Supplementary Material (ESI) for Chemical Communications

List of Electronic Supplementary Information

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2-Dimensional molecular wiring based on toroidal conjugation of hexaarylbenzene

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Experimental part.

General Methods. All manipulations were carried out under an inert atmosphere by using standard Schlenk tube techniques. THF, ether, pentane, hexane, toluene (Na-K alloy) and MeCN, CH_2Cl_2 (P_2O_5) were treated with appropriate drying agents, distilled, and stored under N_2 atmosphere. ^1H and ^{31}P NMR spectra were recorded on a JEOL EX-300 spectrometer (^1H, 300 MHz; ^{31}P, 121.5 MHz). Chemical shifts (downfield from TMS (^1H and ^{13}C) and H_3PO_4 (^{31}P)) and coupling constants are reported in ppm and in Hz, respectively. Solvents for NMR measurements containing 0.5% TMS were dried over molecular sieves, degassed, distilled under reduced pressure, and stored under N_2. IR and UV-vis spectra were obtained on a JASCO FT/IR 4200 spectrometer and a JASCO V-670 spectrometer, respectively. UV light irradiations were performed with an Ushio high pressure mercury lamp. Electrochemical measurements were made with a BAS 100B/W analyzer (observed in CH_2Cl_2; [complex]= ~1 x 10^{-3} M; [NBu_4PF_6]= 0.1 M; Ag/AgCl electrode; reported with respect to the $[FeCp_2]/[FeCp_2]^+$ couple). Simulation of the electrochemical data was performed with ECReact. Elemental analyses were performed at the Center for Advanced Materials Analysis, Technical Department, Tokyo Institute of Technology.

Synthesis of the HAB-iron complexes 1-5. The iron complexes **1** – **5** were prepared following the synthetic routes summarized in Scheme S1. Trimethylsilylacetylene,[1] di(5-bromothien-2-yl)acetylene,[2] 3,4-diphenyl-2,5-dithienylcyclopentadienones,[3] dithien-2-ylethyne,[4] thien-2-yltributyltin [5] were synthesized according to the reported procedures. Other chemicals were purchased and used without further purification.

References

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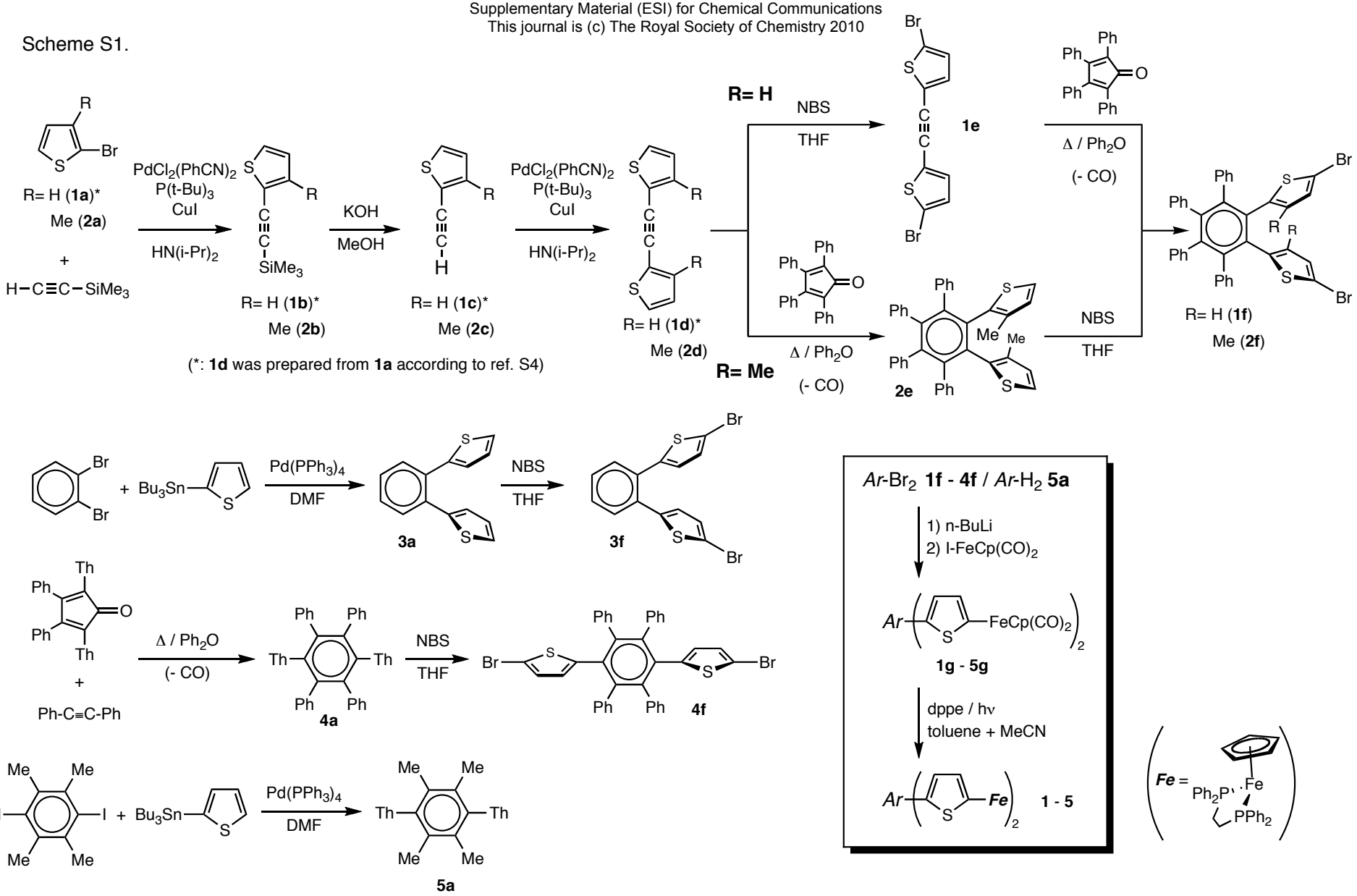
Scheme S1.


R= H (1a)*
Me (2a)
+
H–C≡C–SiMe3
PdCl2(PhCN)2
P(t-Bu)3
CuI
HN(i-Pr)2
SiMe3
R= H (1b)*
Me (2b)
KOH
MeOH
R= H (1c)*
Me (2c)
PdCl2(PhCN)2
P(t-Bu)3
CuI
HN(i-Pr)2
R= H (1d)*
Me (2d)
(*: 1d was prepared from 1a according to ref. S4)
R= H
NBS
THF
1e
Δ / Ph2O
(- CO)
R= Me
Δ / Ph2O
(- CO)
2e
NBS
THF
R= H (1f)
Me (2f)
Br + Bu3Sn
Pd(PPh3)4
DMF
3a
NBS
THF
3f
Th
Δ / Ph2O
(- CO)
4a
NBS
THF
4f
Ph-C≡C-Ph
Me Me
I + Bu3Sn
Pd(PPh3)4
DMF
5a
Ar-Br2 1f - 4f / Ar-H2 5a
1) n-BuLi
2) I-FeCp(CO)2
1g - 5g
dppe / hν
toluene + MeCN
1 - 5
Fe =
Ph2P
PPh2

1,2-di(5-bromothien-2-yl)-3,4,5,6-tetraphenylbenzene (1f). A mixture of 2,3,4,5-tetraphenylcyclopentadien-1-one (811.8 mg, 2.11 mmol) and **1e** (955.5 mg, 2.75 mmol, 1.3 eq) dissolved in degassed diphenyl ether (20 ml) was refluxed for 24 hrs. After the reaction mixture was cooled to room temperature, EtOH was added to precipitate the product, which was collected and washed with EtOH. **1f** was obtained as white powder (936.0 mg, 1.33 mmol, 63% yield). δ_H ($CDCl_3$) 6.24, 6.59 (2H, x 2, d x 2, J = 3.6 Hz, C_4H_2S), 6.72–7.33 (20H, m, Ph).

