Supporting Information for

P_4 Activation by Group 3 Metal Arene Complexes

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1. Experimental Details

General Considerations: All experiments were performed under a dry nitrogen atmosphere using standard Schlenk techniques or an MBraun inert-gas glove box. Solvents were purified using a two-column solid-state purification system by the method of Grubbs[1] and transferred to the glove box without exposure to air. NMR solvents were obtained from Cambridge Isotope Laboratories, freezer-pump-thaw three times, and stored over activated molecular sieves prior to use. Scandium oxide and yttrium oxide were purchased from Stanford Materials Corporation, 4 Meadowpoint, Aliso Viejo, CA 92656, and used as received. **Sc-naph**, **Sc-anth**, and $Y(CH_2Ph)_3(THF)_3$ were prepared following published procedures.[2, 3] Other organic substrates were used as received (for solids) or freezed-pumped-thawed three times and stored over molecular sieves (for liquids). NMR spectra were recorded on Bruker300 or Bruker500 (work supported by the NSF grants CHE-9974928 and CHE-0116853) at room temperature in C_6D_6 unless otherwise specified. Chemical shifts are reported with respect to internal solvent (C_6D_6, C_7D_8, or d_8-tetrahydrofuran). CHN analyses were performed on CE-440 Elemental Analyzer manufactured by EXETER ANALYTICAL, INC.

Synthesis of $[(NN^{fc})Sc]_4P_8$ (Sc_4P_8) and $[(NN^{fc})Sc]_3P_7$ (Sc_3P_7). Sc-naph (0.316 g, 0.286 mmol) was dissolved in 15 mL of toluene in a Schlenk tube and P_4 (0.036 g, 0.291 mmol) was added as a 5 mL toluene solution. The mixture was stirred at 25 °C for 22.5 h. The initial dark blue color turned to green after 15 min stirring. Then the color gradually changed from green to light green and finally to orange. After stirring, the volatiles were removed under reduced pressure. The resulting orange solid was extracted by pentane, diethyl ether and toluene. Based on ^{1}H NMR spectroscopy, pentane extraction was mostly **Sc_3P_7** while diethyl ether and toluene extraction contained mostly **Sc_4P_8**. **Sc_3P_7** was collected as orange micro-crystals precipitated from pentane. Yield: 0.100 g, 31.2 % (based on Sc). The diethyl ether and toluene extraction were combined and dried down under reduced pressure. The resulting yellow solid was further washed with pentane to get clean **Sc_4P_8**. Yield: 0.147 g, 46.8 %. **Sc_4P_8**: ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 4.65, 4.46, 4.07 4.03, 4.01, 3.96, 3.93, and 3.79 (m, 32H, C*H* on Cp rings), 1.20, and 1.19 (s, 72H, SiCC*H*$_3$), and 0.92, 0.37, 0.36, and 0.29 (s, 48H, SiC*H*$_3$). ^{13}C NMR (126 MHz, C_6D_6, 25 °C) δ, ppm: 107.4, and 105.7 (*C*N on Cp rings), 71.3, 71.1, 70.4, 70.1, 69.8, 66.5, and 64.3 (*C*H on Cp rings), 28.5, and 27.7 (SiC*C*H$_3$), 20.6, and 20.1 (Si*C*CH$_3$), and 2.0, 0.4, -1.2, and -1.3 (Si*C*H$_3$). ^{31}P NMR (122 MHz, C_6D_6, 25 °C) δ, ppm: 96.2 (m, 4P, P_{corner}), and 45.7 (m, 4P, P_{inner}). Anal. (%): Calcd. for $C_{88}H_{152}N_8Fe_4Sc_4Si_8P_8$ with half molecule of toluene: C, 48.97; H, 7.01; N, 4.99. Found: C, 48.76; H, 6.60; N, 5.19. **Sc_3P_7**: ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 4.62, 4.03, 3.88, and 3.83 (b, 24H, C*H* on Cp rings), 1.15 (s, 54H, SiCC*H*$_3$), and 0.72, and 0.35 (s, 12H, SiC*H*$_3$). ^{13}C NMR (126 MHz, C_6D_6, 25 °C) δ, ppm: 106.2 (*C*N on Cp rings), 71.3, 69.8, 67.2, and 66.0 (*C*H on Cp rings), 28.1 (SiC*C*H$_3$), 20.3 (Si*C*CH$_3$), and 0.2, and -0.3 (Si*C*H$_3$). ^{31}P NMR (122 MHz, C_6D_6, 25 °C) δ, ppm: 23.2 (m, 3P, P_{edge}), -118.9 (m, 1P, P_{cap}), and -131.4 (m, 3P, P_{bottom}). Anal. (%): Calcd. for $C_{66}H_{114}N_6Fe_3Sc_3Si_6P_7$ with one molecule of hexanes: C, 48.98; H, 7.31; N, 4.75. Found: C, 48.77; H, 7.29; N, 4.89.

Reaction of $(NN^{fc})ScI(THF)_2$ with P_4 and KC_8. $(NN^{fc})ScI(THF)_2$ (0.0496 g, 0.0654 mmol), P_4 (0.0050 g, 0.040 mmol) and KC_8 (0.0115 g, 0.0851 mmol) were dissolved in 5 mL cold THF. The reaction mixture was allowed to stir at -78 °C in a dry ice/acetone bath. Then the volatiles were removed under reduced pressure. The crude reaction mixture was checked by ^{1}H NMR spectroscopy. Further work-up did not give isolable products.

Reaction of Sc-naph with 1.03 equiv of P_4. Sc-naph (0.0295 g, 0.0267 mmol) and P_4 (0.0034 g, 0.0274 mmol) were dissolved in 5 mL of toluene. The reaction mixture was stirred at 25 °C for 45 min until the color turned to light green. Then the volatiles were removed under reduced pressure. The resulting greenish solid was taken into d_8-toluene. After leaving it at 25 °C for 2 days, the reaction reached completion as indicated by no **Sc-naph** left over. Based on integration in ^{31}P NMR spectrum, **Sc_3P_7** and **Sc_4P_8** were formed in a 0.5:1 ratio (27% and 73% yields on Sc, respectively). Assuming all P-atoms in P_4 converted into either **Sc_3P_7** or **Sc_4P_8**, the stoichiometry of P_4 was calculated to be 1.04 equiv, which is very close to the experimental value of 1.03 equiv.

Reaction of Sc-naph with 1.24 equiv of P_4. Sc-naph (0.0265 g, 0.0240 mmol) and P_4 (0.0037 g, 0.0299 mmol) were dissolved in C_6D_6 in a J-Young tube. The reaction mixture was immersed in a 70 °C bath for 10 min to enhance the solubility of **Sc-naph** in C_6D_6. Then the reaction was kept at 25 °C and monitored by ^{1}H NMR spectroscopy. After 2 days at 25 °C, the reaction reached completion as indicated by no **Sc-naph** left over. Based on integration in ^{31}P NMR spectrum, **Sc_3P_7** and **Sc_4P_8** were formed in a 2.1:1 ratio (61% and 39% yields on Sc, respectively), while some P_4 was left over (ratio of **Sc_3P_7** vs left over P_4 is 2.1:0.5). Assuming all P-atoms in consumed P_4 converted into either **Sc_3P_7** or **Sc_4P_8** and including the left over P_4, the stoichiometry of P_4 was calculated to be 1.20 equiv, which is close to the experimental value of 1.24 equiv. Note: further heating of the reaction mixture led to no change.

Reaction of Sc-anth with 0.98 equiv of P_4. Sc-anth (0.0200 g, 0.0173 mmol) and P_4 (0.0021 g, 0.0169 mmol) were dissolved in C_6D_6 in a J-Young tube. The J-Young tube was then immersed in a 50 °C oil bath. The reaction was monitored based on the integration ratio between free anthracene and **Sc-anth**. After 2 days of heating at 50 °C, the reaction reached completion as indicated by no ^{31}P signal for free P_4 and no change in the ratio between free anthracene and **Sc-anth**. Based on integration in ^{1}H NMR spectrum, 10% unreacted **Sc-anth** was left in solution; based on the integration in ^{31}P NMR spectrum, **Sc_3P_7** and **Sc_4P_8** were formed in a 1.5:1 ratio (48% and 42% yields on Sc, respectively). Assuming all P-atoms in P_4 converted to either **Sc_3P_7** or **Sc_4P_8**, the stoichiometry of P_4 was calculated to be 0.98 equiv, which matches perfectly with the experimental value of 0.98 equiv. Note: further heating of the reaction mixture led to no change.

Synthesis of $(NN^{fc})YI(THF)_2$ ($YI(THF)_2$). $Y(CH_2Ph)_3(THF)_3$ (0.869 g, 1.50 mmol) and 1,1'-fc$(NHSi^tBuMe_2)_2$ (0.668 g, 1.50 mmol) were each dissolved in 5 mL THF (tetrahydrofuran) in a vial and cooled down with a dry ice/acetone bath. After cooling for 15 min, the THF solution of 1,1'-fc$(NHSi^tBuMe_2)_2$ was added to the $Y(CH_2Ph)_3(THF)_3$ solution. The mixture was warmed up to 0 °C and stirred for 1 h. Then the volatiles were removed under reduced pressure. The resulting orange solid (**$(NN^{fc})Y(CH_2Ph)(THF)_2$**) was extracted into 12 mL toluene and filtered through Celite. TMSI (trimethylsilyl iodide) (0.601 g, 3.00 mmol) was added as a toluene solution to crude **$(NN^{fc})Y(CH_2Ph)(THF)_2$** (toluene solution). The reaction mixture was stirred at 25 °C for 4 h. The volatiles were removed under reduced pressure. The remaining oily yellow powder was dissolved in a minimum amount of diethyl ether and layered with pentane. After storing in a freezer at -35 °C overnight, hexagonal orange crystals of **$YI(THF)_2$** were collected by decanting and washing with cold pentane. Yield: 0.768 g, 63.7 %. ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 4.07 and 3.10 (b, 8H, C*H* on Cp rings), 4.06 (b, 8H, CH_2O), 1.40 (m, 8H, CH_2CH_2), 1.02 (s, 18H, $SiCCH_3$), and 0.44 (s, 12H, $SiCH_3$). ^{13}C NMR (126 MHz, C_6D_6, 25 °C) δ, ppm: 102.9 (*C*N on Cp rings), 72.6 (CH_2O), 67.6, and 67.1 (*C*H on Cp rings), 28.0 ($SiCCH_3$), 25.0 (CH_2CH_2O), 20.6 ($SiCCH_3$), and -1.0 ($SiCH_3$). Anal. (%): Calcd. for $C_{30}H_{54}N_2FeIO_2Si_2Y$: C, 44.90; H, 6.78; N, 3.49. Found: C, 44.70; H, 6.56; N, 3.47.

Synthesis of [(NN^{fc})Y(THF)]$_2$(μ-$C_{10}H_8$) (Y-naph). YI(THF)$_2$ (0.410 g, 0.511 mmol) and 0.5 equiv of naphthalene (0.0350 g, 0.273 mmol) were dissolved in 10 mL of THF. The solution was cooled down to -78 °C using a dry ice/acetone bath. Then KC_8 (0.125 g, 0.925 mmol) was added to the solution. The color immediately turned to dark red. The reaction mixture was allowed to stir at room temperature for 2 h. 6 mL of hexanes was added to the reaction mixture to minimize the solubility of salt KI. The solution was then filtered through Celite. The solid left on Celite was washed with 4 mL THF/hexanes (3:1 ratio). After removing volatiles under reduced pressure, the remaining reddish-purple solid was transferred into a vial using 18 mL THF. The THF was removed under reduced pressure, resulting in a reddish-purple solid. 6 mL of diethyl ether was added and the mixture was kept at -35 °C. After one day, the diethyl ether solution was filtered and **Y-naph** was collected as a reddish-purple solid on the medium frit. Yield: 0.214 g, 62.6 %. ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 5.09 and 3.94 (t, 8H, C*H* of naphthalene), 4.33, 4.13 and 3.87 (b, 24H, C*H* on Cp rings and CH_2O), 1.42 (b, 8H, CH_2CH$_2$O), 1.07 (s, 36H, SiCCH_3), and 0.22 and 0.13 (s, 24H, SiCH_3). ^{1}H NMR (500 MHz, C_4D_8O, 25 °C) δ, ppm: 5.01 and 3.66 (t, 8H, C*H* of naphthalene), 4.25, and 3.83 (b, 16H, C*H* on Cp rings), 0.73 (s, 36H, SiCCH_3), and -0.03 (s, 24H, SiCH_3). ^{13}C NMR (126 MHz, C_4D_8O, 25 °C) δ, ppm: 158.3, 118.3 and 94.3 (*C* and *C*H on naphthalene), 108.4 (*C*N on Cp rings), signals of *C*H on Cp rings were covered by solvent C_4D_8O peaks, 28.5 (SiC*C*H$_3$), 21.2 (Si*C*CH$_3$) and -1.7 (Si*C*H$_3$). Anal. (%): Calcd. for $C_{62}H_{100}N_4Fe_2O_2Si_4Y_2$: C, 55.77; H, 7.55; N, 4.20. Found: C, 55.22; H, 7.20; N, 4.53.

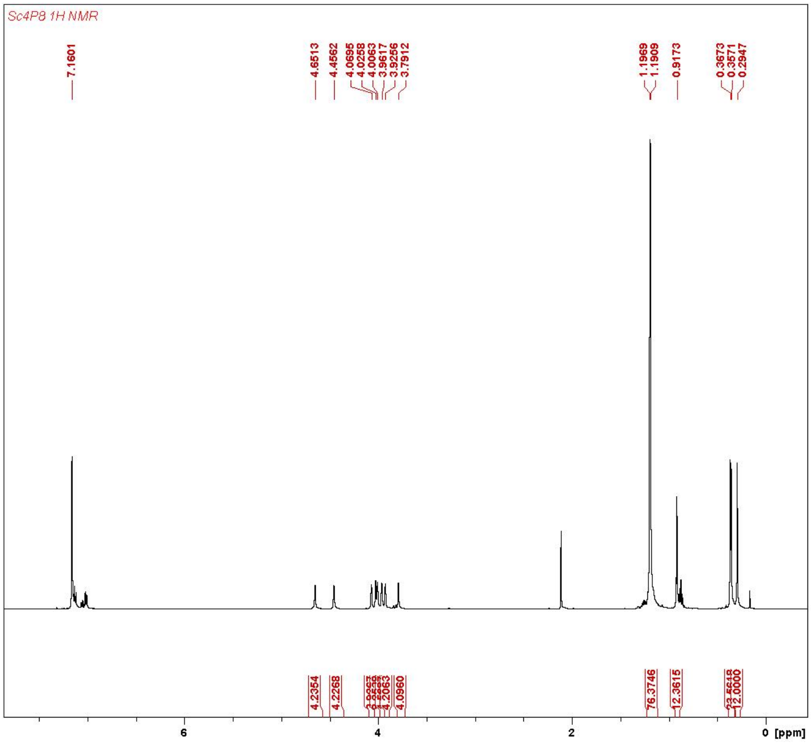
Synthesis of [(NN^{fc})Y(THF)]$_3$P$_7$ (Y$_3$P$_7$). Y-naph (0.150 g, 0.112 mmol) was dissolved in 10 mL of THF and cooled down to -78 °C with a dry ice/acetone bath for 15 min. P_4 (0.0189 g, 0.153 mmol) was then added as a THF solution. The color of solution gradually changed from reddish-purple to orange. After stirring for 1 h at 25 °C, the volatiles were removed under reduced pressure. The resulting orange solid was washed with pentane until the pentane wash was very light yellow. **Y$_3$P$_7$** was isolated as a yellow powder. Yield: 0.106 g, 69.7%. ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 4.18, 3.94, and 3.41 (b, 24H, C*H* on Cp rings), 4.04 (b, 12H, CH_2O), 1.48 (b, 12H, CH_2CH$_2$), 1.19 (s, 54H, SiCCH_3), and 0.61, and 0.28 (s, 24H, SiCH_3). Due to low solubility of **Y$_3$P$_7$** in C_6D_6, the ^{13}C NMR experiment was performed at higher temperature (75 °C). The ^{1}H NMR spectrum at 75 °C is also included here since it was different from that at 25 °C. ^{1}H NMR (500 MHz, C_6D_6, 75 °C) δ, ppm: 4.13, 4.04, and 3.55 (b, 24H, C*H* on Cp rings), 3.95 (b, 12H, CH_2O), 1.55 (b, 12H, CH_2CH$_2$), 1.13 (s, 54H, SiCCH_3), and 0.55, and 0.29 (s, 24H, SiCH_3). ^{13}C NMR (126 MHz, C_6D_6, 75 °C) δ, ppm: 106.1 (*C*N on Cp rings), 70.3, 69.1, and 66.4 (*C*H on Cp rings), 68.4 (*C*H$_2$O), 28.3 (SiC*C*H$_3$), 25.5 (*C*H$_2$CH$_2$O), 20.6 (Si*C*CH$_3$), and -0.5 (Si*C*H$_3$). ^{31}P NMR (122 MHz, C_6D_6, 25 °C) δ, ppm: -20.4 (b, 3P, P_{edge}), -81.8 (b, 1P, P_{cap}), and -130.4 (b, 3P, P_{bottom}). Anal. (%): Calcd. for $C_{78}H_{138}N_6Fe_3O_3P_7Si_6Y_7$ with 1 molecule of toluene, C_7H_8: C, 48.16; H, 6.94; N, 3.96. Found: C, 47.88; H, 6.99; N, 3.87.

General reaction set-up for M$_3$P$_7$ (M = Sc, Y) and TMSI (trimethylsilyl iodide). 0.015 g **M$_3$P$_7$** was dissolved in C_6D_6 in a J-Young tube. Excess TMSI was added at room temperature and the reaction was monitored by ^{1}H NMR spectroscopy. For M = Sc, no obvious change was observed after 1 h at room temperature; so, the J-Young tube was placed in a 50 °C oil bath. The transformation reached completion after 23 h at 50 °C with the formation of (NN^{fc})ScI and $P_7(TMS)_3$, which was confirmed by ^{31}P NMR spectra. For M = Y, the transformation took place at room temperature and reached completion after 9 h. The formation of $(NN^{fc})YI$ and $P_7(TMS)_3$ were confirmed by ^1H and ^{31}P NMR spectroscopy, respectively.

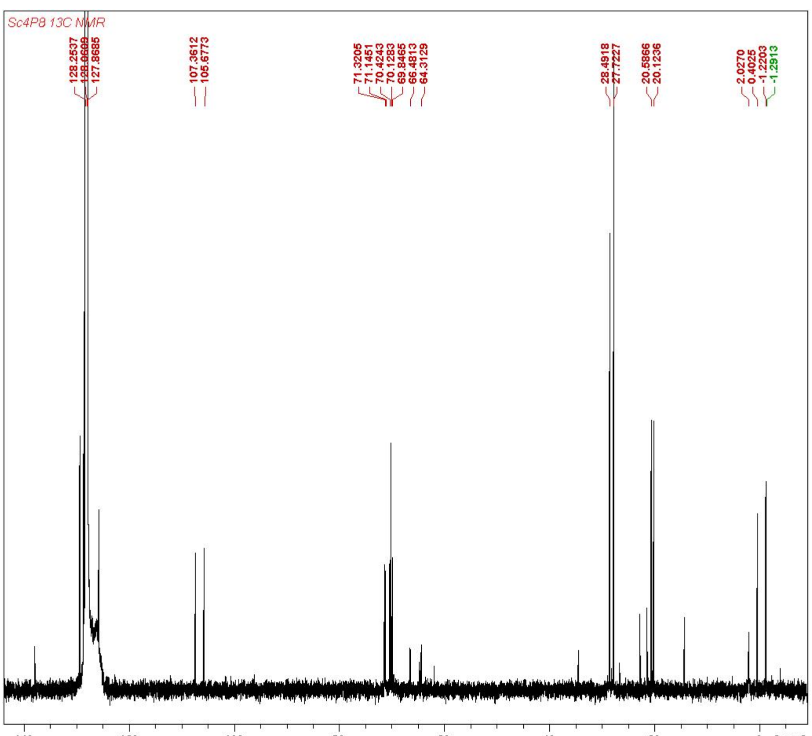
Note: The attempt to transfer the P_8^{4-} unit in **Sc_4P_8** with TMSI was not successful. Even after prolonged heating (2 days) at 100 °C with excess TMSI, **Sc_4P_8** remained intact.

