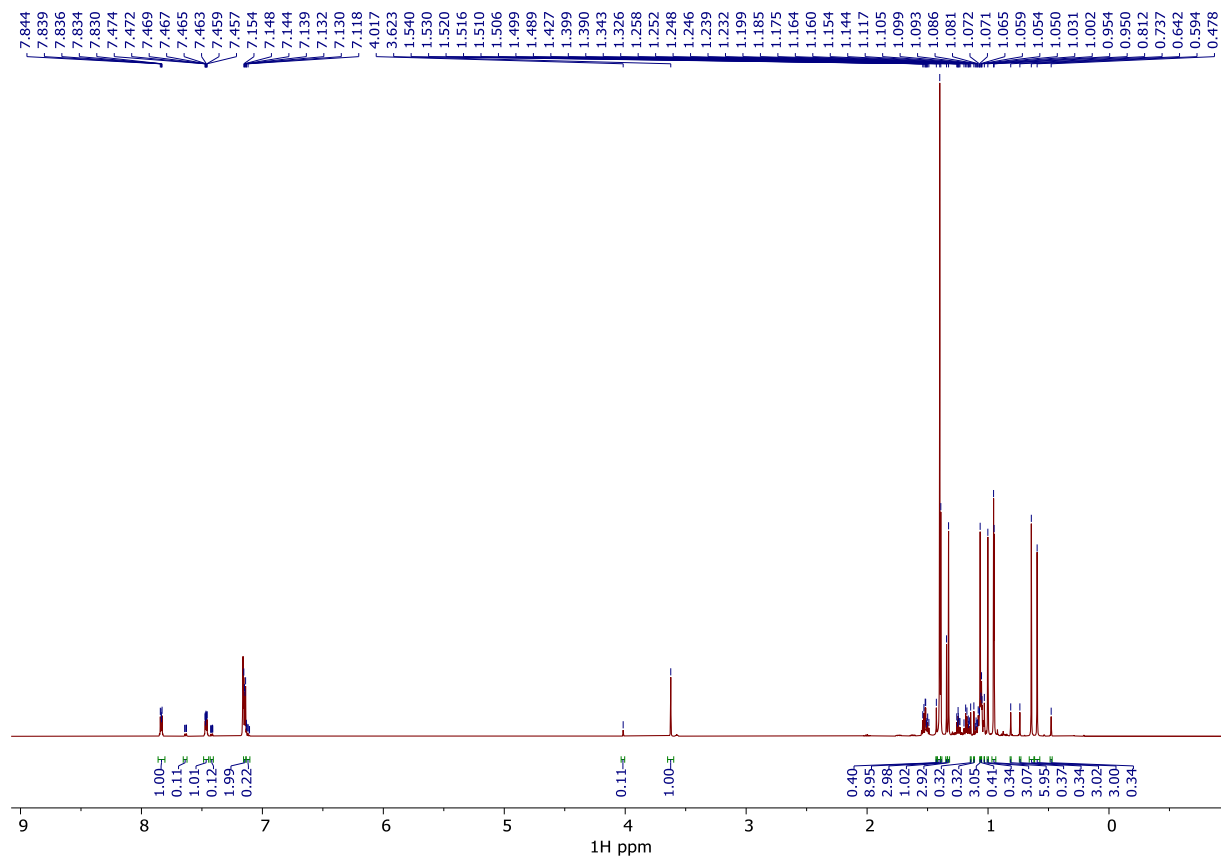


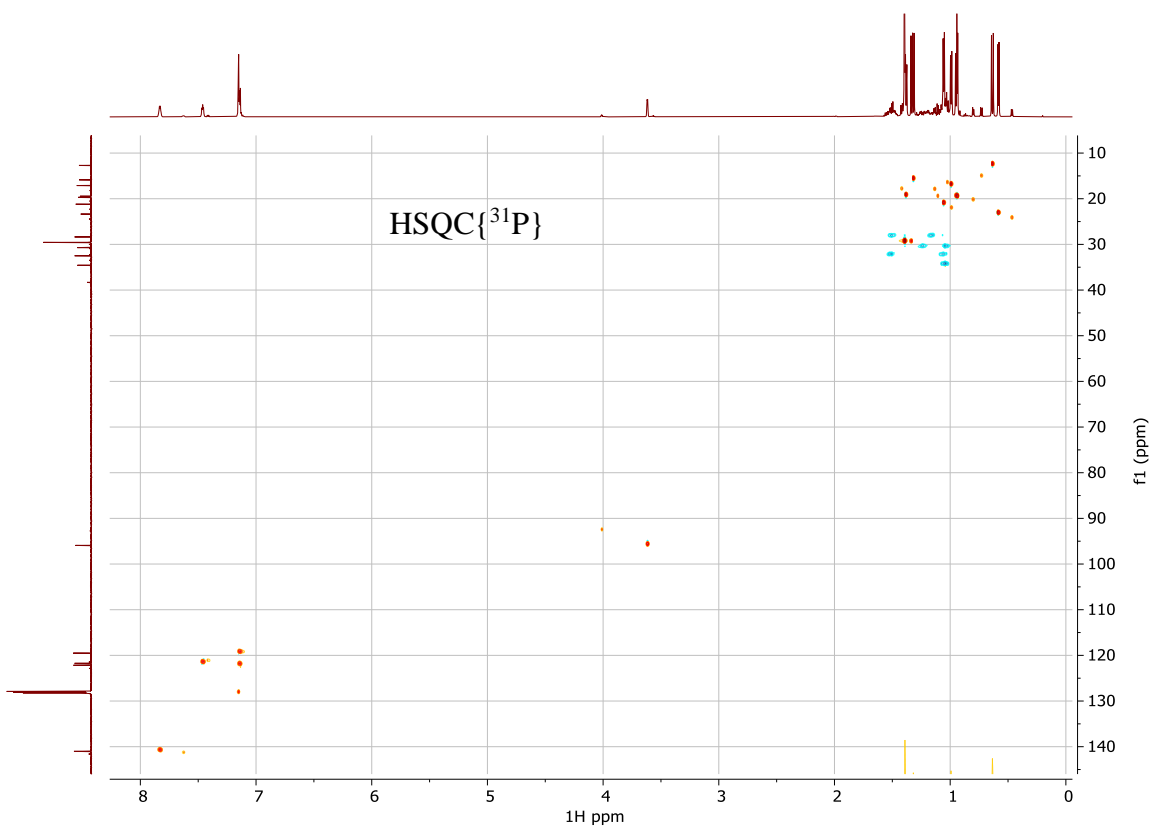
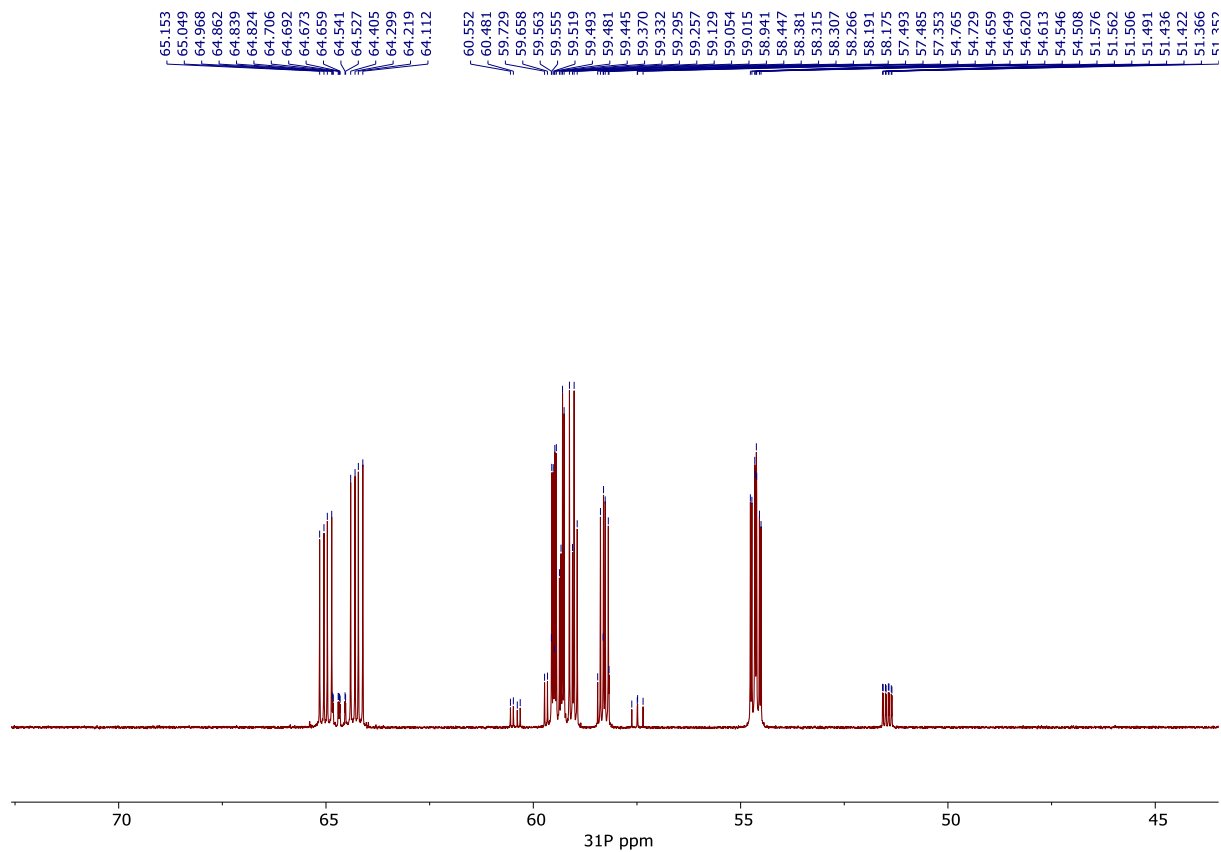
In a nitrogen filled glove box a vial was loaded with a PTFE coated stirring bar, **4** (110 mg, 0.31 mmol), and **1** (110  $\mu$ L, 0.66 mmol). The resulted yellow solution was slowly stirred during which time a gradual color change occurred from dark yellow to green, cyan-green, and blue at which

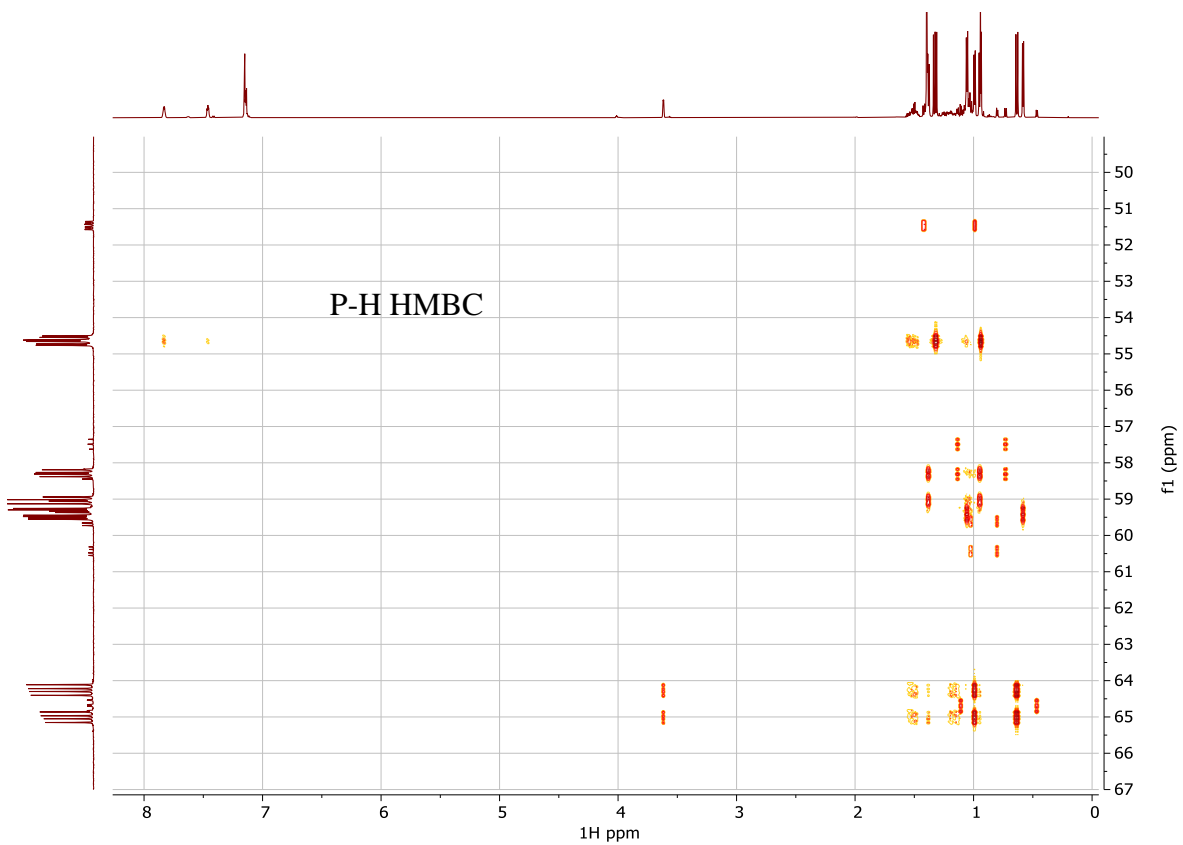
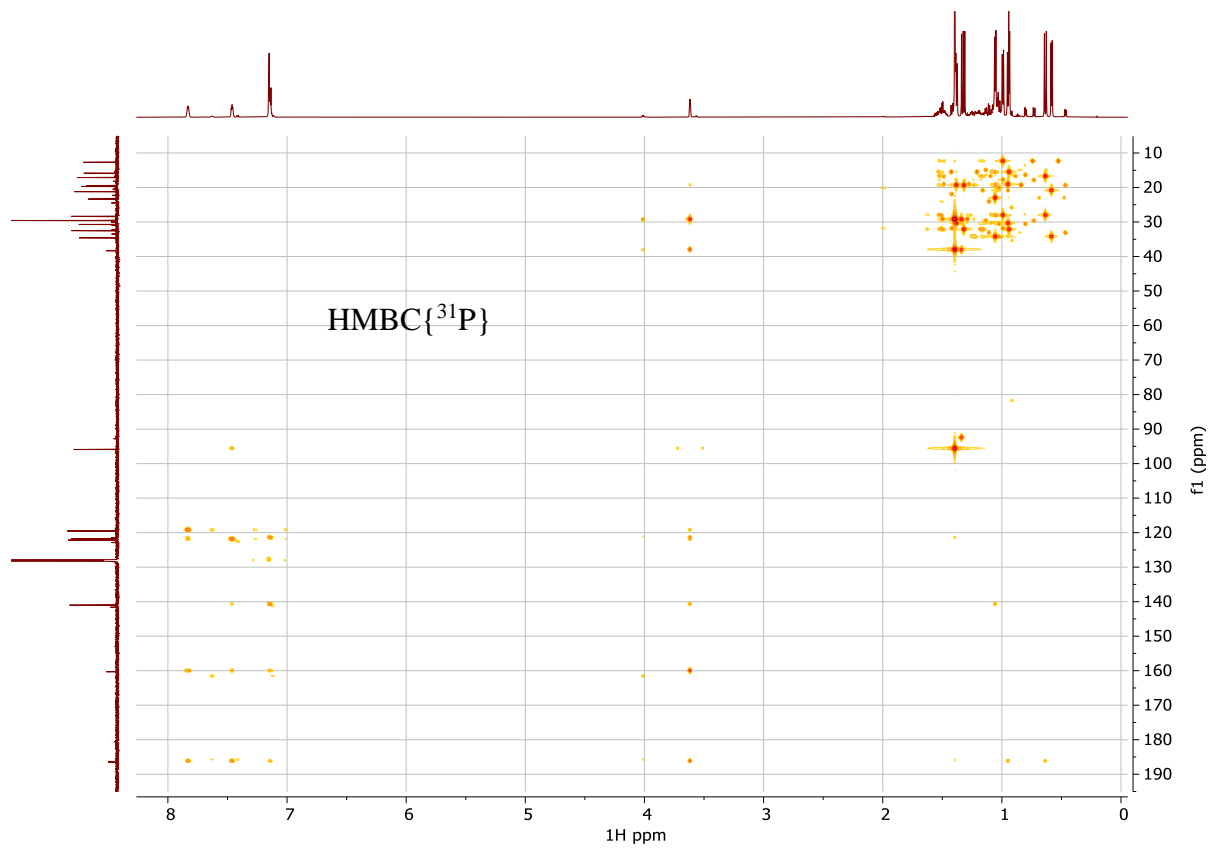
time the viscous solution solidified to give a dark paste (about 4 hours). Pentane (3 mL) was added followed by addition of dmpe (110  $\mu$ L, 0.66 mmol) which resulted in immediate formation of an orange crystalline solid. The mixture was sonicated (1 min), stirred for one hour, and stored at -20  $^{\circ}$ C for 12 hours. The supernatant solution was then decanted while still cold and the isolated solid was washed with cold pentane until the washings are dark orange in color to yield complex **9** as a mixture of two stereoisomers in the form of an orange crystalline solid (80.1 mg, 50% yield). Crystals suitable for an X-ray crystallographic analysis were grown by slowly evaporating a benzene solution of **9**. As expected, complex **9** is also formed quantitative upon reaction of either **5** or **6** with two equivalents of dmpe: in a nitrogen filled glove box an NMR tube was loaded with **6** (10 mg, 0.022 mmol) followed by addition of dmpe (15  $\mu$ L, 0.090 mmol) and  $C_6D_6$ . An immediate color change to purple and then dark orange occurred. Quantitative formation of complex **9** was confirmed from a  $^{31}P$  NMR spectroscopic analysis of the solution. The above reaction was repeated with **5** in the place of **6** resulting in an orange solution whose  $^{31}P\{^1H\}$  NMR spectrum was identical to the one obtained from the crude reaction mixture with **6** again implying formation of **9**.

$^1H\{^{31}P\}$  NMR (600 MHz,  $C_6D_6$ )  $\delta$  = 7.93 – 7.74 (m, 1H, **9a**), 7.63 (dd,  $J$  = 7.2, 1.5 Hz, 0.11H, **9b**), 7.48 – 7.45 (m, 1H, **9a**), 7.42 (dt,  $J$  = 7.3, 1.4 Hz, 0.11H, **9b**), 7.16 – 7.14 (m,  $J$  = 5.6, 3.2 Hz, 2H, **9a**), 7.15 – 7.09 (m, 0.22H, **9b**), 4.02 (s, 0.11H, **9b**), 3.62 (s, 1H, **9a**), 1.43 (s, 0.11H, **9b**), 1.40 (s, 9H, **9a**), 1.39 (s, 3H, **9a**), 1.34 (s, 0.99H, **9b**), 1.33 (s, 3H, **9a**), 1.14 (s, 0.33H, **9b**), 1.12 (s, 0.33H, **9b**), 1.07 (s, 3H, **9a**), 1.05 (s, 0.33H, **9b**), 1.03 (s, 0.33H, **9b**), 1.00 (s, 3H, **9a**), 0.95 (s, 3H, **9a**), 0.95 (s, 3H, **9a**), 0.81 (s, 0.33H, **9b**), 0.74 (s, 0.33H, **9b**), 0.64 (s, 3H, **9a**), 0.59 (s, 3H, **9a**), 0.48 (s, 0.33H, **9b**). Due to the complexity of the spectrum, it was not possible to assign  $CH_2$  signals.  $^{13}C\{^1H, ^{31}P\}$  NMR (151 MHz,  $C_6D_6$ )  $\delta$  = 186.4 ( $C_{Fe}$ , **9a**), 180.6 ( $C_{Fe}$ , **9b**), 160.4 ( $C_q$ , **9b**), 160.3 ( $C_q$ , **9a**), 141.6 (CH, **9b**), 141.0 (CH, **9a**), 122.9 (CH, **9b**), 122.2 (CH, **9a**), 121.7 (CH, **9a**), 121.4 (CH, **9b**), 119.6 (CH, **9b**), 119.5 (CH, **9a**), 95.9 (CH, **9a**), 92.8 (CH, **9b**), 38.3 ( $C_q$ , **9a**), 34.6 ( $CH_2$ , **9a**), 33.5 ( $CH_2$ , **9b**), 32.5 ( $CH_2$ , **9a**), 32.2 ( $CH_2$ , **9b**), 30.9 ( $CH_3$ , **9b**), 30.7 ( $CH_2$ , **9a**), 30.0 ( $CH_2$ , **9b**), 29.6 ( $CH_3$ , **9b**), 29.6 ( $CH_3$ , **9a**), 28.4 ( $CH_2$ , **9a**), 24.5 ( $CH_3$ , **9b**), 23.4 ( $CH_3$ , **9a**), 22.3 ( $CH_3$ , **9b**), 21.2 ( $CH_3$ , **9a**), 20.5 ( $CH_3$ , **9b**), 19.7 ( $CH_3$ , **9a**), 19.7 ( $CH_3$ , **9a**), 19.5 ( $CH_3$ , **9a**), 18.2 ( $CH_3$ , **9b**), 17.1 ( $CH_3$ , **9a**), 15.9 ( $CH_3$ , **9a**), 12.7 ( $CH_3$ , **9a**), five signals from **9b** were not observed due to its low concentration.  $^{31}P$  NMR (243 MHz,  $C_6D_6$ )  $\delta$  = 64.7 (ddd,  $J$  = 40.2, 32.3, 3.5 Hz, 0.11P, **9b**), 64.6 (ddd,  $J$  = 182.2, 45.3, 25.6 Hz, 1P, **9a**), 60.0 (ddd,  $J$  = 199.8, 40.2, 17.1 Hz, 0.11P,

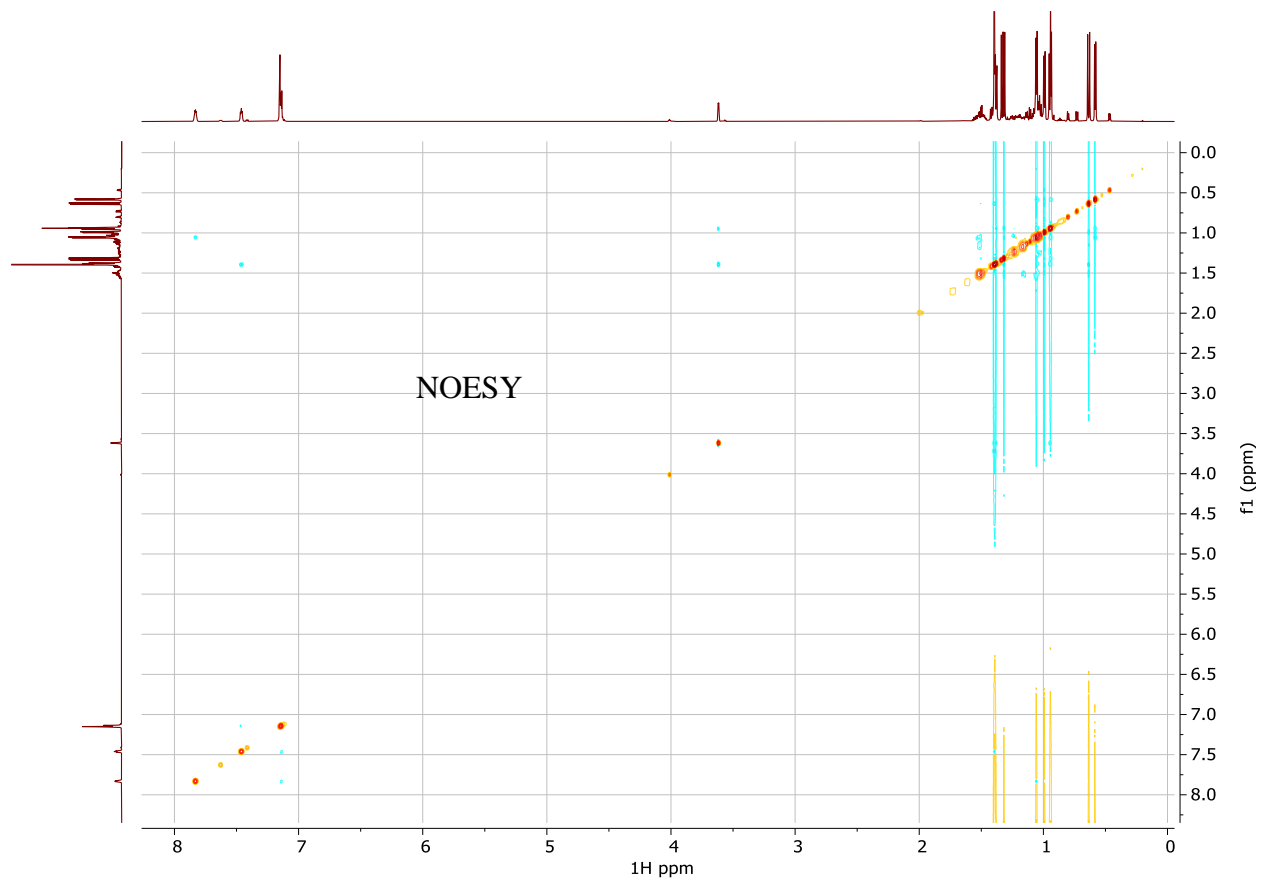
**9b**), 59.4 (ddd,  $J = 45.5, 18.1, 9.0$  Hz, 1P, **9a**), 58.7 (ddd,  $J = 182.3, 27.8, 18.1$  Hz, 1P, **9a**), 58.0 (ddd,  $J = 200.0, 34.0, 32.2$  Hz, 0.11P, **9b**), 54.6 (ddd,  $J = 27.3, 25.6, 9.0$  Hz, 1P, **9a**), 51.5 (ddd,  $J = 33.9, 17.1, 3.5$  Hz, 0.11P, **9b**). **IR** (ATR): 2901, 1562, 1420, 1321, 1106, 924, 886, 709, 689, 639, 445  $\text{cm}^{-1}$ . **HRMS** (H-ESI)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{46}\text{FeOP}_4$   $[\text{M}]^+$ : 518.1849, found: 518.1843. **Anal.** Calcd for  $\text{C}_{23}\text{H}_{46}\text{FeOP}_4$ : C, 53.29%; H, 8.95%. Found: C, 53.37%; H, 8.95%.



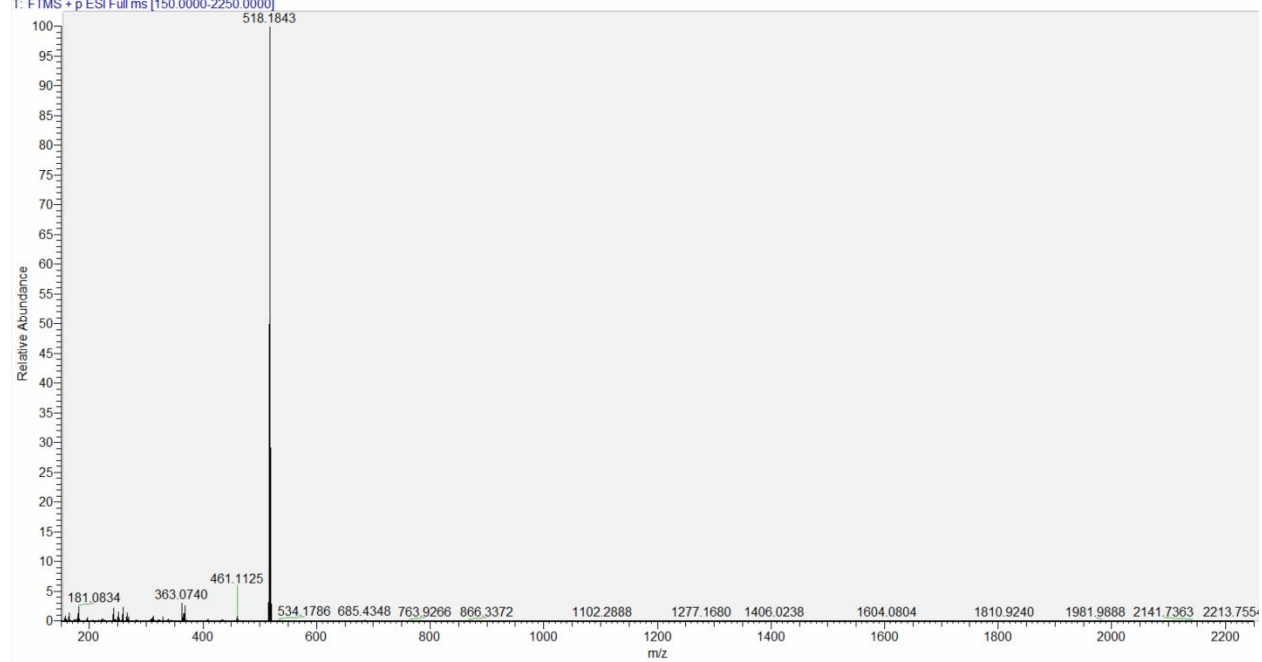




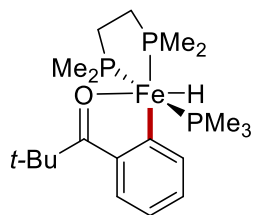




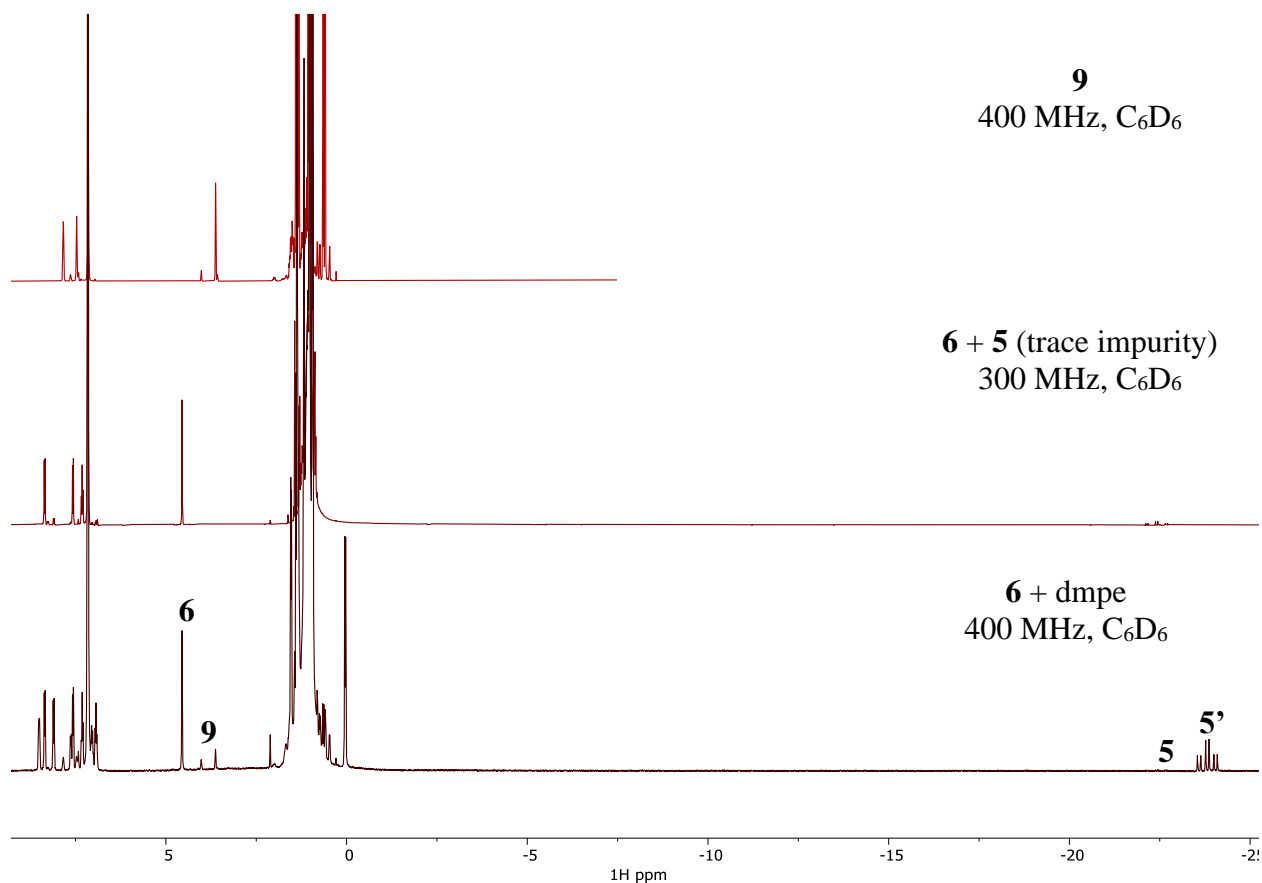
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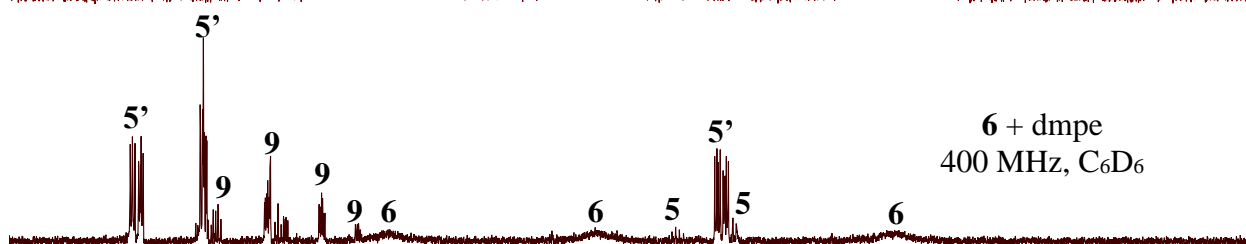
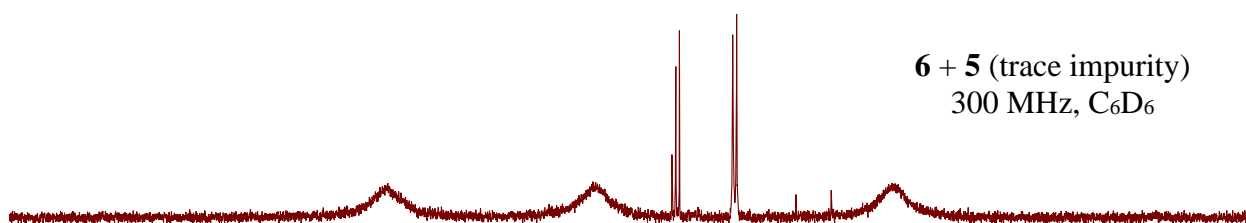
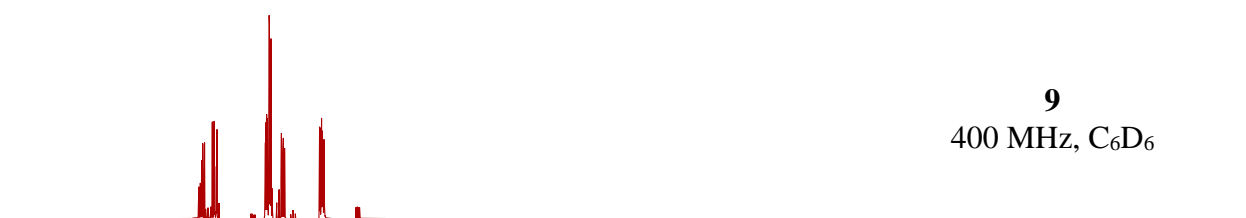


When complex **6** (10.0 mg, 0.0224 mmol) is reacted with one equivalent of dmpe (224  $\mu$ L, 100 mM stock solution in  $C_6D_6$ , 0.0224 mmol) a mixture of **5** (trace), **6**, **9** and a new hydride complex **5'** was formed according to the  $^1H$  and  $^{31}P$  NMR spectra of the crude reaction mixture (see below). A subsequent HESI-MS analysis of the solution confirmed that **5'** is derived from **5** by replacing two  $PMe_3$  ligands by one dmpe ligand. Isolation of **5'** was not possible due to the complexity of the crude reaction mixture in combination with its labile nature.

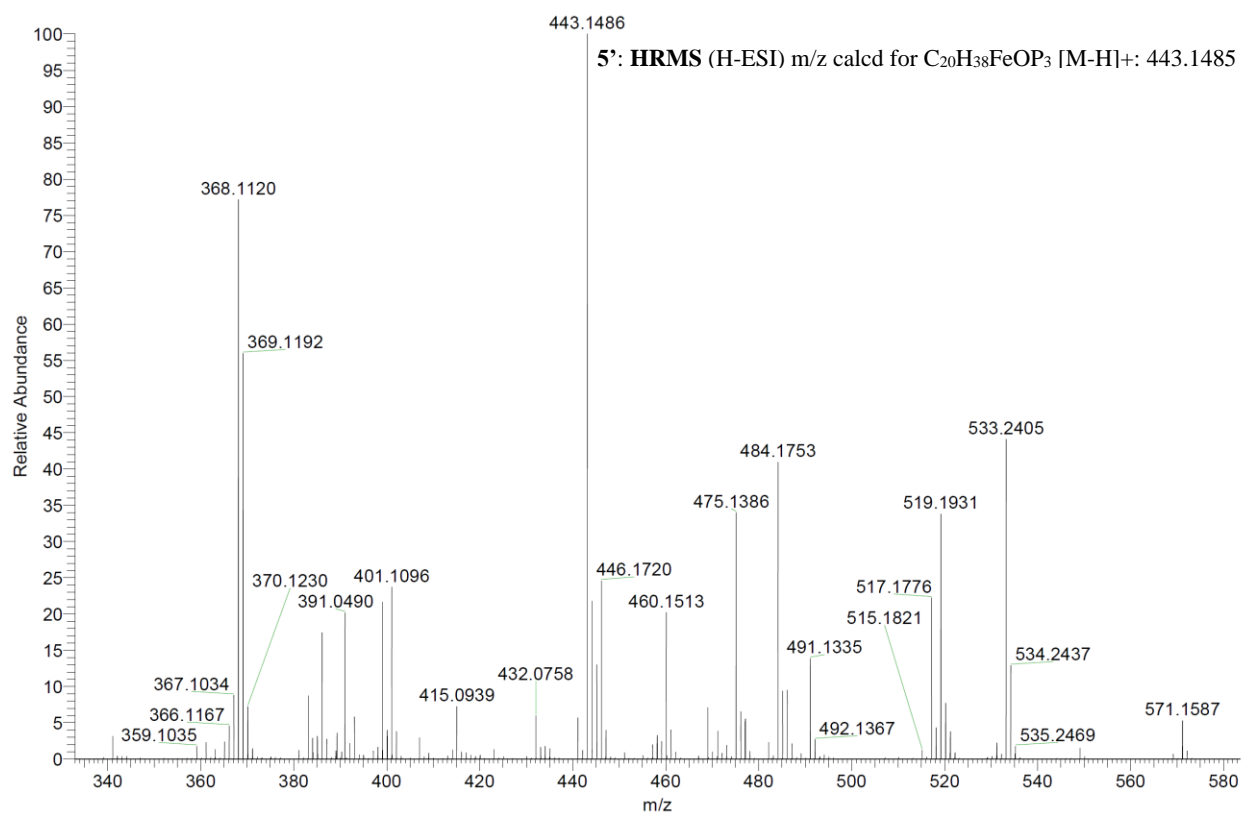


**5'**

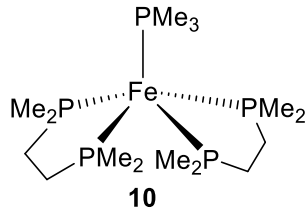




80 70 60 50 40 30 20 10 0 -10 -20  
31P ppm



## 2.4 Complex [Fe(PMe<sub>3</sub>)(dmpe)<sub>2</sub>] (**10**)

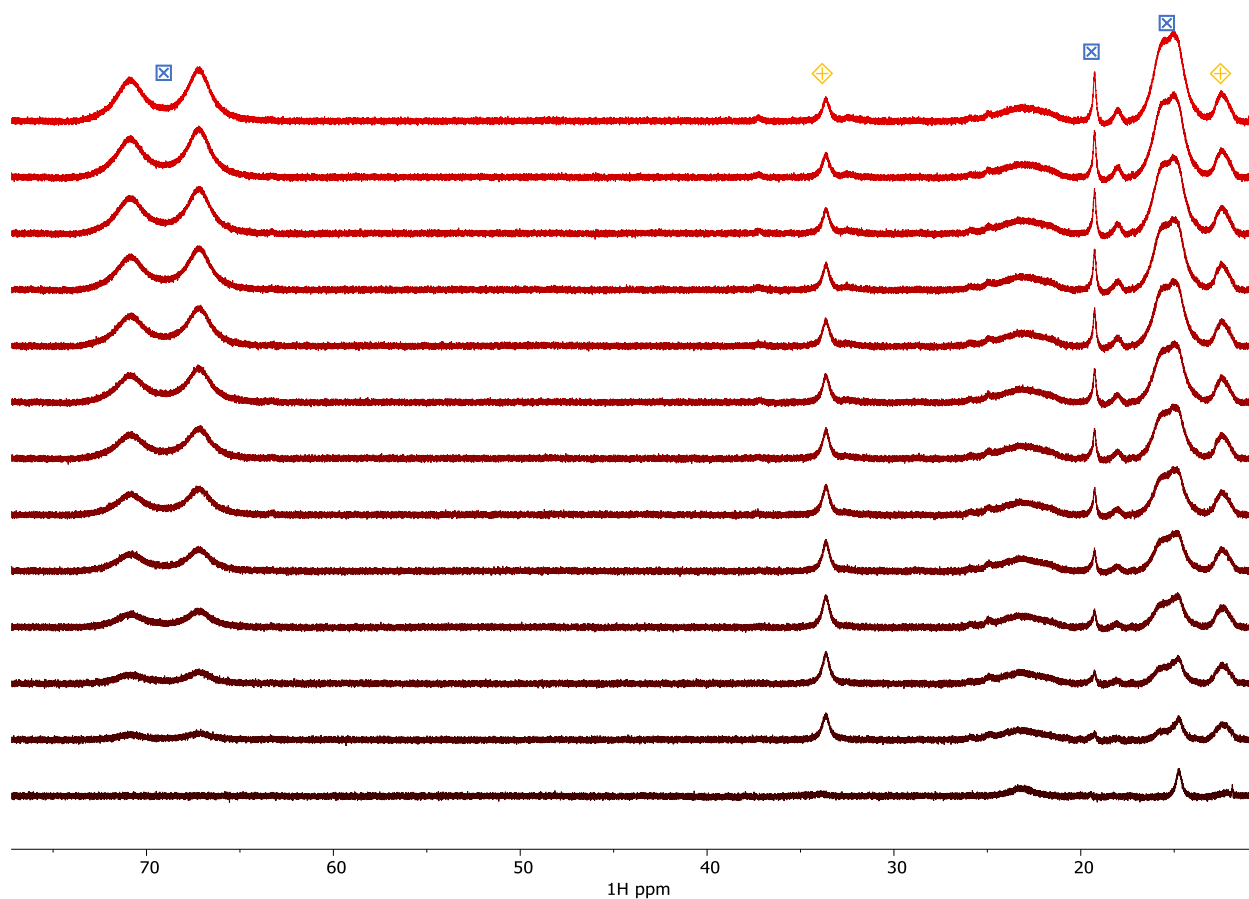


In a nitrogen filled glove box an NMR tube was loaded with, **4** (110 mg, 0.31 mmol), C<sub>6</sub>D<sub>6</sub> (1 mL), and dmpe (110 μL, 0.66 mmol). The solution was brought to a gentle reflux for one minute resulting in a color change from dark brownish yellow to dark red. It was then concentrated to half its volume under reduced pressure and kept at 70 °C for 17 hours. Subsequently, the <sup>31</sup>P{<sup>1</sup>H} NMR spectrum was collected to ensure reaction was complete. The solution was dried under reduced pressure, dissolved in pentane, and stored at -20 °C for 12 hours to yield complex **10** as an orange crystalline solid (59.4 mg, 44% yield). NMR data were identical to the ones previously reported while crystals suitable for an X-ray diffraction study were grown out of a cold (-20 °C) pentane solution of the compound.<sup>5</sup>

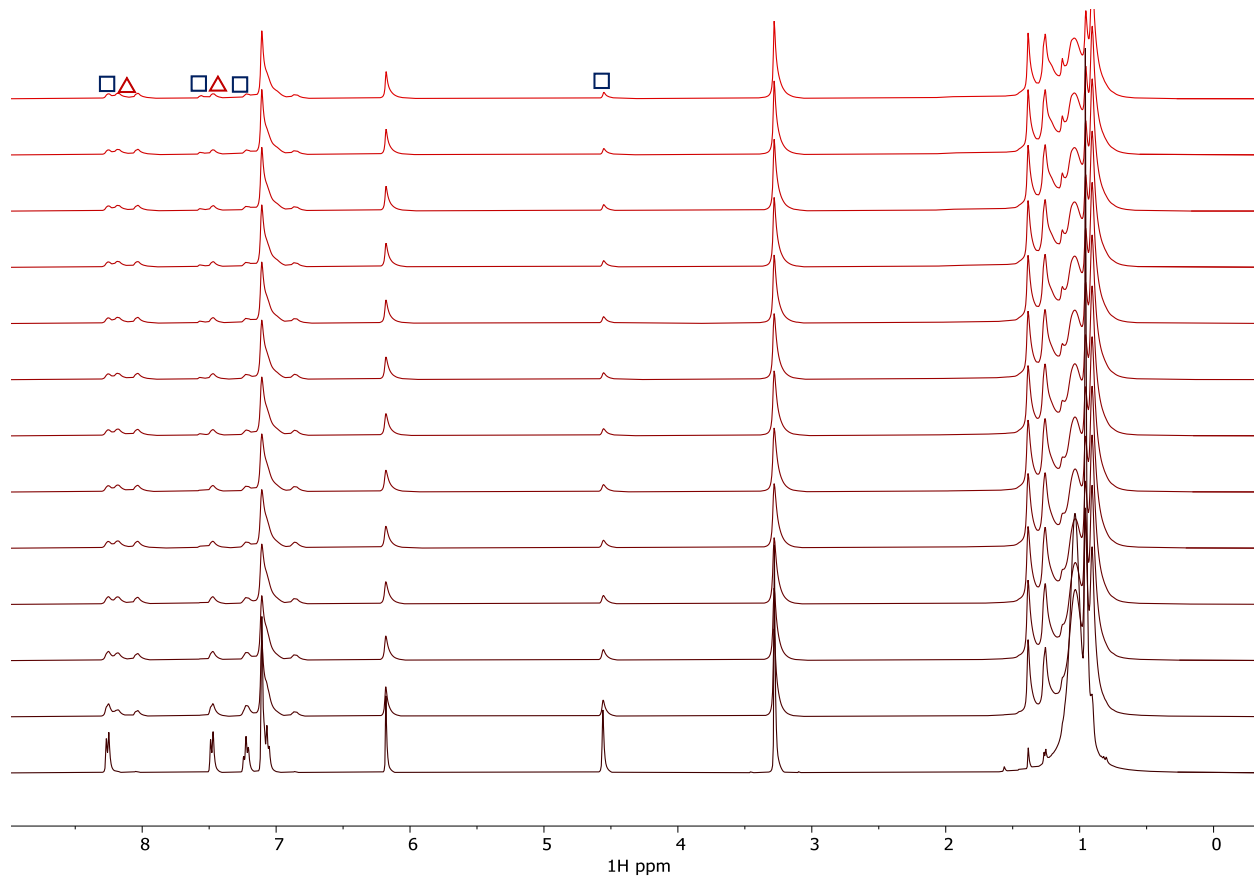
### 3 Exploration of the Equilibrium Between 5 and 6 in Solution

#### 3.1 Monitoring the Speciation of 6 in Solution by *in situ* $^1\text{H}$ NMR Spectroscopy

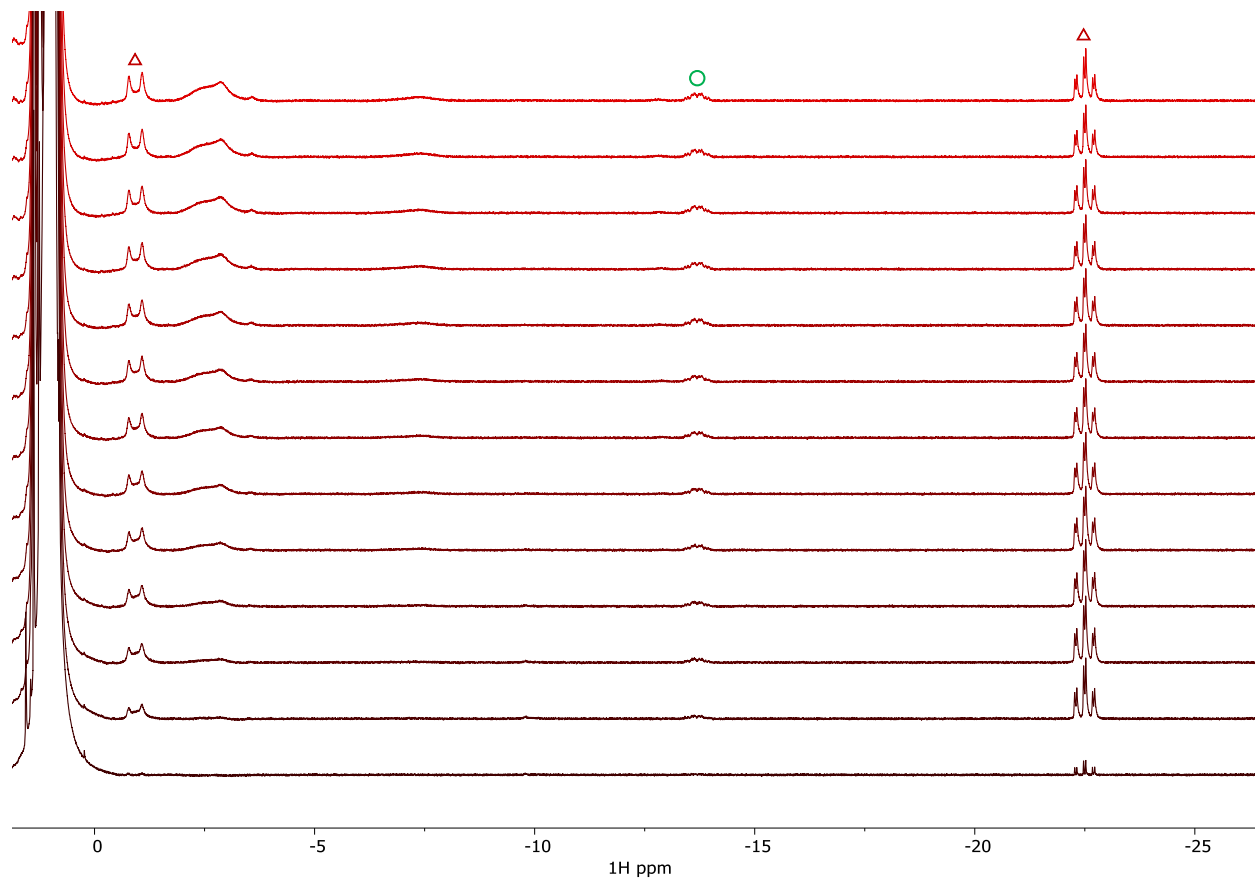
In a nitrogen filled glove box, an airtight NMR tube was loaded with 1,3,5-trimethoxybenzene (25.0  $\mu\text{L}$ , 500 mM stock solution in  $\text{C}_6\text{D}_6$ , 0.0125 mmol) and  $\text{C}_6\text{D}_6$  (475  $\mu\text{L}$ ). The NMR tube was locked and shimmed on the spectrometer and then taken back in the glove box where **6** (22.3 mg, 0.050 mmol) was accurately weighed by difference and placed above the solution inside the NMR tube. Subsequently, the NMR tube was carefully transferred to the spectrometer where it was vigorously shaken to dissolve the solids and measured immediately by collecting an  $^1\text{H}$  NMR spectrum every 5 minutes for a total of 10 h with a relaxation delay of 5 s.



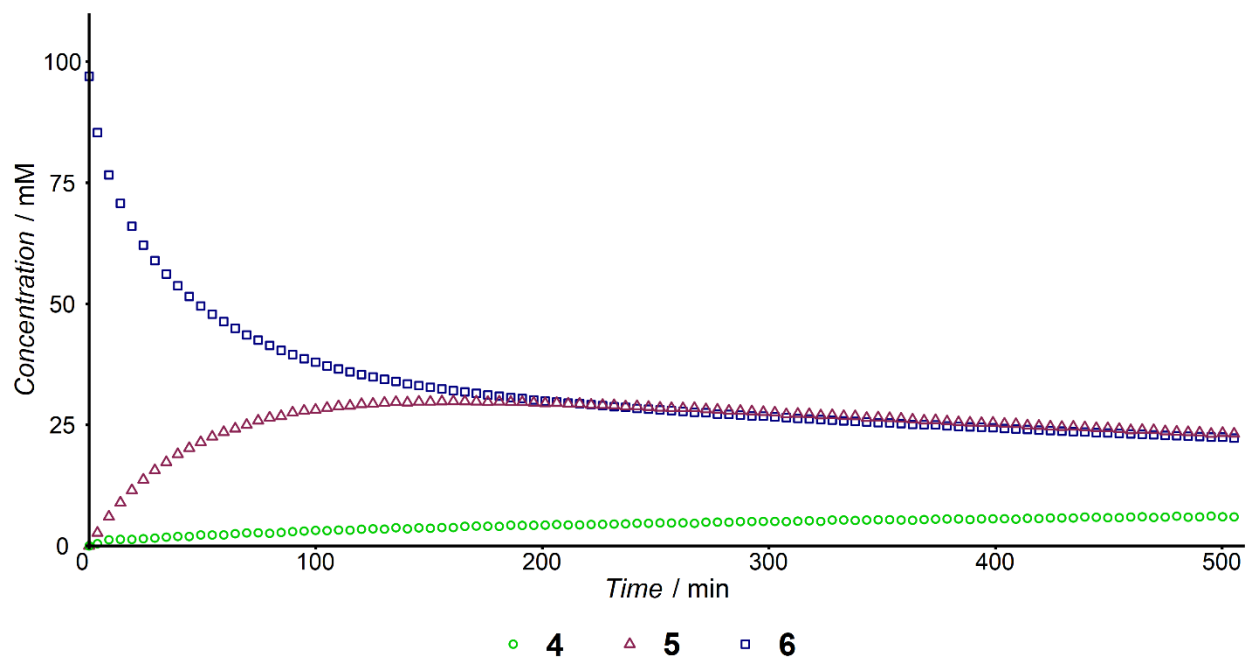
**Figure S1.**  $^1\text{H}$  NMR (400 MHz,  $\text{C}_6\text{D}_6$ , 35  $^\circ\text{C}$ , 80 to 11 ppm region) spectra collected with a time interval of 5 min (only 13 of the 120 collected spectra are presented here for clarity) in the reaction of **6** in  $\text{C}_6\text{D}_6$  (500  $\mu\text{L}$ ). Compound key:  $\boxtimes$  = paramagnetic species 1,  $\diamond$  = paramagnetic species 2.



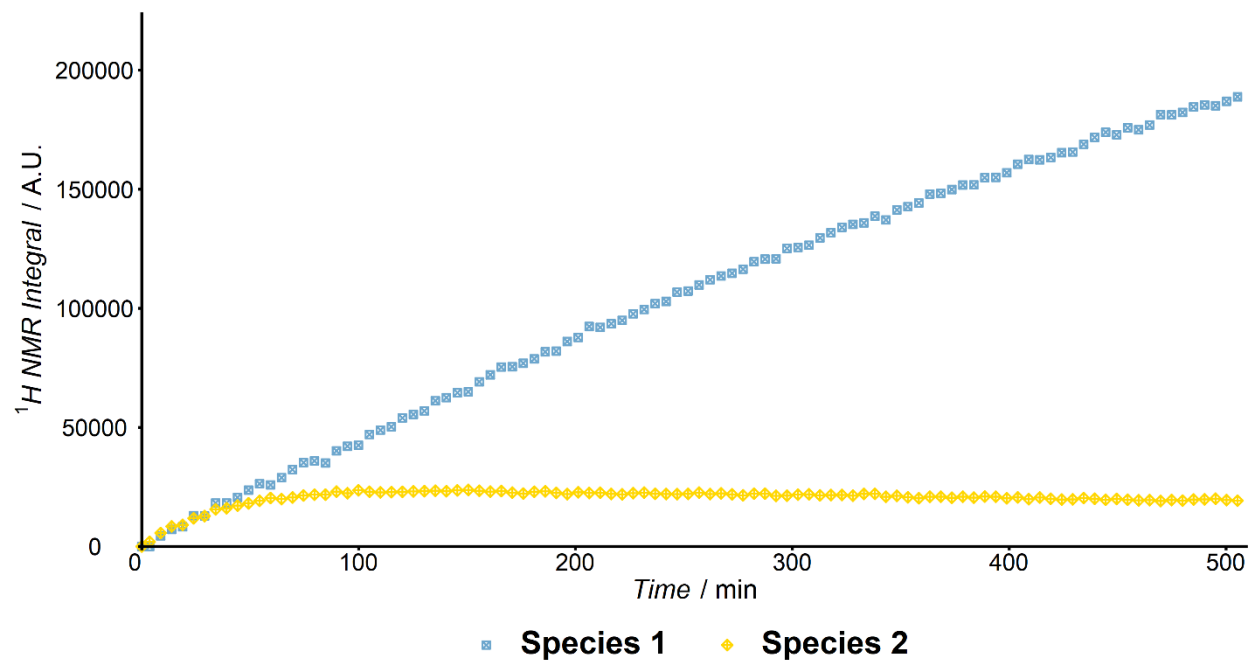
**Figure S2.** <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>, 35 °C, 10 to 0 ppm region) spectra collected with a time interval of 5 min (only 13 of the 120 collected spectra are presented here for clarity) in the reaction of **6** in C<sub>6</sub>D<sub>6</sub> (500 μL). Compound key: △ = **5**, □ = **6**.



**Figure S3.**  $^1\text{H}$  NMR (400 MHz,  $\text{C}_6\text{D}_6$ , 35  $^\circ\text{C}$ , 1 to -25 ppm region) spectra collected with a time interval of 5 min (only 13 of the 120 collected spectra are presented here for clarity) in the reaction of **6** in  $\text{C}_6\text{D}_6$  (500  $\mu\text{L}$ ). Compound key:  $\bigcirc$  = **4**,  $\triangle$  = **5**.



**Figure S4.** Monitoring diamagnetic product formation during the speciation of **6** (97 mM) in  $C_6D_6$  solution at 35.0 °C and a total volume of 500  $\mu$ L.

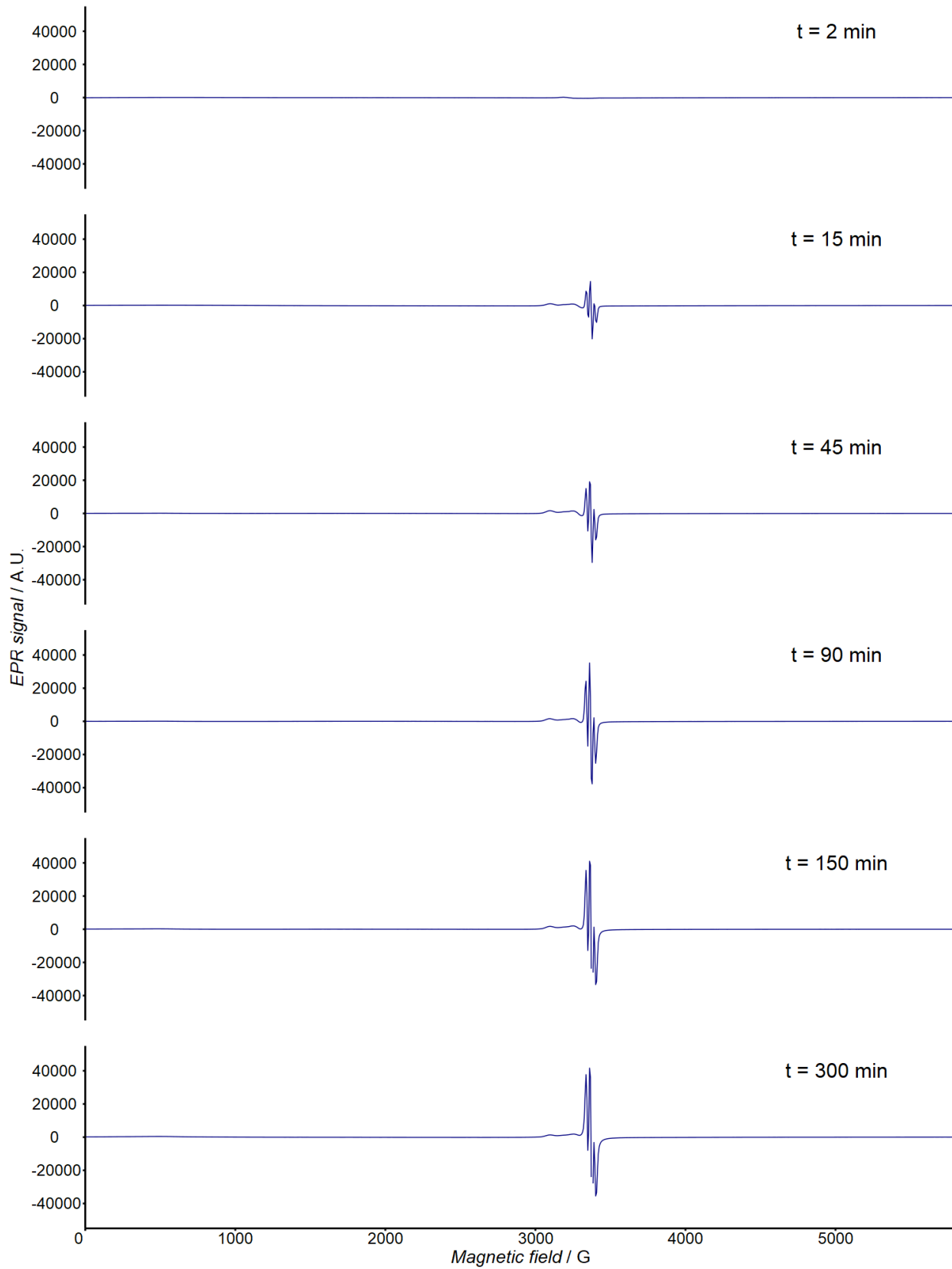


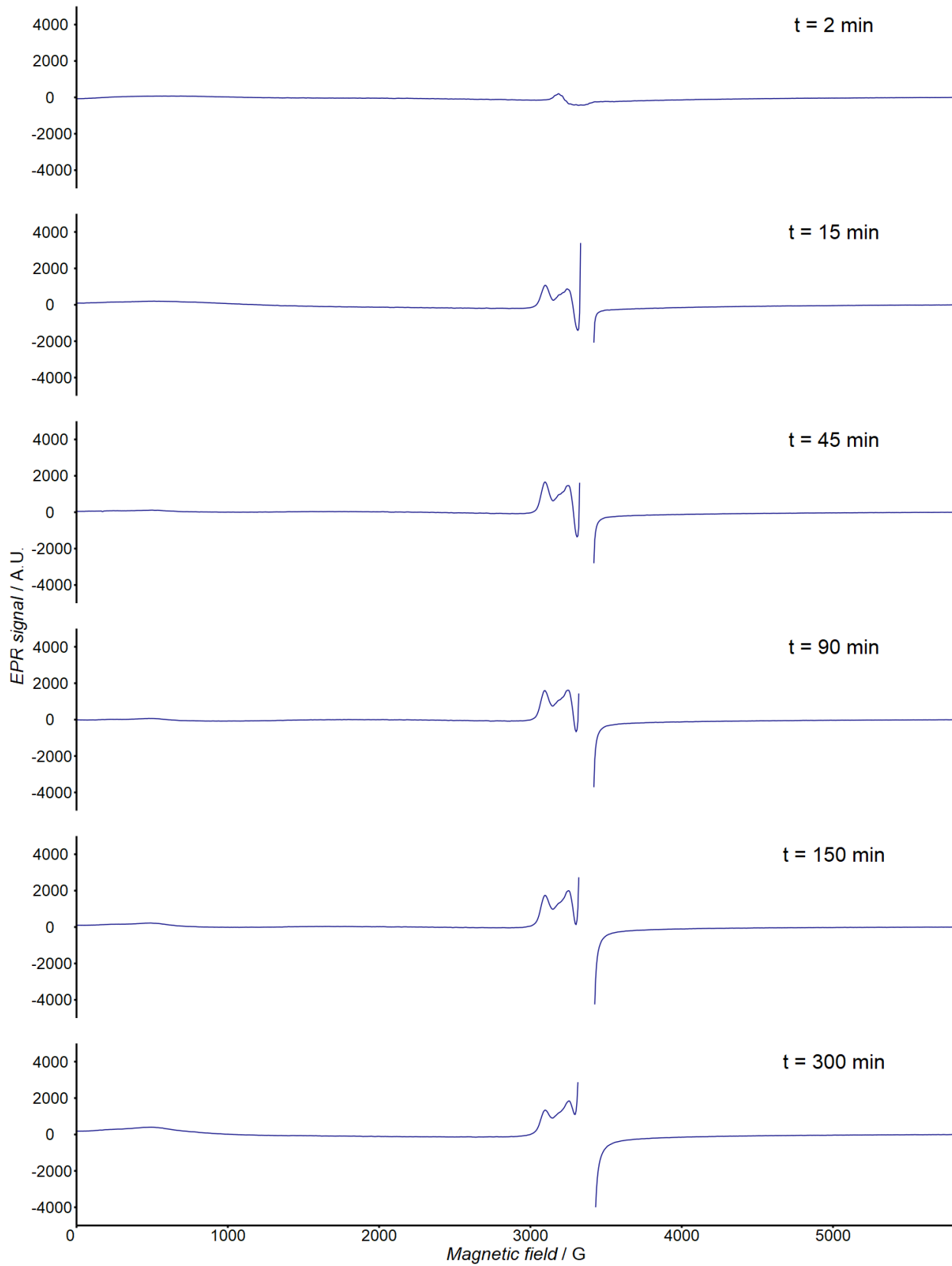
**Figure S5.** Monitoring paramagnetic product formation during the speciation of **6** (97 mM) in  $C_6D_6$  solution at 35.0 °C and a total volume of 500  $\mu$ L.

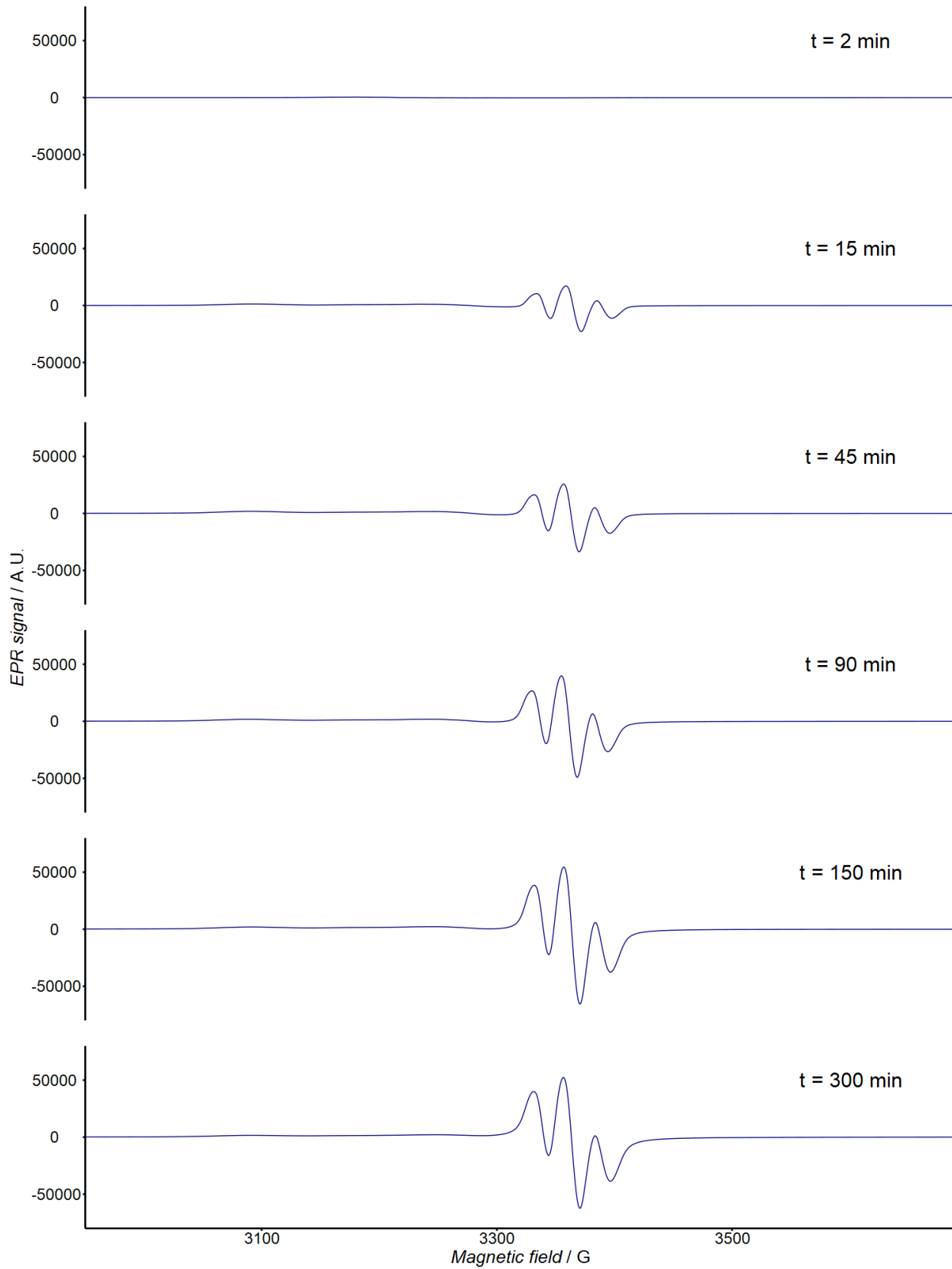


### 3.2 Monitoring the Speciation of **6** in Solution by EPR Spectroscopy

In a nitrogen filled glove box an EPR tube equipped with a J. Youngs tap was loaded with C<sub>6</sub>D<sub>6</sub> (250 μL) followed by addition of iron alkoxide **6** (11.2 mg, 0.025 mmol). The tube was taken to the EPR spectrometer where the solids were immediately dissolved, frozen, and the EPR spectrum of the frozen solution measured at 140 – 150 K. Subsequently, the solution was kept at 35 °C and after 15 minutes the EPR spectrum was collected at 140 K – 150 K. The procedure was repeated at 45, 90, 150, and 300 minutes.

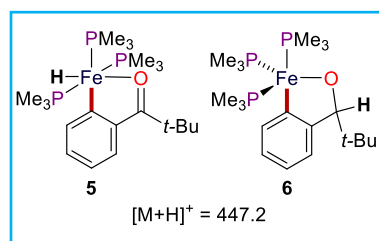
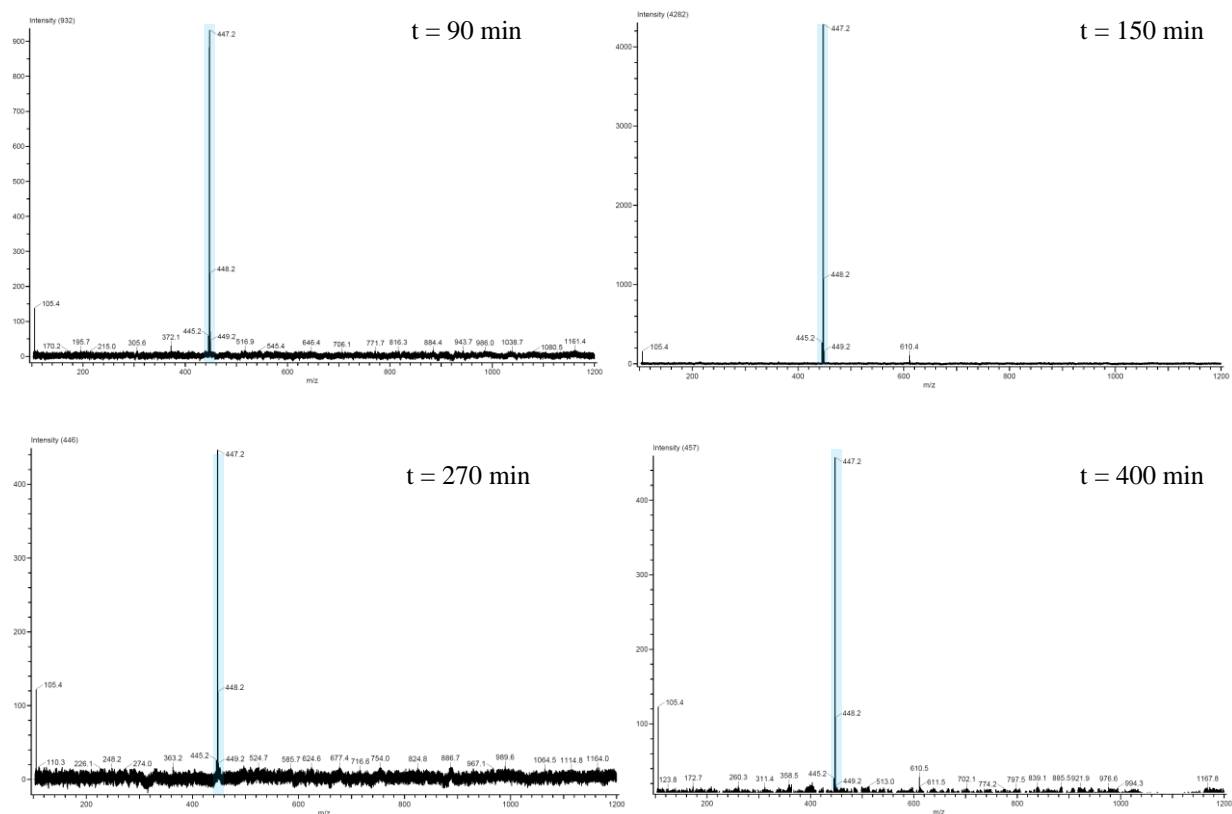


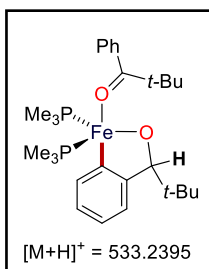
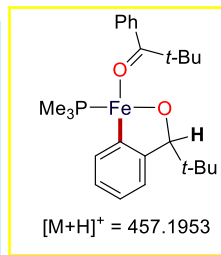
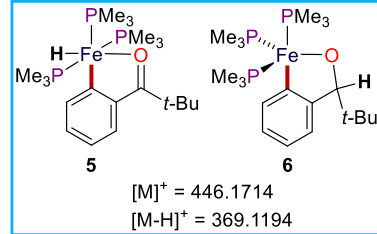
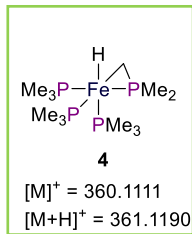
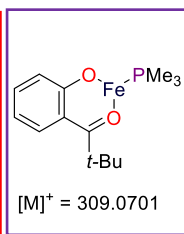
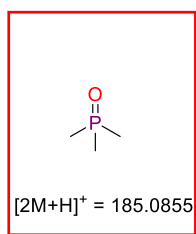
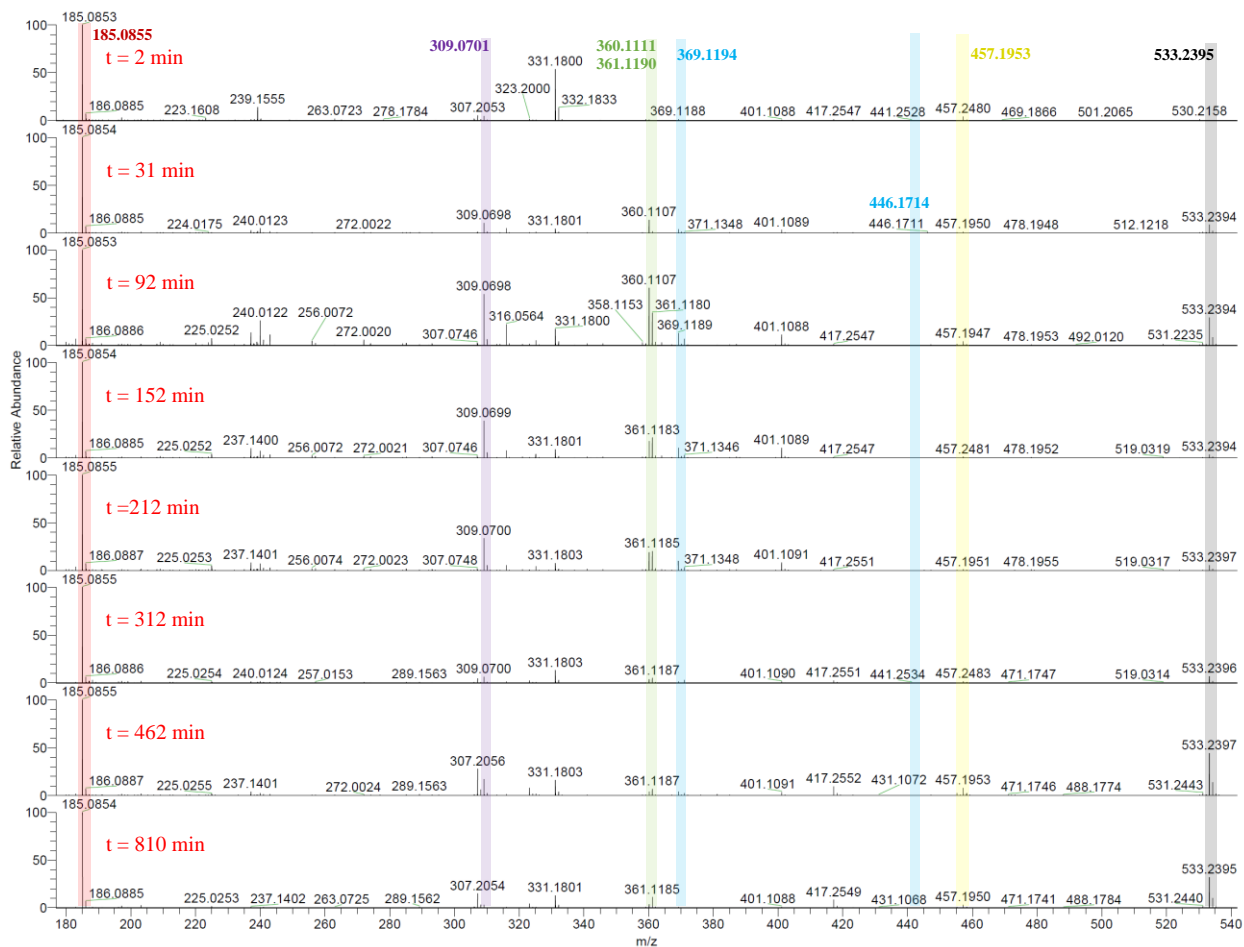




### 3.3 Monitoring the Speciation of **6** in Solution by LIFDI and HESI Mass Spectrometry

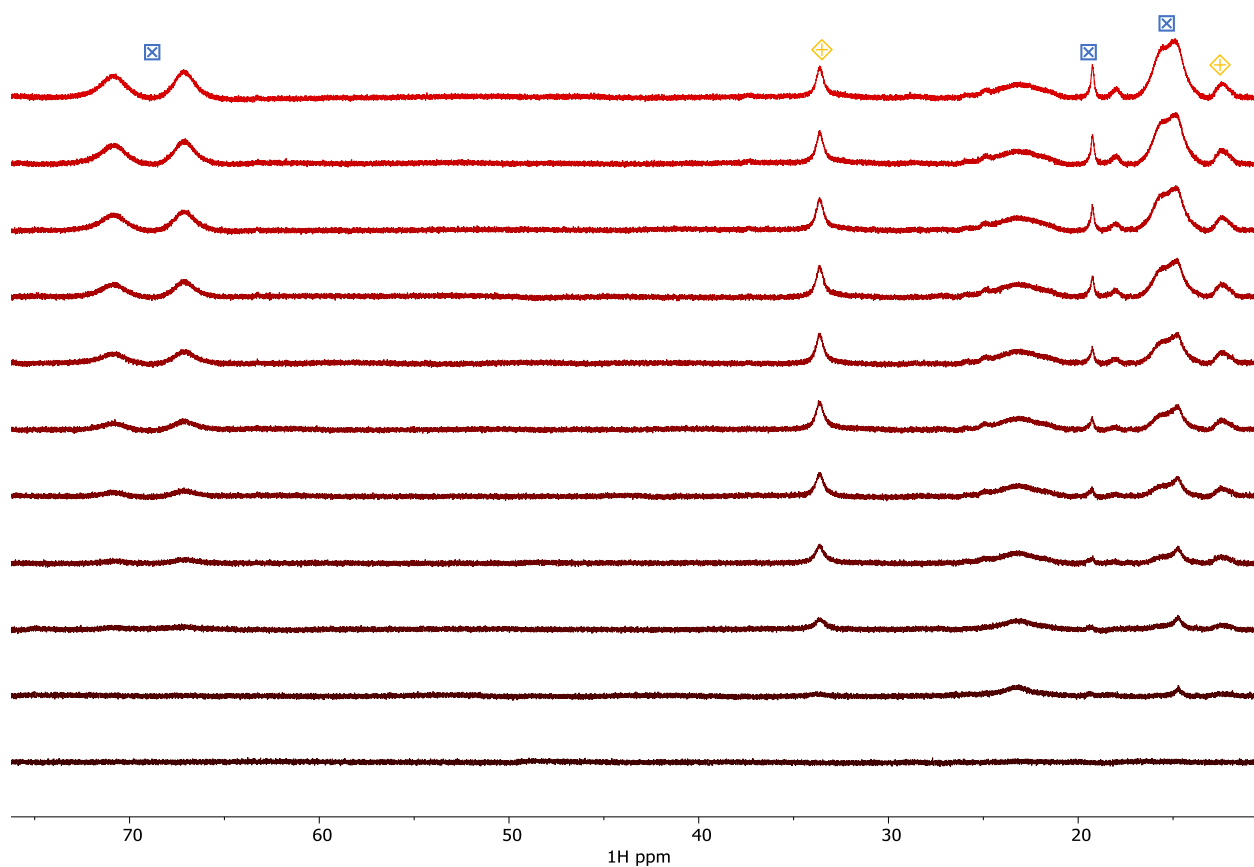
In a nitrogen filled glovebox, alkoxide complex **6** (11.2 mg, 0.025 mmol) was dissolved in toluene (500  $\mu$ L) and the solution was heated at 35  $^{\circ}$ C. Four aliquots (55  $\mu$ L) were collected over a period of seven hours which were diluted with toluene (195  $\mu$ L) sealed in airtight GC vials and measured immediately. For the HESI HR-MS measurements, the experiment was repeated in benzene with the aliquots being injected from within the glovebox after dilution with THF.