3-methyl-2-trimethylsilylethynylthiophene (2b). A mixture of 2-bromo-3-methylthiophene (0.500 ml, 4.44 mmol), $Pd(PhCN)_2Cl_2$ (51.0 mg, 0.133 mmol), CuI (25.3 mg, 0.133 mmol) and P(*t*-Bu)$_3$ (0.537 ml, 0.266 mmol, 10 wt% in toluene) dissolved in diisopropylamine (0.745 ml, 5.33 mmol) was stirred for 5 min. HC≡C-TMS (1.56 ml, 8.88 mmol) was added to the mixture, which was stirred for 13 hrs at room temperature. Then the mixture was passed through a Celite plug and the solvent was removed by a rotary evaporator. Column chromatography (silica gel eluted with hexane) afforded **2b** as yellow solid (825.0 mg, 4.25 mmol, 96% yield). δ_H ($CDCl_3$) 0.24 (9H, s, $SiMe_3$), 2.31(3H, s, C_4H_2SMe, 3H), 6.80, 7.11 (1H x 2, d x 2, J = 5.1 Hz, C_4H_2SMe).

2-ethynyl-3-methylthiophene (2c). A mixture of **2b** (825.0 ml, 4.25 mmol) and KOH (1.333 g, 23.8 mmol) dissolved in MeOH (30 ml) was stirred for 2 hrs at room temperature. After addition of water, the product was extracted with diethyl ether. The organic layer was washed with brine and water, and dried over Na_2SO_4. The volatiles were evaporated and the residue was dissolved in hexane and passed through a short silica gel column chromatography. Evaporation gave **2c** as yellow oil (475.0 mg, 3.89 mmol, 92% yield). δ_H ($CDCl_3$) 2.31(3H, s, Me), 3.44 1H, (s, ≡C-H), 6.82, 7.14 (1H x 2, d x 2, J = 5.1 Hz, C_4H_2S).

1,2-di(3-methylthien-2-yl)ethyne (2d). A mixture of 2-bromo-3-methylthiophene (0.500 ml, 4.44 mmol), $Pd(PhCN)_2Cl_2$ (51.0 mg, 0.133 mmol), CuI (25.3 mg, 0.133 mmol) and P(*t*-Bu)$_3$ (0.537 ml, 0.266 mmol, 10 wt% in toluene) dissolved in diisopropylamine (0.745 ml, 5.33 mmol) was stirred for 5 min, and **2c** (475.0 mg, 3.89 mmol) was added to the mixture. After the mixture was stirred for 12 hrs, the volatiles were evaporated. The residue was purified by silica gel column chromatography eluted with hexane to give **2d** as yellow solid (725.0 mg, 3.33 mmol, 86% yield). δ_H ($CDCl_3$) 2.36 (6H, s, Me), 6.86, 7.18 (2H x 2, d x 2, J = 4.8 Hz, C_4H_2S).

1,2-di(3-methylthien-2-yl)-3,4,5,6-tetraphenylbenzene (2e). **2e** was synthesized in a manner similar to the procedure described for **1f**, starting from 1,2-di(3-methylthien-2-yl)ethyne and 2,3,4,5-tetraphenylcyclopentadien-1-one (49% yield, obtained as a syn/anti mixture). δ_H ($CDCl_3$) one isomer : 1.82 (6H, s, Me), 6.41 (2H, d, J = 4.4 Hz, C_4HS), 6.30-7.20 (20H, m, Ph); the other isomer : 1.84 (6H, s, Me), 6.39 (2H, d, J = 5.0 Hz, C_4H_2S), 6.30-7.20 (22H, m, Ph and C_4H_2S); FAB-MS: *m/z*=574(M^+).

1,2-di(5-bromo-3-methylthien-2-yl)-3,4,5,6-tetraphenylbenzene (2f). To a THF solution (10 ml) of 1,2-di(3-methylthien-2-yl)-3,4,5,6-tetraphenylbenzene (314.6 mg, 0.547 mmol) cooled in an ice bath was added

NBS (194.8 mg, 1.095 mmol). After the mixture was stirred at room temperature for 7 hrs, water was added. The product was extracted with diethyl ether, and the organic layer was washed with water and dried over Na_2SO_4. The residue was purified by silica gel column chromatography (CH_2Cl_2) to give **2f** as white powder (385.0 mg, 0.526 mmol 96% yield, a syn/anti mixture). δ_H ($CDCl_3$) one isomer: 1.76 (6H, s, Me) 6.39 (2H, s, C_4HS), 6.75-7.10 (20H, m, Ph); the other isomer : 1.76 (6H, s, Me) 6.40 (2H, s, C_4HS), 6.75-7.10 (20H, m, Ph).

1,2-dithien-2-ylbenzene (3a). A mixture of 1,2-dibromobenzene (260 μl, 2.16 mmol), 2-thienyltributyltin (2.014 g 5.40 mmol), $Pd(PPh_3)_4$ (249.4 mg, 0.216 mmol) dissolved in DMF (30 ml) was heated at 100°C for 24 hrs. After the reaction mixture was allowed to cool at room temperature, 1M KF aq. (100 ml) was added to the solution and the mixture was stirred for 10 min. The organic layer was extracted with diethyl ether, washed with brine and water, and dried over Na_2SO_4. The solvent was evaporated and the residue was purified by silica gel column chromatography (eluted with hexane) to give **3a** as colorless oil (249.7 mg, 1.030 mmol, 48% yield). δ_H ($CDCl_3$) 6.89 (2H, dd, J = 3.5, 1.0 Hz, C_4H_3S), 6.96 (2H, dd, J = 5.0, 3.5 Hz, C_4H_3S), 7.26 (2H, dd, J = 5.0, 1.0 Hz, C_4H_3S), 7.48-7.53 (4H, m, C_6H_4).

3,6-dithienyl-1,2,4,5-tetraphenylbenzene (4a). **4a** was synthesized in a manner similar to the procedure described for **1f**, starting from diphenylacetylene and 3,4-diphenyl-2,5-dithienylcyclopentadienone (80% yield). δ_H ($CDCl_3$) 6.35 (2H, dd, J = 3.7, 1.1 Hz, C_4H_3S), 6.52 (2H, dd, J = 5.1, 3.7 Hz, C_4H_3S), 6.90-7.00 (22H, m, C_4H_3S and Ph).

1,4-di(5-bromothien-2-yl)-2,3,5,6-tetraphenylbenzene (4f). **4f** was synthesized in a manner similar to the procedure described for **2f**, starting from 3,6-dithien-2-yl-1,2,4,5-tetraphenylbenzene (91% yield). δ_H ($CDCl_3$) 6.08, 6.45 (2H x 2, d x 2, J = 3.7 Hz, C_4H_2S), 6.89-7.00 (20H, m, Ph).