2. NMR Spectra

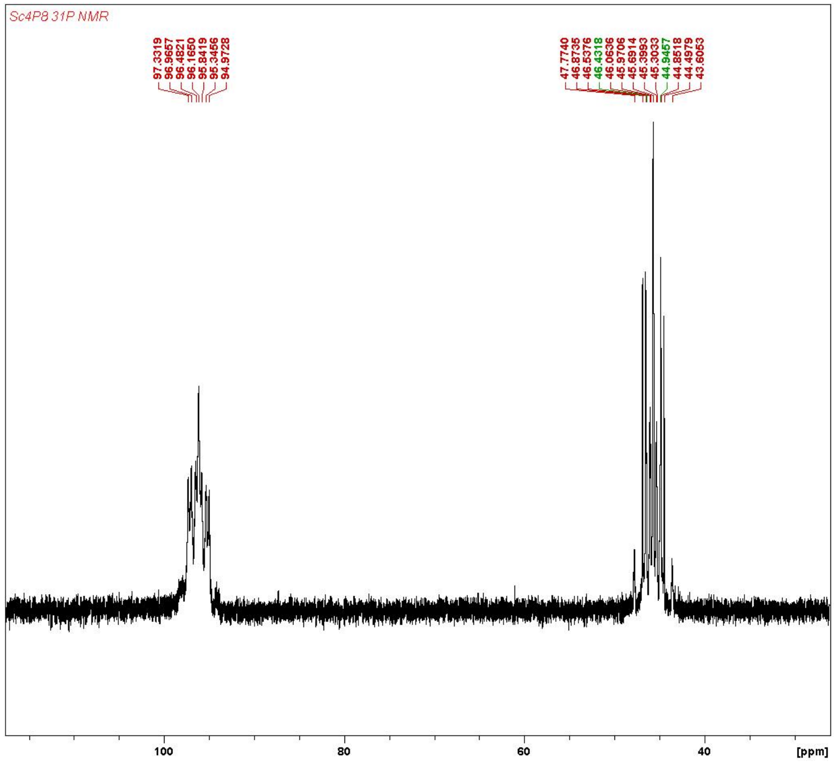
^{1}H NMR spectrum of **Sc_4P_8** (500 MHz, C_6D_6, 25 °C)



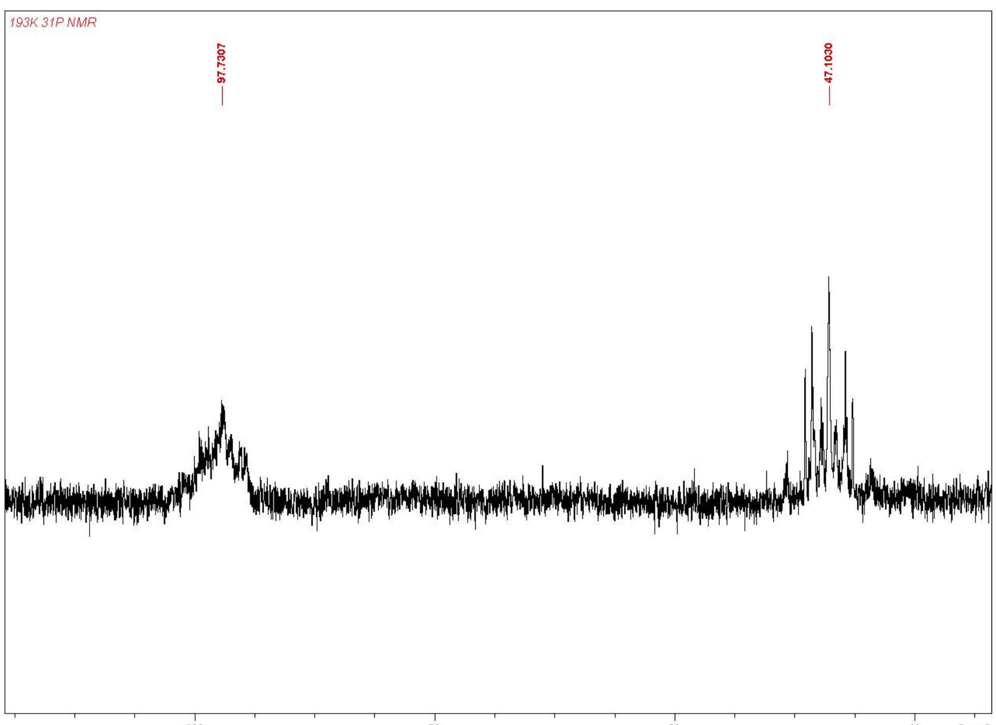
^{13}C NMR spectrum of **Sc_4P_8** (126 MHz, C_6D_6, 25 °C)



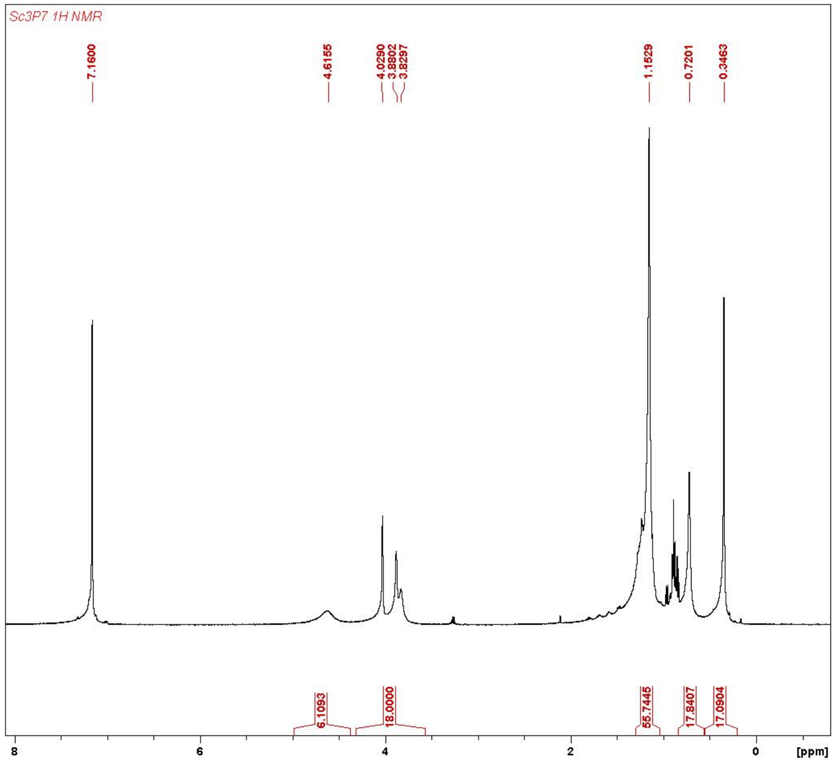
^{31}P NMR spectrum of $\mathbf{Sc_4P_8}$ (203 MHz, C_6D_6, 25 °C)



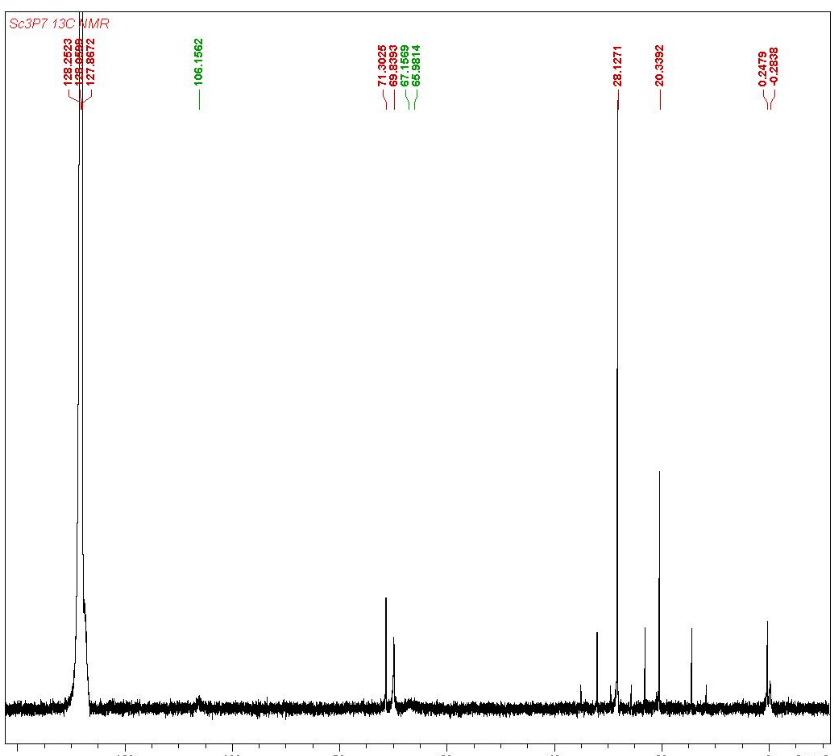
^{31}P NMR spectrum of $\mathbf{Sc_4P_8}$ (122 MHz, C_7D_8, -80 °C)



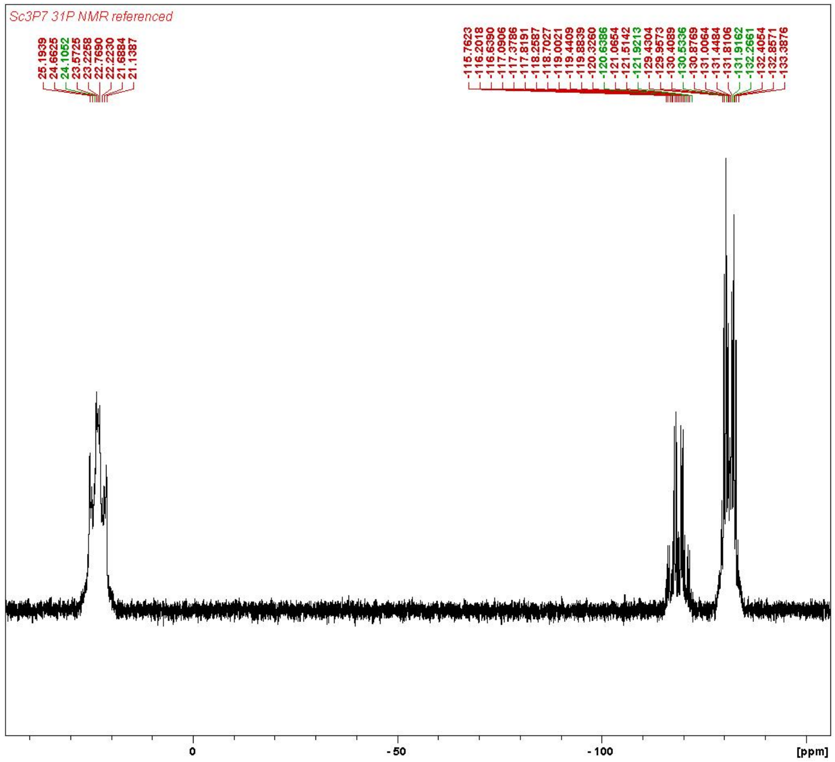
^{1}H NMR spectrum of **Sc_3P_7** (500 MHz, C_6D_6, 25°C)



^{13}C NMR spectrum of **Sc_3P_7** (500 MHz, C_6D_6, 25°C)

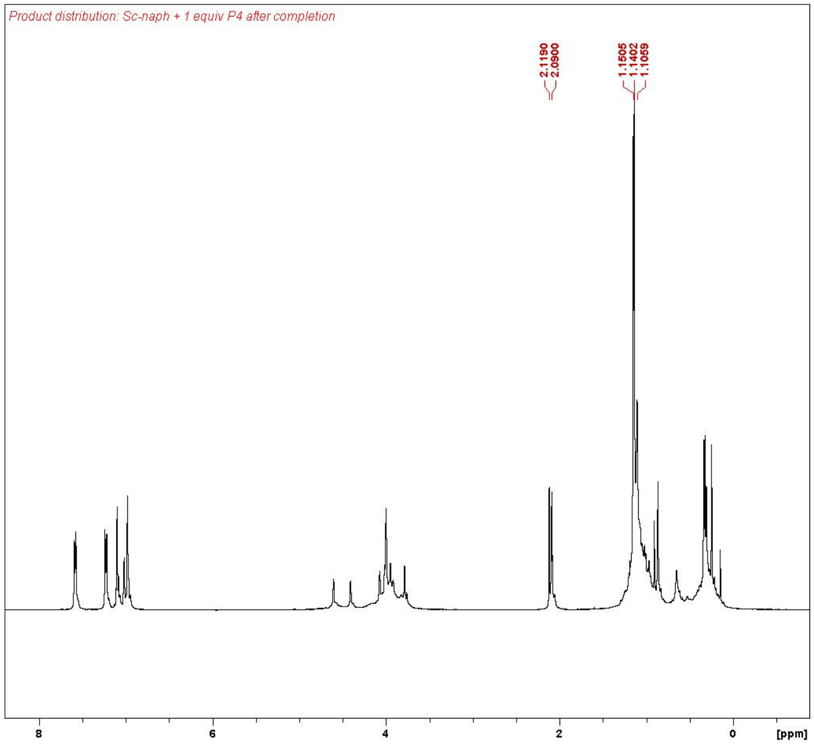


^{31}P NMR spectrum of **Sc_3P_7** (122 MHz, C_6D_6, 25°C)

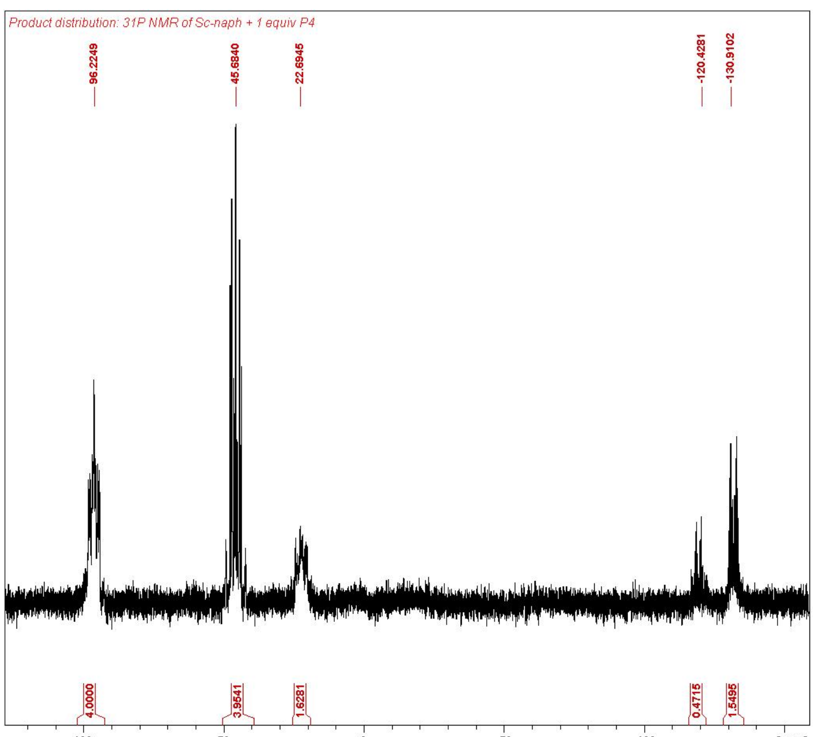


Product distribution of **Sc-naph** with 1.03 equiv of P_4:

^{1}H NMR spectrum (500 MHz, C_7D_8, 25°C)

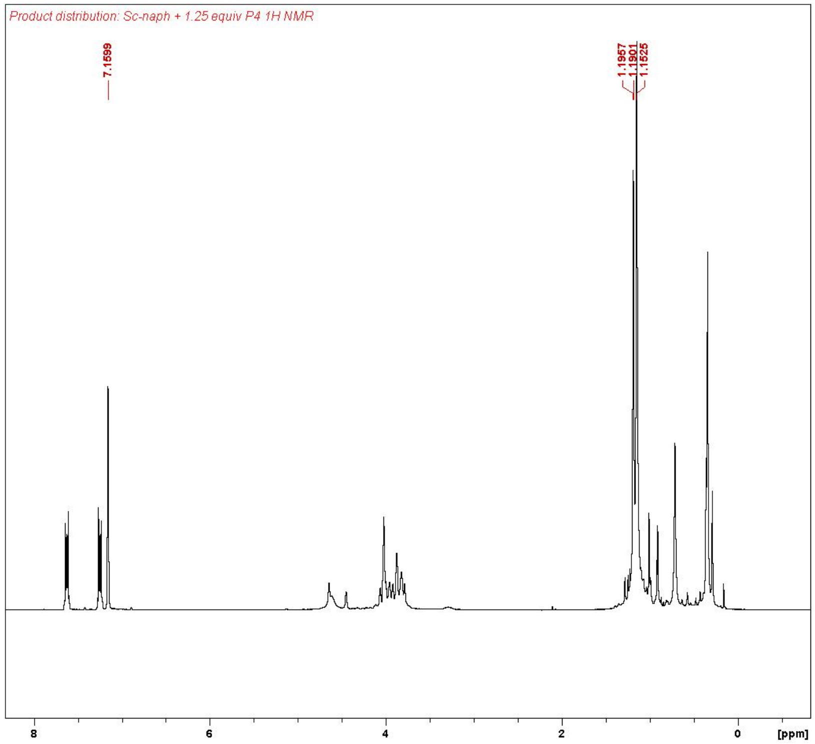


^{31}P NMR spectrum (122 MHz, C_7D_8, 25°C)

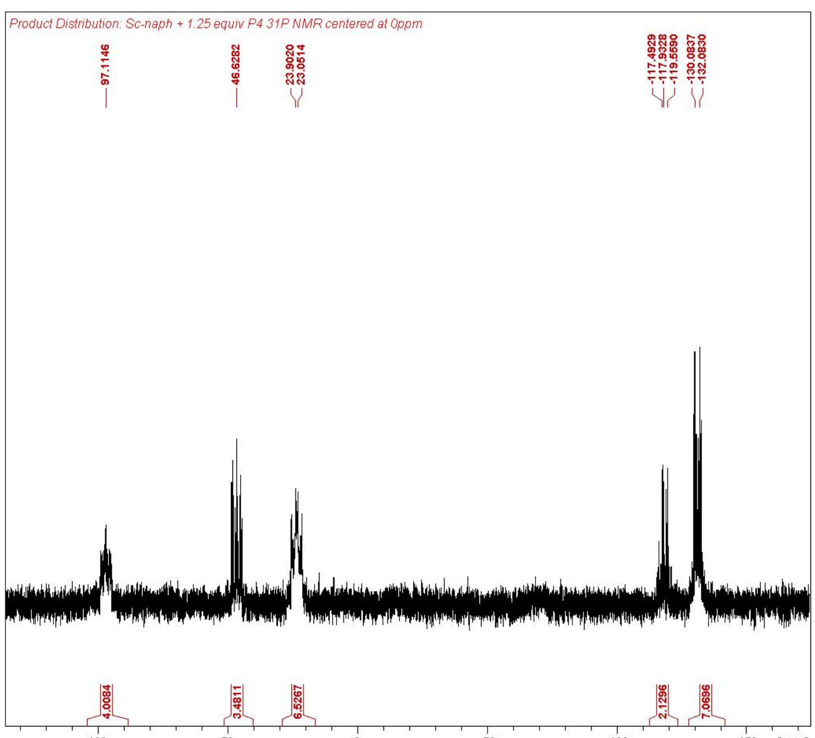


Product distribution of **Sc-naph** with 1.24 equiv of P_4:

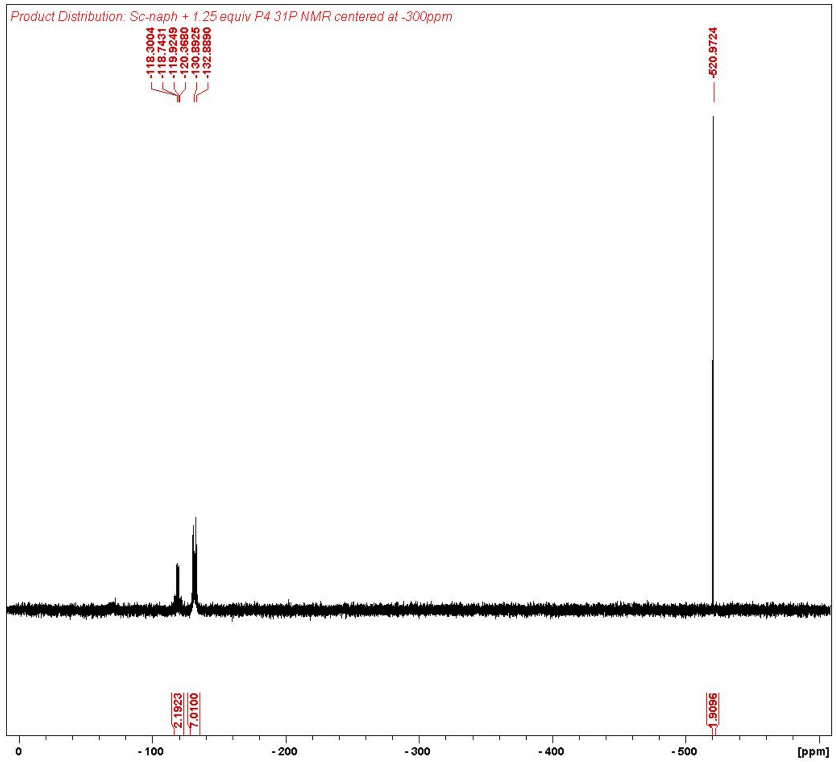
^{1}H NMR spectrum (300 MHz, C_6D_6, 25°C)



^{31}P NMR spectrum (122 MHz, C_6D_6, 25°C, centered at 0 ppm)

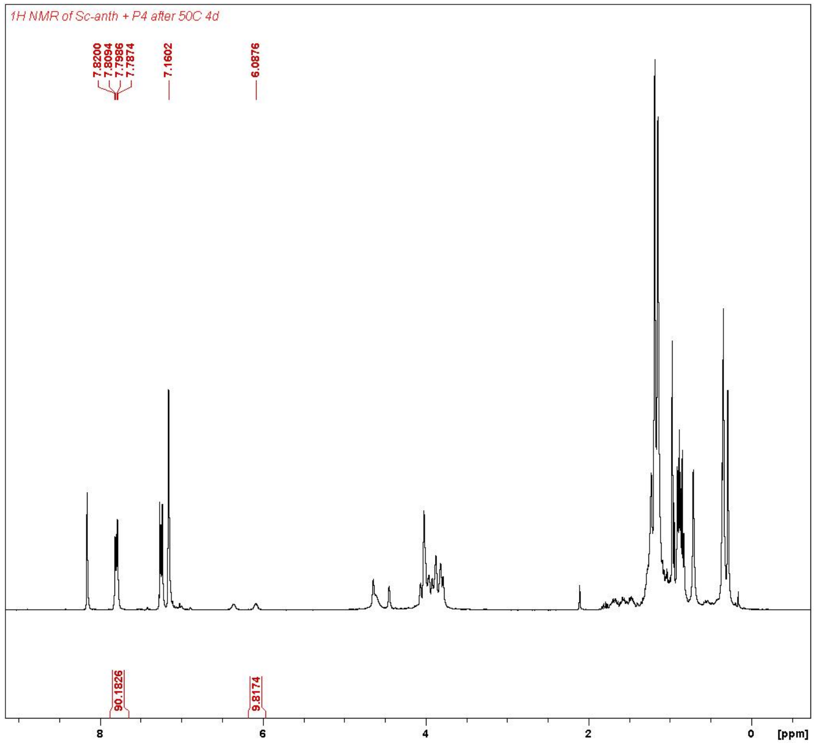


^{31}P NMR spectrum (122 MHz, C_6D_6, 25°C, centered at -300 ppm)