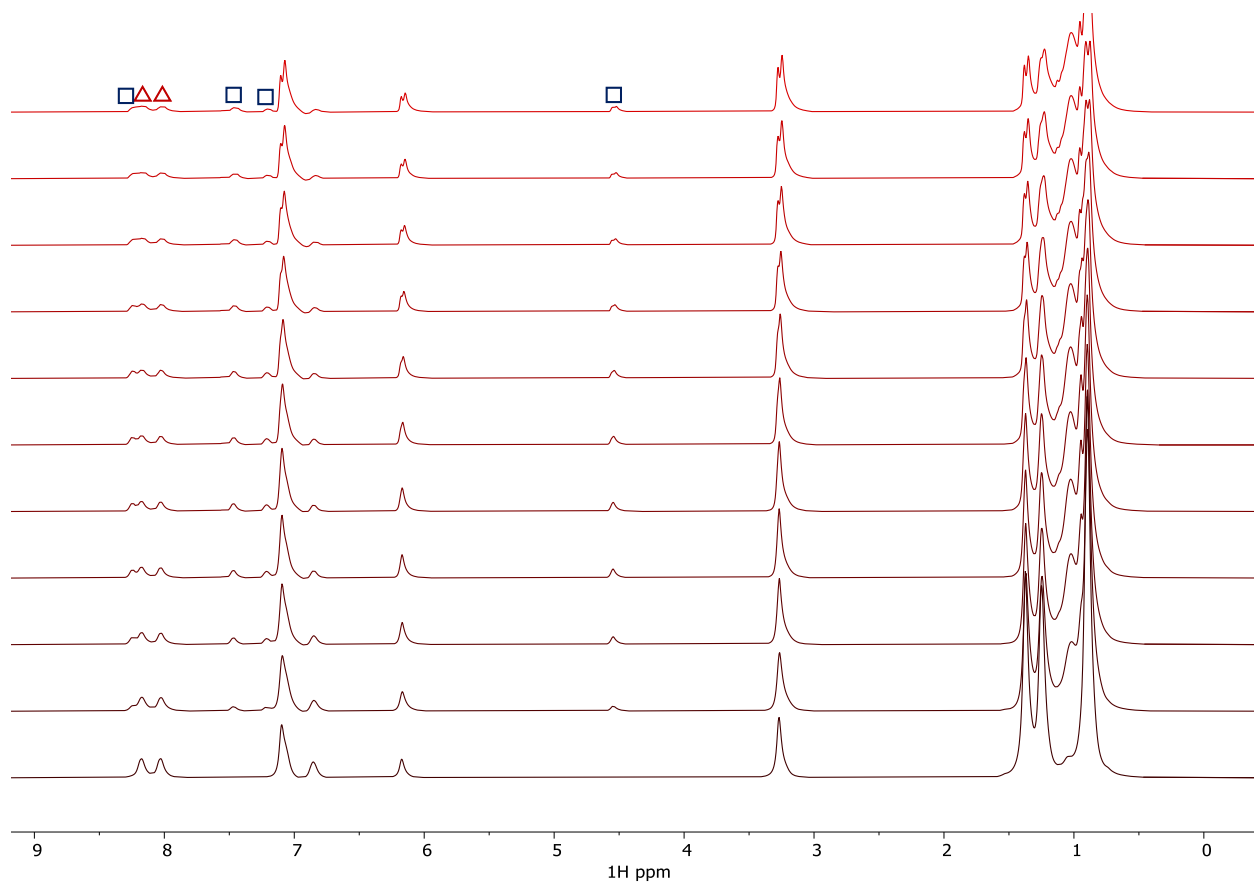


### 3.4 Monitoring the Speciation of **5** in Solution by *in situ* $^1\text{H}$ NMR Spectroscopy

In a nitrogen filled glove box, an airtight NMR tube was loaded with 1,3,5-trimethoxybenzene (25.0  $\mu\text{L}$ , 500 mM stock solution in  $\text{C}_6\text{D}_6$ , 0.0125 mmol) and  $\text{C}_6\text{D}_6$  (475  $\mu\text{L}$ ). The NMR tube was locked and shimmed on the spectrometer and then taken back in the glove box where **5** (22.3 mg, 0.050 mmol) was accurately weighed by difference and placed above the solution inside the NMR tube. Subsequently, the NMR tube was carefully transferred to the spectrometer where it was vigorously shaken to dissolve the solids and measured immediately by collecting an  $^1\text{H}$  NMR spectrum every 5 minutes for a total of 10 h with a relaxation delay of 5 s.

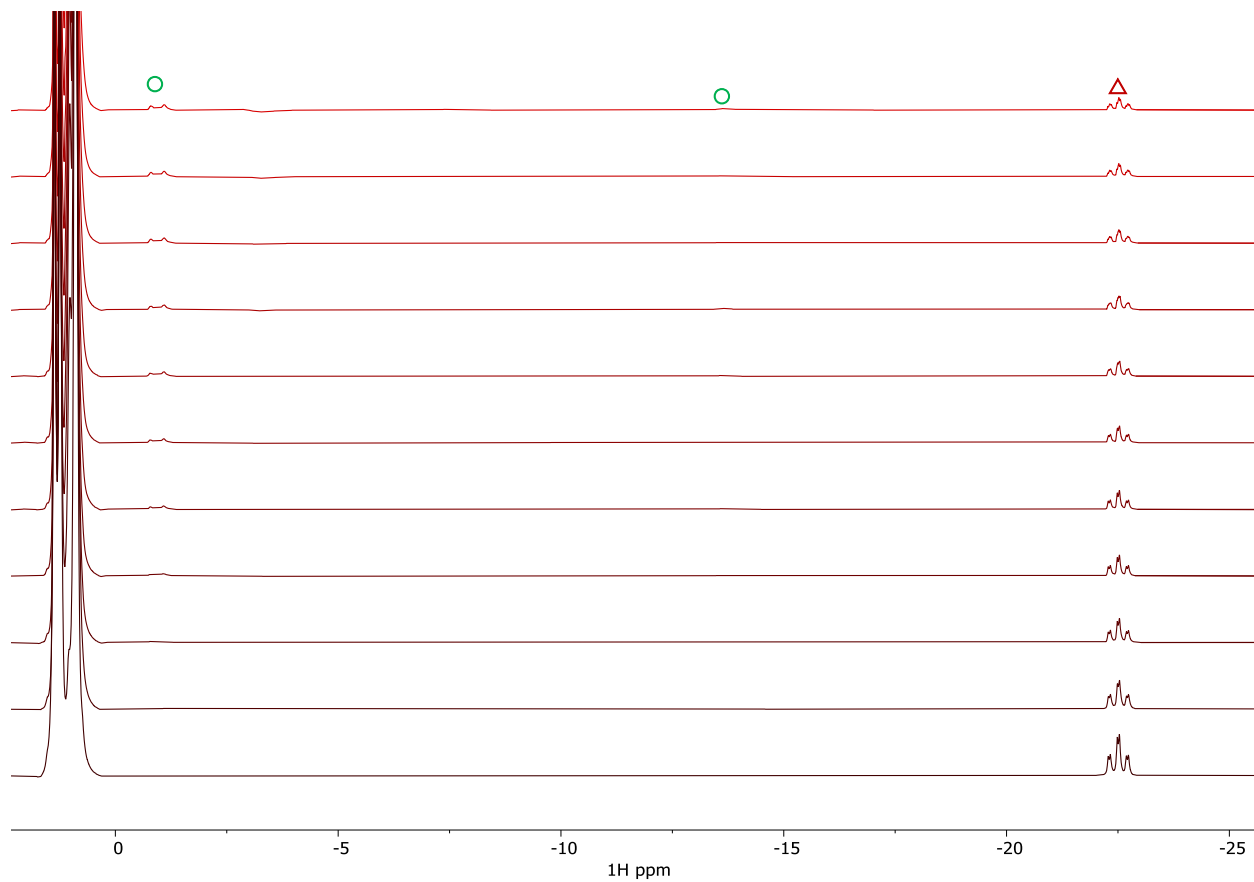


**Figure S6.**  $^1\text{H}$  NMR (400 MHz,  $\text{C}_6\text{D}_6$ , 35  $^\circ\text{C}$ , 80 to 11 ppm region) spectra collected with a time interval of 5 min (only 13 of the 120 collected spectra are presented here for clarity) in the reaction of **5** in  $\text{C}_6\text{D}_6$  (500  $\mu\text{L}$ ). Compound key:  $\boxtimes$  = paramagnetic species **1**,  $\blacklozenge$  = paramagnetic species **2**.

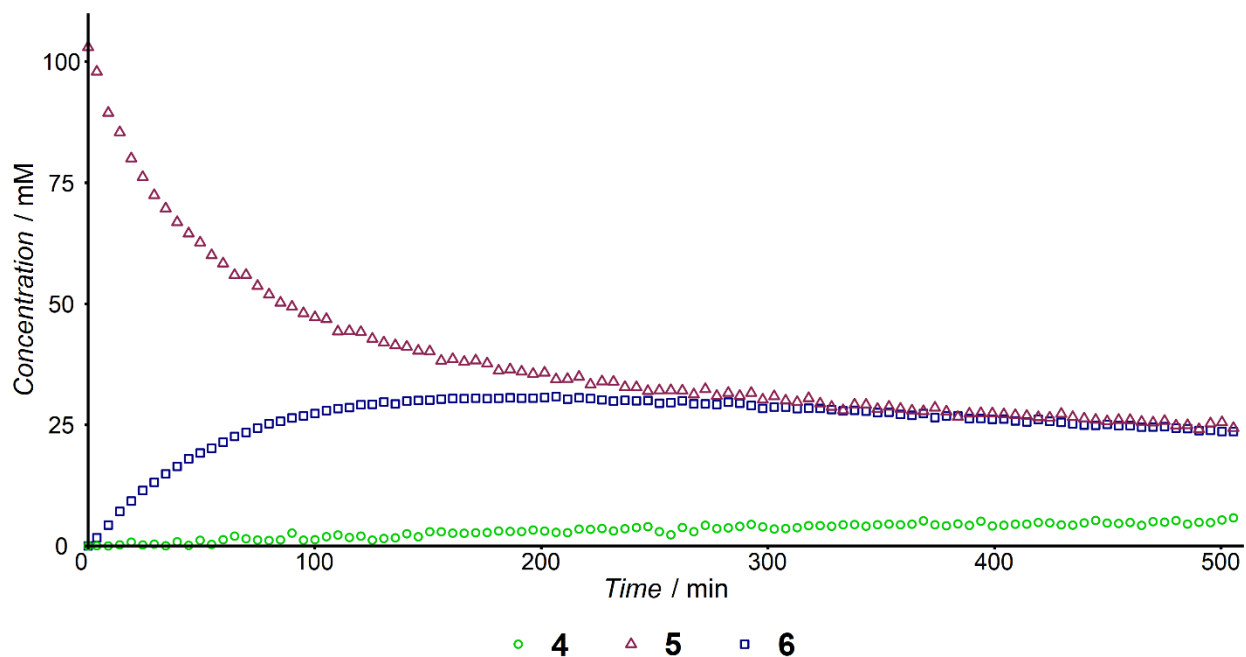


**Figure S7.** <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>, 35 °C, 10 to 0 ppm region) spectra collected with a time interval of 5 min (only 13 of the 120 collected spectra are presented here for clarity) in the reaction of **5** in C<sub>6</sub>D<sub>6</sub> (500 μL). Compound key: Δ = **5**, □ = **6**.

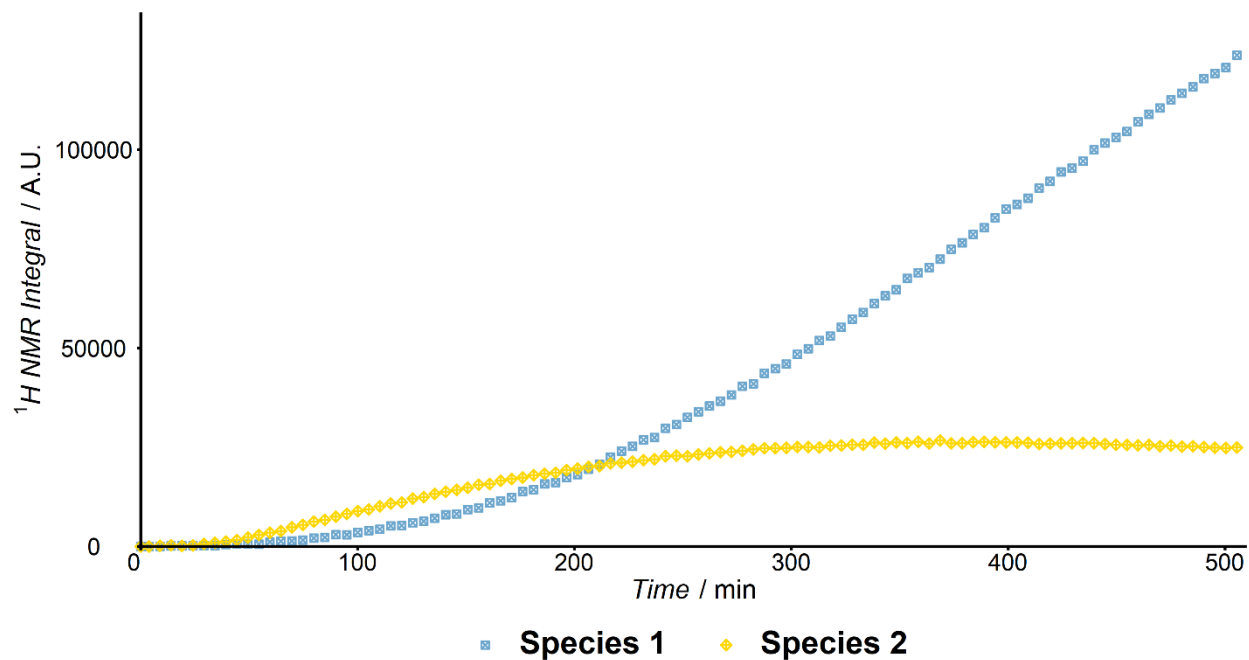




**Figure S8.** <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>, 35 °C, 1 to -25 ppm region) spectra collected with a time interval of 5 min (only 13 of the 120 collected spectra are presented here for clarity) in the reaction of **5** in C<sub>6</sub>D<sub>6</sub> (500 μL). Compound key: ○ = **4**, △ = **5**.



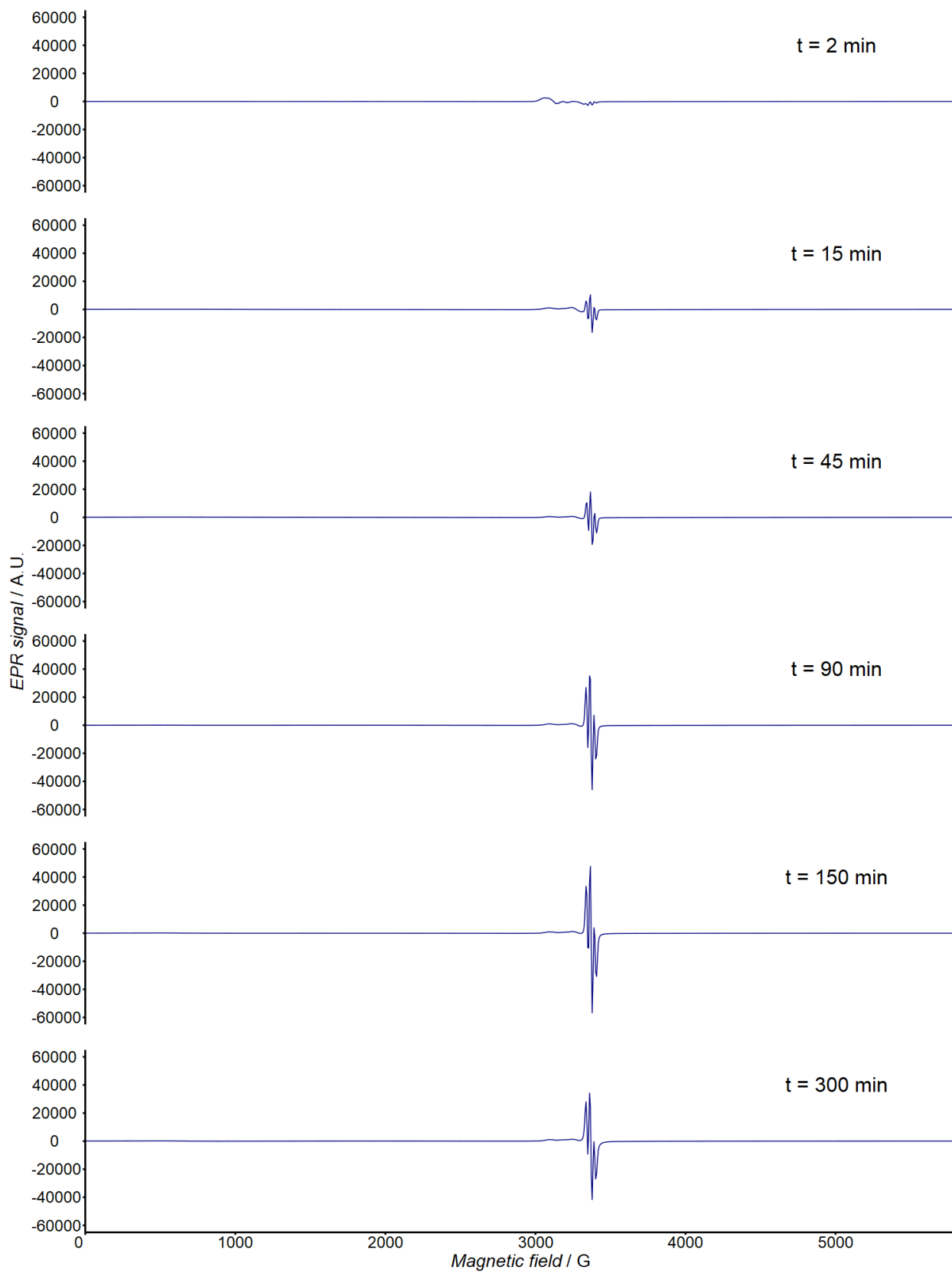
**Figure S9.** Monitoring diamagnetic product formation during the speciation of **5** (103 mM) in  $C_6D_6$  solution at 35.0 °C and a total volume of 500  $\mu$ L.

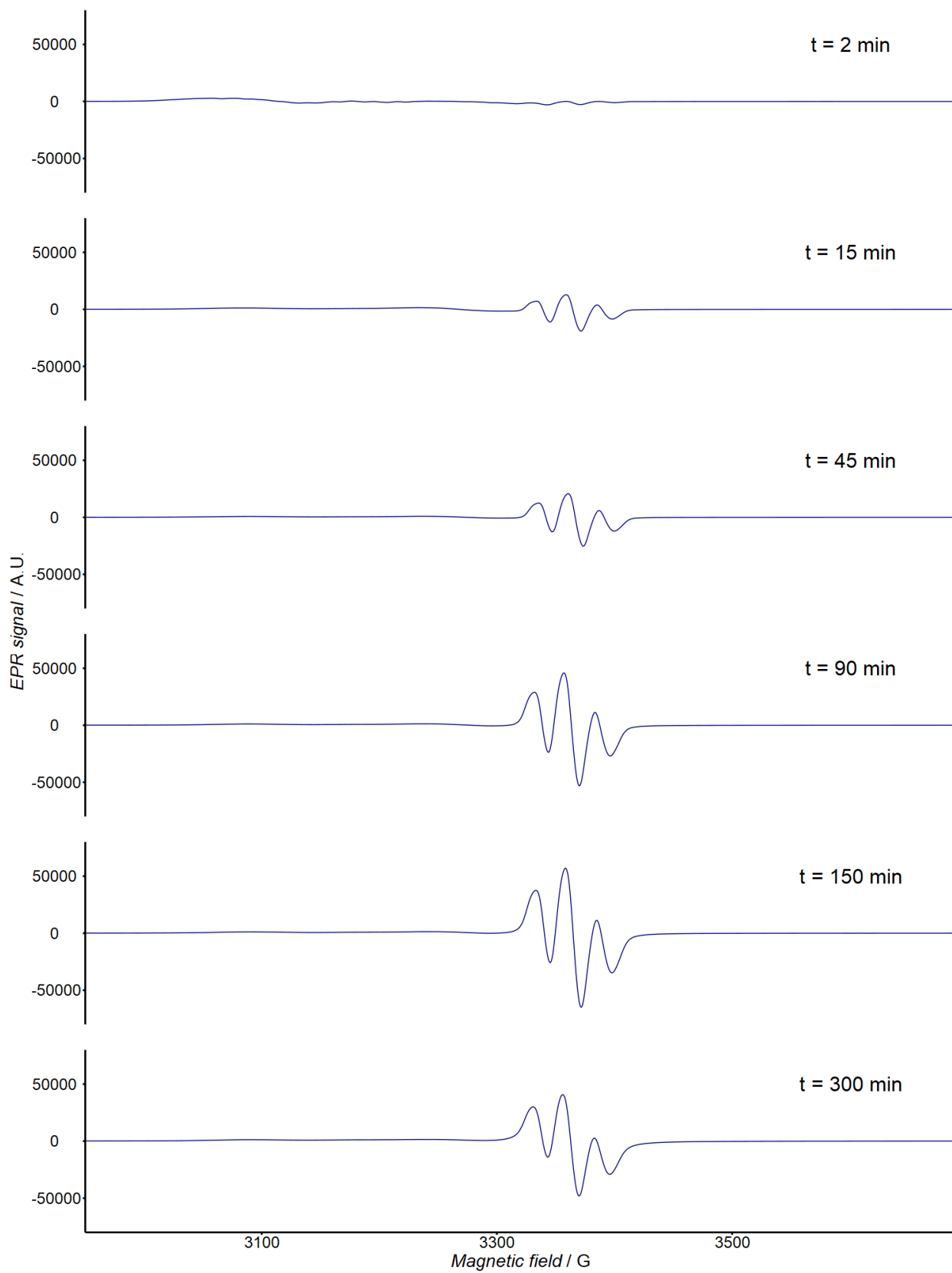


**Figure S10.** Monitoring paramagnetic product formation during the speciation of **5** (103 mM) in  $C_6D_6$  solution at 35.0 °C and a total volume of 500  $\mu$ L.

### 3.5 Monitoring the Speciation of **5** in Solution by EPR Spectroscopy

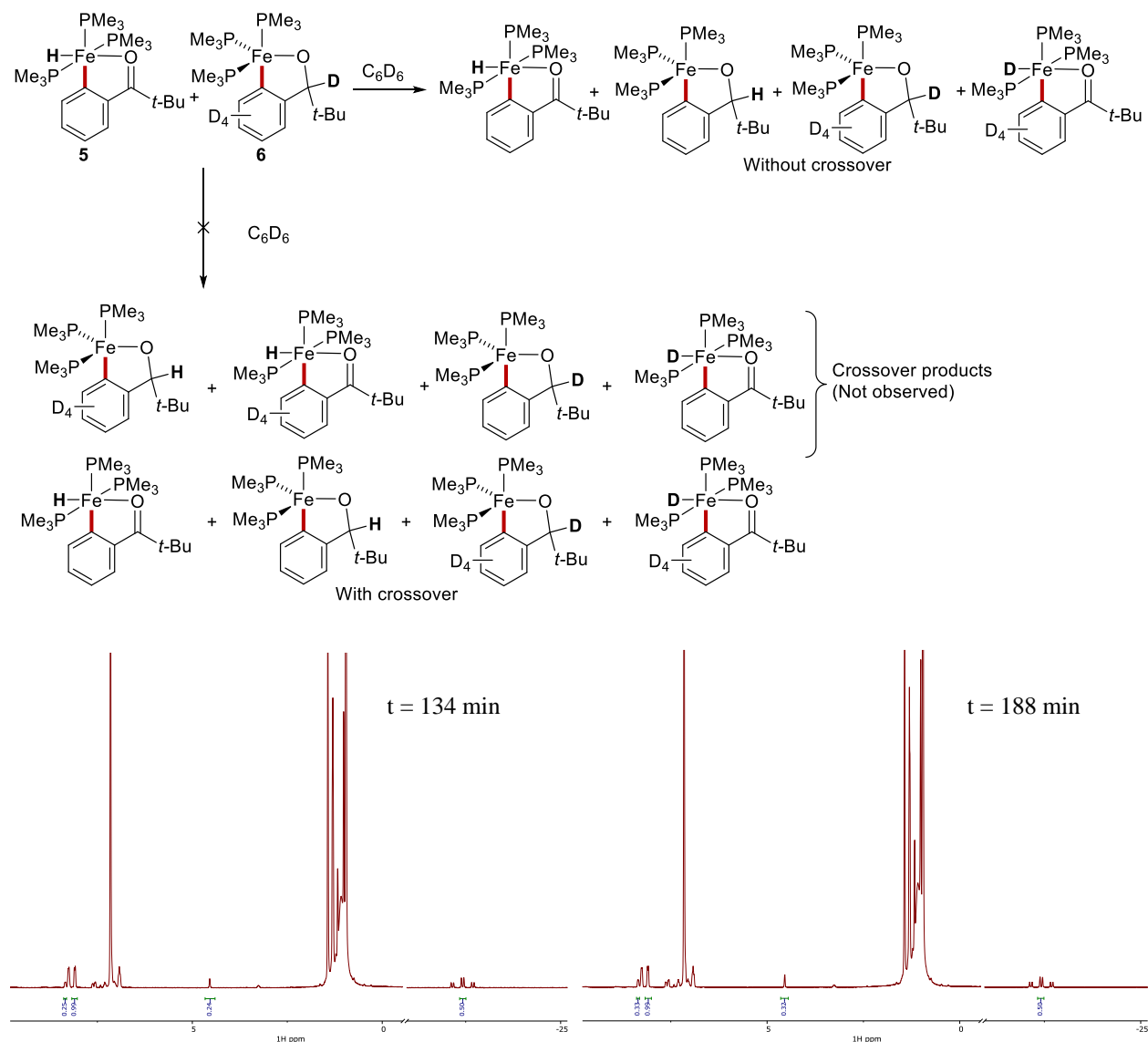
In a nitrogen filled glove box an EPR tube equipped with a J. Youngs tap was loaded with C<sub>6</sub>D<sub>6</sub> (250 μL) followed by addition of iron alkoxide **5** (11.2 mg, 0.025 mmol). The solution was taken to the EPR spectrometer where the solids were immediately dissolved, frozen, and the EPR spectrum of the frozen solution measured at 140 K. Subsequently, the solution was kept at 35 °C and after 15 minutes the EPR spectrum was collected at 140 K. The procedure was repeated at 45, 90, 150, and 300 minutes.

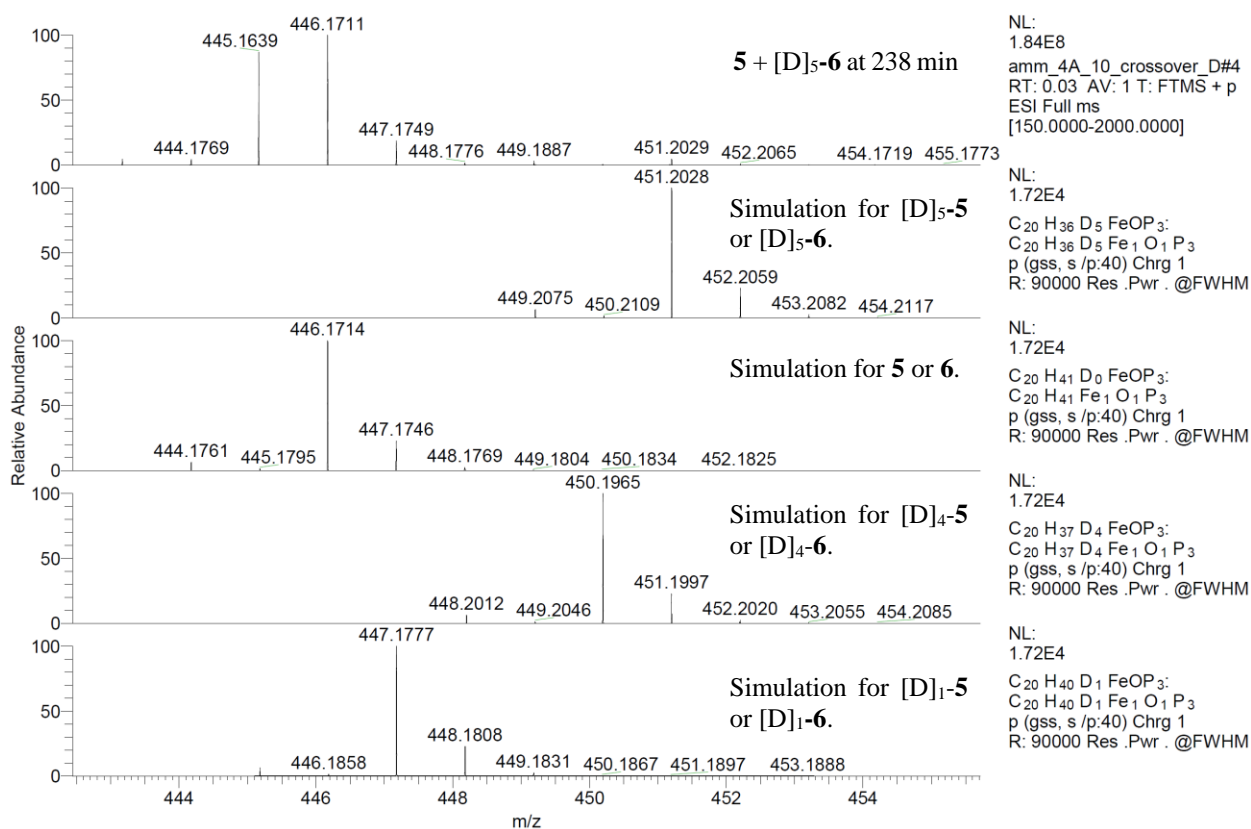
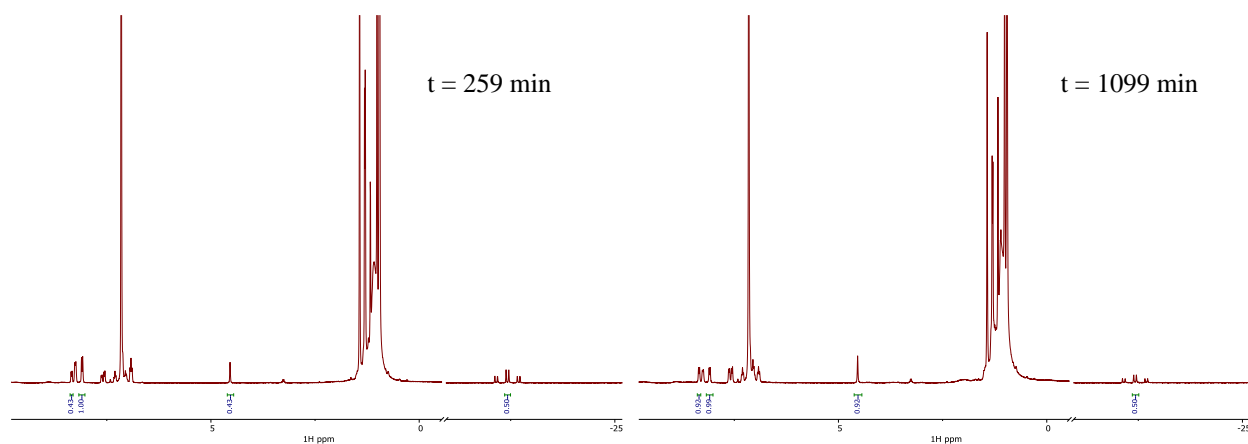




### 3.6 Reaction Between **5** and [D]<sub>5</sub>-**6** (Crossover Experiment)

In a nitrogen filled glove box, an airtight NMR tube was loaded with **5** (10.0 mg, 0.022 mmol), [D]<sub>5</sub>-**6** (10.1 mg, 0.022 mmol), and C<sub>6</sub>D<sub>6</sub> (0.6 μL). The solution was analyzed by <sup>1</sup>H NMR spectroscopy as well as high resolution mass spectrometry over a period of 18 hours. According to the excellent integration of the <sup>1</sup>H NMR spectra as well as the absence of crossover products in the HRMS spectra below, it is concluded that no crossover is observed between **5** and [D]<sub>5</sub>-**6**.





## 4 Catalytic Reaction Monitoring

### 4.1 Catalytic Reaction Monitoring by *in Situ* <sup>1</sup>H NMR Spectroscopy

Stock solutions of precatalyst, 2,2-dimethyl-1-phenylpropan-1-one (**1**), 1,3,5-trimethoxybenzene and 3-(*tert*-butyl)hepta-1,2-diene (**2**) were prepared in C<sub>6</sub>D<sub>6</sub> at 100 mM, 1000 mM, 500 mM, and 1000 mM concentration respectively, by weighing the appropriate amount of compound and diluting to 1.00 mL. The stock solution of complex **4** was passed through a 0.22 μm PTFE milipore

filter before use. All stock solutions were stored at -20 °C inside a nitrogen filled glove box. In a typical experiment a J. Young's tap NMR tube was loaded with 1,3,5-trimethoxybenzene (30.0  $\mu$ L, 500 mM stock solution in C<sub>6</sub>D<sub>6</sub>, 15.0  $\mu$ mol), 2,2-dimethyl-1-phenylpropan-1-one (60.0  $\mu$ L, 500 mM stock solution in C<sub>6</sub>D<sub>6</sub>, 60.0  $\mu$ mol), 3-(*tert*-butyl)hepta-1,2-diene (60.0  $\mu$ L, 500 mM stock solution in C<sub>6</sub>D<sub>6</sub>, 60.0  $\mu$ mol) and C<sub>6</sub>D<sub>6</sub> (390.0  $\mu$ L) with the help of micropipettes. The <sup>1</sup>H NMR spectrum (Varian 400 MHz) of the solution was recorded using a relaxation delay of 35 s to accurately determine the reagent's concentrations at t = 0 min and the NMR spectrometer probe was set to the desired temperature. Subsequently, the NMR tube was taken in the glove box where it was activated with precatalyst (60.0  $\mu$ L, 100 mM, 6.0  $\mu$ mol) and immediately frozen with liquid nitrogen. Once thawed, it was inserted to the spectrometer (Varian 400 MHz) and the time at that moment was noted (t<sub>0</sub>). Proton spectra were collected every 5 or 1.33 min using a relaxation delay of 5 s at 32 or 8 scans (the relaxation delays of the resonances of interest were measured by performing an inversion recovery experiment and were found to be less than 1 s for an endpoint reaction mixture). Lastly, the reaction was quenched with an aqueous HCl solution (1 M), extracted with dichloromethane and the final concentrations of the product and leftover starting materials were determined. The collected data were then stacked in Mestrenova, phased and appropriately baseline corrected (ablative in most cases) before processing to give the desired concentration-time plots. The NMR spectra collected over time are summarized in Table S1 and presented in Figure S11 to S29 below.

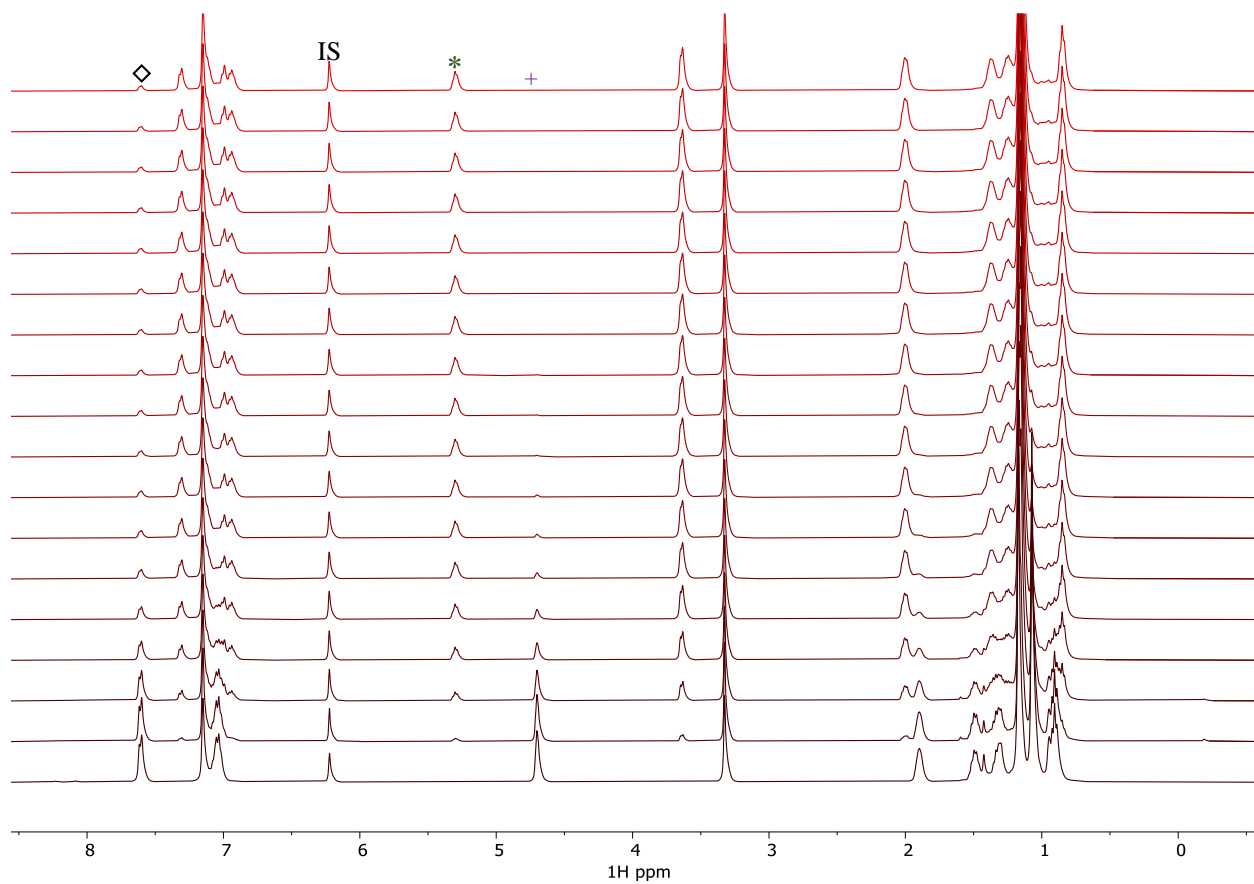
**Table S1.** Summary of catalytic reactions monitored with *in situ* <sup>1</sup>H NMR spectroscopy.<sup>a</sup>

Entry #	Precatalyst (mM)	<b>1</b> (mM)	<b>2</b> (mM)	Temperature (°C)
S1 <sup>b</sup>	<b>4</b> (10.0)	102.3	95.9	35
S2	<b>5</b> (10.0)	95.6	91.3	35
S3	<b>6</b> (10.0)	101.3	98.6	35
S4	<b>6</b> + [D] <sub>5</sub> - <b>6</b> (5.0 + 5.0)	<b>1</b> + [D] <sub>5</sub> - <b>1</b> = 50.0+53.7	92.8	25
S5 <sup>c</sup>	<b>6</b> (10.0)	95.0	95.5	25
S6 <sup>c, d</sup>	<b>6</b> (10.0)	94.9	95.5	25
S7	<b>6</b> (10.0)	93.5	95.6	7

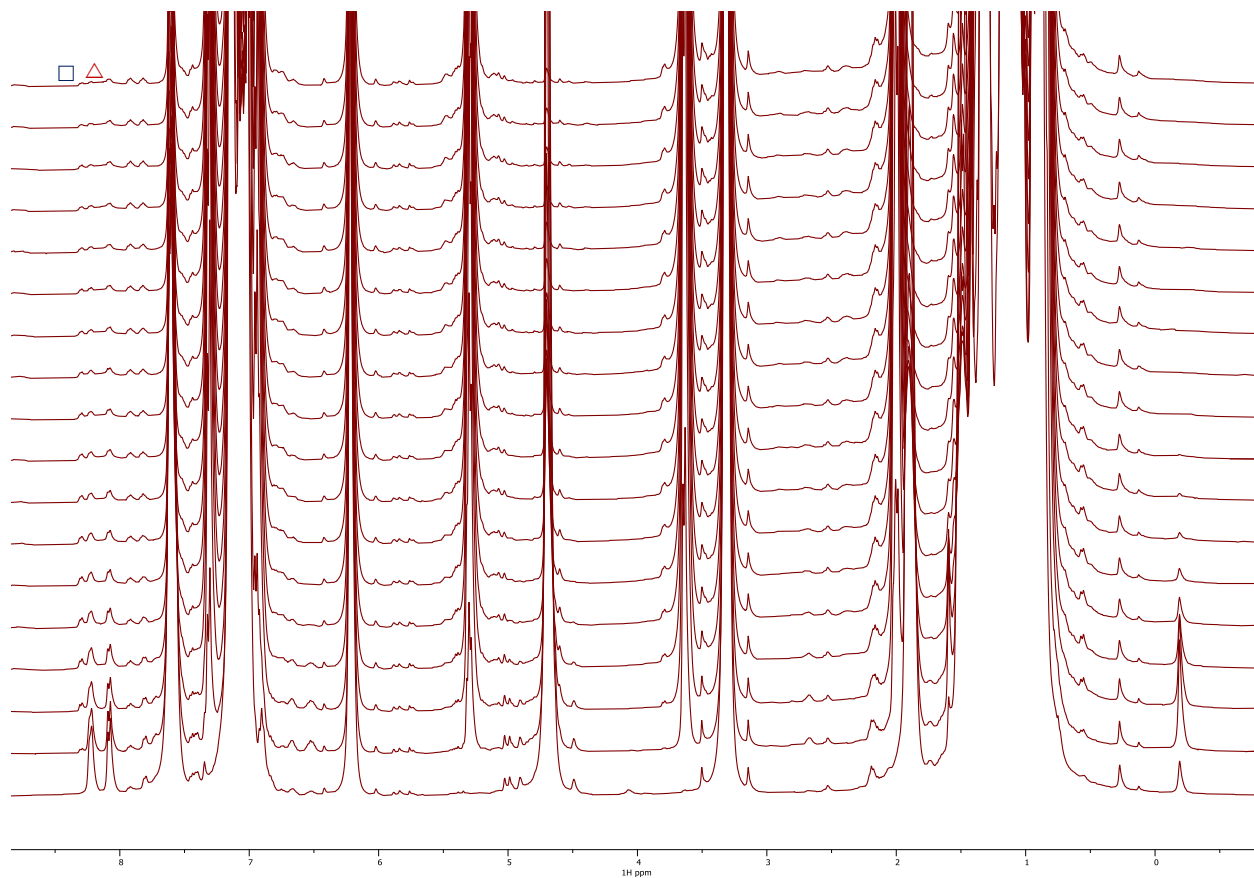
<sup>a</sup> General conditions: Reactions were performed in C<sub>6</sub>D<sub>6</sub> at a total volume of 600  $\mu$ L and monitored with <sup>1</sup>H NMR spectroscopy with a relaxation delay of 5 s at 32 scans per spectrum. Collection of spectra was performed every 5 min.

<sup>b</sup> Data taken from reference.<sup>4</sup> <sup>c</sup> Spectra were collected every 1.33 min at 8 scans instead of 32. <sup>d</sup> The stock solution of **6** used in this run was left to react at 35 °C for 500 min prior to use.

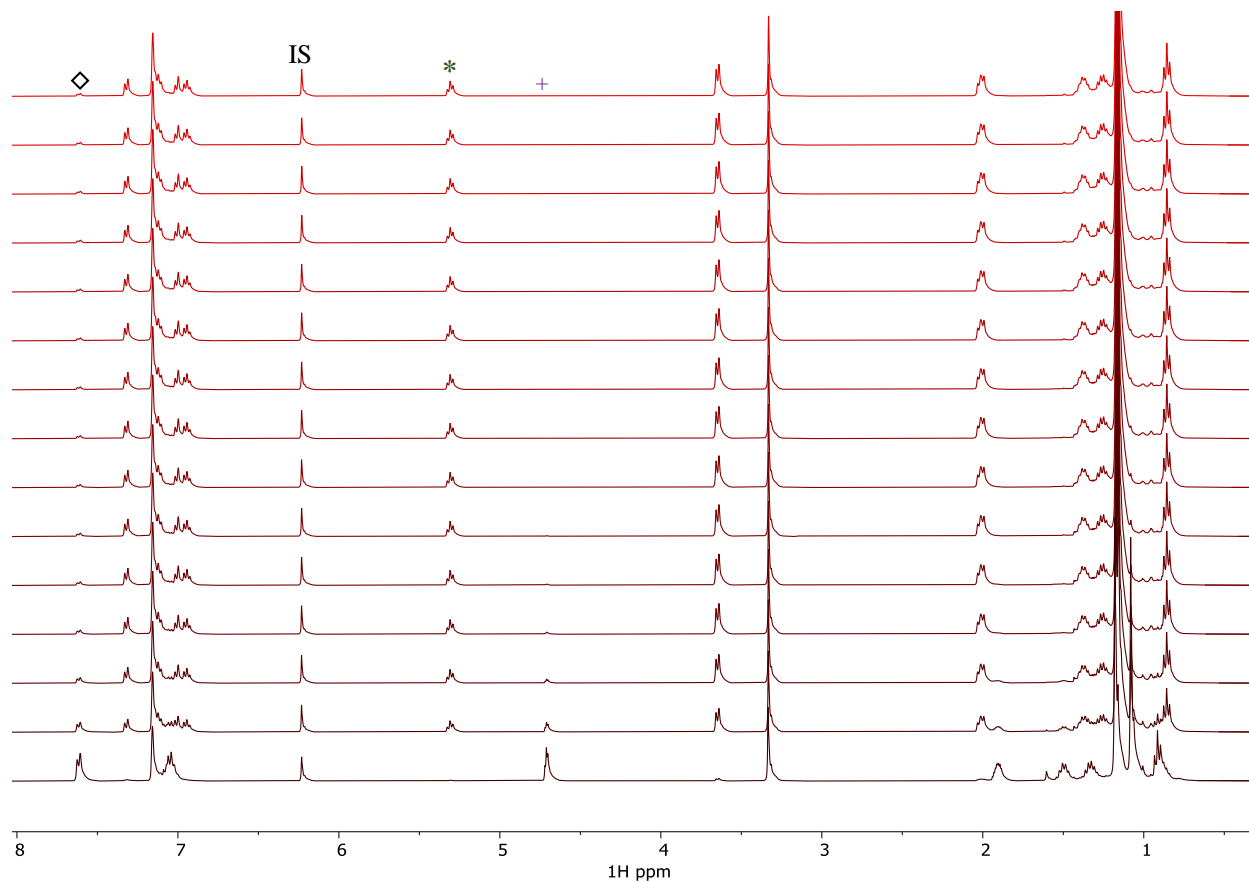




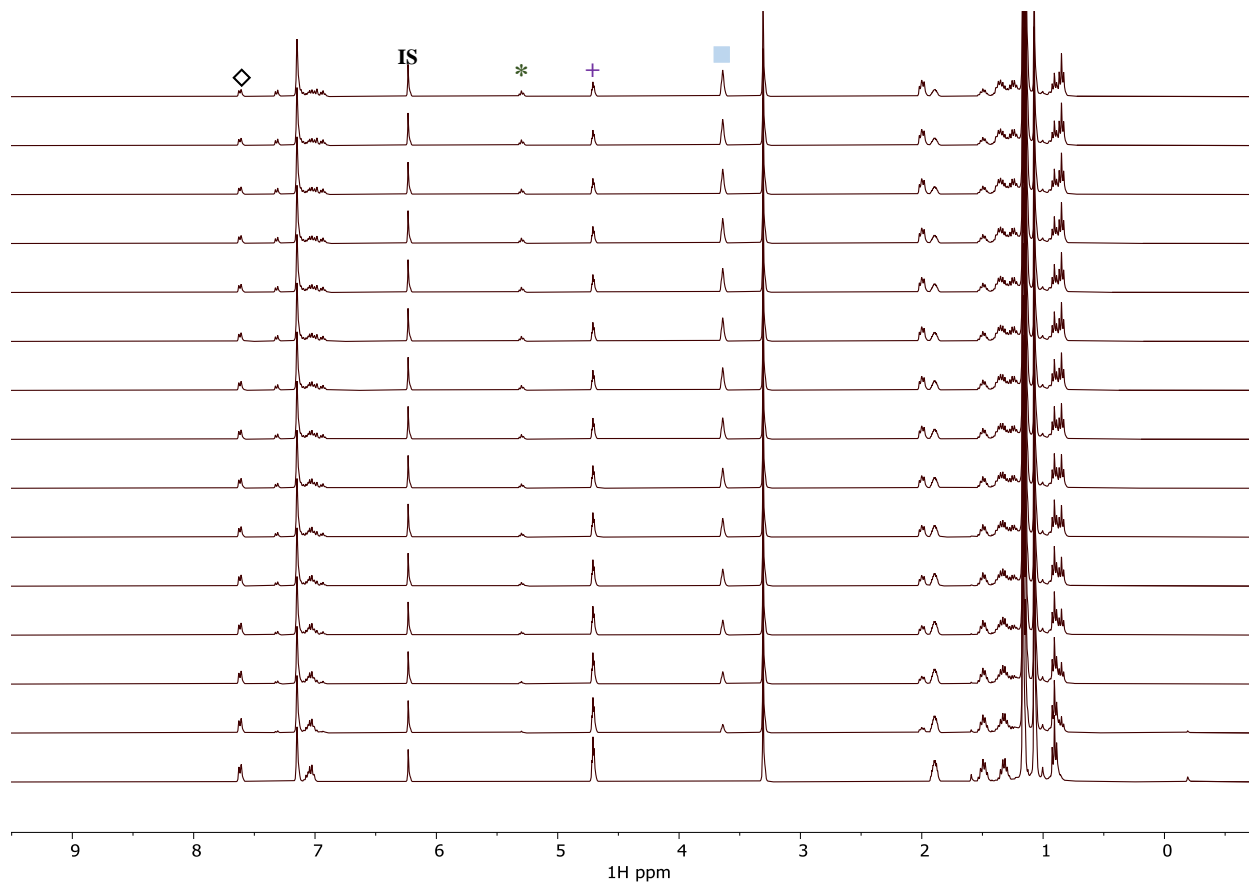
**Figure S11.**  $^1\text{H}$  NMR (400 MHz,  $\text{C}_6\text{D}_6$ ,  $35^\circ\text{C}$ ) spectra collected with a time interval of 5 min (only 18 spectra are presented here for clarity) in the reaction of **1** and **2** catalyzed by **5** (10 mol%) in  $\text{C}_6\text{D}_6$  (600  $\mu\text{L}$ ). Compound key:  $\diamond = \mathbf{1}$ , IS = 1,3,5-trimethoxybenzene,  $+$  = **2**,  $*$  = **3**.



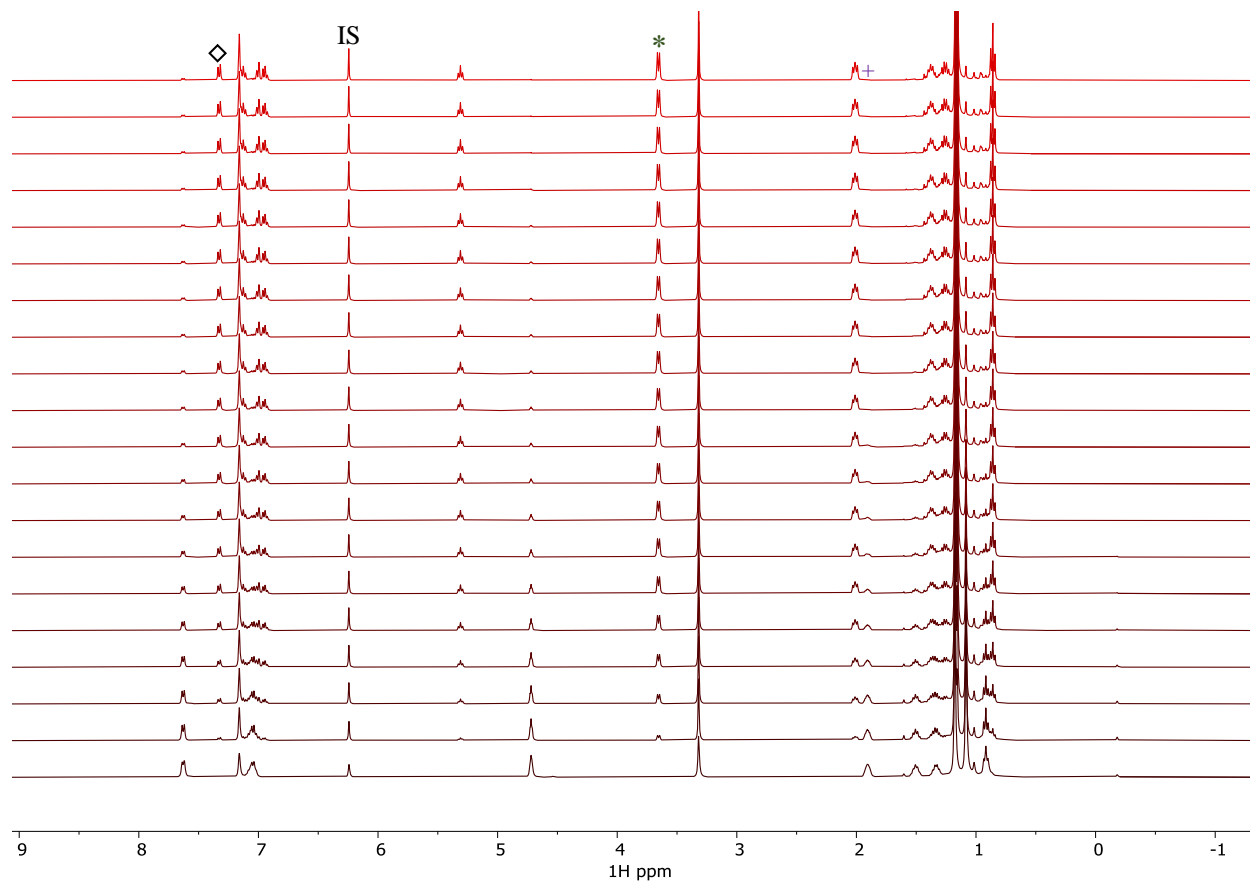
**Figure S12.** <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>, 35 °C) spectra collected with a time interval of 5 min (only 18 spectra are presented here for clarity) in the reaction of **1** and **2** catalyzed by **5** (10 mol%) in C<sub>6</sub>D<sub>6</sub> (600 μL). Compound key: Compound key:  $\triangle = \mathbf{5}$ ,  $\square = \mathbf{6}$ .



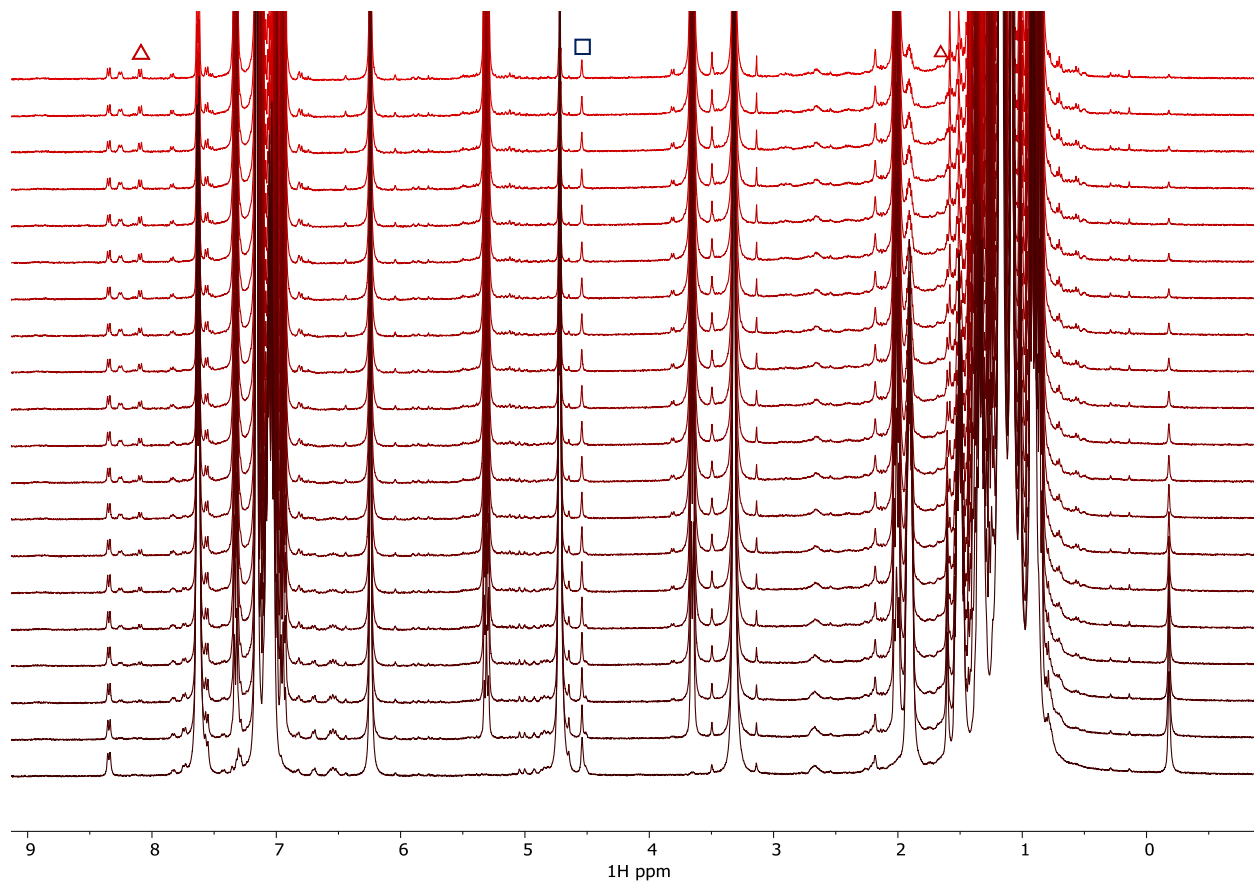
**Figure S13.** <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>, 35 °C) spectra collected with a time interval of 5 min (only 15 spectra are presented here for clarity) in the reaction of **1** and **2** catalyzed by **6** (10 mol%) in C<sub>6</sub>D<sub>6</sub> (600 μL). Compound key: ◇ = **1**, IS = 1,3,5-trimethoxybenzene, + = **2**, \* = **3**.



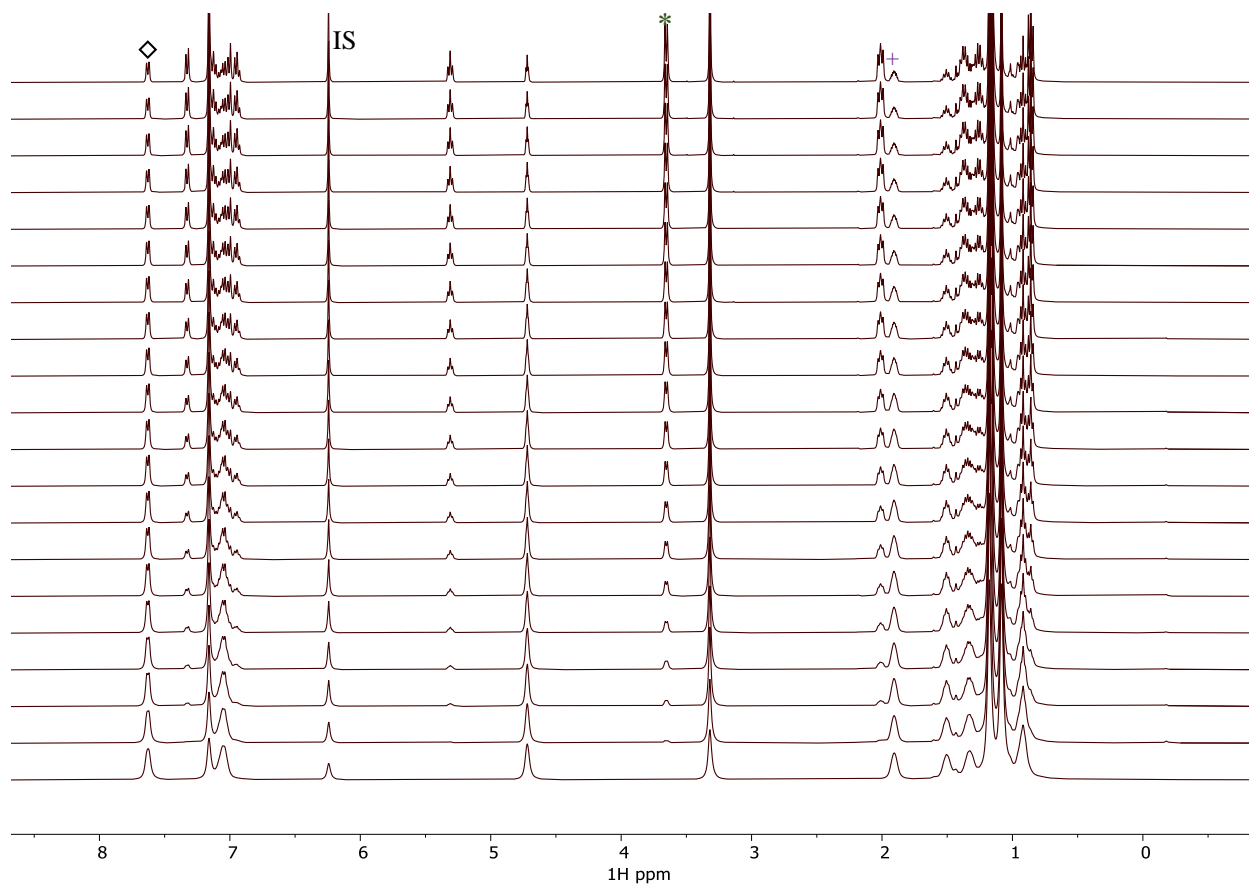
**Figure S14.**  $^1\text{H}$  NMR (400 MHz,  $\text{C}_6\text{D}_6$ ,  $25\text{ }^\circ\text{C}$ ) spectra collected with a time interval of 5 min (only 15 spectra are presented here for clarity) in the reaction of **1** (50.0 mM),  $[\text{D}]_5\text{-1}$  (53.7 mM) and **2** (92.8 mM) catalyzed by a mixture of **6** (5.0 mM) and  $[\text{D}]_5\text{-6}$  (5.0 mM) in  $\text{C}_6\text{D}_6$  (600  $\mu\text{L}$ ). Compound key:  $\diamond$  = **1**, IS = 1,3,5-trimethoxybenzene, + = **2**, \* = **3**,  $\blacksquare$  = **3** +  $[\text{D}]_5\text{-3}$ .



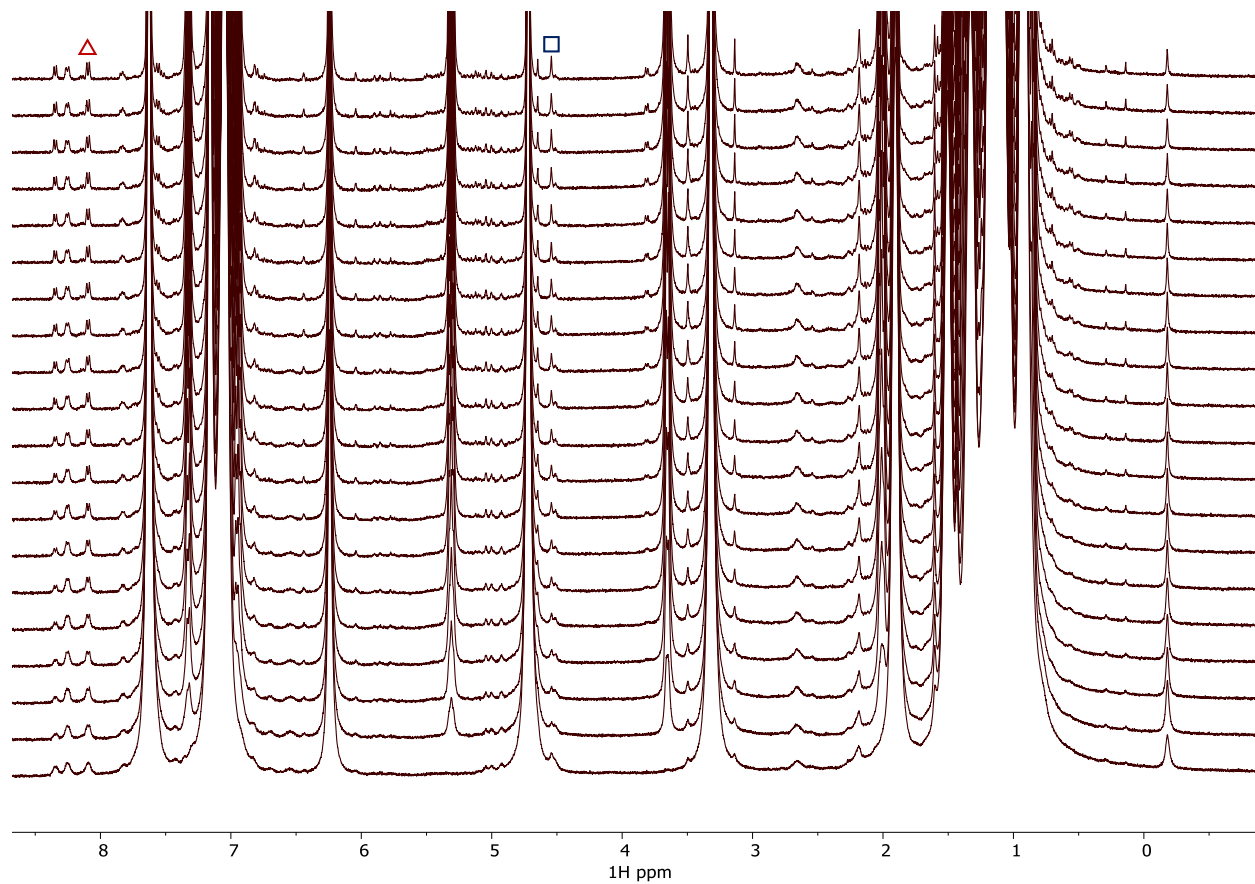
**Figure S15.** <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>, 25 °C) spectra collected with a time interval of 1.33 min (only 20 spectra are presented here for clarity) in the reaction of **1** (95.0 mM) and **2** (95.5 mM) catalyzed by **6** (10.0 mM) in C<sub>6</sub>D<sub>6</sub> (600 μL). Compound key: ◇ = **1**, IS = 1,3,5-trimethoxybenzene, + = **2**, \* = **3**.



**Figure S16.** <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>, 25 °C) spectra collected with a time interval of 1.33 min (only 20 spectra are presented here for clarity) in the reaction of **1** (95.0 mM) and **2** (95.5 mM) catalyzed by **6** (10.0 mM) in C<sub>6</sub>D<sub>6</sub> (600 μL). Compound key: Δ = **5**, □ = **6**.

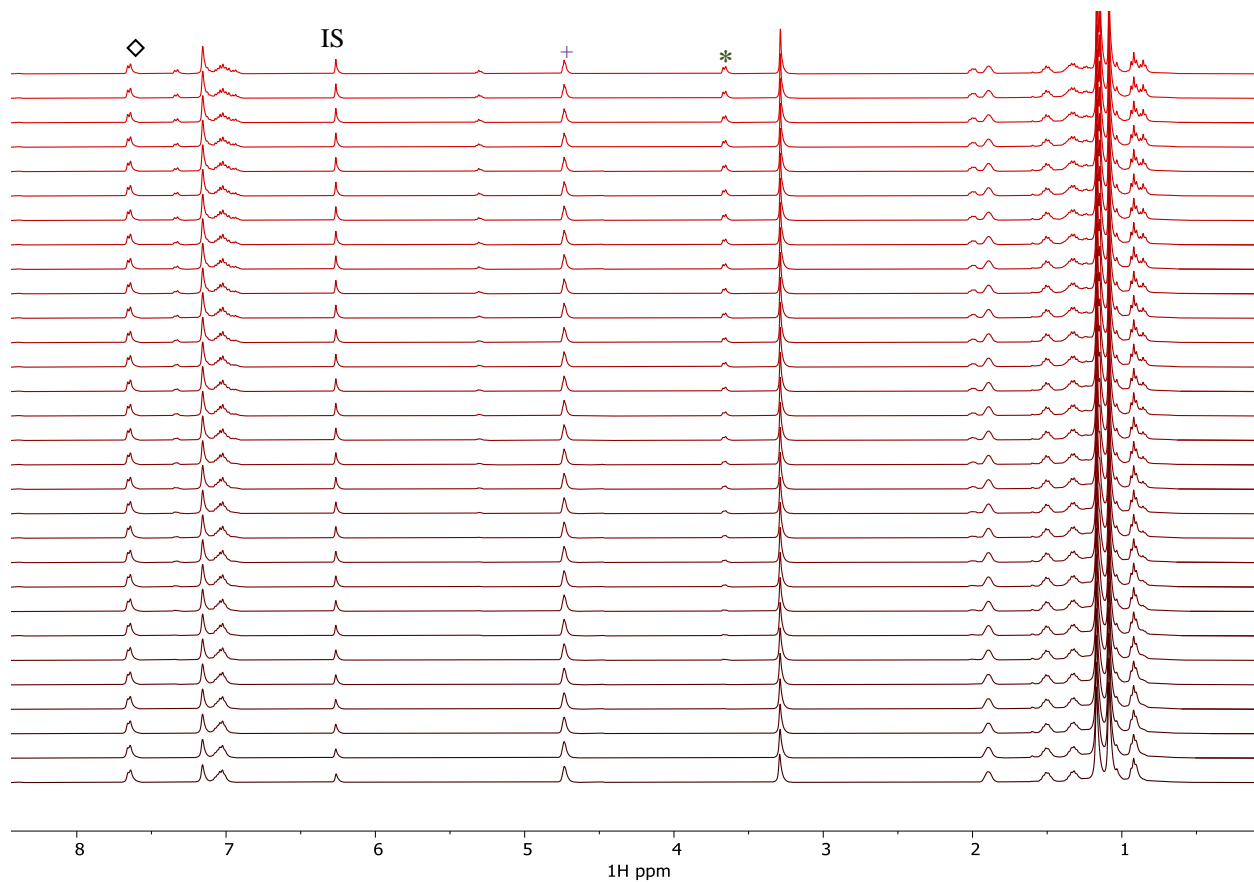


**Figure S17.** <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>, 25 °C) spectra collected with a time interval of 1.33 min (only 20 spectra are presented here for clarity) in the reaction of **1** (95.0 mM) and **2** (95.5 mM) catalyzed by **6** (10.0 mM, incubated in a C<sub>6</sub>D<sub>6</sub> solution for 500 min at 35 °C) in C<sub>6</sub>D<sub>6</sub> (600 μL). Compound key: ◇ = **1**, IS = 1,3,5-trimethoxybenzene, + = **2**, \* = **3**.

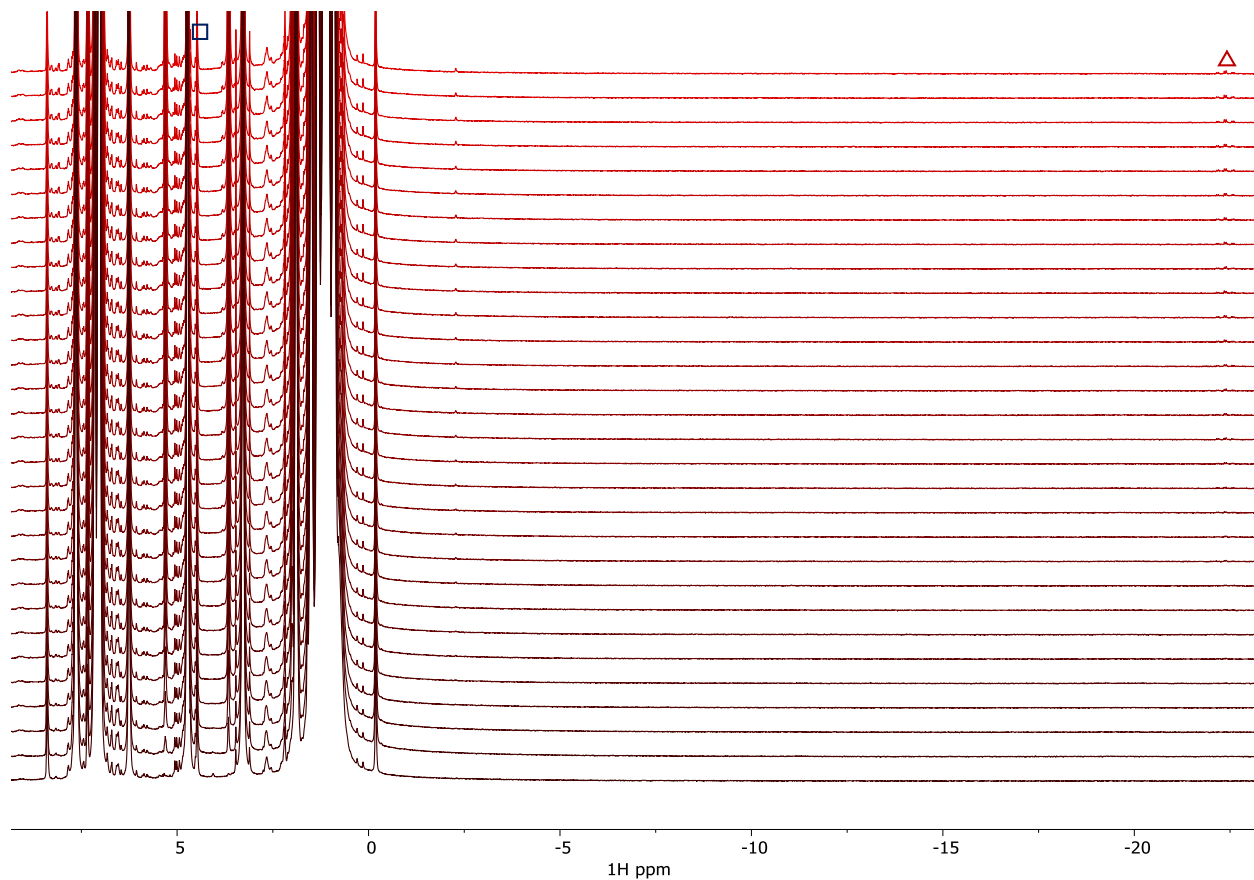


**Figure S18.** <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>, 25 °C) spectra collected with a time interval of 1.33 min (only 20 spectra are presented here for clarity) in the reaction of **1** (95.0 mM) and **2** (95.5 mM) catalyzed by **6** (10.0 mM, incubated in a C<sub>6</sub>D<sub>6</sub> solution for 500 min at 35 °C) in C<sub>6</sub>D<sub>6</sub> (600 μL). Compound key: Δ = **5**, □ = **6**.