1,4-dithien-2-yl-2,3,5,6-tetramethylbenzene (5a). **5a** was synthesized in a manner similar to the procedure described for **1f**, starting from 1,4-diiodo-2,3,5,6-tetramethylbenzene (96% yield). δ_H ($CDCl_3$) 2.05 (12H, s, Me), 6.83 (2H, dd, J = 3.6, 1.2 Hz, C_4H_3S), 7.12 (2H, dd, J = 5.0, 3.6 Hz, C_4H_3S), 7.38 (2H, dd, J = 5.1, 1.2 Hz, C_4H_3S).

***o*-$(Cp(CO)_2Fe\text{-}C_4H_2S)_2C_6Ph_4$ (1g).** To a THF solution of **6** (151.1 mg, 0.214 mmol) was cooled at -78°C was added *n*-BuLi (0.163 ml, 0.429 mmol, 2.64 M in *n*-hexane) dropwise. After the mixture was stirred at -78°C for 30 min, $CpFe(CO)_2I$ (130.0mg, 0.429mmol) was added to the mixture in one portion. The mixture was stirred at room temperature for additional 3 hrs. The solvent was removed in *vacuo* and the residue was extracted with CH_2Cl_2 and passed through an alumina short column. The solvent was concentrated and precipitated by hexane gave **1f** as yellow powder (182.1 mg, 0.203 mmol, 95%yield). δ_H ($CDCl_3$) 4.77 (10H, s, Cp), 6,29, 6.32 (2H x 2, d x 2, J = 2.9 Hz, C_4H_2S), 6.45–7.00 (20H, m, Ph); IR (KBr) 1968, 2022 cm^{-1} (ν(CO)); FD-

MS: *m/z*= 898 (M^+), analysis: found (calcd. for $C_{52}H_{34}Fe_2O_4S_2$) : C, 67.03 (67.00); H, 4.22 (3.75); N, 0.00 (0.00)

Complexes **2g** – **4g** were synthesized in a manner similar to the procedure described for **1g**. Complex **5g** was prepared in a manner similar to the procedure described for **1g**, starting from **5a**.

***o*-(Cp(CO)$_2$Fe-C$_4$HMeS)$_2$C$_6$Ph$_4$ (2g)** (yellow powder, 78%, a syn/anti mixture); δ_H ($CDCl_3$) one isomer: 1.67 (6H, s, *Me*), 4.72 (10H, s, Cp), 6.07 (2H, s, C_4HS), 6.40–7.15 (20H, m, Ph); the other isomer: 1.71 (6H, s, *Me*), 4.74 (10H, s, Cp), 6.05 (2H, s, C_4HS), 6.40–7.15 (20H, m, Ph); IR (KBr) 1970, 2022 cm^{-1} (ν(CO)); FAB-MS: *m/z*= 926 (M^+); analysis: found (calcd. for $C_{54.5}H_{39}ClFe_2O_4S_2$ (**2g**·0.5CH_2Cl_2)): C, 67.55 (67.54); H, 4.29 (4.06); N, 0.00 (0.00).

***o*-(Cp(CO)$_2$Fe-C$_4$H$_2$S)$_2$C$_6$H$_4$ (3g)** (yellow powder, 61% yield); δ_H ($CDCl_3$) 4.94 (10H, s, Cp), 7.19-7.23 (4H, m, C_4H_2S), 7.39-7.45 (4H, m, C_6H_4); IR (KBr) 1968, 2022 cm^{-1} (ν(CO)); FAB-MS: *m/z*= 594 (M^+), analysis: found (calcd. for $C_{28}H_{18}Fe_2O_4S_2$) : C, 56.94 (56.59); H, 3.33 (3.05); N, 0.00 (0.00).

***p*-(Cp(CO)$_2$Fe-C$_4$H$_2$S)$_2$C$_6$Ph$_4$ (4g)** (yellow powder, 56%); δ_H ($CDCl_3$) 4.67 (10H, s, Cp), 6.17, 6.19 (2H x 2, d x 2, *J* = 3.1 Hz, C_4H_2S), 6.85-6.93 (20H, m, Ph); IR (KBr) 1972, 2024 cm^{-1} (ν(CO)); FAB-MS: *m/z*= 898 (M^+); analysis: found (calcd. for $C_{53.5}H_{37}Cl_3Fe_2O_4S_2$ (**4g**·1.5CH_2Cl_2)): C, 62.01 (62.63); H, 3.76 (3.63) ; N, 0.00 (0.00). .

***p*-(Cp(CO)$_2$Fe-C$_4$H$_2$S)$_2$C$_6$Me$_4$ (5g)** (yellow powder, 53%); δ_H ($CDCl_3$) 2.06 (12H, s, Me), 5.01 (10H, s, Cp), 6.73, 6.77 (2H x 2, brs x 2, C_4H_2S); IR (KBr) 1967, 2020 cm^{-1} (ν(CO)); FAB-MS: *m/z*= 650 (M^+); analysis: found (calcd. for $C_{34}H_{30}Cl_2Fe_2O_4S_2$ (**5g**·2CH_2Cl_2)): C, 49.00 (49.79); H, 3.78 (3.69) ; N, 0.00 (0.00).

***o*-(Cp(dppe)Fe-C$_4$H$_2$S)$_2$C$_6$Ph$_4$ (1)** Complex **1** (301.2 mg, 0.335 mmol) and dppe (333.8 mg, 0.838 mmol, 2.5 eq) dissolved in a mixture of toluene/acetonitrile (95/5 ml) was irradiated by a UV lamp for 60 hrs. The progress of the reaction was followed by IR. After consumption of **11** was confirmed, the volatiles were removed under reduced pressure and the residue was subjected to alumina short column chromatography. Recrystallization from CH_2Cl_2 gave **1** as orange crystal (187.7 mg, 0.119 mmol, 35% yield). δ_H (C_6D_6) 2.10-2.47 (8H, m, CH_2), 4.33 (10H, s, Cp s), 5.41, 6.04 (2H x 2, brs x 2, C_4H_2S), 6.65-7.30, 7.45-7.55 (60H, m, Ph); δ_P (C_6D_6) 110.2(s); ESI-MS: *m/z*= 1582 (M^+); UV-vis: λ_{max} / nm (ε / M^{-1} cm^{-1}) (in CH_2Cl_2) = 400 (1.33 x 10^4); CV / mV: -694 ($E_{1/2}^1$), -553 ($E_{1/2}^2$); analysis: found (calcd. for $C_{100}H_{82}Fe_2P_4S_2$): C, 76.11 (75.85); H, 5.30 (5.22); N, 0.00 (0.00).

Complexes **2** – **5** were synthesized in a manner similar to the procedure described for **1**.

***o*-(Cp(dppe)Fe-C$_4$HMeS)$_2$C$_6$Ph$_4$ (2)** (red crystal, 40% yield); δ_H (C_6D_6) 1.80 (6H, s, Me), 1.98-2.75 (8H, m, CH_2), 4.64 (10H, s, Cp), 5.62 (2H, s, C_4HS) 6.76-7.44, 7.95–8.08, (60H, m, Ph); δ_P (C_6D_6) 105.6, 107.2 (d x 2, J_{P-P} = 19.5 Hz); ESI-MS: *m/z*= 1601 (M^+); UV-vis: λ_{max} / nm (ε / M^{-1} cm^{-1}) (in CH_2Cl_2) = 375 (sh, 9.5 x 10^3); CV / mV: -614 ($E_{1/2}^1$), -512 ($E_{1/2}^2$); analysis: found (calcd. for $C_{102}H_{86}Fe_2P_4S_2$): C, 75.76 (76.02); H, 6.17 (5.38); N, 0.00 (0.00).