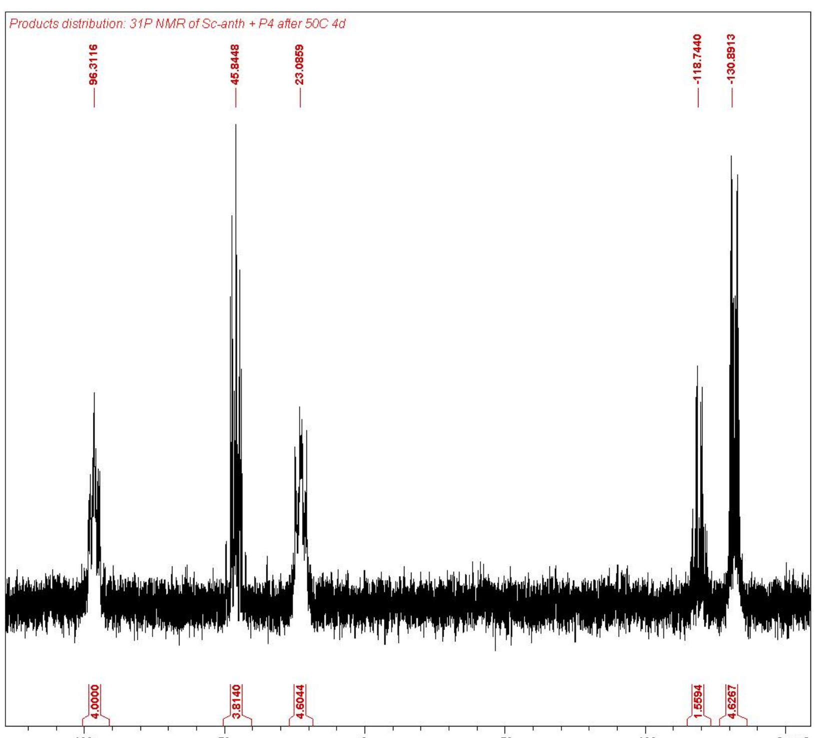


Product distribution of **Sc-anth** with 0.98 equiv of P_4:

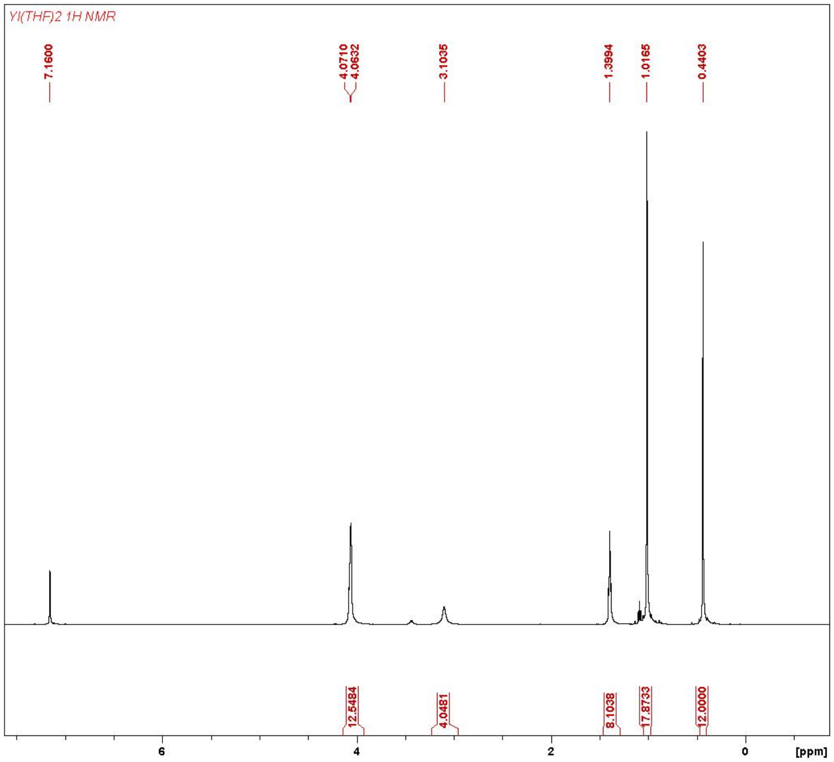
^{1}H NMR spectrum (300 MHz, C_6D_6, 25°C)



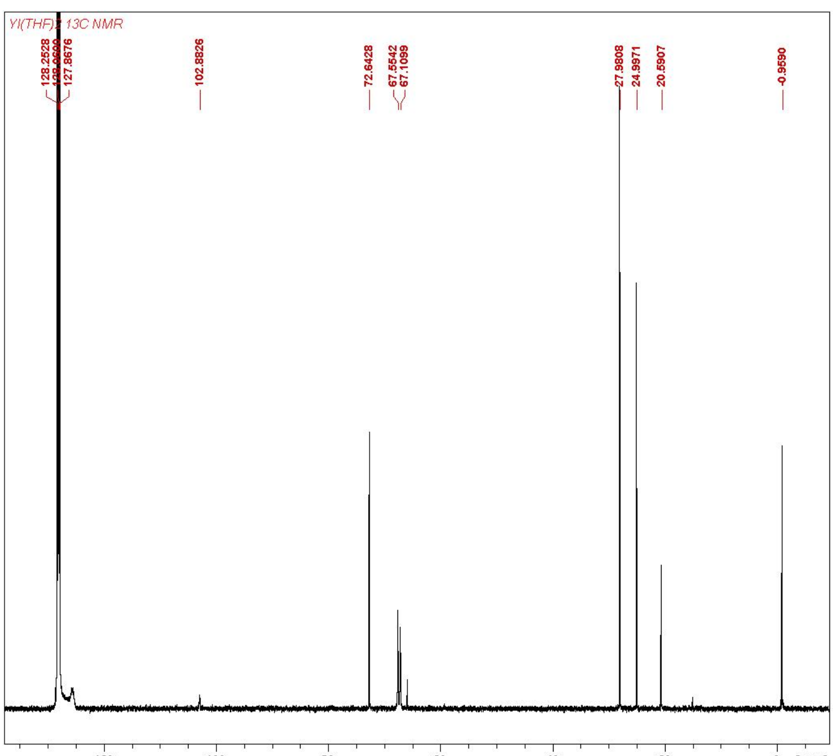
^{31}P NMR spectrum (122 MHz, C_6D_6, 25°C)



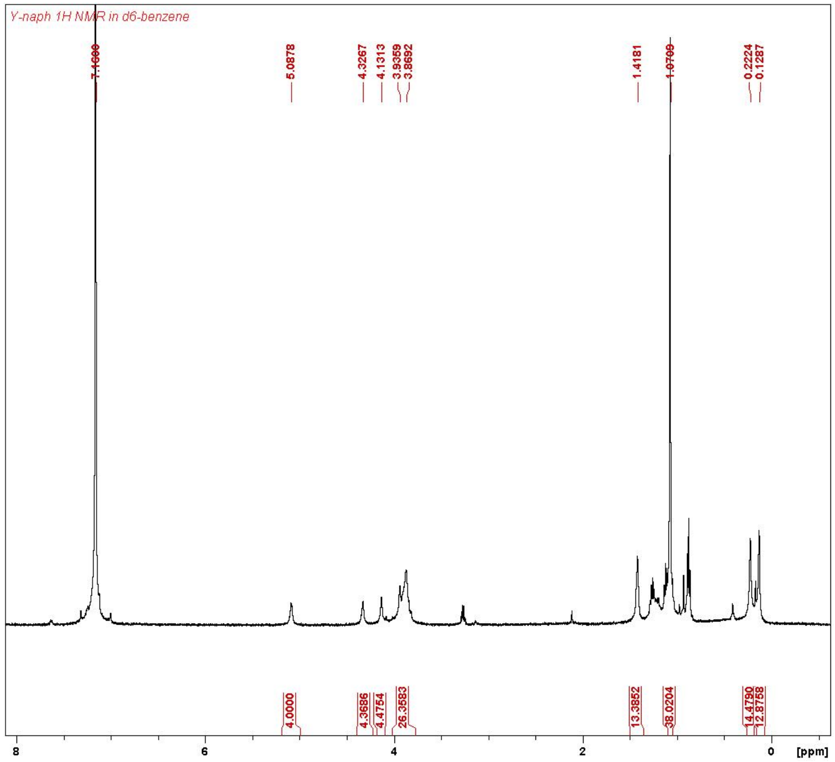
^{1}H NMR spectrum of **(NN^{fc})YI(THF)$_2$** (500 MHz, C_6D_6, 25°C)



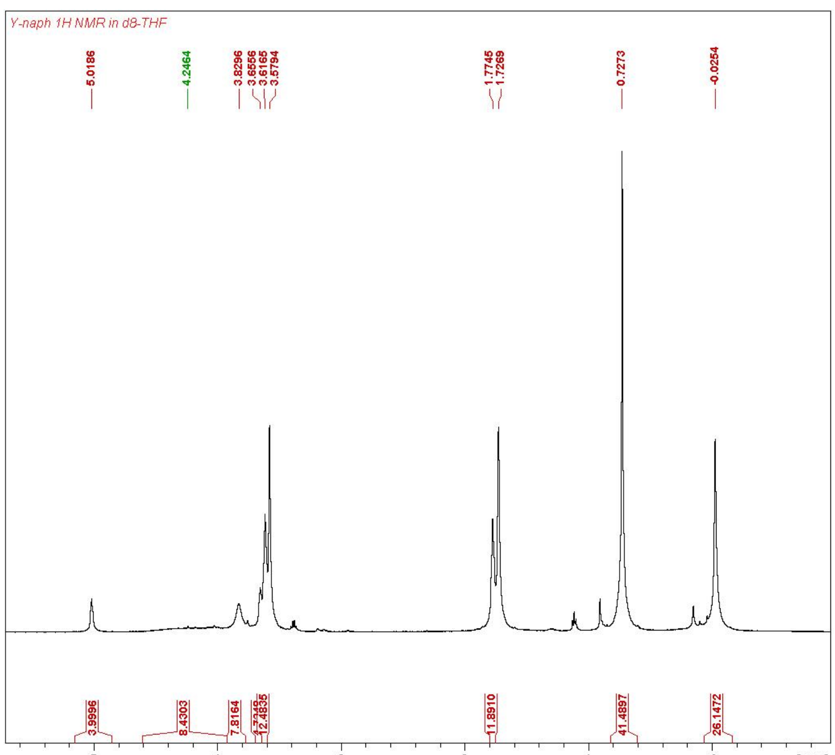
^{13}C NMR spectrum of **(NN^{fc})YI(THF)$_2$** (500 MHz, C_6D_6, 25°C)



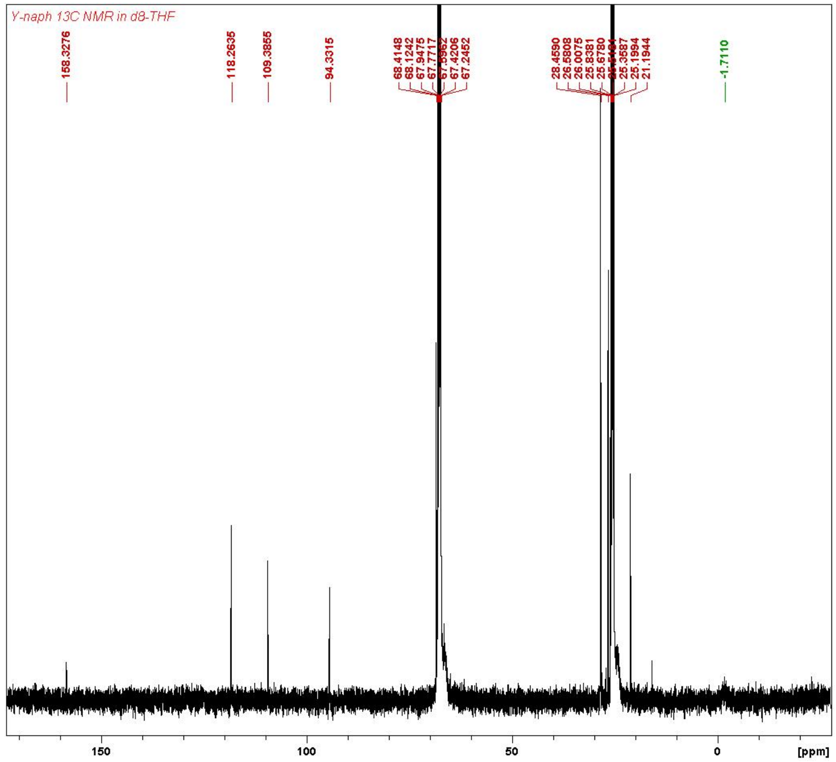
^{1}H NMR spectrum of **Y-naph** (500 MHz, C_6D_6, 25°C)



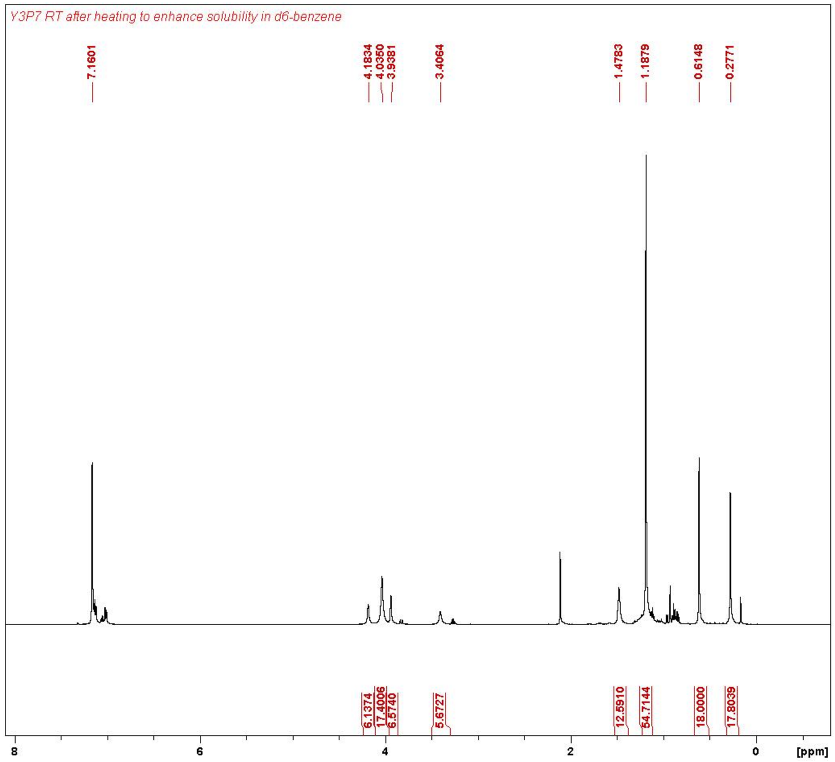
^{1}H NMR spectrum of **Y-naph** (500 MHz, C_4D_8O, 25°C)



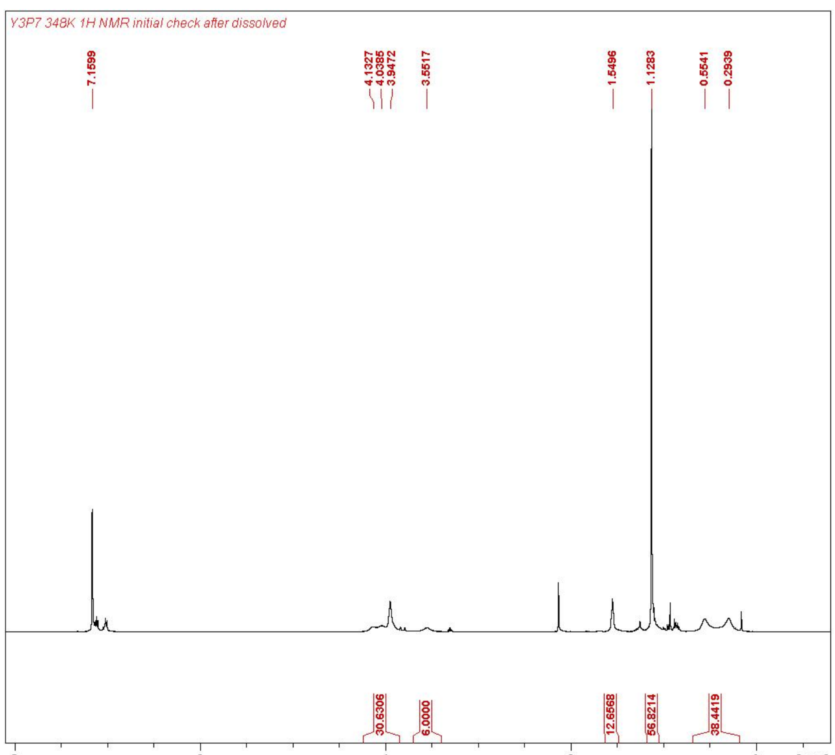
^{13}C NMR spectrum of **Y-naph** (500 MHz, C_4D_8O, 25°C)



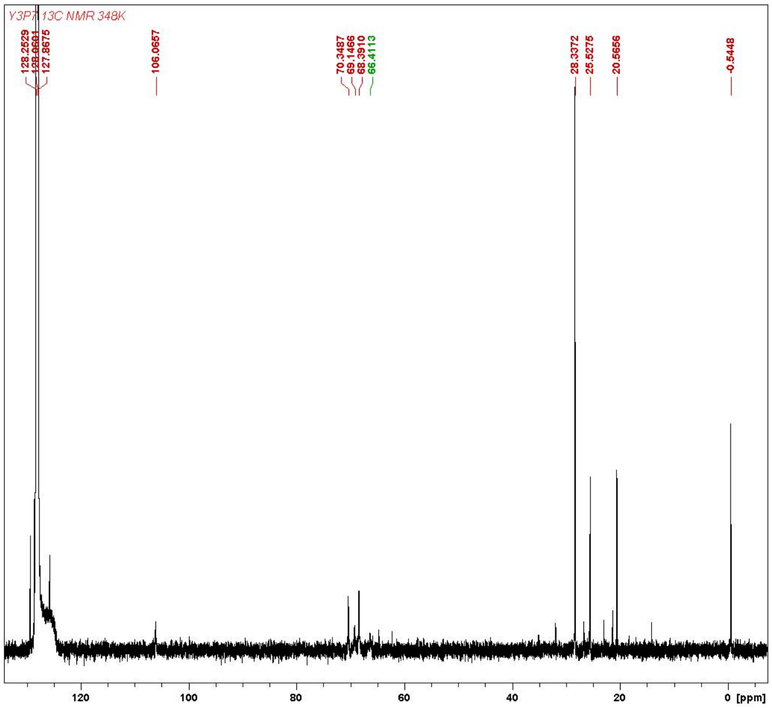
^{1}H NMR spectrum of $\mathbf{Y_3P_7}$ (500 MHz, C_6D_6, 25°C)



^{1}H NMR spectrum of $\mathbf{Y_3P_7}$ (500 MHz, C_6D_6, 75°C)

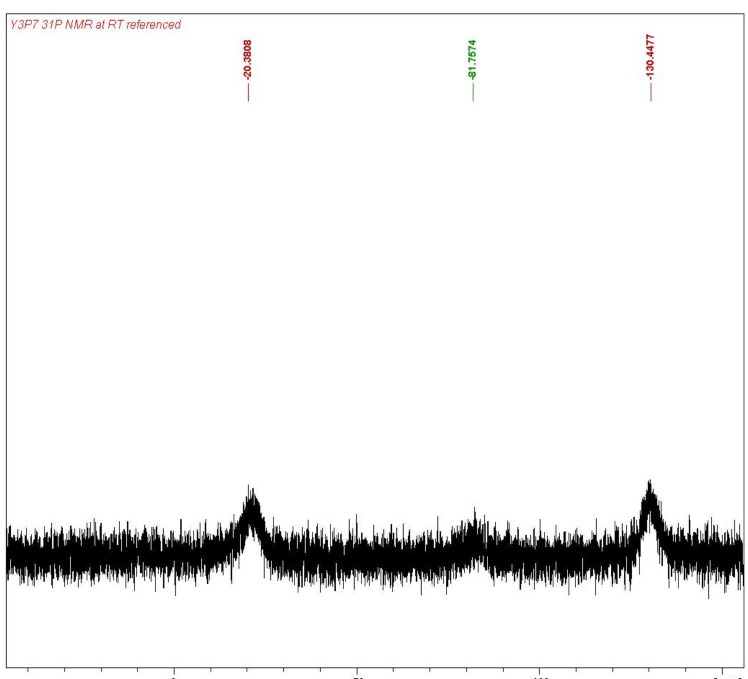


^{13}C NMR spectrum of $\mathbf{Y_3P_7}$ (126 MHz, C_6D_6, 75°C)

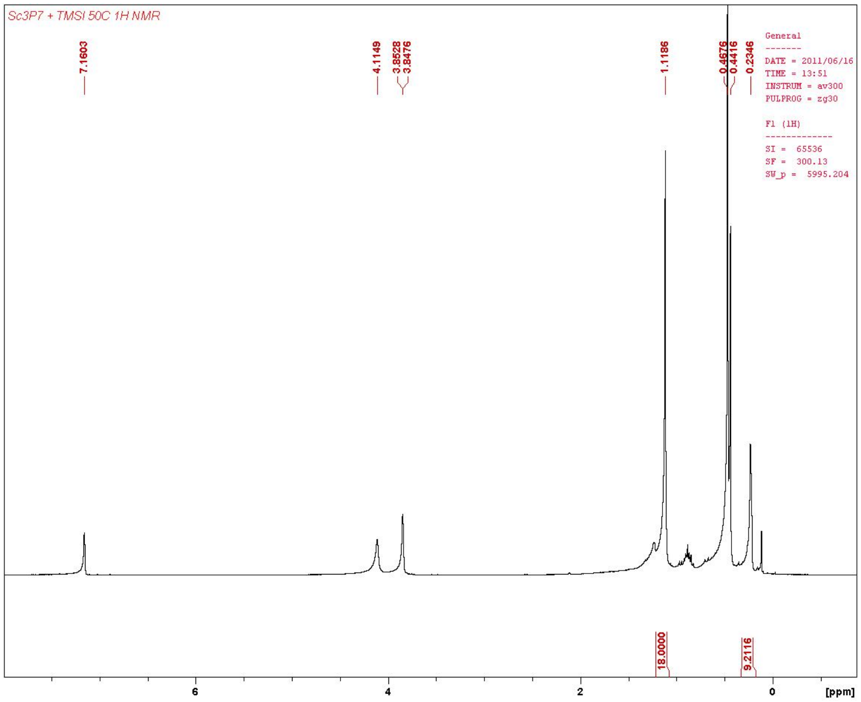


^{31}P NMR spectrum of $\mathbf{Y_3P_7}$ (122 MHz, C_6D_6, 25°C)

Note: The low solubility of $\mathbf{Y_3P_7}$ in C_6D_6 prevents getting a high resolution ^{31}P NMR spectrum. An attempt to use d_8-THF as a solvent resulted in the decomposition of $\mathbf{Y_3P_7}$.