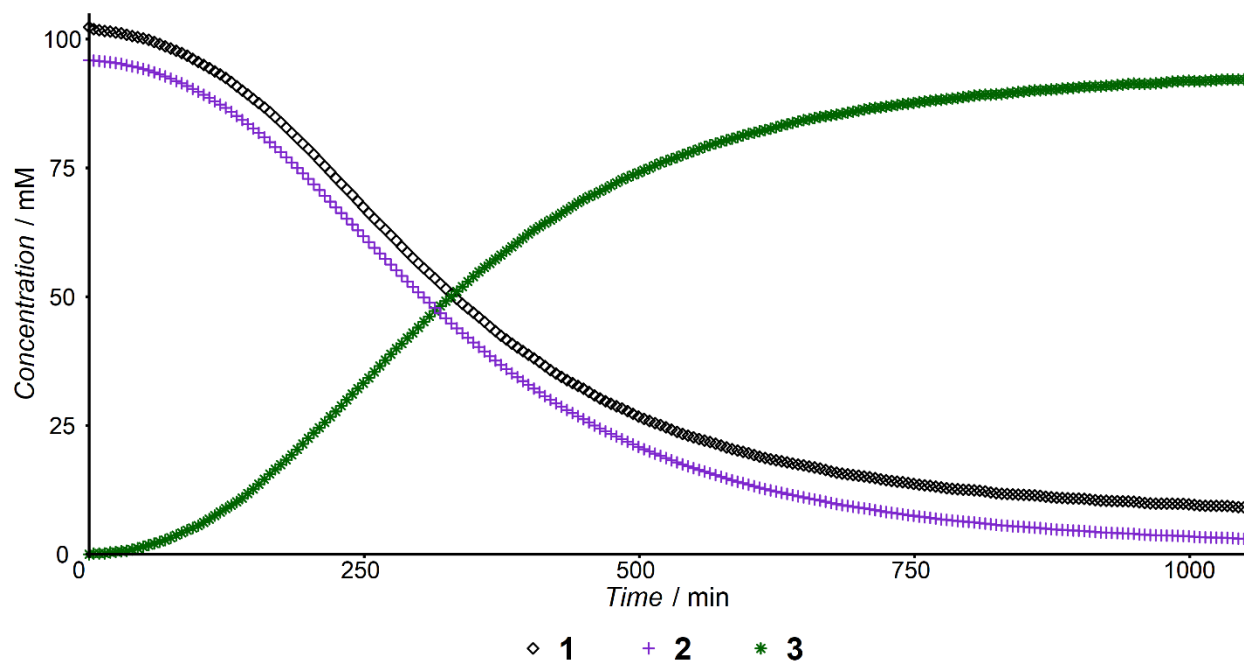




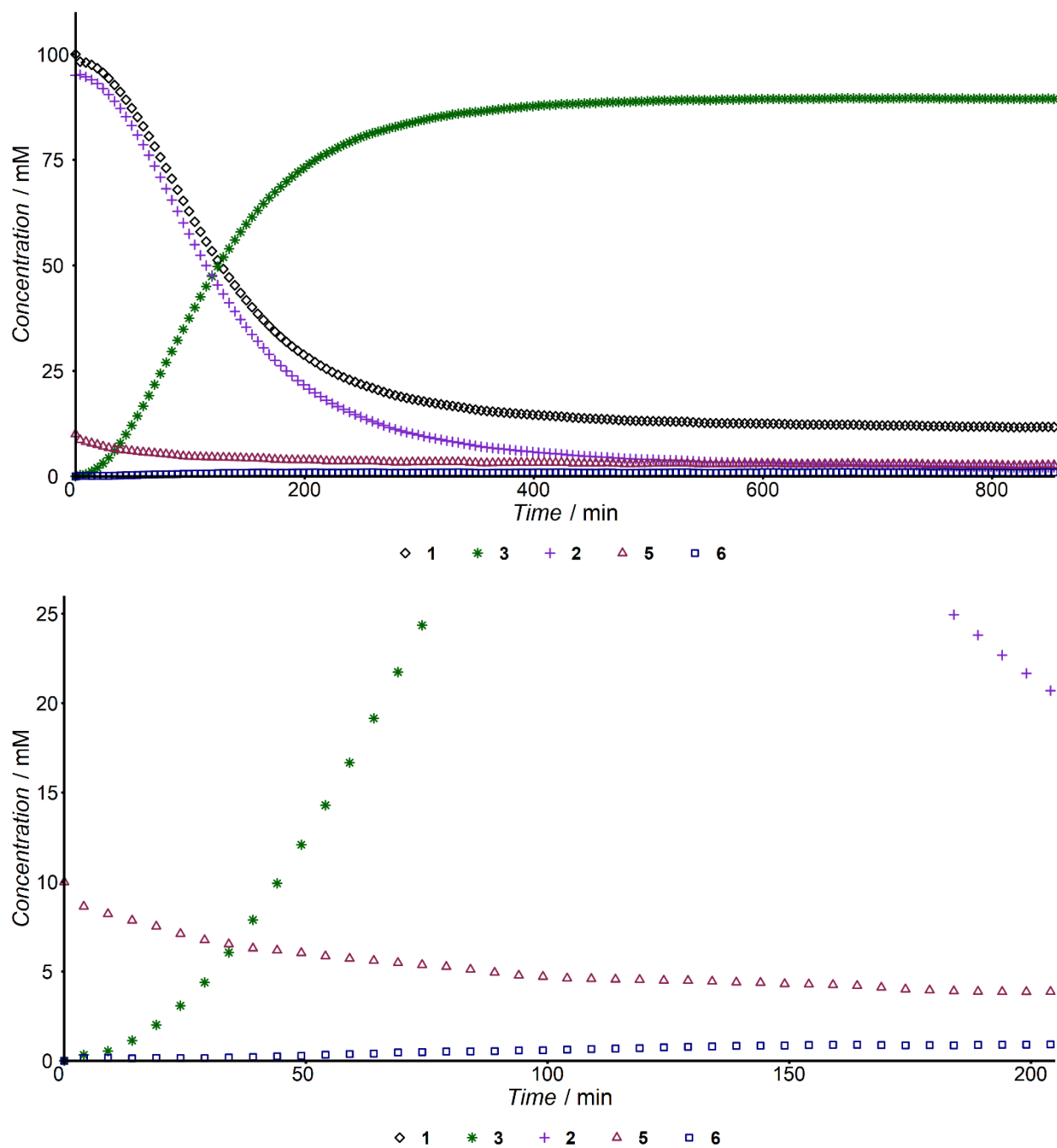
**Figure S19.** <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>, 7 °C) spectra collected with a time interval of 2.15 min (only 30 spectra are presented here for clarity) in the reaction of **1** (93.5 mM) and **2** (95.6 mM) catalyzed by **6** (10.0 mM) in C<sub>6</sub>D<sub>6</sub> (600 μL). Compound key: ◇ = **1**, IS = 1,3,5-trimethoxybenzene, + = **2**, \* = **3**.



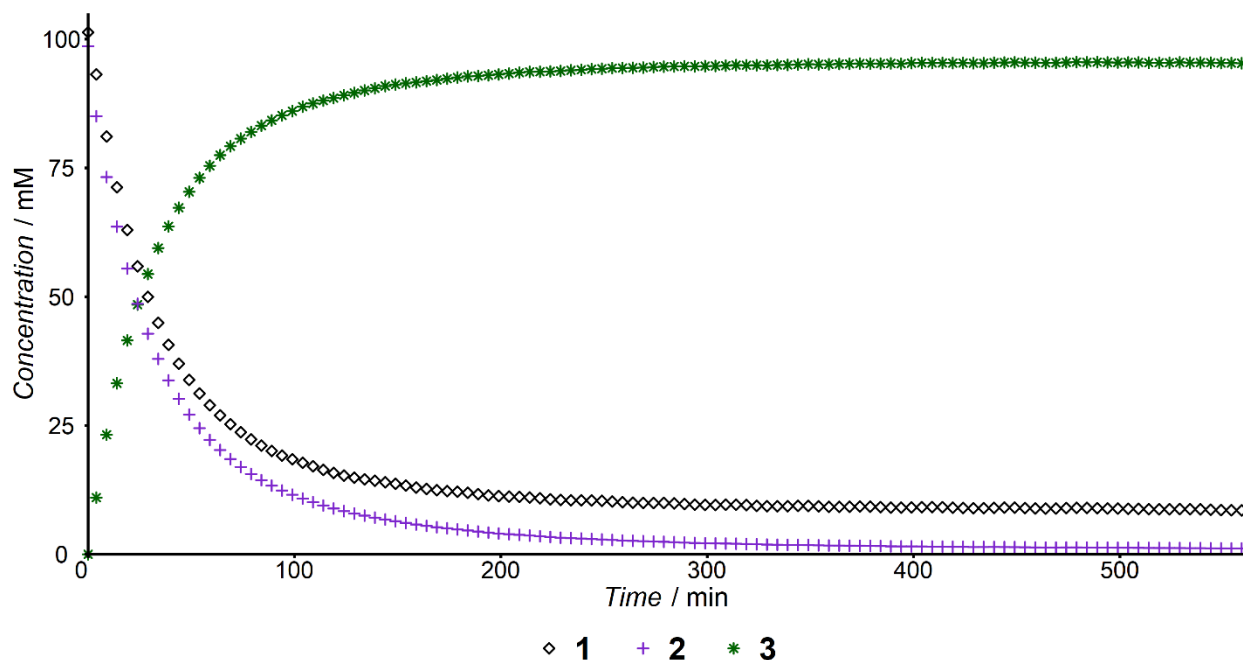
**Figure S20.** <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>, 7 °C) spectra collected with a time interval of 2.15 min (only 30 spectra are presented here for clarity) in the reaction of **1** (93.5 mM) and **2** (95.6 mM) catalyzed by **6** (10.0 mM) in C<sub>6</sub>D<sub>6</sub> (600 μL). Compound key:  $\triangle$  = **5**,  $\square$  = **6**.



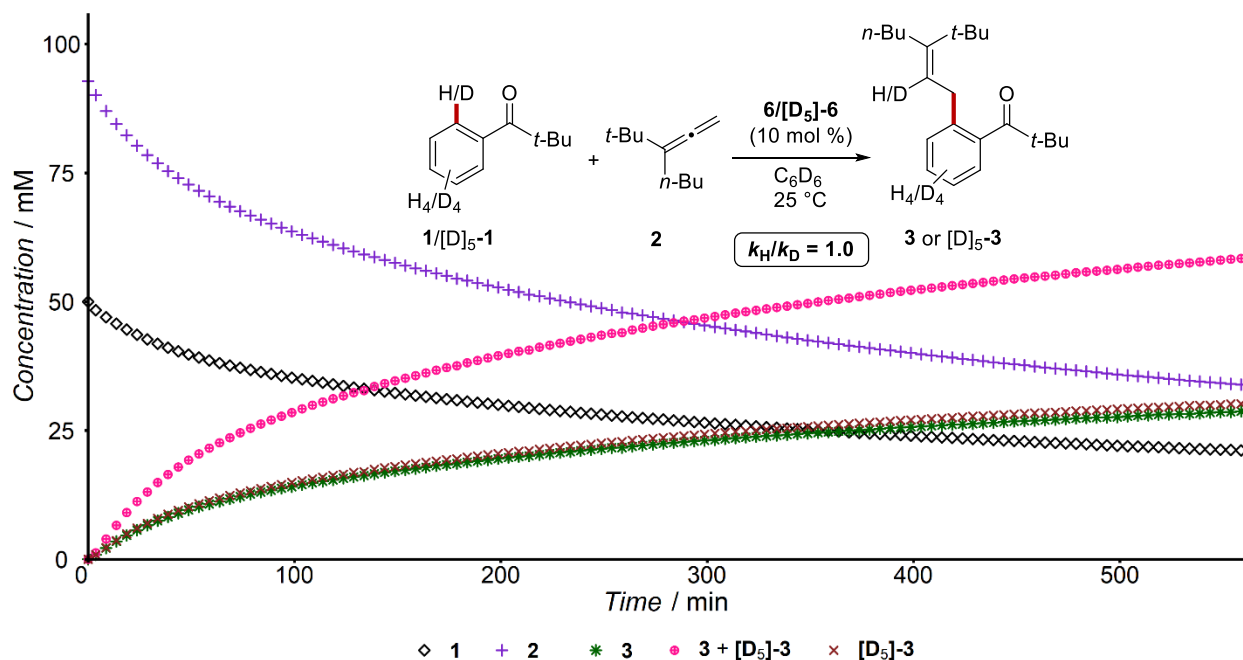
**Figure S21.** Reaction between **1** (102.3 mM) and **2** (95.9 mM) catalyzed by **4** (10.0 mM) at 35.0 °C and a total volume of 600  $\mu$ L (Entry S1, Table S1). Data taken from reference 4.



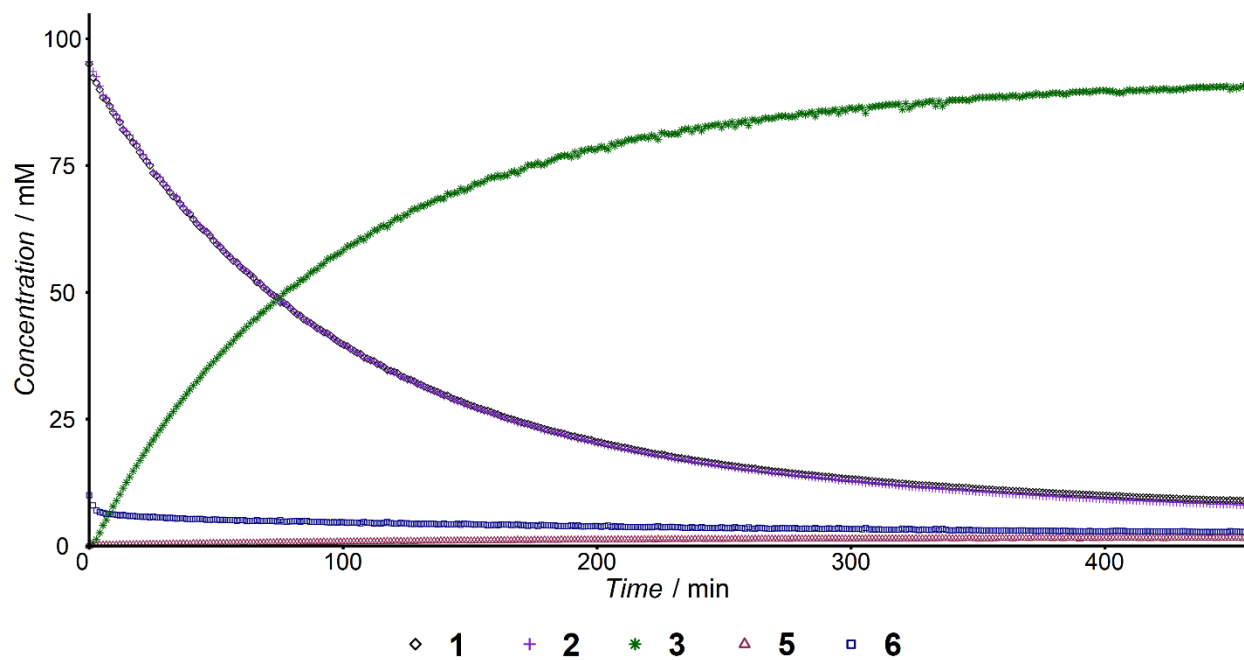
**Figure S22.** Reaction between **1** (95.6 mM) and **2** (91.3 mM) catalyzed by **5** (10.0 mM) at 35.0 °C and a total volume of 600  $\mu$ L (Entry S2, Table S1).



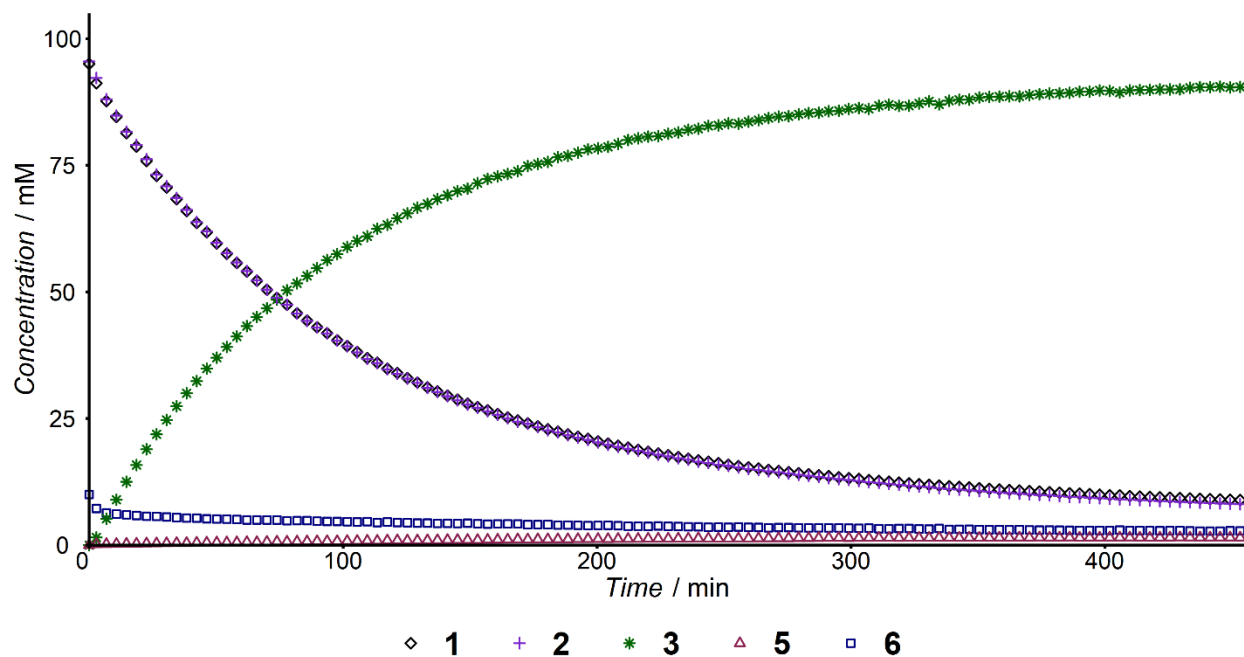
**Figure S23.** Reaction between **1** (101.3 mM) and **2** (98.6 mM) catalyzed by **6** (10.0 mM) at 35.0 °C and a total volume of 600  $\mu$ L (Entry S3, Table S1).



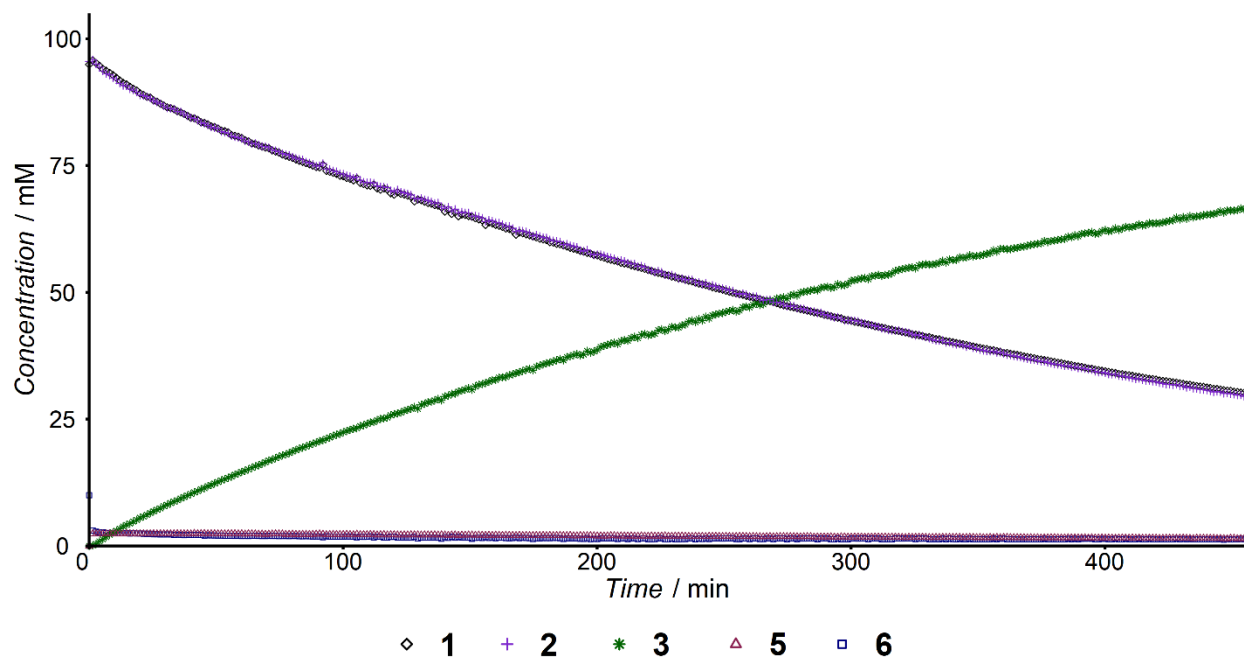
**Figure S24.** Reaction between ketone **1** (50.0 mM),  $[D]_5$ -**1** (53.7 mM) and **2** (92.8 mM) catalyzed by a mixture of **6** (5.0 mM) and  $[D]_5$ -**6** (5.0 mM) at 25.0 °C and a total volume of 600  $\mu$ L (entry S4, Table S1). A  $k_H/k_D$  ratio of 1.0 was calculated by obtaining the initial rates from each of the non-deuterated and deuterated product reaction profiles (by performing a linear regression in the range between 0 and 3.5 mM of product formed where good linearity is observed) followed by subsequent division of the two values.



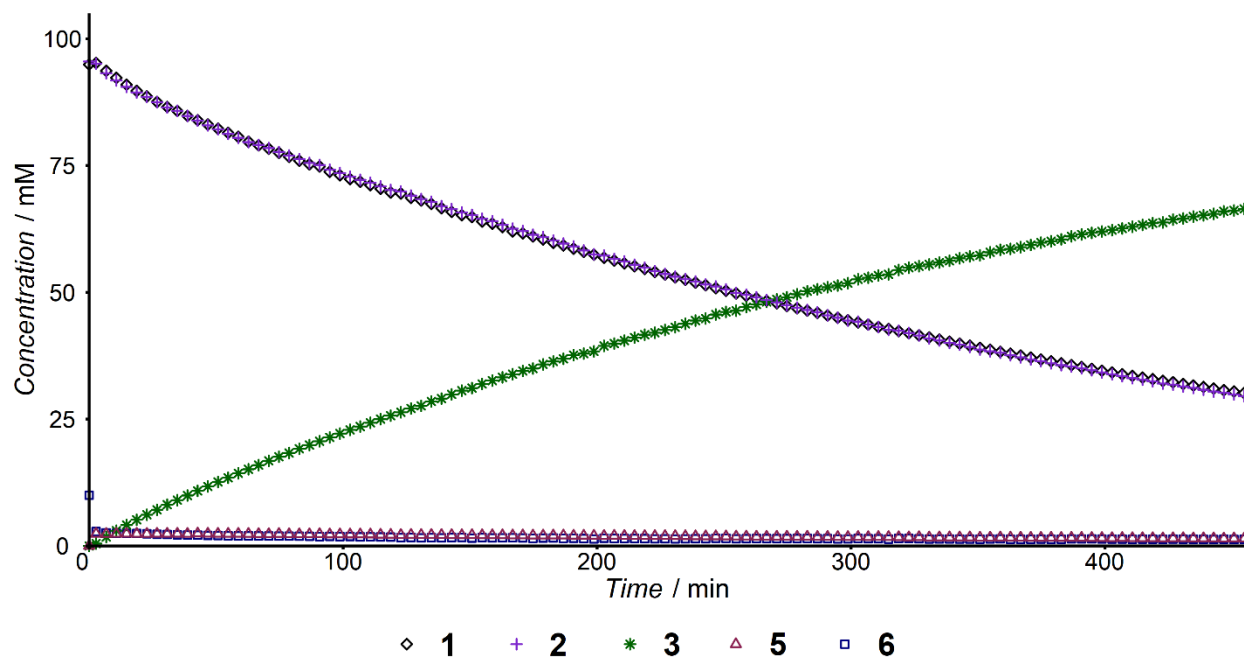
**Figure S25.** Reaction between **1** (95.0 mM) and **2** (95.5 mM) catalyzed by **6** (10.0 mM) at 25.0 °C and a total volume of 600  $\mu$ L (Entry S5, Table S1).



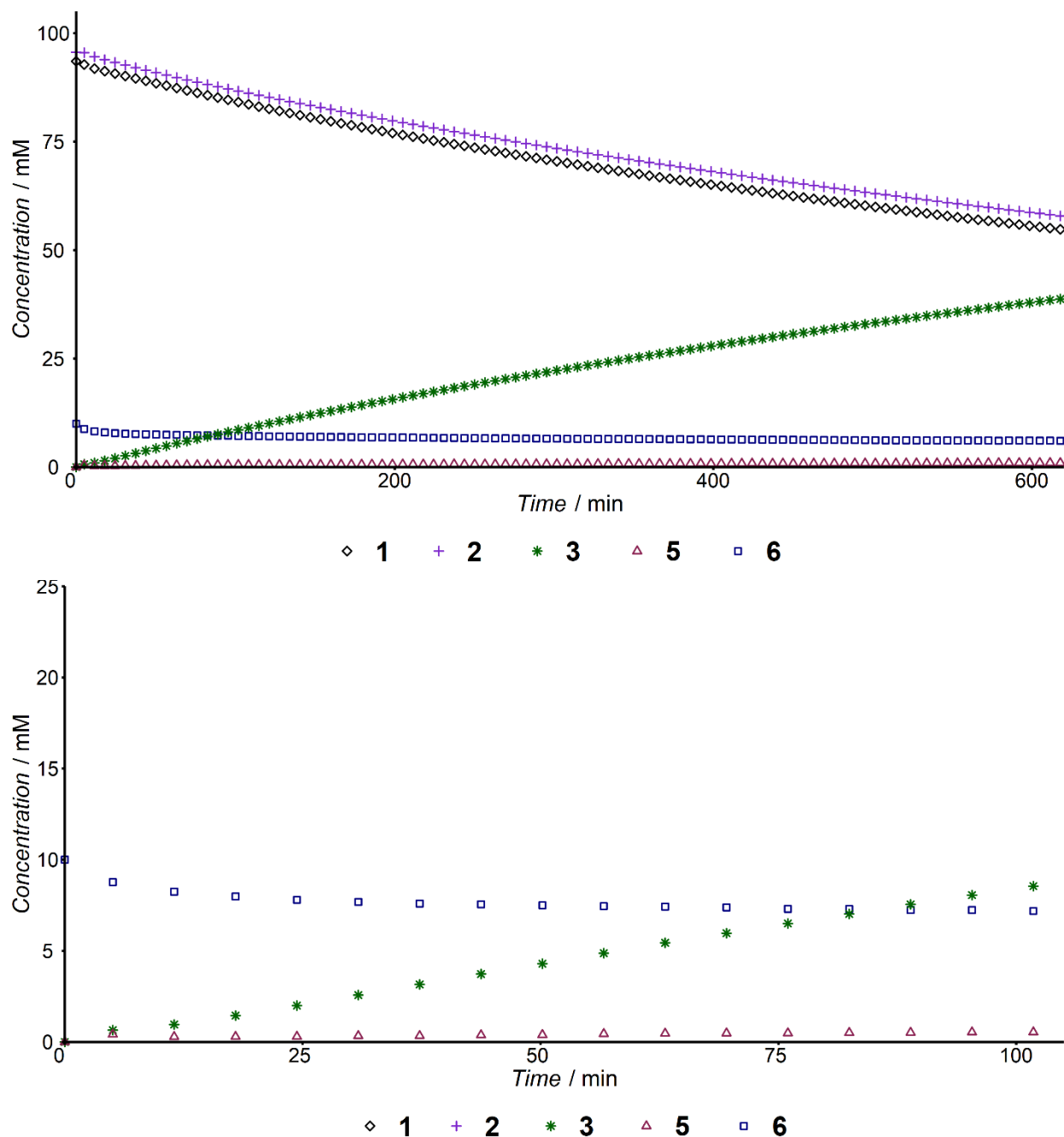
**Figure S26.** Binned data from Figure S25 where the average was obtained every three timepoints.



**Figure S27.** Reaction between **1** (95.0 mM) and **2** (95.5 mM) catalyzed at 25.0 °C by an incubated solution of **6** (10.0 mM) in C<sub>6</sub>D<sub>6</sub> at 35 °C and a total volume of 600 μL (Entry S6, Table S1).



**Figure S28.** Binned data from Figure S27 where the average was obtained every three timepoints.



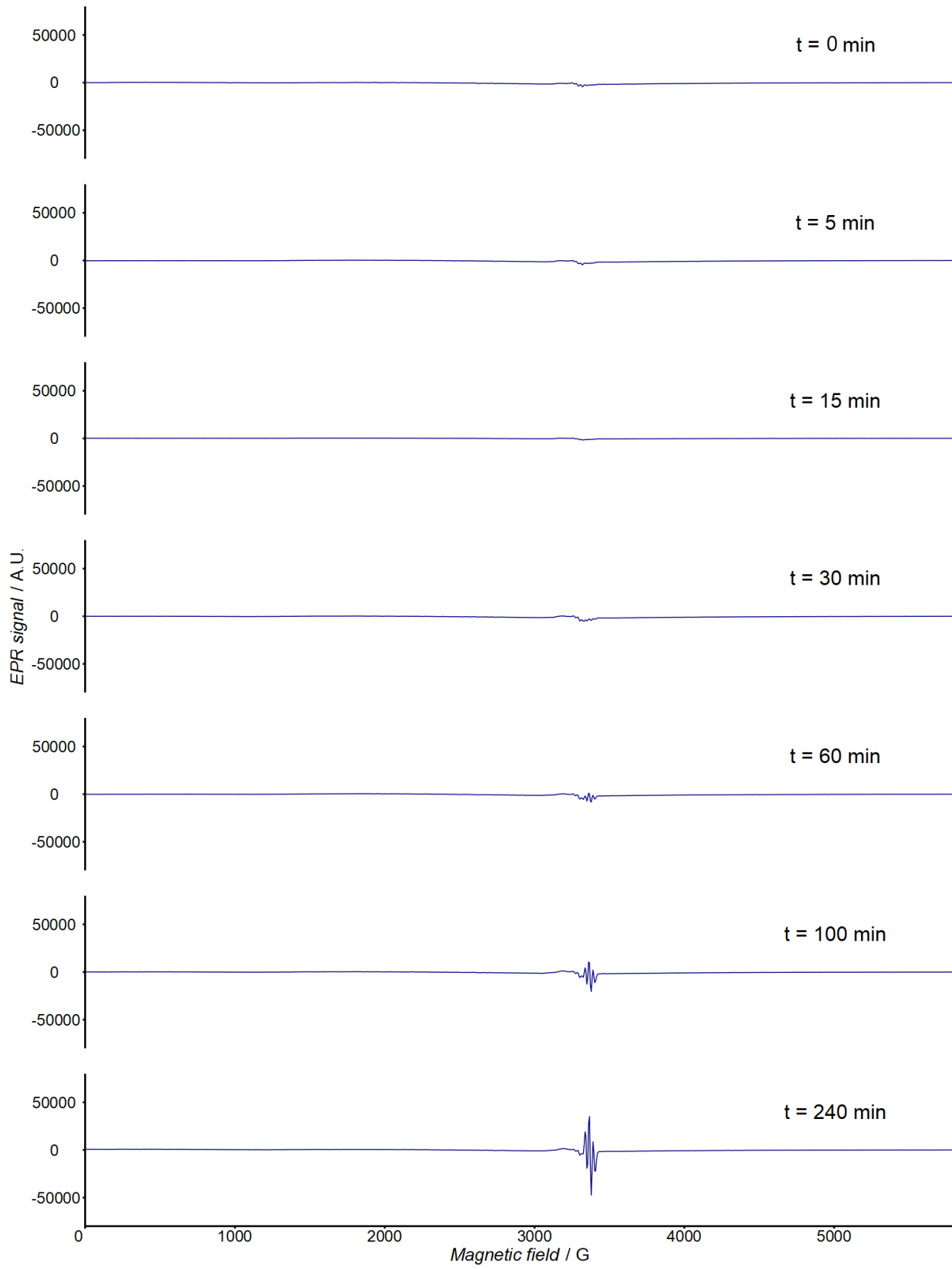
**Figure S29.** Reaction between **1** (93.5 mM) and **2** (95.6 mM) catalyzed by **6** (10.0 mM) at 7 °C and a total volume of 600  $\mu$ L (Entry S5, Table S1) with expansion at the bottom.

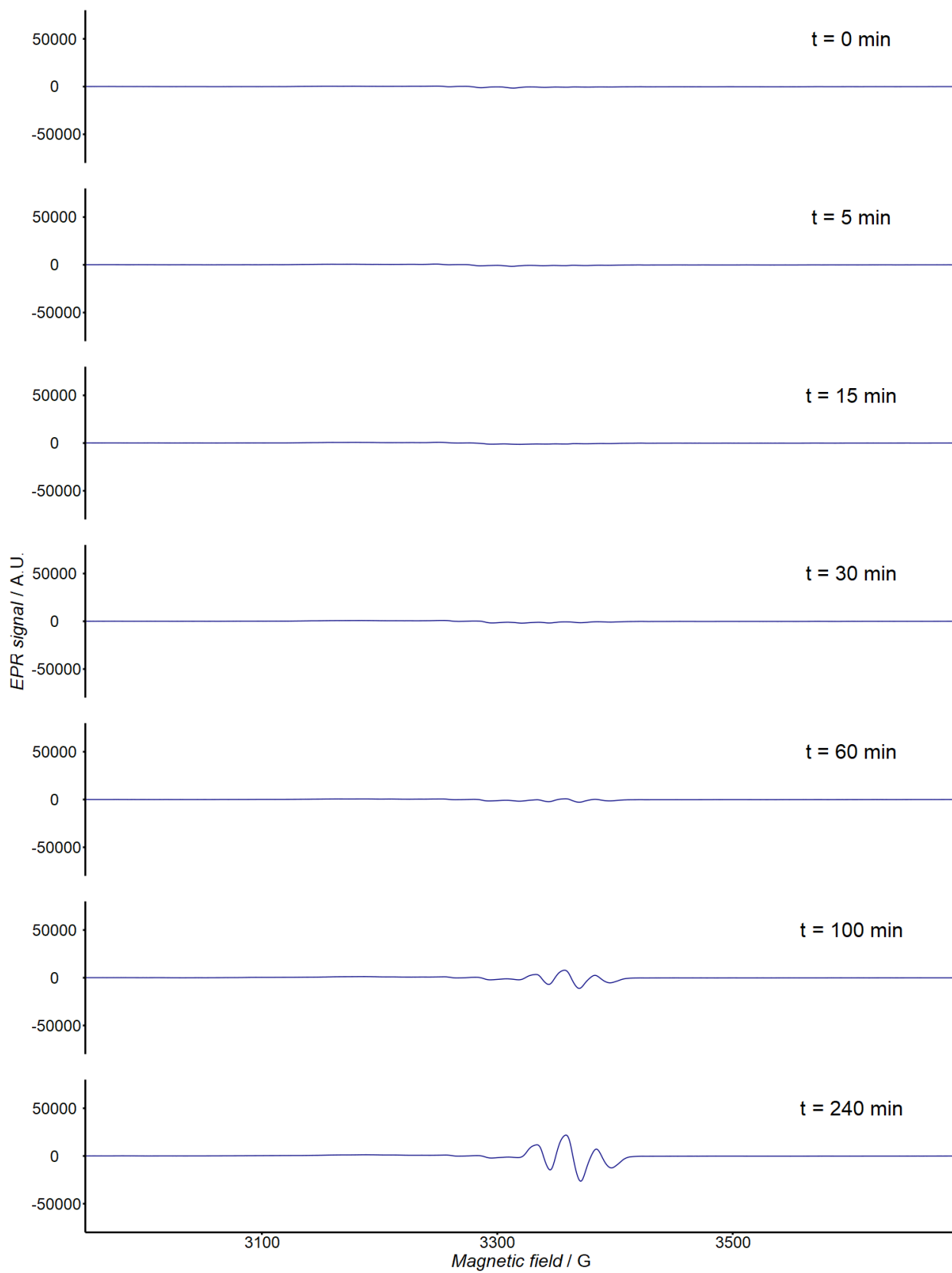
#### 4.2 Catalytic Reaction Monitoring by in Situ EPR Spectroscopy

In a nitrogen filled glove box an EPR tube fitted with a J. Young's tap was loaded with phenone **1** (25.0  $\mu$ L, 0.025 mmol, 1.00 M stock solution in  $C_6D_6$ ), allene **2** (25.0  $\mu$ L, 0.025 mmol, 1.00 M



stock solution in C<sub>6</sub>D<sub>6</sub>), 1,3,5-trimethoxybenzene (12.5 μL, 0.0063 mmol, 500 mM stock solution in C<sub>6</sub>D<sub>6</sub>), and C<sub>6</sub>D<sub>6</sub> (162.5 μL). The solution was then activated by adding **6** (25.0 μL, 0.025 mmol, 100 mM stock solution in C<sub>6</sub>D<sub>6</sub>), immediately frozen, and the EPR spectrum was collected at 140 K. Subsequently, the tube was removed from the spectrometer and kept at 35 °C until further EPR measurement.

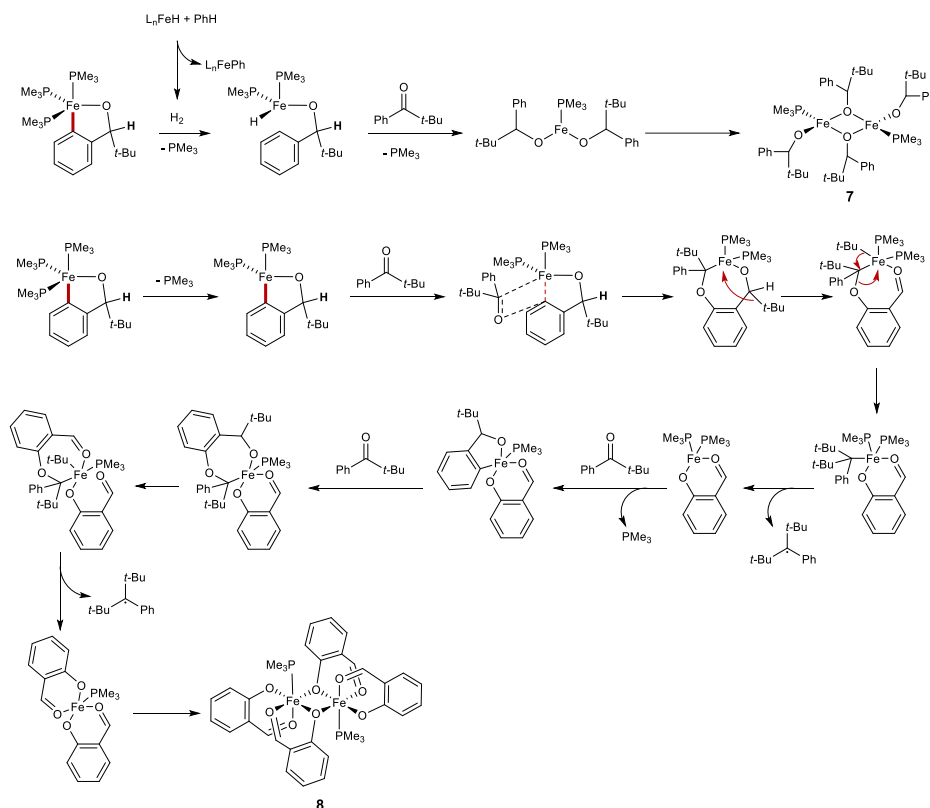




## 5 Stoichiometric reactions

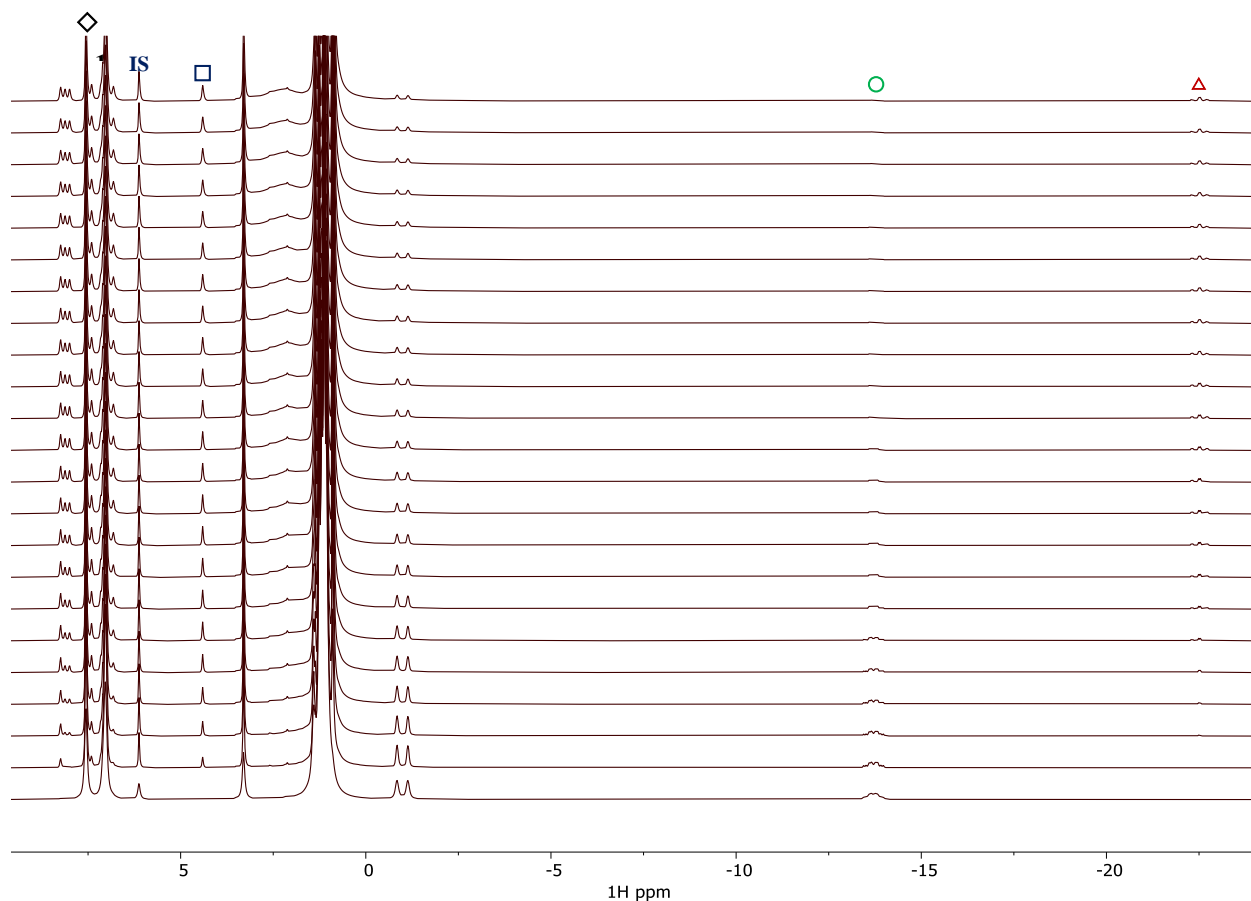
### 5.1 Reaction Between 4 and Excess 1: Isolation of Complex 7 and 8

A Schlenk tube was loaded with **4** (81 mg, 0.22 mmol), **1** (0.5 mL), and a PTFE coated stir bar. After 6 hours of stirring the reaction mixture turned ink blue in color and was dried under reduced pressure for 12 hours. The dark residue was extracted with pentane and the condensed extracts (0.3 mL) were stored at -20 °C. After 12 hours of cooling two types of crystals suitable for an X-ray crystallographic analysis were formed: the previously characterized **5** as well as a lesser amount of **7**. The supernatant solution was subsequently left at room temperature for 12 hours during which time a color change occurred from ink blue to brownish red. After 3 days, crystals suitable for an X-ray crystallographic analysis formed which were found to be complex **8**. A possible mechanism for the formation of **7** and **8** is tentatively proposed in the scheme below. It is possible that hydrogen could be generated by the reaction of the various iron hydride complexes with benzene and immediately react with **6**.<sup>6</sup> It must also be noted that the produced radical is reported as stable and has been previously spectroscopically characterized.<sup>7</sup> However, at this point we cannot rule out formation of such species due to reaction with trace amounts of water/air present in the reaction mixture.

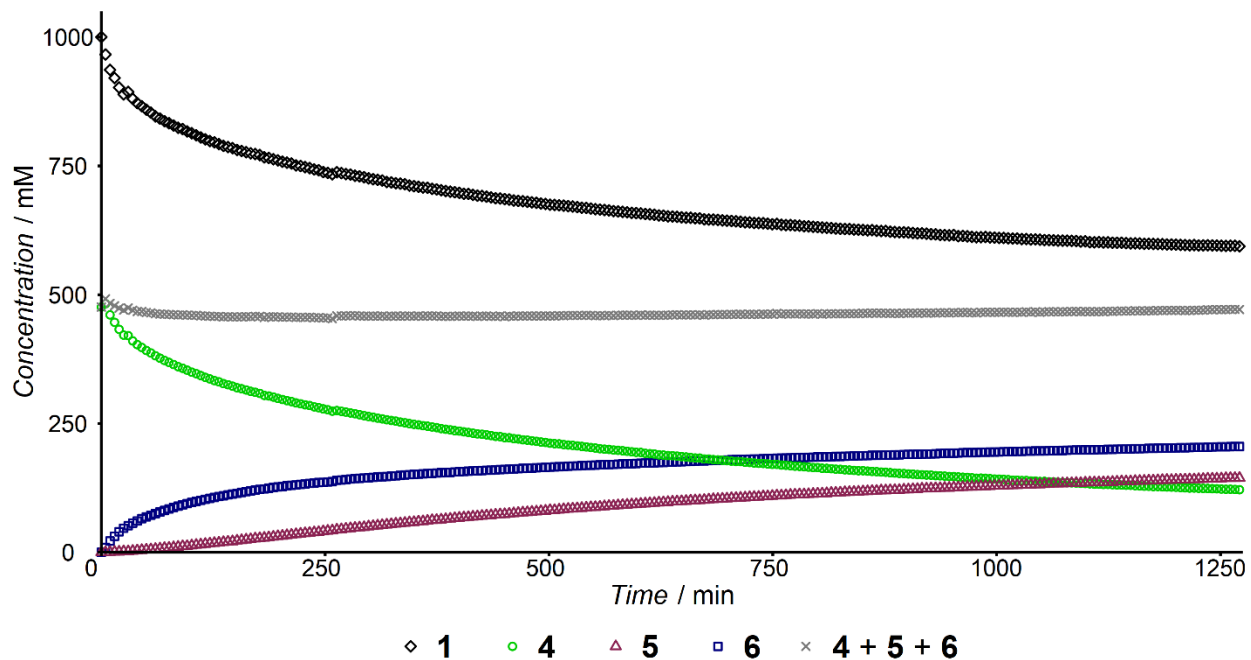


## 5.2 Monitoring of the Reaction Between **1** and **4** by $^1\text{H}$ NMR Spectroscopy

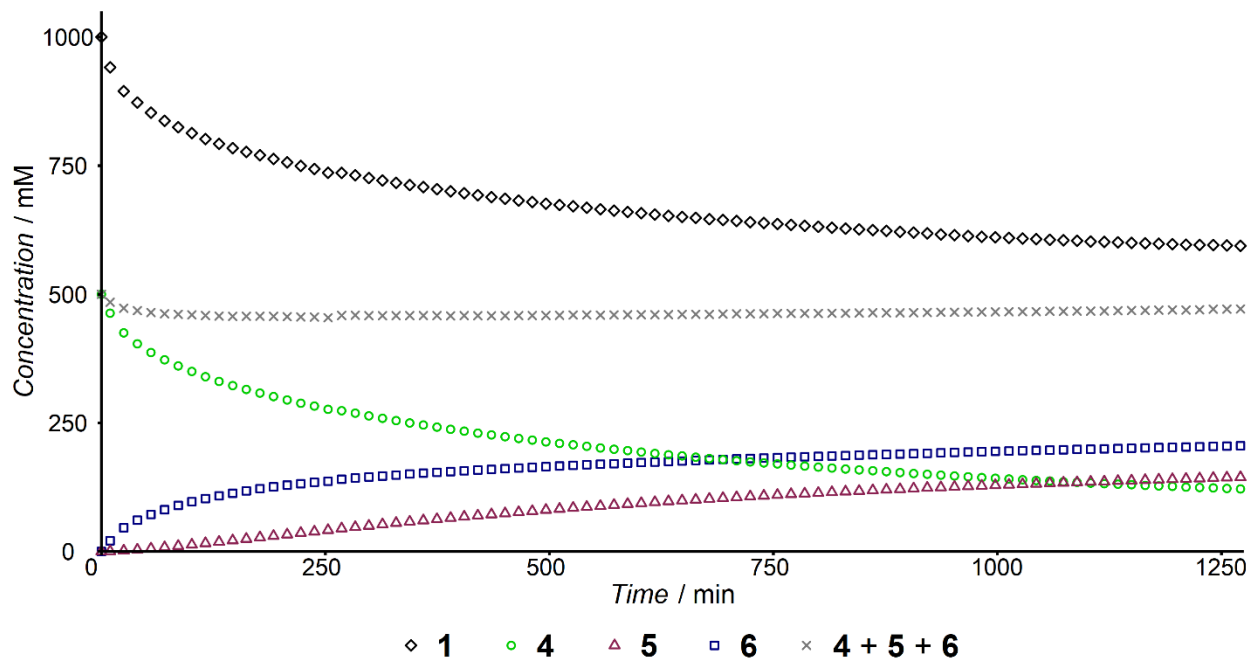
In a nitrogen filled glove box, an airtight NMR tube was loaded with **4** (90.0 mg, 0.250 mmol),  $\text{C}_6\text{D}_6$  (500  $\mu\text{L}$ ), and 1,3,5-trimethoxybenzene (100  $\mu\text{L}$ , 500 mM stock solution in  $\text{C}_6\text{D}_6$ , 0.050 mmol). A first spectrum was collected to lock and shim the spectrometer. Phenone **1** (83.6  $\mu\text{L}$ , 0.500 mmol) was added and the NMR tube was shaken, frozen with liquid nitrogen, and taken to the spectrometer where it was allowed to thaw followed by immediate measurement. Spectra were collected every five minutes. Stacked spectra are presented in Figure S30 below.



**Figure S30.**  $^1\text{H}$  NMR (400 MHz,  $\text{C}_6\text{D}_6$ ,  $30^\circ\text{C}$ ) spectra collected with a time interval of 5 min (only 23 spectra are presented here for clarity) in the reaction of **1** and **4**. Compound key:  $\diamond$  = **1**, **IS** = 1,3,5-trimethoxybenzene,  $\circ$  = **4**,  $\triangle$  = **5**,  $\square$  = **6**.



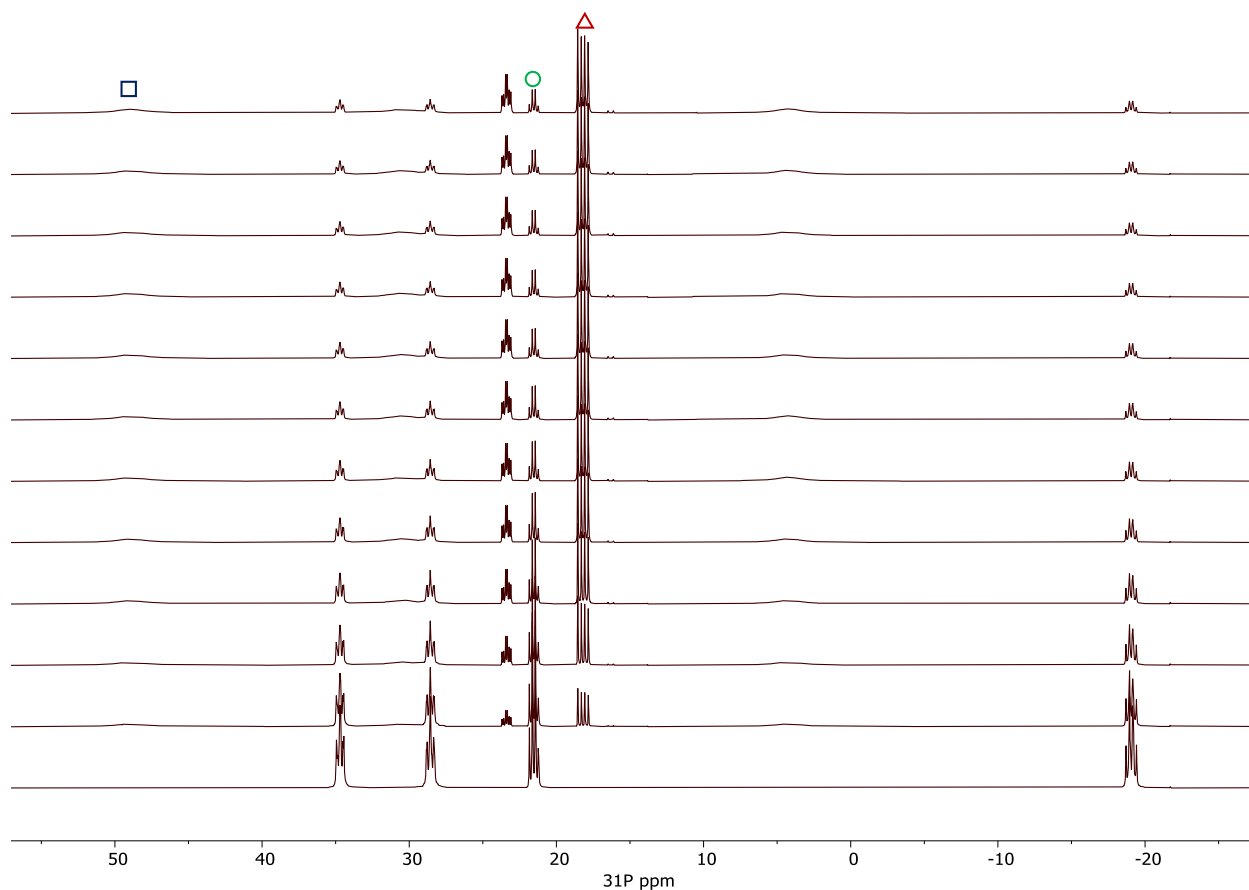
**Figure S31.** Reaction between **1** (1000 mM) and **4** (500 mM) in  $C_6D_6$  at 25.0 °C and a total volume of 500  $\mu$ L.



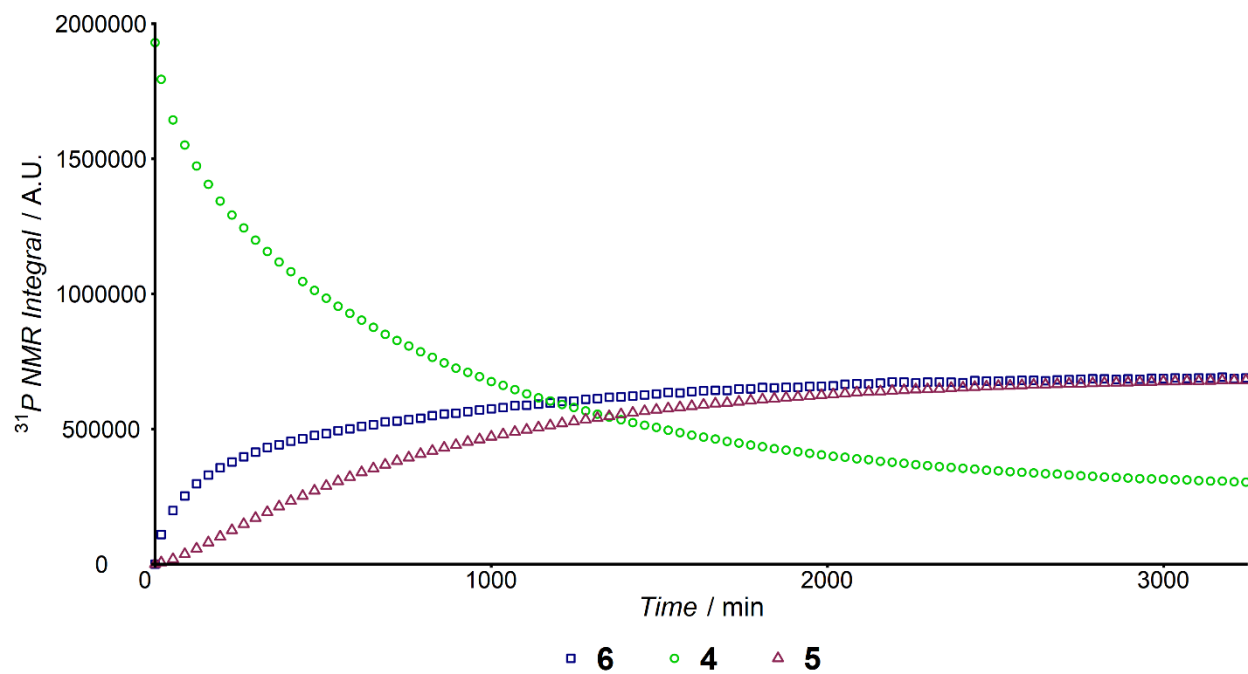
**Figure S32.** Binned data from Figure S31 where the average was obtained every three timepoints.

### 5.3 Monitoring of the Reaction Between **1** or [D]<sub>5</sub>-**1** and **4** by <sup>31</sup>P NMR Spectroscopy and Kinetic Isotope Effect

In a nitrogen filled glove box, an airtight NMR tube was loaded with **4** (90.0 mg, 0.250 mmol), C<sub>6</sub>D<sub>6</sub> (500 μL), and **1** (83.6 μL, 0.500 mmol). The NMR tube was shaken, frozen with liquid nitrogen, and taken to the spectrometer where it was allowed to thaw followed by immediate measurement. Spectra were collected every 35 minutes (1020 scans per spectrum) with a relaxation delay of 1 second. The experiment was then repeated under identical conditions (concentration, volume, temperature, spectrometer, NMR tube used) using [D]<sub>5</sub>-**1** (83.8 μL, 0.500 mmol).

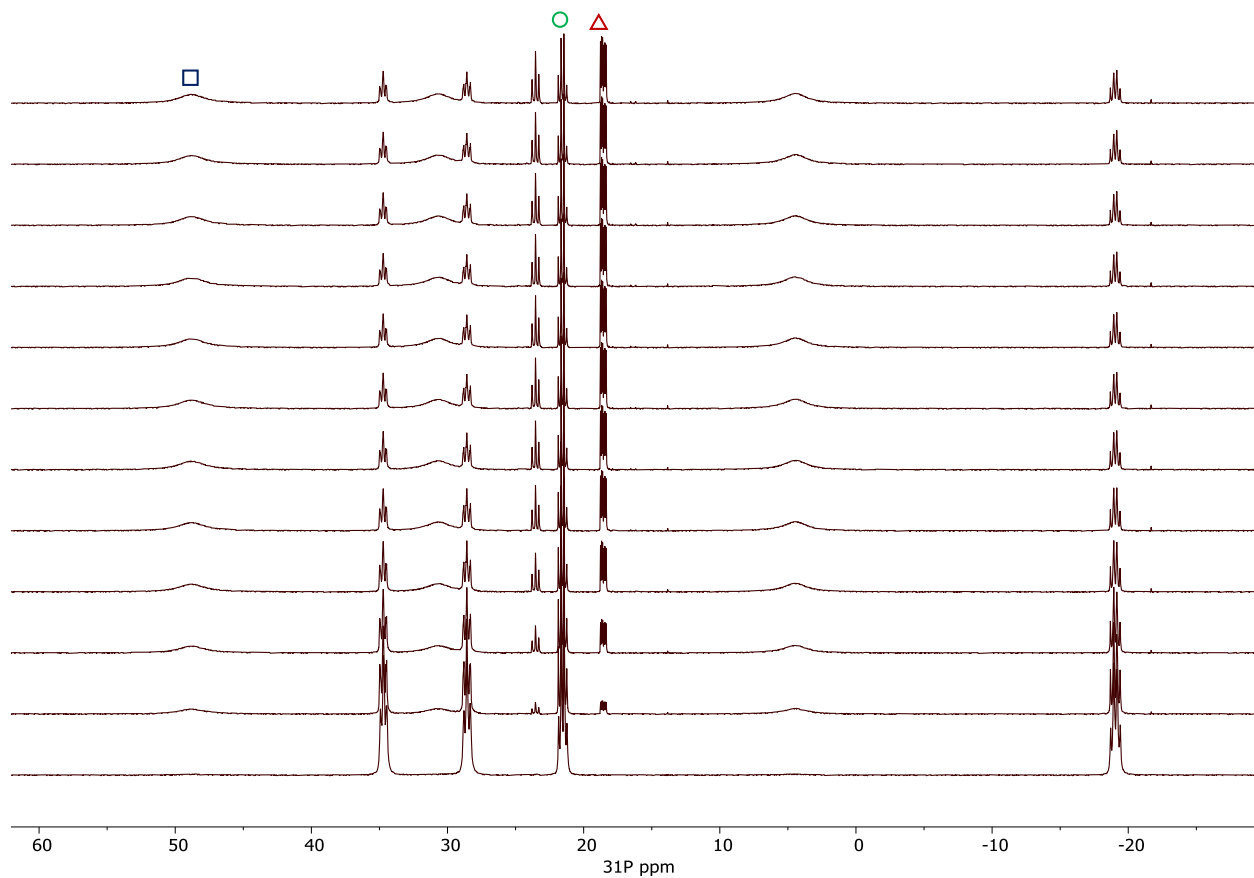


**Figure S33.** <sup>31</sup>P NMR (162 MHz, C<sub>6</sub>D<sub>6</sub>, 25 °C) spectra collected every 35 min (only 10 spectra are presented here for clarity) in the reaction of **1** and **4**. Compound key: ○ = **4**, △ = **5**, □ = **6**.

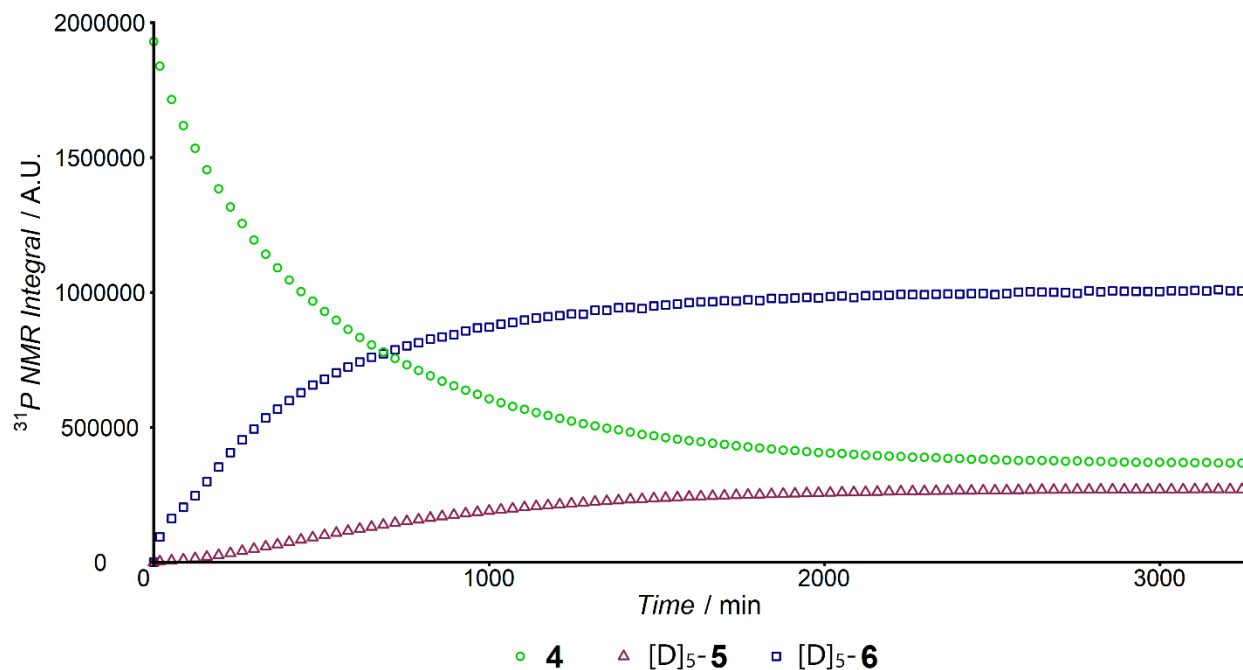


**Figure S34.** Reaction between **1** (1000 mM) and **4** (500 mM) in  $\text{C}_6\text{D}_6$  at 25.0 °C and a total volume of 500  $\mu\text{L}$ .

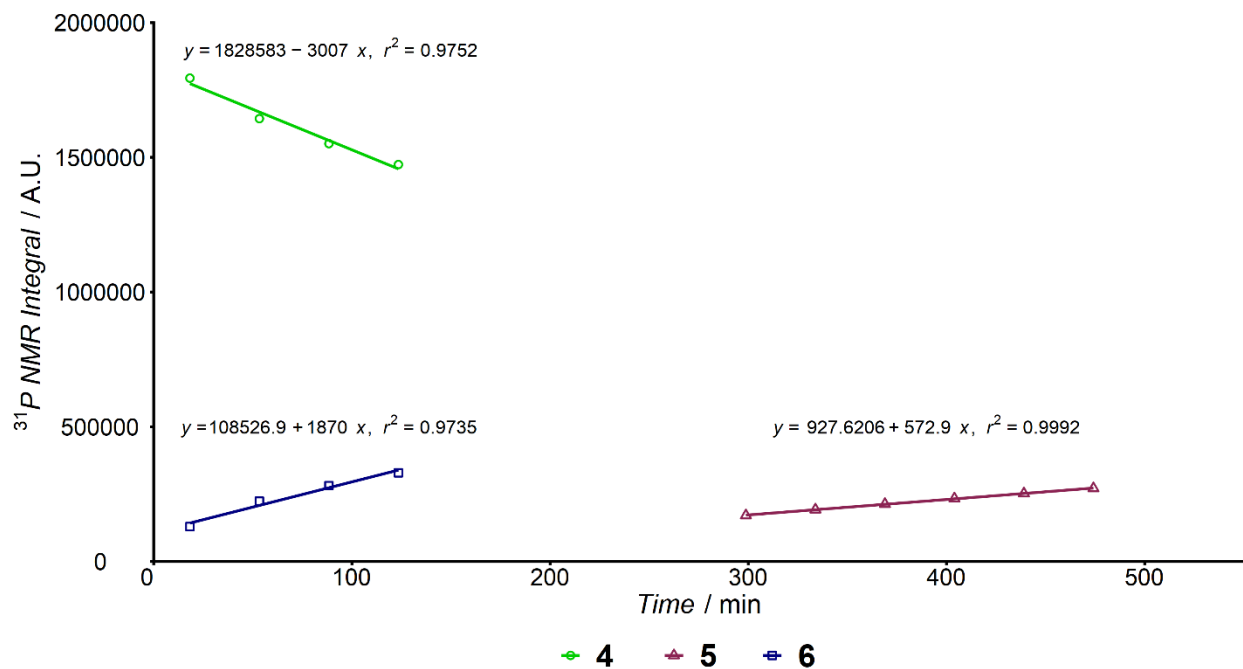




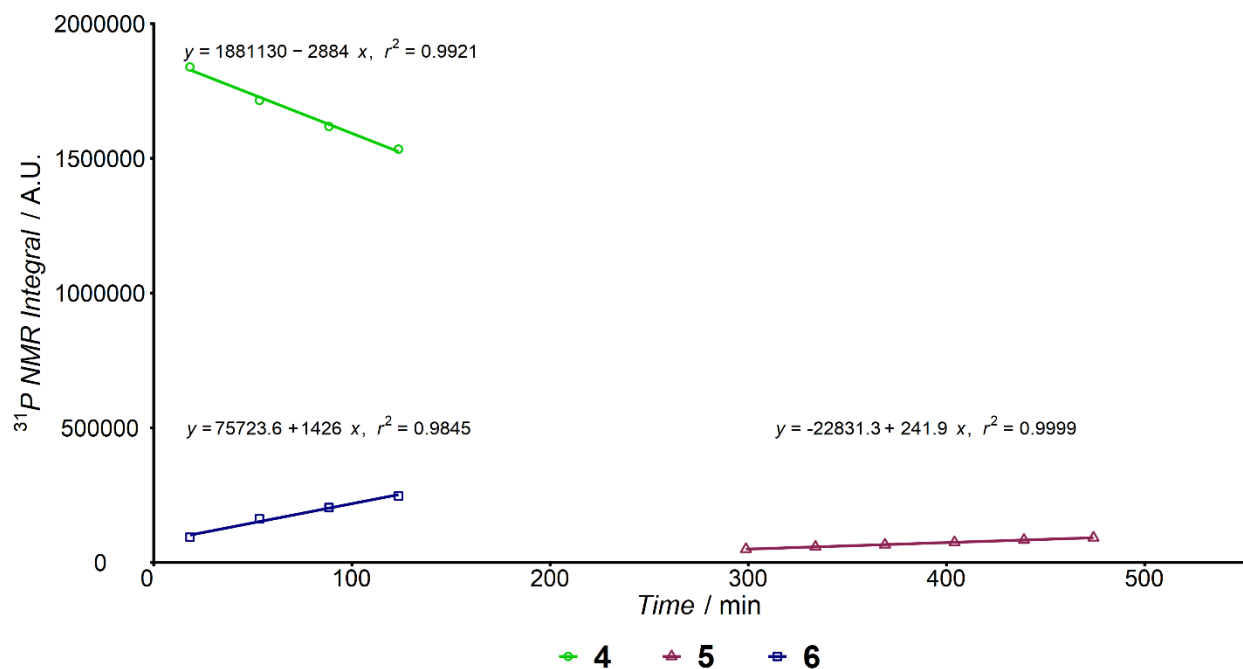
**Figure S35.**  $^{31}\text{P}$  NMR (162 MHz,  $\text{C}_6\text{D}_6$ , 25 °C) spectra collected every 35 min (only 10 spectra are presented here for clarity) in the reaction of  $[\text{D}]_5\text{-1}$  and **4**. Compound key:  $\circ$  = **4**,  $\triangle$  = **5**,  $\square$  = **6**.



**Figure S36.** Reaction between [D]<sub>5</sub>-1 (1000 mM) and 4 (500 mM) in C<sub>6</sub>D<sub>6</sub> at 25.0 °C and a total volume of 500 μL.

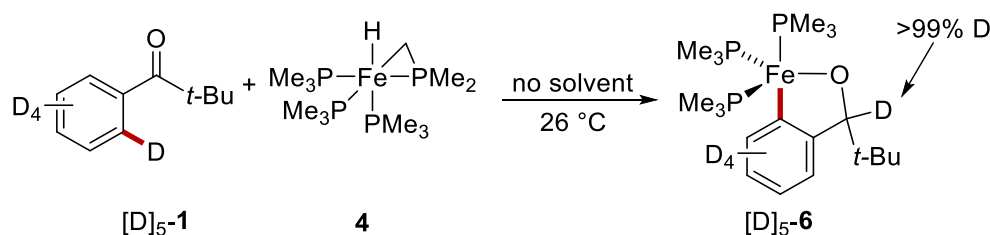


**Figure S37.** Initial rates calculations for the reaction between 1 (1000 mM) and 4 (500 mM) in C<sub>6</sub>D<sub>6</sub> at 25.0 °C and a total volume of 500 μL.

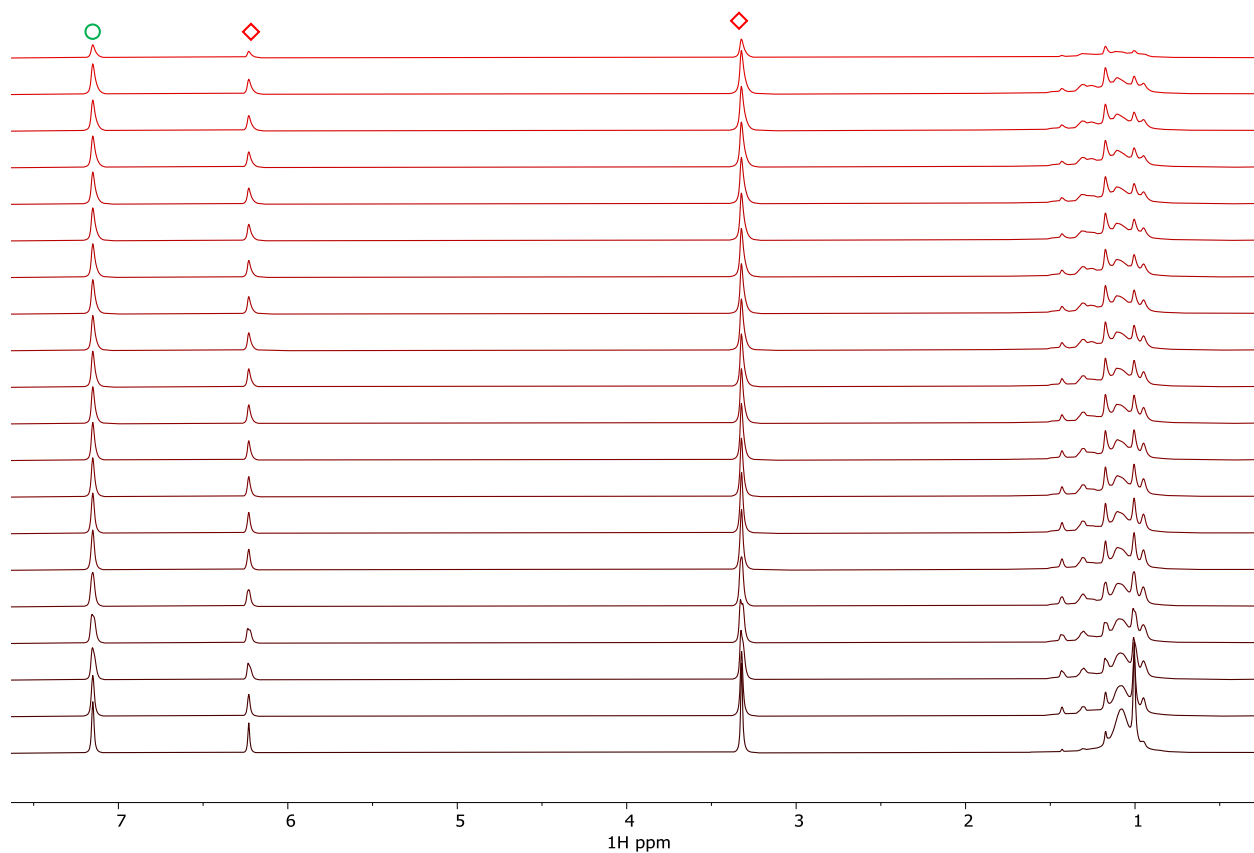


**Figure S38.** Initial rates calculations for the reaction between [D]<sub>5</sub>-1 (1000 mM) and **4** (500 mM) in C<sub>6</sub>D<sub>6</sub> at 25.0 °C and a total volume of 500 μL.

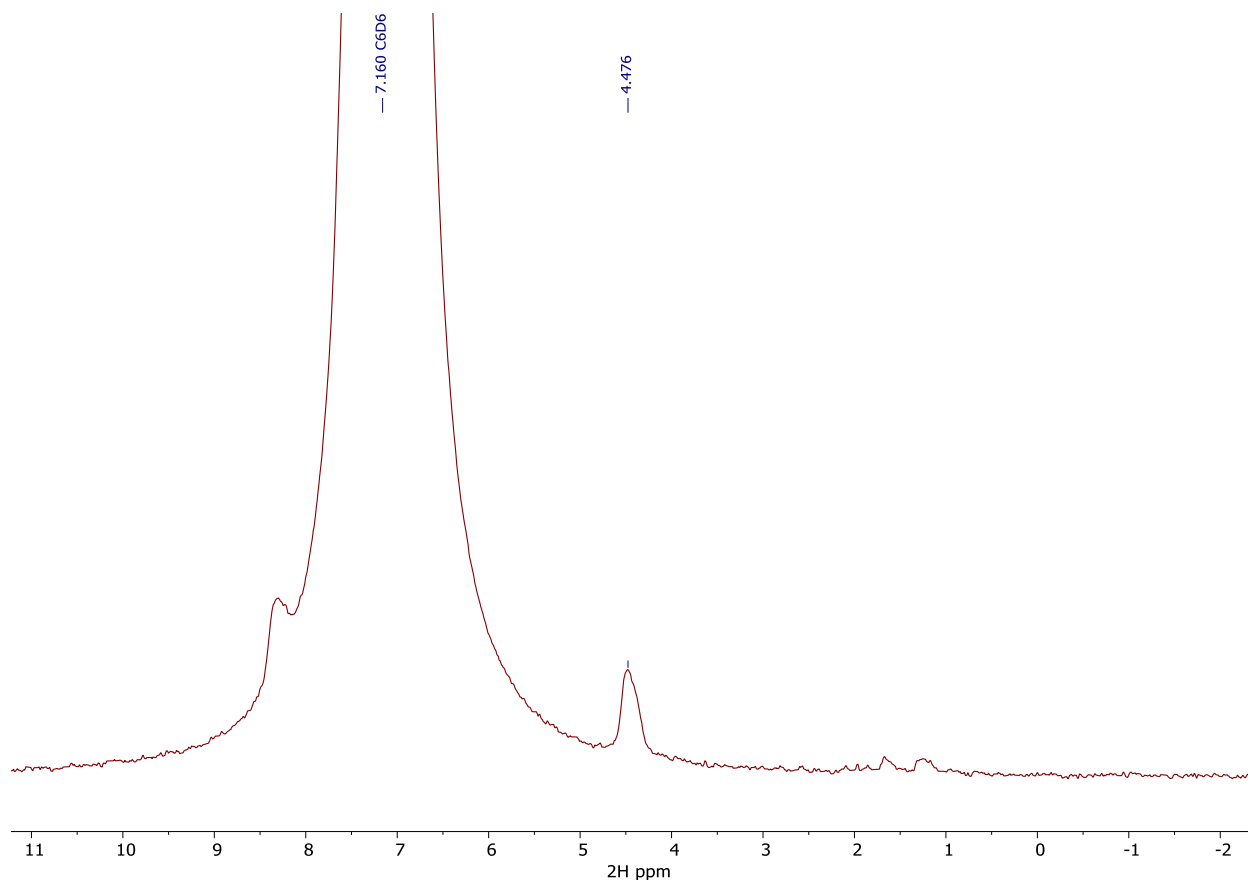
#### 5.4 Reaction Between [D]<sub>5</sub>-1 and **4**: Isolation of [D]<sub>5</sub>-6



In a nitrogen filled glove box a vial was loaded with **4** (50.0 mg, 0.139 mmol), a PTFE coated stir bar, and [D]<sub>5</sub>-1 (50.0 μL, 0.299 mmol). The mixture was stirred until it solidified followed by extraction with pentane. The extracts were then condensed and stored at -20 °C for 12 hours resulting in the formation of [D]<sub>5</sub>-6 as a turquoise solid (25.7 mg, 41% yield). Subsequently, an NMR tube was loaded with 1,3,5-trimethoxy benzene (25 μL, 500 mM s/s in C<sub>6</sub>D<sub>6</sub>, 0.0125 mmol), C<sub>6</sub>D<sub>6</sub> (475 μL), and [D]<sub>5</sub>-6 and the solution was immediately monitored by <sup>1</sup>H NMR spectroscopy over time. Spectra were collected every 5 minutes in the way described in section 3.1 (Figure S39). The same solution was then prepared for a second time and the <sup>2</sup>H-NMR spectrum was collected (Figure S40).