***o*-(Cp(dppe)$_2$Fe-C$_4$H$_2$S)$_2$C$_6$H$_4$ (3)** (orange powder, 61% yield); δ_H (C_6D_6) 2.05-2.20, 2.48-2.65 (8H, m, CH_2), 4.43 (10H, s, Cp), 5.75, 6.70 (2H x 2, d x 2, J = 3.3 Hz, C_4H_2S), 6.95-7.08, 7.40-7.62 (44H, m, C_6H_4, and Ph); δ_P (C_6D_6): 112.6 (s); ESI-MS: *m/z*= 1278 (M^+); UV-vis: λ_{max} / nm (ε / M^{-1} cm^{-1}) (in CH_2Cl_2) = 410 (1.30 x 10^4); CV / mV: -627 ($E_{1/2}^1$), -524 ($E_{1/2}^2$); analysis: found (calcd. for $C_{76.5}H_{67}ClFe_2P_4S_2$ (**3**·0.5CH_2Cl_2)): C, 69.96 (69.53); H 5.15 (5.11).

***p*-(Cp(dppe)Fe-C$_4$H$_2$S)$_2$C$_6$Ph$_4$ (4)** (orange crystal, 56% yield); δ_H (C_6D_6): 1.90-2.32 (8H, m, CH_2), 4.21 (10H, s, Cp), 5.33, 6.10 (2H x 2, brs x 2, C_4H_2S), 6.70-7.44 (60H, m, Ph); δ_P (C_6D_6): 109.2 (brs); ESI-MS: *m/z*= 1582 (M^+); UV-vis: λ_{max} / nm (ε / M^{-1} cm^{-1}) (in CH_2Cl_2) = 405 (1.24 x 10^4); CV / mV: -645 ($E_{1/2}^1$), -565 ($E_{1/2}^2$); analysis: found (calcd. for $C_{100}H_{82}Fe_2P_4S_2$): C, 75.19 (75.85); H, 5.22 (6.04).

***p*-(Cp(dppe)$_2$Fe-C$_4$H$_2$S)$_2$C$_6$Me$_4$ (5)** (orange crystal, 37% yield); δ_H (C_6D_6): 2.20 (12H, s, Me), 2.10-2.71 (8H, m, C*H$_2$*), 4.41 (10H, s, Cp), 5.88, 6.51 (2H x 2, brs x 2, C_4H_2S), 6.77-7.65 (40H, m, Ph); δ_P (C_6D_6): 113.2 (s); ESI-MS: *m/z*= 1334 (M^+); UV-vis: λ_{max} / nm (ε / M^{-1} cm^{-1}) (in CH_2Cl_2) = 337 (2.22 x 10^4); CV / mV: -630 ($E_{1/2}^1$), -570 ($E_{1/2}^2$); analysis: found (calcd. for $C_{80.5}H_{75}ClFe_2P_4S_2$ (**5**·0.5CH_2Cl_2)): C, 69.78 (70.18); H 5.69 (5.49).

Synthesis of dicationic species [1]$^{2+}$(PF$_6$)$_2$ To a mixture of **1** (99.7 mg, 0.063 mmol) and [$FeCp_2$](PF_6) (40.6 mg, 0.123 mmol, 1.95 eq.) cooled at -78°C was slowly added THF (15 ml). After the mixture was stirred at -78°C for 2 hrs, pentane was added to the mixture to precipitate the product **[1]**$^{2+}$(PF_6)$_2$, which was washed with pentane and obtained as green powder (113.3 mg, 0.061mmol, 96%). IR (KBr) 840 cm^{-1} (PF_6); ESI-MS: *m/z*= 1727 (M^+-PF_6); UV-vis: λ_{max} / nm (ε / M^{-1} cm^{-1}) (in CH_2Cl_2) = 417 (1.27 x 10^4), 833 (1.39 x 10^4), 1423 (560); analysis: found (calcd. for $C_{101}H_{84}Cl_2F_{12}Fe_2P_6S_2$ (**[1]**$^{2+}$(PF_6)$_2$·CH_2Cl_2): C: 61.23 (61.95), H: 4.47 (4.32), N: 0.00 (0.00).

Complexes **[2]**$^{2+}$(PF_6)$_2$ – **[5]**$^{2+}$(PF_6)$_2$ were synthesized in a similar to the procedure described for **[1]**$^{2+}$(PF_6)$_2$.

[2]$^{2+}$(PF_6)$_2$ (light green powder, 91% yield); IR(KBr) 840 cm^{-1} (PF_6); ESI-MS: *m/z*= 1423 (M^+-PF_6); UV-vis: λ_{max} / nm (ε / M^{-1} cm^{-1}) (in CH_2Cl_2) = 391 (8.9 x 10^3), 796 (9.6 x 10^3), 1536 (600); analysis: found (calcd. for $C_{104}H_{90}Cl_4F_{12}Fe_2P_6S_2$ (**[2]**$^{2+}$(PF_6)$_2$·2CH_2Cl_2): C: 60.40 (60.31), H: 4.52 (4.38), N: 0.00 (0.00).

[3]$^{2+}$(PF_6)$_2$ (brown powder, 82% yield); IR(KBr) 840 cm^{-1} (PF_6); ESI-MS: *m/z*= 1756 (M+-PF6) ; UV-vis: λ_{max} / nm (ε / M^{-1} cm^{-1}) (in CH_2Cl_2) = 389 (1.08 x 10^4), 450 (sh, 7.2 x 10^3), 827 (1.21 x 10^4), 1492 (600); analysis: found (calcd. for $C_{77}H_{68}Cl_2F_{12}Fe_2P_6S_2$ (**[3]**$^{2+}$(PF_6)$_2$·CH_2Cl_2): C: 56.54 (55.92), H: 4.50 (4.14), N: 0.17 (0.00).

[4]$^{2+}$(PF_6)$_2$ (brown powder, 84% yield); IR(KBr)) 840 cm^{-1} (PF_6); ESI-MS: *m/z*= 1727 (M^+-PF_6); UV-vis: λ_{max} / nm (ε / M^{-1} cm^{-1}) (in CH_2Cl_2) =. 395 (1.08 x 10^4), 426 (1.12 x 10^4), 562 (3.1 x 10^3), 791 (1.40 x 10^4), 1480 (600); analysis: found (calcd. for $C_{101.5}H_{85}Cl_3F_{12}Fe_2P_6S_2$ (**[4]**$^{2+}$(PF_6)$_2$·1.5CH_2Cl_2): C: 60.79 (60.93), H: 4.47 (4.28), N: 0.00 (0.00).

[5]$^{2+}(PF_6)_2$ (dark blue powder, 99% yield); IR(KBr) 840 cm^{-1} (PF_6); ESI-MS: *m/z*= 1479 (M^+-PF_6); UV-vis: λ_{max} / nm (ε / M^{-1} cm^{-1}) (in CH_2Cl_2) = 368 (1.48 x 10^4), 534 (3.6 x 10^3), 717 (1.53 x 10^4), 1550 (300) ; analysis: found (calcd. for $C_{82}H_{78}Cl_4F_{12}Fe_2P_6S_2$ (**[4]**$^{2+}(PF_6)_2 \cdot 2CH_2Cl_2$): C: 54.54 (54.87), H: 4.36 (4.38), N: 0.00 (0.00).