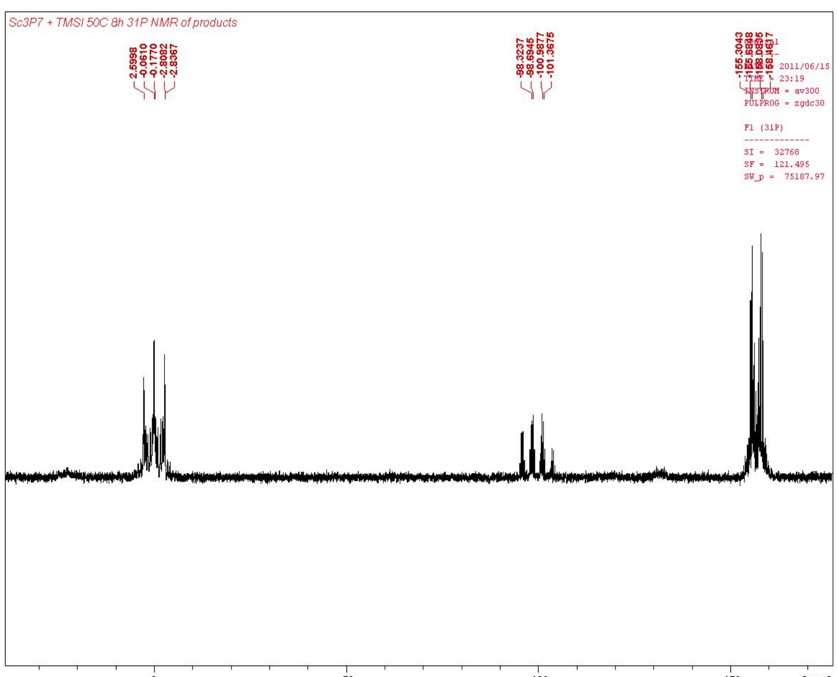


^{1}H NMR spectrum of the reaction mixture of **Sc_3P_7** and excess Me_3SiI after 23 h at 50 °C (300 MHz, C_6D_6, 25 °C)

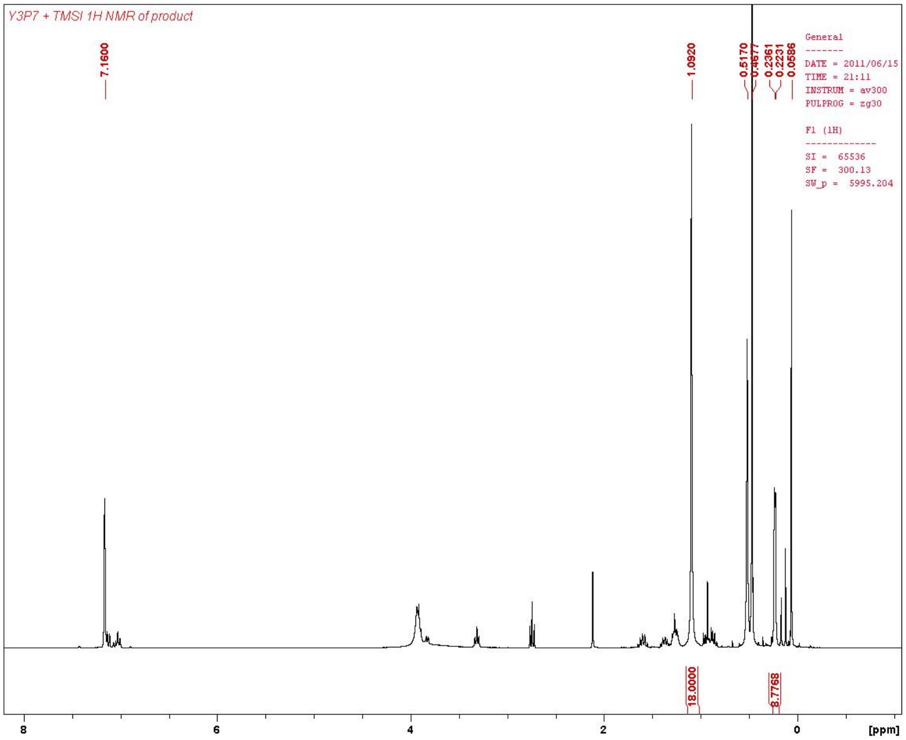


^{31}P NMR spectrum of the reaction mixture of **Sc_3P_7** and excess Me_3SiI after 8 h at 50 °C (122 MHz, C_6D_6, 25 °C)

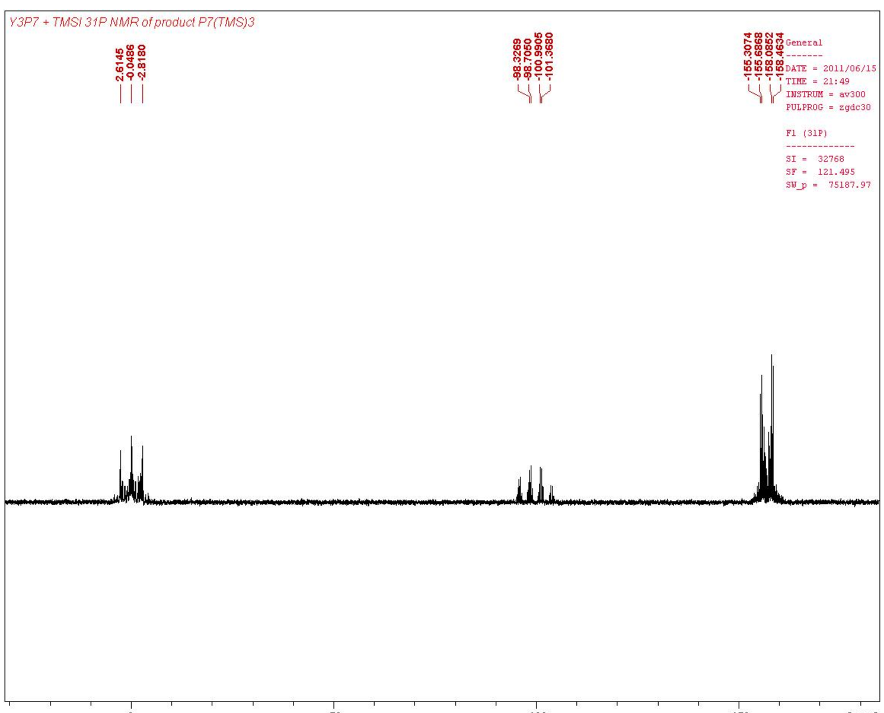
Note: the small, broad peaks belong to unreacted **Sc_3P_7**.



^{1}H NMR spectrum of the reaction mixture of $\mathbf{Y_3P_7}$ and excess Me_3SiI after 9 h at 25 °C (300 MHz, C_6D_6, 25 °C)

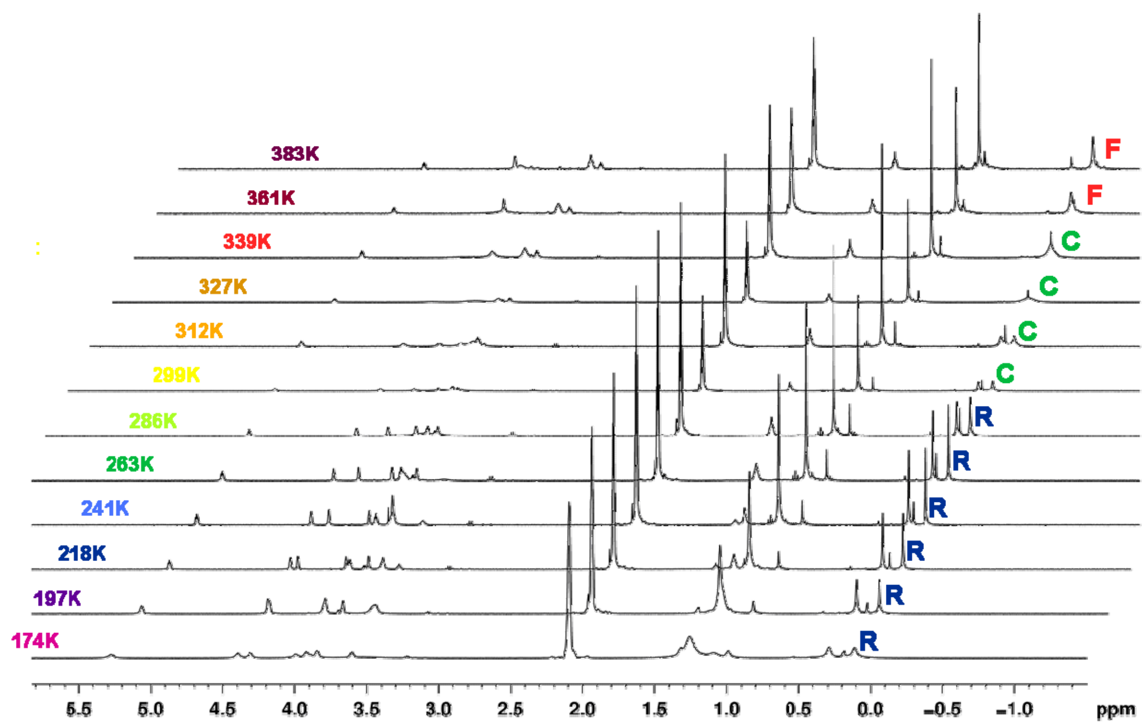


^{31}P NMR spectrum of the reaction mixture of $\mathbf{Y_3P_7}$ and excess Me_3SiI after 9 h at 25 °C (122 MHz, C_6D_6, 25 °C)



3. Variable Temperature ^{1}H NMR spectra of Y-anth (500 MHz, C_7D_8)

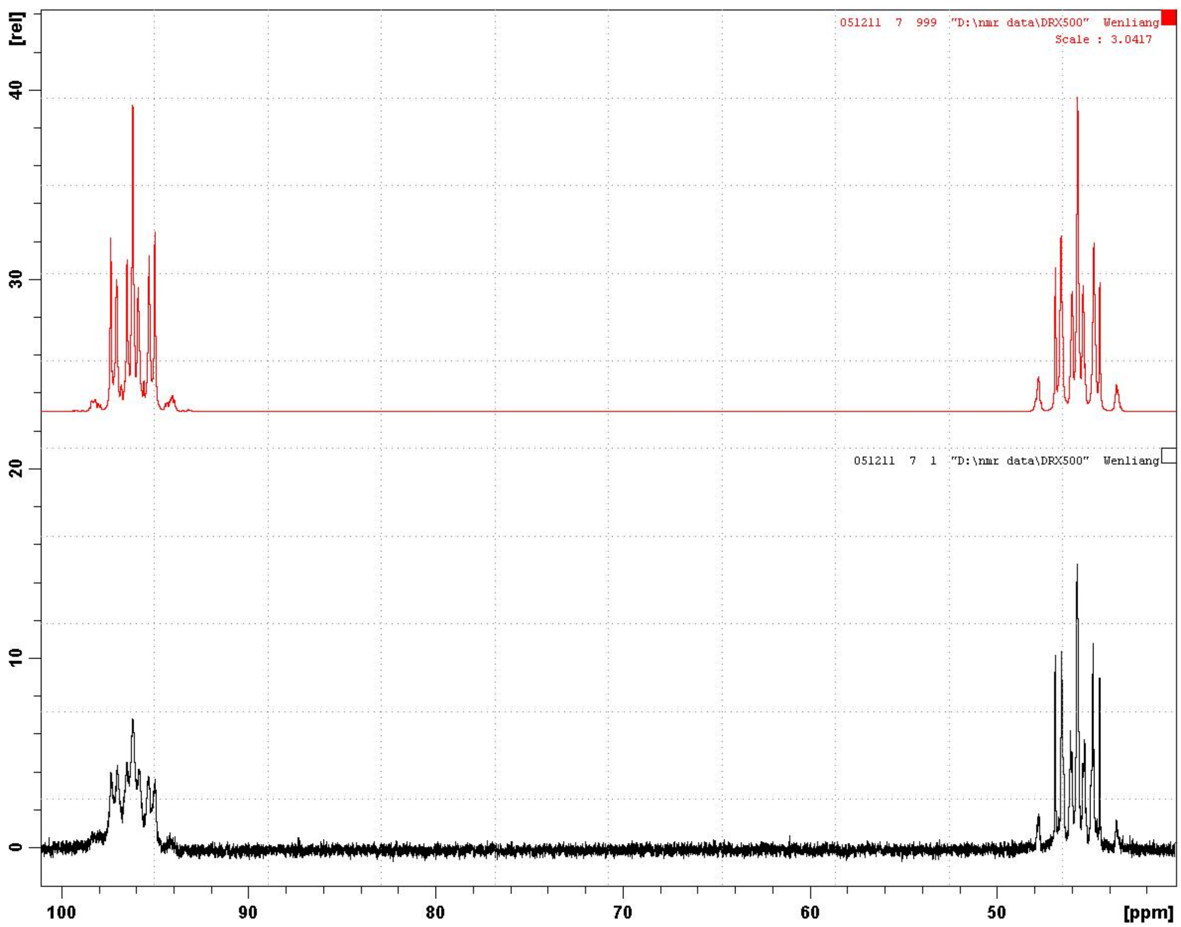
R = Restricted Rotation C = Coalescence F = Free Rotation



4. Simulation of ^{31}P NMR spectra

Note: The simulation was performed with Topspin^{TM} software.

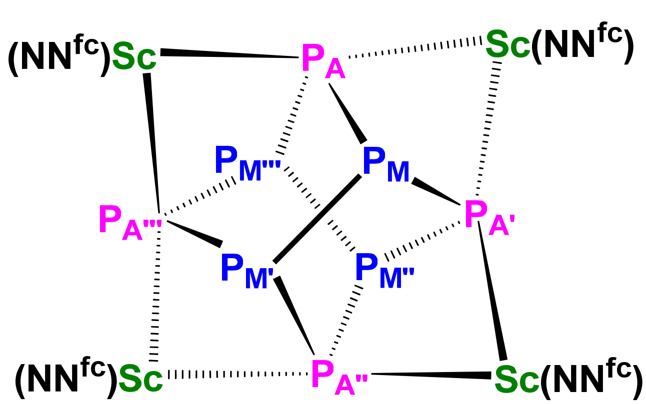
Sc_4P_8: AA'A"A'"MM'M"M'" spin system



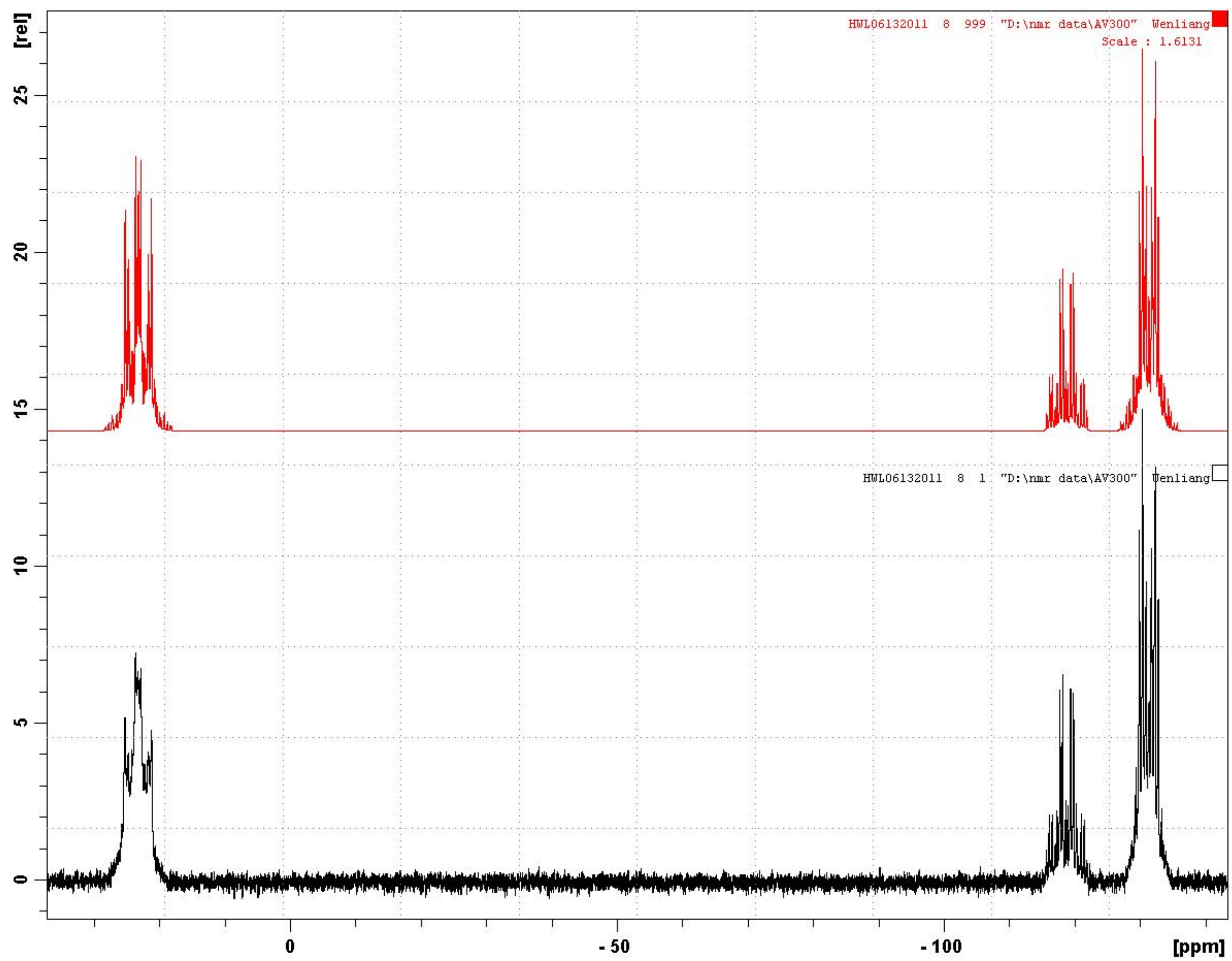
Top: simulated spectrum; bottom: experimental spectrum. $^{1}J_{AM}$ is an abbreviation for $^{1}J_{PA\text{-}PM}$ which was also applied to other J values for **Sc_4P_8**, **Sc_3P_7** and **Y_3P_7**.

$\boxed{\mathbf{Sc_4P_8}}$

$^{1}J_{AM}$ = 255 Hz
$^{1}J_{MM'}$ = 255 Hz
$^{2}J_{AA'}$ = -10 Hz
$^{2}J_{AM'}$ = -15 Hz
$^{2}J_{MM''}$ = -10 Hz
$^{3}J_{AA''}$ = 20 Hz



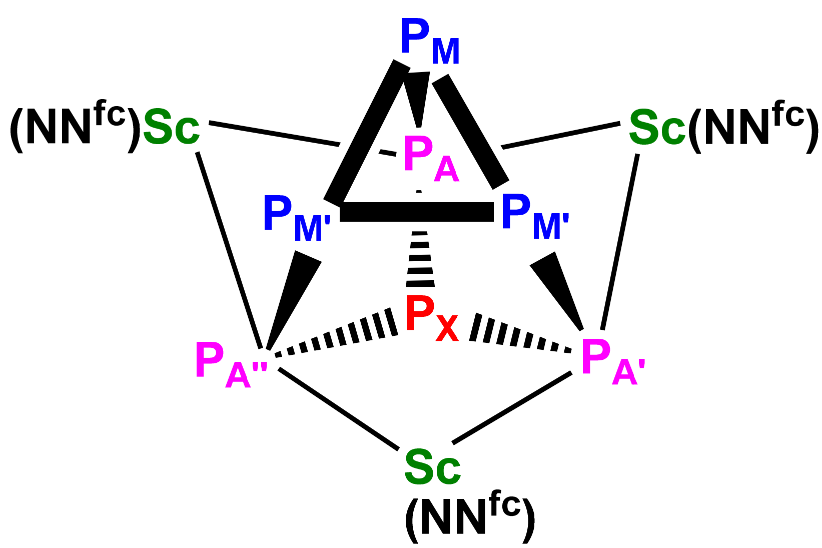
Sc_3P_7: AA'A"MM'M"X spin system



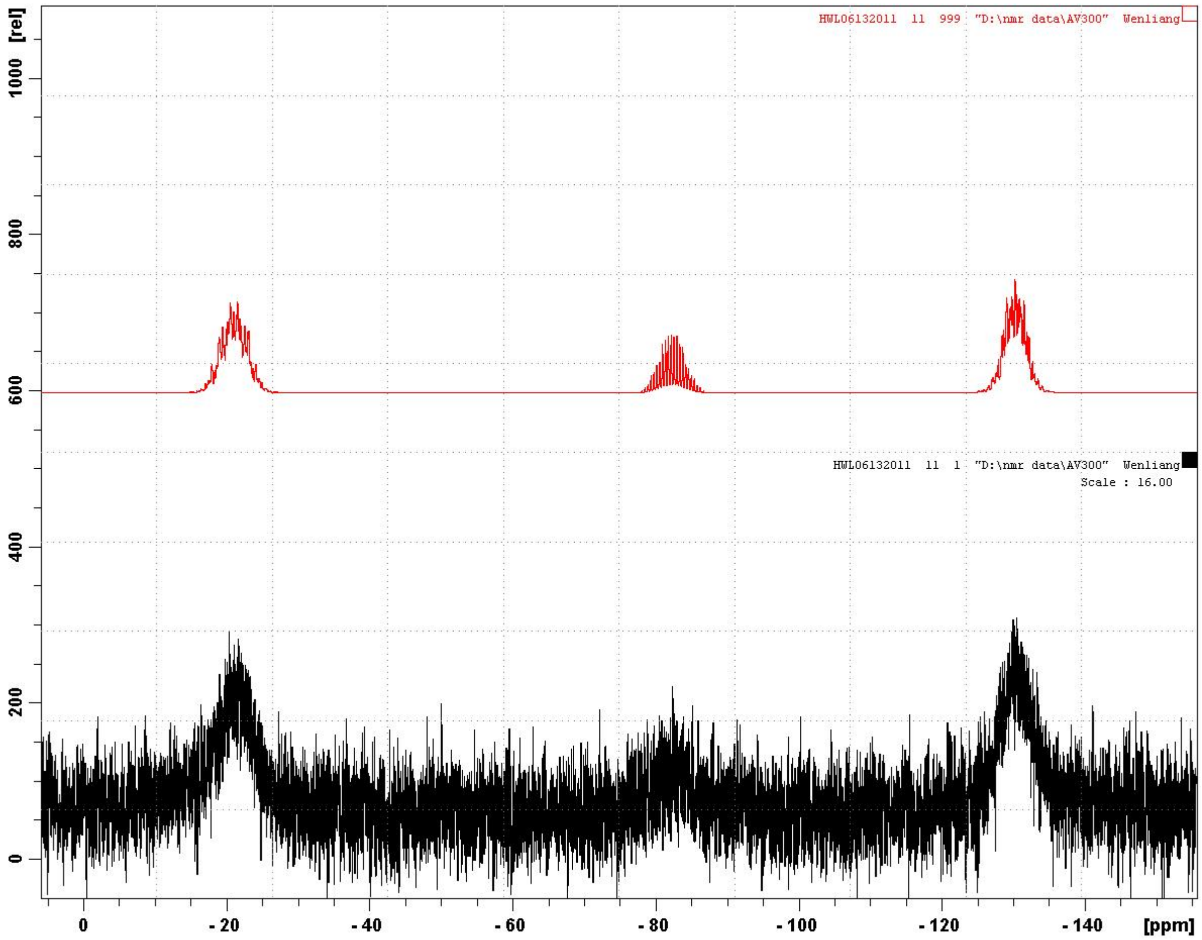
Top: simulated spectrum; bottom: experimental spectrum.