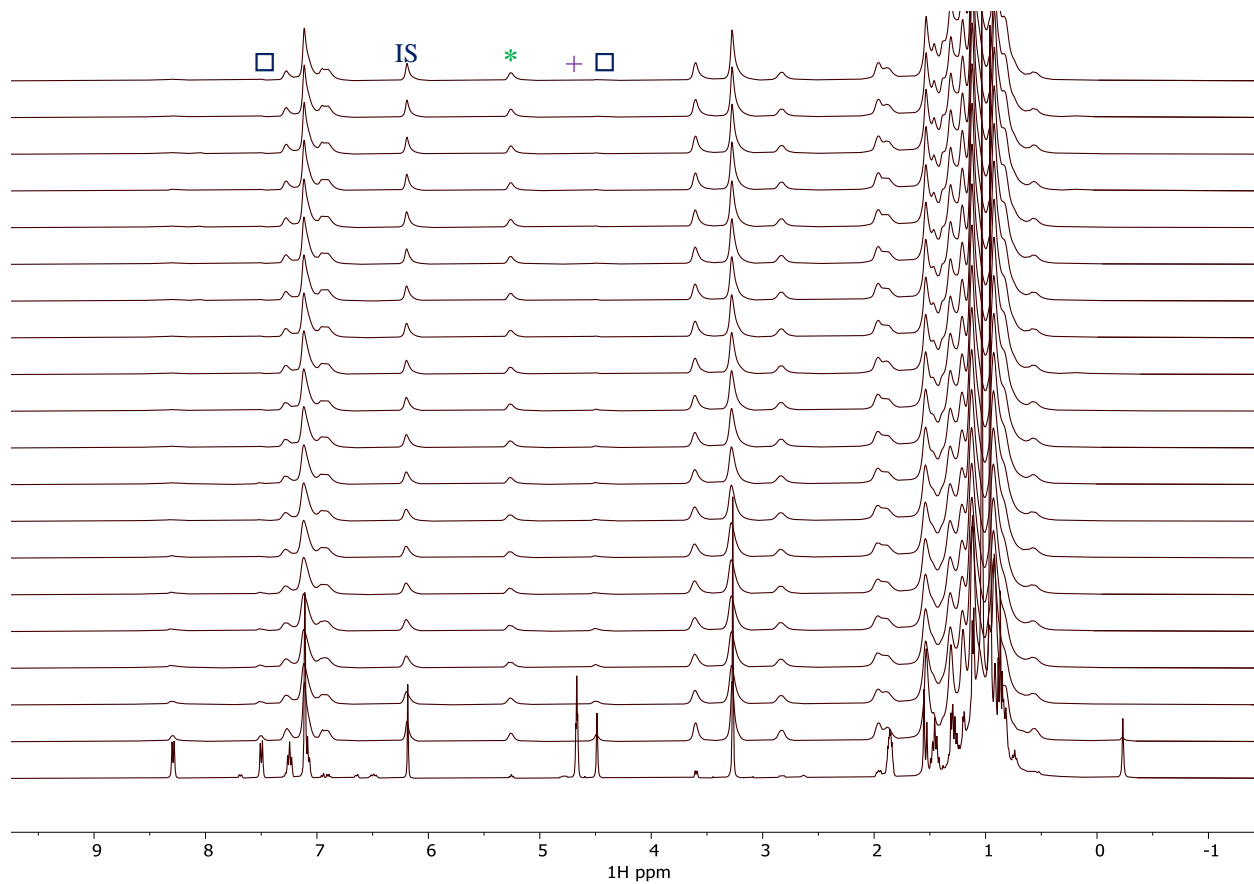
**Figure S39.** <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>, 27 °C) spectra collected with a time interval of 5 min (only 20 of the 300 collected spectra are presented here for clarity) in the reaction of [D]<sub>5</sub>-**6** in C<sub>6</sub>D<sub>6</sub> (500 μL). Compound key: ○ = C<sub>6</sub>D<sub>6</sub>, ◇ = 1,3,5-trimethoxybenzene.



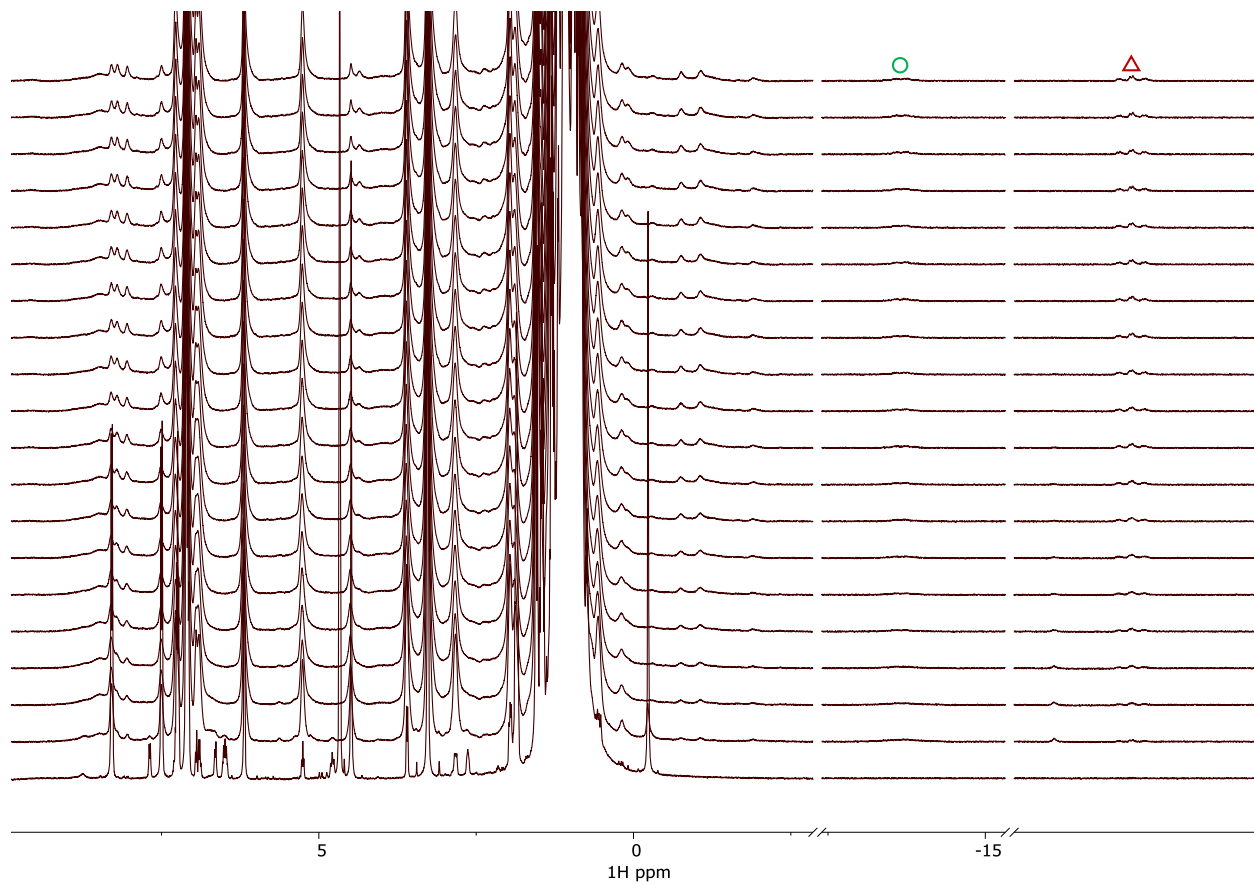
**Figure S40.**  $^2\text{H}$  NMR (400 MHz,  $\text{C}_6\text{D}_6$ , 27  $^\circ\text{C}$ ) spectrum of a freshly prepared  $[\text{D}]_5\text{-6}$  solution (50.0 mM) in  $\text{C}_6\text{D}_6$  (500  $\mu\text{L}$ ).

### 5.5 Reaction Between Allene **2** and Iron Alkoxide **6**

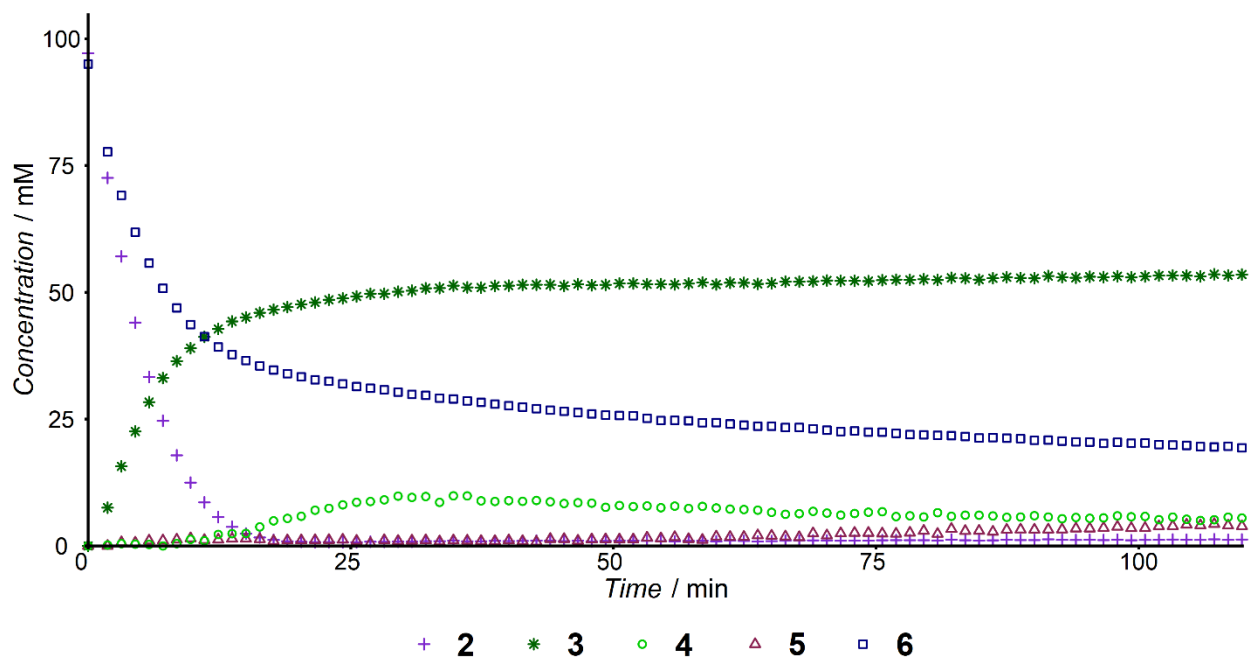
In a nitrogen filled glove box, an airtight NMR tube was loaded with allene **2** (50.0  $\mu\text{L}$ , 1.00 M solution in  $\text{C}_6\text{D}_6$ , 0.050 mmol), 1,3,5-trimethoxybenzene (25.0  $\mu\text{L}$ , 500 mM solution in  $\text{C}_6\text{D}_6$ , 0.0125 mmol), and  $\text{C}_6\text{D}_6$  (425  $\mu\text{L}$ ). The sampled was locked and shimmed and the NMR tube was taken back in the glove box where alkoxide complex **6** (22.3 mg, 0.050 mmol) was added in the top compartment. It was then carefully taken to the spectrometer where the contents were vigorously mixed, and the reaction was monitored by  $^1\text{H}$  NMR spectroscopy at 25  $^\circ\text{C}$  over time.



**Figure S41.** <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>, 25 °C) spectra collected with a time interval of 1.33 min (only 20 spectra are presented here for clarity) in the reaction of **2** (97.1 mM) with **6** (95.0 mM) in C<sub>6</sub>D<sub>6</sub> (500 μL). Compound key: □ = **6**, **IS** = 1,3,5-trimethoxybenzene, \* = **3**, + = **2**.



**Figure S42.** <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>, 25 °C) spectra collected with a time interval of 1.33 min (only 20 spectra are presented here for clarity) in the reaction of **2** (97.1 mM) with **6** (95.0 mM) in C<sub>6</sub>D<sub>6</sub> (500 μL). Compound key: ○ = **4**, △ = **5**.



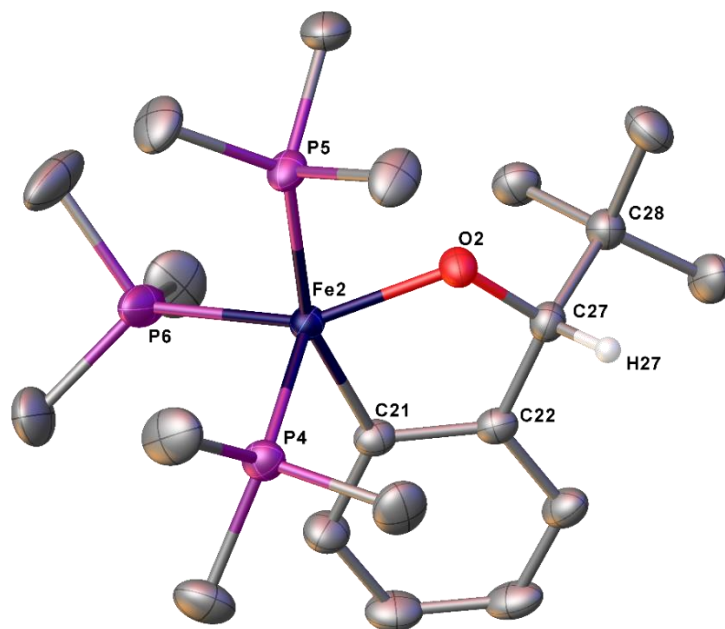
**Figure S43.** Reaction between **2** (97.1 mM) and **6** (95.0 mM) at 25.0 °C and a total volume of 500  $\mu\text{L}$ .

## 6 Crystallographic Information

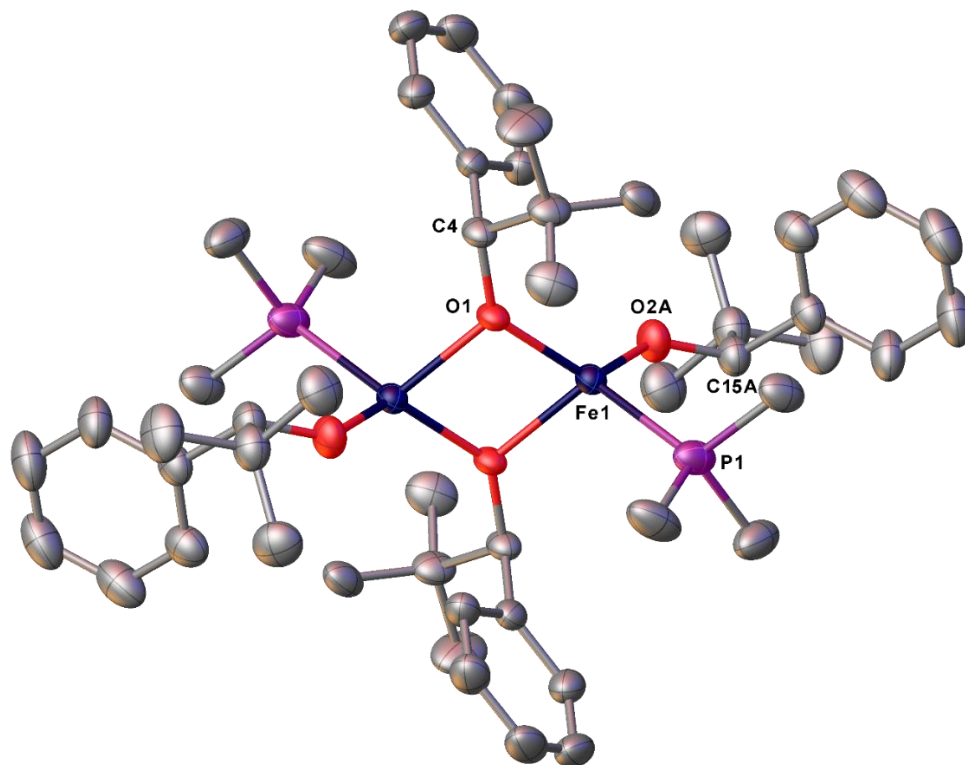
X-ray diffraction experiments for all the compounds were carried out at 100(2) K on a Bruker D8 Venture four-circle-diffractometer from Bruker AXS GmbH equipped with a Photon II detector purchased from Bruker AXS GmbH and using microfocus  $\text{I}\mu\text{S}$  Cu/Mo radiation from Incoatec GmbH with HELIOS mirror optics and single-hole collimator from Bruker AXS GmbH. Intensities were integrated<sup>8</sup> and absorption corrections based on equivalent reflections were applied using SADABS.<sup>9</sup> The structures were all solved using SHELXT<sup>10</sup> and refined against all F2 in SHELXL<sup>11</sup> using Olex 2.<sup>12</sup> All of the non-hydrogen atoms were refined anisotropically while the carbon bound hydrogen atoms were located geometrically and refined using a riding model. Crystal structure and refinement data are given in Table S2. Crystallographic data for the compounds have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication CCDC 2084594 – 2084598. Copies of the data can be obtained free of



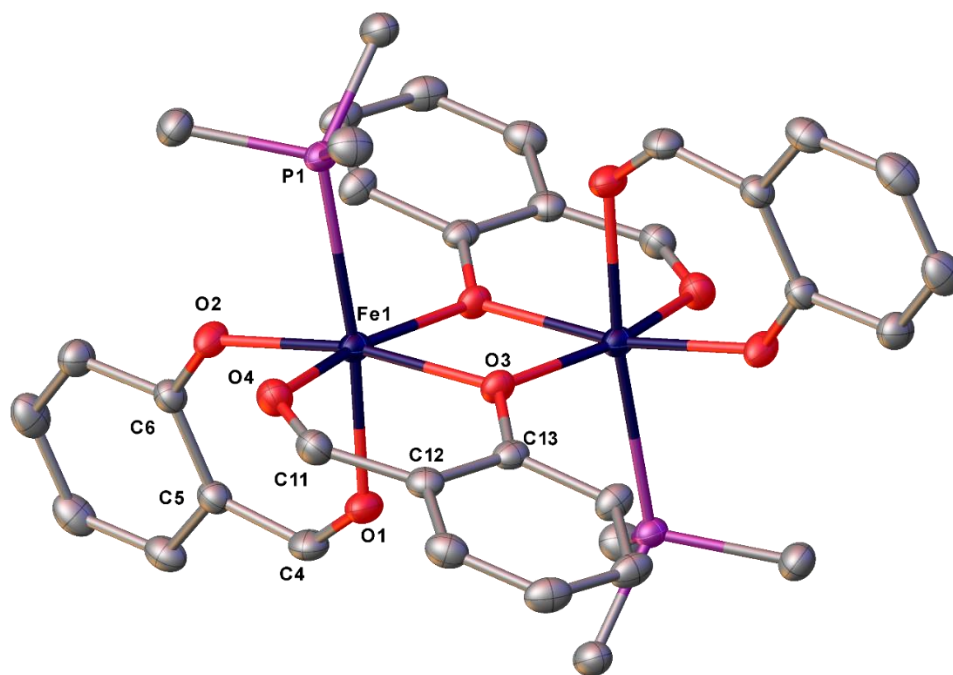
charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax(+44) 1223 336033, e-mail: [deposit@ccdc.cam.ac.uk](mailto:deposit@ccdc.cam.ac.uk))



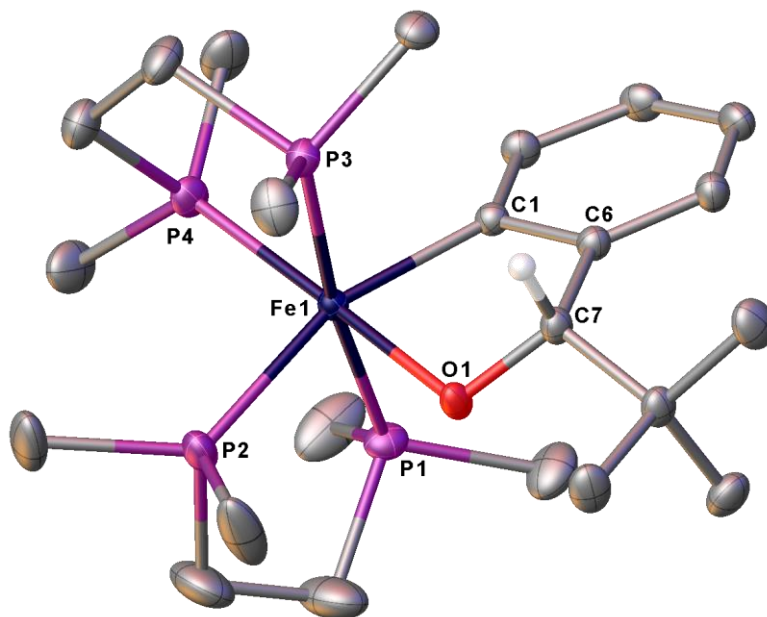
**Figure S44.** Molecular structure of complex **6**. Thermal ellipsoids are drawn at the 50% probability level and H atoms are omitted for clarity.



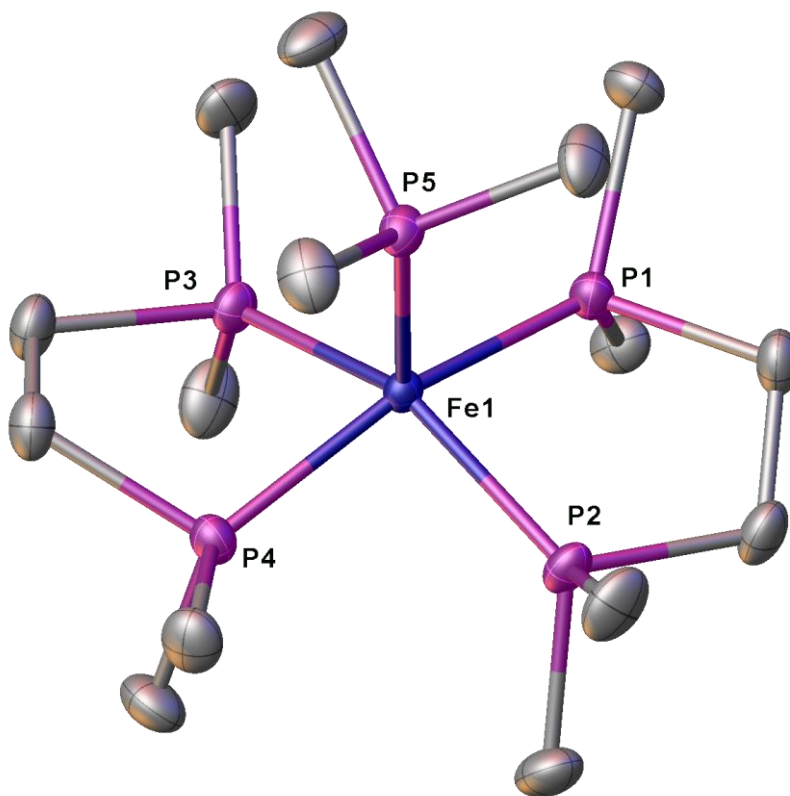
**Figure S45.** Molecular structure of complex **7**. Thermal ellipsoids are drawn at the 50% probability level and H atoms are omitted for clarity.



**Figure S46.** Molecular structure of complex **8**. Thermal ellipsoids are drawn at the 50% probability level and H atoms are omitted for clarity.



**Figure S47.** Molecular structure of complex **9a**. Thermal ellipsoids are drawn at the 50% probability level and H atoms are omitted for clarity.



**Figure S48.** Molecular structure of complex **10**. Thermal ellipsoids are drawn at the 50% probability level and H atoms are omitted for clarity.

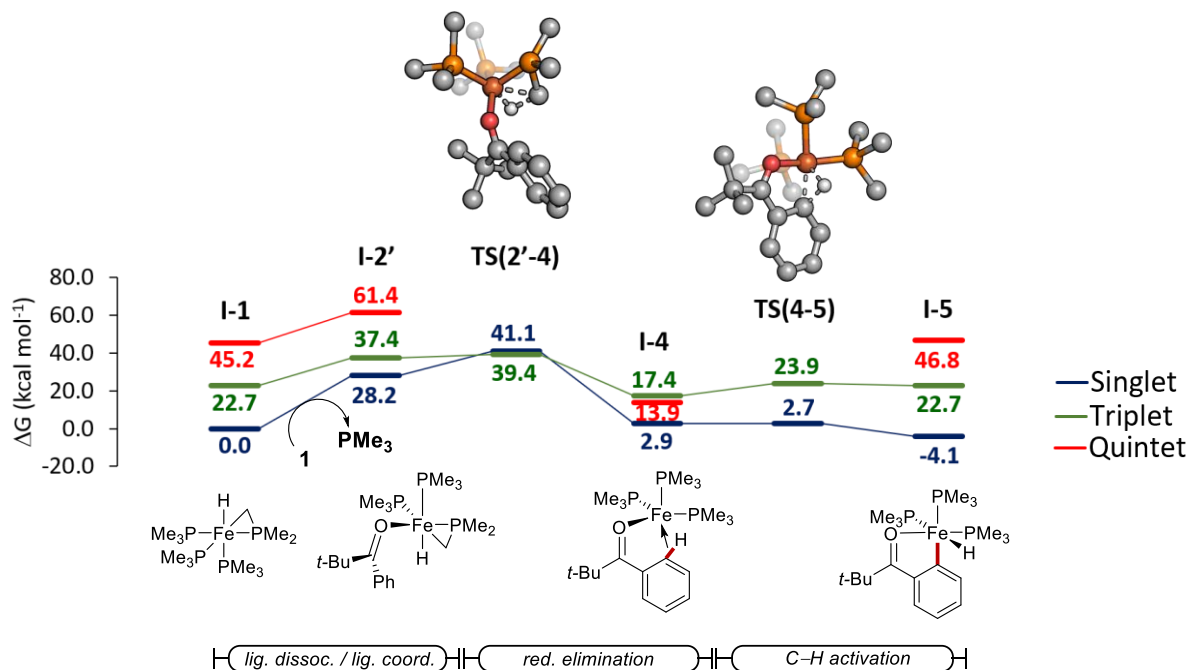
Table S2: Crystal data and structure refinement for complexes **3 – 8**.

Compound	<b>6</b>	<b>7</b>	<b>8</b>	<b>9a</b>	<b>10</b>
CCDC	2084594	2084595	2084596	2084597	2084598
Empirical formula	C <sub>20</sub> H <sub>41</sub> FeOP <sub>3</sub>	C <sub>50</sub> H <sub>78</sub> Fe <sub>2</sub> O <sub>4</sub> P <sub>2</sub>	C <sub>34</sub> H <sub>38</sub> Fe <sub>2</sub> O <sub>8</sub> P <sub>2</sub>	C <sub>23</sub> H <sub>46</sub> FeOP <sub>4</sub>	C <sub>15</sub> H <sub>41</sub> FeP <sub>5</sub>
Formula weight	446.29	916.76	748.28	518.33	432.18
Temperature/K	150.0	150.0	100.0	100.0	100.0
Crystal system	monoclinic	monoclinic	monoclinic	triclinic	orthorhombic
Space group	P2 <sub>1</sub> /c	P2 <sub>1</sub> /c	P2 <sub>1</sub> /c	P-1	Pbca
<i>a</i> /Å	18.0135(10)	12.148(2)	9.6929(12)	9.2828(11)	10.3448(7)
<i>b</i> /Å	15.4791(10)	11.104(2)	14.1709(16)	9.6552(16)	15.4459(10)
<i>c</i> /Å	17.8598(9)	19.365(4)	12.6241(12)	15.772(3)	28.2821(19)
<i>α</i> /°	90	90	90	72.401(5)	90
<i>β</i> /°	100.554(2)	101.252(8)	103.673(4)	89.249(8)	90
<i>γ</i> /°	90	90	90	78.000(7)	90
Volume/Å <sup>3</sup>	4895.6(5)	2562.0(8)	1684.9(3)	1316.1(3)	4519.0(5)
Z	8	2	2	2	8
$\rho_{\text{calc}}/\text{cm}^3$	1.211	1.188	1.475	1.308	1.270
$\mu/\text{mm}^{-1}$	0.818	0.668	1.006	0.829	1.016
F(000)	1920.0	984.0	776.0	556.0	1856.0
Crystal size/mm <sup>3</sup>	0.307 × 0.109 × 0.053	0.358 × 0.346 × 0.238	0.152 × 0.151 × 0.07	0.234 × 0.177 × 0.142	0.311 × 0.181 × 0.054
Radiation	MoK $\alpha$ ( $\lambda = 0.71073$ )	MoK $\alpha$ ( $\lambda = 0.71073$ )	MoK $\alpha$ ( $\lambda = 0.71073$ )	MoK $\alpha$ ( $\lambda = 0.71073$ )	MoK $\alpha$ ( $\lambda = 0.71073$ )
2 $\theta$ range for data collection/°	4.6 to 57.582	5.014 to 57.594	5.194 to 57.42	4.492 to 59.272	4.878 to 59.246
Index ranges	-23 ≤ <i>h</i> ≤ 24, -20 ≤ <i>k</i> ≤ 20, -24 ≤ <i>l</i> ≤ 23	-16 ≤ <i>h</i> ≤ 16, 0 ≤ <i>k</i> ≤ 14, 0 ≤ <i>l</i> ≤ 26	-13 ≤ <i>h</i> ≤ 13, -19 ≤ <i>k</i> ≤ 19, -17 ≤ <i>l</i> ≤ 17	-12 ≤ <i>h</i> ≤ 12, -13 ≤ <i>k</i> ≤ 13, -21 ≤ <i>l</i> ≤ 21	-14 ≤ <i>h</i> ≤ 14, -21 ≤ <i>k</i> ≤ 21, -38 ≤ <i>l</i> ≤ 39
Reflections collected	87355	6842	26293	77224	230519
R <sub>int</sub> / R <sub>sigma</sub>	12593 [R <sub>int</sub> = 0.0291, R <sub>sigma</sub> = 0.0204]	6842 [R <sub>int</sub> = ?, R <sub>sigma</sub> = 0.0293]	4317 [R <sub>int</sub> = 0.0434, R <sub>sigma</sub> = 0.0290]	7411 [R <sub>int</sub> = 0.0212, R <sub>sigma</sub> = 0.0113]	6341 [R <sub>int</sub> = 0.0446, R <sub>sigma</sub> = 0.0146]
Data/restraints/parameters	12593/3/506	6842/96/375	4317/0/211	7411/0/273	6341/0/201
Goodness-of-fit on F <sup>2</sup>	1.055	1.042	1.089	1.045	1.157
Final R indexes [ <i>I</i> ≥ 2 $\sigma$ ( <i>I</i> )]	R <sub>1</sub> = 0.0295, wR <sub>2</sub> = 0.0682	R <sub>1</sub> = 0.0422, wR <sub>2</sub> = 0.0982	R <sub>1</sub> = 0.0418, wR <sub>2</sub> = 0.0904	R <sub>1</sub> = 0.0327, wR <sub>2</sub> = 0.0801	R <sub>1</sub> = 0.0451, wR <sub>2</sub> = 0.1251
Final R indexes [all data]	R <sub>1</sub> = 0.0379, wR <sub>2</sub> = 0.0724	R <sub>1</sub> = 0.0499, wR <sub>2</sub> = 0.1031	R <sub>1</sub> = 0.0521, wR <sub>2</sub> = 0.0986	R <sub>1</sub> = 0.0355, wR <sub>2</sub> = 0.0824	R <sub>1</sub> = 0.0515, wR <sub>2</sub> = 0.1295
Largest diff. peak/hole / e Å <sup>-3</sup>	0.49/-0.37	1.10/-0.59	1.16/-0.61	1.41/-0.55	0.86/-0.59

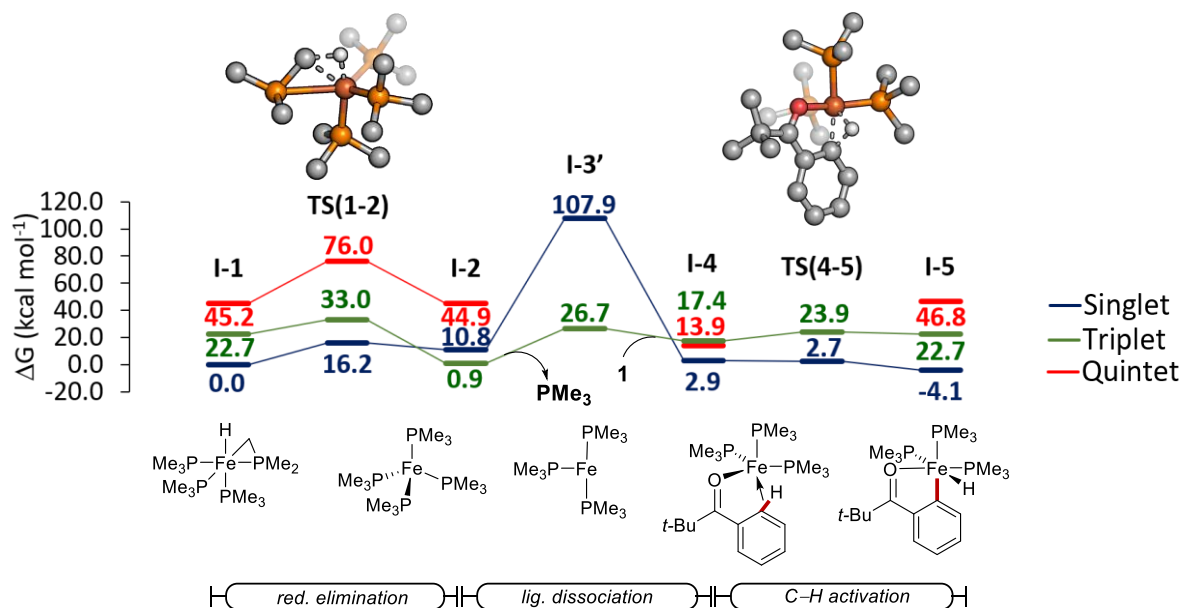
## 7 Computational Details

Calculations were performed using the Gaussian 16, Revision A.03 package.<sup>13</sup> All structures were optimized at the TPSS<sup>14</sup> level of theory in combination with Grimme's D3 dispersion corrections with the Becke-Johnson damping scheme [D3(BJ)]<sup>15,16</sup> in combination with a def2-SVP basis set.<sup>17,18</sup> Analytical frequency calculations were carried out at the same level of theory in order to identify the stationary points either as intermediates (no imaginary frequencies) or transition states (only one imaginary frequency), as well as to provide thermal and non-thermal corrections to the free energy in gas-phase at 308.15 K and 1 atm. The electronic energy was then refined through TPSS<sup>14</sup> single-point calculations on the optimized geometries in combination with a standalone version of Grimme's D4 dispersion corrections<sup>19-21</sup> with a def2-TZVP basis set.<sup>17,18</sup> Solvent effects were included through the use of an implicit solvation model SMD<sup>22</sup> with a dielectric constant of  $\epsilon = 2.2706$ , which corresponds to benzene, the solvent of choice used in the experimental work. Unless otherwise stated, the energies herein provided are based on gas-phase Gibbs free energies with def2-SVP basis set for which the electronic energies were improved at the TPSS-D4/def2-TZVP+SMD(Benzene) level of theory. Open-shell systems were calculated under the unrestricted formalism. 3D structure images were created with PyMOL version 1.8.x.<sup>23</sup>

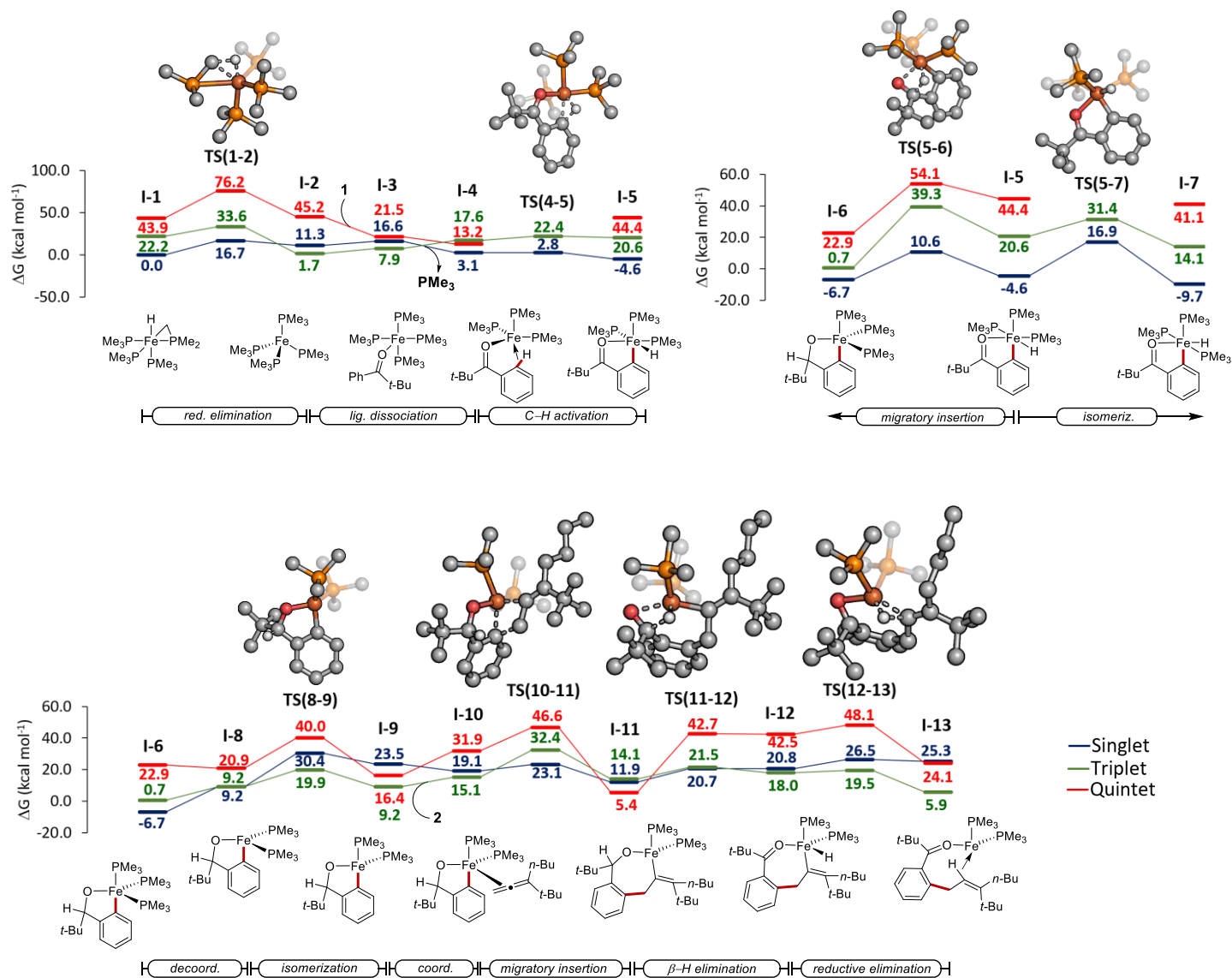
<sup>1</sup>H NMR chemical shift for intermediate **I-5** were calculated at the B3LYP-D3(BJ)+SMD(THF)/def2-TZVP level of theory<sup>24-27</sup> in combination with the gauge-including atomic orbital (GIAO) approach on the optimized geometries using tetramethylsilane (TMS) as reference.<sup>28-32</sup>



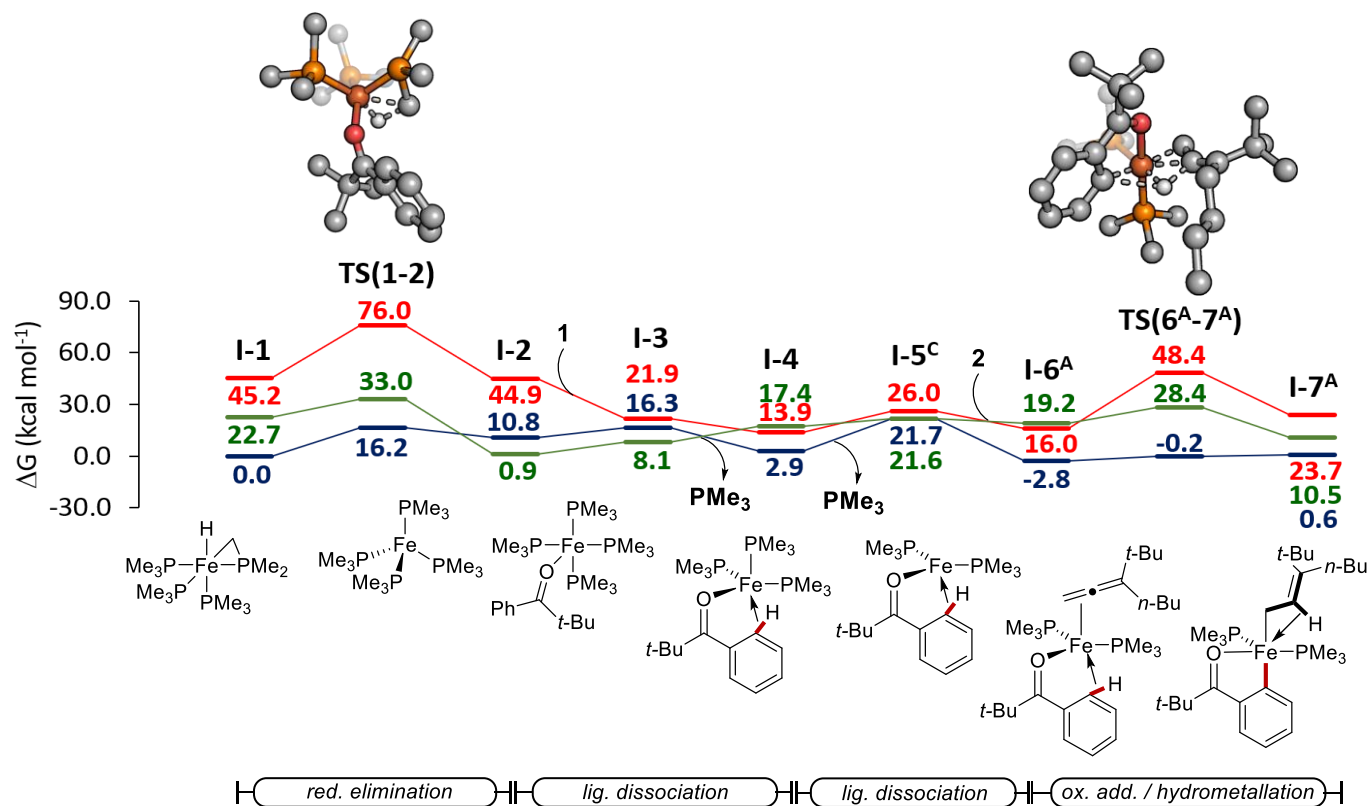
**Figure S49.** Computed relative Gibbs free energies ( $\Delta G_{308.15}$ ) in kcal mol<sup>-1</sup> for an alternative mechanism between **I-4** and the C–H activation elementary steps at the TPSS-D4/def2-TZVP+SMD(Benzene)//TPSS-D3(BJ)/def2-SVP level of theory. In the computed transition state structures non-relevant hydrogens were omitted for clarity.



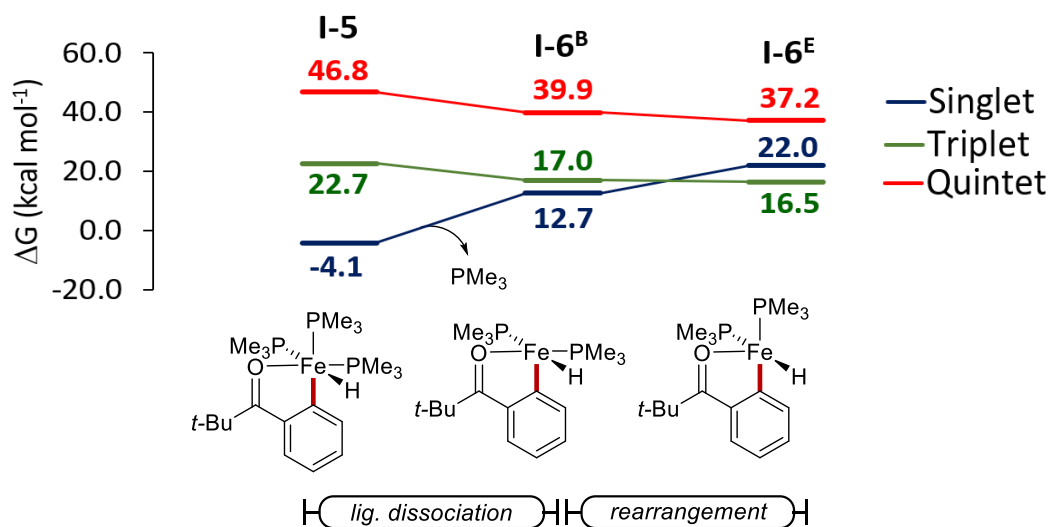
**Figure S50.** Computed relative Gibbs free energies ( $\Delta G_{308.15}$ ) in kcal mol<sup>-1</sup> for an alternative mechanism between **I-4** and the C–H activation elementary steps at the TPSS-D4/def2-TZVP+SMD(Benzene)//TPSS-D3(BJ)/def2-SVP level of theory. In the computed transition state structures non-relevant hydrogens were omitted for clarity.



**Figure S51.** Computed relative Gibbs free energies ( $\Delta G_{308.15}$ ) in kcal mol<sup>-1</sup> at the TPSS-D4/def2-TZVP+SMD(THF)//TPSS-D3(BJ)/def2-SVP level of theory. Energy values are given in respect to **I-1** in the singlet state. In the computed transition state structures non-relevant hydrogens were omitted for clarity.



**Figure S52.** Computed relative Gibbs free energies ( $\Delta G_{308.15}$ ) in kcal mol<sup>-1</sup> at the TPSS-D4/def2-TZVP+SMD(Benzene)//TPSS-D3(BJ)/def2-SVP level of theory for a concerted oxidative addition/hydrometallation mechanism through a dissociative pathway. In the computed transition state structures non-relevant hydrogens were omitted for clarity.



**Figure S53.** Computed relative Gibbs free energies ( $\Delta G_{308.15}$ ) in kcal mol<sup>-1</sup> at the TPSS-D4/def2-TZVP+SMD(Benzene)//TPSS-D3(BJ)/def2-SVP level of theory. Energy values are given in respect to I-1 in the singlet state.



**Table S3.** Calculated electronic energies at the TPSS-D4/def2-TZVP+SMD(Benzene) level of theory and Gibbs free energies with dispersion corrections for all structures in the present study (all in Hartree).<sup>[a]</sup>

Structure	Electronic energy	Total Gibbs Free Energy
<sup>1</sup> I-1	-3108.775529	-3108.386757
<sup>3</sup> I-1	-3108.732957	-3108.350600
<sup>5</sup> I-1	-3108.687291	-3108.314744
<sup>1</sup> TS(1-2)	-3108.748575	-3108.360960
<sup>3</sup> TS(1-2)	-3108.715704	-3108.334125
<sup>3</sup> TS(1-2)	-3108.638978	-3108.265612
<sup>1</sup> I-2	-3108.762158	-3108.369593
<sup>3</sup> I-2	-3108.771294	-3108.385311
<sup>5</sup> I-2	-3108.692285	-3108.315205
<sup>1</sup> I-3	-3611.925648	-3611.325892
<sup>3</sup> I-3	-3611.936353	-3611.338870
<sup>5</sup> I-3	-3611.902086	-3611.316988
<sup>1</sup> I-4	-3150.706275	-3150.213342
<sup>3</sup> I-4	-3152.980941	-3152.490253
<sup>5</sup> I-4	-3150.678407	-3150.195801
<sup>1</sup> TS(4-5)	-3150.703517	-3150.213646
<sup>3</sup> TS(4-5)	-3150.664469	-3150.179908
<sup>1</sup> I-5	-3150.716123	-3150.224444
<sup>3</sup> I-5	-3150.666776	-3150.181729
<sup>5</sup> I-5	-3150.621882	-3150.143318
<sup>1</sup> TS(5-6)	-3150.690155	-3150.200657
<sup>3</sup> TS(5-6)	-3150.636679	-3150.153986
<sup>3</sup> TS(5-6)	-3150.602840	-3150.130363
<sup>1</sup> I-6	-3150.723150	-3150.228733
<sup>3</sup> I-6	-3150.707074	-3150.216594
<sup>5</sup> I-6	-3150.662647	-3150.180380
<sup>1</sup> TS(5-7)	-3150.682015	-3150.190134
<sup>3</sup> TS(5-7)	-3150.650806	-3150.166311
<sup>1</sup> I-7	-3150.725050	-3150.233697
<sup>3</sup> I-7	-3150.679475	-3150.194226
<sup>5</sup> I-7	-3150.627343	-3150.150161
<sup>1</sup> I-8	-2689.454340	-2689.067651
<sup>3</sup> I-8	-2689.449694	-2689.067280
<sup>5</sup> I-8	-2689.428203	-2689.048193
<sup>1</sup> TS(8-9)	-2689.418162	-2689.033325
<sup>3</sup> TS(8-9)	-2689.435725	-2689.050888
<sup>3</sup> TS(8-9)	-2689.403242	-2689.018405
<sup>1</sup> I-9	-2689.429048	-2689.042946
<sup>3</sup> I-9	-2689.449694	-2689.067281
<sup>5</sup> I-9	-2689.434009	-2689.055192

<sup>1</sup> I-10	-3120.910024	-3120.257144
<sup>3</sup> I-10	-3120.912016	-3120.263028
<sup>5</sup> I-10	-3120.876480	-3120.235917
<sup>1</sup> TS(10-11)	-3120.902971	-3120.250439
<sup>3</sup> TS(10-11)	-3120.882343	-3120.236277
<sup>3</sup> TS(10-11)	-3120.854433	-3120.212904
<sup>1</sup> I-11	-3120.925212	-3120.269307
<sup>3</sup> I-11	-3120.916889	-3120.265900
<sup>5</sup> I-11	-3120.922789	-3120.278731
<sup>1</sup> TS(11-12)	-3120.906196	-3120.254715
<sup>3</sup> TS(11-12)	-3120.900245	-3120.253356
<sup>3</sup> TS(11-12)	-3120.860581	-3120.218354
<sup>1</sup> I-12	-3120.906930	-3120.254661
<sup>3</sup> I-12	-3120.906872	-3120.257926
<sup>5</sup> I-12	-3120.862243	-3120.218657
<sup>1</sup> TS(12-13)	-3120.896048	-3120.245646
<sup>3</sup> TS(12-13)	-3120.902302	-3120.255622
<sup>3</sup> TS(12-13)	-3120.847999	-3120.209245
<sup>1</sup> I-13	-3120.898881	-3120.247157
<sup>3</sup> I-13	-3120.933081	-3120.277670
<sup>5</sup> I-13	-3120.895293	-3120.248067
<sup>1</sup> I-2'	-3150.660137	-3150.173073
<sup>3</sup> I-2'	-3150.641684	-3150.158433
<sup>3</sup> I-2'	-3150.596117	-3150.120083
<sup>1</sup> TS(2'-4)	-3150.639082	-3150.152537
<sup>3</sup> TS(2'-4)	-3150.637645	-3150.155126
<sup>1</sup> I-3'	-2647.363409	-2647.081016
<sup>3</sup> I-3'	-2647.488541	-2647.210382
<sup>1</sup> I-6 <sup>A</sup>	-2689.447336	-2689.063822
<sup>3</sup> I-6 <sup>A</sup>	-2689.432865	-2689.057031
<sup>5</sup> I-6 <sup>A</sup>	-2689.392066	-2689.020478
<sup>1</sup> I-7 <sup>A</sup>	-3120.939218	-3120.291904
<sup>3</sup> I-7 <sup>A</sup>	-3120.887873	-3120.249603
<sup>1</sup> TS(7 <sup>A</sup> -8 <sup>A</sup> )	-3120.934271	-3120.288590
<sup>3</sup> TS(7 <sup>A</sup> -8 <sup>A</sup> )	-3120.889219	-3120.244128
<sup>1</sup> I-8 <sup>A</sup>	-3120.937723	-3120.287313
<sup>3</sup> I-8 <sup>A</sup>	-3120.927245	-3120.282169
<sup>5</sup> I-8 <sup>A</sup>	-3120.891952	-3120.252138
<sup>1</sup> I-9 <sup>A</sup>	-3120.945367	-3120.294805
<sup>3</sup> I-9 <sup>A</sup>	-3120.895994	-3120.252443
<sup>5</sup> I-9 <sup>A</sup>	-3120.890989	-3120.252277
<sup>1</sup> TS(9 <sup>A</sup> -10 <sup>A</sup> )	-3120.905244	-3120.257067
<sup>3</sup> TS(9 <sup>A</sup> -10 <sup>A</sup> )	-3120.885038	-3120.238188
<sup>5</sup> TS(9 <sup>A</sup> -10 <sup>A</sup> )	-3120.890748	-3120.245926
<sup>1</sup> I-10 <sup>A</sup>	-3120.913330	-3120.259260
<sup>3</sup> I-10 <sup>A</sup>	-3120.930363	-3120.280863
<sup>5</sup> I-10 <sup>A</sup>	-3120.890748	-3120.245926
<sup>1</sup> I-5 <sup>B</sup>	-2688.941252	-2689.049530

<sup>3</sup> I-5 <sup>B</sup>	-2688.944218	-2689.049664
<sup>5</sup> I-5 <sup>B</sup>	-2688.940323	-2689.042622
<sup>1</sup> I-6 <sup>B</sup>	-3120.766985	-3120.292691
<sup>3</sup> I-6 <sup>B</sup>	-3120.727268	-3120.257618
<sup>5</sup> I-6 <sup>B</sup>	-3120.728494	-3120.262723
<sup>1</sup> TS(6 <sup>B</sup> -7 <sup>B</sup> )	-3120.759187	-3120.288602
<sup>3</sup> TS(6 <sup>B</sup> -7 <sup>B</sup> )	-3120.064980	-3120.243003
<sup>5</sup> TS(6 <sup>B</sup> -7 <sup>B</sup> )	-3120.040931	-3120.211064
<sup>1</sup> I-7 <sup>B</sup>	-3120.759859	-3120.287324
<sup>3</sup> I-7 <sup>B</sup>	-3120.740092	-3120.271478
<sup>5</sup> I-7 <sup>B</sup>	-3120.71912	-3120.250466
<sup>1</sup> I-5 <sup>C</sup>	-3581.177457	-3581.393088
<sup>3</sup> I-5 <sup>C</sup>	-3581.166626	-3581.383403
<sup>1</sup> I-6 <sup>E</sup>	-2689.430833	-2689.048986
<sup>3</sup> I-6 <sup>E</sup>	-2689.433666	-2689.057869
<sup>5</sup> I-6 <sup>E</sup>	-2689.397838	-2689.024879
<b>1</b>	-503.144255	-502.965068
<b>2</b>	-431.439761	-431.204165
<b>PMe<sub>3</sub></b>	-461.214113	-461.133871

<sup>[a]</sup> Indices correspond to the spin state of the respective complexes.

**Table S4.** Calculated electronic energies at the TPSS-D4/def2-TZVP+SMD(THF) level of theory and Gibbs free energies with dispersion corrections for all structures in the present study (all in Hartree).<sup>[a]</sup>

Structure	Electronic energy	Total Gibbs Free Energy
<sup>1</sup> I-1	-3108.776277	-3108.387505
<sup>3</sup> I-1	-3108.734416	-3108.352059
<sup>5</sup> I-1	-3108.690117	-3108.317570
<sup>1</sup> TS(1-2)	-3108.748541	-3108.360926
<sup>3</sup> TS(1-2)	-3108.715485	-3108.333906
<sup>3</sup> TS(1-2)	-3108.639448	-3108.266082
<sup>1</sup> I-2	-3108.762089	-3108.369524
<sup>3</sup> I-2	-3108.770706	-3108.384723
<sup>5</sup> I-2	-3108.692595	-3108.315515
<sup>1</sup> I-3	-3611.926070	-3611.326314
<sup>3</sup> I-3	-3611.937617	-3611.340134
<sup>5</sup> I-3	-3611.903515	-3611.318417
<sup>1</sup> I-4	-3150.706352	-3150.213419
<sup>3</sup> I-4	-3150.681068	-3150.190380
<sup>5</sup> I-4	-3150.680007	-3150.197401
<sup>1</sup> TS(4-5)	-3150.703789	-3150.213918
<sup>3</sup> TS(4-5)	-3150.667308	-3150.182747
<sup>1</sup> I-5	-3150.717370	-3150.225691
<sup>3</sup> I-5	-3150.670590	-3150.185543
<sup>5</sup> I-5	-3150.626204	-3150.147640
<sup>1</sup> TS(5-6)	-3150.691036	-3150.201538
<sup>3</sup> TS(5-6)	-3150.638508	-3150.155815
<sup>3</sup> TS(5-6)	-3150.604723	-3150.132246
<sup>1</sup> I-6	-3150.723558	-3150.229141
<sup>3</sup> I-6	-3150.707821	-3150.217341
<sup>5</sup> I-6	-3150.664241	-3150.181974
<sup>1</sup> TS(5-7)	-3150.683288	-3150.191407
<sup>3</sup> TS(5-7)	-3150.652891	-3150.168396
<sup>1</sup> I-7	-3150.725286	-3150.233933
<sup>3</sup> I-7	-3150.681216	-3150.195967
<sup>5</sup> I-7	-3150.630155	-3150.152973
<sup>1</sup> I-8	-2689.456060	-2689.069371
<sup>3</sup> I-8	-2689.451779	-2689.069365
<sup>5</sup> I-8	-2689.430791	-2689.050781
<sup>1</sup> TS(8-9)	-2689.420416	-2689.035579
<sup>3</sup> TS(8-9)	-2689.437214	-2689.052377
<sup>3</sup> TS(8-9)	-2689.405164	-2689.020327
<sup>1</sup> I-9	-2689.432727	-2689.046625
<sup>3</sup> I-9	-2689.451779	-2689.069366
<sup>5</sup> I-9	-2689.436724	-2689.057907
<sup>1</sup> I-10	-3120.909202	-3120.256322
<sup>3</sup> I-10	-3120.911703	-3120.262715
<sup>5</sup> I-10	-3120.876473	-3120.235910
<sup>1</sup> TS(10-11)	-3120.902414	-3120.249882

<sup>3</sup> TS(10-11)	-3120.881099	-3120.235033
<sup>3</sup> TS(10-11)	-3120.853944	-3120.212415
<sup>1</sup> I-11	-3120.923640	-3120.267735
<sup>3</sup> I-11	-3120.915240	-3120.264251
<sup>5</sup> I-11	-3120.922109	-3120.278051
<sup>1</sup> TS(11-12)	-3120.905176	-3120.253695
<sup>3</sup> TS(11-12)	-3120.899264	-3120.252375
<sup>3</sup> TS(11-12)	-3120.860879	-3120.218652
<sup>1</sup> I-12	-3120.905892	-3120.253623
<sup>3</sup> I-12	-3120.906926	-3120.257980
<sup>5</sup> I-12	-3120.862537	-3120.218951
<sup>1</sup> TS(12-13)	-3120.894948	-3120.244546
<sup>3</sup> TS(12-13)	-3120.902302	-3120.255622
<sup>3</sup> TS(12-13)	-3120.848872	-3120.210118
<sup>1</sup> I-13	-3120.898081	-3120.246357
<sup>3</sup> I-13	-3120.932754	-3120.277343
<sup>5</sup> I-13	-3120.895606	-3120.248380
<b>1</b>	-503.144414	-502.965227
<b>2</b>	-431.438230	-431.202634
<b>PMe<sub>3</sub></b>	-461.214570	-461.134328

<sup>[a]</sup> Indices correspond to the spin state of the respective complexes.

## Cartesian coordinates of the optimized structures

### <sup>1</sup>I-1

Lowest frequency = 35.9849 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

53

Fe	-0.000002	0.043961	-0.272583
C	1.412174	-0.996748	2.642285
H	1.456190	0.070382	2.916842
H	1.299540	-1.607744	3.556662
H	2.364269	-1.260735	2.151529
C	-0.000031	-3.110574	1.389211
H	0.000002	-3.550598	2.403293
H	-0.890588	-3.462028	0.844059
H	0.890458	-3.462075	0.843980
C	-1.412075	-0.996663	2.642331
H	-2.364205	-1.260516	2.151571
H	-1.299493	-1.607721	3.556673
H	-1.455971	0.070457	2.916945
C	-3.542772	0.592658	-0.324549
H	-4.461068	0.205434	-0.802341
H	-3.623995	0.471049	0.768737
H	-3.459553	1.669368	-0.550735
C	-2.664942	-2.034696	-0.886142
H	-3.612785	-2.134725	-1.444935
H	-1.907907	-2.708561	-1.319381
H	-2.840399	-2.333135	0.161092
C	-2.242285	0.034478	-2.769771
H	-3.282688	-0.145866	-3.095724
H	-1.962389	1.077486	-2.988040
H	-1.557677	-0.624970	-3.327761
C	1.413563	2.912736	1.425778
H	2.361913	2.565351	0.992752
H	1.304658	3.997626	1.248702
C	-0.000042	1.986445	-1.100794
H	-0.903187	2.400931	-1.583302
H	0.903069	2.400963	-1.583336
H	-0.000007	-0.962823	-1.437283
C	-1.413577	2.912692	1.425847
H	-1.444173	2.731190	2.515510
H	-1.304751	3.997580	1.248707
H	-2.361946	2.565229	0.992923
P	0.000021	-1.241745	1.444668
P	-0.000010	1.970867	0.676820
P	-2.015239	-0.291541	-0.952350
H	1.444265	2.731179	2.515429
P	2.015233	-0.291522	-0.952361
C	3.542773	0.592629	-0.324509

H	4.461074	0.205379	-0.802269
H	3.459593	1.669341	-0.550700
H	3.623951	0.471020	0.768780
C	2.242296	0.034576	-2.769766
H	3.282697	-0.145774	-3.095721
H	1.557677	-0.624831	-3.327790
H	1.962422	1.077600	-2.987987
C	2.664917	-2.034689	-0.886229
H	1.907878	-2.708527	-1.319507
H	3.612762	-2.134699	-1.445021
H	2.840365	-2.333187	0.160991

### <sup>3</sup>I-1

Lowest frequency = 34.9544 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

53

Fe	0.058145	-0.377350	-0.440934
C	1.598995	0.067794	2.860243
H	1.415589	1.153296	2.915502
H	1.622442	-0.345727	3.885067
H	2.580385	-0.093824	2.383323
C	0.597582	-2.514725	2.175048
H	0.658307	-2.720377	3.259371
H	-0.208834	-3.118376	1.728707
H	1.542238	-2.807260	1.690035
C	-1.191519	-0.418963	2.937370
H	-2.041689	-1.031805	2.594008
H	-0.970886	-0.666972	3.991474
H	-1.471266	0.643415	2.841656
C	-3.448826	0.105380	-0.300644
H	-4.415172	-0.348153	-0.586648
H	-3.429660	0.292800	0.785095
H	-3.340863	1.076737	-0.811517
C	-2.580941	-2.611315	-0.080055
H	-3.594976	-2.869905	-0.434283
H	-1.866030	-3.388218	-0.396565
H	-2.588544	-2.573443	1.022353
C	-2.347093	-1.237559	-2.571131
H	-3.392521	-1.542818	-2.758660
H	-2.138311	-0.296991	-3.107941
H	-1.659471	-2.011855	-2.948657
C	0.800080	3.175056	0.864649
H	1.582768	2.427896	1.063014
H	1.153548	3.859291	0.070508
C	-0.257667	1.505585	-1.214512
H	-1.123237	1.522682	-1.909043
H	0.558063	2.078848	-1.702702
H	0.348569	-1.867554	-0.944818

C	-1.768170	3.794490	-0.136169
H	-1.989026	4.419061	0.748857
H	-1.230960	4.402682	-0.888001
H	-2.728627	3.463467	-0.568537
P	0.265671	-0.719799	1.826557
P	-0.761123	2.285642	0.372487
P	-2.013336	-0.981930	-0.762801
H	0.627063	3.754748	1.788463
P	2.156003	-0.306726	-0.989405
C	3.282963	1.154405	-0.717968
H	4.258326	1.002979	-1.214506
H	2.810309	2.065209	-1.119527
H	3.451656	1.299687	0.362422
C	2.327854	-0.484095	-2.831275
H	3.385273	-0.475604	-3.153049
H	1.851669	-1.429336	-3.138367
H	1.790467	0.349481	-3.313836
C	3.288332	-1.661126	-0.407185
H	2.818270	-2.631846	-0.633266
H	4.278635	-1.602089	-0.893626
H	3.426954	-1.586402	0.685171

H	1.708882	4.266680	-1.084186
H	-0.015363	4.559977	-1.497306
C	0.110295	1.471336	-1.424490
H	-0.722268	1.761691	-2.098986
H	1.053178	1.497066	-2.006894
H	-0.048105	-1.962363	-0.944978
C	-1.536484	2.868775	0.384439
H	-1.665575	3.558323	1.237166
H	-2.065558	3.280509	-0.496091
H	-1.987107	1.896121	0.641362
P	0.084686	-0.368247	1.969405
P	0.270384	2.585367	0.017795
P	-2.434682	-0.835989	-0.749874
H	0.634141	5.048666	0.113433
P	2.394018	-0.836357	-0.757689
C	3.828975	0.325023	-0.509139
H	4.774390	-0.066980	-0.928216
H	3.588204	1.286652	-0.994197
H	3.960332	0.518406	0.568787
C	2.543761	-1.184257	-2.571478
H	3.561245	-1.512530	-2.850931
H	1.809693	-1.965858	-2.827874
H	2.284618	-0.271799	-3.134813
C	3.061124	-2.413841	-0.045605
H	2.303342	-3.200521	-0.199415
H	4.012655	-2.718046	-0.518214
H	3.224394	-2.291864	1.039228

### <sup>5</sup>I-1

Lowest frequency = 17.9850 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

53

Fe	-0.008526	-0.348473	-0.394880
C	1.623493	0.243917	2.797908
H	1.765175	1.295852	2.497433
H	1.564752	0.162073	3.898183
H	2.483863	-0.343267	2.435854
C	0.010254	-2.124087	2.566009
H	0.114440	-2.193342	3.664111
H	-0.951671	-2.566689	2.259749
H	0.814629	-2.699844	2.080241
C	-1.216664	0.416239	3.036161
H	-2.212797	0.092009	2.689869
H	-1.091499	0.143729	4.099764
H	-1.151232	1.511445	2.931762
C	-4.002418	0.138352	-0.451114
H	-4.894124	-0.359535	-0.875731
H	-4.150096	0.272544	0.634764
H	-3.898649	1.138025	-0.906013
C	-2.955970	-2.498642	-0.113934
H	-3.866095	-2.869091	-0.619490
H	-2.122285	-3.200971	-0.278007
H	-3.153986	-2.428629	0.970005
C	-2.558248	-1.086127	-2.581987
H	-3.542819	-1.488587	-2.881935
H	-2.387017	-0.118954	-3.084618
H	-1.756874	-1.779717	-2.884768
C	0.680345	4.282896	-0.682889

### <sup>1</sup>TS(1-2)

Lowest frequency = -869.9385 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

53

Fe	-0.001909	0.080919	-0.310187
C	1.584496	0.227424	2.764089
H	1.873324	1.253029	2.480254
H	1.430084	0.175996	3.857124
H	2.407930	-0.452012	2.489269
C	-0.284961	-1.899604	2.597421
H	-0.176529	-1.872603	3.696786
H	-1.308198	-2.226581	2.348641
H	0.418769	-2.637554	2.180117
C	-1.163370	0.802432	2.814901
H	-2.180286	0.683964	2.411997
H	-1.155346	0.534702	3.887297
H	-0.873320	1.860699	2.701097
C	-3.342029	-0.856904	0.478077
H	-4.187672	-1.450976	0.085405
H	-3.095297	-1.225663	1.488031
H	-3.652560	0.198706	0.565401
C	-1.753775	-2.823507	-0.797417
H	-2.736049	-3.288550	-1.007834
H	-1.050837	-3.063126	-1.613351

H	-1.343604	-3.247296	0.134401
C	-2.728111	-0.599247	-2.247267
H	-3.619143	-1.240754	-2.367398
H	-3.046667	0.457391	-2.268465
H	-2.042570	-0.769766	-3.094729
C	1.172362	3.464033	-0.128751
H	2.143436	2.990452	-0.345182
H	1.018719	4.327710	-0.801072
C	-0.027975	1.397517	-1.927031
H	-0.909993	1.496881	-2.582046
H	0.895153	1.595254	-2.499154
H	-0.033882	-0.119774	-1.834476
C	-1.682846	3.235893	-0.262806
H	-1.883016	3.556279	0.775627
H	-1.596172	4.133137	-0.902520
H	-2.534247	2.620417	-0.597830
P	0.036258	-0.228740	1.826614
P	-0.154873	2.167780	-0.309555
P	-1.840609	-0.958388	-0.642034
H	1.194907	3.826700	0.915067
P	1.939014	-0.764304	-0.676435
C	3.518872	0.200295	-0.345924
H	4.430609	-0.375934	-0.592209
H	3.499452	1.115192	-0.963667
H	3.558452	0.507944	0.711362
C	2.299198	-1.204069	-2.455925
H	3.335083	-1.563798	-2.594962
H	1.592213	-1.987415	-2.777260
H	2.138357	-0.316647	-3.091727
C	2.446859	-2.390093	0.096363
H	1.673765	-3.142806	-0.133044
H	3.424847	-2.740726	-0.282136
H	2.510733	-2.286603	1.192825

H	2.060061	-3.636373	-1.694565
H	0.625188	-3.536524	-0.608637
H	0.529420	-2.882749	-2.265332
C	3.004120	-1.873903	0.467692
H	3.764824	-2.532511	0.009519
H	3.505680	-0.986504	0.889974
H	2.514210	-2.418032	1.293418
C	2.843850	-0.835907	-2.163798
H	3.584608	-1.619180	-2.410043
H	2.228768	-0.619827	-3.054052
H	3.379146	0.089375	-1.889291
C	-3.062641	1.334202	-0.300847
H	-2.197197	1.680256	0.288245
H	-3.146566	1.956722	-1.211581
C	-1.338997	-0.265160	-1.874021
H	-1.182767	-1.227000	-2.396739
H	-1.580600	0.493395	-2.646084
H	0.060350	0.208007	-1.792560
C	-4.236172	-0.662930	-1.919643
H	-5.190039	-0.600374	-1.363904
H	-4.225549	0.113256	-2.708324
H	-4.180258	-1.658121	-2.394105
P	-0.443550	-0.562529	1.858087
P	-2.787742	-0.463273	-0.723852
P	1.709476	-1.331056	-0.766357
H	-3.978333	1.453915	0.304608
P	0.953330	1.963753	-0.165652
C	0.133509	3.350452	0.791786
H	0.718294	4.288635	0.762290
H	-0.869635	3.540397	0.373266
H	0.009784	3.037055	1.843290
C	1.260341	2.872072	-1.764477
H	1.735617	3.859104	-1.614177
H	1.903282	2.248565	-2.408175
H	0.294526	3.009021	-2.281043
C	2.657985	2.094843	0.586861
H	3.360018	1.485043	-0.006362
H	3.024203	3.137741	0.617049
H	2.636764	1.688489	1.611591

### <sup>3</sup>TS(1-2)

Lowest frequency = -674.2478 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

53

Fe	0.028295	-0.026224	-0.262593
C	-1.873831	0.203127	2.776202
H	-2.807204	-0.065149	2.254749
H	-1.919250	-0.156310	3.820319
H	-1.771212	1.301274	2.773789
C	0.896524	-0.244389	3.110723
H	0.629493	-0.654986	4.101339
H	1.844178	-0.692058	2.773599
H	1.042985	0.845028	3.204942
C	-0.807823	-2.358564	2.177547
H	0.062402	-2.965468	1.875197
H	-1.040450	-2.557337	3.239793
H	-1.668639	-2.641772	1.548430
C	1.195723	-3.014948	-1.395758

### <sup>5</sup>TS(1-2)

Lowest frequency = -974.4254 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

53

Fe	-0.047735	0.010830	-0.164211
C	1.175479	-0.829734	3.024977
H	1.637415	0.171120	3.050634
H	0.932478	-1.143635	4.056479
H	1.903444	-1.535419	2.593003
C	-1.130638	-2.395472	2.403309
H	-1.213490	-2.547089	3.496871
H	-2.138270	-2.442212	1.954837



H	-0.526995	-3.210903	1.968260
C	-1.380803	0.395419	2.991022
H	-2.410799	0.421909	2.600560
H	-1.401765	0.088302	4.052547
H	-0.952776	1.407636	2.895116
C	-3.854116	0.468735	0.156243
H	-4.796114	0.376982	-0.415305
H	-3.877027	-0.253112	0.990804
H	-3.783743	1.484780	0.580602
C	-2.811683	-1.560036	-1.522505
H	-3.864451	-1.605252	-1.859846
H	-2.141354	-1.820794	-2.357919
H	-2.651633	-2.295614	-0.714696
C	-2.756869	1.160846	-2.395479
H	-3.716667	0.857264	-2.850149
H	-2.818173	2.223572	-2.104617
H	-1.946202	1.041286	-3.134372
C	2.598241	1.897212	0.697395
H	2.588153	0.799183	0.807239
H	3.256345	2.168691	-0.149592
C	0.516114	1.757885	-1.278473
H	-0.302367	2.356281	-1.717851
H	1.416604	1.862709	-1.913731
H	0.088751	0.459843	-1.803635
C	1.289412	4.305241	0.027831
H	1.674488	4.803972	0.936673
H	2.047792	4.368380	-0.775095
H	0.374149	4.830296	-0.295116
P	-0.347312	-0.752302	1.955340
P	0.847904	2.490598	0.418811
P	-2.344254	0.132268	-0.901620
H	3.001568	2.343347	1.623569
P	1.700967	-1.385333	-1.014307
C	2.987741	-2.283497	0.011334
H	3.618990	-2.952850	-0.601711
H	3.633144	-1.549246	0.523231
H	2.474341	-2.888053	0.778897
C	2.768773	-0.739441	-2.393968
H	3.321905	-1.550963	-2.899669
H	2.120866	-0.227043	-3.124841
H	3.488603	-0.008679	-1.988158
C	0.939422	-2.866073	-1.849436
H	0.299344	-2.502314	-2.670372
H	1.700619	-3.564071	-2.247328
H	0.297926	-3.394849	-1.122663

H	1.807532	1.630657	2.340799
H	1.361171	0.738091	3.845323
H	2.345682	-0.056633	2.568769
C	-0.341369	-1.496012	2.831728
H	-0.231422	-1.330821	3.918612
H	-1.368204	-1.842555	2.627641
H	0.357170	-2.285224	2.512140
C	-1.254023	1.188738	2.691996
H	-2.258642	0.984208	2.290025
H	-1.260170	1.065908	3.790713
H	-0.993906	2.231770	2.443426
C	-3.329648	-0.900841	0.358319
H	-4.115986	-1.602819	0.022625
H	-3.167172	-1.047076	1.440199
H	-3.676455	0.135824	0.205223
C	-1.559577	-2.990509	-0.352330
H	-2.507283	-3.526889	-0.549261
H	-0.784648	-3.353085	-1.049363
H	-1.223724	-3.216368	0.672927
C	-2.425405	-1.137666	-2.298104
H	-3.278871	-1.833950	-2.387358
H	-2.768041	-0.121503	-2.559358
H	-1.642833	-1.434702	-3.017780
C	1.162042	3.495624	-0.529996
H	2.141443	3.007179	-0.660926
H	1.010349	4.257744	-1.316788
C	-0.030627	1.341664	-2.174169
H	-0.917338	1.506765	-2.810891
H	0.884095	1.607990	-2.732035
H	0.015872	0.185413	-2.041024
C	-1.662541	3.268974	-0.639343
H	-1.832382	3.751156	0.340245
H	-1.568981	4.057172	-1.409378
H	-2.533410	2.628819	-0.857724
P	-0.014447	0.066522	1.862692
P	-0.154216	2.165228	-0.526271
P	-1.711976	-1.133749	-0.565957
H	1.161847	4.000794	0.453017
P	1.862081	-0.893070	-0.553107
C	3.497522	0.022413	-0.399830
H	4.376649	-0.616469	-0.610012
H	3.488967	0.865290	-1.113204
H	3.588381	0.443642	0.615114
C	2.139597	-1.585856	-2.273364
H	3.138596	-2.046032	-2.387713
H	1.362831	-2.341605	-2.481101
H	2.034954	-0.775577	-3.016036
C	2.325842	-2.417996	0.422834
H	1.515002	-3.160354	0.338632
H	3.270764	-2.865446	0.063254
H	2.444869	-2.156070	1.488072

### <sup>1</sup>I-2

Lowest frequency = 42.2226 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

53

Fe	-0.005612	0.108063	-0.253524
C	1.519449	0.649994	2.754670

### <sup>3</sup>I-2

Lowest frequency = 42.5518 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

53

Fe	-0.000051	0.000014	-0.269911
C	1.163794	1.676976	2.584582
H	2.195774	1.491596	2.244668
H	1.129216	2.631704	3.141865
H	0.878795	0.857371	3.266741
C	-1.554994	2.165027	2.007914
H	-1.396428	3.005168	2.709740
H	-2.315946	2.461203	1.265139
H	-1.942990	1.296107	2.565293
C	0.454328	3.346094	0.402559
H	-0.203698	3.557513	-0.457999
H	0.359627	4.162950	1.142401
H	1.494728	3.315067	0.034486
C	-2.542230	1.588006	-1.968142
H	-3.515990	1.484913	-2.482438
H	-2.613663	2.395382	-1.219299
H	-1.769431	1.872994	-2.702325
C	-3.553953	-0.334495	-0.127513
H	-4.469910	-0.232149	-0.738525
H	-3.499313	-1.363177	0.267738
H	-3.605385	0.359464	0.726976
C	-2.292417	-1.197221	-2.516661
H	-3.314684	-1.127990	-2.933495
H	-1.559576	-0.993596	-3.316053
H	-2.118393	-2.222410	-2.148806
C	3.553841	0.334829	-0.127786
H	3.605558	-0.359560	0.726336
H	4.469721	0.232980	-0.738997
C	2.542152	-1.587031	-1.969085
H	3.515860	-1.483599	-2.483410
H	2.613737	-2.394723	-1.220594
H	1.769332	-1.871791	-2.703336
C	2.291874	1.198419	-2.516377
H	2.117711	2.223414	-2.148045
H	3.314112	1.129549	-2.933345
H	1.558988	0.995027	-3.315787
P	0.011627	1.667174	1.108949
P	2.010482	-0.011080	-1.117645
P	-2.010683	0.011622	-1.117431
H	3.499060	1.363294	0.268012
P	-0.011463	-1.667763	1.108216
C	1.555290	-2.165776	2.006844
H	1.396912	-3.006253	2.708310
H	2.316228	-2.461499	1.263873
H	1.943186	-1.297036	2.564568
C	-0.453922	-3.346413	0.401045
H	-0.359078	-4.163608	1.140493
H	-1.494331	-3.315369	0.033001
H	0.204127	-3.557308	-0.459626
C	-1.163570	-1.678391	2.583884
H	-2.195616	-1.493217	2.244054

H	-1.128695	-2.633286	3.140864
H	-0.878811	-0.858907	3.266293

**<sup>51</sup>I-2**

Lowest frequency = 20.8786 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

53

Fe	0.160872	0.009129	-0.313390
C	-0.038430	3.526397	0.091774
H	-0.870486	3.587042	-0.628582
H	-0.105906	4.369938	0.803797
H	0.904984	3.599705	-0.474095
C	1.195656	2.161761	2.257242
H	1.007865	3.084187	2.838037
H	1.222311	1.298487	2.942151
H	2.181347	2.235929	1.766755
C	-1.645236	2.077205	1.960623
H	-1.744272	1.208377	2.632634
H	-1.638909	3.008690	2.556152
H	-2.517515	2.077565	1.285387
C	-1.638440	-2.473757	1.567477
H	-1.530623	-3.322379	2.267305
H	-2.157111	-1.640078	2.068773
H	-2.254347	-2.789998	0.708982
C	0.922531	-1.774909	2.578325
H	0.947354	-2.748145	3.103813
H	1.952879	-1.429953	2.390395
H	0.423982	-1.030773	3.222850
C	0.727444	-3.449499	0.285084
H	0.616844	-4.292179	0.992051
H	0.227255	-3.698590	-0.665785
H	1.799820	-3.292968	0.077425
C	-2.706724	1.439428	-1.925366
H	-1.775962	1.663162	-2.472369
H	-3.534750	1.277367	-2.639669
C	-2.448945	-1.403783	-2.134309
H	-2.374330	-2.386027	-1.633189
H	-3.375581	-1.377654	-2.738415
H	-1.567142	-1.290467	-2.785509
C	-4.227065	-0.261010	-0.256805
H	-4.468615	0.554952	0.447396
H	-4.963161	-0.249345	-1.084348
H	-4.319301	-1.216636	0.288495
P	-0.099801	1.870762	0.947581
P	-2.415168	-0.054224	-0.842671
P	0.008227	-1.862631	0.952564
H	-2.955669	2.307695	-1.288628
P	2.377370	0.036718	-0.908491
C	2.964838	1.629380	-1.678470
H	3.948057	1.513191	-2.169946
H	2.218466	1.963678	-2.418077
H	3.048252	2.401731	-0.893945