Synthesis of monocationic species [1]$^+$(PF_6) - [5]$^+$(PF_6). Monocationic species were generated by comproportionation between the corresponding neutral and dicationic species in CH_2Cl_2.

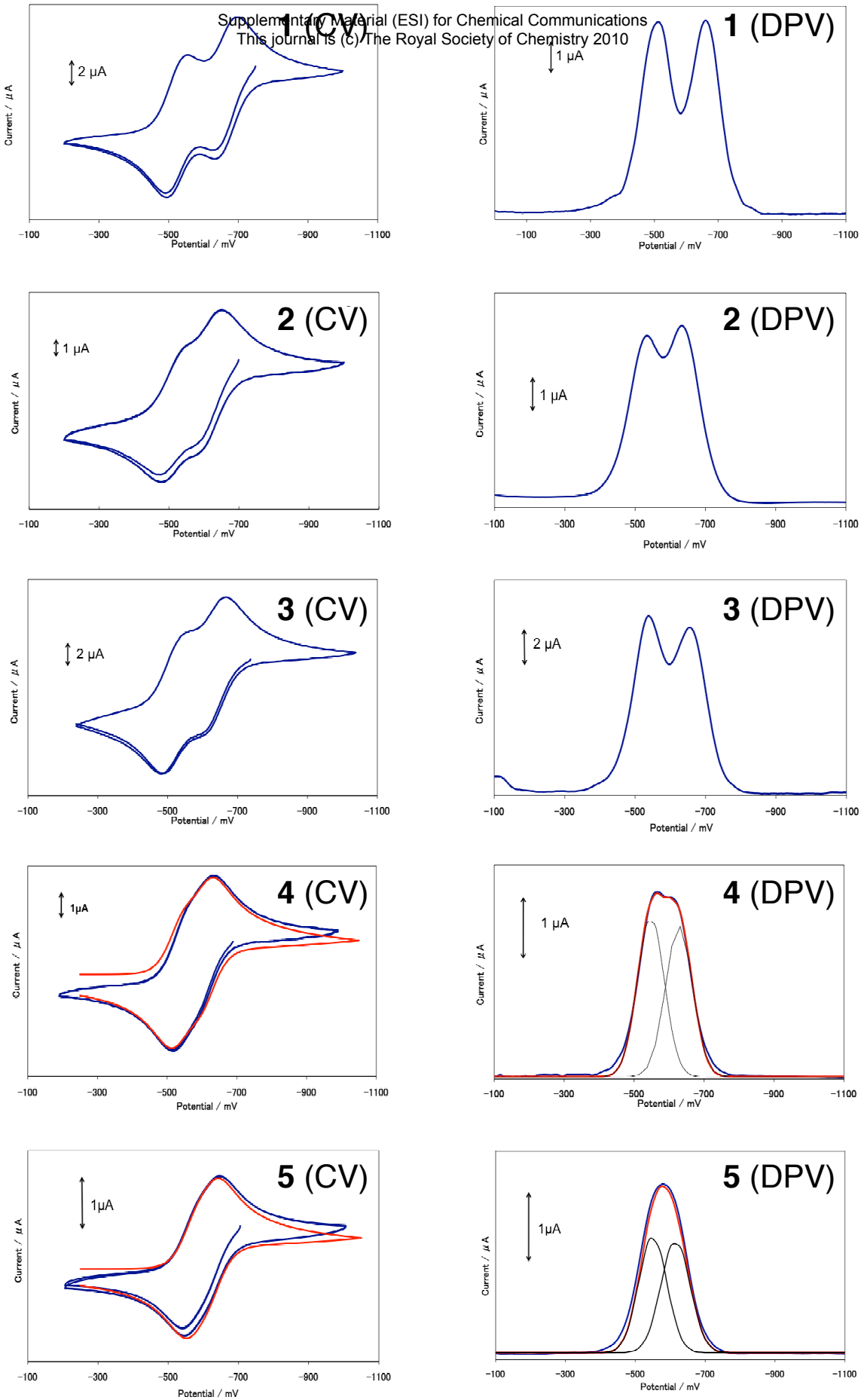


Figure S1. Electrochemical data (CV and DPV) for **1** – **5**. (observed in CH_2Cl_2; [complex]= ~1 x 10^{-3} M; [NBu_4PF_6]= 0.1 M; Ag/AgCl electrode; reported with respect to the $[FeCp_2]/[FeCp_2]^+$ couple)

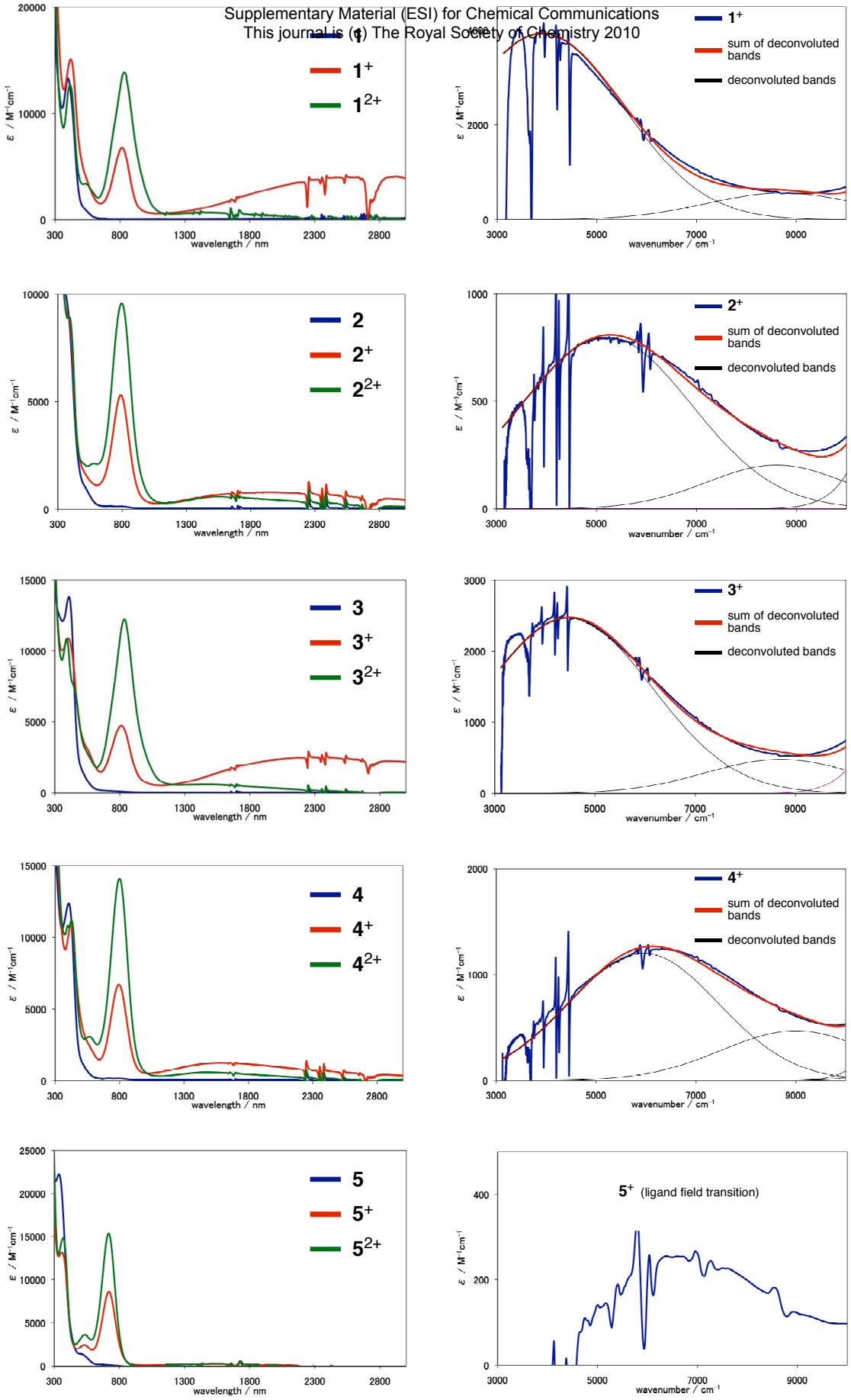


Figure S2. UV-vis and near IR spectra for **1** – **5**.