$\boxed{Sc_3P_7}$

$^1J_{AM}$ = 320 Hz
$^1J_{MM'}$ = 230 Hz
$^1J_{AX}$ = 195 Hz
$^2J_{AA'}$ = -55 Hz
$^2J_{AM'}$ = -12 Hz
$^2J_{MX}$ = -53 Hz



Y_3P_7: AA'A"MM'M"X (YY'Y") spin system



Top: simulated spectrum; bottom: experimental spectrum (see previous note for low resolution explanation). Because of the low resolution, the J_{PP} values were adopted from **Sc_3P_7** and only J_{YP} values were tuned to simulate the spectrum.

$\boxed{Y_3P_7}$

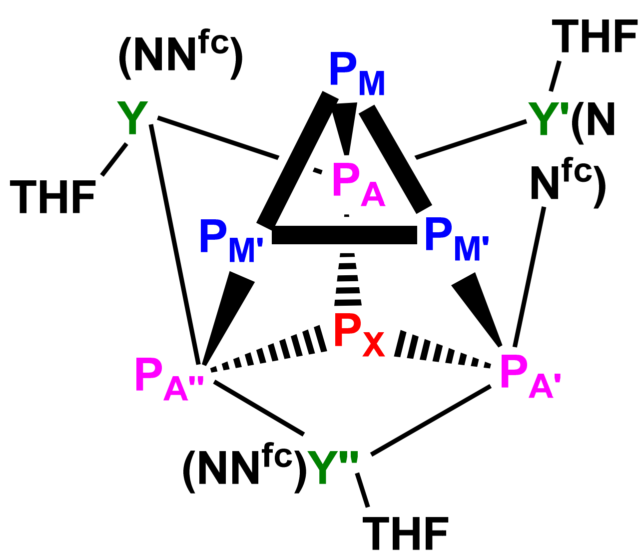
$^1J_{YA}$ = 150 Hz

$^2J_{YA'}$ = -30 Hz

$^2J_{YX}$ = 100 Hz

$^2J_{YM}$ = 125 Hz

$^2J_{YM'}$ = -25 Hz



5. X-ray crystallography

YI(THF)$_2$

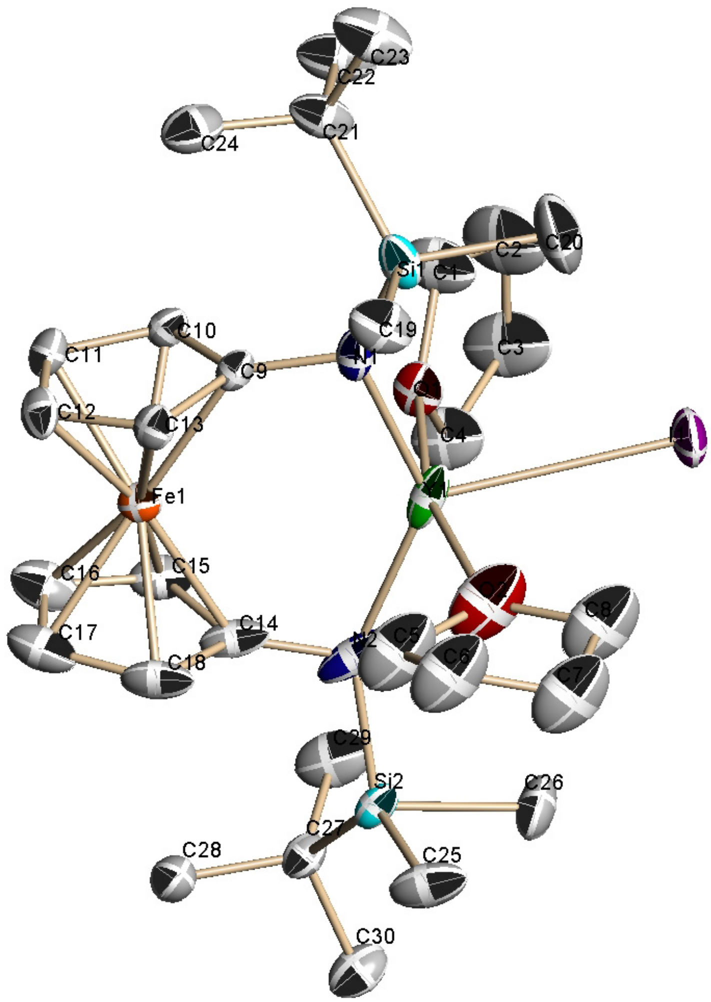


Figure SX1. Thermal-ellipsoid (50% probability) representation of **YI(THF)$_2$**. Hydrogen atoms and disordered counterparts were omitted for clarity.

Single crystals were grown from a diluted diethyl ether solution layered with pentane after storing at -35 °C. The iodide and one of the silyl groups were disordered; this disorder was modeled. A total of 17684 reflections ($-15 \leq h \leq 15$, $-16 \leq k \leq 16$, $-23 \leq l \leq 23$) were collected at T = 100(2) K with $2\theta_{max}$ = 61.50°, of which 9851 were unique. The residual peak and hole electron density were 2.23 and -2.62 eA^{-3}. The least-squares refinement converged normally with residuals of R_1 = 0.0516 and GOF = 1.043. Crystal and refinement data for **YI(THF)$_2$**: formula $C_{30}H_{54}N_2Si_2FeYIO_2$, space group P-1, a = 11.140(3), b = 11.596(3), c = 16.156(5), α = 101.325(3), β = 92.432(3), γ = 118.211(2)°, V = 1781.1(8) Å^3, Z = 2, μ = 2.989 mm^{-1}, F(000) = 820, R_1 = 0.0655 and wR_2 = 0.1329 (based on all 9851 data, I > $2\sigma(I)$).

Y-naph

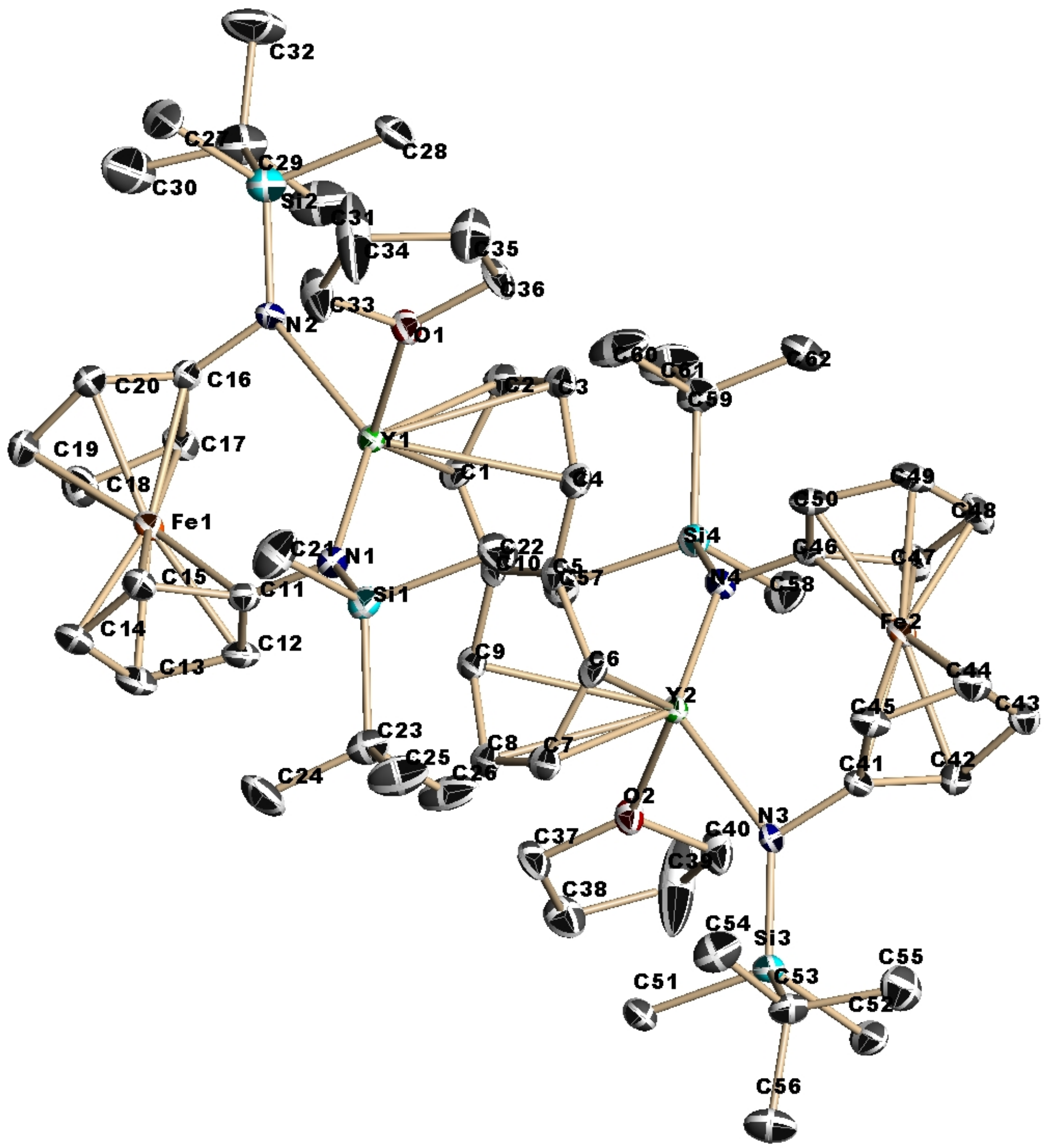


Figure SX2. Thermal-ellipsoid (50% probability) representation of **Y-naph**. Hydrogen and solvent atoms were omitted for clarity.

Single crystals suitable for X-ray diffraction were grown from a concentrated diethyl ether solution stored at -35 °C. A total of 69888 reflections ($-25 \leq h \leq 25$, $-13 \leq k \leq 13$, $-33 \leq l \leq 32$) were collected at T = 100(2) K with $2\theta_{max}$ = 49.00°, of which 11705 were unique. The residual peak and hole electron density were 3.75 and -1.16 eA^{-3}. The least-squares refinement converged normally with residuals of R_1 = 0.0473 and GOF = 1.083. Crystal and refinement data for **Y-naph**: formula $C_{62}H_{100}N_4Si_4Fe_2Y_2O_2(C_7H_8)$, space group $P2_1/n$, a = 22.149(5), b = 11.297(2), c = 28.352(6), β = 94.925(2)°, V = 7068(3) Å^3, Z = 4, μ = 2.141 mm^{-1}, F(000) = 3008, R_1 = 0.0655 and wR_2 = 0.1226 (based on all 11705 data, I > 2σ(I)).

Sc_4P_8

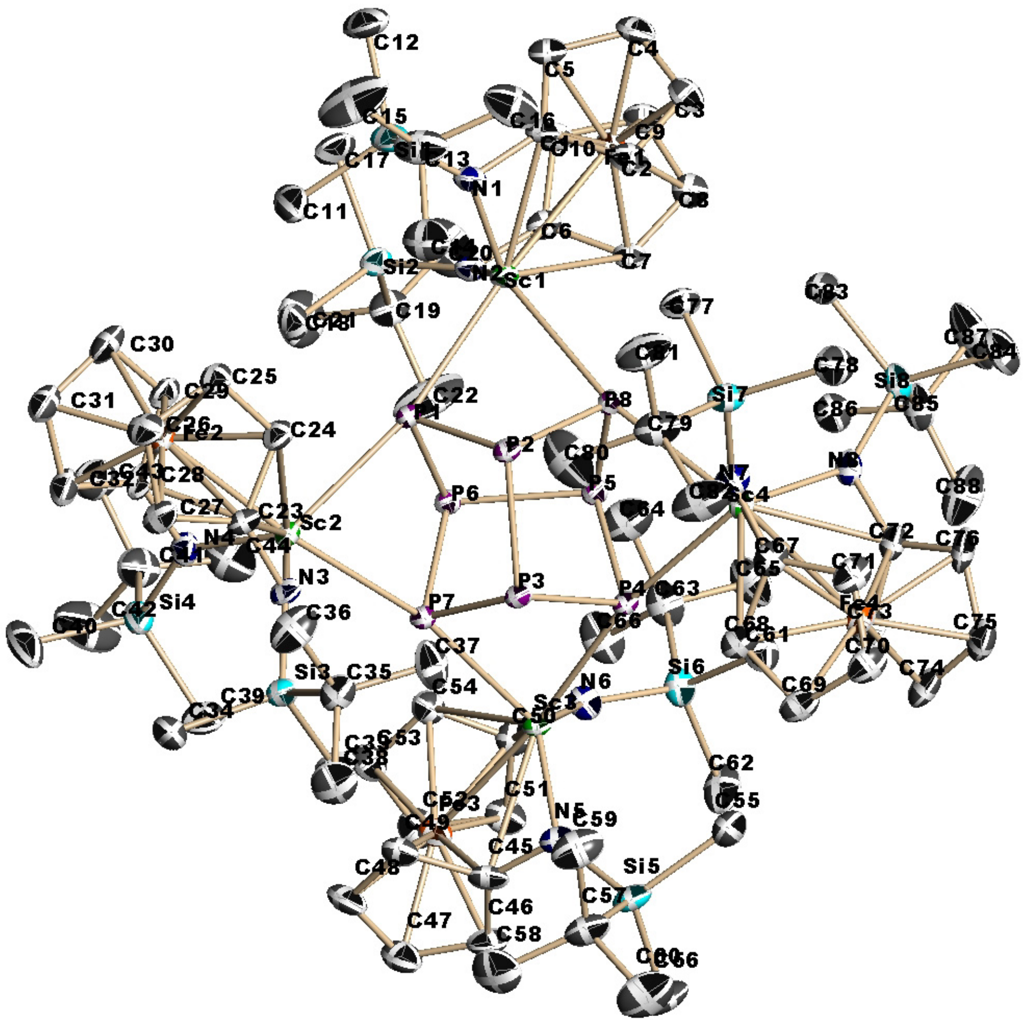


Figure SX3. Thermal-ellipsoid (50% probability) representation of **Sc_4P_8**. Hydrogen and solvent atoms were omitted for clarity. Selected distances [Å] and angles [°]: P1-P2 2.203(2), P1-P6 2.205(2), P2-P3 2.306 (2), P2-P8 2.206(2), P3-P4 2.207(2), P3-P7 2.207(2), P4-P5 2.198(2), P5-P6 2.308(2), P5-P8 2.201(2), P6-P7 2.205(2), Sc1-P1 2.780(2), Sc1-P8 2.762(2), Sc1-N1 2.037(6), Sc1-N2 2.065(5), Sc1-Fe1 2.792(2), Sc2-Fe2 2.823(2), Sc3-Fe3 2.813(2), Sc4-Fe4 2.791(2), P1-Sc1-P8 70.1(1), P1-Sc1-Fe1 175.2(1), P8-Sc1-Fe1 106.3(1), P2-P1-P6 98.5(1), P1-P2-P8 92.4(1), P1-P2-P3 101.8(1).

Single crystals suitable for X-ray diffraction were grown from a toluene solution layered with hexanes stored at -35 °C for a week. Some of the *t*-butyl groups are slightly disordered; this disorder was not modelled. A total of 56284 reflections ($-20 \leq h \leq 21$, $-22 \leq k \leq 22$, $-35 \leq l \leq 35$) were collected at T = 100(2) K with $2\theta_{max}$ = 57.35°, of which 30396 were unique. The residual peak and hole electron density were 1.51 and -0.92 eA^{-3}. The least-squares refinement converged normally with residuals of R_1 = 0.0602 and GOF = 1.005. Crystal and refinement data for **Sc_4P_8**: formula $C_{88}H_{152}N_8Si_8Fe_4Sc_4P_8$ $2(C_7H_3)$, space group P-1, a = 15.581(3), b = 16.495(3), c = 26.449(6), α = 80.486(2), β = 79.606(2), γ = 67.127(2)°, V = 6127(2) $Å^3$, Z = 2, μ = 0.894 mm^{-1}, F(000) = 2492, R_1 = 0.0602 and wR_2 = 0.1698 (based on all 30396 data, I > $2\sigma(I)$).

Sc_3P_7

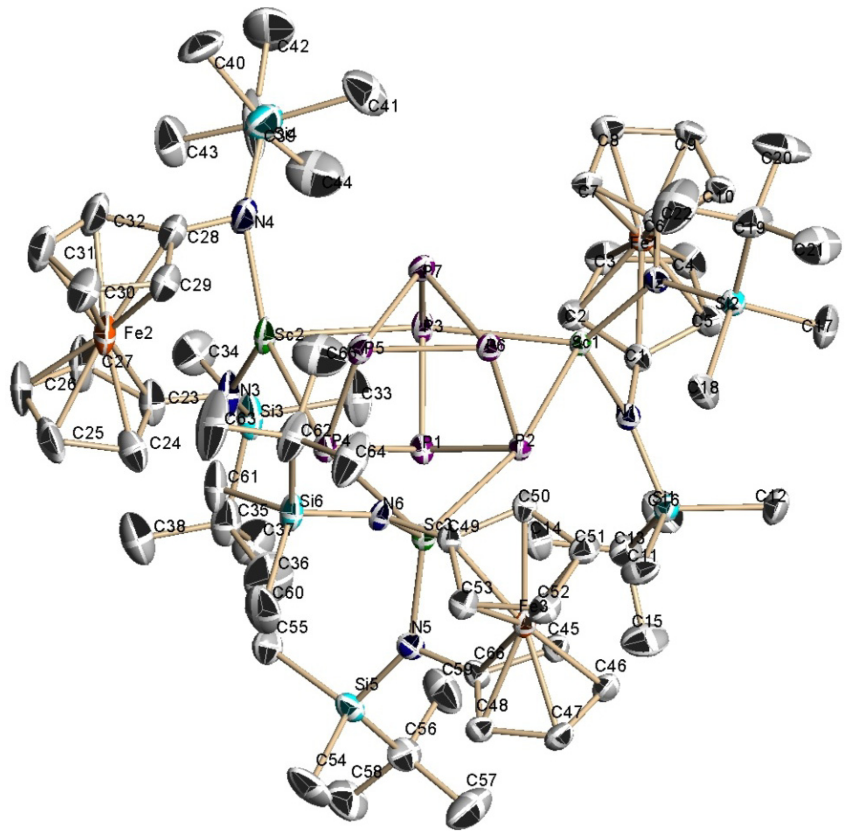


Figure SX4. Thermal-ellipsoid (50% probability) representation of **Sc_3P_7**. Hydrogen atoms were omitted for clarity. Selected distances [Å] and angles [°]: P1-P2 2.197(2), P1-P3 2.204(2), P1-P4 2.196(2), P2-P6 2.197(2), P3-P7 2.197(2), P4-P5 2.194(2), P5-P6 2.226(2), P5-P7 2.234(2), P6-P7 2.228(2), Sc1-P2 2.730(2), Sc1-P3 2.747(2), Sc1-N1 2.028(4), Sc1-N2 2.072(4), Sc1-Fe1 2.803(1), Sc2-Fe2 2.788(1), Sc3-Fe3 2.824(1), P2-P1-P3 99.9(1), P1-P2-P6 100.7(1), P5-P6-P2 103.9(1), P5-P6-P7 60.2(1), N1-Sc1-N2 116.8(2), P2-Sc1-P3 75.9(1), P2-Sc1-Fe1 179.1(1), P3-Sc1-Fe1 104.1(1).

Single crystals suitable for X-ray diffraction were grown from a concentrated hexanes solution with several drops of toluene stored at -35 °C for several days. One of the *t*-butyl groups is disordered and some additional electron density is found that is equidistant from the tertiary carbon, silicon, and nitrogen. As a consequence, it was difficult to get a stable refinement when this electron density was refined as a counterpart to either of them. The unit cell contains large accessible voids; solvent molecules could not be modeled to fit this space (it is possible that some solvent was lost during crystal handling) and the program SQUEEZE was used. A total of 48996 reflections ($-17 \le h \le 17$, $-17 \le k \le 17$, $-27 \le l \le 27$) were collected at $T = 100(2)$ K with $2\theta_{max} = 47.80°$, of which 15016 were unique. The residual peak and hole electron density were 5.11 and -1.13 eA^{-3}. The least-squares refinement converged normally with residuals of R_1 = 0.0577 and GOF = 1.071. Crystal and refinement data for **Sc_3P_7**: formula $C_{66}H_{114}N_6Si_6Fe_3Sc_3P_7$, space group *P*-1, a = 15.3797(15), b = 15.4112(15), c = 24.293(2), α = 101.293(1), β = 93.402(1), γ = 118.660(1)°, V = 4875.4(8) Å^3, Z = 2, μ = 0.854 mm^{-1}, F(000) = 1764, R_1 = 0.0683 and wR_2 = 0.1659 (based on all 15016 data, $I > 2\sigma(I)$).