C	2.758366	-1.161786	-2.285199
H	3.814924	-1.103471	-2.607324
H	2.537330	-2.187557	-1.943881
H	2.093935	-0.938630	-3.135999
C	3.878851	-0.319142	0.180705
H	3.795586	-1.348415	0.571695
H	4.841071	-0.219567	-0.357992
H	3.872225	0.372686	1.040550

O	0.902290	-0.935805	-0.270624
C	2.095002	-3.292415	0.038264
H	1.439158	-3.355710	-0.843103
H	2.711877	-4.207905	0.077220
H	1.449000	-3.272752	0.929667
C	3.829113	-2.177710	-1.345182
H	4.390435	-3.130534	-1.360944
H	3.141661	-2.173320	-2.209490
H	4.547831	-1.356306	-1.486459
C	3.948701	-2.126075	1.212283
H	4.649963	-1.280793	1.274545
H	3.349781	-2.126900	2.140150
H	4.539661	-3.060315	1.189743
H	0.821445	1.565234	0.102585
P	-2.269775	-1.547520	0.298488
P	-0.746078	-0.218556	-2.199647
C	-1.643919	-3.315128	0.334551
H	-2.473762	-4.042675	0.405432
H	-1.059719	-3.513105	-0.576414
H	-0.970810	-3.449525	1.195396
C	-3.388902	-1.672733	1.798586
H	-4.051700	-2.553541	1.717627
H	-2.796805	-1.765328	2.723204
H	-4.013173	-0.765886	1.875014
C	-3.631771	-1.811277	-0.960887
H	-3.199180	-2.060454	-1.942869
H	-4.294535	-2.640308	-0.653085
H	-4.232834	-0.894144	-1.066156
C	-0.377987	-1.932035	-2.817136
H	-0.070344	-1.911321	-3.877095
H	0.436290	-2.333791	-2.197024
H	-1.263957	-2.578756	-2.713761
C	-2.093167	0.255528	-3.397145
H	-2.291964	1.337669	-3.348140
H	-1.783277	0.002499	-4.426373
H	-3.026218	-0.279287	-3.163910
C	0.685130	0.675095	-2.976901
H	0.598552	1.757731	-2.802227
H	1.612494	0.330188	-2.493269
H	0.733360	0.474882	-4.062741

### <sup>1</sup>I-3

Lowest frequency = 29.6161 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

79

Fe	-0.810637	0.028285	0.010236
C	0.250787	-1.418541	2.898794
H	1.056315	-1.806433	2.258204
H	0.629375	-1.288890	3.927884
H	-0.574110	-2.148238	2.907558
C	-1.629100	0.648761	3.473021
H	-1.485183	0.036748	4.380346
H	-1.517915	1.708285	3.750475
H	-2.645811	0.489443	3.089685
C	1.037461	1.268569	2.874234
H	0.911183	2.317022	2.560842
H	1.030361	1.211117	3.977412
H	2.006326	0.914346	2.490640
C	-1.357129	3.207652	-1.331519
H	-2.021541	4.091230	-1.308653
H	-0.333310	3.517732	-1.066979
H	-1.332606	2.812213	-2.358740
C	-2.086999	3.049747	1.339618
H	-2.541541	4.003676	1.017874
H	-2.726104	2.601699	2.114549
H	-1.093763	3.257470	1.771339
C	-3.737224	1.865168	-0.581554
H	-4.159809	2.884728	-0.646616
H	-3.874072	1.358540	-1.549511
H	-4.287999	1.295268	0.186404
P	-0.335556	0.198216	2.194263
P	-1.923319	1.888820	-0.117484
C	1.906118	1.724740	-0.019500
C	2.408006	3.013502	-0.177763
C	3.793075	3.245064	-0.253837
C	4.654616	2.132659	-0.222976
C	4.156388	0.834763	-0.116039
C	2.750270	0.569014	-0.005254
H	1.712832	3.862163	-0.193164
H	4.192185	4.263094	-0.309462
H	5.738592	2.279304	-0.294194
H	4.872962	0.013633	-0.147115
C	2.167899	-0.761978	-0.021899
C	3.018562	-2.057880	-0.025380

### <sup>3</sup>I-3

Lowest frequency = 25.3503 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

79

Fe	-0.812185	0.040548	0.022731
C	0.001771	-1.751715	2.816056
H	0.743035	-2.146464	2.106498
H	0.429105	-1.715977	3.833334
H	-0.878252	-2.414922	2.822950
C	-1.731538	0.361225	3.568879
H	-1.469499	-0.174313	4.498165

H	-1.717720	1.441477	3.776628
H	-2.748381	0.073337	3.264097
C	0.960579	0.894802	2.940123
H	0.848774	1.969717	2.727588
H	1.022807	0.734489	4.031380
H	1.888385	0.550621	2.457172
C	-1.338910	3.300498	-0.989431
H	-2.024265	4.166664	-0.961070
H	-0.366576	3.594442	-0.563003
H	-1.170784	3.014086	-2.039128
C	-2.413516	2.826697	1.535941
H	-2.919386	3.773835	1.276647
H	-3.075447	2.240593	2.191521
H	-1.482768	3.057545	2.080598
C	-3.758096	1.827217	-0.696317
H	-4.211434	2.835168	-0.701843
H	-3.759849	1.427810	-1.721676
H	-4.371656	1.161905	-0.064922
P	-0.477857	-0.052048	2.246064
P	-2.018819	1.857795	-0.010266
C	1.882331	1.725799	0.074196
C	2.349415	3.033312	0.129935
C	3.730729	3.314977	0.110199
C	4.622209	2.226340	0.032958
C	4.163889	0.911624	-0.017146
C	2.759229	0.589706	0.005191
H	1.629692	3.859459	0.195846
H	4.098409	4.345081	0.153612
H	5.703301	2.408714	0.012860
H	4.909770	0.117786	-0.074549
C	2.213953	-0.743028	-0.034941
C	3.089513	-2.019828	-0.097228
O	0.914202	-0.973502	-0.015571
C	2.201163	-3.281471	-0.115434
H	1.529196	-3.297106	-0.987672
H	2.844564	-4.178723	-0.159122
H	1.572529	-3.352435	0.785954
C	3.932802	-2.048776	-1.399071
H	4.548589	-2.967016	-1.438054
H	3.266542	-2.048972	-2.280229
H	4.605318	-1.182777	-1.493268
C	3.993723	-2.130496	1.158540
H	4.672840	-1.272451	1.274621
H	3.369593	-2.185292	2.068313
H	4.607247	-3.049780	1.110271
H	0.794407	1.540795	0.094750
P	-2.337486	-1.578186	0.012362
P	-0.522791	0.041613	-2.192687
C	-1.656630	-3.317417	0.002578
H	-2.463093	-4.073040	0.015307
H	-1.038239	-3.456330	-0.897052
H	-1.002840	-3.461952	0.874992
C	-3.564775	-1.767055	1.411127
H	-4.256579	-2.609893	1.230914
H	-3.033587	-1.946040	2.359782
H	-4.151609	-0.838004	1.514374

C	-3.575508	-1.791275	-1.376263
H	-3.050608	-1.946112	-2.332751
H	-4.227982	-2.663980	-1.191808
H	-4.202837	-0.889953	-1.465766
C	-0.108970	-1.627101	-2.887826
H	0.249045	-1.541579	-3.928606
H	0.676885	-2.061509	-2.252845
H	-0.991024	-2.286653	-2.865607
C	-1.809849	0.577740	-3.429376
H	-2.014565	1.656069	-3.334305
H	-1.447244	0.379835	-4.453360
H	-2.750623	0.029176	-3.271714
C	0.934763	0.983643	-2.851639
H	0.868746	2.047391	-2.578066
H	1.851964	0.577993	-2.396204
H	0.983943	0.880915	-3.950384

### <sup>5</sup>I-3

Lowest frequency = 18.1405 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

79

Fe	-0.832626	0.043291	0.210916
C	0.498576	-1.144558	3.261707
H	1.102465	-1.756786	2.573989
H	1.061504	-0.968679	4.196151
H	-0.425978	-1.696925	3.499152
C	-0.966747	1.258593	3.714962
H	-0.526124	1.111952	4.717784
H	-1.023420	2.340390	3.512227
H	-1.990462	0.850710	3.707393
C	1.653676	1.381233	2.655226
H	1.556092	2.394006	2.232057
H	1.903907	1.444865	3.730163
H	2.465093	0.875100	2.108850
C	-1.401778	3.001711	-1.843759
H	-1.956622	3.952937	-1.931384
H	-0.321052	3.209761	-1.806573
H	-1.600082	2.388636	-2.736914
C	-1.869068	3.446729	0.921107
H	-2.376627	4.356517	0.552482
H	-2.358814	3.115115	1.851601
H	-0.814931	3.681820	1.147089
C	-3.751123	1.976449	-0.624430
H	-4.186321	2.965130	-0.859580
H	-3.938038	1.287420	-1.464503
H	-4.246992	1.568286	0.273000
P	0.072815	0.444162	2.400397
P	-1.915812	2.062651	-0.323480
C	1.785376	1.599793	-0.613126
C	2.209844	2.921726	-0.685957
C	3.578759	3.252073	-0.605944
C	4.505461	2.197097	-0.477119

C	4.090725	0.869381	-0.398490	Fe	0.225832	-0.027408	-0.198963
C	2.698069	0.503768	-0.429858	C	2.524745	1.729185	-2.223233
H	1.468470	3.721964	-0.807553	H	2.503025	2.615418	-1.568773
H	3.912349	4.293286	-0.658724	H	3.516059	1.655532	-2.705123
H	5.578674	2.418688	-0.436672	H	1.755649	1.849674	-3.002615
H	4.858866	0.100235	-0.302075	C	2.445175	-1.070101	-2.539663
C	2.171895	-0.823202	-0.239668	H	3.306226	-0.820673	-3.185269
C	3.057290	-2.080020	-0.054474	H	2.612882	-2.060080	-2.086138
O	0.873273	-1.033147	-0.224208	H	1.522572	-1.123523	-3.141010
C	2.163824	-3.325901	0.115961	C	3.825388	0.165883	-0.338752
H	1.547940	-3.506538	-0.779686	H	3.925415	-0.723821	0.299149
H	2.798383	-4.215180	0.283017	H	4.654622	0.180221	-1.068764
H	1.477849	-3.217301	0.970940	H	3.906681	1.061396	0.301094
C	3.941453	-2.313226	-1.306344	C	2.287003	-2.693833	0.995816
H	4.549049	-3.229987	-1.184786	H	2.226147	-3.768274	1.243539
H	3.305263	-2.440617	-2.200298	H	2.983053	-2.573956	0.150626
H	4.626506	-1.473678	-1.502830	H	2.688092	-2.152010	1.863639
C	3.933564	-1.973904	1.221501	C	0.305179	-3.366594	-0.837215
H	4.599335	-1.097579	1.211720	H	1.272937	-3.604154	-1.307714
H	3.295696	-1.895378	2.119191	H	-0.120266	-4.294876	-0.419841
H	4.561009	-2.878391	1.331316	H	-0.361159	-2.927563	-1.591662
H	0.714917	1.364818	-0.707863	C	-0.336615	-2.817516	1.944097
P	-2.466817	-1.481118	0.682578	H	-0.035102	-3.864566	2.126113
P	-0.950857	-0.603514	-2.308467	H	-0.121222	-2.222526	2.847869
C	-1.821969	-3.196395	1.002984	H	-1.419971	-2.777645	1.760512
H	-2.633037	-3.898994	1.267285	P	2.174913	0.203736	-1.211756
H	-1.299275	-3.555500	0.102861	P	0.587703	-2.089648	0.492456
H	-1.086433	-3.158649	1.821373	C	-0.508226	1.731595	-1.364993
C	-3.466675	-1.219167	2.236743	C	-0.296187	3.144950	-1.265742
H	-4.227796	-2.008278	2.375598	C	-1.048453	3.930843	-0.416840
H	-2.792633	-1.217683	3.109291	C	-2.076076	3.325695	0.374282
H	-3.971064	-0.238537	2.191081	C	-2.312652	1.969635	0.313141
C	-3.874777	-1.893165	-0.471820	C	-1.544408	1.116564	-0.562771
H	-3.473069	-2.264839	-1.428012	H	0.436815	3.619249	-1.927541
H	-4.541810	-2.662860	-0.042260	H	-0.891779	5.013916	-0.371835
H	-4.460512	-0.981745	-0.675620	H	-2.701207	3.954288	1.018682
C	-0.690407	-2.424269	-2.565833	H	-3.130417	1.548112	0.899411
H	-0.456596	-2.659267	-3.620125	C	-1.698929	-0.315635	-0.784504
H	0.147581	-2.719427	-1.916505	C	-3.013123	-1.068441	-0.467901
H	-1.588954	-2.989507	-2.266764	O	-0.874491	-0.779980	-1.728148
C	-2.315353	-0.321906	-3.560697	C	-2.901369	-2.549348	-0.870401
H	-2.485087	0.758987	-3.704331	H	-2.218475	-3.100846	-0.206635
H	-2.067600	-0.768618	-4.541388	H	-3.895876	-3.025326	-0.798544
H	-3.257045	-0.765969	-3.196133	H	-2.532848	-2.649545	-1.903144
C	0.495649	0.035071	-3.281667	C	-3.432261	-0.992345	1.021443
H	0.453105	1.133746	-3.353409	H	-4.105213	-1.833380	1.268393
H	1.421072	-0.229883	-2.744733	H	-2.552856	-1.041991	1.682334
H	0.515831	-0.398138	-4.298500	H	-3.981011	-0.067307	1.261180

**<sup>1</sup>I-4**

Lowest frequency = 43.3897 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

H	2.152303	0.805626	3.728476
H	1.710817	-0.851050	3.219594
H	2.980333	0.047340	2.330105
C	-0.639866	0.972119	3.006567
H	-0.276865	1.465737	3.925809
H	-1.483867	1.543255	2.593213
H	-0.989643	-0.043487	3.253623
C	1.318151	2.611996	1.727167
H	1.497010	2.975641	2.754849
H	2.259615	2.662015	1.153967
H	0.579411	3.254362	1.226747

H	-2.531999	-0.678595	1.827807
C	-1.141999	-1.111821	-0.572386
C	-1.276098	-2.652134	-0.434644
O	-0.413227	-0.700868	-1.629552
C	0.102560	-3.290081	-0.682588
H	0.835847	-2.888963	0.037007
H	0.051965	-4.388737	-0.572467
H	0.461265	-3.050443	-1.696550
C	-1.806299	-3.094530	0.940702
H	-1.763298	-4.195870	1.026203
H	-1.201215	-2.662601	1.756566
H	-2.854861	-2.788983	1.091303
C	-2.259960	-3.130777	-1.530116
H	-3.260213	-2.686617	-1.381033
H	-1.894000	-2.829572	-2.526856
H	-2.364578	-4.231743	-1.513054
H	-2.432263	0.405521	-2.343480
P	1.217974	-0.407033	1.936456
C	2.814719	0.410380	2.461913
H	3.033935	0.243011	3.532421
H	3.645586	0.000034	1.863179
H	2.753664	1.492604	2.266010
C	1.611209	-2.126102	2.553355
H	1.996207	-2.101970	3.589022
H	0.707865	-2.754975	2.515578
H	2.371352	-2.582564	1.897619
C	0.122316	0.175554	3.328087
H	0.577221	-0.016497	4.316493
H	-0.058527	1.257932	3.217428
H	-0.849996	-0.339514	3.267931

### <sup>3</sup>I-4

Lowest frequency = 30.0995 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

66

Fe	0.452789	-0.017694	-0.084878
C	-1.306035	2.958529	0.742152
H	-1.312584	2.689107	1.811023
H	-1.340146	4.058937	0.645071
H	-2.199832	2.519507	0.274043
C	0.019302	2.924106	-1.790067
H	-0.248774	3.996104	-1.800023
H	0.960955	2.780111	-2.346159
H	-0.767146	2.334767	-2.287865
C	1.458056	3.475811	0.627322
H	2.465221	3.266133	0.235219
H	1.183442	4.519175	0.385956
H	1.485927	3.365078	1.725119
C	3.729392	1.197409	-1.152832
H	4.607676	0.930193	-1.767958
H	3.291473	2.128742	-1.549234
H	4.056972	1.380766	-0.116595
C	2.189185	-0.295244	-3.021443
H	1.691849	0.619121	-3.384816
H	3.140660	-0.443443	-3.562450
H	1.502394	-1.136290	-3.203943
C	3.539892	-1.624023	-0.895454
H	4.394984	-1.646723	-1.595368
H	3.924522	-1.599344	0.138468
H	2.943558	-2.542186	-1.019883
P	0.215911	2.268239	-0.064645
P	2.442943	-0.148479	-1.192006
C	-2.906773	0.487625	-1.360647
C	-4.035970	1.292062	-1.170441
C	-4.640611	1.380002	0.094971
C	-4.091422	0.656252	1.165381
C	-2.960973	-0.148177	0.974729
C	-2.344661	-0.256985	-0.294279
H	-4.454105	1.850027	-2.016329
H	-5.523940	2.009448	0.246307
H	-4.541170	0.728225	2.162190

### <sup>5</sup>I-4

Lowest frequency = 25.0437 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

66

Fe	0.794819	-0.017380	-0.151768
C	1.630049	2.938307	-1.978002
H	1.152443	3.526254	-1.176897
H	2.459366	3.519821	-2.419843
H	0.871369	2.740986	-2.754070
C	3.115898	0.620927	-2.736465
H	3.785524	1.360717	-3.212025
H	3.711452	-0.249734	-2.412435
H	2.373527	0.272203	-3.474414
C	3.653933	1.929720	-0.250213
H	4.173139	1.070900	0.206515
H	4.372484	2.507927	-0.859157
H	3.271888	2.572774	0.560778
C	3.698054	-1.933578	0.960989
H	4.075969	-2.958434	1.129242
H	4.333844	-1.437295	0.208064
H	3.771467	-1.363632	1.902728

C	2.058786	-3.022176	-1.132714			
H	2.702231	-2.533501	-1.883188			
H	2.466323	-4.020797	-0.893175	Fe	0.536830	0.021662 -0.196946
H	1.046008	-3.113230	-1.557281	C	3.949406	0.681891 0.209639
C	1.158519	-3.090372	1.589403	H	4.061592	-0.370238 0.505717
H	1.673487	-4.067336	1.632517	H	4.852153	1.003410 -0.339603
H	1.176706	-2.627352	2.590974	H	3.859562	1.291564 1.124890
H	0.105834	-3.242891	1.301095	C	2.660652	2.756273 -1.118270
P	2.215755	1.323122	-1.264723	H	3.710135	2.938695 -1.410124
P	1.939400	-1.934879	0.361987	H	2.001317	3.103248 -1.929699
C	-1.570331	1.576036	-1.035427	H	2.438054	3.334047 -0.206268
C	-1.971918	2.904075	-0.910057	C	3.010293	0.361129 -2.491316
C	-3.177209	3.238794	-0.260458	H	2.237466	0.629210 -3.231197
C	-3.982128	2.191296	0.238288	H	3.968769	0.835813 -2.769935
C	-3.607038	0.856888	0.094280	H	3.130844	-0.733319 -2.511380
C	-2.376482	0.486741	-0.548640	C	3.092029	-2.633949 -0.334465
H	-1.342633	3.698144	-1.329478	H	3.138688	-3.719853 -0.530986
H	-3.489577	4.282958	-0.157911	H	3.750068	-2.118258 -1.052304
H	-4.923551	2.426300	0.748992	H	3.471229	-2.445851 0.684535
H	-4.263265	0.085733	0.505310	C	0.836124	-2.816995 -2.073123
C	-1.883749	-0.852231	-0.723969	H	1.103873	-3.888216 -2.131775
C	-2.751961	-2.123387	-0.637202	H	-0.255235	-2.699749 -2.173637
O	-0.616945	-1.027630	-1.071125	H	1.315029	-2.270311 -2.902278
C	-1.962534	-3.318991	-1.209948	C	0.582125	-3.266969 0.725469
H	-1.056045	-3.520392	-0.617683	H	0.799929	-4.305974 0.419849
H	-2.596621	-4.224039	-1.194300	H	0.991546	-3.097588 1.735037
H	-1.646990	-3.125128	-2.248177	H	-0.503085	-3.099776 0.748821
C	-3.104340	-2.453020	0.836936	C	0.996572	2.133045 2.446526
H	-3.689760	-3.390216	0.893983	H	0.014027	0.728118 -1.525280
H	-2.183476	-2.588627	1.430788	H	0.260162	2.774991 1.935226
H	-3.695224	-1.655528	1.315875	H	0.898525	2.252640 3.540503
C	-4.045701	-1.972704	-1.475154	C	-0.854098	0.001450 2.830140
H	-4.672224	-1.133898	-1.134247	H	-1.077970	-1.073815 2.736384
H	-3.794186	-1.792240	-2.534805	H	-0.783514	0.275444 3.897631
H	-4.648925	-2.898004	-1.415834	H	-1.675496	0.567288 2.359037
H	-0.654412	1.322256	-1.582298	C	1.941581	-0.477991 3.038585
P	0.273907	0.996143	1.833360	H	2.968942	-0.274502 2.696308
C	1.660677	0.830097	3.065689	H	1.838476	-0.138690 4.085542
H	1.413526	1.316204	4.026954	H	1.776300	-1.567610 2.999800
H	1.858983	-0.240070	3.245316	P	2.409532	0.926671 -0.817012
H	2.578049	1.286101	2.656934	P	0.717228	0.373375 1.914833
C	-1.130762	0.264912	2.795239	P	1.327902	-2.038424 -0.454151
H	-1.223470	0.724541	3.795903	C	-0.750000	1.472581 -0.503024
H	-2.059864	0.427758	2.224347	C	-0.591164	2.892077 -0.639557
H	-0.970177	-0.820579	2.900018	C	-1.663653	3.771912 -0.700954
C	-0.097838	2.804489	1.998502	C	-3.000789	3.300614 -0.667847
H	-0.217292	3.098008	3.057131	C	-3.226775	1.939685 -0.541311
H	0.726990	3.385392	1.550735	C	-2.140989	1.023239 -0.433849
H	-1.022134	3.030135	1.442155	H	2.007518	2.455840 2.143432
				H	0.413168	3.312737 -0.674714
				H	-1.471015	4.849369 -0.772412
				H	-3.839495	4.000935 -0.737051
				H	-4.255928	1.571622 -0.508382
				C	-2.241538	-0.387746 -0.243453
				C	-3.514587	-1.244872 -0.213699
				O	-1.112683	-0.995761 -0.127336

**<sup>1</sup>TS(4-5)**Lowest frequency = -785.6491 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

C	-3.140914	-2.728290	-0.025604
H	-2.626852	-2.890635	0.936321
H	-4.058337	-3.342918	-0.034169
H	-2.475478	-3.080807	-0.830250
C	-4.420898	-0.826577	0.972001
H	-5.318170	-1.471204	1.001918
H	-3.883014	-0.943014	1.928725
H	-4.754832	0.219983	0.898387
C	-4.274281	-1.101775	-1.556951
H	-4.590626	-0.064660	-1.749523
H	-3.633318	-1.420306	-2.397520
H	-5.175612	-1.741505	-1.548962

H	1.899712	0.394732	4.070050
H	1.945768	-1.093592	3.070906
P	2.366457	0.849320	-1.099741
P	0.731600	0.702583	1.886884
P	1.432284	-2.108925	-0.092018
C	-0.824546	1.456354	-0.448306
C	-0.671998	2.845823	-0.565062
C	-1.771635	3.731223	-0.591333
C	-3.079396	3.214216	-0.516771
C	-3.284214	1.840396	-0.415598
C	-2.179752	0.926076	-0.376959
H	1.906448	2.856996	1.836319
H	0.329980	3.276414	-0.627745
H	-1.602170	4.810724	-0.674258
H	-3.941541	3.890923	-0.536225
H	-4.307828	1.461838	-0.343405
C	-2.238453	-0.485012	-0.265214
C	-3.479938	-1.379324	-0.332627
O	-1.067025	-1.101566	-0.069414
C	-3.066319	-2.865131	-0.322531
H	-2.527516	-3.127407	0.602933
H	-3.967891	-3.500517	-0.389390
H	-2.410049	-3.103648	-1.176156
C	-4.380592	-1.126498	0.905300
H	-5.271479	-1.781895	0.875506
H	-3.824050	-1.343326	1.834199
H	-4.726329	-0.081444	0.956856
C	-4.274151	-1.114787	-1.636324
H	-4.595870	-0.064858	-1.719797
H	-3.648933	-1.343986	-2.517062
H	-5.175064	-1.755584	-1.674724

### <sup>3</sup>TS(4-5)

Lowest frequency = -540.5506 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

66

Fe	0.522157	-0.008326	-0.284874
C	3.927275	0.940157	-0.081267
H	4.156460	-0.041045	0.361328
H	4.789057	1.274613	-0.686253
H	3.769627	1.660391	0.739567
C	2.408326	2.573150	-1.793746
H	3.354522	2.737496	-2.338930
H	1.556328	2.720488	-2.476512
H	2.335415	3.311480	-0.978673
C	2.996978	-0.044930	-2.608138
H	2.205688	-0.020439	-3.375882
H	3.912979	0.424864	-3.009207
H	3.211142	-1.099500	-2.371852
C	3.207844	-2.593954	0.155609
H	3.304019	-3.693640	0.187831
H	3.845312	-2.206852	-0.655580
H	3.568918	-2.178641	1.111593
C	0.955485	-3.104265	-1.577109
H	1.209823	-4.172314	-1.454222
H	-0.132960	-2.983812	-1.694651
H	1.454261	-2.705074	-2.474754
C	0.637866	-3.090550	1.258960
H	0.868572	-4.165319	1.157018
H	0.990793	-2.737683	2.241478
H	-0.444811	-2.914267	1.177142
C	0.947449	2.502849	2.252018
H	0.128230	0.631367	-1.599731
H	0.129804	3.064611	1.774276
H	0.938976	2.681349	3.341611
C	-0.822499	0.320978	2.811469
H	-0.994951	-0.766795	2.782259
H	-0.776362	0.669032	3.858491
H	-1.657723	0.810735	2.283960
C	2.021029	0.005844	3.042782
H	3.026159	0.272223	2.675923

### <sup>1</sup>I-5

Lowest frequency = 25.6908 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

66

Fe	0.530341	0.012349	-0.237068
C	3.805527	1.276906	0.026996
H	4.163735	0.298040	0.384902
H	4.613170	1.767337	-0.545816
H	3.565686	1.898799	0.906157
C	2.163689	2.765699	-1.721334
H	3.055116	2.958236	-2.343935
H	1.253585	2.855101	-2.335675
H	2.126388	3.523516	-0.922733
C	3.029297	0.246563	-2.507182
H	2.287275	0.275895	-3.321790
H	3.945485	0.777880	-2.820855
H	3.278253	-0.807179	-2.310475
C	3.239849	-2.435242	-0.005880
H	3.405270	-3.525125	-0.077107
H	3.896714	-1.931653	-0.733490



H	3.524172	-2.096720	1.003999
C	1.153562	-2.907830	-1.918316
H	1.491781	-3.959363	-1.884096
H	0.069233	-2.869860	-2.113054
H	1.662918	-2.378566	-2.739109
C	0.671505	-3.239744	0.846527
H	1.014253	-4.268849	0.638284
H	0.922410	-2.983746	1.888962
H	-0.419005	-3.174071	0.721628
C	0.864563	2.082550	2.564146
H	0.396962	-0.041188	-1.773023
H	-0.029656	2.647248	2.257898
H	0.948630	2.089585	3.665313
C	-0.745543	-0.226107	2.885692
H	-0.883788	-1.309875	2.741117
H	-0.648292	-0.004345	3.963349
H	-1.634001	0.291044	2.485024
C	2.104559	-0.417745	2.936694
H	3.079259	-0.063892	2.562567
H	2.011263	-0.144962	4.003238
H	2.078978	-1.516089	2.849207
P	2.264423	1.045042	-1.005624
P	0.736361	0.342305	1.919350
P	1.450047	-2.015256	-0.317293
C	-0.776251	1.458496	-0.293443
C	-0.644422	2.873613	-0.234569
C	-1.729651	3.749801	-0.308336
C	-3.047194	3.260754	-0.437979
C	-3.250024	1.885503	-0.455893
C	-2.148036	0.993038	-0.366867
H	1.749772	2.579706	2.133030
H	0.347189	3.313791	-0.109154
H	-1.555669	4.832155	-0.261277
H	-3.895132	3.950124	-0.506862
H	-4.270677	1.500166	-0.533310
C	-2.234519	-0.446663	-0.300203
C	-3.498560	-1.315181	-0.362157
O	-1.119645	-1.045875	-0.170066
C	-3.108464	-2.803132	-0.260999
H	-2.617162	-3.021372	0.701689
H	-4.016236	-3.427427	-0.335558
H	-2.415904	-3.091618	-1.068265
C	-4.436263	-0.980350	0.825734
H	-5.320806	-1.642093	0.798104
H	-3.916303	-1.143795	1.785826
H	-4.787805	0.062654	0.804911
C	-4.222503	-1.090875	-1.714008
H	-4.552570	-0.048777	-1.845448
H	-3.553768	-1.341973	-2.555488
H	-5.111601	-1.744490	-1.772636

Fe	0.514713	0.006248	-0.278645
C	3.873830	1.089677	-0.031076
H	4.147541	0.112684	0.396950
H	4.727725	1.483019	-0.611143
H	3.659712	1.783111	0.799830
C	2.313610	2.626081	-1.817962
H	3.236232	2.800268	-2.399074
H	1.432109	2.727908	-2.470497
H	2.247647	3.384086	-1.021190
C	3.040552	0.023395	-2.555723
H	2.280294	0.034150	-3.353879
H	3.964228	0.507290	-2.919249
H	3.261757	-1.025861	-2.306517
C	3.259465	-2.534301	0.131985
H	3.386654	-3.631344	0.134871
H	3.909036	-2.105471	-0.648028
H	3.582915	-2.137665	1.109271
C	1.051881	-3.044855	-1.669488
H	1.328175	-4.110366	-1.576696
H	-0.036946	-2.944671	-1.803456
H	1.553589	-2.604822	-2.545748
C	0.679981	-3.137700	1.151014
H	0.951295	-4.200133	1.022553
H	0.991080	-2.806282	2.154960
H	-0.405686	-2.996812	1.044521
C	0.869804	2.417254	2.365434
H	0.305960	0.313404	-1.752838
H	0.028035	2.975365	1.927807
H	0.883309	2.548173	3.461557
C	-0.869617	0.179715	2.817454
H	-1.016441	-0.909538	2.745475
H	-0.844151	0.491997	3.876132
H	-1.706132	0.670752	2.293450
C	1.985955	-0.091501	3.062977
H	2.985508	0.216248	2.713352
H	1.850570	0.247726	4.105718
H	1.936766	-1.192341	3.039763
P	2.343866	0.921364	-1.084362
P	0.687220	0.629553	1.935657
P	1.477107	-2.086366	-0.145953
C	-0.820673	1.461879	-0.385461
C	-0.673854	2.851179	-0.467928
C	-1.777725	3.732831	-0.543163
C	-3.083127	3.207026	-0.546024
C	-3.285245	1.830946	-0.466819
C	-2.175189	0.925960	-0.378661
H	1.809271	2.812376	1.942726
H	0.324936	3.295751	-0.459616
H	-1.612208	4.814787	-0.601980
H	-3.947389	3.878857	-0.607495
H	-4.309064	1.445545	-0.460254
C	-2.227645	-0.484861	-0.279262

**<sup>3</sup>I-5**Lowest frequency = 24.7415 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

C	-3.457612	-1.392437	-0.351121
O	-1.043425	-1.094596	-0.080682
C	-3.032939	-2.873725	-0.285021
H	-2.525839	-3.103954	0.666944
H	-3.926374	-3.519198	-0.363975
H	-2.344319	-3.130432	-1.107004
C	-4.399380	-1.113412	0.849838
H	-5.287354	-1.772078	0.806483
H	-3.873578	-1.306840	1.801641
H	-4.748686	-0.068520	0.865291
C	-4.213793	-1.171061	-1.685861
H	-4.537827	-0.125370	-1.807373
H	-3.560162	-1.420147	-2.540104
H	-5.109906	-1.818145	-1.733885

C	1.761124	-0.528434	3.061829
H	2.799659	-0.377633	2.721294
H	1.669815	-0.177501	4.105732
H	1.537483	-1.608123	3.028586
P	3.062684	0.906196	-0.595257
P	0.607382	0.381078	1.919941
P	1.290970	-2.260479	-0.468475
C	-0.880439	1.498031	-0.547354
C	-0.592573	2.852400	-0.735105
C	-1.611731	3.828473	-0.822153
C	-2.957320	3.419637	-0.795799
C	-3.284919	2.070206	-0.661064
C	-2.268571	1.071807	-0.510084
H	2.040607	2.359023	2.074022
H	0.448563	3.182756	-0.801723
H	-1.352025	4.889072	-0.916943
H	-3.758959	4.161307	-0.891329
H	-4.339861	1.782288	-0.678910
C	-2.469207	-0.329824	-0.297290
C	-3.812328	-1.061525	-0.180376
O	-1.375366	-1.085290	-0.198194
C	-3.566005	-2.562423	0.076775
H	-3.008546	-2.719282	1.015432
H	-4.533954	-3.090079	0.153919
H	-2.983949	-3.015048	-0.742851
C	-4.640697	-0.504332	1.005910
H	-5.609126	-1.033899	1.079150
H	-4.097708	-0.651773	1.956054
H	-4.846261	0.572514	0.900720
C	-4.610620	-0.928662	-1.503265
H	-4.829571	0.121674	-1.752678
H	-4.034848	-1.359249	-2.341076
H	-5.571476	-1.471802	-1.427619

### <sup>5</sup>I-5

Lowest frequency = 26.3609 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

66

Fe	0.331458	-0.058512	-0.403087
C	4.614681	0.863044	0.447877
H	4.864356	-0.182317	0.697917
H	5.478781	1.325810	-0.064197
H	4.431733	1.404294	1.392684
C	3.032492	2.707875	-1.039305
H	4.018676	3.045626	-1.406214
H	2.276610	2.860964	-1.826560
H	2.744916	3.310998	-0.162257
C	3.716324	0.232988	-2.199930
H	2.916154	0.321687	-2.953041
H	4.611171	0.786311	-2.537203
H	3.976394	-0.833737	-2.099122
C	3.016141	-2.694657	0.056985
H	3.179522	-3.786205	0.013047
H	3.755406	-2.199228	-0.591836
H	3.174964	-2.347074	1.090897
C	1.176454	-3.043415	-2.138905
H	1.472852	-4.107631	-2.126216
H	0.130702	-2.951737	-2.476735
H	1.813632	-2.485835	-2.845177
C	0.306624	-3.431275	0.566060
H	0.606939	-4.479205	0.388477
H	0.452808	-3.185920	1.631325
H	-0.753922	-3.273106	0.319375
C	0.998633	2.133468	2.357894
H	0.755821	0.372942	-1.857561
H	0.325205	2.790846	1.784094
H	0.873060	2.315416	3.439808
C	-1.025188	0.126462	2.739299
H	-1.333971	-0.920364	2.588549
H	-0.987582	0.364709	3.816916
H	-1.761848	0.771143	2.231926

### <sup>1</sup>TS(5-6)

Lowest frequency = -420.8499 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

66

Fe	0.310926	-0.026169	0.006905
C	1.584182	-2.361633	2.329766
H	2.585659	-2.348041	1.867716
H	1.685459	-2.555882	3.412526
H	0.999964	-3.175473	1.872946
C	-0.755654	-0.931732	3.109184
H	-0.451733	-1.158156	4.146466
H	-1.328488	0.010193	3.087496
H	-1.407732	-1.729635	2.725300
C	1.723131	0.334083	3.180612
H	1.219578	1.309926	3.278801
H	1.780515	-0.138983	4.176636
H	2.746630	0.500483	2.809868
C	3.755813	0.450301	0.079981

Lowest frequency = -925.8419 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

66

H	4.593660	1.077692	-0.273574
H	3.895227	0.253193	1.155801
H	3.778584	-0.518200	-0.442063
C	2.445558	2.814666	0.843358
H	3.500008	3.122354	0.726646
H	1.800007	3.636141	0.499851
H	2.239618	2.631574	1.907740
C	2.364038	2.065877	-1.853285
H	3.179902	2.809413	-1.829396
H	2.599853	1.294894	-2.599423
H	1.416199	2.542606	-2.148157
C	1.413633	-3.287264	-0.992940
H	-0.476197	1.069565	0.822617
H	0.629343	-3.699336	-0.340599
H	1.515028	-3.933943	-1.882429
C	-0.398153	-1.865332	-2.713451
H	-0.788349	-0.880284	-3.016129
H	-0.024895	-2.426631	-3.587752
H	-1.212121	-2.421763	-2.225759
C	2.328597	-1.292984	-2.753210
H	3.299305	-1.068804	-2.283951
H	2.437154	-2.199194	-3.374758
H	2.048759	-0.453621	-3.410037
P	0.734721	-0.735518	2.014901
P	0.966873	-1.556905	-1.497885
P	2.109137	1.289784	-0.185301
C	-1.333194	-1.143098	0.084177
C	-1.818344	-2.438117	0.336876
C	-3.197996	-2.710185	0.239502
C	-4.106445	-1.691813	-0.086713
C	-3.643250	-0.381713	-0.316488
C	-2.266526	-0.136281	-0.234833
H	2.367930	-3.281651	-0.440962
H	-1.144654	-3.259149	0.619515
H	-3.566540	-3.726742	0.423919
H	-5.177648	-1.912054	-0.152648
H	-4.362203	0.411985	-0.547298
C	-1.422166	1.107120	-0.470572
C	-1.982425	2.517790	-0.155713
O	-0.594558	0.986853	-1.490357
C	-0.848244	3.546580	-0.084631
H	-0.206878	3.479565	-0.978062
H	-1.258857	4.569975	-0.020933
H	-0.231171	3.366299	0.810238
C	-2.913807	2.889845	-1.335684
H	-3.333948	3.899866	-1.179684
H	-2.344008	2.885580	-2.279914
H	-3.752688	2.183510	-1.441048
C	-2.749949	2.524329	1.178378
H	-3.616384	1.844608	1.165803
H	-2.083189	2.207360	2.001264
H	-3.112067	3.543289	1.405135

Fe	0.441583	-0.015782	0.054463
C	2.040745	-2.191697	2.157552
H	3.006467	-1.921525	1.697961
H	2.207459	-2.533636	3.194822
H	1.592218	-3.011676	1.574182
C	-0.513012	-1.293634	3.127202
H	-0.167469	-1.595614	4.131653
H	-1.233349	-0.463236	3.212285
H	-1.020197	-2.133397	2.629302
C	1.727092	0.396889	3.324514
H	1.063512	1.255087	3.519913
H	1.905448	-0.140937	4.272442
H	2.688237	0.771929	2.938498
C	3.645883	1.588918	0.244943
H	4.163311	2.552835	0.091416
H	3.842247	1.242305	1.273262
H	4.060116	0.842635	-0.449401
C	1.472255	3.194509	1.101666
H	2.136142	4.046160	0.868855
H	0.423955	3.498389	0.967712
H	1.618660	2.898830	2.151578
C	1.755932	2.635012	-1.653106
H	2.341408	3.570941	-1.634855
H	2.140939	1.981114	-2.451779
H	0.695255	2.840167	-1.866248
C	1.706202	-3.032168	-1.622750
H	-0.684169	0.646217	1.069086
H	0.725811	-3.495303	-1.439550
H	2.105560	-3.389725	-2.588610
C	0.395400	-0.966733	-3.107027
H	0.256243	0.110074	-3.289429
H	0.795544	-1.469575	-4.005718
H	-0.586446	-1.387281	-2.835309
C	3.176026	-0.784616	-2.402587
H	3.975868	-1.053795	-1.691301
H	3.328033	-1.355958	-3.336086
H	3.258084	0.290149	-2.628950
P	0.908354	-0.720784	2.088817
P	1.515806	-1.186747	-1.653895
P	1.811761	1.756673	-0.022029
C	-0.997093	-1.391758	-0.002024
C	-1.137432	-2.778896	0.149303
C	-2.402086	-3.404878	0.077499
C	-3.548040	-2.634855	-0.162644
C	-3.442610	-1.241191	-0.308373
C	-2.180908	-0.616685	-0.216545
H	2.398864	-3.327392	-0.816787
H	-0.265956	-3.409935	0.370038
H	-2.485198	-4.489813	0.213749
H	-4.529964	-3.116068	-0.236277

<sup>3</sup>TS(5-6)

H	-4.349055	-0.657974	-0.500130
C	-1.835885	0.817582	-0.304302
C	-2.848132	1.964432	-0.197225
O	-0.737199	1.075615	-1.073354
C	-2.103464	3.296790	0.014053
H	-1.362565	3.464337	-0.783095
H	-2.819873	4.137989	0.017605
H	-1.579528	3.288246	0.985860
C	-3.629164	2.047612	-1.535824
H	-4.326652	2.906137	-1.525642
H	-2.921962	2.180008	-2.372562
H	-4.213018	1.131339	-1.724386
C	-3.808422	1.762698	0.993258
H	-4.428752	0.859553	0.890567
H	-3.232997	1.670175	1.931690
H	-4.484346	2.632514	1.085541

H	0.784802	-1.307261	-4.201041
H	-0.520384	-1.224905	-2.944220
C	3.236455	-0.520172	-2.811535
H	4.111606	-0.759840	-2.182929
H	3.326800	-1.069179	-3.767066
H	3.248927	0.562177	-3.024634
P	0.942525	-1.117546	2.219967
P	1.661449	-0.981772	-1.911130
P	1.880784	1.856654	0.177870
C	-1.120176	-1.440062	-0.326518
C	-1.423069	-2.814112	-0.302943
C	-2.746967	-3.289740	-0.331525
C	-3.809449	-2.377249	-0.389120
C	-3.548959	-0.997653	-0.407477
C	-2.220287	-0.529178	-0.384069
H	2.682620	-3.077544	-1.134733
H	-0.616007	-3.559983	-0.241317
H	-2.950343	-4.367453	-0.303362
H	-4.844556	-2.735444	-0.424120
H	-4.393652	-0.304736	-0.464594
C	-1.808333	0.936694	-0.460240
C	-2.749123	2.084445	-0.010294
O	-0.886495	1.222630	-1.306790
C	-1.904861	3.355111	0.189521
H	-1.348431	3.603518	-0.727846
H	-2.553450	4.208008	0.457955
H	-1.182245	3.186218	1.005967
C	-3.744499	2.350413	-1.170954
H	-4.369923	3.230568	-0.935180
H	-3.188136	2.554461	-2.101697
H	-4.415803	1.495788	-1.354913
C	-3.488387	1.777192	1.305116
H	-4.177911	0.923477	1.219515
H	-2.751122	1.541229	2.092974
H	-4.074833	2.658814	1.622174

### <sup>5</sup>TS(5-6)

Lowest frequency = -437.7543 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

66

Fe	0.317308	-0.044126	0.145610
C	1.746997	-2.776917	2.023934
H	2.758111	-2.645123	1.602659
H	1.818814	-3.319058	2.984167
H	1.149057	-3.371701	1.314524
C	-0.604178	-1.554833	3.134370
H	-0.397316	-2.143533	4.046263
H	-1.124315	-0.619223	3.398991
H	-1.257958	-2.123686	2.452943
C	1.961375	-0.380711	3.591329
H	1.508666	0.579217	3.892952
H	2.010941	-1.045233	4.473367
H	2.985590	-0.184332	3.231010
C	3.687546	1.453305	0.317200
H	4.318639	2.359224	0.270830
H	3.864946	0.939271	1.276958
H	3.975690	0.767935	-0.495076
C	1.723090	3.087982	1.552452
H	2.494407	3.876074	1.484940
H	0.723575	3.547960	1.513262
H	1.821828	2.562904	2.516865
C	1.847462	2.946370	-1.315992
H	2.536822	3.805354	-1.229691
H	2.118464	2.345237	-2.199592
H	0.810987	3.289805	-1.457256
C	1.885613	-2.821466	-1.853267
H	-0.823929	0.915541	1.136644
H	0.943987	-3.280577	-1.515723
H	2.150789	-3.225030	-2.847137
C	0.436802	-0.798789	-3.283651
H	0.272515	0.273495	-3.473009

### <sup>1</sup>I-6

Lowest frequency = 35.0395 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

66

Fe	0.434904	-0.030321	0.002808
C	1.212811	3.018471	-1.594725
H	1.845626	3.453643	-0.805676
H	1.576819	3.365538	-2.577837
H	0.175668	3.353770	-1.443958
C	0.320331	0.776709	-3.082649
H	0.721762	1.317305	-3.958794
H	0.344395	-0.308511	-3.263922
H	-0.727121	1.072946	-2.906793
C	3.028295	0.924811	-2.113280
H	3.187556	-0.125845	-2.404710
H	3.254566	1.572468	-2.979116

H	3.721859	1.169176	-1.290511
C	3.590385	-2.019335	-0.094468
H	3.914173	-3.012539	-0.453191
H	4.094238	-1.242865	-0.690898
H	3.902665	-1.907738	0.954740
C	1.471194	-2.692210	-1.873372
H	1.867067	-3.723108	-1.878758
H	0.384334	-2.689752	-2.049550
H	1.968279	-2.113958	-2.670785
C	1.228511	-3.224451	0.916068
H	1.790553	-4.156146	0.725008
H	1.390917	-2.910478	1.960793
H	0.151888	-3.402833	0.773261
C	2.172294	2.535074	1.809962
H	-2.548773	-1.092117	-1.758832
H	1.463554	3.311429	1.484197
H	2.510724	2.768186	2.835153
C	0.195851	0.937400	3.160301
H	-0.183301	-0.078374	3.362711
H	0.673716	1.339132	4.071932
H	-0.659463	1.566456	2.868176
C	2.784607	-0.051827	2.611285
H	3.695702	-0.018365	1.992040
H	3.000031	0.422384	3.585454
H	2.510234	-1.105555	2.783224
P	1.273922	1.162577	-1.538189
P	1.393873	0.838603	1.740734
P	1.739197	-1.862362	-0.237702
C	-1.100612	1.200041	0.085333
C	-1.215883	2.557455	0.477066
C	-2.394735	3.300683	0.314719
C	-3.517810	2.708979	-0.282270
C	-3.458527	1.358989	-0.655452
C	-2.289607	0.606635	-0.438002
H	3.044794	2.551161	1.133922
H	-0.351315	3.074929	0.908355
H	-2.428509	4.349476	0.634131
H	-4.430209	3.291028	-0.453595
H	-4.329424	0.894461	-1.130839
C	-2.169079	-0.864598	-0.735541
C	-2.975043	-1.802630	0.249025
O	-0.807219	-1.225296	-0.658885
C	-2.710092	-3.260012	-0.177693
H	-1.630926	-3.477838	-0.169101
H	-3.222967	-3.964987	0.501874
H	-3.082019	-3.441619	-1.202844
C	-2.487835	-1.573324	1.690274
H	-2.981770	-2.276855	2.384835
H	-1.396540	-1.722854	1.755313
H	-2.708569	-0.543269	2.020002
C	-4.489267	-1.537869	0.169835
H	-4.752894	-0.548110	0.577157
H	-4.853784	-1.594813	-0.872805
H	-5.032910	-2.300467	0.757176

### <sup>3</sup>I-6

Lowest frequency = 37.0602 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

66

Fe	0.405846	-0.064941	-0.033912
C	0.968351	-3.404847	1.131732
H	1.650082	-3.703091	0.317281
H	1.180946	-4.023477	2.021914
H	-0.069916	-3.570962	0.804710
C	0.119106	-1.413076	3.005581
H	0.389820	-2.128148	3.802869
H	0.201018	-0.375778	3.365578
H	-0.923570	-1.574634	2.685999
C	2.887612	-1.702907	2.295189
H	3.167823	-0.730219	2.731353
H	2.917097	-2.469657	3.090719
H	3.630978	-1.964311	1.522289
C	3.849804	1.120489	0.126678
H	4.464386	1.979774	0.450014
H	4.141257	0.231333	0.707505
H	4.058471	0.916035	-0.936201
C	2.026039	2.033594	2.134264
H	2.669440	2.919268	2.278159
H	0.975414	2.257041	2.378498
H	2.371148	1.223325	2.797179
C	1.879625	3.089591	-0.492914
H	2.644078	3.807545	-0.145400
H	1.981761	2.950925	-1.580658
H	0.876805	3.496890	-0.288583
C	1.745362	-2.086146	-2.443490
H	-2.409370	1.089754	2.075354
H	1.090251	-2.865165	-2.023022
H	1.928691	-2.301453	-3.511596
C	-0.441821	-0.478462	-3.422181
H	-0.848387	0.539722	-3.536518
H	-0.102247	-0.848219	-4.406068
H	-1.240104	-1.123928	-3.024416
C	2.135683	0.624463	-3.200283
H	3.114851	0.689426	-2.700140
H	2.275983	0.198565	-4.209814
H	1.723888	1.642391	-3.300431
P	1.195368	-1.604478	1.516168
P	0.958419	-0.419774	-2.208003
P	2.036253	1.454053	0.376052
C	-1.280503	-1.063323	-0.190525
C	-1.604915	-2.311161	-0.771727
C	-2.883950	-2.883305	-0.660446
C	-3.888101	-2.215245	0.054145
C	-3.606902	-0.964673	0.626788
C	-2.333478	-0.384972	0.492188
H	2.701693	-2.103282	-1.894331
H	-0.841902	-2.876713	-1.323846
H	-3.090479	-3.856886	-1.121501

H	-4.881197	-2.664159	0.168006
H	-4.385835	-0.444575	1.196918
C	-1.956083	0.964446	1.064208
C	-2.471158	2.190043	0.211529
O	-0.552906	1.025271	1.188715
C	-1.942595	3.471022	0.883652
H	-0.844229	3.436319	0.955323
H	-2.240606	4.368617	0.311023
H	-2.343092	3.569641	1.909399
C	-1.922238	2.081034	-1.220380
H	-2.118429	3.005084	-1.794871
H	-0.828419	1.907398	-1.193288
H	-2.384393	1.231740	-1.752023
C	-4.008588	2.238051	0.174386
H	-4.427894	1.372052	-0.365184
H	-4.432419	2.248012	1.196014
H	-4.350243	3.155405	-0.339831

H	-0.930335	-1.316415	3.578650
H	-0.476780	0.115421	4.572524
H	-1.509194	0.305909	3.096625
C	2.114350	-0.938524	3.438210
H	3.098860	-0.795645	2.960531
H	2.171498	-0.592896	4.486888
H	1.879234	-2.016624	3.429663
P	1.021667	2.125376	-1.242116
P	0.813448	-0.019976	2.466262
P	2.436783	-1.197025	-0.589811
C	-1.506558	0.914577	0.339316
C	-2.076527	1.994830	1.052122
C	-3.422201	2.381415	0.912747
C	-4.253604	1.690278	0.020791
C	-3.733266	0.600025	-0.694669
C	-2.395504	0.201333	-0.521406
H	2.258957	1.955744	2.349470
H	-1.456846	2.582431	1.748626
H	-3.815346	3.230984	1.485766
H	-5.295817	1.998224	-0.121635
H	-4.376874	0.065860	-1.405296
C	-1.815779	-1.001692	-1.265751
C	-2.178332	-2.394848	-0.616362
O	-0.415007	-0.881559	-1.343367
C	-1.488607	-3.489142	-1.453327
H	-0.400604	-3.317325	-1.479391
H	-1.685856	-4.491624	-1.030384
H	-1.857137	-3.478273	-2.495661
C	-1.654491	-2.437958	0.828086
H	-1.777019	-3.446596	1.264348
H	-0.578801	-2.176436	0.851856
H	-2.194053	-1.712689	1.459757
C	-3.697878	-2.636639	-0.621967
H	-4.224491	-1.914550	0.024443
H	-4.111749	-2.550977	-1.643982
H	-3.923928	-3.653989	-0.252220

### <sup>5</sup>I-6

Lowest frequency = 31.5223 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

66

Fe	0.417089	0.159150	-0.005940
C	0.549715	3.768749	-0.532694
H	1.225298	4.022818	0.302201
H	0.602243	4.566066	-1.295470
H	-0.479069	3.691177	-0.145183
C	-0.087254	2.005105	-2.713574
H	0.040707	2.869101	-3.389973
H	0.128699	1.062576	-3.241337
H	-1.126149	1.955500	-2.347837
C	2.656741	2.553394	-2.029699
H	3.007350	1.700541	-2.635122
H	2.581991	3.444711	-2.679332
H	3.404810	2.747735	-1.241363
C	4.199014	-0.698698	-0.272741
H	4.920606	-1.423326	-0.692190
H	4.381397	0.292008	-0.722280
H	4.368549	-0.616468	0.814910
C	2.441511	-1.499722	-2.413766
H	3.177720	-2.267243	-2.712962
H	1.417610	-1.804902	-2.684571
H	2.665669	-0.555584	-2.938065
C	2.438332	-2.934649	0.059807
H	3.258327	-3.539081	-0.368858
H	2.536283	-2.915932	1.158118
H	1.471057	-3.400512	-0.190317
C	1.298929	1.732060	2.846116
H	-2.234639	-1.029683	-2.298457
H	0.531963	2.408640	2.435496
H	1.400358	1.907951	3.932389
C	-0.668132	-0.246179	3.546424

### <sup>1</sup>TS(5-7)

Lowest frequency = -138.5329 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

66

Fe	-0.573607	0.149115	0.138958
C	-1.484763	2.718850	-1.992655
H	-1.171631	2.121978	-2.866350
H	-2.289490	3.414900	-2.292350
H	-0.608449	3.281310	-1.637633
C	-2.899159	2.660231	0.542957
H	-3.517474	3.420304	0.032598
H	-3.547431	2.033490	1.179859
H	-2.167874	3.160651	1.195729
C	-3.622497	1.000768	-1.541535
H	-4.206750	0.316123	-0.906791

H	-4.232579	1.894760	-1.760984
H	-3.387566	0.500371	-2.494541
C	-2.597798	-1.878192	2.269019
H	-2.681099	-2.234141	3.312365
H	-3.471355	-1.247330	2.030605
H	-2.607281	-2.749483	1.593198
C	-1.163526	0.218302	3.498839
H	-1.293809	-0.367322	4.426973
H	-0.241120	0.819115	3.563606
H	-2.014950	0.909518	3.379150
C	0.245055	-2.065228	2.609507
H	1.211201	-1.534400	2.633528
H	0.004013	-2.441852	3.620037
H	0.340235	-2.911286	1.912587
C	-0.694863	-1.417270	-2.922329
H	-0.893634	1.090988	1.220247
H	0.395689	-1.260711	-2.888266
H	-0.927420	-2.306082	-3.537023
C	-0.590858	-3.239123	-0.723738
H	-1.125854	-3.635387	0.155402
H	-0.715322	-3.948697	-1.560557
H	0.471397	-3.118886	-0.479902
C	-3.045567	-2.151518	-1.461193
H	-3.574809	-1.506771	-2.175409
H	-3.025764	-3.178207	-1.866548
H	-3.603595	-2.154414	-0.511113
P	-2.053017	1.526920	-0.676117
P	-1.291804	-1.579339	-1.171570
P	-1.047820	-0.873294	1.999258
C	0.749244	1.565974	0.169384
C	0.630415	2.955589	0.479582
C	1.707514	3.835149	0.504713
C	3.022679	3.369858	0.249220
C	3.220331	2.023443	-0.001319
C	2.119966	1.111493	-0.034626
H	-1.154436	-0.524020	-3.378099
H	-0.354559	3.372918	0.713576
H	1.538482	4.894541	0.733030
H	3.870982	4.062424	0.269551
H	4.237606	1.657502	-0.168436
C	2.196230	-0.294982	-0.219963
C	3.449983	-1.153159	-0.434213
O	1.049607	-0.897624	-0.172012
C	3.058442	-2.635322	-0.585644
H	2.403917	-2.788856	-1.459422
H	3.968362	-3.245724	-0.724692
H	2.528769	-3.001277	0.309288
C	4.180845	-0.715952	-1.729178
H	5.069142	-1.352756	-1.896090
H	3.512703	-0.822087	-2.601994
H	4.513810	0.332785	-1.687950
C	4.394314	-1.031208	0.789420
H	4.728366	0.004480	0.957277
H	3.880609	-1.371868	1.705614
H	5.289562	-1.663117	0.642072

### <sup>3</sup>TS(5-7)

Lowest frequency = -528.0344 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

66

Fe	-0.594050	0.129004	-0.042864
C	-1.418086	2.409748	-2.385125
H	-1.094003	1.706998	-3.171919
H	-2.171377	3.104028	-2.799351
H	-0.532015	2.964303	-2.040309
C	-2.919064	2.714440	0.077688
H	-3.564606	3.380033	-0.522955
H	-3.532361	2.202450	0.839175
H	-2.158946	3.316104	0.599955
C	-3.656675	0.805791	-1.812946
H	-4.331008	0.342966	-1.074749
H	-4.179951	1.654779	-2.287683
H	-3.412596	0.064035	-2.591212
C	-2.277428	-1.279212	2.915635
H	-2.172377	-1.358745	4.013019
H	-3.222475	-0.759065	2.681781
H	-2.328131	-2.294825	2.489596
C	-0.869467	1.150813	3.278642
H	-0.805748	0.863417	4.343293
H	-0.009759	1.789675	3.013349
H	-1.793694	1.730498	3.112443
C	0.609702	-1.234266	2.819303
H	1.500427	-0.628379	2.583155
H	0.538647	-1.392506	3.910323
H	0.715540	-2.199024	2.300901
C	-1.125870	-2.154595	-2.501068
H	-0.647035	1.333460	0.795060
H	-0.034714	-2.044312	-2.610232
H	-1.435903	-3.163914	-2.825726
C	-0.775666	-3.340626	0.065555
H	-1.117167	-3.427383	1.109954
H	-1.068787	-4.252898	-0.482945
H	0.314927	-3.209272	0.048964
C	-3.314305	-2.314511	-0.623234
H	-3.918684	-1.745413	-1.343092
H	-3.427964	-3.391628	-0.838237
H	-3.694109	-2.109879	0.391189
P	-2.105354	1.411876	-0.974029
P	-1.520041	-1.838467	-0.718480
P	-0.865023	-0.327595	2.157015
C	0.820509	1.571729	0.035725
C	0.740981	2.964044	0.182141
C	1.876683	3.807103	0.191693
C	3.151534	3.228542	0.074276
C	3.287333	1.847407	-0.062187
C	2.145865	0.979461	-0.091043
H	-1.618814	-1.397233	-3.133226
H	-0.239733	3.440145	0.305613

H	1.757377	4.890138	0.304413
H	4.047955	3.859331	0.093478
H	4.292514	1.426652	-0.151532
C	2.157485	-0.429434	-0.287631
C	3.377576	-1.311239	-0.585400
O	0.982611	-1.044912	-0.227628
C	2.934692	-2.774703	-0.785286
H	2.210307	-2.866336	-1.611188
H	3.815201	-3.399050	-1.021672
H	2.463080	-3.176490	0.127102
C	4.077859	-0.842816	-1.886676
H	4.957802	-1.478056	-2.101077
H	3.382388	-0.917240	-2.741314
H	4.416483	0.203252	-1.821995
C	4.371606	-1.280456	0.604672
H	4.744595	-0.265090	0.811972
H	3.881018	-1.652083	1.521589
H	5.242787	-1.928762	0.393558

H	2.452180	1.875643	2.360049
H	3.006414	3.160255	1.236962
H	1.253042	2.778882	1.388659
C	4.145742	0.680961	-0.000444
H	4.377419	0.073483	-0.890180
H	4.779733	1.585952	-0.001028
H	4.377608	0.074512	0.889948
P	0.844607	-0.889809	-2.102119
P	2.335808	1.102983	-0.000500
P	0.844479	-0.887645	2.103028
C	-1.033706	-1.268383	0.000589
C	-1.385316	-2.646454	0.001206
C	-2.709326	-3.087812	0.001346
C	-3.777013	-2.160316	0.000867
C	-3.495565	-0.798666	0.000242
C	-2.147929	-0.341960	0.000079
H	2.451826	1.873192	-2.361844
H	-0.582472	-3.392309	0.001585
H	-2.926879	-4.163113	0.001827
H	-4.814770	-2.510336	0.000981
H	-4.324747	-0.084893	-0.000136
C	-1.705757	1.034026	-0.000590
C	-2.572770	2.299039	-0.001063
O	-0.436417	1.188237	-0.000686
C	-1.664473	3.544723	-0.001610
H	-1.015099	3.564627	-0.892169
H	-2.287909	4.456310	-0.001920
H	-1.014973	3.565317	0.888841
C	-3.454252	2.337092	-1.275179
H	-4.053060	3.265864	-1.289582
H	-2.822829	2.321988	-2.180768
H	-4.146177	1.482194	-1.331451
C	-3.454058	2.338069	1.273160
H	-4.145945	1.483192	1.330208
H	-2.822490	2.323686	2.178660
H	-4.052889	3.266836	1.286933

### <sup>1</sup>I-7

Lowest frequency = 37.2115cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

66

Fe	0.701668	-0.398167	0.000235
C	-0.110496	0.201512	-3.266783
H	0.246370	1.240293	-3.182991
H	-0.032717	-0.133258	-4.316771
H	-1.169080	0.176427	-2.955075
C	0.236662	-2.546026	-2.676130
H	0.453946	-2.674817	-3.751122
H	0.744335	-3.338221	-2.102199
H	-0.847021	-2.631390	-2.505407
C	2.517697	-0.952922	-2.915963
H	3.128422	-1.699322	-2.380598
H	2.433827	-1.245617	-3.977734
H	3.028913	0.020182	-2.855639
C	2.517640	-0.950151	2.916772
H	2.433858	-1.241851	3.978824
H	3.128228	-1.697108	2.382029
H	3.028937	0.022852	2.855484
C	0.236475	-2.543312	2.678561
H	0.453868	-2.671195	3.753639
H	-0.847230	-2.628757	2.508031
H	0.744030	-3.336036	2.105255
C	-0.110418	0.204771	3.266854
H	-0.032372	-0.129006	4.317138
H	0.246368	1.243497	3.182018
H	-1.169078	0.179328	2.955440
C	2.268500	2.349638	-1.386219
H	1.531489	-1.699632	0.001015
H	1.252485	2.777032	-1.391268
H	3.005764	3.159174	-1.240172
C	2.268903	2.351111	1.383935

### <sup>3</sup>I-7

Lowest frequency = 32.5796 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

66

Fe	0.723153	-0.341408	0.000075
C	-0.250966	0.113791	-3.150186
H	0.078423	1.158863	-3.043046
H	-0.234800	-0.180313	-4.214538
H	-1.276173	0.035062	-2.751036
C	0.269844	-2.658129	-2.648609
H	0.454170	-2.776654	-3.730707
H	0.836334	-3.423955	-2.094081
H	-0.800328	-2.785565	-2.430774
C	2.459191	-0.938894	-2.999357
H	3.127847	-1.673567	-2.519477



H	2.343132	-1.197675	-4.066710
H	2.924998	0.055327	-2.922084
C	2.458624	-0.937926	3.000021
H	2.342359	-1.196363	4.067435
H	3.127382	-1.672749	2.520513
H	2.924436	0.056275	2.922512
C	0.269420	-2.657344	2.649318
H	0.453560	-2.775578	3.731479
H	-0.800710	-2.784865	2.431328
H	0.836028	-3.423298	2.095088
C	-0.251612	0.114673	3.150045
H	-0.235622	-0.179158	4.214476
H	0.077732	1.159740	3.042717
H	-1.276744	0.035782	2.750735
C	2.278468	2.386275	-1.391496
H	1.687104	-1.562353	0.000393
H	1.249478	2.780805	-1.378806
H	2.998817	3.212405	-1.256625
C	2.278175	2.386714	1.391042
H	2.462305	1.907921	2.365460
H	2.998357	3.212949	1.255925
H	1.249100	2.781022	1.378170
C	4.183752	0.718145	0.000208
H	4.407267	0.108181	-0.890536
H	4.829174	1.614564	0.000168
H	4.407100	0.108376	0.891126
P	0.823715	-0.979060	-2.117089
P	2.385026	1.160384	-0.000022
P	0.823325	-0.978399	2.117445
C	-1.034086	-1.259241	0.000085
C	-1.361825	-2.618487	0.000235
C	-2.700040	-3.081812	0.000246
C	-3.748725	-2.142870	0.000108
C	-3.475075	-0.774676	-0.000044
C	-2.122750	-0.293412	-0.000068
H	2.462532	1.907116	-2.365746
H	-0.553576	-3.360953	0.000366
H	-2.913736	-4.156833	0.000365
H	-4.790874	-2.483697	0.000119
H	-4.312169	-0.070157	-0.000147
C	-1.689913	1.060725	-0.000234
C	-2.555798	2.323172	-0.000442
O	-0.356709	1.258291	-0.000262
C	-1.659839	3.579081	-0.000580
H	-1.010408	3.606414	-0.891145
H	-2.292175	4.485511	-0.000721
H	-1.010470	3.606651	0.890023
C	-3.442096	2.367329	-1.272118
H	-4.069906	3.278265	-1.274694
H	-2.809607	2.383170	-2.177348
H	-4.107503	1.492053	-1.342426
C	-3.442203	2.367691	1.271145
H	-4.107603	1.492425	1.341661
H	-2.809793	2.383815	2.176425
H	-4.070030	3.278616	1.273397

### <sup>5</sup>I-7

Lowest frequency = 16.6704 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

66

Fe	0.800856	-0.624088	-0.000172
C	-0.292443	0.046985	-3.116519
H	-0.020625	1.097172	-2.929496
H	-0.293256	-0.161140	-4.201036
H	-1.294454	-0.124893	-2.689734
C	0.385869	-2.736586	-2.753416
H	0.475520	-2.827114	-3.850119
H	1.038848	-3.480185	-2.267468
H	-0.654210	-2.919358	-2.442698
C	2.482751	-0.845995	-3.127389
H	3.213532	-1.552132	-2.700235
H	2.353036	-1.050236	-4.204969
H	2.871446	0.175990	-2.998676
C	2.483015	-0.847336	3.126818
H	2.353381	-1.051890	4.204348
H	3.213751	-1.553364	2.699402
H	2.871720	0.174678	2.998356
C	0.386149	-2.737855	2.752201
H	0.475871	-2.828846	3.848860
H	-0.653945	-2.920532	2.441471
H	1.039119	-3.481229	2.265895
C	-0.292241	0.045551	3.116474
H	-0.293025	-0.163011	4.200907
H	-0.020459	1.095825	2.929882
H	-1.294254	-0.126186	2.689638
C	2.132852	2.530215	-1.401753
H	2.222416	-1.519552	-0.000553
H	1.078293	2.847766	-1.396767
H	2.794438	3.407233	-1.283335
C	2.132775	2.529624	1.402869
H	2.353804	2.043153	2.366599
H	2.794454	3.406636	1.284928
H	1.078251	2.847296	1.397891
C	4.144850	1.010807	0.000282
H	4.403428	0.411062	-0.888641
H	4.738738	1.942390	0.000496
H	4.403409	0.410668	0.888944
P	0.885673	-1.045838	-2.214674
P	2.320407	1.332198	0.000307
P	0.885880	-1.046868	2.214141
C	-1.093099	-1.272132	-0.000251
C	-1.436025	-2.625552	-0.000448
C	-2.785718	-3.058704	-0.000390
C	-3.800020	-2.081655	-0.000116
C	-3.491647	-0.719634	0.000076
C	-2.129793	-0.262715	-0.000005
H	2.354063	2.044186	-2.365663
H	-0.641240	-3.386520	-0.000644

H	-3.031000	-4.126479	-0.000553
H	-4.852775	-2.389017	-0.000065
H	-4.316439	-0.001435	0.000262
C	-1.662417	1.095240	0.000107
C	-2.558211	2.347770	0.000511
O	-0.361061	1.295757	-0.000194
C	-1.680073	3.615049	0.000680
H	-1.030967	3.651593	-0.889845
H	-2.322909	4.514291	0.000972
H	-1.030739	3.651188	0.891058
C	-3.440958	2.384373	-1.272953
H	-4.077028	3.289852	-1.278015
H	-2.804821	2.407952	-2.175747
H	-4.098952	1.504390	-1.350436
C	-3.440625	2.383813	1.274220
H	-4.098609	1.503805	1.351490
H	-2.804254	2.406987	2.176860
H	-4.076683	3.289296	1.279849

C	0.729989	-2.330854	2.523334
C	2.015417	-2.633400	2.047071
C	2.505940	-1.970663	0.910320
C	1.721361	-1.011596	0.248201
H	-4.029737	0.610721	0.974038
H	-1.088508	-1.214042	2.214845
H	0.347748	-2.826217	3.424212
H	2.634305	-3.378502	2.558869
H	3.505807	-2.216146	0.535562
C	2.168142	-0.183142	-0.937900
C	3.248849	0.916990	-0.616779
O	1.017559	0.476479	-1.451513
C	3.489345	1.722447	-1.909599
H	2.549285	2.175437	-2.262487
H	4.230494	2.523237	-1.732973
H	3.877483	1.069358	-2.712898
C	2.726165	1.850519	0.489439
H	3.448233	2.664572	0.681893
H	1.765184	2.300097	0.185172
H	2.562848	1.297219	1.430692
C	4.574885	0.275703	-0.169788
H	4.480837	-0.212116	0.814383
H	4.924324	-0.476807	-0.901035
H	5.357024	1.052193	-0.087024

### <sup>1</sup>I-8

Lowest frequency = 32.3353 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

53

Fe	-0.493867	0.406717	-0.534463
C	-2.769192	-2.235263	-0.012742
H	-3.446137	-1.696789	0.668167
H	-3.351787	-2.961046	-0.607155
H	-2.014994	-2.769113	0.586802
C	-1.013983	-2.239504	-2.257069
H	-1.692337	-3.005798	-2.673901
H	-0.539249	-1.671025	-3.073138
H	-0.217439	-2.724903	-1.668255
C	-3.301342	-0.472706	-2.214381
H	-2.901453	0.170466	-3.016860
H	-3.844263	-1.321320	-2.668379
H	-4.005320	0.124359	-1.609476
C	-3.266244	0.894413	1.718332
H	2.598504	-0.829979	-1.734361
H	-3.026193	0.009077	2.330231
H	-3.680336	1.680640	2.374577
C	-0.767142	2.137997	2.293649
H	0.096707	2.710797	1.919245
H	-1.385635	2.781250	2.945125
H	-0.380585	1.279933	2.868212
C	-2.389173	3.064994	0.101347
H	-3.109303	2.819656	-0.698300
H	-2.889024	3.698099	0.856527
H	-1.552446	3.628016	-0.346339
P	-1.896402	-1.050305	-1.139648
P	-1.728519	1.486335	0.845466
C	0.378063	-0.746553	0.673115
C	-0.076103	-1.409091	1.837601

### <sup>3</sup>I-8

Lowest frequency = 27.3357 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

53

Fe	0.557783	0.087882	-0.304736
C	4.041917	-0.571895	-1.252563
H	4.732995	-1.384732	-1.538783
H	3.953621	0.137896	-2.092820
H	4.462501	-0.031650	-0.387208
C	1.948413	-2.294598	-2.267582
H	2.709368	-3.076189	-2.441627
H	0.966433	-2.741080	-2.040456
H	1.845003	-1.668726	-3.169722
C	2.720523	-2.468612	0.490952
H	3.465998	-3.214039	0.161367
H	3.085331	-1.961639	1.399624
H	1.768376	-2.971140	0.728261
C	2.438030	2.995489	0.146862
H	-2.316578	-2.030145	-1.078883
H	1.817251	3.534970	-0.587817
H	2.836330	3.714891	0.884467
C	0.228399	2.678269	1.973275
H	-0.336310	1.991582	2.624998
H	0.754744	3.428300	2.590153
H	-0.491250	3.173818	1.303008
C	2.571877	1.078865	2.282072
H	3.458050	0.617942	1.814330

H	2.897685	1.902452	2.942626
H	2.059805	0.311907	2.887734
P	2.360046	-1.219588	-0.825914
P	1.410810	1.678999	0.960096
C	-1.107060	1.016414	-0.720254
C	-1.334875	2.346919	-1.132154
C	-2.593038	2.770761	-1.590973
C	-3.658503	1.859140	-1.645219
C	-3.461972	0.527468	-1.246328
C	-2.204374	0.107826	-0.780708
H	3.275092	2.520188	-0.391425
H	-0.511791	3.075844	-1.120169
H	-2.741464	3.807974	-1.915009
H	-4.639747	2.181478	-2.011995
H	-4.289276	-0.187393	-1.325607
C	-1.859589	-1.304723	-0.368065
C	-2.365773	-1.721690	1.064652
O	-0.446755	-1.436109	-0.421057
C	-1.818171	-3.131677	1.359407
H	-0.717064	-3.126901	1.322663
H	-2.143587	-3.475997	2.358330
H	-2.181167	-3.859762	0.610688
C	-1.841804	-0.733556	2.121246
H	-2.099743	-1.078532	3.139411
H	-0.742460	-0.645775	2.044854
H	-2.271888	0.272113	1.971700
C	-3.904080	-1.754556	1.104326
H	-4.333728	-0.746676	0.974943
H	-4.310459	-2.409094	0.310793
H	-4.252754	-2.148183	2.076740

C	-0.277101	3.003851	1.639910
H	0.587147	3.456531	1.128908
H	-0.790082	3.770537	2.247206
H	0.089427	2.185578	2.281196
C	-1.985200	3.776715	-0.550630
H	-2.788239	3.487268	-1.249528
H	-2.354335	4.570278	0.124254
H	-1.139300	4.166161	-1.142263
P	-2.030758	-1.669217	-0.823217
P	-1.420741	2.276577	0.386066
C	0.368232	-0.521398	1.033802
C	0.077805	-0.831975	2.381642
C	0.965959	-1.562614	3.191135
C	2.178810	-2.020850	2.656311
C	2.506802	-1.716746	1.324674
C	1.631219	-0.955192	0.530404
H	-3.727768	1.530073	0.765006
H	-0.877832	-0.512068	2.825895
H	0.704913	-1.788944	4.232675
H	2.865283	-2.615670	3.269541
H	3.447136	-2.093207	0.904109
C	1.940878	-0.571262	-0.916366
C	2.988158	0.597207	-1.077183
O	0.745792	-0.204694	-1.571975
C	3.143282	0.870821	-2.585967
H	2.164315	1.110945	-3.030853
H	3.838523	1.712686	-2.760887
H	3.546046	-0.018281	-3.105664
C	2.456283	1.855793	-0.373998
H	3.127464	2.717416	-0.545103
H	1.455383	2.108712	-0.769360
H	2.366862	1.689772	0.713405
C	4.356070	0.212458	-0.487088
H	4.309203	0.098161	0.608927
H	4.725995	-0.736090	-0.919136
H	5.100741	0.997283	-0.715027

### <sup>5</sup>I-8

Lowest frequency = 23.0840 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

53

Fe	-0.703003	0.234349	-0.505622
C	-2.873754	-2.336428	0.680615
H	-3.698356	-1.664031	0.973389
H	-3.275139	-3.350714	0.506923
H	-2.133733	-2.362519	1.497894
C	-0.814420	-2.988258	-1.240759
H	-1.306857	-3.965890	-1.387488
H	-0.277492	-2.679456	-2.151772
H	-0.082258	-3.046644	-0.418384
C	-3.329049	-1.876238	-2.132629
H	-2.893777	-1.606374	-3.109701
H	-3.705788	-2.914339	-2.175422
H	-4.171969	-1.193675	-1.928830
C	-2.914672	1.891452	1.417270
H	2.380969	-1.449754	-1.442946
H	-2.654805	1.088858	2.127570
H	-3.263272	2.777461	1.977839

### <sup>1</sup>TS(8-9)

Lowest frequency = -193.1189 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

53

Fe	0.621740	0.041265	-0.310990
C	4.428666	-0.338740	-0.508261
H	5.157823	-1.102000	-0.836133
H	4.660194	0.617019	-1.008677
H	4.525781	-0.191427	0.580630
C	2.826657	-1.256150	-2.707391
H	3.656035	-1.959341	-2.905372
H	1.872059	-1.705610	-3.027527
H	2.984359	-0.331784	-3.288559
C	2.564979	-2.516690	-0.127344
H	3.342668	-3.202057	-0.511074

H	2.667991	-2.419065	0.965919
H	1.556470	-2.906564	-0.342696
C	2.359812	2.634539	1.088551
H	-2.122100	-1.912937	-1.331950
H	1.980508	3.329496	0.320338
H	2.551929	3.197566	2.019916
C	-0.246951	2.233250	2.181240
H	-1.007343	1.530330	2.553278
H	0.148902	2.832739	3.020032
H	-0.725912	2.890120	1.437596
C	1.852875	0.374998	2.790983
H	2.795375	-0.105920	2.479219
H	2.055571	1.056652	3.636818
H	1.152709	-0.411701	3.118501
P	2.686501	-0.841761	-0.906583
P	1.104452	1.281068	1.349073
C	-0.913889	1.007220	-0.819423
C	-0.999951	2.360051	-1.224626
C	-2.196631	2.898637	-1.720945
C	-3.340687	2.090334	-1.833140
C	-3.283834	0.743255	-1.438638
C	-2.094356	0.208386	-0.917620
H	3.303496	2.195828	0.724262
H	-0.110515	3.005426	-1.169112
H	-2.236671	3.949510	-2.033444
H	-4.270651	2.504103	-2.238787
H	-4.170301	0.111598	-1.564732
C	-1.860858	-1.224388	-0.497995
C	-2.628415	-1.745342	0.766778
O	-0.457265	-1.362224	-0.270801
C	-2.150461	-3.184908	1.044281
H	-1.060141	-3.202582	1.201563
H	-2.650286	-3.593080	1.941742
H	-2.384802	-3.848849	0.191667
C	-2.299096	-0.850097	1.972583
H	-2.769662	-1.241711	2.892745
H	-1.206788	-0.810873	2.122703
H	-2.663511	0.178062	1.803929
C	-4.148608	-1.755178	0.525478
H	-4.551589	-0.733221	0.432069
H	-4.406591	-2.316752	-0.391535
H	-4.661924	-2.242745	1.374413