Details of X-ray crystallography. Single crystals were obtained by recrystallization from CH_2Cl_2-hexane (**1**·3CH_2Cl_2), CH_2Cl_2-MeOH (**2**·2MeOH·CH_2Cl_2), and CH_2Cl_2-pentane (**3**·2CH_2Cl_2). Diffraction measurements were made on a Rigaku RAXIS IV imaging plate area detector with Mo Kα radiation (λ= 0.71069 Å) at –60°C. Indexing was performed from 3 oscillation images, which were exposed for 3 min. The crystal-to-detector distance was 110 mm ($2\theta_{max}$= 55°). In the reduction of data, Lorentz and polarization corrections and empirical absorption corrections were made.[6] The crystallographic data are summarized in Table S1. Neutral scattering factors were obtained from the standard source.[7]

The structure of **1** was solved by using the teXsan structure solving program system obtained from the Rigaku Corp., Tokyo, Japan.[8] The structure was solved by a combination of the direct methods (SHELXS-86)[9] and Fourier synthesis (DIRDIF94).[10] Least-squares refinements were carried out using SHELXL-97 [9] (refined on F^2) linked to teXsan.

The structures of **2** and **5** were solved by using the Win GX package.[11] The structure was solved by the direct methods (SHELXS-86),[9] and least-squares refinements were carried out using SHELXL-97 [9] (refined on F^2) .

Unless otherwise stated, all non-hydrogen atoms were refined anisotropically, methyl hydrogen atoms were refined using riding models, and other hydrogen atoms were fixed at the calculated positions.

1 and **2**: The solvent molecules were refined isotropically and hydrogen atoms attached to them were not included in the refinement. For **2** with the large R_{int}, we repeated data collection a couple of times but the present data was the best among them. The large R_{int} value should be due to the low quality of the crystal.

5: The solvent molecules were refined anisotropically and hydrogen atoms attached to them were not included in the refinement.

The crystallographic data have been deposited at the CSD: CCDC767557 (**1**), CCDC767558 (**2**), and CCDC767559 (**5**).

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S10) Beurskens, P. T.; Admiraal, G.; Beurskens, G.; Bosman, W. P.; Garcia-Granda, S.; Gould, R. O.; Smits, J. M. M.; Smykalla, C. *The DIRDIF program system, Technical Report of the Crystallography Laboratory*, University of Nijmegen, Nijmegen, The Netherland, 1992.

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Table S1. Crystallographic data for DTE complexes.

complex	**1**	**2**	**5**
solvate	$3CH_2Cl_2$	$2MeOH{\cdot}CH_2Cl_2$	$2CH_2Cl_2$
formula	$C_{103}H_{88}Cl_6Fe_2P_4S_2$	$C_{105}H_{86}Cl_2Fe_2O_2P_4S_2$	$C_{82}H_{74}Cl_4Fe_2P_4S_2$
formula weight	1838.26	1750.34	1500.91
crystal system	triclinic	monoclinic	triclinic
space group	*P-1*	$P2_1/n$	*P-1*
a / Å	17.548(3)	17.354(3)	9.048(3)
b / Å	17.970(2)	25.1295(17)	11.720(6)
c / Å	18.225(3)	20.621(3)	17.902(8)
α / deg	104.363(8)	90	86.243(14)
β / deg	105.373(6)	99.251(2)	80.025(19)
γ / deg	115.240(6)	90	73.990(18)
V/ $Å^3$	4562(1)	8876(2)	1796.9(13)
Z	2	4	1
d_{calcd} / $g{\cdot}cm^{-3}$	1.338	1.310	1.387
μ / mm^{-1}	0.657	0.557	0.745
no of diffractions collected	37206	68496	14757
no of variable	1009	1020	425
R1 for data	0.0887	0. 0794	0.0616
with $I > 2\sigma(I)$	(for 10679 data)	(for 6721 data)	(for 4066 data)
wR2	0. 2555	0.1911	0.1588
	(for all 19008 data)	(for all 19008 data)	(for all 7513 data)

Table S2. Interatomic distances (Å) and bond angles (deg) for **1**.

ATOM	ATOM	DISTANCE	ATOM	ATOM	DISTANCE
Fe(1)	P(1)	2.163(2)	P(4)	C(241)	1.844(9)
Fe(1)	P(2)	2.161(2)	P(4)	C(251)	1.842(7)
Fe(1)	C(14)	2.009(5)	C(1)	C(2)	1.422(9)
Fe(1)	C(100)	2.102(8)	C(1)	C(6)	1.398(8)
Fe(1)	C(101)	2.102(7)	C(1)	C(11)	1.483(7)
Fe(1)	C(102)	2.104(8)	C(2)	C(3)	1.408(7)
Fe(1)	C(103)	2.118(7)	C(2)	C(21)	1.491(8)
Fe(1)	C(104)	2.124(8)	C(3)	C(4)	1.399(8)
Fe(2)	P(3)	2.163(2)	C(3)	C(31)	1.49(1)
Fe(2)	P(4)	2.160(2)	C(4)	C(5)	1.40(1)
Fe(2)	C(24)	1.985(7)	C(4)	C(41)	1.488(7)
Fe(2)	C(200)	2.098(9)	C(5)	C(6)	1.396(7)
Fe(2)	C(201)	2.104(9)	C(5)	C(51)	1.500(8)
Fe(2)	C(202)	2.117(5)	C(6)	C(61)	1.505(9)
Fe(2)	C(203)	2.111(5)	C(11)	C(12)	1.36(1)
Fe(2)	C(204)	2.086(8)	C(12)	C(13)	1.419(6)
Cl(1)	C(301)	1.81(1)	C(13)	C(14)	1.37(1)
Cl(2)	C(301)	1.77(1)	C(21)	C(22)	1.359(6)
Cl(3)	C(302)	1.64(2)	C(22)	C(23)	1.413(9)
Cl(4)	C(302)	1.66(3)	C(23)	C(24)	1.380(9)
Cl(5)	C(303)	1.68(5)	C(31)	C(32)	1.39(1)
Cl(6)	C(303)	1.61(3)	C(31)	C(36)	1.369(8)
S(1)	C(11)	1.722(6)	C(32)	C(33)	1.41(1)
S(1)	C(14)	1.730(6)	C(33)	C(34)	1.37(1)
S(2)	C(21)	1.715(7)	C(34)	C(35)	1.37(1)
S(2)	C(24)	1.747(5)	C(35)	C(36)	1.40(1)
P(1)	C(111)	1.848(8)	C(41)	C(42)	1.37(1)
P(1)	C(121)	1.817(8)	C(41)	C(46)	1.383(9)
P(1)	C(131)	1.852(5)	C(42)	C(43)	1.398(8)
P(2)	C(112)	1.860(7)	C(43)	C(44)	1.37(1)
P(2)	C(141)	1.825(7)	C(44)	C(45)	1.39(1)
P(2)	C(151)	1.840(6)	C(45)	C(46)	1.383(8)
P(3)	C(211)	1.843(6)	C(51)	C(52)	1.39(1)
P(3)	C(221)	1.831(8)	C(51)	C(56)	1.39(1)
P(3)	C(231)	1.849(8)	C(52)	C(53)	1.37(1)
P(4)	C(212)	1.863(6)	C(53)	C(54)	1.36(2)

Table S2. Interatomic distances (Å) and bond angles (deg) for **1**.