Y_3P_7

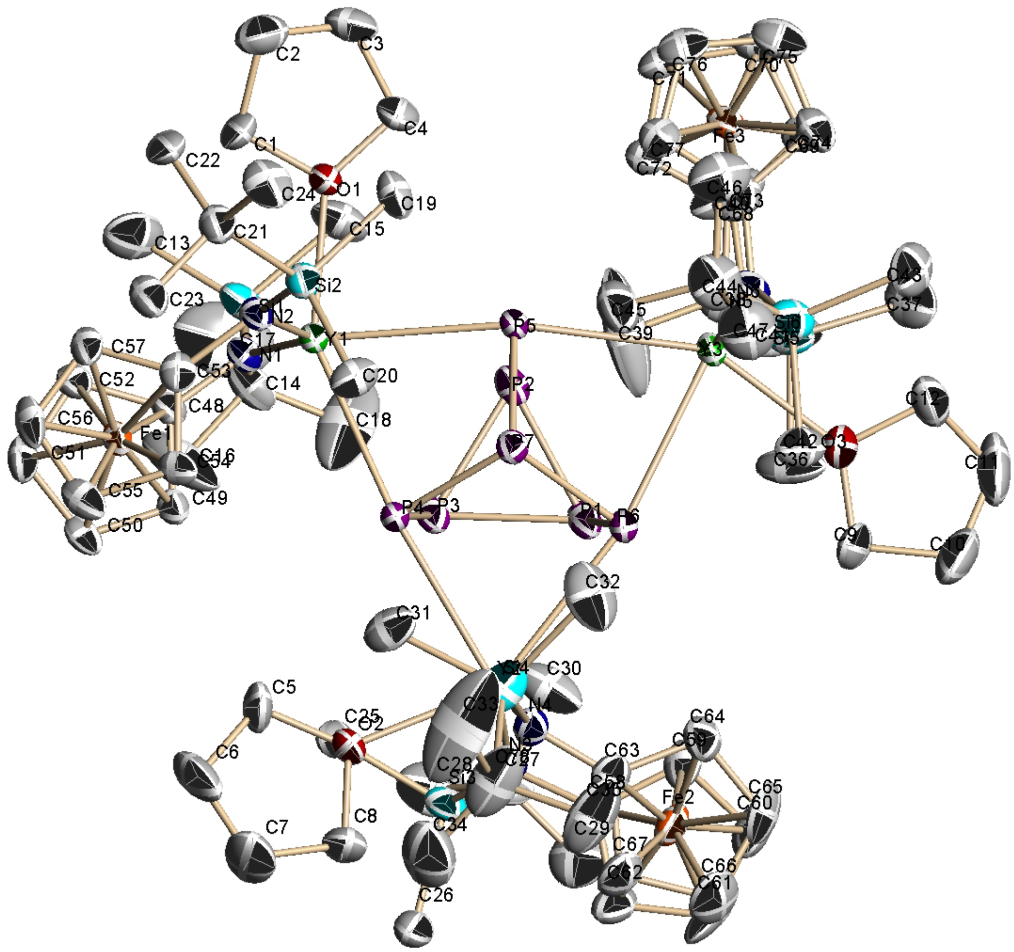


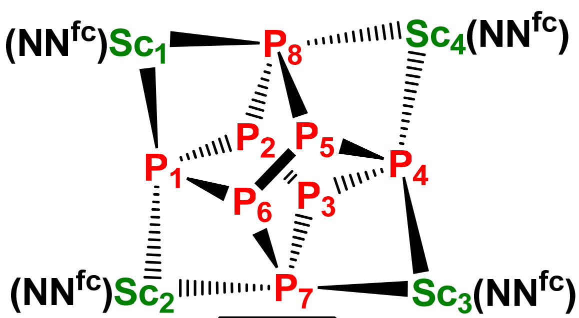
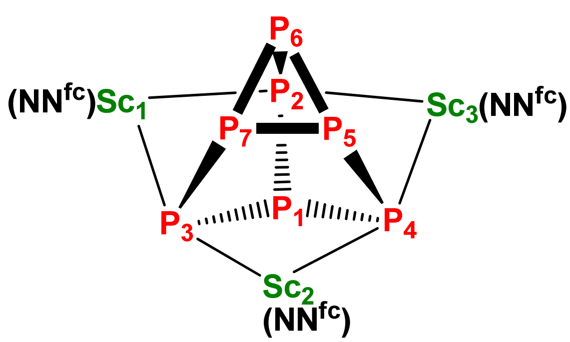
Figure SX5. Thermal-ellipsoid (50% probability) representation of $\mathbf{Y_3P_7}$. Hydrogen atoms were omitted for clarity. Selected distances [Å] and angles [°]: P1-P6 2.176(3), P1-P2 2.246(3), P1-P3 2.236(3), P2-P5 2.182(3), P2-P3 2.231(3), P3-P4 2.175(3), P4-P7 2.187(3), P5-P7 2.188(3), P6-P7 2.186(3), Y1-P4 2.910(2), Y1-P5 2.952(2), Y1-N1 2.204(6), Y1-N2 2.223(6), Y1-O1 2.358(5), Y1-Fe1 3.243(1), Y2-Fe2 3.262(1), Y3-Fe3 3.337(1), P2-P1-P3 59.7(1), P2-P1-P6 105.7(1), P4-P7-P5 99.2(1), N1-Y1-N2 130.4(2), P4-Y1-P5 69.3(1), P5-Y1-O1 82.3(1), O1-Y1-Fe1 121.5(1), Fe1-Y1-P4 86.6(1).

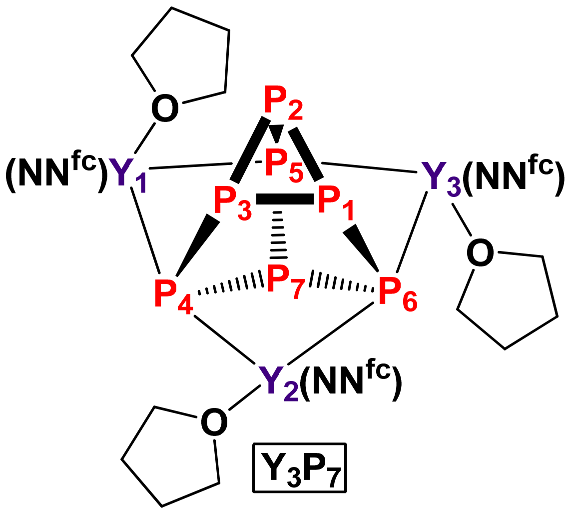
Single crystals suitable for X-ray diffraction were grown from a toluene solution layered with hexanes. Some of the *t*-butyl groups are disordered; this disorder was not modeled. The unit cell contains large accessible voids; solvent molecules could not be modeled to fit this space (it is possible that some solvent was lost during crystal handling) and the program SQUEEZE was used. A total of 104336 reflections ($-60 \leq h \leq 62$, $-28 \leq k \leq 28$, $-31 \leq l \leq 31$) were collected at T = 100(2) K with $2\theta_{max}$ = 56.67°, of which 28887 were unique. The residual peak and hole electron density were 1.47 and -1.68 eA^{-3}. The least-squares refinement converged normally with residuals of R_1 = 0.0850 and GOF = 1.036. Crystal and refinement data for $\mathbf{Y_3P_7}$: formula $C_{78}H_{138}N_6Si_6Fe_3Y_3P_7O_3$, space group *C*2/c, a = 46.711(11), b = 21.615(5), c = 23.922(6), β = 104.938(2)°, V = 23337(10) Å^3, Z = 8, μ = 2.033 mm^{-1}, F(000) = 8448, R_1 = 0.1365 and wR_2 = 0.2697 (based on all 28887 data, I > 2σ(*I*)).

Electronic Supplementary Material (ESI) for Chemical Communications

6. DFT calculations

Table SX1. Comparison of metrical parameters from calculated (ADF) and X-ray crystal structures (experimental) for **Sc_4P_8**, **Sc_3P_7**, and **Y_3P_7**.

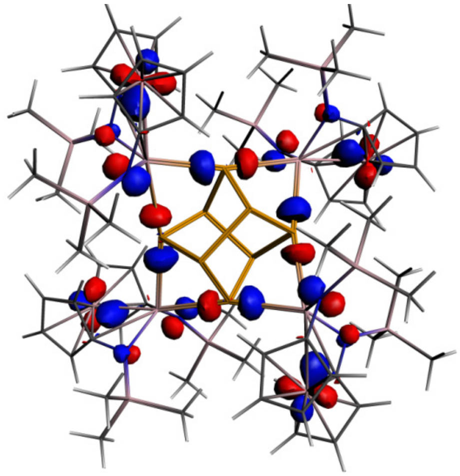
Complex	Parameter	ADF	Experimental
 Sc_4P_8	P1–P2	2.23 Å	2.20 Å
	P1–P6	2.23 Å	2.20 Å
	P2–P3	2.34 Å	2.31 Å
	P2–P8	2.23 Å	2.21 Å
	P3–P4	2.23 Å	2.21 Å
	P3–P7	2.23 Å	2.21 Å
	P4–P5	2.23 Å	2.20 Å
	P5–P6	2.37 Å	2.31 Å
	P5–P8	2.23 Å	2.20 Å
	P6–P7	2.23 Å	2.20 Å
	Sc1–P1	2.84 Å	2.78 Å
	Sc1–P8	2.83 Å	2.76 Å
	Sc1–N$_{fc}$	2.08 Å	2.04 Å
	Sc1–N$_{fc}$	2.10 Å	2.06 Å
	Sc1–Fe1	2.81 Å	2.79 Å
	Sc2–Fe2	2.83 Å	2.82 Å
	Sc3–Fe3	2.83 Å	2.81 Å
	Sc4–Fe4	2.83 Å	2.79 Å
	P1Sc1P8	69.5°	70.1°
	P1Sc1Fe1	172.7°	175.2°
	P8Sc1Fe1	105.1°	106.3°
	P2P1P6	99.2°	98.5°
	P1P2P8	92.6°	92.4°
	P1P2P3	101.1°	101.8°
 Sc_3P_7	P1–P2	2.23 Å	2.20 Å
	P1–P3	2.24 Å	2.20 Å
	P1–P4	2.24 Å	2.20 Å
	P2–P6	2.23 Å	2.20 Å
	P3–P7	2.23 Å	2.20 Å
	P4–P5	2.23 Å	2.19 Å
	P5–P6	2.27 Å	2.23 Å
	P5–P7	2.27 Å	2.23 Å
	P6–P7	2.27 Å	2.23 Å
	Sc1–P2	2.83 Å	2.73 Å
	Sc1–P3	2.83 Å	2.75 Å
	Sc1–N$_{fc}$	2.07 Å	2.03 Å
	Sc1–N$_{fc}$	2.11 Å	2.07 Å
	Sc1–Fe1	2.83 Å	2.80 Å
	Sc2–Fe2	2.84 Å	2.79 Å
	Sc3–Fe3	2.84 Å	2.82 Å
	P2Sc1P3	74.4°	75.9°
	P2Sc1Fe1	179.1°	179.1°
	P3Sc1Fe1	105.4°	104.1°
	P2P1P3	99.8°	99.9°
	P1P2P6	100.6°	100.7°
	P5P6P2	104.5°	103.9°
	P5P6P7	60.1°	60.2°
	N$_{fc}$Sc1N$_{fc}$	118.0°	116.8°



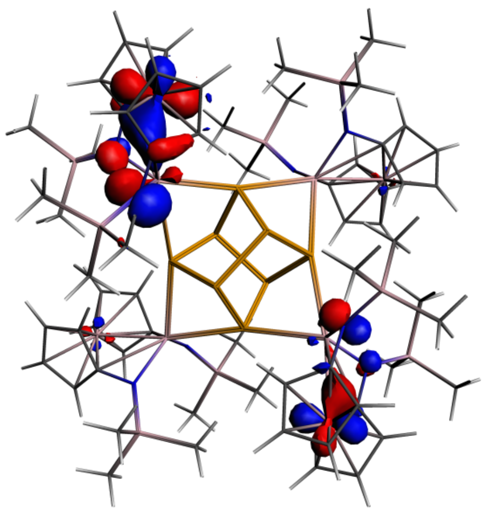
P1–P2	2.28 Å	2.25 Å
P1–P6	2.22 Å	2.18 Å
P1–P3	2.28 Å	2.24 Å
P2–P5	2.22 Å	2.18 Å
P2–P3	2.28 Å	2.23 Å
P3–P4	2.22 Å	2.17 Å
P4–P7	2.23 Å	2.19 Å
P5–P7	2.23 Å	2.19 Å
P6–P7	2.23 Å	2.19 Å
Y1–P4	3.01 Å	2.91 Å
Y1–P5	3.03 Å	2.95 Å
Y1–N_{fc}	2.24 Å	2.20 Å
Y1–N_{fc}	2.25 Å	2.22 Å
Y1–O1	2.48 Å	2.36 Å
Y1–Fe1	3.41 Å	3.24 Å
Y2–Fe2	3.43 Å	3.26 Å
Y3–Fe3	3.42 Å	3.34 Å
P2P1P3	59.9°	59.7°
P2P1P6	104.3°	105.7°
P4P7P5	100.0°	99.2°
P4Y1P5	68.8°	69.3°
P5Y1O1	81.9°	82.3°
O1Y1Fe1	116.8°	121.5°
P4Y1Fe1	92.6°	86.6°
N_{fc}Y1N_{fc}	127.1°	130.4°