C	2.826658	-1.256150	-2.707390
H	3.656035	-1.959342	-2.905371
H	1.872060	-1.705610	-3.027527
H	2.984360	-0.331785	-3.288559
C	2.564979	-2.516689	-0.127344
H	3.342668	-3.202057	-0.511073
H	2.667990	-2.419063	0.965920
H	1.556470	-2.906564	-0.342695
C	2.359812	2.634539	1.088551
H	-2.122100	-1.912937	-1.331950
H	1.980508	3.329495	0.320338
H	2.551929	3.197567	2.019916
C	-0.246951	2.233250	2.181240
H	-1.007343	1.530330	2.553279
H	0.148902	2.832739	3.020032
H	-0.725912	2.890120	1.437596
C	1.852875	0.374999	2.790983
H	2.795375	-0.105920	2.479219
H	2.055572	1.056652	3.636817
H	1.152709	-0.411701	3.118502
P	2.686501	-0.841761	-0.906583
P	1.104452	1.281068	1.349072
C	-0.913889	1.007220	-0.819422
C	-0.999952	2.360051	-1.224626
C	-2.196632	2.898637	-1.720945
C	-3.340688	2.090334	-1.833139
C	-3.283834	0.743255	-1.438637
C	-2.094356	0.208386	-0.917620
H	3.303496	2.195828	0.724261
H	-0.110515	3.005426	-1.169111
H	-2.236671	3.949510	-2.033443
H	-4.270652	2.504103	-2.238787
H	-4.170301	0.111597	-1.564732
C	-1.860858	-1.224389	-0.497995
C	-2.628415	-1.745342	0.766778
O	-0.457265	-1.362224	-0.270802
C	-2.150461	-3.184908	1.044281
H	-1.060140	-3.202583	1.201563
H	-2.650285	-3.593080	1.941742
H	-2.384802	-3.848849	0.191666
C	-2.299095	-0.850097	1.972583
H	-2.769661	-1.241712	2.892746
H	-1.206787	-0.810873	2.122703
H	-2.663510	0.178062	1.803930
C	-4.148607	-1.755178	0.525478
H	-4.551589	-0.733221	0.432070
H	-4.406591	-2.316752	-0.391535
H	-4.661923	-2.242745	1.374414

### <sup>3</sup>TS(8-9)

Lowest frequency = -193.1192 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

53

Fe	0.621740	0.041265	-0.310991
C	4.428666	-0.338739	-0.508261
H	5.157823	-1.102000	-0.836132
H	4.660194	0.617019	-1.008677
H	4.525781	-0.191427	0.580630

### <sup>5</sup>TS(8-9)

Lowest frequency = -193.1193 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

53

**<sup>1</sup>H-9**Lowest frequency = 27.1307 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

53

Fe	0.621740	0.041265	-0.310990
C	4.428666	-0.338740	-0.508261
H	5.157823	-1.102000	-0.836133
H	4.660194	0.617019	-1.008677
H	4.525781	-0.191427	0.580630
C	2.826657	-1.256149	-2.707391
H	3.656035	-1.959341	-2.905372
H	1.872059	-1.705610	-3.027527
H	2.984359	-0.331784	-3.288558
C	2.564979	-2.516690	-0.127344
H	3.342668	-3.202057	-0.511074
H	2.667991	-2.419065	0.965919
H	1.556470	-2.906564	-0.342696
C	2.359812	2.634539	1.088551
H	-2.122100	-1.912937	-1.331950
H	1.980508	3.329496	0.320338
H	2.551929	3.197566	2.019916
C	-0.246951	2.233250	2.181240
H	-1.007343	1.530330	2.553278
H	0.148902	2.832739	3.020032
H	-0.725912	2.890120	1.437596
C	1.852875	0.374998	2.790983
H	2.795375	-0.105920	2.479219
H	2.055571	1.056652	3.636818
H	1.152709	-0.411701	3.118501
P	2.686501	-0.841761	-0.906583
P	1.104452	1.281068	1.349073
C	-0.913889	1.007220	-0.819423
C	-0.999951	2.360051	-1.224626
C	-2.196631	2.898637	-1.720945
C	-3.340687	2.090334	-1.833140
C	-3.283834	0.743255	-1.438638
C	-2.094356	0.208386	-0.917620
H	3.303496	2.195828	0.724262
H	-0.110515	3.005426	-1.169112
H	-2.236671	3.949510	-2.033444
H	-4.270651	2.504103	-2.238787
H	-4.170301	0.111598	-1.564732
C	-1.860858	-1.224388	-0.497995
C	-2.628415	-1.745342	0.766778
O	-0.457265	-1.362224	-0.270801
C	-2.150461	-3.184908	1.044281
H	-1.060141	-3.202582	1.201563
H	-2.650286	-3.593080	1.941742
H	-2.384802	-3.848849	0.191667
C	-2.299096	-0.850097	1.972583
H	-2.769662	-1.241711	2.892745
H	-1.206788	-0.810873	2.122703
H	-2.663511	0.178062	1.803929
C	-4.148608	-1.755178	0.525478
H	-4.551589	-0.733221	0.432069
H	-4.406591	-2.316752	-0.391535
H	-4.661924	-2.242745	1.374413

Fe	0.588730	0.336676	-0.591461
C	4.207687	-0.041359	-0.846294
H	4.988286	-0.785151	-1.086246
H	4.241580	0.767303	-1.596916
H	4.428363	0.398052	0.141820
C	2.501654	-1.697335	-2.458718
H	3.362449	-2.381449	-2.569306
H	1.558246	-2.266417	-2.502993
H	2.506214	-0.966373	-3.285237
C	2.722619	-2.226260	0.328505
H	3.539415	-2.901058	0.016682
H	2.917792	-1.860293	1.349110
H	1.760234	-2.762915	0.327537
C	2.101151	2.978459	0.697276
H	-1.931143	-2.065128	-1.259115
H	1.551020	3.609912	-0.021299
H	2.339480	3.581028	1.592059
C	-0.294950	2.308575	2.108378
H	-0.927880	1.531330	2.562570
H	0.126554	2.952967	2.900013
H	-0.923418	2.902212	1.426326
C	2.051514	0.730093	2.493353
H	3.031429	0.409932	2.103764
H	2.205952	1.443392	3.322482
H	1.517514	-0.156430	2.873706
P	1.052117	1.498482	1.131848
P	2.512415	-0.801378	-0.833886
C	-1.173658	1.042610	-0.796693
C	-1.593355	2.354480	-1.120638
C	-2.932611	2.644287	-1.426009
C	-3.890363	1.617990	-1.413331
C	-3.504258	0.306815	-1.089911
C	-2.166840	0.020792	-0.766391
H	3.038137	2.642417	0.223048
H	-0.859522	3.174671	-1.151893
H	-3.230000	3.668315	-1.683386
H	-4.934310	1.834550	-1.666498
H	-4.253359	-0.492399	-1.118675
C	-1.618044	-1.356843	-0.459201
C	-2.057657	-2.015461	0.897589
O	-0.195925	-1.292939	-0.508800
C	-1.349003	-3.379604	1.013578
H	-0.255296	-3.250771	1.005372
H	-1.638771	-3.887479	1.951625
H	-1.621981	-4.039236	0.169434
C	-1.634112	-1.113276	2.066769
H	-1.842255	-1.598978	3.037524
H	-0.553070	-0.902731	1.999180
H	-2.179036	-0.154171	2.032306

C	-3.580056	-2.240114	0.940063
H	-4.131109	-1.285608	0.967564
H	-3.926098	-2.816870	0.062317
H	-3.851272	-2.812312	1.846123

H	-2.143722	-3.475998	2.358190
H	-2.181205	-3.859773	0.610547
C	-1.841937	-0.733560	2.121113
H	-2.099947	-1.078530	3.139263
H	-0.742588	-0.645782	2.044797
H	-2.272008	0.272109	1.971533
C	-3.904146	-1.754566	1.104064
H	-4.333787	-0.746687	0.974650
H	-4.310473	-2.409108	0.310507
H	-4.252882	-2.148190	2.076458

### <sup>3</sup>I-9

Lowest frequency = 27.3342 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

53

Fe	0.557804	0.087880	-0.304708
C	4.041988	-0.571848	-1.252309
H	4.733103	-1.384670	-1.538480
H	3.953711	0.137926	-2.092581
H	4.462512	-0.031576	-0.386941
C	1.948586	-2.294634	-2.267398
H	2.709570	-3.076211	-2.441383
H	0.966604	-2.741134	-2.040318
H	1.845211	-1.668784	-3.169557
C	2.720571	-2.468570	0.491176
H	3.466092	-3.213971	0.161639
H	3.085316	-1.961567	1.399856
H	1.768436	-2.971137	0.728450
C	2.437994	2.995504	0.147027
H	-2.316499	-2.030162	-1.079042
H	1.817271	3.534971	-0.587710
H	2.836220	3.714917	0.884661
C	0.228231	2.678269	1.973279
H	-0.336510	1.991580	2.624972
H	0.754526	3.428312	2.590185
H	-0.491382	3.173801	1.302962
C	2.571701	1.078889	2.282249
H	3.457924	0.617995	1.814572
H	2.897436	1.902477	2.942837
H	2.059602	0.311911	2.887862
P	1.410724	1.679008	0.960186
P	2.360114	-1.219581	-0.825731
C	-1.107017	1.016404	-0.720337
C	-1.334810	2.346907	-1.132255
C	-2.592944	2.770743	-1.591162
C	-3.658401	1.859117	-1.645479
C	-3.461892	0.527446	-1.246574
C	-2.204323	0.107811	-0.780866
H	3.275110	2.520212	-0.391184
H	-0.511732	3.075837	-1.120213
H	-2.741353	3.807955	-1.915209
H	-4.639621	2.181449	-2.012323
H	-4.289186	-0.187419	-1.325909
C	-1.859560	-1.304734	-0.368196
C	-2.365837	-1.721698	1.064489
O	-0.446723	-1.436114	-0.421094
C	-1.818250	-3.131683	1.359283
H	-0.717141	-3.126907	1.322599

### <sup>5</sup>I-9

Lowest frequency = 24.7575 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

53

Fe	-0.520053	-0.058041	-0.224734
C	-1.806324	3.239267	-0.367114
H	-2.057380	4.175636	0.162496
H	-0.901474	3.390965	-0.978813
H	-2.639640	2.963546	-1.035938
C	-0.171107	2.560364	1.913333
H	-0.495065	3.503099	2.389076
H	0.068952	1.806747	2.681263
H	0.735898	2.728969	1.309497
C	-2.967245	1.908264	1.912304
H	-3.130208	2.912378	2.344880
H	-3.863662	1.615744	1.338459
H	-2.829649	1.182282	2.732112
C	-3.927655	-0.615027	-1.382101
H	2.331991	-0.314512	1.979009
H	-3.727745	-0.209164	-2.388379
H	-4.749944	-1.350357	-1.443480
C	-2.187748	-2.858313	-1.802566
H	-1.368322	-3.484570	-1.411945
H	-3.116349	-3.455043	-1.850549
H	-1.910492	-2.529049	-2.818407
C	-2.951829	-2.132199	0.875173
H	-3.264906	-1.329397	1.562802
H	-3.790920	-2.832994	0.716334
H	-2.100946	-2.661934	1.334688
P	-2.373916	-1.370712	-0.710663
P	-1.470376	1.853498	0.810270
C	1.100573	0.873721	-0.928648
C	1.392232	1.857492	-1.896256
C	2.645535	2.492342	-1.958170
C	3.638630	2.164497	-1.024099
C	3.383543	1.181580	-0.053246
C	2.142108	0.523980	-0.012368
H	-4.232126	0.219364	-0.728441
H	0.624342	2.146156	-2.628154
H	2.842410	3.252865	-2.723873
H	4.608449	2.674631	-1.046276

H	4.157644	0.938500	0.685226
C	1.838889	-0.571544	1.014790
C	2.389325	-1.992472	0.605711
O	0.439451	-0.666957	1.235702
C	1.957894	-2.986845	1.701418
H	0.860441	-2.988907	1.802406
H	2.301719	-4.009193	1.458490
H	2.388069	-2.704182	2.679919
C	1.783496	-2.416842	-0.743185
H	2.053706	-3.461614	-0.983229
H	0.679290	-2.347302	-0.699876
H	2.129418	-1.765727	-1.564085
C	3.924654	-1.979773	0.503467
H	4.271153	-1.328130	-0.316341
H	4.384569	-1.626000	1.445017
H	4.301110	-3.000840	0.308814

C	3.831350	-2.272382	-1.303849
C	3.011392	-1.217942	-0.859624
H	-2.009682	-1.991311	0.824812
H	0.033578	-2.912725	-0.789724
H	1.510444	-4.779635	-1.451549
H	3.958441	-4.373862	-1.825306
H	4.886053	-2.095080	-1.533406
C	3.448299	0.227013	-0.721146
C	4.634147	0.598186	0.238331
O	2.303463	0.989495	-0.349523
C	4.867990	2.118348	0.115918
H	3.950911	2.676212	0.360837
H	5.674267	2.442454	0.798683
H	5.163447	2.388559	-0.914518
C	4.266800	0.242279	1.686823
H	5.067314	0.553773	2.382134
H	3.332039	0.750173	1.976980
H	4.119935	-0.845858	1.793173
C	5.938415	-0.122214	-0.152472
H	5.892557	-1.201497	0.065056
H	6.168656	0.010109	-1.225740
H	6.781322	0.298713	0.425431
C	-0.484025	-0.177695	-2.032414
C	-1.546033	0.039154	-1.182297
H	-0.261751	-1.185984	-2.405714
H	-0.034645	0.643779	-2.611098
C	-2.861440	0.171875	-0.980592
C	-3.821099	0.163621	-2.211163
C	-3.110197	0.659929	-3.487348
C	-4.325036	-1.277580	-2.468010
C	-5.022096	1.104942	-1.958926
H	-2.671038	1.661454	-3.332438
H	-2.303151	-0.022590	-3.797682
H	-3.837028	0.724318	-4.316951
H	-4.893900	-1.675283	-1.612430
H	-4.984831	-1.301503	-3.355430
H	-3.470831	-1.951381	-2.654087
H	-5.675809	1.120742	-2.849205
H	-5.636994	0.784281	-1.101975
H	-4.681722	2.139175	-1.771145
C	-3.454323	0.339280	0.407438
C	-4.429059	-0.753598	0.892840
H	-3.973099	1.314371	0.483992
H	-2.606331	0.389395	1.106166
C	-4.741864	-0.626549	2.390470
H	-5.375139	-0.705169	0.322878
H	-4.005716	-1.754956	0.691227
C	-5.724053	-1.689349	2.894698
H	-3.796606	-0.693938	2.963118
H	-5.147730	0.384326	2.592084
H	-5.927075	-1.574062	3.973908
H	-6.689783	-1.624430	2.360962
H	-5.323491	-2.706905	2.733354

### <sup>1</sup>H-10

Lowest frequency = 20.1212 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe	0.644907	0.238212	-0.168519
C	-1.598212	3.153148	0.577392
H	-1.543301	4.255542	0.617762
H	-2.304003	2.849115	-0.211722
H	-1.970439	2.778363	1.544158
C	0.507532	3.392271	-1.322178
H	0.426254	4.482862	-1.166099
H	1.540830	3.120504	-1.590600
H	-0.166955	3.093268	-2.142979
C	1.114983	3.280420	1.471546
H	1.012295	4.378900	1.422287
H	0.829166	2.937014	2.479638
H	2.159753	2.990047	1.282382
C	-1.215147	-2.200603	1.553939
H	3.755974	0.590437	-1.728724
H	-0.662835	-3.093643	1.223517
H	-1.652971	-2.395955	2.548313
C	1.340898	-1.590322	2.579717
H	2.058366	-0.830553	2.922945
H	0.926066	-2.121815	3.454703
H	1.864287	-2.299726	1.920089
C	-0.721977	0.253758	3.015351
H	-1.621439	0.803977	2.700824
H	-0.972055	-0.378432	3.885959
H	0.047144	0.984594	3.315331
P	-0.026162	-0.775950	1.624881
P	0.066469	2.434197	0.201555
C	1.613020	-1.420470	-0.647985
C	1.109864	-2.722081	-0.887821
C	1.937451	-3.783350	-1.283443
C	3.305979	-3.558980	-1.492371

**<sup>3</sup>I-10**Lowest frequency = 16.1201 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	0.538435	0.106489	0.009682
C	-1.594131	2.487294	2.044990
H	-1.503073	3.469605	2.541636
H	-2.372103	2.546330	1.267824
H	-1.894989	1.734589	2.790152
C	0.289136	3.504872	0.169673
H	0.260186	4.443618	0.750260
H	1.274219	3.365628	-0.303132
H	-0.491834	3.530862	-0.608885
C	1.208839	2.341040	2.619702
H	1.085531	3.352742	3.045108
H	1.070362	1.594037	3.419387
H	2.221736	2.227545	2.204989
C	-0.976802	-2.939123	1.170594
H	3.512236	1.181588	-1.740650
H	-0.363232	-3.542159	0.484296
H	-1.204529	-3.534705	2.071934
C	1.492067	-2.201353	2.336100
H	2.096785	-1.445051	2.860058
H	1.220381	-3.007298	3.040904
H	2.088430	-2.611009	1.505263
C	-0.891279	-0.942132	3.208469
H	-1.915597	-0.595412	2.998377
H	-0.939630	-1.803656	3.897840
H	-0.338335	-0.124124	3.698516
P	-0.027084	-1.411595	1.628757
P	0.012760	2.027843	1.243313
C	1.541119	-1.232355	-1.015816
C	1.061483	-2.438003	-1.573222
C	1.862798	-3.234849	-2.406233
C	3.164715	-2.819934	-2.720994
C	3.650414	-1.607056	-2.210078
C	2.862157	-0.818885	-1.349949
H	-1.913159	-2.669511	0.660478
H	0.025754	-2.750240	-1.391340
H	1.463845	-4.166556	-2.825310
H	3.792248	-3.423611	-3.386277
H	4.641229	-1.260848	-2.520353
C	3.244577	0.562318	-0.850281
C	4.486449	0.666834	0.111785
O	2.118675	1.150531	-0.225686
C	4.680977	2.159124	0.448043
H	3.764420	2.580809	0.889287
H	5.516730	2.294082	1.158963
H	4.911192	2.738577	-0.464934
C	4.212425	-0.130115	1.395096
H	5.030829	0.000124	2.126556
H	3.270265	0.211302	1.854024
H	4.115992	-1.206435	1.171037

C	5.775666	0.147218	-0.550476
H	5.753712	-0.946391	-0.688247
H	5.941975	0.620683	-1.536019
H	6.646846	0.386293	0.086824
C	-0.362749	0.751231	-1.966734
C	-1.442886	0.685298	-1.131565
H	-0.195223	-0.026599	-2.723785
H	0.294895	1.628108	-2.019232
C	-2.753956	0.738376	-0.880083
C	-3.699667	1.359985	-1.952905
C	-3.043708	2.598977	-2.599364
C	-3.971935	0.308256	-3.054930
C	-5.034934	1.815639	-1.323980
H	-2.828500	3.369747	-1.837731
H	-2.097157	2.338666	-3.099602
H	-3.722457	3.038096	-3.352642
H	-4.464266	-0.589967	-2.645897
H	-4.626168	0.730203	-3.840531
H	-3.024107	-0.006050	-3.524802
H	-5.668920	2.280347	-2.099929
H	-5.604443	0.977533	-0.888929
H	-4.867766	2.567429	-0.532097
C	-3.340454	0.138248	0.381851
C	-4.122443	-1.171865	0.159748
H	-4.001962	0.858557	0.899407
H	-2.492513	-0.066131	1.056133
C	-4.619630	-1.798049	1.470266
H	-4.989684	-0.993389	-0.502011
H	-3.475271	-1.887728	-0.382702
C	-5.354600	-3.126826	1.263202
H	-3.760258	-1.954684	2.150508
H	-5.284957	-1.077213	1.984306
H	-5.708664	-3.547323	2.220768
H	-6.233491	-2.997332	0.605706
H	-4.693243	-3.875362	0.789755

**<sup>5</sup>I-10**Lowest frequency = 15.0744 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

84

scf done: -3119.206122

Fe	0.422445	0.006107	0.204202
C	-1.798835	-2.882558	-1.873949
H	-1.703118	-3.935244	-2.197450
H	-2.565624	-2.818632	-1.085039
H	-2.129962	-2.272554	-2.731021
C	0.133941	-3.498009	0.119535
H	0.077456	-4.528583	-0.274680
H	1.134330	-3.286705	0.528112
H	-0.614609	-3.368690	0.919656
C	0.989375	-2.777472	-2.523296
H	0.905231	-3.858396	-2.737800
H	0.793077	-2.213594	-3.451726



H	2.011408	-2.546449	-2.184927
C	-1.047442	2.963765	-1.575938
H	3.369310	-1.114247	1.776247
H	-0.486168	3.578199	-0.854186
H	-1.134492	3.513216	-2.530012
C	1.416057	1.958190	-2.596200
H	1.993460	1.093808	-2.959796
H	1.201954	2.640275	-3.438148
H	2.014549	2.473371	-1.827996
C	-1.011286	0.648590	-3.292285
H	-2.026605	0.317731	-3.021775
H	-1.076474	1.388805	-4.109424
H	-0.442643	-0.227043	-3.646618
P	-0.147373	1.363934	-1.811457
P	-0.190318	-2.239843	-1.196950
C	1.719114	1.511177	0.803059
C	1.494916	2.854381	1.169485
C	2.445374	3.599826	1.885494
C	3.637417	2.982545	2.291508
C	3.879379	1.642269	1.955952
C	2.951712	0.912494	1.185919
H	-2.051160	2.773842	-1.167130
H	0.539292	3.338966	0.922416
H	2.246283	4.645109	2.152215
H	4.371747	3.537030	2.887017
H	4.789597	1.161695	2.329063
C	3.154024	-0.564401	0.828162
C	4.364385	-0.890884	-0.130923
O	1.982690	-1.092100	0.247079
C	4.409239	-2.422749	-0.303695
H	3.445300	-2.798773	-0.679822
H	5.208057	-2.713135	-1.010586
H	4.611601	-2.919562	0.663100
C	4.130563	-0.215388	-1.491206
H	4.927965	-0.483674	-2.208043
H	3.159751	-0.534059	-1.904327
H	4.115059	0.883111	-1.383103
C	5.718200	-0.432301	0.441578
H	5.808071	0.666083	0.457965
H	5.872981	-0.812022	1.468587
H	6.538149	-0.825997	-0.186916
C	-0.264606	-0.345316	2.117985
C	-1.329903	-0.414770	1.220211
H	-0.141943	0.526733	2.776123
H	0.329909	-1.228535	2.393132
C	-2.655890	-0.574152	1.066853
C	-3.529153	-1.011059	2.279197
C	-2.838124	-2.155944	3.051615
C	-3.709629	0.196993	3.229689
C	-4.914883	-1.527071	1.831949
H	-2.694254	-3.036269	2.399832
H	-1.852029	-1.846586	3.432922
H	-3.458861	-2.463217	3.912790
H	-4.224595	1.032614	2.725968
H	-4.306652	-0.091088	4.115120
H	-2.727721	0.560795	3.577539

H	-5.490943	-1.851277	2.716900
H	-5.508096	-0.753482	1.316308
H	-4.820259	-2.396411	1.157098
C	-3.325003	-0.227225	-0.247165
C	-4.080482	1.117906	-0.217982
H	-4.028416	-1.018215	-0.568303
H	-2.530524	-0.169053	-1.010618
C	-4.686992	1.501745	-1.574678
H	-4.887407	1.084664	0.536906
H	-3.383634	1.906093	0.125766
C	-5.403186	2.856750	-1.553426
H	-3.888826	1.519396	-2.342142
H	-5.392855	0.709676	-1.891962
H	-5.836290	3.102096	-2.539007
H	-6.223774	2.861017	-0.813158
H	-4.706013	3.669835	-1.279533

### <sup>1</sup>TS(10-11)

Lowest frequency = -201.5236 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe	-0.415261	0.051784	-0.444982
C	1.603073	3.064874	-1.614165
H	1.548854	4.149360	-1.412994
H	2.574911	2.689592	-1.260032
H	1.535715	2.908463	-2.702177
C	0.267483	3.033602	0.913587
H	0.311957	4.133974	0.833864
H	-0.631138	2.712141	1.459151
H	1.158846	2.657358	1.439705
C	-1.199215	3.153052	-1.585031
H	-1.039150	4.245042	-1.546981
H	-1.260618	2.830182	-2.638511
H	-2.130869	2.878379	-1.071816
C	1.766360	-2.403719	-1.646839
H	-2.635789	0.067452	2.002494
H	2.289803	-2.766941	-2.548244
H	2.501095	-2.139770	-0.869310
C	-0.191494	-1.368295	-3.536772
H	-0.651061	-0.458613	-3.960715
H	0.457463	-1.836046	-4.298741
H	-1.001444	-2.058818	-3.254838
C	2.123588	0.079534	-2.882467
H	2.843952	0.469334	-2.148357
H	2.655440	-0.571616	-3.598337
H	1.684690	0.925490	-3.433631
P	0.776245	-0.872852	-2.026633
P	0.173965	2.238717	-0.748937
C	-1.682987	-1.496381	-0.247395
C	-1.665724	-2.756939	-0.907297
C	-2.832020	-3.461938	-1.209412
C	-4.076482	-2.957162	-0.806333

C	-4.124499	-1.750452	-0.091584
C	-2.966038	-1.016479	0.197018
H	1.136956	-3.213428	-1.248642
H	-0.707189	-3.207074	-1.176843
H	-2.765224	-4.415161	-1.746043
H	-5.000457	-3.500199	-1.030500
H	-5.097733	-1.376290	0.232700
C	-2.881920	0.303137	0.934841
C	-4.139029	1.236521	1.022923
O	-1.809012	1.013025	0.361772
C	-3.669877	2.582564	1.619673
H	-2.981092	3.104864	0.939063
H	-4.541423	3.235348	1.808824
H	-3.143649	2.426475	2.579110
C	-4.749819	1.495255	-0.367549
H	-5.535837	2.269794	-0.305573
H	-3.971801	1.847994	-1.065368
H	-5.199211	0.587223	-0.801410
C	-5.189167	0.655933	1.995127
H	-5.626639	-0.294390	1.651572
H	-4.740327	0.477451	2.989360
H	-6.018820	1.374415	2.124375
C	-0.334874	-1.378944	1.044116
C	0.808073	-0.481162	0.854226
H	-0.087719	-2.449617	0.991526
H	-0.977282	-1.172212	1.911817
C	2.005535	-0.299867	1.461291
C	2.402470	-1.044655	2.765357
C	1.189177	-1.270538	3.696019
C	3.010589	-2.426033	2.413898
C	3.432147	-0.223256	3.576925
H	0.639595	-0.327558	3.862072
H	0.485227	-2.012863	3.288808
H	1.533282	-1.651204	4.675110
H	3.916157	-2.324809	1.792679
H	3.285895	-2.982062	3.330629
H	2.280721	-3.034168	1.850894
H	3.687553	-0.760665	4.508039
H	4.371266	-0.055364	3.024254
H	3.018105	0.761722	3.857109
C	3.012695	0.645587	0.829502
C	4.304197	0.016828	0.265543
H	3.304900	1.452117	1.532597
H	2.491869	1.139136	-0.006485
C	5.212695	1.043102	-0.426337
H	4.877527	-0.479401	1.069826
H	4.039041	-0.782399	-0.452246
C	6.489087	0.427918	-1.010333
H	4.646261	1.548868	-1.234038
H	5.476742	1.838111	0.298102
H	7.122674	1.190354	-1.496911
H	7.091692	-0.058457	-0.221658
H	6.247875	-0.342580	-1.765553

### <sup>3</sup>TS(10-11)

Lowest frequency = -282.9032 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	-0.215212	-0.275351	0.236151
C	1.626839	-2.654968	2.381218
H	1.432613	-3.597091	2.924433
H	2.445347	-2.814104	1.661983
H	1.939699	-1.881127	3.102127
C	-0.227993	-3.551376	0.378784
H	-0.230376	-4.507447	0.931886
H	-1.211407	-3.373215	-0.085063
H	0.543954	-3.573469	-0.408845
C	-1.197135	-2.305964	2.784900
H	-1.245953	-3.345282	3.154747
H	-0.988979	-1.630806	3.631568
H	-2.147829	-2.012975	2.312213
C	0.972915	3.054134	1.383709
H	-2.760297	-1.120813	-1.698844
H	0.610801	3.520179	0.454916
H	0.880253	3.775695	2.214727
C	-1.698277	2.233083	2.052208
H	-2.367333	1.416952	2.368000
H	-1.668369	3.020360	2.826283
H	-2.090540	2.647214	1.108484
C	0.575221	1.142489	3.443199
H	1.616546	0.780893	3.391931
H	0.533089	2.027447	4.103369
H	-0.048325	0.342172	3.874092
P	-0.021830	1.529402	1.726756
P	0.100080	-2.106247	1.482903
C	-1.177003	1.192558	-1.174859
C	-0.691964	2.461476	-1.537936
C	-1.575784	3.510047	-1.827317
C	-2.958126	3.275079	-1.786785
C	-3.443475	1.993660	-1.475091
C	-2.573623	0.930128	-1.171451
H	2.032249	2.779757	1.254293
H	0.391099	2.628441	-1.595560
H	-1.187707	4.501468	-2.088554
H	-3.663526	4.082832	-2.009582
H	-4.524784	1.840070	-1.456591
C	-2.941982	-0.501195	-0.779430
C	-4.410721	-0.850229	-0.362490
O	-2.060637	-0.913763	0.239815
C	-4.417562	-2.341080	0.045581
H	-3.767780	-2.514526	0.916480
H	-5.444683	-2.663924	0.295974
H	-4.051877	-2.975728	-0.783040
C	-4.855247	-0.008866	0.847928
H	-5.856481	-0.322486	1.195734
H	-4.139280	-0.150277	1.675304
H	-4.895815	1.068419	0.614574

C	-5.387937	-0.704115	-1.548604
H	-5.545874	0.339178	-1.863197
H	-5.018255	-1.266185	-2.426018
H	-6.375655	-1.118835	-1.276319
C	0.147275	-0.244238	-2.052762
C	1.194247	-0.567108	-1.120381
H	0.318514	0.532801	-2.804694
H	-0.576983	-1.011722	-2.364545
C	2.537124	-0.742606	-1.176977
C	3.287105	-0.966979	-2.514530
C	2.484777	-1.913218	-3.434582
C	3.479685	0.391931	-3.234254
C	4.672105	-1.611375	-2.282155
H	2.311827	-2.884937	-2.938949
H	1.502242	-1.488944	-3.698213
H	3.037335	-2.094640	-4.374713
H	4.078475	1.087460	-2.622597
H	3.998279	0.251737	-4.201566
H	2.505889	0.870359	-3.435472
H	5.170493	-1.786570	-3.252592
H	5.335586	-0.968016	-1.679673
H	4.578428	-2.585329	-1.769673
C	3.324428	-0.599298	0.112040
C	4.065882	0.746796	0.251036
H	4.049958	-1.423162	0.259107
H	2.589000	-0.652435	0.933570
C	4.638333	0.970394	1.657413
H	4.885224	0.817055	-0.489273
H	3.357972	1.560144	0.001785
C	5.351996	2.317472	1.816881
H	3.815133	0.897190	2.395794
H	5.336398	0.146229	1.902178
H	5.751087	2.448082	2.838266
H	6.197368	2.405435	1.110379
H	4.663485	3.158593	1.614276

H	1.953648	2.923257	-1.183193
C	-0.643204	0.111526	3.615446
H	2.548385	-1.262652	-1.795714
H	-0.162658	-0.874814	3.707593
H	-0.504412	0.676016	4.554320
C	1.850768	1.265180	2.738851
H	2.373762	1.875596	1.985210
H	1.899617	1.759820	3.725056
H	2.347036	0.281154	2.783995
C	-0.641693	2.690733	2.373591
H	-1.708862	2.642091	2.100133
H	-0.544028	3.064919	3.408155
H	-0.139817	3.389163	1.684527
P	0.109760	1.009840	2.185525
P	-0.405074	2.440118	-1.230396
C	1.370103	-1.581815	0.787824
C	1.167151	-2.349845	1.949367
C	2.249163	-2.798515	2.720628
C	3.556840	-2.514346	2.302013
C	3.770338	-1.805013	1.106955
C	2.696505	-1.331868	0.332297
H	-1.720652	-0.033969	3.430267
H	0.143290	-2.605453	2.255880
H	2.072594	-3.373828	3.637273
H	4.414609	-2.856308	2.891007
H	4.800258	-1.615577	0.796025
C	2.771990	-0.531401	-0.976848
C	4.114928	0.145557	-1.409711
O	1.748087	0.441025	-0.940567
C	3.823060	0.932677	-2.707396
H	3.078888	1.723747	-2.532109
H	4.751012	1.395073	-3.090244
H	3.425649	0.262061	-3.491363
C	4.609925	1.129852	-0.333730
H	5.509144	1.669461	-0.682462
H	3.822636	1.872522	-0.119063
H	4.860686	0.620472	0.611722
C	5.192075	-0.905113	-1.756836
H	5.564851	-1.460037	-0.882284
H	4.795218	-1.642830	-2.478181
H	6.060637	-0.409606	-2.227412
C	-0.114226	-2.051588	-0.664913
C	-1.215988	-1.135002	-0.813328
H	-0.245031	-2.981924	-0.092576
H	0.575762	-2.177344	-1.514160
C	-2.544133	-1.190458	-1.068239
C	-3.265998	-2.493623	-1.496390
C	-2.475097	-3.187454	-2.627178
C	-3.344481	-3.441156	-0.272332
C	-4.700025	-2.234341	-2.004899
H	-2.398462	-2.529144	-3.510452
H	-1.451965	-3.441245	-2.304803
H	-2.978331	-4.123391	-2.932786
H	-3.920148	-2.979469	0.548524
H	-3.838305	-4.392719	-0.546192
H	-2.337174	-3.676166	0.110449

### <sup>5</sup>TS(10-11)

Lowest frequency = -289.3016 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

84

Fe	0.159123	0.036756	0.001294
C	-1.798922	3.671678	-1.338720
H	-1.632549	4.403611	-2.150360
H	-2.748023	3.141756	-1.525066
H	-1.890686	4.213238	-0.381293
C	-0.349177	1.790702	-2.960597
H	-0.335408	2.597431	-3.715650
H	0.561392	1.174716	-3.033664
H	-1.221559	1.135284	-3.122539
C	1.062843	3.570650	-1.204571
H	1.097843	4.239401	-2.083684
H	1.047262	4.185006	-0.287363

H	-5.166876	-3.188750	-2.309056
H	-5.339717	-1.785195	-1.225147
H	-4.703246	-1.563440	-2.882295
C	-3.351087	0.070033	-0.796819
C	-3.868264	0.148338	0.653710
H	-4.197032	0.191730	-1.497394
H	-2.671731	0.926900	-0.948065
C	-4.536807	1.486033	0.996530
H	-4.574121	-0.680595	0.856130
H	-2.999601	-0.014970	1.321614
C	-4.967442	1.587630	2.464397
H	-3.834337	2.308850	0.758449
H	-5.414473	1.638653	0.338741
H	-5.445066	2.559004	2.683594
H	-5.688061	0.790978	2.724398
H	-4.098894	1.479974	3.140830

C	-2.724843	2.027028	-1.370713
C	-2.179874	0.718135	-1.351959
H	2.186696	2.636804	0.291572
H	0.823305	1.490661	-2.842550
H	-0.214293	3.757691	-2.919705
H	-2.506458	4.098516	-1.938520
H	-3.720956	2.195940	-0.960840
C	-2.914718	-0.535663	-0.840349
C	-4.419809	-0.458802	-0.426089
O	-2.156955	-1.046075	0.230628
C	-4.825394	-1.907303	-0.064741
H	-4.210022	-2.282467	0.768146
H	-5.889867	-1.946741	0.228628
H	-4.681562	-2.582808	-0.927811
C	-4.636360	0.411717	0.828628
H	-5.668295	0.288038	1.203562
H	-3.936700	0.097687	1.620715
H	-4.477332	1.487071	0.646891
C	-5.299464	-0.000614	-1.606649
H	-5.119818	1.046146	-1.900457
H	-5.115454	-0.632914	-2.494608
H	-6.368202	-0.096700	-1.342326
C	-0.124714	-0.804716	-1.926056
C	0.851785	-0.689284	-0.741732
H	0.386284	-0.899353	-2.902282
H	-0.814375	-1.659274	-1.820930
C	2.177398	-1.011951	-0.756848
C	2.857214	-1.885033	-1.854550
C	1.981047	-3.103301	-2.236261
C	3.162117	-1.051141	-3.125401
C	4.190234	-2.483559	-1.340701
H	1.760770	-3.712333	-1.341819
H	1.022605	-2.818911	-2.693799
H	2.518299	-3.743630	-2.960560
H	3.828024	-0.203547	-2.892782
H	3.656281	-1.674396	-3.895324
H	2.238912	-0.639992	-3.568103
H	4.626848	-3.135244	-2.119189
H	4.938647	-1.711631	-1.097995
H	4.026728	-3.099906	-0.438874
C	3.069204	-0.412502	0.318779
C	4.008313	0.704825	-0.183520
H	3.686660	-1.170894	0.839927
H	2.397251	0.021513	1.077256
C	4.765155	1.411431	0.949791
H	4.744246	0.298270	-0.901688
H	3.409923	1.440119	-0.755109
C	5.676313	2.541941	0.458737
H	4.036009	1.817403	1.678426
H	5.362922	0.663630	1.506826
H	6.211068	3.026974	1.294607
H	6.433515	2.162217	-0.251425
H	5.092496	3.321049	-0.065249

## <sup>1</sup>H-11

Lowest frequency = 18.1904 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe	-0.552915	-0.095732	0.401904
C	1.413300	-1.883953	2.824070
H	1.265084	-2.709654	3.542239
H	2.186011	-2.172376	2.096050
H	1.752654	-0.989893	3.366754
C	-0.449664	-3.254806	1.190338
H	-0.378570	-4.051210	1.952038
H	-1.445813	-3.242770	0.723053
H	0.312480	-3.412151	0.409438
C	-1.413032	-1.539399	3.290549
H	-1.334780	-2.423443	3.948419
H	-1.276920	-0.624987	3.892657
H	-2.408611	-1.507184	2.819832
C	1.186071	3.015244	0.548503
H	-2.896988	-1.264115	-1.687514
H	0.674992	3.302310	-0.382926
H	1.282699	3.897841	1.205527
C	-1.300728	2.640476	1.881655
H	-1.959116	1.994418	2.486128
H	-1.028559	3.539574	2.464344
H	-1.849128	2.942839	0.975272
C	1.087980	1.617547	3.012821
H	2.092894	1.180887	2.895080
H	1.188667	2.637353	3.423924
H	0.513719	1.001692	3.724653
P	0.207761	1.665971	1.370829
P	-0.170518	-1.580696	1.916724
C	-0.870003	0.531982	-1.901225
C	-0.183233	1.650402	-2.440384
C	-0.757770	2.917077	-2.475184
C	-2.040208	3.107617	-1.926078

**<sup>3</sup>I-11**Lowest frequency = 26.8471 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	-0.393744	0.037450	0.380748
C	1.439839	-1.010301	3.295513
H	1.266304	-1.555983	4.240197
H	2.191175	-1.547215	2.695072
H	1.823268	-0.002254	3.523362
C	-0.617934	-2.674752	2.220183
H	-0.638765	-3.157847	3.213262
H	-1.620913	-2.711924	1.764965
H	0.100265	-3.200006	1.568545
C	-1.333033	-0.260502	3.580894
H	-1.381661	-0.916908	4.467869
H	-1.047423	0.755472	3.900878
H	-2.311851	-0.220389	3.076295
C	0.473436	3.463649	-0.407190
H	-2.553809	-1.876996	-0.633980
H	-0.098060	3.332372	-1.339983
H	0.407604	4.514932	-0.072912
C	-1.870355	3.022372	1.186452
H	-2.354779	2.454872	1.996990
H	-1.814241	4.092869	1.454540
H	-2.480669	2.894969	0.277986
C	0.741030	2.855150	2.368187
H	1.793596	2.539111	2.276199
H	0.701288	3.952614	2.491927
H	0.315915	2.376372	3.265574
P	-0.198411	2.294882	0.866647
P	-0.131396	-0.892277	2.322298
C	-0.647546	-0.535685	-1.899105
C	0.159869	0.229504	-2.783665
C	-0.312080	1.386729	-3.398523
C	-1.608576	1.842978	-3.102133
C	-2.399516	1.138298	-2.193324
C	-1.962604	-0.063960	-1.582909
H	1.526358	3.211341	-0.612602
H	1.177077	-0.120690	-2.985469
H	0.327137	1.938573	-4.095749
H	-1.997115	2.753730	-3.570738
H	-3.395382	1.515720	-1.957707
C	-2.777071	-0.789902	-0.497075
C	-4.342046	-0.744572	-0.520082
O	-2.276514	-0.337797	0.734988
C	-4.793742	-1.817964	0.497595
H	-4.386523	-1.588231	1.496225
H	-5.896024	-1.857212	0.563544
H	-4.431104	-2.819344	0.200610
C	-4.910509	0.607309	-0.042807
H	-5.984100	0.503894	0.197556
H	-4.374022	0.929662	0.864397
H	-4.826100	1.406255	-0.798387

C	-4.866979	-1.123224	-1.916482
H	-4.613525	-0.363248	-2.675112
H	-4.435676	-2.085814	-2.248767
H	-5.966564	-1.234779	-1.900112
C	0.025640	-1.777775	-1.280006
C	0.997689	-1.132359	-0.288478
H	0.501241	-2.375828	-2.080222
H	-0.715273	-2.433045	-0.788970
C	2.350091	-1.251647	-0.209148
C	3.189566	-2.361339	-0.900111
C	2.555132	-3.747715	-0.632614
C	3.297200	-2.124344	-2.427833
C	4.626878	-2.415959	-0.331071
H	2.498185	-3.938697	0.453759
H	1.535663	-3.826747	-1.040910
H	3.165708	-4.547938	-1.091430
H	3.744317	-1.138886	-2.643456
H	3.932590	-2.898769	-2.897957
H	2.309627	-2.161931	-2.916596
H	5.182505	-3.243812	-0.807871
H	5.187757	-1.485311	-0.521925
H	4.621617	-2.597387	0.758128
C	3.073792	-0.127683	0.518821
C	3.634395	0.936331	-0.447437
H	3.889091	-0.484880	1.176345
H	2.319360	0.369479	1.155103
C	4.303387	2.120263	0.263513
H	4.364347	0.477550	-1.141630
H	2.797811	1.294511	-1.078433
C	4.818238	3.194952	-0.700805
H	3.582395	2.574500	0.971191
H	5.139759	1.745771	0.885379
H	5.297714	4.031108	-0.161574
H	5.561915	2.775084	-1.402544
H	3.993406	3.613777	-1.306554

**<sup>5</sup>I-11**Lowest frequency = 14.0757 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

84

Fe	-0.121478	-0.570488	-0.167661
C	1.809289	-3.544217	-1.537337
H	1.700724	-4.403680	-2.223127
H	2.656218	-2.920468	-1.868927
H	2.034517	-3.914174	-0.522617
C	0.004112	-2.122681	-3.271151
H	0.031363	-3.022576	-3.911870
H	-0.977547	-1.628640	-3.363335
H	0.778839	-1.408082	-3.596936
C	-1.045847	-3.764492	-1.153402
H	-1.084914	-4.546362	-1.932847
H	-0.860967	-4.236435	-0.173293

H	-2.002447	-3.218858	-1.102744
C	0.452431	-0.033628	3.321385
H	-2.274084	0.944629	-1.588391
H	-0.258999	0.795730	3.174936
H	0.359505	-0.431741	4.347955
C	-1.552311	-1.950572	2.590553
H	-1.846492	-2.800649	1.954096
H	-1.544855	-2.259862	3.651090
H	-2.283949	-1.142702	2.433975
C	1.224476	-2.703681	2.584055
H	2.271915	-2.418220	2.393275
H	1.103007	-2.939858	3.656807
H	0.998705	-3.604172	1.987662
P	0.101191	-1.326844	2.046878
P	0.271203	-2.509821	-1.481252
C	-1.179977	2.252997	0.387886
C	-0.831538	3.065859	1.485101
C	-1.583029	3.079170	2.665476
C	-2.710779	2.253418	2.765874
C	-3.070141	1.439790	1.684147
C	-2.334986	1.424478	0.480933
H	1.471443	0.360552	3.171182
H	0.059056	3.699545	1.403324
H	-1.289256	3.726467	3.498987
H	-3.313402	2.242903	3.680720
H	-3.952139	0.803835	1.777321
C	-2.664317	0.461291	-0.665431
C	-4.162427	0.166276	-1.021501
O	-1.973701	-0.751275	-0.437785
C	-4.127598	-0.536701	-2.398320
H	-3.547241	-1.472356	-2.332803
H	-5.149305	-0.779041	-2.742173
H	-3.652088	0.108979	-3.159581
C	-4.842535	-0.798943	-0.028091
H	-5.750803	-1.234041	-0.483136
H	-4.148919	-1.617793	0.225592
H	-5.158641	-0.303719	0.905049
C	-4.944561	1.485800	-1.146827
H	-5.026319	2.004713	-0.176684
H	-4.444681	2.173152	-1.854297
H	-5.966531	1.297379	-1.523765
C	-0.247880	2.271707	-0.819514
C	0.776439	1.137967	-0.729069
H	0.208614	3.276091	-0.866010
H	-0.835689	2.157457	-1.750852
C	2.110311	1.241375	-1.013353
C	2.845993	2.493717	-1.571924
C	2.125641	3.033032	-2.833096
C	2.924140	3.596633	-0.485497
C	4.296201	2.178861	-2.012955
H	2.055040	2.241514	-3.600102
H	1.106279	3.387701	-2.622538
H	2.694464	3.878697	-3.263089
H	3.477271	3.233985	0.398156
H	3.447372	4.490035	-0.876166
H	1.923498	3.909258	-0.147246

H	4.768872	3.100269	-2.398972
H	4.920236	1.810459	-1.181481
H	4.320588	1.427873	-2.822022
C	2.960855	0.018254	-0.689945
C	3.691217	0.103437	0.663966
H	3.694878	-0.206974	-1.486996
H	2.281006	-0.854909	-0.630714
C	4.545602	-1.134383	0.967250
H	4.329186	1.006534	0.707570
H	2.923338	0.235948	1.450126
C	5.173016	-1.112358	2.365615
H	3.919491	-2.041667	0.853042
H	5.341524	-1.222817	0.202381
H	5.786889	-2.011314	2.552333
H	5.822209	-0.227374	2.495367
H	4.394580	-1.066802	3.149871

### <sup>1</sup>TS(11-12)

Lowest frequency = -317.8303 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe	-0.646459	-0.501759	-0.123884
C	1.372024	-3.040215	-1.694933
H	1.514715	-3.460485	-2.705981
H	2.327507	-2.628119	-1.341114
H	1.057664	-3.853118	-1.020861
C	0.527023	-0.800139	-3.268419
H	0.841744	-1.468047	-4.089313
H	-0.329366	-0.186993	-3.593601
H	1.345699	-0.117011	-2.992963
C	-1.297056	-2.873783	-2.419311
H	-0.912398	-3.453179	-3.277345
H	-1.607536	-3.557153	-1.613008
H	-2.174985	-2.291560	-2.722295
C	0.686100	-0.432269	3.030096
H	-1.347920	0.217746	-1.310783
H	-0.197939	0.145852	3.339416
H	1.077631	-0.999192	3.893423
C	-1.033021	-2.666857	2.444937
H	-1.352490	-3.426943	1.713512
H	-0.610807	-3.158853	3.339299
H	-1.917847	-2.077314	2.726557
C	1.659812	-2.710144	1.627185
H	2.536015	-2.239515	1.159961
H	1.913623	-2.994931	2.663346
H	1.405280	-3.620766	1.063376
P	0.208354	-1.551777	1.637685
P	0.021725	-1.752159	-1.763581
C	-1.303590	1.769685	1.057439
C	-1.194246	2.433741	2.299859
C	-1.962302	2.064918	3.406268
C	-2.835248	0.963433	3.317741

C	-2.940490	0.274360	2.112372
C	-2.221120	0.681784	0.957964
H	1.447730	0.275847	2.665125
H	-0.483378	3.263302	2.383689
H	-1.869662	2.620840	4.345544
H	-3.427529	0.654360	4.185528
H	-3.609402	-0.585136	2.008984
C	-2.560978	-0.097814	-0.329964
C	-3.666626	0.505547	-1.250378
O	-2.573664	-1.391291	-0.124198
C	-3.749564	-0.300681	-2.554916
H	-3.952032	-1.361574	-2.339295
H	-4.559323	0.092317	-3.194820
H	-2.802636	-0.226203	-3.118595
C	-5.000779	0.353149	-0.482257
H	-5.842314	0.672366	-1.122731
H	-5.159335	-0.699434	-0.192876
H	-5.011183	0.974902	0.429565
C	-3.436220	1.987875	-1.579827
H	-3.327263	2.597851	-0.666562
H	-2.534072	2.120931	-2.202479
H	-4.297505	2.380659	-2.149226
C	-0.368255	2.179299	-0.071974
C	0.593368	1.020904	-0.340795
H	0.139730	3.106082	0.246406
H	-0.950042	2.425962	-0.976541
C	1.907315	1.220471	-0.660313
C	2.544878	2.597558	-1.037719
C	1.642477	3.405710	-2.006758
C	2.848038	3.446386	0.223269
C	3.876939	2.406343	-1.809231
H	1.335798	2.775422	-2.860140
H	0.731734	3.795793	-1.530912
H	2.201152	4.273968	-2.403266
H	3.561950	2.928021	0.885760
H	3.288040	4.423151	-0.056295
H	1.934461	3.640949	0.809736
H	4.289243	3.396131	-2.076752
H	4.644315	1.878092	-1.220953
H	3.717488	1.845796	-2.747414
C	2.840798	0.024011	-0.646154
C	3.871439	0.006421	0.504124
H	3.387405	-0.100542	-1.602843
H	2.200659	-0.863006	-0.528654
C	4.908590	-1.117630	0.366615
H	4.406206	0.971244	0.566317
H	3.330195	-0.092258	1.464505
C	5.857161	-1.220445	1.565821
H	4.390219	-2.087052	0.222693
H	5.491544	-0.953695	-0.560640
H	6.603069	-2.023379	1.428932
H	6.405402	-0.272967	1.719675
H	5.298015	-1.433762	2.495459

### <sup>3</sup>TS(11-12)

Lowest frequency = -501.2520 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	-0.515274	-0.622493	0.041716
C	1.840192	-3.550789	0.022612
H	2.062540	-4.462587	-0.560389
H	2.716076	-2.883896	-0.003495
H	1.649157	-3.837862	1.069491
C	0.776149	-2.654321	-2.464725
H	1.155140	-3.628034	-2.823827
H	-0.119033	-2.368482	-3.040819
H	1.540794	-1.875542	-2.622418
C	-0.862455	-4.090801	-0.556386
H	-0.430802	-5.019694	-0.970144
H	-1.124265	-4.242954	0.503713
H	-1.783235	-3.833241	-1.097031
C	0.577686	1.257021	2.772008
H	-1.210303	-0.418453	-1.325211
H	-0.346527	1.845593	2.648917
H	0.891398	1.274526	3.831097
C	-1.052504	-1.018632	3.369499
H	-1.297040	-2.073248	3.163937
H	-0.711400	-0.903628	4.413760
H	-1.960895	-0.421475	3.200078
C	1.708186	-1.387842	2.847641
H	2.606762	-1.188302	2.246165
H	1.901990	-1.098881	3.895775
H	1.494626	-2.468305	2.809170
P	0.246504	-0.462219	2.177310
P	0.338789	-2.688119	-0.663814
C	-1.614781	2.154676	0.085884
C	-1.704968	3.347232	0.826909
C	-2.579057	3.478405	1.915312
C	-3.372836	2.387255	2.296211
C	-3.300972	1.194767	1.566814
C	-2.451719	1.064576	0.445213
H	1.354921	1.712635	2.137336
H	-1.047882	4.181425	0.554715
H	-2.622429	4.419270	2.474380
H	-4.046025	2.463389	3.157046
H	-3.907308	0.332224	1.859563
C	-2.458864	-0.297217	-0.260972
C	-3.499090	-0.478431	-1.409049
O	-2.301678	-1.319332	0.585490
C	-3.332011	-1.869244	-2.036543
H	-3.483422	-2.652941	-1.277669
H	-4.064790	-2.014273	-2.849760
H	-2.317732	-1.979546	-2.459063
C	-4.909956	-0.383367	-0.781415
H	-5.674839	-0.604737	-1.547267
H	-5.018975	-1.113716	0.038659
H	-5.108324	0.626088	-0.383426

C	-3.350145	0.601877	-2.492291	H	-1.567132	-2.881157	-3.008194
H	-3.422617	1.616460	-2.063301	C	-0.392825	-0.948998	3.319726
H	-2.378238	0.507558	-3.009492	H	-1.407120	-0.455245	-1.624000
H	-4.148895	0.493225	-3.247684	H	-1.408046	-0.579180	3.111383
C	-0.545622	2.028790	-0.984429	H	-0.372503	-1.521013	4.264615
C	0.483839	0.937606	-0.662371	C	-1.005179	-3.447073	2.004363
H	-0.076942	3.021174	-1.095424	H	-0.694382	-4.207477	1.266579
H	-1.023316	1.792268	-1.951967	H	-0.979628	-3.894082	3.014540
C	1.789345	0.997000	-1.068887	H	-2.023065	-3.107814	1.758053
C	2.382622	2.058045	-2.052268	C	1.715870	-2.695233	2.489998
C	1.452582	2.302978	-3.269404	H	2.436528	-1.881147	2.664837
C	2.648364	3.398247	-1.320555	H	1.569239	-3.250243	3.434532
C	3.721901	1.577074	-2.669088	H	2.143350	-3.377125	1.736094
H	1.139455	1.341882	-3.714118	P	0.114869	-1.980451	1.875167
H	0.546869	2.871163	-3.016194	P	0.447729	-2.235157	-1.792429
H	1.994594	2.879621	-4.041426	C	-1.403742	2.417295	0.236859
H	3.385775	3.267138	-0.510381	C	-1.277250	3.596514	0.994556
H	3.044167	4.155487	-2.024178	C	-1.943832	3.763315	2.214700
H	1.726792	3.801314	-0.868492	C	-2.736558	2.720689	2.714011
H	4.101836	2.351103	-3.359986	C	-2.870846	1.541703	1.972644
H	4.505289	1.395432	-1.916148	C	-2.238778	1.380982	0.719947
H	3.582594	0.649112	-3.251524	H	0.283644	-0.081001	3.397159
C	2.759887	-0.045775	-0.536087	H	-0.622078	4.392146	0.621143
C	3.801958	0.488191	0.470760	H	-1.827700	4.693605	2.781348
H	3.299184	-0.564547	-1.353321	H	-3.247540	2.822973	3.677715
H	2.154101	-0.812138	-0.023882	H	-3.479561	0.718407	2.358530
C	4.876667	-0.546790	0.832644	C	-2.489416	0.049215	0.014367
H	4.301946	1.390383	0.075048	C	-3.730158	-0.009199	-0.927187
H	3.275425	0.821838	1.384916	O	-2.285101	-1.002489	0.787156
C	5.848607	-0.060675	1.913179	C	-3.858291	-1.414842	-1.529786
H	4.391053	-1.484691	1.169130	H	-3.886181	-2.179593	-0.736693
H	5.437181	-0.815180	-0.084078	H	-4.776846	-1.489710	-2.138625
H	6.619982	-0.818210	2.138401	H	-2.984839	-1.616269	-2.172465
H	6.365207	0.863252	1.594983	C	-4.982938	0.259642	-0.051537
H	5.313499	0.166401	2.853560	H	-5.894498	0.124567	-0.660774

### <sup>5</sup>TS(11-12)

Lowest frequency = -349.2257 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

84

Fe	-0.473972	-0.625144	-0.237113
C	1.850165	-3.383326	-1.370810
H	2.178977	-3.967513	-2.249001
H	2.701274	-2.800180	-0.982771
H	1.517947	-4.081070	-0.583027
C	1.092852	-1.376706	-3.292900
H	1.402070	-2.094191	-4.073363
H	0.298953	-0.715426	-3.675704
H	1.948919	-0.748357	-2.999658
C	-0.762088	-3.438972	-2.504838
H	-0.274234	-4.118433	-3.226082
H	-1.212987	-4.029641	-1.689628

H	-1.567132	-2.881157	-3.008194
C	-0.392825	-0.948998	3.319726
H	-1.407120	-0.455245	-1.624000
H	-1.408046	-0.579180	3.111383
H	-0.372503	-1.521013	4.264615
C	-1.005179	-3.447073	2.004363
H	-0.694382	-4.207477	1.266579
H	-0.979628	-3.894082	3.014540
H	-2.023065	-3.107814	1.758053
C	1.715870	-2.695233	2.489998
H	2.436528	-1.881147	2.664837
H	1.569239	-3.250243	3.434532
H	2.143350	-3.377125	1.736094
P	0.114869	-1.980451	1.875167
P	0.447729	-2.235157	-1.792429
C	-1.403742	2.417295	0.236859
C	-1.277250	3.596514	0.994556
C	-1.943832	3.763315	2.214700
C	-2.736558	2.720689	2.714011
C	-2.870846	1.541703	1.972644
C	-2.238778	1.380982	0.719947
H	0.283644	-0.081001	3.397159
H	-0.622078	4.392146	0.621143
H	-1.827700	4.693605	2.781348
H	-3.247540	2.822973	3.677715
H	-3.479561	0.718407	2.358530
C	-2.489416	0.049215	0.014367
C	-3.730158	-0.009199	-0.927187
O	-2.285101	-1.002489	0.787156
C	-3.858291	-1.414842	-1.529786
H	-3.886181	-2.179593	-0.736693
H	-4.776846	-1.489710	-2.138625
H	-2.984839	-1.616269	-2.172465
C	-4.982938	0.259642	-0.051537
H	-5.894498	0.124567	-0.660774
H	-5.025339	-0.449903	0.793105
H	-4.988177	1.287101	0.348854
C	-3.664258	1.041506	-2.044912
H	-3.547746	2.060175	-1.635023
H	-2.811112	0.828704	-2.713803
H	-4.592511	1.018622	-2.644018
C	-0.518550	2.212498	-0.977010
C	0.499674	1.121511	-0.643905
H	-0.069801	3.185250	-1.237044
H	-1.120333	1.889287	-1.843231
C	1.853143	1.220056	-0.813236
C	2.601248	2.396776	-1.515628
C	1.992073	2.670956	-2.914298
C	2.545776	3.676259	-0.642570
C	4.096723	2.081075	-1.768602
H	2.049048	1.763368	-3.540490
H	0.938125	2.979970	-2.870912
H	2.559489	3.472609	-3.422928
H	3.048130	3.508922	0.325761
H	3.056600	4.514245	-1.153640
H	1.511287	3.984919	-0.428030



H	4.570046	2.945662	-2.268118
H	4.655763	1.891285	-0.837355
H	4.222272	1.206496	-2.431050
C	2.722761	0.116389	-0.228359
C	3.382582	0.497054	1.115411
H	3.511814	-0.202237	-0.936016
H	2.081038	-0.767107	-0.047000
C	4.545285	-0.427250	1.502572
H	3.752241	1.538383	1.079490
H	2.598369	0.490574	1.897395
C	5.089765	-0.163811	2.910703
H	4.221664	-1.483005	1.419826
H	5.357563	-0.305590	0.759429
H	5.941033	-0.825690	3.149196
H	5.434677	0.881192	3.013640
H	4.309175	-0.329427	3.676342

C	-2.965079	0.853060	1.946178
C	-2.223544	0.904088	0.737079
H	1.371509	1.069950	2.419139
H	-0.560015	3.831139	1.345427
H	-1.987208	3.789395	3.380682
H	-3.515977	1.836170	3.794150
H	-3.625979	-0.006525	2.093584
C	-2.560063	-0.221044	-0.264722
C	-3.623779	0.097967	-1.350007
O	-2.556587	-1.405959	0.274683
C	-3.685625	-1.039213	-2.379738
H	-3.880785	-2.001188	-1.880555
H	-4.492461	-0.846836	-3.108988
H	-2.732705	-1.108992	-2.932710
C	-4.982086	0.167807	-0.606465
H	-5.803141	0.300330	-1.333615
H	-5.160311	-0.763466	-0.042322
H	-5.009472	1.017122	0.097891
C	-3.381827	1.427644	-2.079051
H	-3.294312	2.272638	-1.374680
H	-2.464838	1.379916	-2.691342
H	-4.229074	1.638415	-2.756049
C	-0.364336	2.073028	-0.662669
C	0.604613	0.893317	-0.615363
H	0.144443	3.049506	-0.589990
H	-0.930655	2.074864	-1.609508
C	1.924754	1.008099	-0.946345
C	2.575751	2.255582	-1.629665
C	1.699274	2.802975	-2.786870
C	2.852589	3.383058	-0.603063
C	3.924434	1.887166	-2.301717
H	1.406172	1.982802	-3.465711
H	0.781241	3.299420	-2.442269
H	2.272129	3.546500	-3.371836
H	3.549735	3.040330	0.180519
H	3.301652	4.265599	-1.098312
H	1.926354	3.709733	-0.101059
H	4.346134	2.784910	-2.788933
H	4.676473	1.516953	-1.586740
H	3.784281	1.118030	-3.081768
C	2.852665	-0.150580	-0.628291
C	3.857920	0.109052	0.515159
H	3.420107	-0.498599	-1.514888
H	2.209126	-0.987659	-0.317710
C	4.873579	-1.028713	0.693957
H	4.411223	1.049812	0.343531
H	3.295589	0.266648	1.455177
C	5.797825	-0.834968	1.900877
H	4.337254	-1.994162	0.792080
H	5.476368	-1.118096	-0.230736
H	6.528705	-1.657963	1.991861
H	6.363293	0.111310	1.818946
H	5.217422	-0.793184	2.840964

## <sup>1</sup>H-12

Lowest frequency = 29.2837 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe	-0.653932	-0.522022	-0.064197
C	1.367059	-3.418986	-0.725645
H	1.546279	-4.123481	-1.556755
H	2.315934	-2.931541	-0.460536
H	0.999380	-3.989156	0.142547
C	0.656238	-1.735104	-2.934180
H	1.055722	-2.608307	-3.478562
H	-0.188450	-1.300647	-3.493497
H	1.430458	-0.958515	-2.833730
C	-1.256130	-3.447160	-1.610933
H	-0.833975	-4.272584	-2.210874
H	-1.646095	-3.834736	-0.656532
H	-2.087588	-2.981208	-2.152420
C	0.632361	0.487530	2.993299
H	-1.070209	-0.220572	-1.493212
H	-0.256577	1.118403	3.146343
H	1.053607	0.199880	3.972885
C	-1.087862	-1.819767	3.099037
H	-1.409580	-2.761332	2.625281
H	-0.657458	-2.026421	4.095023
H	-1.971956	-1.174596	3.203794
C	1.596627	-2.107782	2.328846
H	2.470945	-1.807816	1.735398
H	1.857736	-2.065835	3.400852
H	1.332985	-3.144828	2.070490
P	0.149508	-0.993207	1.996020
P	0.055156	-2.193752	-1.245375
C	-1.326079	1.991773	0.517701
C	-1.257467	3.000780	1.502765
C	-2.047662	2.970886	2.655309
C	-2.902226	1.878357	2.888062

**<sup>3</sup>I-12**Lowest frequency = 24.6176 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	-0.186118	-0.705496	-0.299731
C	2.453763	-3.250628	-0.035525
H	2.639331	-4.336896	-0.109896
H	3.092750	-2.728571	-0.765632
H	2.728544	-2.903646	0.971540
C	0.544709	-3.676209	-2.065823
H	0.963769	-4.697915	-2.036905
H	-0.513117	-3.721752	-2.363767
H	1.089912	-3.072509	-2.809884
C	-0.230002	-4.080644	0.642913
H	0.093186	-5.116313	0.437115
H	-0.069663	-3.856168	1.709955
H	-1.303393	-3.964344	0.423989
C	0.532231	1.187294	2.732117
H	0.119281	-0.553282	-1.780896
H	-0.279611	1.885794	2.479366
H	0.653758	1.145980	3.828782
C	-1.362098	-0.962638	3.035373
H	-1.749805	-1.919029	2.650467
H	-1.111050	-1.051367	4.106930
H	-2.144813	-0.201368	2.899305
C	1.423523	-1.479181	2.937487
H	2.425561	-1.237780	2.546953
H	1.402164	-1.254512	4.018503
H	1.239972	-2.556433	2.796845
P	0.124409	-0.480234	2.049586
P	0.680159	-2.861652	-0.409217
C	-2.055165	1.822713	0.507139
C	-2.588542	2.688221	1.483991
C	-3.721184	2.345559	2.233366
C	-4.340225	1.104606	2.021166
C	-3.815023	0.229991	1.063325
C	-2.684222	0.575655	0.291669
H	1.461180	1.546057	2.261864
H	-2.094167	3.651614	1.658978
H	-4.112455	3.040001	2.984719
H	-5.221851	0.816765	2.604225
H	-4.270347	-0.753253	0.910142
C	-2.152706	-0.445077	-0.684223
C	-2.724635	-0.420096	-2.131509
O	-1.904662	-1.637732	-0.140395
C	-2.181977	-1.602194	-2.947138
H	-2.407812	-2.556734	-2.443539
H	-2.645898	-1.612388	-3.949647
H	-1.088937	-1.516548	-3.062690
C	-4.265581	-0.573596	-2.032357
H	-4.699851	-0.623480	-3.047454
H	-4.534959	-1.502342	-1.499060
H	-4.726045	0.278565	-1.504743

C	-2.404448	0.895846	-2.860198
H	-2.835792	1.762047	-2.328751
H	-1.313516	1.034938	-2.947183
H	-2.839847	0.877885	-3.875850
C	-0.839377	2.254265	-0.282450
C	0.282338	1.241846	-0.500551
H	-0.457577	3.176148	0.188674
H	-1.195039	2.563782	-1.282039
C	1.548702	1.633092	-0.839583
C	2.042758	3.111612	-1.000132
C	1.136534	3.928647	-1.957808
C	2.129189	3.818156	0.377037
C	3.460207	3.184809	-1.624500
H	0.968831	3.372692	-2.896993
H	0.155107	4.169502	-1.525613
H	1.627409	4.887226	-2.209266
H	2.866731	3.315317	1.026973
H	2.448452	4.870582	0.254295
H	1.163111	3.818735	0.907425
H	3.771406	4.243343	-1.685102
H	4.218385	2.652397	-1.026804
H	3.476240	2.773933	-2.648825
C	2.600443	0.555780	-1.051994
C	3.544340	0.337289	0.150454
H	3.209533	0.769693	-1.949730
H	2.069696	-0.393690	-1.266348
C	4.846786	-0.393480	-0.201287
H	3.799289	1.307518	0.616923
H	2.991012	-0.226366	0.923701
C	5.684966	-0.763694	1.026917
H	4.614913	-1.307593	-0.780721
H	5.440995	0.246976	-0.881880
H	6.628551	-1.262677	0.743499
H	5.942577	0.134570	1.617616
H	5.129916	-1.449702	1.693798

**<sup>5</sup>I-12**Lowest frequency = 17.5204 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

84

Fe	-0.505924	-0.695389	-0.325106
C	2.147439	-3.425658	-0.893171
H	2.582510	-4.087932	-1.663148
H	2.931327	-2.750944	-0.511003
H	1.782199	-4.044286	-0.055390
C	1.462985	-1.698749	-3.095634
H	1.871213	-2.484960	-3.754635
H	0.672294	-1.134504	-3.614937
H	2.264353	-0.996233	-2.816229
C	-0.358365	-3.760528	-2.214491
H	0.217591	-4.480606	-2.822184
H	-0.831477	-4.289005	-1.369491

H	-1.153234	-3.307451	-2.827223
C	-0.235896	-0.441471	3.251712
H	-1.074871	-0.882320	-1.921820
H	-1.266249	-0.154578	2.992781
H	-0.188519	-0.813699	4.290882
C	-0.755384	-3.170257	2.460633
H	-0.412314	-4.051874	1.891223
H	-0.715908	-3.402321	3.540293
H	-1.786368	-2.931337	2.158314
C	1.926064	-2.252345	2.788942
H	2.627740	-1.404090	2.799324
H	1.781503	-2.607007	3.825936
H	2.375166	-3.064354	2.192964
P	0.311273	-1.718352	2.034261
P	0.729008	-2.415986	-1.561468
C	-1.655986	2.332814	0.166966
C	-1.646595	3.544124	0.882423
C	-2.369630	3.698037	2.072301
C	-3.104281	2.617167	2.579421
C	-3.121422	1.405369	1.878936
C	-2.422658	1.252687	0.662537
H	0.402997	0.451625	3.147365
H	-1.041738	4.375754	0.502498
H	-2.345312	4.652366	2.609566
H	-3.660869	2.715473	3.517888
H	-3.684881	0.553613	2.272776
C	-2.489167	-0.104163	-0.015012
C	-3.655199	-0.351522	-1.013208
O	-2.132462	-1.121076	0.757763
C	-3.648535	-1.813516	-1.484355
H	-3.705253	-2.504990	-0.627762
H	-4.508194	-1.997667	-2.153099
H	-2.713678	-2.015722	-2.032857
C	-4.981186	-0.097947	-0.244682
H	-5.835252	-0.345772	-0.900155
H	-5.043833	-0.736535	0.653892
H	-5.079884	0.955987	0.064200
C	-3.597514	0.593786	-2.223704
H	-3.592896	1.651999	-1.908023
H	-2.688340	0.389682	-2.815893
H	-4.482087	0.436444	-2.867186
C	-0.741550	2.149742	-1.028174
C	0.335292	1.123248	-0.680039
H	-0.342116	3.140301	-1.300304
H	-1.316145	1.781826	-1.894920
C	1.679122	1.295190	-0.874709
C	2.332256	2.469453	-1.671603
C	1.654290	2.621897	-3.057351
C	2.243392	3.795928	-0.874425
C	3.831170	2.216143	-1.972138
H	1.718187	1.672832	-3.617998
H	0.592590	2.897413	-2.989626
H	2.169591	3.404068	-3.645373
H	2.800844	3.718535	0.074957
H	2.679711	4.626780	-1.460576
H	1.204362	4.061574	-0.625847

H	4.234511	3.071699	-2.543262
H	4.439745	2.113277	-1.058643
H	3.974931	1.310407	-2.587233
C	2.635313	0.290794	-0.250281
C	3.336550	0.812660	1.023922
H	3.410645	-0.036579	-0.968832
H	2.058167	-0.610252	0.030194
C	4.577310	-0.006418	1.405828
H	3.634424	1.869055	0.893633
H	2.599656	0.815730	1.850049
C	5.185236	0.400314	2.752500
H	4.318589	-1.083097	1.423659
H	5.334774	0.104700	0.605389
H	6.090052	-0.188360	2.985495
H	5.467357	1.468946	2.753561
H	4.463604	0.249501	3.576711

### <sup>1</sup>TS(12-13)

Lowest frequency = -780.6367 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe	-0.627742	-0.525589	-0.063980
C	1.433690	-3.296133	-1.078182
H	1.582224	-3.938918	-1.963594
H	2.373709	-2.770188	-0.857635
H	1.172606	-3.936177	-0.221167
C	0.491108	-1.567542	-3.122807
H	0.781339	-2.422272	-3.759039
H	-0.362268	-1.041645	-3.579605
H	1.331405	-0.857901	-3.052225
C	-1.262698	-3.406010	-1.713557
H	-0.892188	-4.142287	-2.448609
H	-1.473164	-3.906797	-0.755032
H	-2.193931	-2.944890	-2.060162
C	0.621051	0.071083	3.096702
H	-0.227359	0.311828	-1.272500
H	-0.266373	0.701707	3.263467
H	0.977921	-0.328422	4.062953
C	-1.095109	-2.220068	2.886431
H	-1.418801	-3.092551	2.295438
H	-0.698007	-2.552692	3.862304
H	-1.971951	-1.573801	3.043100
C	1.622253	-2.420917	2.156993
H	2.498660	-2.064844	1.596895
H	1.878868	-2.482264	3.229606
H	1.363926	-3.429846	1.799261
P	0.172879	-1.281207	1.912433
P	0.024562	-2.113213	-1.408965
C	-1.414066	1.924306	0.882169
C	-1.475470	2.700904	2.060239
C	-2.360651	2.400632	3.098631
C	-3.184308	1.264381	3.005442

C	-3.119919	0.471243	1.861744
C	-2.284532	0.804457	0.762548
H	1.403433	0.698608	2.637538
H	-0.797337	3.556492	2.156532
H	-2.394077	3.037072	3.989712
H	-3.868511	1.007102	3.821325
H	-3.735049	-0.427547	1.757593
C	-2.433926	-0.131101	-0.463914
C	-3.357919	0.326220	-1.617407
O	-2.512212	-1.387371	-0.043771
C	-3.371289	-0.740007	-2.723116
H	-3.736179	-1.701367	-2.328305
H	-4.034077	-0.424369	-3.548651
H	-2.358632	-0.889294	-3.131991
C	-4.790890	0.453327	-1.042119
H	-5.506703	0.702541	-1.846788
H	-5.104821	-0.498209	-0.579496
H	-4.844644	1.246983	-0.276758
C	-2.936717	1.675557	-2.217829
H	-2.950749	2.476083	-1.458171
H	-1.923114	1.615232	-2.651798
H	-3.637411	1.966164	-3.021451
C	-0.366894	2.282365	-0.157306
C	0.558638	1.099707	-0.443713
H	0.203805	3.136412	0.236219
H	-0.864746	2.631498	-1.077645
C	1.879928	1.279667	-0.793886
C	2.545607	2.648163	-1.133232
C	1.651678	3.525024	-2.050370
C	2.904025	3.442365	0.150420
C	3.853473	2.439874	-1.941922
H	1.273724	2.932114	-2.901870
H	0.788093	3.962127	-1.529703
H	2.246229	4.365149	-2.453853
H	3.618910	2.882472	0.776343
H	3.364271	4.414967	-0.108624
H	2.011143	3.643022	0.766404
H	4.294162	3.424265	-2.181513
H	4.613999	1.863854	-1.391181
H	3.652374	1.920779	-2.895580
C	2.775935	0.058116	-0.808805
C	3.800214	0.011212	0.347918
H	3.319647	-0.067930	-1.765840
H	2.113825	-0.812721	-0.689636
C	4.750456	-1.192239	0.271814
H	4.407645	0.933747	0.369038
H	3.246462	-0.000783	1.305610
C	5.707143	-1.283121	1.465693
H	4.161676	-2.128259	0.201451
H	5.329378	-1.133553	-0.670346
H	6.389605	-2.146731	1.376284
H	6.325585	-0.370755	1.548575
H	5.147984	-1.391418	2.413287

### <sup>3</sup>TS(12-13)

Lowest frequency = -555.7832 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	-0.253737	-0.710442	-0.241433
C	2.474243	-3.199314	0.034279
H	2.681202	-4.281378	-0.045579
H	3.153174	-2.656538	-0.642191
H	2.674196	-2.867638	1.063378
C	0.728815	-3.642292	-2.120291
H	1.206013	-4.637827	-2.076151
H	-0.302108	-3.750199	-2.488489
H	1.283794	-3.000943	-2.825606
C	-0.208704	-4.095225	0.541510
H	0.147197	-5.120690	0.338052
H	-0.092585	-3.874112	1.615509
H	-1.276677	-3.998865	0.289940
C	0.577644	1.251763	2.659974
H	0.042297	-0.071722	-1.595612
H	-0.239972	1.927473	2.362717
H	0.699060	1.278772	3.757253
C	-1.298808	-0.883913	3.086932
H	-1.650048	-1.888034	2.801396
H	-1.050797	-0.853918	4.162617
H	-2.106957	-0.169547	2.871193
C	1.467900	-1.414532	3.012516
H	2.477189	-1.206014	2.621597
H	1.441089	-1.141258	4.082533
H	1.269680	-2.495329	2.919568
P	0.178695	-0.452408	2.063772
P	0.718938	-2.835512	-0.445838
C	-2.038246	1.894343	0.339176
C	-2.494555	2.884285	1.231439
C	-3.584639	2.661500	2.083705
C	-4.237771	1.421016	2.058952
C	-3.790207	0.424191	1.183286
C	-2.700387	0.644571	0.313524
H	1.503433	1.594396	2.171308
H	-1.973382	3.848977	1.259476
H	-3.915703	3.449906	2.768238
H	-5.087260	1.227887	2.723239
H	-4.273577	-0.557752	1.176519
C	-2.227097	-0.492152	-0.557696
C	-2.864347	-0.644999	-1.967010
O	-1.940204	-1.619697	0.096511
C	-2.192771	-1.800229	-2.722299
H	-2.276987	-2.736804	-2.147018
H	-2.669704	-1.944917	-3.708482
H	-1.121750	-1.579233	-2.873944
C	-4.361178	-0.991123	-1.757580
H	-4.843507	-1.190795	-2.731991
H	-4.465585	-1.892067	-1.128112
H	-4.902154	-0.160228	-1.273232

C	-2.763743	0.638482	-2.807230	H	-1.557297	-3.886211	-1.531066
H	-3.209317	1.500924	-2.281175	C	0.341606	0.629835	2.996595
H	-1.711490	0.869675	-3.046985	H	-0.274068	0.012466	-1.945042
H	-3.308627	0.507272	-3.759684	H	-0.646972	1.081986	2.815623
C	-0.862860	2.203650	-0.566339	H	0.521798	0.551846	4.083845
C	0.295269	1.208755	-0.640043	C	-0.945707	-1.934926	3.079031
H	-0.487691	3.195075	-0.272308	H	-0.930657	-2.994921	2.773997
H	-1.253673	2.327664	-1.592535	H	-0.813228	-1.862757	4.173188
C	1.576268	1.600849	-0.939469	H	-1.914160	-1.509832	2.777118
C	2.061920	3.072474	-1.139738	C	1.894887	-1.785782	2.966155
C	1.244255	3.801858	-2.238698	H	2.808175	-1.305155	2.583294
C	2.007620	3.865771	0.191732	H	1.862972	-1.675599	4.065521
C	3.534143	3.136443	-1.622729	H	1.939045	-2.859432	2.717813
H	1.228563	3.199888	-3.164337	P	0.387785	-1.027686	2.175611
H	0.202906	4.000079	-1.947878	P	0.549951	-2.723053	-1.120832
H	1.713366	4.776090	-2.471582	C	-1.813788	2.112268	0.452866
H	2.695765	3.421665	0.932272	C	-1.978735	3.133638	1.404563
H	2.316099	4.915864	0.029708	C	-2.799061	2.966126	2.530941
H	1.001067	3.873593	0.639491	C	-3.469656	1.749462	2.724018
H	3.837884	4.195439	-1.705454	C	-3.325998	0.724769	1.780858
H	4.232669	2.646251	-0.924739	C	-2.515169	0.891220	0.635547
H	3.659720	2.676802	-2.618062	H	1.099487	1.283693	2.534396
C	2.625551	0.513295	-1.083109	H	-1.423106	4.069536	1.272638
C	3.506510	0.307204	0.169960	H	-2.896362	3.774705	3.263364
H	3.281185	0.711737	-1.950756	H	-4.104699	1.600134	3.604205
H	2.098877	-0.437444	-1.306654	H	-3.849377	-0.227570	1.916066
C	4.850763	-0.374794	-0.116673	C	-2.376511	-0.266431	-0.320176
H	3.702152	1.279907	0.659319	C	-3.273744	-0.322826	-1.582234
H	2.928416	-0.283439	0.902231	O	-2.091401	-1.442030	0.242750
C	5.633276	-0.729039	1.152131	C	-2.898143	-1.544181	-2.435749
H	4.683816	-1.289941	-0.716838	H	-3.030771	-2.474722	-1.861885
H	5.457947	0.293548	-0.757989	H	-3.536645	-1.589693	-3.335864
H	6.609621	-1.187809	0.915837	H	-1.842851	-1.461391	-2.749519
H	5.822915	0.170787	1.765720	C	-4.725215	-0.498955	-1.060663
H	5.069368	-1.444407	1.779150	H	-5.417345	-0.625767	-1.912943

### <sup>5</sup>TS(12-13)

Lowest frequency = -796.8109 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