ATOM	ATOM	DISTANCE	ATOM	ATOM	DISTANCE
C(54)	C(55)	1.35(2)	C(154)	C(155)	1.379(9)
C(55)	C(56)	1.40(1)	C(155)	C(156)	1.39(1)
C(61)	C(62)	1.39(1)	C(200)	C(201)	1.43(1)
C(61)	C(66)	1.39(1)	C(200)	C(204)	1.38(1)
C(62)	C(63)	1.39(1)	C(201)	C(202)	1.41(1)
C(63)	C(64)	1.36(1)	C(202)	C(203)	1.40(1)
C(64)	C(65)	1.39(1)	C(203)	C(204)	1.40(1)
C(65)	C(66)	1.37(1)	C(211)	C(212)	1.54(1)
C(100)	C(101)	1.40(1)	C(221)	C(222)	1.38(1)
C(100)	C(104)	1.424(7)	C(221)	C(226)	1.379(7)
C(101)	C(102)	1.414(9)	C(222)	C(223)	1.38(1)
C(102)	C(103)	1.41(1)	C(223)	C(224)	1.393(9)
C(103)	C(104)	1.42(1)	C(224)	C(225)	1.33(1)
C(111)	C(112)	1.52(1)	C(225)	C(226)	1.39(1)
C(121)	C(122)	1.39(1)	C(231)	C(232)	1.403(7)
C(121)	C(126)	1.41(1)	C(231)	C(236)	1.38(1)
C(122)	C(123)	1.40(1)	C(232)	C(233)	1.38(1)
C(123)	C(124)	1.38(1)	C(233)	C(234)	1.37(1)
C(124)	C(125)	1.34(1)	C(234)	C(235)	1.377(9)
C(125)	C(126)	1.38(2)	C(235)	C(236)	1.39(1)
C(131)	C(132)	1.38(1)	C(241)	C(242)	1.392(9)
C(131)	C(136)	1.367(9)	C(241)	C(246)	1.397(9)
C(132)	C(133)	1.378(8)	C(242)	C(243)	1.39(2)
C(133)	C(134)	1.38(1)	C(243)	C(244)	1.38(1)
C(134)	C(135)	1.33(1)	C(244)	C(245)	1.39(1)
C(135)	C(136)	1.390(7)	C(245)	C(246)	1.38(1)
C(141)	C(142)	1.376(8)	C(251)	C(252)	1.39(1)
C(141)	C(146)	1.42(1)	C(251)	C(256)	1.40(1)
C(142)	C(143)	1.39(1)	C(252)	C(253)	1.39(1)
C(143)	C(144)	1.38(1)	C(253)	C(254)	1.38(2)
C(144)	C(145)	1.36(1)	C(254)	C(255)	1.36(2)
C(145)	C(146)	1.37(1)	C(255)	C(256)	1.38(1)
C(151)	C(152)	1.392(7)			
C(151)	C(156)	1.38(1)	C(11)	C(21)	2.90(1)
C(152)	C(153)	1.39(1)	C(11)	C(61)	2.892(7)
C(153)	C(154)	1.38(1)	C(21)	C(31)	2.898(7)

Table S2. Interatomic distances (Å) and bond angles (deg) for **1**.

ATOM	ATOM	DISTANCE	ATOM	ATOM	DISTANCE
C(31)	C(41)	2.870(7)			
C(41)	C(51)	2.92(1)			
C(51)	C(61)	2.924(7)			
Fe(1)	Fe(2)	9.220(2)			

Table S2. Interatomic distances (Å) and bond angles (deg) for **1**. (cont'd.)

ATOM	ATOM	ATOM	ANGLE	ATOM	ATOM	ATOM	ANGLE
P(1)	Fe(1)	P(2)	86.41(8)	P(4)	Fe(2)	C(200)	104.1(2)
P(1)	Fe(1)	C(14)	84.8(2)	P(4)	Fe(2)	C(201)	91.3(2)
P(1)	Fe(1)	C(100)	96.7(2)	P(4)	Fe(2)	C(202)	116.2(2)
P(1)	Fe(1)	C(101)	117.4(2)	P(4)	Fe(2)	C(203)	154.5(3)
P(1)	Fe(1)	C(102)	156.7(2)	P(4)	Fe(2)	C(204)	141.1(2)
P(1)	Fe(1)	C(103)	148.4(3)	C(24)	Fe(2)	C(200)	159.5(2)
P(1)	Fe(1)	C(104)	110.6(2)	C(24)	Fe(2)	C(201)	127.1(3)
P(2)	Fe(1)	C(14)	92.5(2)	C(24)	Fe(2)	C(202)	94.9(3)
P(2)	Fe(1)	C(100)	132.3(2)	C(24)	Fe(2)	C(203)	95.8(2)
P(2)	Fe(1)	C(101)	98.1(2)	C(24)	Fe(2)	C(204)	128.5(3)
P(2)	Fe(1)	C(102)	94.8(2)	C(200)	Fe(2)	C(201)	39.8(4)
P(2)	Fe(1)	C(103)	125.1(3)	C(200)	Fe(2)	C(202)	65.8(3)
P(2)	Fe(1)	C(104)	160.5(2)	C(200)	Fe(2)	C(203)	65.0(3)
C(14)	Fe(1)	C(100)	135.2(3)	C(200)	Fe(2)	C(204)	38.4(4)
C(14)	Fe(1)	C(101)	155.8(2)	C(201)	Fe(2)	C(202)	39.1(3)
C(14)	Fe(1)	C(102)	118.4(2)	C(201)	Fe(2)	C(203)	65.3(3)
C(14)	Fe(1)	C(103)	90.4(2)	C(201)	Fe(2)	C(204)	65.5(4)
C(14)	Fe(1)	C(104)	98.3(2)	C(202)	Fe(2)	C(203)	38.7(3)
C(100)	Fe(1)	C(101)	39.0(3)	C(202)	Fe(2)	C(204)	65.3(3)
C(100)	Fe(1)	C(102)	65.5(3)	C(203)	Fe(2)	C(204)	38.9(3)
C(100)	Fe(1)	C(103)	65.5(3)	C(11)	S(1)	C(14)	95.4(3)
C(100)	Fe(1)	C(104)	39.4(2)	C(21)	S(2)	C(24)	96.0(3)
C(101)	Fe(1)	C(102)	39.3(2)	Fe(1)	P(1)	C(111)	108.1(2)
C(101)	Fe(1)	C(103)	65.7(2)	Fe(1)	P(1)	C(121)	120.8(2)
C(101)	Fe(1)	C(104)	66.0(3)	Fe(1)	P(1)	C(131)	121.2(2)
C(102)	Fe(1)	C(103)	39.0(3)	C(111)	P(1)	C(121)	105.2(3)
C(102)	Fe(1)	C(104)	65.8(3)	C(111)	P(1)	C(131)	100.1(3)
C(103)	Fe(1)	C(104)	39.2(3)	C(121)	P(1)	C(131)	98.7(3)
P(3)	Fe(2)	P(4)	87.47(7)	Fe(1)	P(2)	C(112)	111.0(3)
P(3)	Fe(2)	C(24)	86.6(2)	Fe(1)	P(2)	C(141)	122.3(2)
P(3)	Fe(2)	C(200)	108.1(3)	Fe(1)	P(2)	C(151)	114.6(3)
P(3)	Fe(2)	C(201)	146.2(3)	C(112)	P(2)	C(141)	103.7(3)
P(3)	Fe(2)	C(202)	156.2(2)	C(112)	P(2)	C(151)	105.3(3)
P(3)	Fe(2)	C(203)	117.5(3)	C(141)	P(2)	C(151)	97.9(3)
P(3)	Fe(2)	C(204)	95.3(2)	Fe(2)	P(3)	C(211)	109.2(3)
P(4)	Fe(2)	C(24)	90.4(2)	Fe(2)	P(3)	C(221)	121.2(2)