Selected molecular orbitals for Sc_4P_8

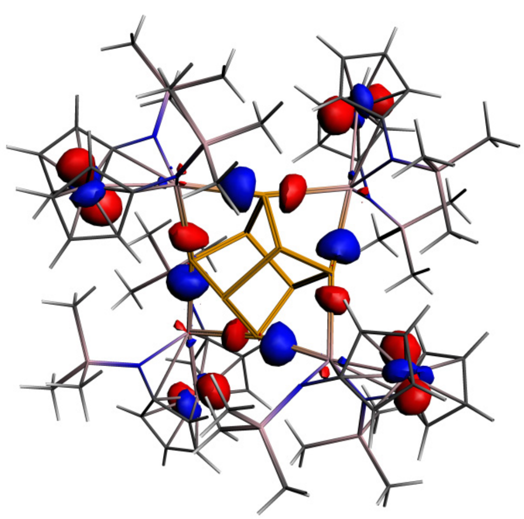
HOMO



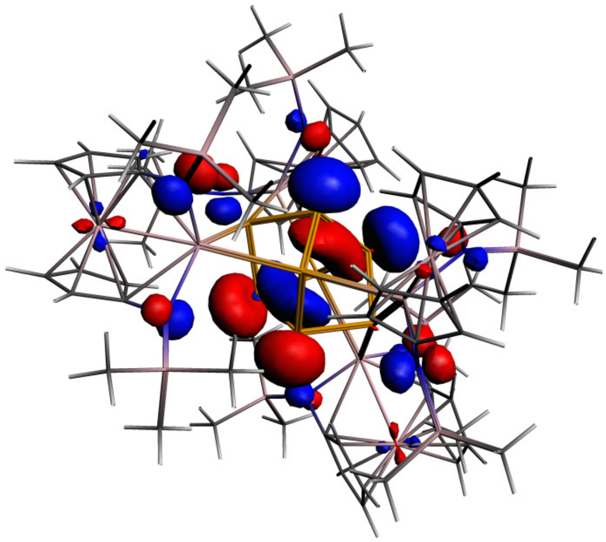
HOMO-1



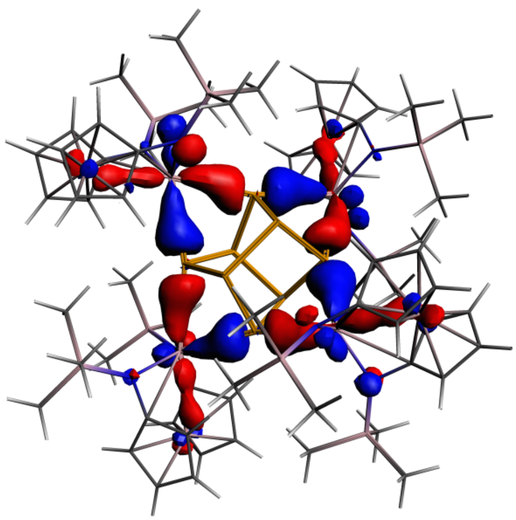
HOMO-8



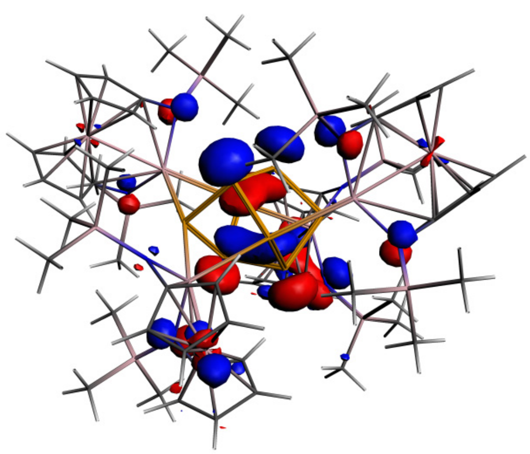
HOMO-12



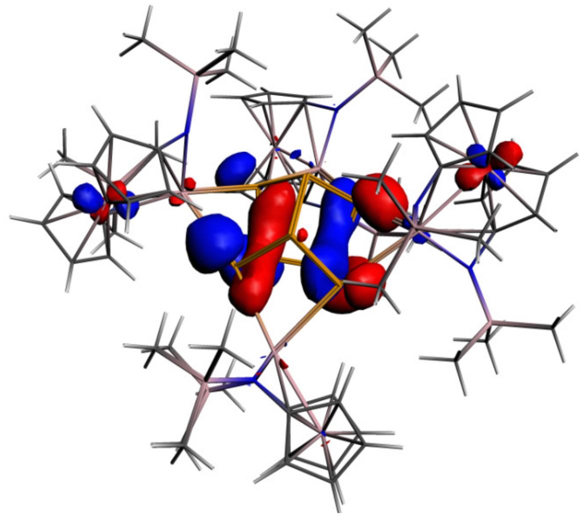
HOMO-15



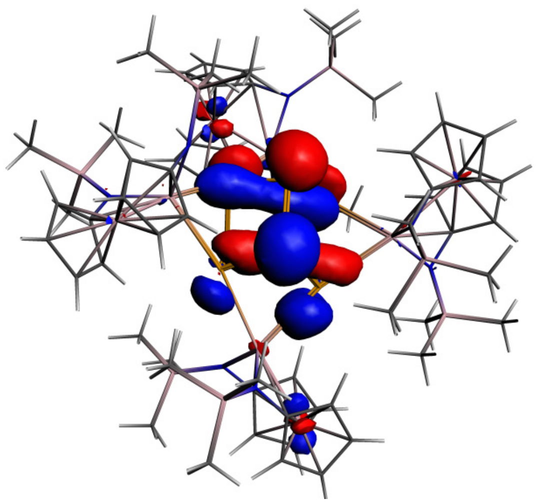
HOMO-20



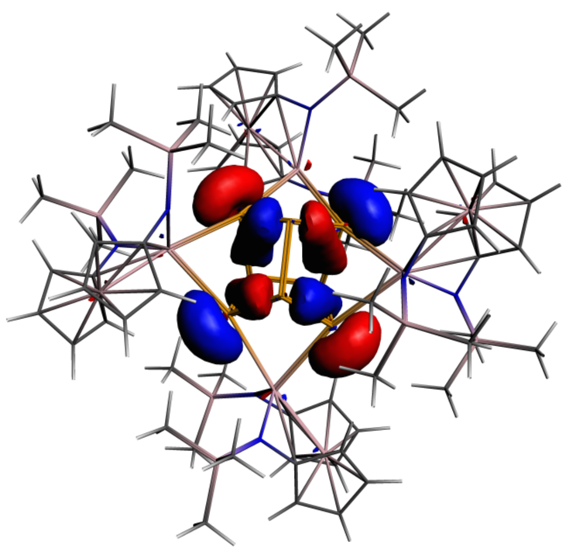
HOMO-22



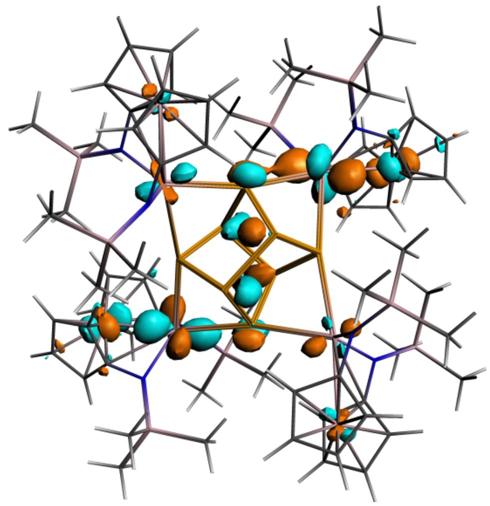
HOMO-23



HOMO-24

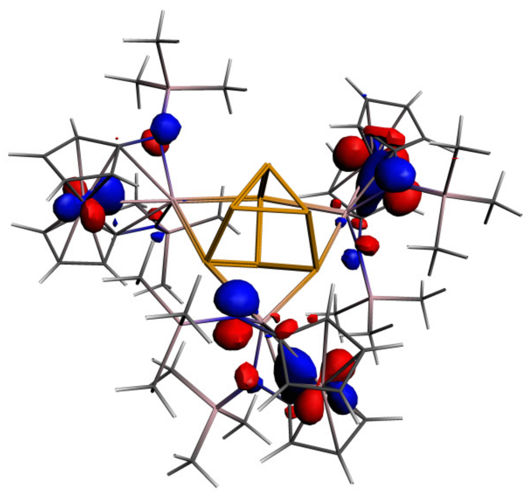


LUMO

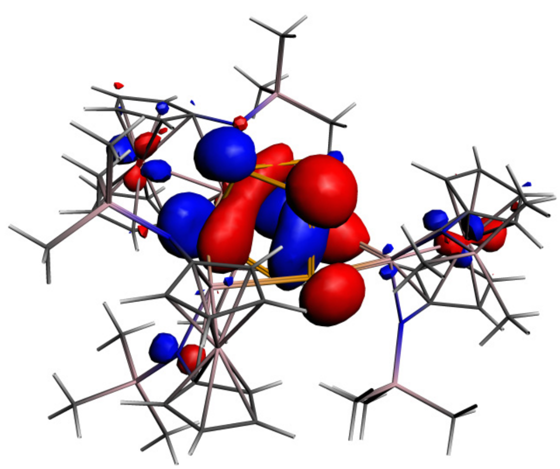


Selected molecular orbitals for Sc_3P_7

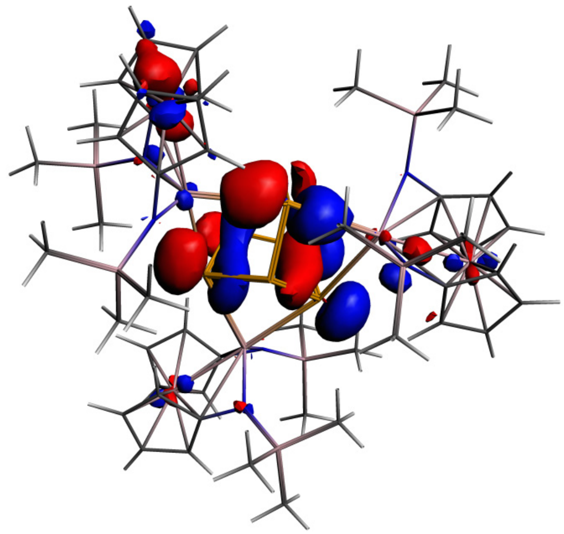
HOMO



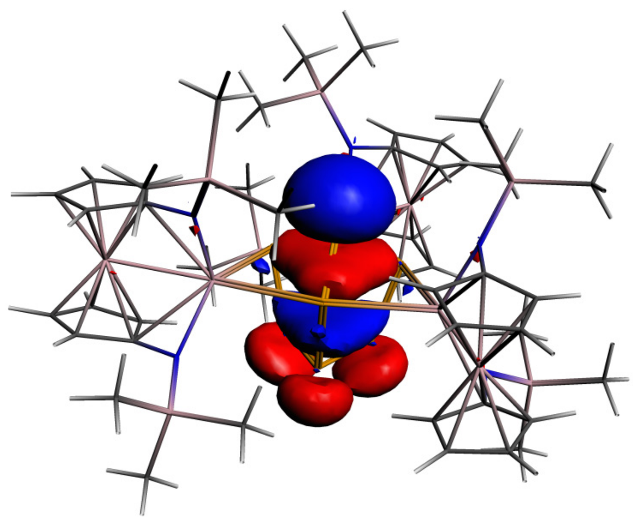
HOMO-15



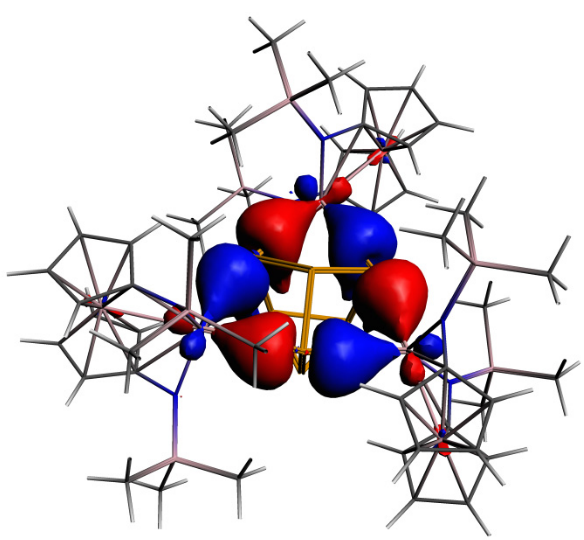
HOMO-16



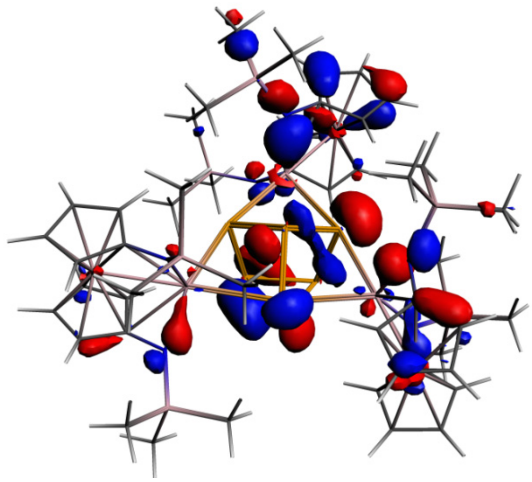
HOMO-17



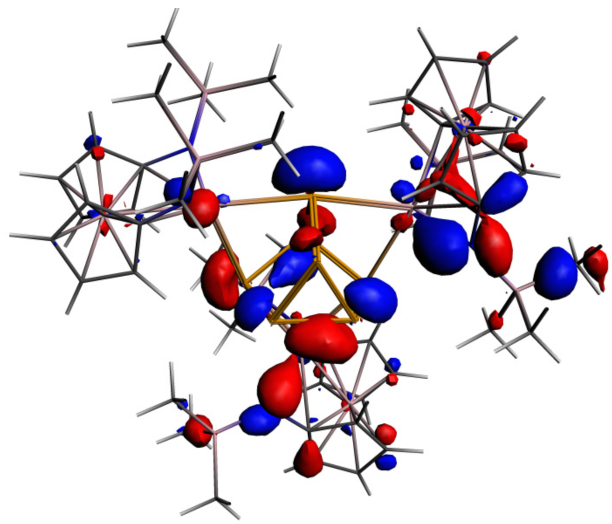
HOMO-18



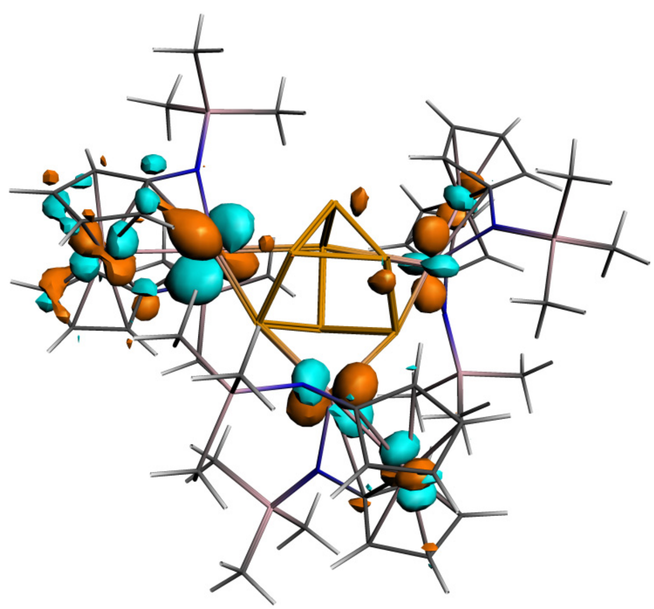
HOMO-22



HOMO-25

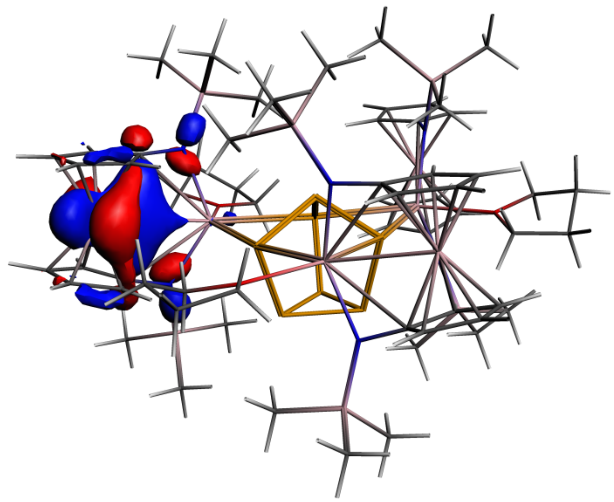


LUMO

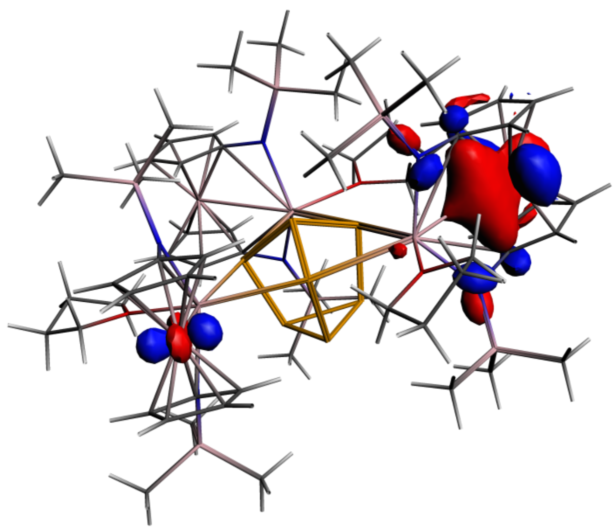


Selected molecular orbitals for Y_3P_7

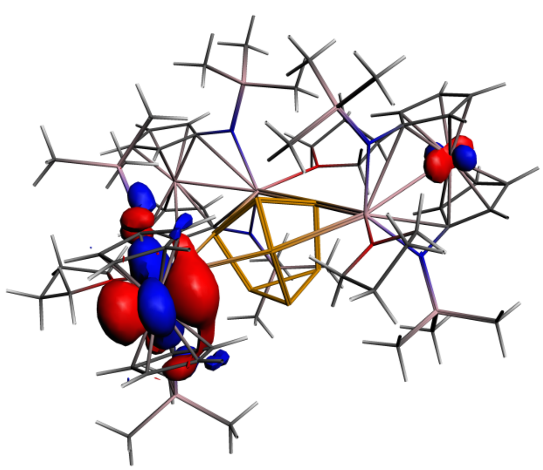
HOMO



HOMO-1



HOMO-2



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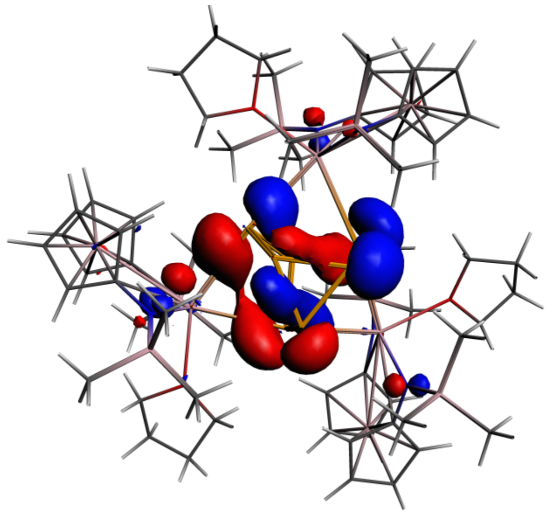

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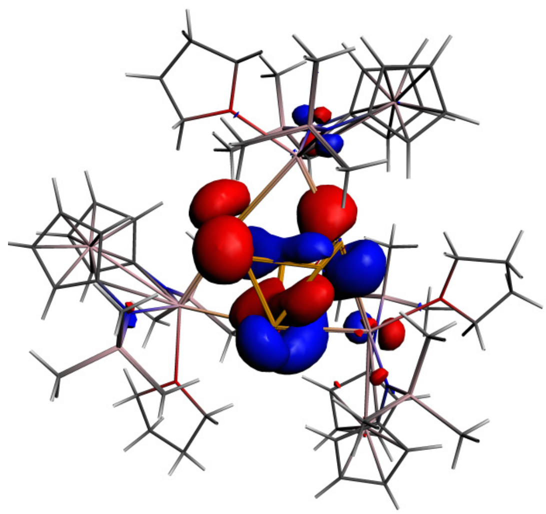
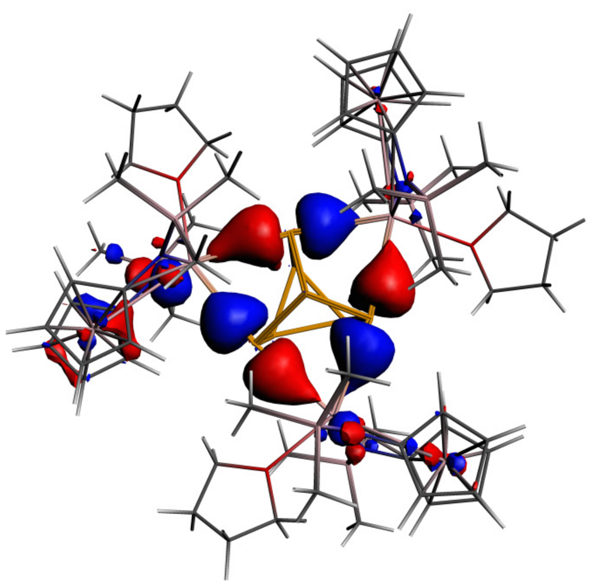
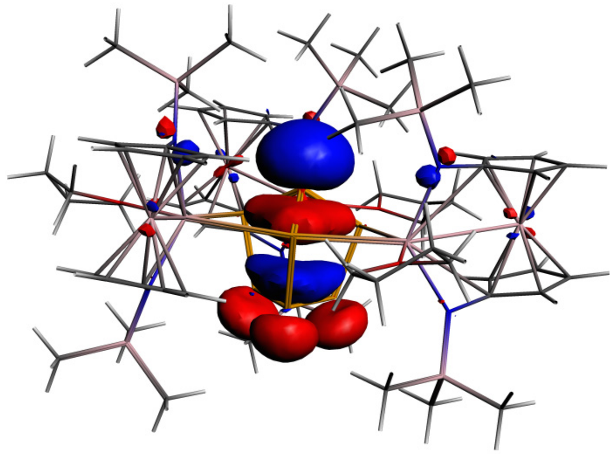


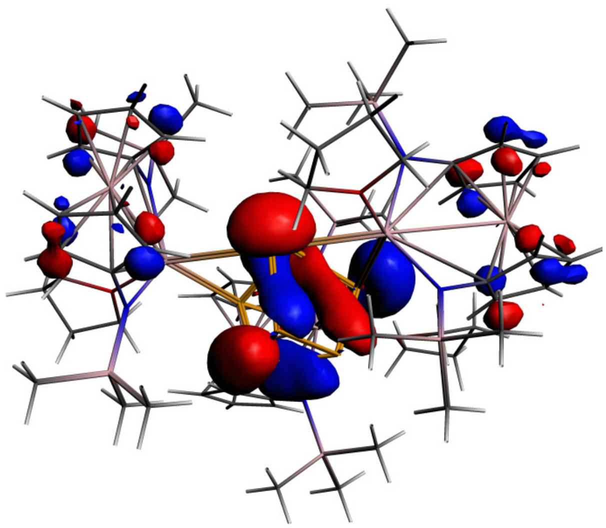
HOMO-23



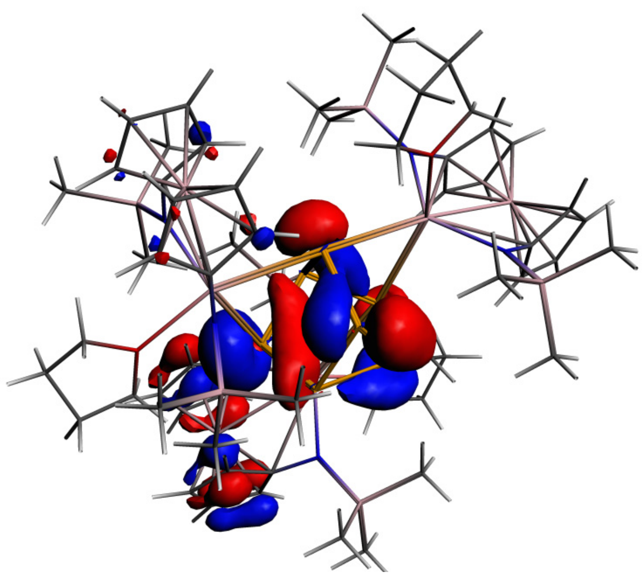
HOMO-24



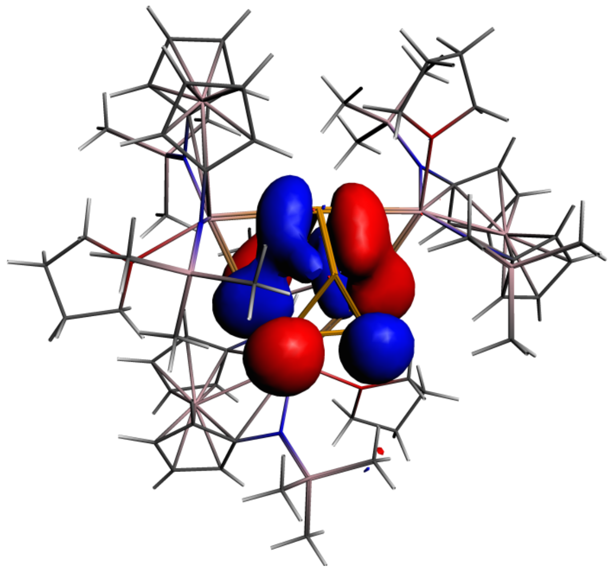
HOMO-28



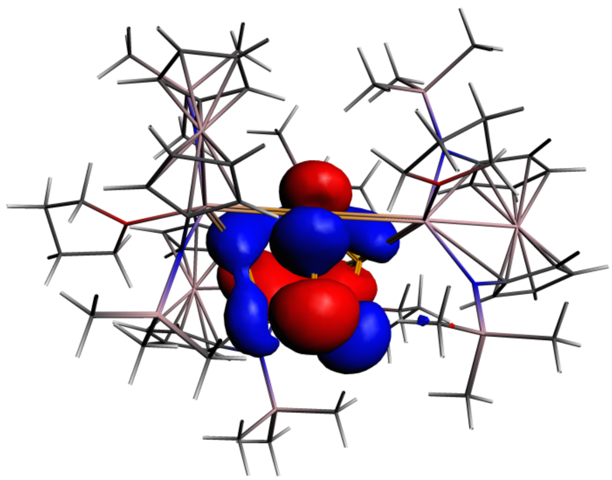
HOMO-29



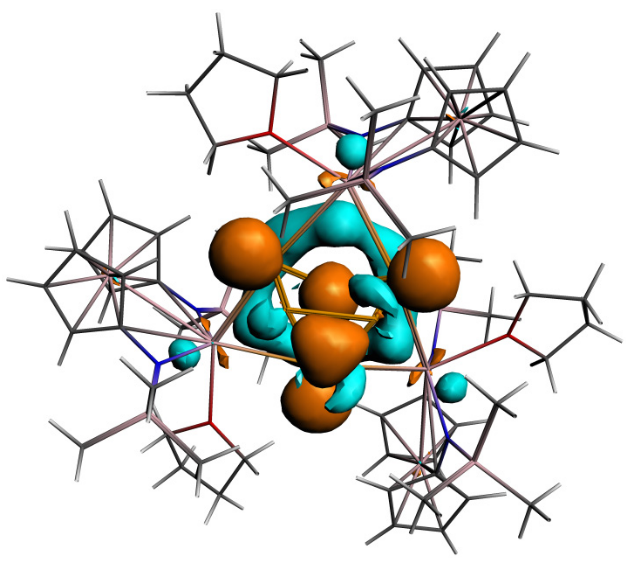
HOMO-30



HOMO-31



LUMO



Optimized coordinates for Sc_4P_8

Atom	X	Y	Z (Angstrom)
1.Sc	12.472902	6.504389	17.175533
2.Sc	8.185080	7.720193	20.617740
3.Sc	6.943944	2.351905	19.371015
4.Sc	12.480336	1.819336	20.336931
5.P	10.297130	6.832616	18.974639
6.P	11.320125	5.504621	20.448505
7.P	9.518847	4.143454	21.162068
8.P	9.759661	2.376135	19.820600
9.P	10.338328	3.429938	17.938318
10.P	8.933899	5.336180	18.029705
11.P	7.842000	4.970206	19.939736
12.P	12.213109	4.236566	18.841622
13.Fe	14.511593	5.843545	15.350629
14.Fe	8.892469	10.366678	21.325117
15.Fe	4.212100	2.671026	18.704129
16.Fe	12.444578	-0.443943	22.033909
17.Si	14.171879	9.495721	18.359123
18.Si	10.404185	7.798715	14.477869
19.Si	7.313452	6.968824	24.064572
20.Si	5.017281	8.706183	19.138508
21.Si	6.259781	0.022225	22.062475
22.Si	7.495282	0.207538	16.472923
23.Si	14.885282	3.492901	22.503381
24.Si	14.563923	0.195231	17.845554
25.N	13.929755	7.898469	17.681180
26.N	11.461190	6.690410	15.339097
27.N	8.248704	7.596454	22.715978
28.N	6.675387	8.806993	19.695067
29.N	6.019164	1.338173	20.931776
30.N	6.885271	1.542622	17.436498
31.N	13.481834	2.546298	22.034066
32.N	13.396472	0.391200	19.137119
33.C	14.923780	7.201052	16.977347
34.C	15.378650	5.853279	17.290351
35.H	15.078225	5.293090	18.172630
36.C	16.330270	5.438589	16.307932
37.H	16.854919	4.487596	16.289218
38.C	16.479495	6.508870	15.365116
39.H	17.131176	6.504692	14.495099
40.C	15.595726	7.571274	15.746421
41.H	15.455635	8.510030	15.219221
42.C	12.446860	5.949701	14.684703
43.C	12.818895	4.587333	15.046146
44.H	12.260989	3.957905	15.739434
45.C	13.925484	4.170980	14.240107
46.H	14.398389	3.193278	14.261257
47.C	14.265866	5.259959	13.373058
48.H	15.064024	5.259998	12.635111
49.C	13.400315	6.361793	13.671313
50.H	13.433453	7.342551	13.208597
51.C	12.473454	10.305278	18.533158
52.H	12.015627	10.470317	17.545874
53.H	12.568362	11.287031	19.023960
54.H	11.778523	9.697299	19.131707
55.C	15.243786	10.602836	17.247962
56.H	14.777525	10.763122	16.264010
57.H	16.245858	10.177648	17.086989
58.H	15.375954	11.590887	17.718251
59.C	14.994187	9.378508	20.063145
60.H	14.392978	8.763010	20.749485
61.H	12.979461	-1.347788	24.665215
62.C	13.698538	0.406433	23.455782