84

Fe	-0.385078	-0.635298	-0.167335	H	-5.051676	0.381506	-0.480606
C	2.088472	-3.508862	-0.441609	C	-3.210377	0.940409	-2.454206
H	2.334523	-4.441742	-0.979226	H	-3.442960	1.848474	-1.871677
H	2.934516	-2.808047	-0.529437	H	-2.208710	1.041806	-2.906839
H	1.938511	-3.737116	0.626254	H	-3.953174	0.863085	-3.268774
C	0.956360	-2.664905	-2.923157	C	-0.811743	2.281874	-0.673858
H	1.296848	-3.644138	-3.304606	C	0.260340	1.190515	-0.703071
H	0.064860	-2.332798	-3.478996	H	-0.355994	3.276746	-0.553015
H	1.745238	-1.909287	-3.075998	H	-1.341657	2.299691	-1.639096
C	-0.627762	-4.142759	-1.001751	C	1.603322	1.469046	-0.960404
H	-0.196169	-5.065376	-1.428656	C	2.153771	2.796308	-1.557629
H	-0.877718	-4.304756	0.059890	C	1.254938	3.306131	-2.715866
				C	2.284266	3.888766	-0.463678
				C	3.555664	2.602208	-2.192744
				H	1.044201	2.487043	-3.425500
				H	0.292209	3.709431	-2.371820
				H	1.773711	4.115150	-3.262463
				H	2.996324	3.575198	0.319386
				H	2.650711	4.837485	-0.900537
				H	1.318300	4.089866	0.028614

H	3.904901	3.567465	-2.601455
H	4.313054	2.258585	-1.469752
H	3.521111	1.879318	-3.026544
C	2.596583	0.344322	-0.741248
C	3.544162	0.562252	0.458383
H	3.205695	0.146169	-1.646085
H	2.023403	-0.585400	-0.549661
C	4.631707	-0.511400	0.595018
H	4.031017	1.551301	0.380655
H	2.934815	0.606744	1.380273
C	5.568331	-0.277042	1.785829
H	4.156674	-1.507089	0.688931
H	5.222111	-0.545741	-0.341282
H	6.342792	-1.061220	1.855429
H	6.080981	0.698255	1.700289
H	5.008706	-0.271760	2.739563

C	-2.889536	0.817731	1.976234
C	-2.176676	1.051049	0.767925
H	1.751091	0.436438	2.595994
H	-0.256889	3.657203	1.904222
H	-1.633828	3.307965	3.943417
H	-3.323311	1.444981	4.001026
H	-3.588659	-0.023630	1.978263
C	-2.450533	0.066170	-0.380200
C	-3.455871	0.463487	-1.487575
O	-2.567865	-1.163980	0.170377
C	-3.740564	-0.753214	-2.382907
H	-4.144988	-1.585240	-1.785062
H	-4.476694	-0.486541	-3.162761
H	-2.823293	-1.101513	-2.883513
C	-4.784364	0.880000	-0.807463
H	-5.554122	1.108260	-1.568025
H	-5.163301	0.064315	-0.167448
H	-4.646273	1.776692	-0.178335
C	-2.956732	1.628959	-2.356967
H	-2.832417	2.549795	-1.760872
H	-1.991047	1.381814	-2.832789
H	-3.688888	1.850537	-3.155032
C	-0.278051	2.344132	-0.424994
C	0.668177	1.186310	-0.667098
H	0.278694	3.264192	-0.205422
H	-0.872370	2.536586	-1.332132
C	2.004788	1.283475	-0.950527
C	2.782713	2.618517	-1.119776
C	2.074360	3.555817	-2.134564
C	2.956918	3.328276	0.247832
C	4.198103	2.392796	-1.711614
H	1.918404	3.030043	-3.092820
H	1.097281	3.920841	-1.788933
H	2.709201	4.439588	-2.328849
H	3.533316	2.695232	0.944088
H	3.500968	4.282678	0.120326
H	1.988673	3.547245	0.725918
H	4.702789	3.369717	-1.814386
H	4.835142	1.757974	-1.075883
H	4.147400	1.937186	-2.715538
C	2.786388	-0.006624	-1.066276
C	3.661068	-0.290199	0.174753
H	3.420179	-0.026417	-1.972176
H	2.056432	-0.826997	-1.150120
C	4.578962	-1.509753	0.019697
H	4.283504	0.590252	0.416023
H	2.987958	-0.425563	1.039139
C	5.428189	-1.783025	1.266313
H	3.970956	-2.404403	-0.217496
H	5.239601	-1.354901	-0.855555
H	6.084417	-2.659937	1.126355
H	6.069752	-0.915416	1.505839
H	4.790108	-1.976375	2.147810

### <sup>1</sup>H-13

Lowest frequency = 20.8065 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe	-0.686583	-0.536798	-0.007469
C	1.152584	-3.366422	-1.197196
H	1.147723	-4.065036	-2.052526
H	2.110534	-2.825358	-1.185571
H	1.065063	-3.946686	-0.266721
C	-0.070602	-1.737354	-3.137914
H	0.005685	-2.633152	-3.780179
H	-0.914694	-1.114443	-3.471525
H	0.853854	-1.142584	-3.236179
C	-1.634586	-3.461181	-1.369546
H	-1.444050	-4.213177	-2.155340
H	-1.648504	-3.952125	-0.382474
H	-2.604936	-2.971462	-1.511327
C	0.858586	-0.042730	3.031862
H	0.152898	0.260756	-1.165196
H	0.083984	0.731970	3.151025
H	1.110958	-0.467195	4.020787
C	-1.124044	-2.090594	2.908641
H	-1.611124	-2.894720	2.333436
H	-0.724082	-2.491579	3.857533
H	-1.882920	-1.322443	3.119963
C	1.501663	-2.666476	2.109560
H	2.401240	-2.474467	1.506877
H	1.786102	-2.729083	3.175362
H	1.078861	-3.638103	1.805136
P	0.214511	-1.335712	1.861034
P	-0.290962	-2.191384	-1.343086
C	-1.192292	2.078051	0.758440
C	-1.018497	2.869113	1.916867
C	-1.784595	2.669011	3.066445
C	-2.728142	1.624900	3.098980

**<sup>3</sup>I-13**Lowest frequency = 33.1550 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	0.018580	-0.335634	0.108944
C	3.449816	-2.232125	0.839101
H	4.019517	-3.128294	0.534397
H	4.075400	-1.340264	0.679083
H	3.220085	-2.309653	1.914252
C	2.558634	-2.399096	-1.837521
H	3.141945	-3.336485	-1.877801
H	1.739107	-2.447853	-2.572581
H	3.215164	-1.556732	-2.109644
C	1.181514	-3.780651	0.271024
H	1.982251	-4.541140	0.267786
H	0.702508	-3.738045	1.261691
H	0.412237	-4.063167	-0.462193
C	-0.250691	1.333947	3.258092
H	-0.041922	0.065440	-2.375105
H	-1.310436	1.074466	3.095825
H	-0.009822	1.251413	4.333225
C	0.636629	-1.341496	3.310394
H	1.362661	-2.105870	2.988751
H	0.809070	-1.109168	4.376191
H	-0.376520	-1.746237	3.161945
C	2.493417	0.744335	2.781607
H	2.696659	1.752755	2.387937
H	2.571815	0.766325	3.883545
H	3.258865	0.062809	2.379926
P	0.801070	0.175511	2.250718
P	1.862085	-2.103704	-0.137683
C	-2.911748	1.004220	-0.788151
C	-3.934668	1.952582	-0.619411
C	-4.800291	1.900582	0.482006
C	-4.640482	0.891725	1.444789
C	-3.652328	-0.084127	1.266341
C	-2.808377	-0.058868	0.137725
H	-0.093928	2.373620	2.931155
H	-4.028833	2.771115	-1.343902
H	-5.579831	2.660713	0.601816
H	-5.295340	0.858120	2.322725
H	-3.528741	-0.897047	1.990263
C	-1.839598	-1.178162	-0.109322
C	-2.310784	-2.274917	-1.138150
O	-1.148212	-1.607775	0.954490
C	-1.271673	-2.523977	-2.246639
H	-0.269681	-2.660961	-1.814681
H	-1.528797	-3.426394	-2.832403
H	-1.220326	-1.669921	-2.942985
C	-2.532898	-3.573563	-0.326210
H	-2.856599	-4.390101	-0.997266
H	-1.615975	-3.878066	0.197735
H	-3.317124	-3.421827	0.436062

C	-3.658396	-1.921027	-1.805047
H	-4.453682	-1.773594	-1.055990
H	-3.599069	-1.006364	-2.416418
H	-3.961202	-2.749989	-2.470830
C	-1.897643	1.131602	-1.913820
C	-0.427297	0.775511	-1.626820
H	-1.974135	2.152640	-2.331977
H	-2.207708	0.457803	-2.734837
C	0.610796	1.607772	-1.086317
C	0.331408	3.040662	-0.548116
C	0.178448	3.998743	-1.763136
C	-0.955553	3.126074	0.299970
C	1.487261	3.592425	0.313713
H	1.105604	4.049068	-2.360444
H	-0.639497	3.676277	-2.428935
H	-0.050429	5.021777	-1.412111
H	-1.096098	2.214168	0.900630
H	-0.908784	3.994734	0.980973
H	-1.852377	3.250879	-0.319311
H	1.218216	4.596668	0.687391
H	1.675478	2.943535	1.183815
H	2.425469	3.694263	-0.256028
C	1.997315	1.408933	-1.715239
C	3.210417	1.137577	-0.811738
H	2.225402	2.306008	-2.330372
H	1.927197	0.574183	-2.438042
C	4.523268	1.036559	-1.600905
H	3.318839	1.922917	-0.048091
H	3.016014	0.209516	-0.246236
C	5.753665	0.800245	-0.717691
H	4.445324	0.228612	-2.355790
H	4.663245	1.969785	-2.180928
H	6.681587	0.762057	-1.314944
H	5.865458	1.607196	0.029362
H	5.676045	-0.153045	-0.163774

**<sup>5</sup>I-13**Lowest frequency = 33.1550 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

84

Fe	-0.093972	-0.566010	0.030385
C	2.864171	-2.560103	1.266812
H	3.460742	-3.466753	1.061339
H	3.528296	-1.682089	1.247524
H	2.428593	-2.643047	2.275332
C	2.454687	-2.712202	-1.542782
H	3.015905	-3.661151	-1.471989
H	1.754872	-2.765215	-2.392700
H	3.162084	-1.888800	-1.732189
C	0.620899	-3.976027	0.263057
H	1.341745	-4.810340	0.327759
H	0.017330	-3.913381	1.181049

H	-0.069375	-4.150062	-0.576413
C	-1.190339	0.988197	3.102471
H	0.365806	0.275057	-2.111385
H	-2.175524	0.552298	2.874342
H	-1.060106	1.070378	4.196576
C	-0.164470	-1.621298	3.384258
H	0.658156	-2.338933	3.236538
H	-0.243067	-1.377128	4.458501
H	-1.098497	-2.082697	3.025055
C	1.657221	0.605010	3.082968
H	1.842613	1.596076	2.636325
H	1.586966	0.710309	4.180385
H	2.512172	-0.044372	2.833530
P	0.104777	-0.106352	2.356421
P	1.497973	-2.365966	0.014829
C	-2.477978	1.419434	-0.677286
C	-3.274123	2.526173	-0.331412
C	-4.297291	2.428413	0.623560
C	-4.537791	1.198836	1.255883
C	-3.765206	0.083750	0.912684
C	-2.748856	0.168909	-0.064019
H	-1.157356	1.989923	2.647930
H	-3.073217	3.493011	-0.809260
H	-4.892875	3.311014	0.880607
H	-5.329305	1.109965	2.008698
H	-3.939009	-0.886650	1.390829
C	-1.978823	-1.069470	-0.424788
C	-2.441489	-1.861751	-1.699668
O	-1.564962	-1.810614	0.624461
C	-1.259416	-2.160113	-2.642195
H	-0.445202	-2.659779	-2.092783
H	-1.571843	-2.822957	-3.471315
H	-0.852090	-1.232884	-3.081803
C	-3.044510	-3.196905	-1.203664
H	-3.371242	-3.810398	-2.063389
H	-2.308679	-3.761906	-0.611379
H	-3.920527	-3.011577	-0.557777
C	-3.536195	-1.114544	-2.489124
H	-4.422864	-0.925643	-1.861591
H	-3.185566	-0.143432	-2.875154
H	-3.849593	-1.725787	-3.355385
C	-1.346705	1.573134	-1.683800
C	0.075757	1.036233	-1.358566
H	-1.296719	2.637305	-1.970467
H	-1.645052	1.038889	-2.604680
C	1.207429	1.882525	-1.084408
C	1.138449	3.311319	-0.520580
C	0.883549	4.299476	-1.696205
C	0.041318	3.470394	0.549180
C	2.460549	3.756197	0.154279
H	1.678632	4.209247	-2.457696
H	-0.081659	4.105151	-2.191417
H	0.876724	5.344217	-1.331658
H	0.272483	2.828433	1.414319
H	-0.000000	4.517113	0.902693
H	-0.957897	3.192640	0.192094

H	2.360369	4.802637	0.494505
H	2.688646	3.138408	1.039875
H	3.324029	3.712369	-0.530722
C	2.552642	1.405827	-1.594399
C	3.504738	0.760755	-0.564126
H	3.090153	2.252188	-2.071512
H	2.385233	0.666035	-2.401680
C	4.863752	0.384977	-1.170945
H	3.664776	1.440559	0.289803
H	2.999693	-0.129154	-0.143899
C	5.832069	-0.270795	-0.180294
H	4.708073	-0.286294	-2.039093
H	5.326522	1.301788	-1.585665
H	6.814782	-0.465927	-0.644656
H	5.998163	0.376207	0.700464
H	5.441195	-1.237038	0.185813

### **<sup>1</sup>H-2'**

Lowest frequency = 17.7771 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

66

Fe	-1.006461	0.021233	-0.269600
C	0.440569	-0.416341	2.769783
H	0.966916	0.523836	2.537648
H	0.292281	-0.502205	3.860987
H	1.068416	-1.253728	2.424899
C	-1.921527	-1.987782	2.593619
H	-1.799509	-2.023975	3.691576
H	-2.998452	-2.033426	2.357393
H	-1.431677	-2.868247	2.144720
C	-2.093476	0.831998	2.887222
H	-3.116273	0.966942	2.501896
H	-2.138885	0.545917	3.953956
H	-1.562642	1.793349	2.786275
C	-4.494728	0.170311	0.181124
H	-5.446850	-0.117275	-0.300520
H	-4.475479	-0.255115	1.199166
H	-4.448895	1.268355	0.267446
C	-3.439670	-2.273916	-0.766887
H	-4.514006	-2.442799	-0.963178
H	-2.835580	-2.774408	-1.540862
H	-3.171440	-2.711982	0.206901
C	-3.584617	-0.049984	-2.501864
H	-4.574563	-0.494076	-2.708390
H	-3.648446	1.043502	-2.629711
H	-2.842634	-0.438767	-3.217996
C	0.429442	3.288879	0.220306
H	1.340136	2.672401	0.280377
H	0.587179	4.114164	-0.496948
C	-0.705240	1.360973	-1.828243
H	-1.435245	1.537400	-2.632689
H	0.326745	1.360915	-2.217985



H	-1.020192	-1.276596	-1.078993
C	-2.395743	3.365710	-0.377646
H	-2.733487	3.650158	0.634858
H	-2.118572	4.277925	-0.935169
H	-3.232798	2.870877	-0.896254
P	-1.185003	-0.433254	1.862043
P	-0.974300	2.183650	-0.276875
P	-3.015873	-0.461967	-0.779984
C	4.292274	-0.401203	0.710390
C	5.424610	0.400454	0.903074
C	5.553744	1.620526	0.222984
C	4.532626	2.044035	-0.642578
C	3.391147	1.255658	-0.820594
C	3.257516	0.015681	-0.154856
H	0.229823	3.713454	1.220846
H	6.209339	0.071350	1.592768
H	6.445201	2.239801	0.368267
H	4.626629	2.993567	-1.180444
H	2.590356	1.580432	-1.491871
C	1.988091	-0.749227	-0.333614
C	1.950279	-2.210881	-0.813804
O	0.936763	-0.081836	-0.194641
C	0.958666	-3.016038	0.052373
H	-0.000191	-2.469523	0.109028
H	0.780660	-4.007601	-0.400501
H	1.360944	-3.170627	1.070015
C	1.421770	-2.111391	-2.273480
H	1.273918	-3.127222	-2.682516
H	0.459882	-1.570876	-2.285028
H	2.148402	-1.580116	-2.913492
C	3.319970	-2.913895	-0.836816
H	4.076826	-2.328463	-1.386171
H	3.704500	-3.114319	0.177638
H	3.208311	-3.888479	-1.344536
H	4.196645	-1.339722	1.262598

H	2.823944	-2.297112	1.889947
C	4.259833	0.299908	-0.838635
H	4.965164	0.772584	-1.545798
H	4.540393	0.597739	0.185997
H	4.347309	-0.796572	-0.916632
C	2.706360	2.661804	-0.987143
H	3.593310	3.025615	-1.536534
H	1.803075	3.162418	-1.371802
H	2.809165	2.919106	0.079910
C	2.490115	0.708123	-3.028113
H	3.332611	1.273542	-3.463414
H	2.564723	-0.344359	-3.349045
H	1.537568	1.115482	-3.404485
C	-0.082614	-3.524324	0.052054
H	-1.012262	-3.096981	0.456681
H	-0.335796	-4.267788	-0.723816
C	-0.056998	-1.072585	-1.673178
H	0.238638	-0.913788	-2.720238
H	-1.148489	-1.138545	-1.538905
H	0.323203	1.036556	-1.170585
C	2.237300	-3.021472	-1.615190
H	2.964039	-3.480554	-0.922196
H	1.808488	-3.807211	-2.261801
H	2.771286	-2.289292	-2.241321
P	1.683621	-0.143971	1.914845
P	0.917184	-2.143945	-0.659020
P	2.496417	0.821971	-1.172145
C	-4.217300	0.257435	-0.714476
C	-5.198727	-0.714947	-0.912773
C	-5.086150	-1.993264	-0.334363
C	-3.956859	-2.276470	0.459691
C	-2.968757	-1.315763	0.657847
C	-3.053421	-0.008984	0.075050
H	0.473770	-4.021041	0.866129
H	-6.066598	-0.475491	-1.538455
H	-5.862309	-2.748876	-0.494233
H	-3.857414	-3.259835	0.935672
H	-2.104723	-1.521793	1.295139
C	-1.968643	0.913735	0.314156
C	-2.024762	2.434051	0.061786
O	-0.857796	0.422617	0.830493
C	-0.806277	3.097920	0.737333
H	0.131787	2.657670	0.363099
H	-0.807199	4.183095	0.528776
H	-0.835776	2.951542	1.831084
C	-1.960062	2.738478	-1.458313
H	-1.938654	3.831029	-1.631970
H	-1.044759	2.294739	-1.888796
H	-2.823992	2.322638	-2.002087
C	-3.298402	3.059817	0.682439
H	-4.225434	2.658741	0.244698
H	-3.330631	2.866053	1.769073
H	-3.293879	4.154917	0.527534
H	-4.336826	1.225908	-1.205360

### <sup>3</sup>I-2'

Lowest frequency = 17.3747 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

66

Fe	0.771256	0.010356	-0.159012
C	0.469520	-0.781323	3.153844
H	0.200052	-1.816303	2.884667
H	0.880798	-0.760252	4.178327
H	-0.437488	-0.161905	3.078707
C	2.266017	1.412938	2.735362
H	2.546852	1.242852	3.790166
H	3.137897	1.813254	2.190788
H	1.453877	2.156416	2.686091
C	3.114394	-1.283005	2.212355
H	3.988584	-0.971723	1.620165
H	3.389677	-1.305939	3.281586

**<sup>5</sup>I-2'**Lowest frequency = 18.4704 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

66

Fe	0.918935	0.032001	-0.611346
C	-1.195386	-0.497972	2.412997
H	-1.596277	-1.327057	1.808231
H	-1.238258	-0.754698	3.486585
H	-1.832134	0.378486	2.212513
C	0.984670	1.211128	3.090747
H	0.704493	0.930957	4.122069
H	2.069719	1.402331	3.057382
H	0.458247	2.139212	2.812597
C	1.446311	-1.572903	2.604909
H	2.518580	-1.493190	2.361979
H	1.318766	-1.636501	3.700412
H	1.056466	-2.493288	2.138760
C	4.549819	0.386815	1.405301
H	5.450222	1.027011	1.356070
H	4.105382	0.482323	2.410798
H	4.853228	-0.665782	1.267219
C	3.141317	2.665963	0.414283
H	4.134509	3.143243	0.494863
H	2.578156	3.113409	-0.420642
H	2.575332	2.846990	1.342163
C	4.394309	0.865388	-1.387200
H	5.271461	1.514746	-1.217564
H	4.744721	-0.156623	-1.611691
H	3.818308	1.237148	-2.250033
C	0.057187	-3.341373	-1.579030
H	-0.793634	-2.746349	-1.948517
H	0.438218	-3.991070	-2.385707
C	1.643557	-0.934884	-2.272225
H	2.663361	-0.779103	-2.648334
H	0.874863	-0.856595	-3.056360
H	1.392854	1.258051	-1.477445
C	2.863502	-3.137726	-0.685109
H	2.727002	-3.759837	0.216051
H	3.118320	-3.785356	-1.542130
H	3.691355	-2.433959	-0.498481
P	0.531758	-0.129417	1.886024
P	1.340551	-2.146229	-1.013161
P	3.282957	0.841328	0.098667
C	-4.496431	0.555632	0.309092
C	-5.529357	-0.265939	0.758903
C	-5.425075	-1.670521	0.717665
C	-4.237252	-2.235251	0.211581
C	-3.195810	-1.427451	-0.234512
C	-3.275259	0.010500	-0.212146
H	-0.289923	-3.960610	-0.734522
H	-6.438297	0.199555	1.158631
H	-6.244755	-2.304845	1.070691
H	-4.129624	-3.326047	0.162273

H	-2.278432	-1.871687	-0.625289
C	-2.116167	0.742013	-0.656661
C	-1.966506	2.243385	-0.979433
O	-1.017918	0.033864	-0.880103
C	-0.968660	2.857155	0.035095
H	-0.021596	2.282831	0.037367
H	-0.727265	3.903528	-0.228874
H	-1.393002	2.846141	1.055816
C	-1.360217	2.348855	-2.404198
H	-1.167902	3.408093	-2.656668
H	-0.411744	1.791668	-2.455840
H	-2.058904	1.933593	-3.152161
C	-3.257638	3.085184	-0.964130
H	-4.050582	2.629178	-1.580361
H	-3.646917	3.240592	0.055921
H	-3.034756	4.084161	-1.381009
H	-4.628981	1.633217	0.390543

**<sup>1</sup>TS(2'-4)**Lowest frequency = -794.0310 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

66

Fe	0.898716	-0.009795	-0.140831
C	0.270339	-1.210323	2.966613
H	-0.249508	-2.039289	2.459536
H	0.681681	-1.558165	3.930633
H	-0.459880	-0.403966	3.134353
C	2.422333	0.660670	2.960064
H	2.618982	0.251956	3.967791
H	3.375955	0.991386	2.515042
H	1.759685	1.538111	3.045210
C	2.817168	-1.998584	1.972149
H	3.725541	-1.776956	1.391467
H	3.094477	-2.202078	3.021986
H	2.341484	-2.893203	1.536881
C	4.401834	0.147264	-0.488487
H	5.203535	0.709918	-1.000406
H	4.603433	0.159892	0.596216
H	4.418757	-0.901565	-0.830459
C	3.083760	2.643641	-0.305360
H	4.041214	3.009896	-0.720271
H	2.263044	3.292279	-0.653893
H	3.117225	2.703459	0.795125
C	2.885141	1.118706	-2.671066
H	3.818749	1.653341	-2.919844
H	2.888730	0.140891	-3.181661
H	2.025320	1.699922	-3.044396
C	-0.633000	-3.174931	-0.848826
H	-1.518257	-2.636505	-0.474851
H	-0.878219	-3.676725	-1.802451
C	0.067126	-0.517476	-1.944499
H	0.513226	-0.282117	-2.922871
H	-1.036054	-0.459949	-1.983037

H	0.356865	0.847942	-1.293257
C	1.962479	-2.841302	-2.093117
H	2.497121	-3.586834	-1.477798
H	1.480348	-3.358610	-2.942095
H	2.703489	-2.120742	-2.475999
P	1.612821	-0.591165	1.846277
P	0.730783	-1.929807	-1.046430
P	2.717031	0.883568	-0.827341
C	-4.259328	0.607445	-0.702813
C	-5.441955	-0.124988	-0.846357
C	-5.602524	-1.364535	-0.206728
C	-4.547693	-1.867925	0.577423
C	-3.360065	-1.149997	0.712236
C	-3.180146	0.117458	0.085166
H	-0.347648	-3.938694	-0.103337
H	-6.246461	0.274770	-1.473991
H	-6.531728	-1.932473	-0.320779
H	-4.658463	-2.830745	1.089471
H	-2.541283	-1.534634	1.326169
C	-1.885854	0.793808	0.237870
C	-1.718761	2.329012	0.135434
O	-0.910471	0.054311	0.635219
C	-0.450804	2.744616	0.903196
H	0.429712	2.174111	0.540287
H	-0.264267	3.824373	0.768124
H	-0.559563	2.537601	1.982204
C	-1.609982	2.830386	-1.325501
H	-1.556355	3.935425	-1.343835
H	-0.696075	2.427521	-1.795213
H	-2.471859	2.519795	-1.939446
C	-2.912741	3.028516	0.841276
H	-3.871270	2.864061	0.325799
H	-3.021005	2.660066	1.876340
H	-2.728344	4.116992	0.879939
H	-4.158678	1.552016	-1.242448

H	2.773419	-2.452125	1.820975
C	4.259065	0.303548	-0.750139
H	4.981326	0.813368	-1.413110
H	4.534000	0.516301	0.297023
H	4.321851	-0.786022	-0.909405
C	2.753998	2.704734	-0.772976
H	3.654969	3.079236	-1.292197
H	1.867818	3.244958	-1.143936
H	2.845901	2.905290	0.307041
C	2.517752	0.890090	-2.920683
H	3.385903	1.448803	-3.312305
H	2.551170	-0.139419	-3.314191
H	1.588778	1.364573	-3.278875
C	-0.165622	-3.519216	-0.276227
H	-1.053052	-3.106830	0.227653
H	-0.491867	-4.131815	-1.135056
C	-0.108203	-0.913575	-1.712672
H	0.164790	-0.716207	-2.761097
H	-1.199295	-1.012802	-1.588619
H	0.152903	0.649115	-1.299820
C	2.080588	-2.937093	-1.985299
H	2.774747	-3.575451	-1.410517
H	1.551762	-3.559775	-2.728897
H	2.674655	-2.170993	-2.508858
P	1.651521	-0.295880	1.945000
P	0.897285	-2.103069	-0.820044
P	2.510314	0.877569	-1.057605
C	-4.199296	0.288842	-0.644854
C	-5.177474	-0.690406	-0.823853
C	-5.046104	-1.966653	-0.244709
C	-3.899830	-2.240779	0.527941
C	-2.914469	-1.273509	0.707412
C	-3.020203	0.033130	0.126261
H	0.389414	-4.157210	0.434135
H	-6.058363	-0.457603	-1.433656
H	-5.820043	-2.727721	-0.388517
H	-3.783271	-3.223895	1.000473
H	-2.032980	-1.477882	1.320426
C	-1.937906	0.963274	0.345016
C	-1.978545	2.470168	0.019038
O	-0.826950	0.495179	0.878296
C	-0.741689	3.144224	0.647207
H	0.180850	2.655329	0.296581
H	-0.715624	4.214525	0.373543
H	-0.764879	3.063472	1.747606
C	-1.918656	2.692611	-1.515275
H	-1.899126	3.773789	-1.749387
H	-1.001921	2.231848	-1.926075
H	-2.781246	2.244708	-2.035164
C	-3.235679	3.149199	0.616059
H	-4.174111	2.747573	0.203990
H	-3.263372	3.006835	1.710611
H	-3.210871	4.235662	0.410585
H	-4.336553	1.255915	-1.133680

### <sup>3</sup>TS(2'-4)

Lowest frequency = -667.3487 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

66

Fe	0.781131	-0.027318	-0.097757
C	0.412890	-0.983152	3.132359
H	0.129251	-1.995650	2.799298
H	0.809517	-1.030055	4.161859
H	-0.480924	-0.341789	3.083706
C	2.226445	1.218039	2.845470
H	2.485512	1.001098	3.897112
H	3.110448	1.637654	2.335994
H	1.417082	1.965768	2.811797
C	3.069084	-1.459767	2.200724
H	3.950957	-1.125139	1.633124
H	3.333008	-1.540149	3.270082

**PMe<sub>3</sub>**Lowest frequency = 180.2515 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

13

P	-2.028118	0.285559	-0.950517
C	-3.545409	-0.609243	-0.329721
H	-4.463776	-0.306259	-0.867098
H	-3.403162	-1.697584	-0.449961
H	-3.676564	-0.403221	0.747085
C	-2.236189	-0.021780	-2.780933
H	-3.249444	0.238810	-3.140630
H	-1.493923	0.575756	-3.338751
H	-2.042765	-1.087101	-2.997354
C	-2.670895	2.037513	-0.873672
H	-1.945336	2.714946	-1.357204
H	-3.652594	2.149451	-1.371381
H	-2.767995	2.345565	0.182190

**1**Lowest frequency = 18.8183 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

26

C	4.542702	0.375473	0.611838
C	5.634980	-0.500466	0.552858
C	5.458254	-1.822954	0.123824
C	4.179107	-2.267561	-0.247563
C	3.091401	-1.393354	-0.188276
C	3.250732	-0.056458	0.241865
H	6.629101	-0.145491	0.844294
H	6.314038	-2.505113	0.078863
H	4.032759	-3.299569	-0.583938
H	2.084774	-1.714274	-0.471894
C	1.993302	0.785598	0.259892
C	1.985112	2.272243	0.704270
O	0.939776	0.263372	-0.093209
C	0.537415	2.789716	0.589855
H	-0.143589	2.205882	1.229936
H	0.497974	3.848835	0.900160
H	0.168404	2.708315	-0.445297
C	2.431567	2.400866	2.182325
H	2.335914	3.454208	2.501423
H	1.786553	1.788708	2.836523
H	3.474324	2.090089	2.350190
C	2.880736	3.124283	-0.229767
H	3.945679	2.849338	-0.180711
H	2.553074	3.022871	-1.279104
H	2.791877	4.188845	0.051864
H	4.714282	1.398531	0.950204

**2**Lowest frequency = 40.1815cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

31

C	0.301671	0.161611	-1.190004
C	1.606723	0.011081	-1.104463
H	-0.232829	0.908524	-0.585936
H	-0.306594	-0.450760	-1.870800
C	2.913499	-0.161029	-1.011163
C	3.882024	0.661924	-1.899332
C	3.212938	0.983258	-3.252462
C	4.220175	1.996025	-1.188342
C	5.183019	-0.123901	-2.167990
H	2.964473	0.056306	-3.798077
H	2.279525	1.552937	-3.107691
H	3.893299	1.586663	-3.880067
H	4.710332	1.828068	-0.215280
H	4.902098	2.600729	-1.814556
H	3.300514	2.579539	-1.011080
H	5.839010	0.462178	-2.835964
H	5.746423	-0.324020	-1.240555
H	4.972980	-1.089699	-2.660657
C	3.442728	-1.160781	0.013792
C	4.152868	-0.540057	1.232459
H	4.133464	-1.866796	-0.485657
H	2.590226	-1.762325	0.374474
C	4.560862	-1.590124	2.275972
H	5.054493	0.012649	0.907762
H	3.481932	0.207404	1.697444
C	5.271182	-0.986877	3.493038
H	3.659146	-2.141776	2.606475
H	5.218525	-2.341388	1.796134
H	5.550255	-1.765104	4.224975
H	6.195152	-0.458910	3.193672
H	4.623108	-0.255184	4.009174

**TMS**Lowest frequency = 145.6760 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

17

Si	8.954168	3.357142	-0.056317
C	7.058745	3.357028	-0.056393
H	6.657877	4.387754	-0.056743
H	6.658014	2.841334	-0.948892
H	6.658035	2.841917	0.836450
C	9.585814	4.250855	1.491247
H	9.233732	3.752656	2.413698
H	10.691215	4.268298	1.520779

H	9.233184	5.298644	1.520793
C	9.586132	1.570188	-0.056146
H	9.234409	1.020588	-0.949067
H	10.691535	1.536074	-0.055478
H	9.233332	1.020471	0.836276
C	9.586007	4.250740	-1.603806
H	10.691405	4.267164	-1.633884
H	9.232997	3.753071	-2.526190
H	9.234337	5.298860	-1.632881

H	-3.442902	2.000231	0.825147
C	-2.067652	-0.104949	-0.520198
C	-3.521441	-0.481708	-0.821242
O	-1.152117	-0.868334	-0.986221
C	-3.546736	-1.771071	-1.666610
H	-3.077423	-2.610010	-1.126485
H	-4.592724	-2.041442	-1.895943
H	-2.999037	-1.635724	-2.613190
C	-4.293350	-0.740756	0.497106
H	-5.332578	-1.038026	0.267441
H	-3.822071	-1.559536	1.068157
H	-4.327187	0.148980	1.145420
C	-4.196836	0.654725	-1.630142
H	-4.231745	1.602059	-1.069152
H	-3.648828	0.837798	-2.570395
H	-5.232978	0.366382	-1.884155

**<sup>1</sup>I-6<sup>A</sup>**

Lowest frequency = 39.8766 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

53

Fe	0.648119	-0.327781	-0.679572
C	3.961450	0.607316	0.305318
H	4.185569	-0.399685	0.696966
H	4.884696	1.035960	-0.124140
H	3.634449	1.242298	1.145958
C	2.647375	2.224940	-1.641631
H	3.682481	2.577141	-1.797530
H	2.094764	2.236170	-2.594267
H	2.127318	2.896322	-0.939098
C	3.539856	-0.418096	-2.303546
H	2.919792	-0.447605	-3.214547
H	4.507077	0.065515	-2.530121
H	3.726019	-1.454857	-1.972947
C	1.617259	-0.784417	2.679911
H	0.630919	0.333369	-2.095151
H	0.989106	0.078123	2.956999
H	1.618864	-1.521774	3.501868
C	-0.631747	-2.271487	1.786303
H	-1.097816	-2.886912	0.999479
H	-0.456194	-2.884590	2.687886
H	-1.324362	-1.448308	2.032347
C	2.004900	-3.041117	0.943927
H	3.036025	-2.733931	0.698345
H	2.019308	-3.649269	1.866293
H	1.621654	-3.658106	0.112876
P	2.605815	0.495930	-0.975895
P	0.934538	-1.529042	1.126950
C	-0.122619	1.031968	0.313225
C	0.454161	2.063393	1.107826
C	-0.322619	3.028211	1.747681
C	-1.734370	3.014301	1.640769
C	-2.351281	2.012525	0.899506
C	-1.578311	1.017346	0.243126
H	2.644305	-0.425992	2.511702
H	1.543356	2.103410	1.230378
H	0.166109	3.809800	2.342506
H	-2.333649	3.781106	2.142197

**<sup>3</sup>I-6<sup>A</sup>**

Lowest frequency = 15.3596 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

53

Fe	0.783755	0.202769	-0.566868
C	3.311363	-1.935295	0.700129
H	2.509571	-2.483480	1.223791
H	4.119258	-2.639433	0.430673
H	3.713807	-1.171679	1.387661
C	4.072578	-0.352179	-1.581364
H	4.872847	-1.097998	-1.735374
H	3.775270	0.077784	-2.551986
H	4.453059	0.464151	-0.944476
C	2.255616	-2.565033	-1.879650
H	1.934594	-2.198826	-2.868271
H	3.145473	-3.211717	-1.985332
H	1.425260	-3.145577	-1.443148
C	2.910107	2.220387	1.444457
H	0.837479	0.203877	-2.139163
H	3.143069	2.873041	0.585754
H	2.996254	2.806116	2.377579
C	0.155135	2.995386	1.552144
H	-0.899492	2.676415	1.585659
H	0.431986	3.489188	2.500873
H	0.259716	3.708566	0.718190
C	0.987025	0.565550	2.805124
H	1.667838	-0.301150	2.809705
H	1.180340	1.194313	3.692799
H	-0.047034	0.184870	2.837835
P	2.575661	-1.102838	-0.790457
P	1.208039	1.509848	1.223725
C	-0.855731	1.120428	-0.953481
C	-1.088999	2.386545	-1.552110
C	-2.375752	2.862315	-1.800088
C	-3.510644	2.083971	-1.466440

C	-3.337422	0.839735	-0.873176
C	-2.029025	0.349066	-0.596569
H	3.646894	1.399509	1.462705
H	-0.229553	3.000914	-1.849220
H	-2.514877	3.842651	-2.272642
H	-4.517767	2.458073	-1.678990
H	-4.220297	0.243616	-0.624173
C	-1.702159	-0.873719	0.105219
C	-2.683349	-1.897035	0.695777
O	-0.454766	-1.102503	0.277669
C	-1.884179	-3.030556	1.370671
H	-1.244827	-2.640015	2.179381
H	-2.582857	-3.771703	1.798010
H	-1.228673	-3.539859	0.645279
C	-3.573867	-1.219852	1.768367
H	-4.246524	-1.969986	2.222401
H	-2.950429	-0.789189	2.571951
H	-4.192272	-0.410452	1.350417
C	-3.553646	-2.512034	-0.428776
H	-4.173226	-1.759127	-0.940375
H	-2.916307	-2.997406	-1.188166
H	-4.225906	-3.278690	-0.002550

P	3.022092	0.639584	-0.760052
P	0.847054	-1.884126	0.979828
C	-0.254159	1.170705	0.284124
C	0.288756	2.198790	1.086050
C	-0.507395	3.050535	1.865494
C	-1.904053	2.884330	1.880432
C	-2.488737	1.878698	1.107404
C	-1.683850	1.026329	0.310751
H	2.629399	-0.851365	2.295044
H	1.377793	2.344502	1.109906
H	-0.046654	3.845230	2.465274
H	-2.532791	3.537316	2.495349
H	-3.575016	1.758797	1.140957
C	-2.199801	-0.055103	-0.558042
C	-3.684331	-0.310907	-0.885688
O	-1.352021	-0.816430	-1.085614
C	-3.768631	-1.438448	-1.934476
H	-3.321610	-2.370617	-1.552844
H	-4.827058	-1.628988	-2.186330
H	-3.227119	-1.164794	-2.854408
C	-4.437044	-0.776666	0.387462
H	-5.482661	-1.020975	0.127134
H	-3.968985	-1.686127	0.803084
H	-4.454193	-0.011750	1.179562
C	-4.337302	0.961719	-1.479704
H	-4.349514	1.804250	-0.771276
H	-3.794292	1.287586	-2.383768
H	-5.380548	0.739913	-1.768407

### <sup>5</sup>I-6<sup>A</sup>

Lowest frequency = 22.6004 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

53

Fe	0.713311	-0.299480	-0.780669
C	4.190054	1.244192	0.568475
H	4.498357	0.391643	1.198396
H	5.094650	1.717551	0.143399
H	3.673203	1.975453	1.213126
C	2.893919	2.150129	-1.822971
H	3.885768	2.550743	-2.099588
H	2.330733	1.875380	-2.729891
H	2.319490	2.921598	-1.282494
C	4.171716	-0.426589	-1.745648
H	3.628634	-0.772548	-2.639729
H	5.087027	0.117416	-2.041162
H	4.453375	-1.309464	-1.145538
C	1.587028	-1.142660	2.504695
H	1.189512	-0.518517	-2.353312
H	1.020978	-0.231050	2.759262
H	1.565764	-1.847216	3.355277
C	-0.765581	-2.525940	1.621836
H	-1.281371	-3.068635	0.812699
H	-0.632917	-3.190322	2.494365
H	-1.390810	-1.663113	1.907796
C	1.835935	-3.438480	0.780775
H	2.869922	-3.170204	0.505123
H	1.848234	-4.044697	1.704741
H	1.406449	-4.034749	-0.041897

### <sup>1</sup>I-6<sup>E</sup>

Lowest frequency = 26.5472 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

53

Fe	-0.788841	-0.383601	-0.605246
C	-3.766224	0.426645	-2.147297
H	-4.562361	1.181467	-2.278117
H	-3.192310	0.327771	-3.083414
H	-4.232002	-0.548382	-1.920130
C	-2.118957	2.610912	-1.260113
H	-3.000811	3.260339	-1.404265
H	-1.477960	3.022485	-0.463552
H	-1.525755	2.563807	-2.187173
C	-3.822010	1.266716	0.572247
H	-4.573824	2.008422	0.246151
H	-4.339870	0.343321	0.880868
H	-3.279672	1.666886	1.445975
C	-0.915684	-3.346729	1.029168
H	-0.689912	0.155569	-2.058805
H	0.024787	-3.597441	0.511231
H	-0.969118	-3.891824	1.988312
C	0.416963	-1.246078	2.469830
H	0.392208	-0.200702	2.820006

H	0.345588	-1.924799	3.337723
H	1.370101	-1.412721	1.941626
C	-2.426489	-1.390195	2.448015
H	-3.351755	-1.657090	1.909846
H	-2.307075	-2.064052	3.315803
H	-2.523278	-0.352421	2.807235
P	-0.979789	-1.507776	1.283922
P	-2.594854	0.886607	-0.780600
C	0.923804	-1.108970	-0.975125
C	1.299325	-2.322130	-1.613621
C	2.637609	-2.664374	-1.814335
C	3.678865	-1.802526	-1.393193
C	3.364163	-0.598731	-0.770640
C	2.004847	-0.246063	-0.552652
H	-1.760566	-3.660992	0.391680
H	0.521503	-3.010648	-1.972720
H	2.890458	-3.609866	-2.310256
H	4.724656	-2.079628	-1.562406
H	4.174275	0.066691	-0.456164
C	1.496139	0.941318	0.086647
C	2.286332	2.109495	0.682312
O	0.215449	1.011851	0.164560
C	1.311935	3.146407	1.276565
H	0.676603	2.696110	2.057057
H	1.886217	3.976665	1.724186
H	0.648076	3.559386	0.499758
C	3.215348	1.600919	1.813483
H	3.773496	2.450820	2.245983
H	2.625987	1.132257	2.620289
H	3.944645	0.858821	1.453009
C	3.117537	2.792555	-0.433419
H	3.855105	2.107568	-0.880463
H	2.457362	3.153603	-1.240766
H	3.660121	3.659898	-0.015656

C	-1.590394	-3.231447	0.845139
H	-1.107866	-0.550696	-2.054230
H	-0.869042	-3.670467	0.137259
H	-1.655235	-3.865641	1.747584
C	0.525790	-1.823918	2.198999
H	0.939215	-0.853725	2.522898
H	0.353244	-2.463860	3.082479
H	1.257303	-2.297410	1.524398
C	-2.194947	-1.079295	2.642330
H	-3.222319	-1.000856	2.246904
H	-2.176322	-1.828736	3.454650
H	-1.906623	-0.095901	3.051747
P	-1.035164	-1.515143	1.254408
P	-2.672919	1.059308	-0.722290
C	0.821031	-1.074499	-0.973704
C	1.070399	-2.349407	-1.548340
C	2.362278	-2.815600	-1.792455
C	3.488812	-2.014782	-1.485723
C	3.302370	-0.759013	-0.920878
C	1.990219	-0.281985	-0.640350
H	-2.577536	-3.186912	0.355076
H	0.218108	-2.975610	-1.839675
H	2.510293	-3.803003	-2.247147
H	4.499344	-2.378708	-1.699770
H	4.178351	-0.143370	-0.696033
C	1.654656	0.941366	0.053225
C	2.624523	1.974358	0.644417
O	0.402870	1.158131	0.220964
C	1.813241	3.092075	1.331030
H	1.183081	2.685774	2.139273
H	2.503421	3.839464	1.761250
H	1.147478	3.597708	0.612536
C	3.536066	1.308394	1.706047
H	4.206777	2.066404	2.149737
H	2.928864	0.872842	2.519022
H	4.157315	0.504656	1.281603
C	3.476375	2.607262	-0.484672
H	4.102332	1.865182	-1.004587
H	2.825904	3.086859	-1.236563
H	4.141447	3.381417	-0.060692

### <sup>3</sup>I-6<sup>E</sup>

Lowest frequency = 18.0407 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

53

Fe	-0.825008	-0.176450	-0.560090
C	-4.275689	0.183437	-1.032037
H	-5.111095	0.890612	-1.182204
H	-4.161933	-0.449714	-1.927582
H	-4.503526	-0.471027	-0.173293
C	-2.618375	2.261223	-2.129776
H	-3.539384	2.868505	-2.194150
H	-1.748612	2.925108	-1.989570
H	-2.472432	1.697907	-3.065839
C	-3.106427	2.179811	0.692328
H	-3.960423	2.839775	0.455547
H	-3.351187	1.573176	1.579931
H	-2.220002	2.792553	0.928804

### <sup>5</sup>I-6<sup>E</sup>

Lowest frequency = 22.3263 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

53

Fe	-0.758302	-0.121182	-0.621286
C	-4.351934	-0.099038	-0.603858
H	-5.254812	0.533375	-0.672156
H	-4.356346	-0.836600	-1.423649
H	-4.362705	-0.646134	0.353847
C	-3.073764	1.901295	-2.243647
H	-4.028029	2.456515	-2.211264

H	-2.235664	2.611091	-2.345278	C	0.868229	-4.077028	-0.228773
H	-3.062034	1.227747	-3.116370	H	1.217891	-4.253107	0.801669
C	-2.998195	2.159657	0.625978	H	0.334946	-4.977449	-0.581420
H	-3.913547	2.765175	0.501393	H	1.748686	-3.913006	-0.871375
H	-3.026308	1.647256	1.601633	C	-0.845124	-2.712916	-2.032566
H	-2.107860	2.810145	0.606665	H	-1.091943	-3.754908	-2.302074
C	-1.506989	-3.090963	0.907296	H	-1.740235	-2.082699	-2.142450
H	-1.298156	-0.780742	-1.936028	H	-0.070285	-2.324577	-2.711880
H	-0.836424	-3.472187	0.119694	C	-1.719854	-3.305996	0.611280
H	-1.500871	-3.782823	1.768367	H	-2.519991	-2.547937	0.636077
C	0.710832	-1.764208	2.175859	H	-2.079398	-4.220984	0.109168
H	1.132520	-0.825915	2.571143	H	-1.439862	-3.551634	1.649297
H	0.605125	-2.499807	2.993092	C	3.604010	-1.984351	0.894796
H	1.396748	-2.147780	1.403242	H	-0.338810	-0.297318	-0.927268
C	-1.977837	-1.011848	2.854498	H	4.003825	-1.305098	0.125195
H	-3.029819	-0.911721	2.536466	H	4.371475	-2.162929	1.668435
H	-1.911337	-1.792288	3.634146	C	2.869697	0.221149	2.503176
H	-1.652012	-0.048026	3.281937	H	2.100736	0.769261	3.070453
P	-0.916249	-1.406597	1.382891	H	3.676367	-0.107369	3.181586
P	-2.803933	0.902145	-0.715066	H	3.290778	0.898915	1.742510
C	0.861645	-1.080280	-1.116818	C	1.804844	-2.361407	3.079636
C	1.110065	-2.325505	-1.694101	H	1.324670	-3.292468	2.735390
C	2.420658	-2.852339	-1.777939	H	2.756112	-2.610182	3.581929
C	3.500272	-2.080339	-1.312460	H	1.129382	-1.874761	3.800774
C	3.292898	-0.810195	-0.769016	P	-0.256748	-2.589379	-0.278424
C	1.974464	-0.266147	-0.639136	P	2.086126	-1.220431	1.642052
H	-2.528207	-3.022826	0.496108	C	1.666931	-0.258022	-1.095661
H	0.272726	-2.914647	-2.087920	C	2.262386	-1.114481	-2.056587
H	2.591192	-3.845563	-2.208178	C	3.160794	-0.653230	-3.023306
H	4.522399	-2.469939	-1.385331	C	3.515056	0.710108	-3.086023
H	4.161368	-0.230677	-0.443148	C	2.965402	1.594882	-2.162320
C	1.623359	0.997226	-0.059549	C	2.061580	1.128838	-1.173039
C	2.565844	2.034744	0.557471	H	3.353859	-2.940299	0.409287
O	0.320379	1.345070	-0.097294	H	2.033294	-2.185764	-2.044955
C	1.740227	3.226027	1.087811	H	3.598024	-1.360120	-3.738988
H	1.010068	2.894643	1.845141	H	4.214743	1.068059	-3.848187
H	2.415448	3.969871	1.548416	H	3.241511	2.651956	-2.207625
H	1.178718	3.712587	0.273949	C	1.431691	1.933755	-0.140190
C	3.346488	1.424444	1.749456	C	1.524794	3.452102	0.054844
H	4.042789	2.171260	2.174332	O	0.695607	1.292794	0.666668
H	2.647851	1.118511	2.548547	C	0.652465	3.858314	1.259706
H	3.930969	0.537948	1.456409	H	1.002768	3.373872	2.185884
C	3.553686	2.569434	-0.512195	H	0.699940	4.953272	1.394660
H	4.186322	1.769595	-0.929290	H	-0.396787	3.561529	1.106717
H	2.998585	3.029580	-1.347967	C	2.986833	3.880449	0.334689
H	4.216541	3.337550	-0.071438	H	3.024916	4.971617	0.502502
				H	3.370031	3.383998	1.243208
				H	3.667399	3.639745	-0.496956
				C	0.977471	4.160134	-1.211321
				H	1.574496	3.936321	-2.109491
				H	-0.062707	3.847242	-1.407334
				H	0.985345	5.253746	-1.055133
				C	-0.675272	-0.586107	2.115939
				C	-1.411141	-0.133315	1.006985
				H	-0.294798	0.167924	2.826432
				H	-0.910158	-1.551743	2.586857

**<sup>1</sup>I-7<sup>A</sup>**

Lowest frequency = 10.3215 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe 0.385653 -0.608734 0.349787



C	-2.505000	0.539964	0.606757
C	-3.579729	0.997260	1.627898
C	-3.634253	0.086221	2.870246
C	-3.214866	2.434574	2.076962
C	-4.994391	1.014169	1.004881
H	-3.818628	-0.963236	2.579215
H	-2.694254	0.118463	3.441904
H	-4.453694	0.409997	3.538207
H	-3.169768	3.122000	1.213287
H	-3.965674	2.830581	2.787062
H	-2.227510	2.441553	2.569349
H	-5.727259	1.372031	1.751166
H	-5.055324	1.685992	0.131786
H	-5.302206	0.002912	0.685666
C	-2.642632	1.010039	-0.832497
C	-3.463492	0.090809	-1.760702
H	-1.622166	1.086982	-1.248462
H	-3.073911	2.030642	-0.862637
C	-3.235960	0.389671	-3.248787
H	-3.183390	-0.958308	-1.549506
H	-4.541803	0.163120	-1.530795
C	-4.030603	-0.531278	-4.181559
H	-3.500780	1.445855	-3.452774
H	-2.154071	0.299861	-3.469187
H	-3.843744	-0.294434	-5.244104
H	-3.756108	-1.590414	-4.020566
H	-5.117641	-0.440652	-4.001532

H	-3.619594	0.728790	-1.031374
C	-2.396498	-2.429564	-2.827598
H	-1.919504	-3.395474	-2.595059
H	-3.420183	-2.610537	-3.201506
H	-1.803000	-1.933559	-3.613457
P	0.285064	-3.056366	0.327700
P	-2.395392	-1.357378	-1.314118
C	-1.387452	0.176998	1.088683
C	-1.864115	-0.413901	2.287007
C	-2.529148	0.319897	3.273809
C	-2.735419	1.703043	3.111266
C	-2.275950	2.324807	1.951097
C	-1.617022	1.585968	0.935439
H	-3.176205	-3.207519	0.097629
H	-1.704723	-1.484704	2.455817
H	-2.883034	-0.182532	4.182360
H	-3.250101	2.284857	3.882875
H	-2.449054	3.396510	1.828436
C	-1.149372	2.159017	-0.344506
C	-1.075263	3.672190	-0.662153
O	-0.775619	1.363480	-1.225986
C	-0.375721	3.844269	-2.025455
H	-0.935996	3.336767	-2.827089
H	-0.301338	4.919116	-2.268794
H	0.637613	3.413282	-2.004427
C	-2.501674	4.267726	-0.774402
H	-2.434628	5.323577	-1.093139
H	-3.089456	3.720656	-1.532436
H	-3.059259	4.234943	0.174560
C	-0.239683	4.412211	0.410641
H	-0.693049	4.366452	1.412760
H	0.771776	3.975710	0.478081
H	-0.135671	5.475525	0.128647
C	0.649538	-0.962337	-2.089714
C	1.341530	-0.331528	-1.050092
H	0.223203	-0.343793	-2.893121
H	0.863999	-2.002608	-2.382590
C	2.378009	0.419594	-0.643222
C	3.595484	0.705209	-1.550845
C	3.641237	-0.229508	-2.773475
C	3.511050	2.168155	-2.052267
C	4.908308	0.514326	-0.753714
H	3.670224	-1.287672	-2.459829
H	2.759561	-0.093544	-3.419434
H	4.546502	-0.020390	-3.372417
H	3.469161	2.883579	-1.212172
H	4.394695	2.421087	-2.667654
H	2.606237	2.309721	-2.667529
H	5.780011	0.722942	-1.400954
H	4.966638	1.194118	0.113609
H	4.996508	-0.522918	-0.384520
C	2.339865	1.097828	0.721370
C	2.737605	0.210697	1.915823
H	1.305923	1.444862	0.895162
H	2.980109	2.000307	0.716893
C	2.443056	0.867645	3.270504

### <sup>3</sup>I-7A

Lowest frequency = 13.7662 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	-0.452287	-0.853658	-0.305784
C	-0.311505	-4.639776	-0.450838
H	-0.122553	-4.596583	-1.537168
H	0.202931	-5.525387	-0.034994
H	-1.397975	-4.749798	-0.293662
C	0.129726	-3.490801	2.124924
H	0.681388	-4.417651	2.364648
H	0.527627	-2.659389	2.730206
H	-0.933891	-3.630100	2.382201
C	2.110771	-3.258218	0.083967
H	2.636075	-2.465232	0.637893
H	2.451218	-4.251370	0.427863
H	2.353536	-3.135509	-0.984348
C	-3.610623	-2.249279	-0.233944
H	0.482831	-0.573672	0.837666
H	-3.803164	-1.631953	0.659340
H	-4.561186	-2.445669	-0.761031
C	-3.427252	0.066003	-1.891377
H	-2.861774	0.635415	-2.645657
H	-4.386657	-0.278545	-2.316390

H	2.159127	-0.730145	1.847305
H	3.806158	-0.069369	1.851190
C	2.768205	-0.039088	4.462655
H	3.012965	1.814132	3.354093
H	1.372415	1.148223	3.299355
H	2.542296	0.455056	5.424248
H	2.177536	-0.973295	4.419376
H	3.836915	-0.322765	4.471587

C	-0.238661	3.475944	-1.103222
O	-0.337707	1.085694	-1.095755
C	0.388686	3.200519	-2.484885
H	-0.314762	2.664284	-3.142412
H	0.657732	4.159009	-2.962891
H	1.294795	2.581976	-2.391677
C	-1.511924	4.336065	-1.302264
H	-1.245185	5.276035	-1.817765
H	-2.247432	3.802325	-1.929427
H	-2.002725	4.594321	-0.351102
C	0.801415	4.227981	-0.233861
H	0.410970	4.484670	0.763317
H	1.705473	3.610668	-0.095635
H	1.096814	5.164395	-0.740248
C	0.345544	-1.504100	-1.814951
C	1.228378	-0.951204	-0.851330
H	0.253144	-0.933199	-2.754508
H	0.271979	-2.590293	-1.962675
C	2.466305	-0.442471	-0.674106
C	3.603565	-0.688393	-1.688078
C	3.366868	-1.948462	-2.543921
C	3.688258	0.543351	-2.624479
C	4.958365	-0.865774	-0.962290
H	3.229572	-2.836954	-1.902625
H	2.473395	-1.849223	-3.178755
H	4.239188	-2.124214	-3.199841
H	3.862995	1.471584	-2.051869
H	4.517438	0.430029	-3.347873
H	2.746682	0.661273	-3.187477
H	5.764127	-1.017055	-1.703555
H	5.224998	0.017429	-0.357082
H	4.937872	-1.746726	-0.296790
C	2.732015	0.513210	0.482664
C	3.141757	-0.141285	1.815057
H	1.807570	1.090062	0.665365
H	3.503969	1.250331	0.189791
C	3.190430	0.860387	2.976476
H	2.406090	-0.930420	2.052204
H	4.118825	-0.648707	1.712163
C	3.542233	0.211316	4.319733
H	3.924190	1.657235	2.743057
H	2.206153	1.362264	3.052571
H	3.564868	0.954123	5.136812
H	2.800827	-0.563207	4.589816
H	4.533343	-0.277246	4.280421

**<sup>1</sup>TS(7A-8A)**

Lowest frequency = -454.4635 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe	-0.644339	-0.652596	-0.229721
C	-2.469829	-3.174039	1.451689
H	-3.075460	-3.441372	0.570514
H	-2.330933	-4.076800	2.071998
H	-3.021367	-2.419029	2.033535
C	0.115499	-2.537581	2.507888
H	-0.116404	-3.444492	3.093489
H	1.190916	-2.528428	2.266586
H	-0.111832	-1.638026	3.100619
C	-0.120778	-4.046847	0.142773
H	0.929477	-3.859651	-0.137594
H	-0.163963	-4.890570	0.853822
H	-0.683695	-4.310704	-0.767553
C	-4.131699	-0.550488	-0.456246
H	0.636041	-0.593383	0.575491
H	-4.086740	0.456779	-0.009927
H	-4.996129	-0.617453	-1.140810
C	-2.704371	0.342139	-2.738733
H	-1.832427	0.250448	-3.405630
H	-3.633501	0.157648	-3.306173
H	-2.721735	1.366197	-2.333483
C	-2.888525	-2.447011	-2.228200
H	-2.917547	-3.288931	-1.517332
H	-3.853643	-2.398001	-2.762820
H	-2.078234	-2.635671	-2.950905
P	-0.820598	-2.500790	0.904354
P	-2.528450	-0.859174	-1.337774
C	-1.337421	0.516344	1.177719
C	-1.947769	0.256317	2.435766
C	-2.353461	1.263875	3.314270
C	-2.171733	2.624471	2.987485
C	-1.589697	2.948407	1.766629
C	-1.183849	1.925455	0.869107
H	-4.259560	-1.274769	0.363281
H	-2.120816	-0.777798	2.753000
H	-2.819475	0.994632	4.270365
H	-2.486518	3.411494	3.680443
H	-1.451943	4.001607	1.506384
C	-0.594138	2.139023	-0.437106

**<sup>3</sup>TS(7A-8A)**

Lowest frequency = -322.9143 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	-0.968110	-0.486501	-0.211058
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C	-3.456384	-0.932468	2.240684
H	-4.239926	-0.467530	1.620317
H	-3.928550	-1.666453	2.917426
H	-2.968166	-0.138890	2.824565
C	-1.263457	-2.845263	2.264840
H	-1.926854	-3.462153	2.896035
H	-0.624853	-3.503687	1.651570
H	-0.606222	-2.234993	2.904229
C	-3.337311	-3.026997	0.347563
H	-2.734622	-3.753160	-0.220024
H	-3.911120	-3.561223	1.125355
H	-4.039451	-2.543303	-0.347717
C	-3.028467	2.206757	-0.644633
H	0.398563	-1.209445	0.529697
H	-2.060991	2.725621	-0.730346
H	-3.802961	2.741092	-1.223548
C	-2.484357	0.658259	-3.039121
H	-2.547810	-0.334000	-3.516991
H	-3.210403	1.341913	-3.513375
H	-1.458921	1.041139	-3.150544
C	-4.590397	-0.097265	-1.300839
H	-5.013981	-0.205897	-0.289165
H	-5.199508	0.635468	-1.860203
H	-4.648756	-1.070709	-1.815775
P	-2.227180	-1.750924	1.116562
P	-2.817636	0.469926	-1.232165
C	-0.481594	0.754850	1.285992
C	-0.550523	0.673883	2.683452
C	-0.150224	1.723817	3.541286
C	0.334356	2.918696	2.985112
C	0.475680	3.036220	1.601753
C	0.125870	1.958664	0.729272
H	-3.301761	2.188623	0.423502
H	-0.926715	-0.236810	3.163868
H	-0.230595	1.606299	4.627721
H	0.614063	3.757378	3.632748
H	0.861658	3.972595	1.189411
C	0.405323	1.896626	-0.679149
C	1.223497	2.899357	-1.507110
O	-0.062726	0.852215	-1.324478
C	1.410109	2.355653	-2.938296
H	0.441686	2.227515	-3.449712
H	2.021453	3.064241	-3.525569
H	1.914385	1.376995	-2.925910
C	0.453085	4.243312	-1.599816
H	1.023551	4.967165	-2.210965
H	-0.529126	4.091643	-2.081475
H	0.278609	4.695360	-0.610029
C	2.630164	3.132802	-0.899889
H	2.585569	3.454722	0.152087
H	3.224752	2.205059	-0.942280
H	3.165853	3.909329	-1.476413
C	-0.462236	-2.195540	-1.217455
C	0.698941	-1.702452	-0.503595
H	-0.461296	-2.036356	-2.306249
H	-0.891451	-3.171660	-0.942625

C	2.040011	-1.530938	-0.664901
C	2.906136	-2.301319	-1.667318
C	2.146160	-3.438182	-2.377208
C	3.424821	-1.307467	-2.738129
C	4.111220	-2.930310	-0.922441
H	1.699878	-4.135112	-1.647638
H	1.337906	-3.052324	-3.017322
H	2.845823	-4.006264	-3.016726
H	3.993732	-0.478483	-2.283171
H	4.091973	-1.828024	-3.449430
H	2.581796	-0.874486	-3.302808
H	4.756345	-3.469732	-1.639364
H	4.731730	-2.169653	-0.419558
H	3.765621	-3.650512	-0.160235
C	2.723095	-0.515418	0.236984
C	2.747357	-0.885755	1.733251
H	2.186100	0.446164	0.141040
H	3.756983	-0.329854	-0.102664
C	3.223730	0.276292	2.613252
H	1.724220	-1.165847	2.046687
H	3.382831	-1.779222	1.890947
C	3.198810	-0.054007	4.108781
H	4.247942	0.571946	2.310283
H	2.573491	1.149643	2.420104
H	3.537087	0.803998	4.716252
H	2.173175	-0.307556	4.432519
H	3.851674	-0.915156	4.344922

### <sup>1</sup>I-8<sup>A</sup>

Lowest frequency = 25.7487 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe	-0.926136	-0.377987	-0.250552
C	-3.881136	-0.936361	1.550313
H	-4.559706	-0.852991	0.685610
H	-4.342019	-1.608515	2.295250
H	-3.755828	0.065832	1.988032
C	-1.509520	-2.205360	2.587108
H	-2.241015	-2.799472	3.162933
H	-0.638559	-2.838218	2.346751
H	-1.160370	-1.357505	3.195727
C	-2.803031	-3.264740	0.346635
H	-1.921247	-3.909828	0.199041
H	-3.483403	-3.749020	1.069362
H	-3.315847	-3.155718	-0.621106
C	-3.533433	1.731599	-1.024788
H	0.196809	-1.277084	0.567491
H	-2.854078	2.559841	-0.762137
H	-4.244983	2.063281	-1.802599
C	-1.880922	0.963518	-3.206684
H	-1.225726	0.215158	-3.679738
H	-2.729328	1.197795	-3.873452

H	-1.290762	1.875016	-3.029937
C	-3.776686	-0.881432	-2.206174
H	-4.389922	-1.266317	-1.375914
H	-4.442130	-0.389314	-2.937313
H	-3.267184	-1.731584	-2.689039
P	-2.239286	-1.605734	0.982217
P	-2.489243	0.302946	-1.584581
C	-0.752725	1.066440	1.053773
C	-1.263078	1.260230	2.370907
C	-0.924889	2.343488	3.183228
C	-0.037649	3.341731	2.723637
C	0.494743	3.224722	1.445659
C	0.158809	2.115751	0.621670
H	-4.086464	1.452555	-0.114004
H	-1.959468	0.530082	2.797036
H	-1.352841	2.421473	4.190491
H	0.225921	4.191483	3.361747
H	1.181947	3.995389	1.085584
C	0.676205	1.883142	-0.708357
C	1.626171	2.781297	-1.517650
O	0.275753	0.815424	-1.272253
C	1.890195	2.138529	-2.894423
H	0.961294	2.038828	-3.478082
H	2.595885	2.769162	-3.463520
H	2.322624	1.132345	-2.783241
C	0.968815	4.167425	-1.740497
H	1.625692	4.790989	-2.373235
H	-0.000084	4.058438	-2.259152
H	0.787289	4.705786	-0.797324
C	2.986252	2.932186	-0.789821
H	2.884729	3.368654	0.215637
H	3.477554	1.950339	-0.684695
H	3.650272	3.585605	-1.383800
C	-0.357892	-1.915089	-1.485940
C	0.651369	-1.674883	-0.471974
H	-0.041348	-1.654403	-2.507340
H	-0.939593	-2.849209	-1.464835
C	2.005474	-1.631923	-0.328251
C	2.997956	-2.430327	-1.184291
C	2.308334	-3.381073	-2.180958
C	3.901263	-1.454967	-1.979951
C	3.879481	-3.292778	-0.243495
H	1.607625	-4.058434	-1.664599
H	1.741509	-2.828320	-2.945845
H	3.071572	-3.993843	-2.694553
H	4.441908	-0.760089	-1.314083
H	4.653410	-2.017759	-2.562740
H	3.297114	-0.856070	-2.682615
H	4.621257	-3.861947	-0.833223
H	4.432641	-2.677448	0.486494
H	3.257247	-4.012504	0.316878
C	2.587560	-0.720480	0.749364
C	2.133552	-0.993520	2.194305
H	2.304889	0.321594	0.506732
H	3.690793	-0.746921	0.717837
C	2.555953	0.117463	3.164519

H	1.032522	-1.065104	2.222542
H	2.525511	-1.973478	2.530248
C	2.048404	-0.108115	4.592579
H	3.660398	0.209074	3.167464
H	2.162025	1.079707	2.785720
H	2.363722	0.707309	5.267397
H	0.944085	-0.148193	4.610771
H	2.427654	-1.059182	5.010532

### <sup>3</sup>I-8<sup>A</sup>

Lowest frequency = 9.0594 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	-0.874004	-0.630945	0.233579
C	-2.646253	-0.215387	3.257523
H	-2.653359	-1.309204	3.400658
H	-2.676598	0.280091	4.244619
H	-3.538343	0.072279	2.680796
C	-1.150422	2.099835	2.425817
H	-1.164053	2.442824	3.475568
H	-0.250124	2.494575	1.924293
H	-2.035187	2.482849	1.892773
C	0.157416	-0.112779	3.621904
H	1.110705	0.370956	3.353494
H	-0.174540	0.272697	4.602209
H	0.328420	-1.199348	3.696549
C	-4.057336	-2.013858	-0.931881
H	1.760579	-0.759782	1.725096
H	-4.114350	-1.203446	-1.675982
H	-4.448773	-2.950438	-1.367088
C	-1.678526	-3.188266	-1.890501
H	-0.683392	-3.610589	-1.682758
H	-2.374349	-4.003210	-2.158356
H	-1.588170	-2.489971	-2.738960
C	-2.521915	-3.647548	0.808257
H	-3.013723	-3.254333	1.713918
H	-3.142996	-4.454880	0.380952
H	-1.538126	-4.052427	1.093100
P	-1.117625	0.249984	2.313951
P	-2.294723	-2.258960	-0.402794
C	-2.203083	0.762336	-0.256289
C	-3.572192	0.920232	0.092320
C	-4.335356	2.022104	-0.295990
C	-3.763693	3.051124	-1.078792
C	-2.425829	2.960249	-1.443365
C	-1.640272	1.846171	-1.036857
H	-4.683706	-1.735500	-0.069867
H	-4.061671	0.150449	0.698796
H	-5.387559	2.090970	0.006385
H	-4.366367	3.909982	-1.392010
H	-1.985357	3.758439	-2.047305
C	-0.227229	1.664531	-1.280639



C	-0.999020	-2.519998	-2.263823
C	0.361246	-2.205546	-2.918748
C	-0.766311	-3.625120	-1.201523
C	-1.925947	-3.088418	-3.373849
H	0.244032	-1.532968	-3.783926
H	1.058321	-1.743232	-2.203090
H	0.811672	-3.145865	-3.288004
H	-1.713058	-4.043030	-0.821133
H	-0.188967	-4.457920	-1.643284
H	-0.204099	-3.226195	-0.341451
H	-1.474214	-3.990411	-3.828510
H	-2.915252	-3.372121	-2.974179
H	-2.079115	-2.337912	-4.168708
C	-2.850068	-1.680671	-0.699706
C	-3.835473	-0.581348	-0.295612
H	-2.408085	-2.083454	0.236564
H	-3.426726	-2.523741	-1.131388
C	-4.913069	-1.083252	0.675278
H	-3.282280	0.240309	0.191025
H	-4.314714	-0.149389	-1.196889
C	-5.875517	0.019665	1.130370
H	-5.485821	-1.903867	0.200300
H	-4.415554	-1.528334	1.558966
H	-6.642770	-0.368139	1.823947
H	-5.332116	0.830452	1.650300
H	-6.398955	0.473579	0.268616

### **<sup>1</sup>H-9A**

Lowest frequency = 21.9381 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe	0.624448	-0.647815	-0.086667
C	2.353710	-3.685326	0.647653
H	1.858724	-3.772948	1.629234
H	2.516887	-4.698484	0.239684
H	3.332350	-3.198784	0.791013
C	2.200081	-2.980747	-2.099332
H	2.497229	-4.040048	-2.192384
H	1.546203	-2.709519	-2.942734
H	3.092920	-2.337972	-2.141921
C	-0.114013	-3.892070	-0.697144
H	-0.831860	-3.509037	-1.440851
H	0.248281	-4.887314	-1.010400
H	-0.640569	-3.983252	0.268154
C	2.626067	-0.938101	2.800595
H	-0.949290	-1.297831	0.139864
H	3.352608	-0.285323	2.289268
H	2.638813	-0.729242	3.885058
C	0.650455	1.055801	2.858603
H	-0.363396	1.408330	2.615231
H	0.785113	1.023039	3.954161
H	1.374644	1.765159	2.423918

C	-0.108018	-1.694294	3.176741
H	0.049993	-2.751145	2.901779
H	0.127544	-1.560771	4.247923
H	-1.169633	-1.452294	3.005415
P	1.287518	-2.682316	-0.506555
P	0.941039	-0.608932	2.090280
C	2.291008	0.185368	-0.452901
C	3.617706	-0.331619	-0.510574
C	4.724264	0.457025	-0.825620
C	4.579404	1.837861	-1.095132
C	3.316678	2.411952	-1.006805
C	2.186274	1.619070	-0.671576
H	2.923526	-1.983881	2.634684
H	3.796634	-1.391212	-0.293533
H	5.721403	0.000969	-0.863489
H	5.451403	2.447948	-1.352041
H	3.204920	3.484944	-1.188537
C	0.845533	2.100725	-0.438473
C	0.313539	3.533181	-0.574048
O	0.016137	1.214158	-0.056695
C	-1.191866	3.545001	-0.237652
H	-1.371117	3.224299	0.801292
H	-1.589631	4.567315	-0.365323
H	-1.749903	2.858539	-0.894662
C	1.046152	4.480111	0.409219
H	0.626225	5.498639	0.325241
H	0.908129	4.139424	1.450070
H	2.127906	4.538107	0.211304
C	0.497204	4.014158	-2.035363
H	1.556193	4.045729	-2.336483
H	-0.033070	3.341540	-2.731850
H	0.075683	5.029287	-2.148129
C	-0.263616	-0.706910	-1.884302
C	-1.335788	-0.896195	-0.905075
H	-0.085644	-1.531093	-2.596504
H	-0.245064	0.262079	-2.405425
C	-2.676638	-0.734437	-0.787622
C	-3.640473	-0.453745	-1.952035
C	-2.925180	-0.072168	-3.261445
C	-4.467850	-1.740603	-2.208035
C	-4.606833	0.701743	-1.590871
H	-2.332796	0.849687	-3.139865
H	-2.248485	-0.870361	-3.604844
H	-3.678020	0.104384	-4.051408
H	-5.023302	-2.054626	-1.307009
H	-5.203047	-1.571865	-3.016547
H	-3.805366	-2.571095	-2.508510
H	-5.310273	0.875512	-2.425333
H	-5.205998	0.478630	-0.691597
H	-4.050520	1.638348	-1.412186
C	-3.289078	-0.883456	0.599865
C	-3.112743	0.375255	1.471695
H	-2.805111	-1.734807	1.118424
H	-4.362563	-1.138987	0.534738
C	-3.737556	0.248543	2.866795
H	-2.030466	0.583661	1.548739

H	-3.545558	1.249939	0.953128
C	-3.520357	1.490932	3.738473
H	-4.822716	0.051111	2.764227
H	-3.318079	-0.640731	3.378545
H	-3.991108	1.379747	4.731276
H	-2.443380	1.682043	3.896446
H	-3.948867	2.390521	3.259968

O	-0.066008	1.148063	0.087790
C	-1.337106	3.469551	0.090026
H	-1.492089	3.067571	1.105006
H	-1.782134	4.479809	0.039314
H	-1.870660	2.806855	-0.609881
C	0.857970	4.462638	0.778408
H	0.422044	5.478565	0.742926
H	0.718206	4.067075	1.799744
H	1.941215	4.550963	0.595783
C	0.308140	4.142513	-1.679936
H	1.362824	4.202910	-1.994617
H	-0.226049	3.514568	-2.414782
H	-0.122307	5.160949	-1.717166
C	-0.327256	-0.470972	-1.975756
C	-1.391215	-0.863584	-1.045438
H	-0.047992	-1.199260	-2.754959
H	-0.360574	0.555055	-2.362911
C	-2.719500	-0.670805	-0.848018
C	-3.708448	-0.143623	-1.897710
C	-3.021307	0.452086	-3.140376
C	-4.592784	-1.334183	-2.353907
C	-4.617649	0.951757	-1.286841
H	-2.401864	1.324631	-2.875995
H	-2.378418	-0.287196	-3.644849
H	-3.791541	0.783744	-3.860103
H	-5.128397	-1.794073	-1.505029
H	-5.348317	-0.991838	-3.084729
H	-3.974327	-2.113484	-2.832469
H	-5.340184	1.300821	-2.046411
H	-5.195646	0.578922	-0.424142
H	-4.021859	1.819471	-0.956536
C	-3.281218	-1.059398	0.513667
C	-3.012063	0.003198	1.598116
H	-2.811992	-2.009306	0.839441
H	-4.366481	-1.260128	0.454545
C	-3.560787	-0.385168	2.976837
H	-1.921215	0.174275	1.644764
H	-3.444082	0.971482	1.287304
C	-3.236100	0.643547	4.066202
H	-4.657885	-0.521428	2.908911
H	-3.154794	-1.375219	3.267920
H	-3.658402	0.349163	5.043187
H	-2.144215	0.758296	4.192043
H	-3.643938	1.637325	3.806676

### **<sup>3</sup>I-9A**

Lowest frequency = 13.9044 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	0.612155	-0.633200	-0.234267
C	2.481845	-3.663167	0.334091
H	2.102458	-3.741333	1.366176
H	2.642019	-4.679711	-0.066031
H	3.443399	-3.125740	0.350968
C	1.973040	-3.012252	-2.401111
H	2.316857	-4.054194	-2.521957
H	1.200119	-2.795969	-3.155833
H	2.811217	-2.316027	-2.561054
C	-0.138279	-3.963401	-0.727395
H	-0.925039	-3.602430	-1.410715
H	0.201875	-4.963414	-1.049673
H	-0.569697	-4.033256	0.285776
C	2.916530	-0.902072	2.526162
H	-0.975577	-1.479575	-0.148106
H	3.523960	-0.219780	1.909223
H	3.076116	-0.688665	3.597542
C	0.829537	0.984948	2.873397
H	-0.217193	1.281904	2.711319
H	1.059068	0.948980	3.952766
H	1.471953	1.728407	2.374228
C	0.277527	-1.816472	3.240131
H	0.481073	-2.858270	2.938467
H	0.602278	-1.674079	4.286426
H	-0.809972	-1.647351	3.173727
P	1.258685	-2.740724	-0.712027
P	1.140266	-0.650504	2.078638
C	2.260058	0.286396	-0.603605
C	3.534132	-0.230234	-0.867408
C	4.645634	0.606347	-1.126750
C	4.466135	2.002933	-1.116327
C	3.218775	2.565125	-0.839751
C	2.087287	1.733295	-0.559871
H	3.230891	-1.934861	2.314388
H	3.698981	-1.314982	-0.877030
H	5.628140	0.171264	-1.340473
H	5.317926	2.662500	-1.320666
H	3.120051	3.654570	-0.823177
C	0.762997	2.134126	-0.225252
C	0.163763	3.543310	-0.258221

### **<sup>5</sup>I-9A**

Lowest frequency = 11.2182 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

84

Fe	0.513914	-0.717085	-0.501743
C	1.277685	-4.403512	0.300844
H	0.842152	-4.303452	1.309224

H	1.163907	-5.450063	-0.036018
H	2.350140	-4.155745	0.368670
C	1.091055	-3.796214	-2.494123
H	0.923565	-4.879331	-2.634518
H	0.576499	-3.240937	-3.296211
H	2.168987	-3.578977	-2.571259
C	-1.270630	-3.905144	-0.921128
H	-1.825748	-3.404999	-1.732264
H	-1.263878	-4.994660	-1.106189
H	-1.793276	-3.697617	0.026552
C	1.411015	-1.083523	2.751663
H	-2.453481	-1.237188	-1.457233
H	2.089489	-0.240793	2.539833
H	1.223677	-1.148948	3.838904
C	-0.850372	0.657124	2.645004
H	-1.864243	0.853265	2.263698
H	-0.885733	0.523719	3.741060
H	-0.216593	1.519517	2.388144
C	-1.217570	-2.176961	2.536905
H	-0.798033	-3.163567	2.280020
H	-1.271008	-2.087441	3.636809
H	-2.237118	-2.114022	2.123048
P	0.447716	-3.205587	-0.854244
P	-0.161117	-0.837412	1.797874
C	2.562340	-0.520611	-0.444391
C	3.542591	-1.501176	-0.719963
C	4.917164	-1.278885	-0.558891
C	5.375038	-0.032358	-0.096268
C	4.451802	0.977416	0.177152
C	3.062105	0.752462	0.000265
H	1.907888	-2.003363	2.401911
H	3.228996	-2.492224	-1.073672
H	5.637095	-2.075011	-0.786141
H	6.445875	0.149685	0.044582
H	4.826260	1.941324	0.530767
C	2.020514	1.777666	0.215765
C	2.285309	3.239876	0.637392
O	0.825049	1.432299	0.040152
C	0.942285	3.992692	0.723310
H	0.271767	3.538248	1.470493
H	1.129250	5.041064	1.015785
H	0.415611	3.983824	-0.242974
C	2.943481	3.276217	2.040890
H	3.057433	4.325789	2.366592
H	2.304522	2.760490	2.779829
H	3.936232	2.801519	2.064541
C	3.166373	3.957833	-0.416144
H	4.165126	3.507789	-0.520172
H	2.678086	3.930498	-1.405694
H	3.294175	5.016679	-0.127516
C	-0.641314	-0.401439	-2.212187
C	-2.000873	-0.258007	-1.696209
H	-0.533832	-1.305636	-2.837929
H	-0.184033	0.461416	-2.711276
C	-2.853844	0.785651	-1.414627
C	-2.650996	2.286938	-1.670966