63.H	14.776049	0.278123	23.457059
64.H	15.120628	10.374544	20.518133
65.C	12.971099	-0.667236	19.954762
66.C	11.582323	-1.038644	20.185967
67.H	10.735832	-0.604734	19.659893
68.H	15.991051	8.916311	19.989111
69.C	11.533303	-2.103254	21.137804
70.H	10.635373	-2.599044	21.495178
71.C	12.880969	-2.408896	21.521403
72.C	11.348980	9.105169	13.460434
73.H	12.154702	9.571598	14.047289
74.H	10.658582	9.905582	13.147298
75.H	11.789089	8.683223	12.544795
76.C	9.380119	8.714072	15.769937
77.H	8.807126	8.013239	16.395254
78.H	8.665337	9.396280	15.284554
79.H	10.021328	9.319122	16.428318
80.C	9.272332	6.837280	13.304875
81.H	9.857415	6.277828	12.557605
82.H	16.168437	5.270056	21.313514
83.C	16.422336	2.423663	22.861576
84.H	14.221239	3.862425	24.894096
85.H	8.593726	7.514545	12.761098
86.H	16.330561	1.860610	23.802023
87.C	12.990406	1.502804	22.821650
88.C	11.573154	1.228196	23.023761
89.H	8.659041	6.112297	13.861278
90.C	15.280305	1.902298	17.467715
91.H	15.867435	2.278022	18.319805
92.H	14.501640	2.646271	17.241882
93.C	8.986821	8.779174	22.803456
94.C	10.279847	8.984730	22.162249
95.H	10.870587	8.195552	21.697481
96.C	10.701682	10.336349	22.372697
97.H	11.638999	10.772417	22.039454
98.C	9.684937	10.994902	23.138755
99.H	9.707375	12.030440	23.468685
100.C	8.616907	10.065998	23.363556
101.H	7.686788	10.275058	23.881786
102.C	7.366218	10.020287	19.840696
103.C	8.643269	10.336224	19.216549
104.H	9.139730	9.705009	18.484008
105.C	9.076535	11.623449	19.660074
106.H	9.986320	12.131300	19.353198
107.C	8.088494	12.127222	20.569909
108.H	8.124979	13.084744	21.083306
109.C	7.061943	11.137411	20.713398
110.H	6.186608	11.207648	21.351983
111.C	6.349100	5.474420	23.433699
112.H	5.633883	5.760438	22.647861
113.H	5.774773	5.013979	24.252530
114.H	7.024155	4.708391	23.023481
115.C	6.052366	8.221779	24.753314
116.H	5.460295	8.684326	23.949084
117.H	6.534689	9.023909	25.331217
118.H	5.350261	7.711501	25.432932
119.C	8.467778	6.451011	25.471502
120.H	9.063714	7.304905	25.830804
121.H	8.692217	1.596560	14.770877
122.H	14.451576	-0.609932	15.464074
123.H	13.182735	-3.172741	22.233593
124.H	9.167899	5.671278	25.135196
125.C	13.760024	-1.510000	20.832981
126.H	14.840202	-1.466511	20.934751

127.H	13.307592	-1.504034	16.491620
128.H	7.898695	6.054469	26.327977
129.H	8.332446	-0.022948	14.117059
130.C	15.305814	4.634164	21.060868
131.H	14.460461	5.294974	20.817153
132.C	4.295152	7.085817	19.789488
133.H	4.245860	7.090438	20.889059
134.H	4.887026	6.211324	19.479471
135.H	3.270015	6.947305	19.410594
136.C	3.948803	10.136673	19.786433
137.H	3.890561	10.133601	20.885496
138.H	2.921196	10.044867	19.398593
139.H	4.336009	11.115857	19.466815
140.C	4.948805	8.709176	17.243683
141.H	3.913922	8.608504	16.878031
142.H	15.954918	1.848041	16.598463
143.C	16.002713	-0.948876	18.326338
144.H	16.549663	-0.562412	19.199797
145.H	5.358652	9.646061	16.835218
146.H	16.718849	-1.022533	17.491641
147.H	15.661823	-1.968913	18.558572
148.C	13.732066	-0.507277	16.292803
149.H	5.540589	7.879460	16.828007
150.H	12.910905	0.142920	15.954812
151.H	15.568339	4.061467	20.158487
152.H	7.048732	1.206466	14.212759
153.C	4.766752	1.902182	20.645084
154.C	3.583974	1.263870	20.099996
155.H	3.489195	0.202487	19.891546
156.C	2.570451	2.258638	19.906327
157.H	1.567162	2.079369	19.527762
158.C	3.116864	3.534924	20.265685
159.H	2.603101	4.490620	20.221172
160.C	4.457831	3.323620	20.712082
161.H	5.133519	4.079718	21.104102
162.C	5.656655	2.154593	17.170461
163.C	4.352947	1.554401	16.957142
164.H	4.159444	0.487668	16.908408
165.C	3.382126	2.596987	16.802275
166.H	2.322603	2.454859	16.604839
167.C	4.039307	3.857306	16.989734
168.H	3.574853	4.837785	16.937740
169.C	5.427617	3.593615	17.217567
170.H	6.216010	4.341020	17.306490
171.C	7.902610	-0.805706	21.628766
172.H	7.847561	-1.296648	20.645005
173.H	8.145836	-1.580675	22.373072
174.H	8.739843	-0.092046	21.602893
175.C	4.893485	-1.293526	21.956485
176.H	4.842890	-1.742371	20.952658
177.H	3.902563	-0.881210	22.198885
178.H	5.097707	-2.105169	22.673761
179.C	6.331045	0.673484	23.841219
180.H	5.385800	1.165164	24.119649
181.H	17.312849	3.066702	22.955214
182.H	16.613666	1.707451	22.047843
183.C	14.493422	4.513747	24.048449
184.H	7.137667	1.413216	23.957860
185.H	13.648406	5.193807	23.862461
186.H	10.766308	1.895701	22.721576
187.C	11.430253	0.034682	23.800054
188.H	6.508503	-0.142682	24.560328
189.H	10.493442	-0.400480	24.135676
190.H	15.360497	5.120112	24.356831

191.C	12.745663	-0.456253	24.088891
192.C	9.040447	-0.451186	17.332983
193.H	8.807594	-0.831093	18.339203
194.H	9.808109	0.331402	17.427384
195.H	9.477300	-1.281752	16.757151
196.C	6.256633	-1.232550	16.328624
197.H	5.877499	-1.539983	17.315417
198.H	6.749988	-2.107480	15.874255
199.H	5.396113	-0.979437	15.691736
200.C	7.932631	0.801060	14.730141

Optimized coordinates for Sc_3P_7

Atom	X	Y	Z (Angstrom)
1.Sc	8.765765	0.762348	7.361533
2.Sc	10.154918	-3.978483	4.733041
3.Sc	14.143565	-0.791913	6.992072
4.Fe	5.977845	1.246575	7.358250
5.Fe	11.119839	-6.369964	3.548489
6.Fe	15.884104	1.018982	8.314267
7.P	11.101453	-0.844588	5.503949
8.P	11.548119	0.249803	7.401263
9.P	9.102261	-1.706239	6.022210
10.P	12.392008	-2.651599	5.794025
11.P	11.766702	-3.276603	7.839546
12.P	11.167342	-1.357055	8.900343
13.P	9.573129	-2.686708	7.972829
14.Si	9.461548	3.774168	5.401611
15.Si	8.969149	2.050092	10.763083
16.Si	9.230669	-2.541527	1.506972
17.Si	7.111293	-5.697413	5.629825
18.Si	15.554997	-0.055965	3.713722
19.Si	16.153564	-3.607900	8.181333
20.N	8.631771	2.380175	6.078510
21.N	8.382469	1.090689	9.411763
22.N	10.037083	-3.525518	2.720725
23.N	8.848623	-5.428268	5.568658
24.N	15.088443	0.120775	5.398816
25.N	15.282741	-2.084354	8.213815
26.C	7.239963	2.240817	5.937279
27.C	6.572167	1.098395	5.328776
28.H	7.085420	0.279786	4.829388
29.C	5.159025	1.272689	5.429863
30.H	4.401645	0.591322	5.051049
31.C	4.919089	2.514923	6.104867
32.H	3.944105	2.933310	6.341404
33.C	6.184541	3.093485	6.447778
34.H	6.340689	4.019462	6.993015
35.C	7.022863	0.849892	9.220016
36.C	6.486828	-0.371299	8.629178
37.H	7.066344	-1.274294	8.438139
38.C	5.067320	-0.247715	8.488730
39.H	4.394330	-1.013302	8.113651
40.C	4.695822	1.047955	8.974027
41.H	3.686807	1.451005	9.004290
42.C	5.886722	1.738789	9.373074
43.H	5.938153	2.755975	9.746675
44.C	11.283664	3.654168	5.881444
45.H	11.419512	3.649096	6.973030
46.H	11.839321	4.513220	5.474206
47.C	14.901618	1.399502	2.690682
48.H	11.737522	2.738010	5.475030
49.C	8.760960	5.411768	6.068195
50.H	8.784294	5.446199	7.168226

51.H	7.722436	5.572764	5.742208
52.H	9.356652	6.260199	5.693919
53.C	9.302390	3.779628	3.513596
54.H	9.744776	2.870051	3.079164
55.H	17.910557	2.954958	7.918094
56.C	16.979294	1.389537	6.597712
57.H	13.804290	1.459186	2.750777
58.H	9.817461	4.650446	3.076648
59.H	17.829455	0.791972	6.282933
60.C	15.676245	-1.020682	9.025042
61.C	14.747031	-0.117312	9.694474
62.H	8.246758	3.823338	3.201494
63.C	18.007211	-3.410031	7.782656
64.H	18.166654	-2.777616	6.896163
65.H	18.450961	-4.396979	7.572499
66.C	8.401966	3.868987	10.696039
67.H	8.599374	4.312906	9.708312
68.H	8.949609	4.462850	11.446103
69.H	7.329712	3.985730	10.913400
70.C	10.857164	2.039378	10.712231
71.H	11.247951	1.015256	10.806323
72.H	11.257849	2.634415	11.548283
73.H	11.249473	2.465371	9.776274
74.C	8.372790	1.295027	12.394290
75.H	7.273105	1.260711	12.443431
76.H	15.081509	-1.813467	2.012962
77.H	13.704472	-1.642576	3.124169
78.H	8.728687	1.883479	13.255338
79.H	15.311547	2.356819	3.049441
80.H	13.672218	-0.281283	9.772737
81.C	15.483651	0.917736	10.355119
82.H	8.745448	0.265468	12.506733
83.H	15.062001	1.712352	10.963958
84.H	15.178397	1.292694	1.629414
85.C	16.874986	0.686978	10.102351
86.C	10.833325	-4.622778	2.345222
87.C	12.239165	-4.793038	2.682893
88.H	12.845965	-4.042942	3.184062
89.C	12.688632	-6.056423	2.194243
90.H	13.695957	-6.454359	2.283046
91.C	11.578741	-6.697536	1.552105
92.H	11.595266	-7.676597	1.080077
93.C	10.435135	-5.841390	1.668328
94.H	9.433470	-6.053949	1.307203
95.C	9.731909	-6.446166	5.227279
96.C	11.123209	-6.493874	5.663510
97.H	11.556474	-5.838887	6.420100
98.C	11.767099	-7.628629	5.072405
99.H	12.791469	-7.945135	5.247481
100.C	10.801618	-8.292751	4.247236
101.H	10.975593	-9.192280	3.662301
102.C	9.578958	-7.546303	4.294886
103.H	8.670180	-7.777013	3.747954
104.C	8.147889	-1.285962	2.411089
105.H	7.392076	-1.777810	3.041591
106.H	7.619708	-0.647980	1.685478
107.H	8.756620	-0.631197	3.053091
108.C	8.133832	-3.584548	0.356582
109.H	7.401482	-4.181870	0.920951
110.H	8.731253	-4.270639	-0.262494
111.H	7.573585	-2.928139	-0.329118
112.C	10.506963	-1.630165	0.445119
113.C	15.997984	-4.475932	9.857272
114.H	11.138207	-0.973855	1.063047

115.H	17.697427	1.296724	10.467310
116.H	16.416734	-3.856150	10.665807
117.C	16.995211	-0.460522	9.251925
118.H	10.012118	-1.006472	-0.317017
119.H	17.919312	-0.862283	8.849906
120.C	17.443532	-0.146241	3.506726
121.H	14.941917	-4.671776	10.097447
122.H	11.167867	-2.337987	-0.079582
123.H	17.874548	-0.973304	4.091284
124.H	17.935399	0.787500	3.817724
125.H	17.700050	-0.315359	2.448236
126.C	15.606345	1.158256	6.194661
127.C	6.322408	-5.742211	3.896828
128.C	6.724769	-7.328076	6.517583
129.H	7.154030	-8.197428	5.998360
130.H	5.635956	-7.480988	6.578341
131.H	7.123257	-7.321420	7.542481
132.C	6.328935	-4.266522	6.582481
133.H	6.511214	-3.299315	6.089297
134.H	6.733453	-4.205214	7.604143
135.H	5.238633	-4.408879	6.653198
136.H	5.226644	-5.839977	3.962810
137.C	15.395284	-4.692432	6.832754
138.H	14.331056	-4.891944	7.025970
139.H	18.570477	-2.975805	8.621952
140.H	6.692523	-6.582950	3.290059
141.H	15.919361	-5.660944	6.796273
142.H	15.475997	-4.228521	5.838098
143.H	6.545256	-4.815443	3.345914
144.H	16.534653	-5.438403	9.859110
145.C	14.803292	-1.664152	3.068157
146.H	15.157913	-2.537018	3.636890
147.C	14.810539	2.161346	6.888829
148.H	13.734047	2.272407	6.785374
149.C	15.676317	2.997061	7.656612
150.H	15.373357	3.841663	8.269352
151.C	17.018768	2.531128	7.463799

Optimized coordinates for Y_3P_7

Atom	X	Y	Z (Angstrom)
1.Y	-1.604576	16.479178	13.266666
2.Y	2.942218	13.001026	11.344716
3.Y	3.360407	19.025014	11.016889
4.Fe	-3.456117	13.977418	14.658819
5.Fe	6.223205	12.358615	10.592591
6.Fe	2.573586	22.221264	11.933443
7.Si	-4.288806	16.485388	10.646638
8.Si	-0.433277	17.094052	16.729574
9.Si	2.316691	11.746955	7.873948
10.Si	4.012146	12.506192	14.861066
11.Si	2.535047	20.219342	7.562051
12.Si	5.436667	19.003862	14.081231
13.P	1.860380	15.963106	9.287288
14.P	0.163804	17.312867	9.994869
15.P	-0.045600	15.049634	10.144119
16.P	0.472894	14.555547	12.241336
17.P	0.744009	17.953831	12.036328
18.P	3.304989	15.971445	10.968761
19.P	1.924216	16.183640	12.703949
20.N	-3.425131	15.930592	12.064362
21.N	-1.334050	16.269176	15.483196
22.N	3.275503	12.249715	9.249460
23.N	4.231331	12.587323	13.129913
24.N	2.704781	20.325958	9.301487

25.N	4.333890	19.696818	12.919480
26.O	-2.443990	18.797633	13.575352
27.O	1.477908	11.074323	11.879103
28.O	5.555896	18.664300	9.933436
29.C	-3.647815	18.951780	14.400187
30.H	-3.520510	18.304200	15.276744
31.H	-4.511539	18.608653	13.810704
32.C	-3.720602	20.439421	14.719421
33.H	-3.086723	20.676968	15.586461
34.H	-4.745312	20.765999	14.939715
35.C	-3.146125	21.070059	13.439328
36.H	-3.909307	21.090049	12.647426
37.H	-2.779134	22.093929	13.588346
38.C	-2.018784	20.109857	13.070543
39.H	-1.851023	20.016361	11.991767
40.H	-1.068298	20.366589	13.558159
41.C	0.063172	10.949289	12.264363
42.H	-0.549377	11.308155	11.428582
43.H	-0.097773	11.603334	13.130448
44.C	-0.153050	9.468521	12.583851
45.H	-0.869684	9.331597	13.404435
46.H	-0.537683	8.935673	11.702445
47.C	1.261714	8.971221	12.935521
48.H	1.380478	7.886851	12.809845
49.H	1.520356	9.231467	13.972879
50.C	2.126121	9.763369	11.965606
51.H	3.153574	9.936570	12.311087
52.H	2.143586	9.314036	10.959887
53.C	6.262055	17.492857	9.404733
54.H	5.882274	17.290398	8.391551
55.H	6.020238	16.645160	10.056330
56.C	7.730381	17.896689	9.390419
57.H	8.178443	17.750890	10.384840
58.H	8.310794	17.317484	8.660513
59.C	7.651669	19.393825	9.045128
60.H	8.550975	19.952638	9.336836
61.H	7.498868	19.528933	7.964247
62.C	6.419090	19.850930	9.823139
63.H	6.660868	20.173013	10.846340
64.H	5.838486	20.635342	9.321358
65.C	-6.145256	16.732925	10.994541
66.H	-6.314077	17.474213	11.791542
67.H	-6.631034	15.793905	11.300630
68.H	-6.659380	17.093985	10.089068
69.C	-4.109207	15.266219	9.205869
70.C	-3.574146	18.161614	10.134029
71.H	-2.500764	18.100347	9.896406
72.H	-3.714924	18.913626	10.925213
73.H	-4.085755	18.529781	9.231268
74.H	-4.525418	14.280008	9.468034
75.C	4.380116	22.253031	12.965732
76.H	5.361370	22.412675	12.526741
77.C	3.496930	23.267846	13.457066
78.H	-4.633810	15.624679	8.305498
79.H	3.682517	24.339023	13.443627
80.C	2.311600	22.623115	13.950352
81.H	1.444652	23.122986	14.376292
82.H	-3.047457	15.123908	8.950187
83.C	2.471599	21.213222	13.771587
84.H	1.767259	20.436553	14.056224
85.C	4.624174	10.849800	15.574033
86.C	0.412123	18.575646	15.912912
87.H	-0.324501	19.272505	15.489480
88.H	1.080418	18.254259	15.101456

89.H	1.021313	19.131460	16.641464
90.C	0.883099	15.981729	17.517835
91.H	0.424874	15.093594	17.980315
92.H	1.440027	16.519559	18.302010
93.H	1.607147	15.633358	16.766146
94.C	-1.569738	17.732193	18.118181
95.H	-2.319664	18.443145	17.735365
96.C	2.957700	22.782374	9.967536
97.H	3.938256	22.973789	9.540359
98.C	2.116178	23.742682	10.615944
99.H	-2.109049	16.903733	18.602592
100.H	2.350555	24.791294	10.781049
101.C	0.916218	23.070982	11.032054
102.H	0.085872	23.526529	11.566424
103.H	-0.987294	18.249507	18.898304
104.C	1.017109	21.702905	10.624873
105.H	0.275883	20.921376	10.766626
106.C	3.775565	20.956503	13.190430
107.C	0.508814	11.647065	8.427746
108.H	0.133539	12.615126	8.795168
109.H	0.377028	10.898186	9.224193
110.H	-0.131103	11.349712	7.581770
111.C	2.823793	10.024636	7.233773
112.H	2.726081	9.254751	8.016366
113.H	3.865512	10.013485	6.877991
114.H	2.181649	9.725264	6.389039
115.C	2.467220	12.974827	6.436542
116.H	1.834126	12.675879	5.585237
117.C	-1.616199	13.742352	15.642540
118.H	-0.665958	13.458773	15.198927
119.C	-2.603691	12.863230	16.186931
120.H	3.505695	13.036516	6.075843
121.H	-2.552479	11.777427	16.212644
122.C	-3.682916	13.667650	16.689148
123.H	-4.591163	13.297498	17.158847
124.H	2.161603	13.984043	6.753855
125.C	-3.360771	15.041252	16.444231
126.H	-3.973914	15.899677	16.705732
127.C	4.671945	12.226608	9.104213
128.C	2.156616	12.655672	15.198951
129.H	1.597191	11.825916	14.744260
130.H	1.752943	13.596627	14.798102
131.H	1.954339	12.643491	16.279865
132.C	4.917877	13.907711	15.758991
133.H	4.552493	14.889391	15.421446
134.H	6.001101	13.867212	15.564788
135.H	4.768661	13.846016	16.849129
136.H	4.472999	10.809820	16.665627
137.C	-3.380414	13.446747	12.628784
138.H	-2.498036	13.185842	12.050711
139.C	-4.223157	12.555265	13.365258
140.H	4.088993	9.994687	15.130622
141.H	-4.088924	11.481827	13.473744
142.C	-5.283026	13.331875	13.946039
143.H	-6.085802	12.948293	14.570492
144.H	5.698669	10.707628	15.381958
145.C	-5.080715	14.700742	13.579027
146.H	-5.708760	15.540847	13.862569
147.C	-2.052577	15.113463	15.826859
148.C	3.396725	18.637266	6.982634
149.H	4.480133	18.682126	7.170933
150.H	3.252946	18.504680	5.898829
151.H	2.995312	17.737483	7.474230
152.C	3.361622	21.688336	6.675491

153.H	4.439792	21.743195	6.892850
154.H	2.909154	22.646744	6.972079
155.H	3.246338	21.590232	5.583826
156.C	0.712818	20.168379	7.042730
157.H	0.203914	19.304079	7.496441
158.C	5.534163	13.373447	8.889608
159.H	5.174795	14.397322	8.834191
160.C	6.880056	12.920504	8.711750
161.H	0.183064	21.078000	7.368058
162.H	7.750761	13.543122	8.519632
163.C	6.882783	11.489423	8.841026
164.H	7.754031	10.843544	8.764149
165.H	0.609260	20.092077	5.948535
166.C	5.541394	11.067688	9.113060
167.H	5.208821	10.044850	9.266883
168.C	5.540000	12.494552	12.625070
169.C	5.993994	17.333363	13.387811
170.H	5.138482	16.654532	13.257210
171.H	6.704938	16.843674	14.069498
172.H	6.487769	17.447113	12.411156
173.C	6.976107	20.092908	14.337961
174.H	7.538559	20.229823	13.400911
175.H	7.659002	19.638138	15.073541
176.H	6.701059	21.090646	14.713274
177.C	4.619903	18.731554	15.767412
178.H	3.758791	18.052587	15.679921
179.C	6.407144	13.602512	12.271322
180.H	6.124352	14.648473	12.347050
181.C	7.681113	13.087569	11.873542
182.H	4.257399	19.681649	16.189780
183.H	8.543178	13.673904	11.563397
184.C	7.619322	11.653928	11.943130
185.H	8.424636	10.967284	11.693767
186.H	5.327481	18.290849	16.487581
187.C	6.303051	11.288853	12.375112
188.H	5.936841	10.277121	12.529416
189.C	2.270301	21.508457	9.920352
190.C	-3.921704	14.789961	12.714352

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