C	-1.288393	2.642011	-2.296024
C	-3.745919	2.796316	-2.647243
C	-2.773434	3.059352	-0.331725
H	-0.456798	2.310332	-1.657135
H	-1.176485	2.191311	-3.296138
H	-1.219309	3.739593	-2.413789
H	-4.764505	2.656198	-2.246292
H	-3.608620	3.876753	-2.838708
H	-3.681020	2.263537	-3.612158
H	-2.642928	4.144567	-0.500800
H	-3.761950	2.912250	0.137945
H	-1.995205	2.724366	0.373853
C	-4.189343	0.388997	-0.782883
C	-4.100734	-0.002337	0.704346
H	-4.615474	-0.471380	-1.336040
H	-4.928648	1.203610	-0.883270
C	-5.432904	-0.472177	1.303095
H	-3.340596	-0.799658	0.809744
H	-3.722590	0.859371	1.285983
C	-5.327521	-0.867064	2.780987
H	-6.185981	0.331851	1.187685
H	-5.813322	-1.330134	0.714322
H	-6.302686	-1.188223	3.187940
H	-4.615427	-1.701197	2.921620
H	-4.968810	-0.020042	3.394441

#### <sup>1</sup>TS(9<sup>A</sup>-10<sup>A</sup>)

Lowest frequency = -317.6665 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe	0.295942	0.273526	0.086005
C	1.476201	3.049725	1.680246
H	0.778638	3.734858	1.171062
H	1.766583	3.487979	2.652055
H	2.370864	2.932554	1.046511
C	1.912756	0.607095	3.043370
H	2.115425	1.257421	3.912827
H	1.530706	-0.369922	3.380834
H	2.847921	0.419258	2.488849
C	-0.706158	1.764316	3.042851
H	-1.145207	0.814694	3.393181
H	-0.366102	2.350343	3.915786
H	-1.486929	2.327959	2.506439
C	0.479809	3.047222	-1.970103
H	-0.961273	-0.365365	0.853750
H	1.161554	2.485854	-2.626219
H	-0.082408	3.793306	-2.559236
C	-1.629915	1.271802	-2.630568
H	-2.423931	0.580371	-2.305607
H	-2.072786	2.112133	-3.194493
H	-0.943629	0.713919	-3.290914
C	-1.883597	3.038093	-0.387806
H	-1.348534	3.685995	0.326968



H	-2.368673	3.674114	-1.150074
H	-2.656920	2.484714	0.166048
P	0.690758	1.377505	1.883260
P	-0.668248	1.847959	-1.145085
C	1.296134	-1.336564	0.563266
C	1.027206	-2.298225	1.615443
C	1.997705	-3.149441	2.092078
C	3.324273	-3.124980	1.549012
C	3.656209	-2.189800	0.589909
C	2.692464	-1.236295	0.122005
H	1.092249	3.559949	-1.212205
H	0.006301	-2.359456	2.015909
H	1.758298	-3.856703	2.895310
H	4.075529	-3.833879	1.912375
H	4.682350	-2.159023	0.211746
C	2.936318	-0.074089	-0.649019
C	4.255029	0.349513	-1.312204
O	1.931664	0.748719	-0.778799
C	4.035643	1.633468	-2.137323
H	3.671257	2.459015	-1.505446
H	4.989218	1.939143	-2.603766
H	3.294123	1.469504	-2.936995
C	5.312656	0.651433	-0.219409
H	6.255079	0.992784	-0.685847
H	4.953110	1.451320	0.452049
H	5.534843	-0.232885	0.398702
C	4.762100	-0.758606	-2.266711
H	4.962735	-1.705668	-1.741662
H	4.013638	-0.961518	-3.052586
H	5.697981	-0.434984	-2.758032
C	0.060727	-1.623861	-0.738895
C	-1.182913	-1.026313	-0.179232
H	0.174420	-2.710627	-0.658388
H	0.313524	-1.325095	-1.771262
C	-2.495316	-1.393756	-0.166161
C	-2.991040	-2.674496	-0.880717
C	-2.416450	-2.802120	-2.310066
C	-2.547619	-3.888412	-0.022902
C	-4.529856	-2.728170	-1.014516
H	-2.687471	-1.920922	-2.917726
H	-1.320172	-2.892608	-2.313186
H	-2.830929	-3.700387	-2.803371
H	-2.989670	-3.831075	0.987738
H	-2.875588	-4.837297	-0.487063
H	-1.451195	-3.919901	0.091239
H	-4.822087	-3.703424	-1.442884
H	-5.040684	-2.627129	-0.042043
H	-4.906192	-1.941914	-1.690724
C	-3.439109	-0.619897	0.738315
C	-4.433680	0.346543	0.060606
H	-2.815682	-0.021492	1.430523
H	-4.010497	-1.324529	1.375735
C	-5.146852	1.258771	1.068753
H	-3.889946	0.966632	-0.674597
H	-5.188939	-0.213764	-0.516581
C	-6.105556	2.254941	0.407467

H	-5.698681	0.633659	1.797625
H	-4.388416	1.810133	1.660096
H	-6.606240	2.894556	1.155483
H	-5.565842	2.916476	-0.294938
H	-6.890197	1.730169	-0.167495

### <sup>3</sup>TS(9<sup>A</sup>-10<sup>A</sup>)

Lowest frequency = -265.2241cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	0.436644	-0.345577	0.614013
C	0.325227	-2.646579	3.132832
H	0.499435	-1.829829	3.853285
H	-0.233829	-3.457812	3.632885
H	1.306583	-3.025200	2.799737
C	-1.024607	-3.609093	0.821584
H	-1.836528	-4.104654	1.381291
H	-1.364216	-3.419376	-0.208756
H	-0.157952	-4.287123	0.790844
C	-2.258164	-1.621119	2.343026
H	-2.950451	-1.477031	1.498234
H	-2.621848	-2.453961	2.970933
H	-2.240140	-0.697248	2.936814
C	1.943079	1.382479	2.972984
H	-0.833904	0.735142	-0.433267
H	2.598427	1.606034	2.117010
H	2.003205	2.196050	3.718086
C	-0.209664	2.880832	1.768625
H	-1.290906	2.932002	1.557644
H	0.047425	3.635520	2.533326
H	0.348616	3.070960	0.839847
C	-0.723279	1.112423	3.935825
H	-0.548317	0.157421	4.458893
H	-0.405507	1.941003	4.593879
H	-1.804713	1.213017	3.742790
P	-0.574781	-1.990928	1.642237
P	0.217603	1.168257	2.328087
C	1.700633	-1.346444	-0.488405
C	1.946287	-2.753408	-0.548632
C	3.175464	-3.291080	-0.909894
C	4.246583	-2.440456	-1.296611
C	4.063238	-1.067240	-1.295004
C	2.829756	-0.482513	-0.875892
H	2.277933	0.437639	3.433859
H	1.127359	-3.441480	-0.331259
H	3.311747	-4.378699	-0.911722
H	5.209537	-2.867625	-1.596193
H	4.895289	-0.418687	-1.584494
C	2.541209	0.902772	-0.762605
C	3.323402	2.078966	-1.360744
O	1.447146	1.191288	-0.103573
C	2.506196	3.376835	-1.194883

H	2.351305	3.617965	-0.130425	C	1.279743	-3.621318	-0.756930
H	3.046890	4.217287	-1.665729	H	1.359854	-4.566576	-1.322898
H	1.514565	3.285354	-1.668389	H	2.107789	-2.948792	-1.027851
C	4.669730	2.256700	-0.611563	H	1.355241	-3.833306	0.322331
H	5.212555	3.134582	-1.008279	C	-0.273626	-2.659848	-2.948475
H	4.494166	2.420858	0.466312	H	0.519644	-1.951001	-3.240292
H	5.323113	1.375673	-0.715566	H	-0.073608	-3.644640	-3.407643
C	3.576388	1.851584	-2.870917	H	-1.234329	-2.268565	-3.320779
H	4.157827	0.935529	-3.060508	C	-4.300710	-1.796054	0.411527
H	2.617767	1.759611	-3.411171	H	1.276882	0.303606	-0.307480
H	4.131835	2.707121	-3.297804	H	-4.098330	-1.476963	1.447714
C	0.117536	-0.926359	-1.461818	H	-5.377591	-1.677977	0.196292
C	-1.094497	-0.219244	-0.956116	C	-4.081020	0.899909	-0.484527
H	-0.083063	-1.925666	-1.855736	H	-3.601331	1.631666	-1.153684
H	0.654250	-0.323232	-2.213371	H	-5.162200	0.840477	-0.703837
C	-2.451304	-0.335561	-1.122432	H	-3.924111	1.233697	0.554206
C	-3.239083	-1.302512	-2.018572	C	-3.913002	-1.226331	-2.389995
C	-2.359975	-2.229290	-2.880300	H	-3.657480	-2.277958	-2.605573
C	-4.167723	-2.193475	-1.151749	H	-5.008980	-1.103833	-2.462450
C	-4.123847	-0.478391	-2.992780	H	-3.429237	-0.589533	-3.150469
H	-1.657510	-1.654954	-3.506595	P	-0.321774	-2.758572	-1.095679
H	-1.779069	-2.937353	-2.266275	P	-3.271558	-0.744121	-0.711407
H	-3.004931	-2.826866	-3.549357	C	-1.339480	0.249525	1.463763
H	-4.850652	-1.589507	-0.529686	C	-2.022362	-0.198843	2.613091
H	-4.787736	-2.841362	-1.798307	C	-2.716761	0.690779	3.446891
H	-3.579639	-2.843266	-0.482411	C	-2.650104	2.081615	3.182636
H	-4.712513	-1.159044	-3.634674	C	-1.964115	2.563473	2.071975
H	-4.835283	0.171352	-2.455591	C	-1.347397	1.680964	1.121016
H	-3.499376	0.157028	-3.644471	H	-4.021695	-2.857503	0.307717
C	-3.273017	0.714530	-0.369790	H	-1.978745	-1.264169	2.876618
C	-3.157070	2.139794	-0.947943	H	-3.279094	0.314738	4.308580
H	-2.936635	0.749280	0.684397	H	-3.143863	2.788914	3.858419
H	-4.339754	0.428377	-0.334520	H	-1.942517	3.642813	1.899075
C	-3.947072	3.183461	-0.147080	C	-0.834455	2.041516	-0.162488
H	-2.087398	2.424548	-0.971240	C	-0.538096	3.470281	-0.650702
H	-3.494794	2.145540	-2.000952	O	-0.577513	1.073433	-1.032342
C	-3.763659	4.612159	-0.671125	C	0.184242	3.401444	-2.013037
H	-5.021934	2.915874	-0.157443	H	-0.438010	2.894088	-2.767323
H	-3.636206	3.136151	0.916025	H	0.410300	4.424690	-2.364617
H	-4.345879	5.340418	-0.079293	H	1.129170	2.839773	-1.933612
H	-2.701196	4.914606	-0.629661	C	-1.854049	4.265207	-0.854056
H	-4.090791	4.694199	-1.723693	H	-1.631560	5.286157	-1.216709

**<sup>5</sup>TS(9<sup>A</sup>-10<sup>A</sup>)**

Lowest frequency = -317.1413 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

84

Fe	-0.904606	-0.701270	-0.206605
C	-1.517611	-4.154738	-0.828724
H	-2.512065	-3.860942	-1.201959
H	-1.192826	-5.073601	-1.348727
H	-1.601467	-4.359445	0.252168

C	1.279743	-3.621318	-0.756930
H	1.359854	-4.566576	-1.322898
H	2.107789	-2.948792	-1.027851
H	1.355241	-3.833306	0.322331
C	-0.273626	-2.659848	-2.948475
H	0.519644	-1.951001	-3.240292
H	-0.073608	-3.644640	-3.407643
H	-1.234329	-2.268565	-3.320779
C	-4.300710	-1.796054	0.411527
H	1.276882	0.303606	-0.307480
H	-4.098330	-1.476963	1.447714
H	-5.377591	-1.677977	0.196292
C	-4.081020	0.899909	-0.484527
H	-3.601331	1.631666	-1.153684
H	-5.162200	0.840477	-0.703837
H	-3.924111	1.233697	0.554206
C	-3.913002	-1.226331	-2.389995
H	-3.657480	-2.277958	-2.605573
H	-5.008980	-1.103833	-2.462450
H	-3.429237	-0.589533	-3.150469
P	-0.321774	-2.758572	-1.095679
P	-3.271558	-0.744121	-0.711407
C	-1.339480	0.249525	1.463763
C	-2.022362	-0.198843	2.613091
C	-2.716761	0.690779	3.446891
C	-2.650104	2.081615	3.182636
C	-1.964115	2.563473	2.071975
C	-1.347397	1.680964	1.121016
H	-4.021695	-2.857503	0.307717
H	-1.978745	-1.264169	2.876618
H	-3.279094	0.314738	4.308580
H	-3.143863	2.788914	3.858419
H	-1.942517	3.642813	1.899075
C	-0.834455	2.041516	-0.162488
C	-0.538096	3.470281	-0.650702
O	-0.577513	1.073433	-1.032342
C	0.184242	3.401444	-2.013037
H	-0.438010	2.894088	-2.767323
H	0.410300	4.424690	-2.364617
H	1.129170	2.839773	-1.933612
C	-1.854049	4.265207	-0.854056
H	-1.631560	5.286157	-1.216709
H	-2.488798	3.768642	-1.609253
H	-2.440522	4.352334	0.074447
C	0.388814	4.205175	0.348532
H	-0.063159	4.298040	1.348891
H	1.339698	3.655411	0.461058
H	0.619699	5.222322	-0.019737
C	0.448894	-0.554115	1.520789
C	1.558046	-0.367604	0.519705
H	0.376653	-1.549325	1.983010
H	0.576661	0.180632	2.330519
C	2.867787	-0.740862	0.492581
C	3.679194	-1.489288	1.565251
C	2.835916	-2.019042	2.741103
C	4.440613	-2.696839	0.959457

C	4.723849	-0.496818	2.143877
H	2.315152	-1.206962	3.272421
H	2.085018	-2.753642	2.404361
H	3.498447	-2.526582	3.465432
H	5.098536	-2.399848	0.125532
H	5.075695	-3.162391	1.734811
H	3.742867	-3.465467	0.588226
H	5.326818	-0.995084	2.925105
H	5.417325	-0.133751	1.366208
H	4.223371	0.377180	2.595254
C	3.665487	-0.207186	-0.704997
C	3.801320	1.328656	-0.722034
H	3.169291	-0.521920	-1.643962
H	4.675240	-0.652855	-0.735299
C	4.525418	1.867214	-1.962508
H	2.791004	1.773496	-0.667096
H	4.329814	1.660397	0.191775
C	4.626594	3.397207	-1.977198
H	5.539831	1.424946	-2.019400
H	3.990528	1.522794	-2.869643
H	5.148798	3.760733	-2.879864
H	3.623051	3.859313	-1.957578
H	5.180207	3.767231	-1.094798

H	-1.808569	2.504276	1.063722
P	0.788002	-0.149843	2.180161
P	0.500956	2.358277	0.228209
C	0.714356	-1.907810	-0.725985
C	0.499060	-3.137494	-0.022902
C	1.520403	-3.881555	0.534450
C	2.849244	-3.379210	0.469007
C	3.094868	-2.145794	-0.094160
C	2.062454	-1.351593	-0.712758
H	2.207330	3.306988	1.744953
H	-0.522476	-3.535222	-0.008970
H	1.313561	-4.847860	1.006212
H	3.678699	-3.963420	0.882310
H	4.120229	-1.774377	-0.109981
C	2.292179	0.000874	-1.237474
C	3.686900	0.622116	-1.481977
O	1.246936	0.529877	-1.858298
C	3.499055	1.947714	-2.246625
H	2.884861	2.659766	-1.676933
H	4.484201	2.411381	-2.434070
H	2.995567	1.776909	-3.211256
C	4.425500	0.912852	-0.155997
H	5.345903	1.495167	-0.346856
H	3.770563	1.487139	0.519078
H	4.716163	-0.006345	0.377592
C	4.531304	-0.303895	-2.395176
H	4.755642	-1.276388	-1.929247
H	3.995698	-0.499704	-3.340441
H	5.492416	0.183921	-2.640849
C	-0.455265	-1.547834	-1.669450
C	-1.448844	-0.741022	-0.875741
H	-0.877675	-2.464404	-2.100353
H	-0.069948	-0.922214	-2.487271
C	-2.727439	-0.932770	-0.460593
C	-3.625763	-2.175187	-0.635487
C	-3.131512	-3.221071	-1.655209
C	-3.728999	-2.870623	0.748923
C	-5.047857	-1.758117	-1.092844
H	-2.967186	-2.773306	-2.649746
H	-2.200977	-3.714653	-1.334107
H	-3.898987	-4.009071	-1.760091
H	-4.134439	-2.190805	1.518088
H	-4.396214	-3.750062	0.688551
H	-2.734285	-3.211093	1.085576
H	-5.691275	-2.653752	-1.158851
H	-5.529108	-1.055609	-0.392623
H	-5.017608	-1.287239	-2.090951
C	-3.367469	0.223412	0.307420
C	-3.873505	1.361172	-0.601443
H	-2.623137	0.639056	1.007141
H	-4.201253	-0.136189	0.936324
C	-4.634564	2.456658	0.157748
H	-3.002895	1.802330	-1.124213
H	-4.520810	0.949321	-1.396768
C	-5.039733	3.635879	-0.733588
H	-5.535437	2.012826	0.624819

### <sup>1</sup>H-10<sup>A</sup>

Lowest frequency = 11.2182 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe	0.772434	0.167094	0.041004
C	1.584459	1.125379	3.292997
H	1.096000	2.107229	3.197074
H	1.527758	0.808077	4.349548
H	2.644103	1.232112	3.005710
C	1.604169	-1.627776	2.953654
H	1.506686	-1.569991	4.052198
H	1.135492	-2.553880	2.590989
H	2.670254	-1.651764	2.679008
C	-0.872573	-0.300620	3.030154
H	-1.426284	-1.131774	2.561895
H	-0.764084	-0.493849	4.112860
H	-1.457693	0.621950	2.887622
C	1.836893	3.557522	0.739658
H	-1.052895	0.282239	-0.616610
H	2.682314	3.502194	0.038248
H	1.439052	4.588192	0.744339
C	-0.033631	3.115398	-1.378467
H	-0.996168	2.664612	-1.673011
H	-0.152302	4.209406	-1.288126
H	0.704824	2.858457	-2.150713
C	-0.864011	3.006908	1.320855
H	-0.647687	2.814080	2.383691
H	-0.988685	4.094746	1.177255

H	-4.011544	2.824600	0.996561
H	-5.596500	4.401909	-0.165625
H	-4.150259	4.122147	-1.174606
H	-5.682182	3.300895	-1.568322

H	4.446592	-0.542362	-3.762619
H	2.667500	-0.764497	-3.871451
C	4.725522	-0.666790	-1.082487
H	5.665854	-0.796112	-1.649665
H	4.582111	0.410778	-0.890986
H	4.843854	-1.169825	-0.111267
C	3.740822	-2.708280	-2.236614
H	3.797877	-3.334336	-1.330903
H	2.903576	-3.082159	-2.851297
H	4.676963	-2.847059	-2.807904
C	-0.857839	-1.616262	-0.305680
C	-2.006192	-0.823897	0.265759
H	-1.108741	-2.689179	-0.388857
H	-0.622483	-1.270383	-1.326589
C	-3.332551	-1.075206	0.381353
C	-4.014804	-2.384039	-0.085854
C	-3.759806	-2.601029	-1.597713
C	-3.464055	-3.577973	0.734835
C	-5.546514	-2.367477	0.125717
H	-4.179373	-1.763349	-2.182855
H	-2.685536	-2.667981	-1.829221
H	-4.243319	-3.534964	-1.939434
H	-3.673347	-3.433592	1.809314
H	-3.947850	-4.518924	0.413525
H	-2.375396	-3.697170	0.619245
H	-5.975424	-3.311404	-0.254956
H	-5.814862	-2.289032	1.193281
H	-6.033934	-1.538799	-0.415401
C	-4.182643	0.042560	0.974057
C	-4.766642	1.005580	-0.080687
H	-3.552085	0.634753	1.663222
H	-5.006298	-0.363370	1.587518
C	-5.594371	2.145425	0.527823
H	-3.930313	1.431118	-0.666523
H	-5.386760	0.444487	-0.805521
C	-6.118763	3.134647	-0.519152
H	-6.443244	1.717653	1.096223
H	-4.973237	2.685457	1.269890
H	-6.708837	3.944041	-0.054190
H	-5.284994	3.601671	-1.075447
H	-6.765750	2.626932	-1.257706

### <sup>3</sup>I-10<sup>A</sup>

Lowest frequency = 13.7702 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	1.336400	0.509230	-0.132997
C	3.229080	3.235978	1.161366
H	2.355422	3.889405	0.999685
H	3.791183	3.600486	2.040021
H	3.875980	3.292719	0.269395
C	4.183343	0.741036	2.142343
H	4.471494	1.273181	3.066603
H	3.983377	-0.318606	2.368024
H	5.011270	0.796605	1.418058
C	1.613476	1.666621	2.937136
H	1.365213	0.656681	3.303221
H	2.148821	2.229564	3.722861
H	0.672986	2.184859	2.687912
C	0.851545	3.394119	-1.774103
H	-1.667785	0.148365	0.660151
H	1.436810	2.874430	-2.551248
H	0.161690	4.110488	-2.255458
C	-1.274103	1.549299	-2.096619
H	-1.995512	0.842200	-1.657579
H	-1.813263	2.402453	-2.545073
H	-0.692885	1.017084	-2.866850
C	-1.134344	3.167893	0.297696
H	-0.492330	3.714342	1.009372
H	-1.726322	3.895106	-0.286619
H	-1.821174	2.524631	0.872649
P	2.651394	1.483983	1.404565
P	-0.078037	2.111748	-0.802224
C	0.396394	-1.480817	0.568004
C	0.190041	-1.642604	1.972877
C	1.174073	-2.091662	2.844103
C	2.429338	-2.490515	2.313058
C	2.715167	-2.288200	0.975164
C	1.774247	-1.664704	0.078114
H	1.549317	3.940962	-1.120705
H	-0.826098	-1.471678	2.350453
H	0.957481	-2.212580	3.910868
H	3.175575	-2.963155	2.962054
H	3.688448	-2.600183	0.590486
C	2.174861	-1.038194	-1.187282
C	3.535471	-1.210297	-1.901380
O	1.227497	-0.395857	-1.863849
C	3.489032	-0.417890	-3.225261
H	3.332341	0.657242	-3.033559

### <sup>5</sup>I-10<sup>A</sup>

Lowest frequency = 18.7758 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

84

Fe	-0.763592	-0.501184	0.183266
C	-1.553091	-0.561395	3.416540
H	-1.404232	-1.653801	3.385151
H	-1.493013	-0.212576	4.463598
H	-2.556405	-0.339212	3.015328
C	-0.582393	2.043781	2.748643

H	-0.558108	2.213363	3.840167
H	0.187958	2.661161	2.261824
H	-1.559318	2.343922	2.337746
C	1.269196	-0.047323	3.308147
H	2.095748	0.513308	2.842673
H	1.155803	0.278560	4.358148
H	1.521019	-1.118658	3.283397
C	-1.445852	-4.056707	0.572670
H	0.882413	-0.218256	-1.181061
H	-2.218775	-3.983137	-0.208314
H	-1.001892	-5.068776	0.549250
C	0.624148	-3.335308	-1.269348
H	1.577144	-2.802615	-1.422076
H	0.807366	-4.424789	-1.269595
H	-0.054553	-3.055975	-2.091854
C	1.079170	-3.326846	1.576854
H	0.632536	-3.238359	2.582024
H	1.364333	-4.380520	1.406271
H	1.982754	-2.698008	1.539562
P	-0.285221	0.268371	2.340308
P	-0.148307	-2.744971	0.308391
C	-1.016818	2.123017	-1.047554
C	-0.965066	3.439595	-0.557758
C	-1.986073	4.025424	0.202983
C	-3.118029	3.242347	0.512309
C	-3.200853	1.929884	0.067254
C	-2.182837	1.303659	-0.738884
H	-1.929310	-3.894637	1.551270
H	-0.094870	4.050001	-0.825616
H	-1.905938	5.064067	0.538510
H	-3.937242	3.661159	1.107870
H	-4.080913	1.348096	0.343508
C	-2.315249	-0.085396	-1.188320
C	-3.679840	-0.829933	-1.284010
O	-1.280771	-0.668594	-1.803690
C	-3.466725	-2.089010	-2.150680
H	-2.700248	-2.746306	-1.713508
H	-4.416252	-2.648948	-2.230469
H	-3.122427	-1.819291	-3.161499
C	-4.172865	-1.296150	0.108356
H	-5.055941	-1.955598	0.010652
H	-3.371425	-1.861096	0.618873
H	-4.454653	-0.457173	0.765952
C	-4.752286	0.033960	-1.990725
H	-4.990192	0.956808	-1.439191
H	-4.401337	0.326373	-2.995719
H	-5.687927	-0.543559	-2.109084
C	0.141199	1.684176	-1.953147
C	1.172357	0.851963	-1.217538
H	0.584592	2.588277	-2.388784
H	-0.255858	1.066054	-2.771076
C	2.381540	1.107348	-0.648006
C	3.132591	2.450108	-0.536251
C	2.787210	3.473503	-1.638909
C	2.782036	3.068552	0.841328
C	4.667814	2.247128	-0.607369

H	2.886128	3.027937	-2.643566
H	1.769236	3.876097	-1.534759
H	3.483308	4.328910	-1.572559
H	3.055084	2.388286	1.667552
H	3.326575	4.019004	0.991801
H	1.700047	3.271354	0.902570
H	5.170102	3.218721	-0.453865
H	5.042829	1.555301	0.164670
H	4.973424	1.863353	-1.596137
C	3.036893	-0.101551	0.018602
C	3.879471	-0.963851	-0.941610
H	2.227008	-0.727483	0.440786
H	3.663715	0.208623	0.875782
C	4.533576	-2.176348	-0.265735
H	3.224084	-1.301396	-1.767665
H	4.662834	-0.345905	-1.416064
C	5.335004	-3.048896	-1.238361
H	5.193157	-1.824784	0.551902
H	3.751179	-2.791499	0.218866
H	5.798330	-3.909522	-0.724389
H	4.686468	-3.444347	-2.041443
H	6.142757	-2.468362	-1.720157

### **<sup>1</sup>I-5<sup>B</sup>**

Lowest frequency = 27.2287 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

53

Fe	0.652993	-0.349112	-0.601116
C	3.940919	0.778607	0.314448
H	4.092446	-0.029385	1.049579
H	4.911459	1.025717	-0.151747
H	3.559185	1.665513	0.847731
C	2.926493	1.610092	-2.205703
H	3.992333	1.783228	-2.441172
H	2.383825	1.344368	-3.128328
H	2.485670	2.540307	-1.808336
C	3.653580	-1.130173	-1.783421
H	3.114925	-1.456032	-2.689913
H	4.671957	-0.808444	-2.066717
H	3.721756	-1.989277	-1.095091
C	1.334113	-0.058017	2.681878
H	0.140655	1.152771	-1.273462
H	0.591663	0.756925	2.661411
H	1.301135	-0.570080	3.660388
C	-0.601870	-2.012994	1.975866
H	-0.917087	-2.834896	1.312340
H	-0.452357	-2.394277	3.001405
H	-1.397750	-1.249602	1.982718
C	2.176572	-2.594717	1.630154
H	3.197227	-2.226780	1.427739
H	2.126852	-2.953710	2.674136
H	1.973791	-3.438200	0.947898

P	2.690527	0.242648	-0.962380
P	0.941945	-1.234981	1.298374
C	-0.226425	1.292498	-0.134152
C	0.283484	2.510821	0.447899
C	-0.519469	3.356494	1.187643
C	-1.911419	3.083498	1.360311
C	-2.468842	1.948401	0.795860
C	-1.668627	1.023993	0.061631
H	2.331669	0.384504	2.537676
H	1.343357	2.755778	0.307984
H	-0.088241	4.255977	1.642831
H	-2.533461	3.772207	1.941241
H	-3.531483	1.739926	0.954148
C	-2.063665	-0.209202	-0.521865
C	-3.481920	-0.722950	-0.788996
O	-1.070147	-0.939573	-0.958721
C	-3.405787	-2.009225	-1.636731
H	-2.832508	-2.794215	-1.116950
H	-4.426096	-2.385402	-1.830745
H	-2.910166	-1.818998	-2.603009
C	-4.192282	-1.058533	0.547359
H	-5.211876	-1.435539	0.346795
H	-3.640296	-1.840526	1.096254
H	-4.278066	-0.178152	1.204845
C	-4.294486	0.340107	-1.568451
H	-4.398197	1.278689	-1.000751
H	-3.800659	0.577968	-2.526643
H	-5.307578	-0.044050	-1.787750

H	-0.014324	2.957537	2.566496
H	-0.685013	2.681508	0.913518
C	1.829936	0.674569	3.011327
H	2.780789	0.129234	2.895770
H	1.991526	1.562138	3.649459
H	1.105414	0.003479	3.503389
P	2.676180	-1.154780	-0.603096
P	1.167510	1.139637	1.336581
C	-0.422428	0.619154	-1.107980
C	-0.046747	1.820413	-1.794087
C	-0.940776	2.864635	-1.967534
C	-2.298836	2.723320	-1.563235
C	-2.731434	1.538411	-0.983736
C	-1.826673	0.469009	-0.725880
H	3.365368	2.007622	0.658252
H	0.979556	1.908673	-2.167912
H	-0.610515	3.796233	-2.441282
H	-3.004024	3.546098	-1.719659
H	-3.778489	1.448441	-0.681715
C	-2.103921	-0.741790	-0.009175
C	-3.485319	-1.317930	0.330548
O	-1.069662	-1.413189	0.379119
C	-3.309999	-2.750513	0.875053
H	-2.682341	-2.757171	1.780301
H	-4.299195	-3.175098	1.123037
H	-2.824195	-3.400679	0.128481
C	-4.146650	-0.453401	1.436202
H	-5.117056	-0.894517	1.728796
H	-3.502646	-0.415528	2.332295
H	-4.328505	0.581899	1.104973
C	-4.388646	-1.373072	-0.924506
H	-4.575386	-0.375371	-1.352184
H	-3.922334	-1.994007	-1.709104
H	-5.364571	-1.822623	-0.665380

### <sup>3</sup>I-5<sup>B</sup>

Lowest frequency = 25.6844 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

53

Fe	0.675207	-0.628291	0.109282
C	4.152558	-1.199967	0.541141
H	3.940951	-1.888628	1.377095
H	5.070398	-1.532308	0.022376
H	4.325334	-0.194037	0.960657
C	3.383245	-0.098067	-1.968994
H	4.376277	-0.455286	-2.298979
H	2.688631	-0.113814	-2.825968
H	3.469650	0.943064	-1.616354
C	2.875006	-2.837535	-1.392551
H	2.145330	-2.931114	-2.214888
H	3.895148	-3.003179	-1.786483
H	2.644585	-3.614760	-0.643570
C	2.370511	2.455499	0.818905
H	0.128864	-0.322556	-1.525334
H	2.022799	2.892519	-0.131800
H	2.449458	3.255458	1.577076
C	-0.285087	2.191888	1.817178
H	-1.073334	1.537268	2.226037

### <sup>5</sup>I-5<sup>B</sup>

Lowest frequency = 16.5162 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

53

Fe	0.726109	0.029355	-0.322439
C	3.073925	-1.961689	1.014528
H	2.192808	-2.589216	1.231230
H	3.969110	-2.602603	0.919641
H	3.214055	-1.257149	1.851449
C	4.359584	-0.197983	-0.865914
H	5.191246	-0.925848	-0.874284
H	4.323079	0.319076	-1.840162
H	4.547161	0.557075	-0.083074
C	2.718141	-2.386628	-1.790569
H	2.690472	-1.953347	-2.804962
H	3.595507	-3.052657	-1.699212
H	1.787204	-2.957703	-1.636016

C	1.651250	3.249088	0.389816
H	-0.108778	0.087672	-2.120617
H	1.085778	3.538957	-0.511876
H	1.677856	4.100960	1.092765
C	-0.781396	2.485739	1.699215
H	-1.347061	1.714377	2.247830
H	-0.636256	3.371041	2.344669
H	-1.366503	2.761563	0.806198
C	1.744846	1.605905	2.749102
H	2.797010	1.343764	2.544709
H	1.711381	2.540837	3.337557
H	1.295116	0.790805	3.341705
P	2.724603	-1.014988	-0.543782
P	0.828924	1.765639	1.140368
C	-0.880307	0.729807	-1.620301
C	-1.089169	2.017513	-2.148185
C	-2.246253	2.743921	-1.845015
C	-3.248402	2.119649	-1.052647
C	-3.084882	0.837047	-0.547605
C	-1.886150	0.074981	-0.781893
H	2.680418	2.987738	0.090563
H	-0.329421	2.445408	-2.813881
H	-2.395091	3.754721	-2.237316
H	-4.176574	2.660593	-0.834626
H	-3.890684	0.408296	0.052300
C	-1.554519	-1.196637	-0.212774
C	-2.484442	-2.068110	0.649354
O	-0.325055	-1.659064	-0.412905
C	-1.767883	-3.397241	0.968015
H	-0.832505	-3.219279	1.522908
H	-2.429387	-4.036990	1.580198
H	-1.506854	-3.937919	0.043671
C	-2.782777	-1.353219	1.993254
H	-3.410171	-1.994150	2.640689
H	-1.838760	-1.144629	2.527981
H	-3.308470	-0.395123	1.850310
C	-3.801187	-2.399431	-0.094904
H	-4.378986	-1.498180	-0.354255
H	-3.584410	-2.939362	-1.032966
H	-4.441874	-3.045466	0.533890

H	2.122489	-1.905715	1.763673
H	0.605465	-2.154159	2.668050
C	1.605720	-3.417275	-0.815812
H	2.415274	-2.698143	-1.022056
H	2.015162	-4.311734	-0.315317
H	1.146672	-3.718771	-1.771869
C	-3.630542	-2.003702	-0.515943
H	-0.274058	-0.208897	1.221175
H	-3.960653	-1.257547	0.225442
H	-4.462434	-2.233110	-1.205299
C	-2.998182	0.055133	-2.353457
H	-2.266023	0.537938	-3.020235
H	-3.859755	-0.311272	-2.938780
H	-3.348606	0.802096	-1.622439
C	-1.976688	-2.574077	-2.789030
H	-1.521667	-3.496315	-2.391100
H	-2.950184	-2.821809	-3.247715
H	-1.303849	-2.164934	-3.559508
P	0.341502	-2.588831	0.258520
P	-2.169124	-1.322323	-1.433794
C	-1.491878	-0.170124	1.263691
C	-2.021482	-0.992953	2.314014
C	-3.059406	-0.567853	3.127356
C	-3.600124	0.739197	2.994214
C	-3.082902	1.598389	2.034448
C	-2.046101	1.177224	1.159028
H	-3.348347	-2.919149	0.027330
H	-1.607966	-1.995015	2.464914
H	-3.463059	-1.244584	3.889343
H	-4.411512	1.068485	3.650934
H	-3.498661	2.605257	1.940120
C	-1.471017	1.920028	0.074173
C	-1.610023	3.421046	-0.212478
O	-0.708075	1.244849	-0.702004
C	-0.675326	3.796507	-1.379897
H	-0.943809	3.247476	-2.296940
H	-0.753300	4.879872	-1.579771
H	0.371655	3.550577	-1.143498
C	-3.064639	3.770992	-0.615766
H	-3.136945	4.850133	-0.841688
H	-3.362124	3.214133	-1.521005
H	-3.791945	3.542064	0.179566
C	-1.187989	4.226510	1.041546
H	-1.835818	4.018931	1.908420
H	-0.150439	3.979694	1.326472
H	-1.238179	5.308940	0.825214
C	0.624200	-0.644820	-2.120822
C	1.391930	-0.205977	-1.013268
H	0.262028	0.118079	-2.831997
H	0.823660	-1.616302	-2.596808
C	2.492007	0.479454	-0.644092
C	3.526559	0.942289	-1.705850
C	3.711579	-0.110838	-2.817296
C	2.988408	2.252688	-2.332930
C	4.918578	1.226380	-1.100969
H	4.060531	-1.069164	-2.391846

### **<sup>1</sup>I-6<sup>B</sup>**

Lowest frequency = 18.1026 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe	-0.392796	-0.632176	-0.361785
C	-0.791941	-4.041393	0.554888
H	-1.305615	-4.314800	-0.381588
H	-0.220971	-4.915885	0.913968
H	-1.556952	-3.782197	1.304715
C	1.250753	-2.566981	1.875367
H	1.586822	-3.577910	2.166837

H	2.770599	-0.300676	-3.356257
H	4.464474	0.235799	-3.549355
H	2.861102	3.033692	-1.562004
H	3.685491	2.642015	-3.099586
H	2.006548	2.078777	-2.804233
H	5.600513	1.587127	-1.892811
H	4.878747	2.003936	-0.318926
H	5.362368	0.315298	-0.663362
C	2.607086	0.992914	0.783565
C	3.641028	0.317147	1.712210
H	1.608184	0.870522	1.241442
H	2.803418	2.085487	0.774130
C	3.350632	0.574428	3.197770
H	3.644516	-0.773610	1.521340
H	4.664340	0.659722	1.479995
C	4.360256	-0.090898	4.139577
H	3.334452	1.667167	3.379133
H	2.329382	0.214964	3.432874
H	4.123044	0.111191	5.199261
H	4.368796	-1.187854	3.999937
H	5.385811	0.274685	3.947827

P	-2.776812	-0.888772	-0.943322
C	-0.870052	0.218803	1.305174
C	-1.339346	-0.410396	2.471493
C	-2.104631	0.286785	3.413241
C	-2.325168	1.676732	3.219045
C	-1.848620	2.330263	2.090079
C	-1.157510	1.621550	1.052789
H	-3.681966	0.858370	0.505355
H	-1.065576	-1.452398	2.660884
H	-2.477713	-0.215772	4.311137
H	-2.884748	2.245843	3.970085
H	-2.063184	3.394996	1.967375
C	-0.862633	2.117062	-0.252543
C	-0.710397	3.593712	-0.651894
O	-0.714464	1.243962	-1.216935
C	-0.041152	3.665719	-2.040932
H	-0.662200	3.175088	-2.806929
H	0.109009	4.722802	-2.325557
H	0.936508	3.156250	-2.029450
C	-2.095589	4.284204	-0.745554
H	-1.975958	5.335961	-1.065300
H	-2.732080	3.774300	-1.490097
H	-2.631999	4.281458	0.217601
C	0.193726	4.334848	0.361509
H	-0.224334	4.325677	1.381109
H	1.189932	3.860952	0.401782
H	0.324250	5.389257	0.055229
C	0.870196	-0.631215	-2.254709
C	1.459247	-0.236516	-1.030185
H	0.572927	0.156386	-2.965236
H	1.138430	-1.590055	-2.728807
C	2.524772	0.270390	-0.392514
C	3.863238	0.562418	-1.113622
C	3.865919	0.067179	-2.570224
C	4.110177	2.091390	-1.118858
C	5.018696	-0.144398	-0.363709
H	3.694012	-1.021547	-2.621247
H	3.082513	0.562596	-3.165869
H	4.844350	0.283446	-3.036665
H	4.135774	2.505812	-0.095976
H	5.077246	2.326601	-1.601210
H	3.309606	2.608572	-1.675367
H	5.984225	0.067474	-0.859194
H	5.100391	0.195369	0.683205
H	4.867723	-1.238635	-0.358885
C	2.463884	0.612271	1.095176
C	2.414514	-0.607808	2.031249
H	1.573947	1.238359	1.287553
H	3.331104	1.235709	1.376976
C	2.212680	-0.233895	3.504915
H	1.583502	-1.264531	1.708369
H	3.338192	-1.207560	1.914050
C	2.074196	-1.453830	4.421816
H	3.060848	0.393468	3.842553
H	1.307055	0.396213	3.589830
H	1.934769	-1.156820	5.476244

### <sup>3</sup>I-6<sup>B</sup>

Lowest frequency = 19.9902 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	-0.462525	-0.643862	-0.764370
C	-0.518531	-3.654072	1.118608
H	-1.585387	-3.502067	1.342583
H	-0.311542	-4.736106	1.039398
H	0.075540	-3.240526	1.950698
C	1.732256	-3.319049	-0.549553
H	1.801878	-4.417547	-0.461913
H	2.173512	-2.999312	-1.506707
H	2.303294	-2.842421	0.261064
C	-0.782708	-3.916725	-1.721121
H	-0.493342	-3.560599	-2.724082
H	-0.432868	-4.955740	-1.587897
H	-1.882751	-3.899173	-1.652295
C	-3.774451	0.616879	-0.565765
H	0.079448	-0.217120	0.875864
H	-3.376688	1.461751	-1.147838
H	-4.835415	0.447611	-0.821109
C	-3.302280	-1.235423	-2.688326
H	-2.873745	-2.191530	-3.029160
H	-4.402295	-1.269285	-2.785814
H	-2.903196	-0.431434	-3.329463
C	-3.716926	-2.150828	0.032034
H	-3.542126	-1.952930	1.103324
H	-4.799598	-2.084952	-0.174880
H	-3.368420	-3.169426	-0.203198
P	-0.041343	-2.775318	-0.450552



H	1.201064	-2.067417	4.131085
H	2.968731	-2.101685	4.368286

### <sup>5</sup>I-6<sup>B</sup>

Lowest frequency = 15.9330 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

84

Fe	0.390524	-0.751549	-0.385920
C	-1.125235	-3.291299	1.811152
H	-1.297089	-3.923056	0.924265
H	-0.974434	-3.941153	2.691636
H	-2.015384	-2.660105	1.964460
C	0.683092	-1.583635	3.225432
H	0.677948	-2.415503	3.951980
H	1.666827	-1.088553	3.236694
H	-0.076899	-0.840485	3.515944
C	1.697846	-3.456526	1.342797
H	2.664080	-2.928862	1.278335
H	1.710762	-4.143517	2.207229
H	1.552388	-4.039506	0.418787
C	-2.705978	-2.037482	-1.528226
H	-1.111295	0.126941	1.578459
H	-3.063689	-0.994952	-1.516230
H	-3.241316	-2.610447	-2.306340
C	-0.781490	-1.425218	-3.569924
H	0.253574	-1.538101	-3.932825
H	-1.466807	-1.978382	-4.236605
H	-1.036649	-0.353656	-3.586872
C	-0.508614	-3.830553	-2.065810
H	-0.678168	-4.380407	-1.125201
H	-1.141596	-4.272313	-2.856073
H	0.552331	-3.942891	-2.346124
P	0.344572	-2.201195	1.510545
P	-0.879843	-2.029859	-1.821985
C	-2.191567	0.256704	1.463378
C	-3.065031	-0.216351	2.439750
C	-4.453398	-0.000552	2.334545
C	-4.933143	0.732032	1.228451
C	-4.068000	1.224403	0.254167
C	-2.651503	0.990717	0.316946
H	-2.919563	-2.468775	-0.536979
H	-2.662962	-0.740561	3.315890
H	-5.139885	-0.372850	3.101465
H	-6.008046	0.923324	1.129382
H	-4.494424	1.783042	-0.581507
C	-1.688512	1.416211	-0.660716
C	-1.941637	2.484837	-1.744811
O	-0.443976	0.968782	-0.583404
C	-0.608832	2.817757	-2.449131
H	-0.169224	1.925305	-2.923359
H	-0.784333	3.582965	-3.226816
H	0.133260	3.206969	-1.733520

C	-2.930906	1.979900	-2.827745
H	-3.067537	2.752801	-3.606813
H	-2.540568	1.072111	-3.319181
H	-3.923878	1.735642	-2.418693
C	-2.479236	3.787431	-1.100086
H	-3.437061	3.631087	-0.578662
H	-1.754400	4.173253	-0.362028
H	-2.630692	4.563391	-1.873469
C	2.140488	-1.367112	-1.353881
C	2.306066	-0.284157	-0.482635
H	2.176058	-1.197634	-2.442041
H	2.380873	-2.399598	-1.058667
C	3.014310	0.794036	-0.103802
C	4.515930	0.953526	-0.427968
C	5.087841	-0.272131	-1.161124
C	4.712041	2.201319	-1.324263
C	5.297233	1.134905	0.896794
H	4.947892	-1.191779	-0.567561
H	4.598645	-0.422993	-2.137303
H	6.170134	-0.133021	-1.335977
H	4.350697	3.120065	-0.831582
H	5.783644	2.342282	-1.557669
H	4.162234	2.084779	-2.274668
H	6.373790	1.280731	0.691437
H	4.942587	2.010758	1.466763
H	5.185205	0.241980	1.537034
C	2.332410	1.948273	0.623505
C	1.591322	1.558213	1.907945
H	1.592937	2.390085	-0.069237
H	3.063886	2.741726	0.858314
C	0.732299	2.695571	2.471502
H	0.945534	0.689312	1.675658
H	2.320379	1.213834	2.668247
C	0.022633	2.343152	3.783392
H	1.369381	3.589638	2.623902
H	-0.019367	2.974919	1.709029
H	-0.549294	3.202877	4.174652
H	-0.692289	1.514744	3.635924
H	0.746462	2.036538	4.561460

### <sup>1</sup>TS(6<sup>B</sup>-7<sup>B</sup>)

Lowest frequency = -454.3619 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe	-0.644150	-0.652649	-0.229866
C	-2.468232	-3.175685	1.450916
H	-3.073816	-3.442831	0.569651
H	-2.328741	-4.078745	2.070655
H	-3.020150	-2.421374	2.033310
C	0.116520	-2.537702	2.507480
H	-0.114811	-3.444906	3.092854
H	1.191958	-2.527737	2.266310

H	-0.111509	-1.638437	3.100384
C	-0.118533	-4.046601	0.141958
H	0.931613	-3.858638	-0.138302
H	-0.161208	-4.890524	0.852801
H	-0.681232	-4.310601	-0.768466
C	-4.131582	-0.552456	-0.455954
H	0.636313	-0.592960	0.575201
H	-4.087277	0.454814	-0.009576
H	-4.996078	-0.619999	-1.140378
C	-2.705067	0.341789	-2.738293
H	-1.833154	0.250860	-3.405334
H	-3.634156	0.156937	-3.305683
H	-2.723009	1.365693	-2.332677
C	-2.887456	-2.447656	-2.228695
H	-2.915736	-3.289840	-1.518112
H	-3.852718	-2.399118	-2.763097
H	-2.077183	-2.635506	-2.951631
P	-0.819420	-2.501189	0.903850
P	-2.528259	-0.859904	-1.337770
C	-1.337856	0.515653	1.177780
C	-1.948315	0.255045	2.435653
C	-2.354557	1.262208	3.314354
C	-2.173325	2.622963	2.987954
C	-1.591255	2.947456	1.767260
C	-1.184863	1.924902	0.869530
H	-4.258775	-1.276869	0.363557
H	-2.121011	-0.779227	2.752566
H	-2.820620	0.992527	4.270303
H	-2.488532	3.409676	3.681071
H	-1.453910	4.000781	1.507305
C	-0.595155	2.139037	-0.436592
C	-0.240123	3.476267	-1.102320
O	-0.338279	1.085980	-1.095503
C	0.387445	3.201433	-2.483999
H	-0.315760	2.665127	-3.141730
H	0.656204	4.160142	-2.961727
H	1.293757	2.583175	-2.390872
C	-1.513676	4.335983	-1.301243
H	-1.247227	5.276195	-1.816453
H	-2.248927	3.802152	-1.928628
H	-2.004662	4.593791	-0.350055
C	0.799607	4.228433	-0.232655
H	0.408967	4.484727	0.764549
H	1.703859	3.611389	-0.094495
H	1.094743	5.165079	-0.738766
C	0.346012	-1.503301	-1.815344
C	1.228687	-0.950356	-0.851600
H	0.253324	-0.932151	-2.754721
H	0.272894	-2.589479	-1.963398
C	2.466504	-0.441383	-0.674270
C	3.603715	-0.686595	-1.688478
C	3.367428	-1.946572	-2.544571
C	3.687695	0.545409	-2.624601
C	4.958734	-0.863534	-0.962996
H	3.230625	-2.835271	-1.903455
H	2.473810	-1.847577	-3.179237

H	4.239719	-2.121794	-3.200672
H	3.862136	1.473576	-2.051794
H	4.516790	0.432624	-3.348178
H	2.745960	0.663054	-3.187388
H	5.764413	-1.014265	-1.704463
H	5.225085	0.019648	-0.357633
H	4.938789	-1.744659	-0.297708
C	2.732071	0.513943	0.482823
C	3.142563	-0.140888	1.814824
H	1.807378	1.090239	0.666040
H	3.503547	1.251595	0.190019
C	3.190785	0.860272	2.976702
H	2.407512	-0.930661	2.051763
H	4.119963	-0.647577	1.711490
C	3.543387	0.210825	4.319569
H	3.923908	1.657764	2.743483
H	2.206160	1.361397	3.053266
H	3.565674	0.953263	5.136992
H	2.802618	-0.564371	4.589467
H	4.534847	-0.276989	4.279787

### <sup>3</sup>TS(6<sup>B</sup>-7<sup>B</sup>)

Lowest frequency = -694.5332 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	-0.979710	-0.518888	-0.326007
C	-2.515938	-2.530017	2.106531
H	-3.544525	-2.209024	1.875806
H	-2.548768	-3.556479	2.512331
H	-2.102889	-1.841937	2.859032
C	-0.032880	-3.507198	0.992547
H	-0.338993	-4.501608	1.361965
H	0.595101	-3.619890	0.092895
H	0.572162	-2.999214	1.760149
C	-2.449014	-3.667051	-0.488329
H	-1.880515	-3.892408	-1.404419
H	-2.633244	-4.604780	0.064953
H	-3.414731	-3.227205	-0.780924
C	-3.486346	1.569249	0.569350
H	0.482953	-0.563673	0.225587
H	-2.672747	2.304825	0.466874
H	-4.461869	2.041123	0.356670
C	-3.375504	0.903226	-2.258144
H	-3.362345	0.093680	-3.007427
H	-4.327123	1.458153	-2.331852
H	-2.518628	1.569982	-2.438119
C	-4.723087	-0.811956	-0.429057
H	-4.802509	-1.276898	0.566729
H	-5.594075	-0.149882	-0.579603
H	-4.747304	-1.605326	-1.194366
P	-1.497805	-2.459447	0.554901
P	-3.152165	0.168067	-0.580521

C	-0.278045	0.285572	1.385254
C	-0.047832	-0.222401	2.670340
C	0.274523	0.602281	3.767489
C	0.389989	1.992750	3.565086
C	0.216409	2.541082	2.296881
C	-0.096471	1.718281	1.165257
H	-3.468005	1.190193	1.604491
H	-0.096483	-1.303067	2.845754
H	0.442816	0.164265	4.756966
H	0.627668	2.651238	4.408435
H	0.311365	3.623381	2.173279
C	-0.212185	2.148257	-0.192009
C	0.199047	3.508795	-0.771757
O	-0.663509	1.259341	-1.063949
C	0.094413	3.464423	-2.310634
H	-0.943266	3.284471	-2.637566
H	0.428250	4.430143	-2.731298
H	0.720581	2.658664	-2.726303
C	-0.743946	4.626873	-0.257442
H	-0.454842	5.602264	-0.691403
H	-1.786982	4.418384	-0.555472
H	-0.719373	4.723438	0.840194
C	1.668663	3.832656	-0.402627
H	1.831851	3.843172	0.686856
H	2.345202	3.076854	-0.837203
H	1.954417	4.822769	-0.803840
C	-0.260842	-1.488610	-1.943220
C	0.828016	-1.004785	-1.163090
H	-0.558303	-0.877207	-2.811273
H	-0.391126	-2.569708	-2.104258
C	2.149353	-0.739490	-1.168632
C	3.057918	-1.098977	-2.364884
C	2.398025	-2.077946	-3.353512
C	3.385439	0.216424	-3.116861
C	4.372595	-1.746444	-1.867449
H	2.100651	-3.012968	-2.847999
H	1.501777	-1.643048	-3.822384
H	3.114710	-2.332526	-4.155318
H	3.882397	0.948060	-2.456306
H	4.060357	0.016141	-3.969582
H	2.460710	0.679016	-3.502665
H	5.029515	-1.969232	-2.727784
H	4.930375	-1.083455	-1.185003
H	4.169153	-2.693811	-1.337844
C	2.796814	-0.004530	-0.002015
C	3.113199	-0.887441	1.219601
H	2.121034	0.802136	0.329467
H	3.724516	0.492824	-0.337971
C	3.637832	-0.073571	2.408811
H	2.184657	-1.405753	1.521165
H	3.837462	-1.678621	0.947045
C	3.850428	-0.919727	3.668020
H	4.587162	0.421757	2.123694
H	2.914992	0.734264	2.627884
H	4.231559	-0.309771	4.506220
H	2.898584	-1.377570	3.993995

H	4.573309	-1.737453	3.488781
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**<sup>5</sup>TS(6<sup>B</sup>-7<sup>B</sup>)**

Lowest frequency = -914.2629 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

84

Fe	-0.993765	-0.516271	-0.427754
C	-2.430213	-3.166528	1.744886
H	-3.432043	-2.732213	1.590651
H	-2.531389	-4.250278	1.933200
H	-1.980662	-2.677942	2.624142
C	0.086323	-3.902237	0.525044
H	-0.188057	-4.960508	0.684198
H	0.750407	-3.817726	-0.351969
H	0.645132	-3.533548	1.401176
C	-2.313963	-3.804968	-1.033242
H	-1.731716	-3.822659	-1.969386
H	-2.495575	-4.842363	-0.699802
H	-3.279306	-3.314484	-1.239453
C	-3.572064	1.299985	0.850890
H	0.564029	-0.512492	0.090284
H	-2.744537	2.026908	0.896525
H	-4.540731	1.826178	0.778012
C	-3.582096	1.307086	-2.042334
H	-3.589804	0.708603	-2.969340
H	-4.537001	1.854711	-1.950826
H	-2.730645	2.004799	-2.077876
C	-4.841520	-0.830900	-0.596703
H	-4.854057	-1.490930	0.287216
H	-5.744510	-0.194026	-0.576581
H	-4.871743	-1.460956	-1.502294
P	-1.395875	-2.825229	0.245019
P	-3.288851	0.193576	-0.599711
C	-0.192451	0.142669	1.334815
C	0.005690	-0.584823	2.513003
C	0.280261	0.046602	3.743441
C	0.401092	1.453870	3.766119
C	0.243778	2.208158	2.606863
C	-0.068968	1.593352	1.347283
H	-3.541924	0.697984	1.774297
H	-0.023163	-1.680610	2.486064
H	0.423537	-0.545813	4.652953
H	0.629537	1.964683	4.708803
H	0.344724	3.294746	2.671971
C	-0.281979	2.248308	0.091701
C	0.004050	3.728746	-0.215024
O	-0.732536	1.514122	-0.900106
C	-0.200814	3.982365	-1.722771
H	-1.245737	3.796448	-2.021788
H	0.047540	5.032912	-1.960088
H	0.440723	3.318718	-2.325199
C	-0.963992	4.654799	0.564046

H	-0.763811	5.715139	0.320113	C	-2.802495	-3.265186	0.346050
H	-2.010807	4.434989	0.287854	H	-1.920610	-3.910078	0.198200
H	-0.872292	4.535151	1.655747	H	-3.482691	-3.749759	1.068746
C	1.475802	4.069138	0.129137	H	-3.315450	-3.156033	-0.621604
H	1.706618	3.898292	1.192845	C	-3.533940	1.731333	-1.024031
H	2.160012	3.440807	-0.467747	H	0.196993	-1.277084	0.567118
H	1.689812	5.129302	-0.102789	H	-2.854775	2.559661	-0.761163
C	-0.112123	-1.117957	-2.159267	H	-4.245602	2.063077	-1.801713
C	0.957709	-0.765342	-1.288588	C	-1.881345	0.964308	-3.206236
H	-0.425015	-0.384538	-2.919082	H	-1.226002	0.216240	-3.679549
H	-0.264403	-2.167376	-2.453426	H	-2.729832	1.198603	-3.872895
C	2.267777	-0.448228	-1.252428	H	-1.291381	1.875884	-3.029235
C	3.180845	-0.537205	-2.495161	C	-3.776654	-0.881383	-2.206198
C	2.536869	-1.297007	-3.669001	H	-4.389804	-1.266596	-1.376026
C	3.486139	0.912424	-2.952958	H	-4.442204	-0.389220	-2.937209
C	4.503975	-1.255514	-2.136002	H	-3.266982	-1.731313	-2.689273
H	2.252384	-2.321305	-3.372232	P	-2.238986	-1.606225	0.981962
H	1.635888	-0.785528	-4.041852	P	-2.489445	0.303094	-1.584311
H	3.258430	-1.367959	-4.502910	C	-0.752815	1.066151	1.054064
H	3.979866	1.494287	-2.155527	C	-1.263166	1.259565	2.371252
H	4.156434	0.905096	-3.832330	C	-0.925089	2.342671	3.183823
H	2.552930	1.434056	-3.227175	C	-0.037979	3.341129	2.724448
H	5.167332	-1.283105	-3.019436	C	0.494388	3.224496	1.446426
H	5.048960	-0.743230	-1.325550	C	0.158565	2.115684	0.622179
H	4.312752	-2.295794	-1.818611	H	-4.086871	1.451885	-0.113311
C	2.901420	0.060906	0.035918	H	-1.959466	0.529234	2.797216
C	3.184801	-1.040448	1.074731	H	-1.353030	2.420366	4.191114
H	2.227083	0.802758	0.497333	H	0.225503	4.190761	3.362755
H	3.840367	0.596862	-0.189492	H	1.181482	3.995339	1.086514
C	3.691748	-0.476279	2.407504	C	0.675918	1.883471	-0.707934
H	2.245976	-1.597029	1.251309	C	1.625756	2.781927	-1.517040
H	3.908746	-1.772803	0.668222	O	0.275557	0.815850	-1.272079
C	3.860286	-1.550024	3.487166	C	1.889799	2.139527	-2.893981
H	4.655041	0.045757	2.242468	H	0.960884	2.039854	-3.477622
H	2.975416	0.288735	2.760468	H	2.595387	2.770386	-3.462954
H	4.232127	-1.118359	4.433328	H	2.322357	1.133370	-2.783062
H	2.893084	-2.040709	3.701612	C	0.968253	4.168043	-1.739518
H	4.572842	-2.334462	3.170411	H	1.625049	4.791836	-2.372113

**<sup>1</sup>I-7<sup>B</sup>**

Lowest frequency = 25.7363 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

84

Fe	-0.926114	-0.377974	-0.250612
C	-3.880918	-0.937276	1.550320
H	-4.559562	-0.853838	0.685681
H	-4.341626	-1.609683	2.295137
H	-3.755766	0.064841	1.988258
C	-1.509008	-2.206084	2.586668
H	-2.240382	-2.800390	3.162446
H	-0.638000	-2.838800	2.346105
H	-1.159891	-1.358306	3.195415

C	-2.802495	-3.265186	0.346050
H	-1.920610	-3.910078	0.198200
H	-3.482691	-3.749759	1.068746
H	-3.315450	-3.156033	-0.621604
C	-3.533940	1.731333	-1.024031
H	0.196993	-1.277084	0.567118
H	-2.854775	2.559661	-0.761163
H	-4.245602	2.063077	-1.801713
C	-1.881345	0.964308	-3.206236
H	-1.226002	0.216240	-3.679549
H	-2.729832	1.198603	-3.872895
H	-1.291381	1.875884	-3.029235
C	-3.776654	-0.881383	-2.206198
H	-4.389804	-1.266596	-1.376026
H	-4.442204	-0.389220	-2.937209
H	-3.266982	-1.731313	-2.689273
P	-2.238986	-1.606225	0.981962
P	-2.489445	0.303094	-1.584311
C	-0.752815	1.066151	1.054064
C	-1.263166	1.259565	2.371252
C	-0.925089	2.342671	3.183823
C	-0.037979	3.341129	2.724448
C	0.494388	3.224496	1.446426
C	0.158565	2.115684	0.622179
H	-4.086871	1.451885	-0.113311
H	-1.959466	0.529234	2.797216
H	-1.353030	2.420366	4.191114
H	0.225503	4.190761	3.362755
H	1.181482	3.995339	1.086514
C	0.675918	1.883471	-0.707934
C	1.625756	2.781927	-1.517040
O	0.275557	0.815850	-1.272079
C	1.889799	2.139527	-2.893981
H	0.960884	2.039854	-3.477622
H	2.595387	2.770386	-3.462954
H	2.322357	1.133370	-2.783062
C	0.968253	4.168043	-1.739518
H	1.625049	4.791836	-2.372113
H	-0.000648	4.059088	-2.258178
H	0.786694	4.706145	-0.796204
C	2.985844	2.932768	-0.789213
H	2.884311	3.369027	0.216336
H	3.477219	1.950935	-0.684295
H	3.649801	3.586356	-1.383076
C	-0.357816	-1.914695	-1.486444
C	0.651498	-1.674624	-0.472502
H	-0.041383	-1.653716	-2.507805
H	-0.939422	-2.848878	-1.465522
C	2.005607	-1.631547	-0.328870
C	2.998111	-2.429719	-1.185095
C	2.308498	-3.380513	-2.181722
C	3.901154	-1.454163	-1.980810
C	3.879892	-3.292084	-0.244461
H	1.607986	-4.058028	-1.665296
H	1.741454	-2.827804	-2.946478
H	3.071757	-3.993119	-2.695483

H	4.441742	-0.759218	-1.314964
H	4.653342	-2.016790	-2.563706
H	3.296820	-0.855342	-2.683379
H	4.621654	-3.861139	-0.834318
H	4.433082	-2.676705	0.485465
H	3.257836	-4.011907	0.315985
C	2.587638	-0.720254	0.748900
C	2.134184	-0.994088	2.193866
H	2.304413	0.321783	0.506784
H	3.690873	-0.746193	0.717010
C	2.556206	0.116790	3.164367
H	1.033202	-1.066329	2.222349
H	2.526789	-1.973946	2.529351
C	2.049146	-0.109563	4.592478
H	3.660600	0.209013	3.167065
H	2.161656	1.078948	2.785996
H	2.364169	0.705813	5.267493
H	0.944854	-0.150282	4.610941
H	2.429041	-1.060554	5.010015

C	-0.416135	-2.529875	1.440991
C	0.288187	-3.098020	2.506129
C	1.104816	-2.297025	3.330958
C	1.214463	-0.939242	3.052388
C	0.513087	-0.360568	1.958956
H	-3.275903	0.489100	2.570174
H	-1.023442	-3.213359	0.838302
H	0.203965	-4.173805	2.702583
H	1.653907	-2.736953	4.169810
H	1.864023	-0.325585	3.681445
C	0.656890	1.017524	1.531104
C	1.457116	2.121702	2.242659
O	0.048189	1.332226	0.451854
C	1.273945	3.458644	1.497504
H	0.216315	3.770565	1.492590
H	1.862094	4.243495	2.004443
H	1.609279	3.387349	0.452078
C	0.944972	2.311096	3.693896
H	1.515768	3.121095	4.182433
H	-0.120418	2.600729	3.695316
H	1.048055	1.401828	4.305362
C	2.968416	1.772855	2.242860
H	3.191843	0.850774	2.800299
H	3.332362	1.638497	1.211104
H	3.536820	2.600539	2.703543
C	-0.652752	0.149254	-2.340054
C	0.690680	-0.352076	-2.026591
H	-0.752628	1.206524	-2.616060
H	-1.186355	-0.476926	-3.075223
C	1.933844	0.228724	-1.932217
C	2.329900	1.603490	-2.517649
C	1.225411	2.684024	-2.418478
C	3.591183	2.188062	-1.835734
C	2.660669	1.369248	-4.016670
H	0.438254	2.535473	-3.173906
H	0.756447	2.680509	-1.422313
H	1.667387	3.680745	-2.601421
H	4.470157	1.530242	-1.933147
H	3.845863	3.155056	-2.304895
H	3.417389	2.372909	-0.761653
H	2.975969	2.313415	-4.500447
H	3.478659	0.635891	-4.133033
H	1.774096	0.981284	-4.546813
C	3.076712	-0.581399	-1.337277
C	2.755576	-1.990688	-0.829201
H	3.494553	-0.010785	-0.482707
H	3.914058	-0.641445	-2.065549
C	3.943043	-2.648473	-0.112162
H	1.899953	-1.941269	-0.131671
H	2.436121	-2.634424	-1.672402
C	3.614772	-4.047460	0.421592
H	4.811174	-2.702346	-0.798906
H	4.257019	-1.999534	0.729050
H	4.480081	-4.499440	0.938627
H	2.773767	-4.003952	1.136485
H	3.320568	-4.727095	-0.399644

### <sup>3</sup>I-7<sup>B</sup>

Lowest frequency = 15.6048 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

84

Fe	-1.140502	-0.039921	-0.337128
C	-3.587870	-2.422137	0.223680
H	-4.306674	-1.658935	0.565784
H	-4.146935	-3.268458	-0.213948
H	-3.017472	-2.765013	1.099659
C	-1.646774	-3.098013	-1.827879
H	-2.387905	-3.877112	-2.078948
H	-1.156623	-2.755107	-2.754401
H	-0.872730	-3.522357	-1.169910
C	-3.713060	-1.241602	-2.334943
H	-3.207535	-0.839258	-3.226929
H	-4.278355	-2.148336	-2.614387
H	-4.417343	-0.483234	-1.962503
C	-2.861760	1.435593	2.184633
H	0.676308	-1.418965	-1.762988
H	-1.828965	1.525636	2.557518
H	-3.465691	2.284207	2.554050
C	-2.465771	3.108373	-0.139347
H	-2.549435	3.203458	-1.235294
H	-3.158597	3.820040	0.344764
H	-1.427190	3.334329	0.145797
C	-4.654734	1.313304	-0.021786
H	-5.088897	0.343344	0.271788
H	-5.172620	2.116426	0.532913
H	-4.824794	1.462764	-1.101076
P	-2.453614	-1.627396	-1.020360
P	-2.828872	1.352655	0.333740
C	-0.369977	-1.148862	1.113313

**<sup>5</sup>I-7<sup>B</sup>**Lowest frequency = 13.8716 cm<sup>-1</sup>

Charge = 0, Multiplicity = 5

84

Fe	-1.274775	-0.081631	-0.205368
C	-3.949835	-2.411299	1.142306
H	-4.487436	-1.543553	1.562003
H	-4.677910	-3.208585	0.905553
H	-3.245331	-2.774388	1.909192
C	-2.430398	-3.483069	-1.055792
H	-3.272192	-4.187152	-1.185831
H	-1.958883	-3.296960	-2.035608
H	-1.671689	-3.936812	-0.397949
C	-4.379251	-1.486396	-1.532383
H	-3.950014	-1.181143	-2.501428
H	-5.032382	-2.364853	-1.684306
H	-4.983751	-0.651114	-1.145680
C	-2.519761	2.050615	2.231801
H	0.470427	-1.711261	-1.527508
H	-1.452277	2.187471	2.464559
H	-3.086093	2.946191	2.545346
C	-2.223881	3.365738	-0.316234
H	-2.414663	3.341803	-1.402498
H	-2.792920	4.197078	0.137431
H	-1.143965	3.506763	-0.156647
C	-4.537776	1.778206	0.229182
H	-4.985464	0.916843	0.753477
H	-4.961075	2.710643	0.644776
H	-4.801466	1.711037	-0.839847
P	-2.994016	-1.855782	-0.351731
P	-2.690014	1.730396	0.414695
C	-0.077363	-0.977840	1.223558
C	-0.158890	-2.322172	1.658394
C	0.763933	-2.906877	2.535800
C	1.843154	-2.150103	3.024037
C	1.958749	-0.811398	2.648687
C	1.009010	-0.219669	1.777552
H	-2.883278	1.170321	2.787916
H	-0.970699	-2.959533	1.286557
H	0.655460	-3.957622	2.832094
H	2.586197	-2.601902	3.689422
H	2.805242	-0.236819	3.032120
C	1.054619	1.199932	1.363338
C	1.998904	2.265629	1.974152
O	0.249058	1.582692	0.489267
C	1.603241	3.653611	1.429679
H	0.566665	3.910139	1.706039
H	2.275684	4.419508	1.854562
H	1.677176	3.691203	0.331732
C	1.856495	2.307725	3.516687
H	2.461708	3.141155	3.916265

H	0.804906	2.485571	3.804024
H	2.184672	1.380025	4.007670
C	3.463683	1.985636	1.552074
H	3.830859	1.006948	1.897021
H	3.557119	2.012024	0.453188
H	4.122798	2.767521	1.970151
C	-0.958399	-0.307341	-2.276352
C	0.414490	-0.719695	-1.998637
H	-1.115703	0.611913	-2.859077
H	-1.597317	-1.119453	-2.663398
C	1.628128	-0.085601	-2.172138
C	1.795848	1.206338	-3.008821
C	0.975413	2.388338	-2.439028
C	3.264064	1.689964	-3.074281
C	1.344068	0.910001	-4.462655
H	-0.091941	2.146656	-2.336652
H	1.337447	2.662436	-1.436482
H	1.070983	3.269050	-3.102008
H	3.928522	0.949974	-3.551288
H	3.314641	2.617419	-3.672696
H	3.667986	1.917848	-2.072625
H	1.452027	1.811024	-5.096161
H	1.960442	0.104586	-4.899967
H	0.291662	0.584778	-4.495299
C	2.884943	-0.703328	-1.582839
C	2.753094	-2.072542	-0.907961
H	3.312947	0.002353	-0.838708
H	3.665102	-0.780982	-2.366662
C	4.073599	-2.553651	-0.290157
H	1.983725	-2.030757	-0.117236
H	2.402169	-2.817674	-1.649216
C	3.970786	-3.950849	0.331355
H	4.869494	-2.546923	-1.061449
H	4.391143	-1.827954	0.484492
H	4.927940	-4.267654	0.783242
H	3.197594	-3.971529	1.119668
H	3.691858	-4.703408	-0.429258

**<sup>1</sup>I-5<sup>C</sup>**Lowest frequency = 13.0871 cm<sup>-1</sup>

Charge = 0, Multiplicity = 1

97

Fe	1.083574	0.308370	0.102744
C	4.099517	-1.426050	-0.629232
H	4.625850	-0.528072	-0.989194
H	4.834371	-2.108189	-0.166641
H	3.634496	-1.935589	-1.489289
C	2.477917	-2.665433	1.293366
H	3.398741	-3.062078	1.756015
H	1.662295	-2.623225	2.031490
H	2.165471	-3.330895	0.477127
C	3.921463	-0.393262	1.990876

H	3.339314	-0.308670	2.922143	H	-3.824850	-2.050114	3.568665
H	4.733440	-1.125975	2.141485	H	-3.589012	-1.027779	2.115787
H	4.367505	0.587576	1.772068	H	-1.882572	-3.468660	4.458894
C	0.784209	-1.482610	-3.080540	H	-1.522205	-4.168221	2.857985
H	-1.221682	-0.566500	-0.946766	H	-0.248516	-3.291094	3.751333
H	-0.211305	-1.864719	-2.810920	C	-1.463107	-2.840509	0.461657
H	0.824645	-1.316668	-4.172236	C	-0.344020	-3.508165	-0.341628
C	0.037108	1.254877	-3.094590	H	-2.197226	-2.392025	-0.233167
H	0.102327	2.263424	-2.657292	H	-2.026151	-3.642727	0.971411
H	0.351467	1.295283	-4.152586	C	-0.849895	-4.425257	-1.462590
H	-1.009758	0.924165	-3.046006	H	0.321880	-2.722759	-0.742412
C	2.704773	0.552746	-3.064679	H	0.269456	-4.111068	0.353023
H	3.582041	0.003366	-2.697019	C	0.267467	-5.219473	-2.149165
H	2.582197	0.350020	-4.143780	H	-1.598205	-5.128822	-1.046836
H	2.888437	1.631872	-2.934663	H	-1.394485	-3.825787	-2.218920
P	2.788455	-0.966232	0.613219	H	-0.124352	-5.867630	-2.953293
P	1.142651	0.090684	-2.133585	H	1.018309	-4.544564	-2.598155
C	-2.191154	-0.236003	-1.343650	H	0.795237	-5.864889	-1.423030
C	-2.945132	-1.019544	-2.221757	P	2.305914	2.170232	0.223226
C	-4.176770	-0.557495	-2.709324	C	1.658561	3.651383	-0.711147
C	-4.649714	0.698972	-2.303585	H	0.571193	3.730514	-0.565715
C	-3.901391	1.482738	-1.419557	H	2.146149	4.586578	-0.382091
C	-2.651545	1.031963	-0.924706	H	1.853327	3.509431	-1.787483
H	1.528310	-2.249270	-2.807216	C	4.091443	2.352764	-0.313475
H	-2.572351	-2.001605	-2.529048	H	4.446894	3.380862	-0.119927
H	-4.763739	-1.172165	-3.399952	H	4.746384	1.651527	0.226543
H	-5.607169	1.074875	-2.679309	H	4.182776	2.142346	-1.389947
H	-4.295477	2.458855	-1.136182	C	2.464353	2.910857	1.926196
C	-1.758941	1.831551	-0.044728	H	3.006239	3.873770	1.908435
C	-2.299925	3.041584	0.763661	H	1.458871	3.060284	2.346339
O	-0.545165	1.549814	0.065413	H	2.995195	2.202968	2.581527
C	-1.252574	3.478853	1.803742				
H	-0.317811	3.800243	1.323217				
H	-1.651786	4.325876	2.388095				
H	-1.013856	2.656636	2.497560				
C	-2.553104	4.253764	-0.172580				
H	-2.879638	5.119067	0.431544				
H	-1.622846	4.537742	-0.694834				
H	-3.321927	4.066259	-0.937219				
C	-3.580749	2.643180	1.540764				
H	-4.427017	2.385319	0.887465				
H	-3.378342	1.772627	2.188332				
H	-3.890442	3.484733	2.185608				
C	0.594078	0.167617	2.025447				
C	-0.096407	-0.836080	1.242919				
H	0.060300	1.060730	2.383585				
H	1.302520	-0.189172	2.794958				
C	-1.013388	-1.802179	1.492477				
C	-1.749265	-1.965896	2.856692				
C	-1.470610	-0.839682	3.868399				
C	-3.281169	-1.967484	2.608924				
C	-1.327821	-3.303053	3.515767				
H	-0.409016	-0.794063	4.155309				
H	-1.754674	0.143983	3.460068				
H	-2.065569	-1.016983	4.783942				
H	-3.605842	-2.805392	1.969896				

### <sup>3</sup>I-5C

Lowest frequency = 13.0871 cm<sup>-1</sup>

Charge = 0, Multiplicity = 3

97

Fe	1.083574	0.308370	0.102744
C	4.099517	-1.426050	-0.629232
H	4.625850	-0.528072	-0.989194
H	4.834371	-2.108189	-0.166641
H	3.634496	-1.935589	-1.489289
C	2.477917	-2.665433	1.293366
H	3.398741	-3.062078	1.756015
H	1.662295	-2.623225	2.031490
H	2.165471	-3.330895	0.477127
C	3.921463	-0.393262	1.990876
H	3.339314	-0.308670	2.922143
H	4.733440	-1.125975	2.141485
H	4.367505	0.587576	1.772068
C	0.784209	-1.482610	-3.080540
H	-1.221682	-0.566500	-0.946766
H	-0.211305	-1.864719	-2.810920

H	0.824645	-1.316668	-4.172236	C	-1.013388	-1.802179	1.492477
C	0.037108	1.254877	-3.094590	C	-1.749265	-1.965896	2.856692
H	0.102327	2.263424	-2.657292	C	-1.470610	-0.839682	3.868399
H	0.351467	1.295283	-4.152586	C	-3.281169	-1.967484	2.608924
H	-1.009758	0.924165	-3.046006	C	-1.327821	-3.303053	3.515767
C	2.704773	0.552746	-3.064679	H	-0.409016	-0.794063	4.155309
H	3.582041	0.003366	-2.697019	H	-1.754674	0.143983	3.460068
H	2.582197	0.350020	-4.143780	H	-2.065569	-1.016983	4.783942
H	2.888437	1.631872	-2.934663	H	-3.605842	-2.805392	1.969896
P	2.788455	-0.966232	0.613219	H	-3.824850	-2.050114	3.568665
P	1.142651	0.090684	-2.133585	H	-3.589012	-1.027779	2.115787
C	-2.191154	-0.236003	-1.343650	H	-1.882572	-3.468660	4.458894
C	-2.945132	-1.019544	-2.221757	H	-1.522205	-4.168221	2.857985
C	-4.176770	-0.557495	-2.709324	H	-0.248516	-3.291094	3.751333
C	-4.649714	0.698972	-2.303585	C	-1.463107	-2.840509	0.461657
C	-3.901391	1.482738	-1.419557	C	-0.344020	-3.508165	-0.341628
C	-2.651545	1.031963	-0.924706	H	-2.197226	-2.392025	-0.233167
H	1.528310	-2.249270	-2.807216	H	-2.026151	-3.642727	0.971411
H	-2.572351	-2.001605	-2.529048	C	-0.849895	-4.425257	-1.462590
H	-4.763739	-1.172165	-3.399952	H	0.321880	-2.722759	-0.742412
H	-5.607169	1.074875	-2.679309	H	0.269456	-4.111068	0.353023
H	-4.295477	2.458855	-1.136182	C	0.267467	-5.219473	-2.149165
C	-1.758941	1.831551	-0.044728	H	-1.598205	-5.128822	-1.046836
C	-2.299925	3.041584	0.763661	H	-1.394485	-3.825787	-2.218920
O	-0.545165	1.549814	0.065413	H	-0.124352	-5.867630	-2.953293
C	-1.252574	3.478853	1.803742	H	1.018309	-4.544564	-2.598155
H	-0.317811	3.800243	1.323217	H	0.795237	-5.864889	-1.423030
H	-1.651786	4.325876	2.388095	P	2.305914	2.170232	0.223226
H	-1.013856	2.656636	2.497560	C	1.658561	3.651383	-0.711147
C	-2.553104	4.253764	-0.172580	H	0.571193	3.730514	-0.565715
H	-2.879638	5.119067	0.431544	H	2.146149	4.586578	-0.382091
H	-1.622846	4.537742	-0.694834	H	1.853327	3.509431	-1.787483
H	-3.321927	4.066259	-0.937219	C	4.091443	2.352764	-0.313475
C	-3.580749	2.643180	1.540764	H	4.446894	3.380862	-0.119927
H	-4.427017	2.385319	0.887465	H	4.746384	1.651527	0.226543
H	-3.378342	1.772627	2.188332	H	4.182776	2.142346	-1.389947
H	-3.890442	3.484733	2.185608	C	2.464353	2.910857	1.926196
C	0.594078	0.167617	2.025447	H	3.006239	3.873770	1.908435
C	-0.096407	-0.836080	1.242919	H	1.458871	3.060284	2.346339
H	0.060300	1.060730	2.383585	H	2.995195	2.202968	2.581527
H	1.302520	-0.189172	2.794958				



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