Table S2. Interatomic distances (Å) and bond angles (deg) for **1**. (cont'd.)

ATOM	ATOM	ATOM	ANGLE	ATOM	ATOM	ATOM	ANGLE
Fe(2)	P(3)	C(231)	119.2(2)	S(2)	C(21)	C(2)	121.1(4)
C(211)	P(3)	C(221)	104.0(3)	S(2)	C(21)	C(22)	109.2(5)
C(211)	P(3)	C(231)	103.1(3)	C(2)	C(21)	C(22)	129.3(6)
C(221)	P(3)	C(231)	97.7(4)	C(21)	C(22)	C(23)	112.4(6)
Fe(2)	P(4)	C(212)	111.1(2)	C(22)	C(23)	C(24)	117.7(4)
Fe(2)	P(4)	C(241)	121.0(2)	Fe(2)	C(24)	S(2)	118.9(3)
Fe(2)	P(4)	C(251)	114.6(2)	Fe(2)	C(24)	C(23)	136.4(4)
C(212)	P(4)	C(241)	103.7(3)	S(2)	C(24)	C(23)	104.6(5)
C(212)	P(4)	C(251)	102.7(3)	C(3)	C(31)	C(32)	119.2(5)
C(241)	P(4)	C(251)	101.5(4)	C(3)	C(31)	C(36)	122.3(6)
C(2)	C(1)	C(6)	119.3(5)	C(32)	C(31)	C(36)	118.5(7)
C(2)	C(1)	C(11)	119.5(5)	C(31)	C(32)	C(33)	120.0(6)
C(6)	C(1)	C(11)	121.1(6)	C(32)	C(33)	C(34)	120.1(9)
C(1)	C(2)	C(3)	119.9(5)	C(33)	C(34)	C(35)	120.4(9)
C(1)	C(2)	C(21)	119.8(4)	C(34)	C(35)	C(36)	119.4(7)
C(3)	C(2)	C(21)	120.2(6)	C(31)	C(36)	C(35)	121.5(7)
C(2)	C(3)	C(4)	120.0(6)	C(4)	C(41)	C(42)	122.6(5)
C(2)	C(3)	C(31)	119.6(5)	C(4)	C(41)	C(46)	118.9(7)
C(4)	C(3)	C(31)	120.3(5)	C(42)	C(41)	C(46)	118.3(5)
C(3)	C(4)	C(5)	119.7(5)	C(41)	C(42)	C(43)	120.6(7)
C(3)	C(4)	C(41)	118.6(6)	C(42)	C(43)	C(44)	120.0(9)
C(5)	C(4)	C(41)	121.6(5)	C(43)	C(44)	C(45)	120.1(6)
C(4)	C(5)	C(6)	120.7(5)	C(44)	C(45)	C(46)	119.0(7)
C(4)	C(5)	C(51)	119.0(5)	C(41)	C(46)	C(45)	121.9(8)
C(6)	C(5)	C(51)	120.3(6)	C(5)	C(51)	C(52)	120.6(7)
C(1)	C(6)	C(5)	120.3(6)	C(5)	C(51)	C(56)	121.5(7)
C(1)	C(6)	C(61)	118.9(4)	C(52)	C(51)	C(56)	117.9(6)
C(5)	C(6)	C(61)	120.8(5)	C(51)	C(52)	C(53)	121.5(9)
S(1)	C(11)	C(1)	122.1(5)	C(52)	C(53)	C(54)	120(1)
S(1)	C(11)	C(12)	108.8(3)	C(53)	C(54)	C(55)	119.7(8)
C(1)	C(11)	C(12)	129.1(5)	C(54)	C(55)	C(56)	121.5(9)
C(11)	C(12)	C(13)	113.1(6)	C(51)	C(56)	C(55)	119.0(9)
C(12)	C(13)	C(14)	115.9(6)	C(6)	C(61)	C(62)	120.9(7)
Fe(1)	C(14)	S(1)	117.3(4)	C(6)	C(61)	C(66)	120.7(6)
Fe(1)	C(14)	C(13)	135.8(5)	C(62)	C(61)	C(66)	118.3(7)
S(1)	C(14)	C(13)	106.7(4)	C(61)	C(62)	C(63)	119.9(8)
C(62)	C(63)	C(64)	121.1(8)	C(131)	C(136)	C(135)	121.1(7)
C(63)	C(64)	C(65)	119.7(8)	P(2)	C(141)	C(142)	121.6(6)
C(64)	C(65)	C(66)	119.7(8)	P(2)	C(141)	C(146)	120.4(4)
C(61)	C(66)	C(65)	121.3(7)	C(142)	C(141)	C(146)	118.0(7)
Fe(1)	C(100)	C(101)	70.5(4)	C(141)	C(142)	C(143)	119.6(8)
Fe(1)	C(100)	C(104)	71.2(4)	C(142)	C(143)	C(144)	121.0(6)
C(101)	C(100)	C(104)	109.0(6)	C(143)	C(144)	C(145)	120.4(8)
Fe(1)	C(101)	C(100)	70.5(4)	C(144)	C(145)	C(146)	119.2(9)
Fe(1)	C(101)	C(102)	70.5(4)	C(141)	C(146)	C(145)	121.7(6)
C(100)	C(101)	C(102)	107.7(5)	P(2)	C(151)	C(152)	123.2(6)
Fe(1)	C(102)	C(101)	70.3(4)	P(2)	C(151)	C(156)	119.1(3)
Fe(1)	C(102)	C(103)	71.0(5)	C(152)	C(151)	C(156)	117.2(6)
C(101)	C(102)	C(103)	108.4(8)	C(151)	C(152)	C(153)	120.8(8)
Fe(1)	C(103)	C(102)	70.0(4)	C(152)	C(153)	C(154)	120.6(6)
Fe(1)	C(103)	C(104)	70.6(4)	C(153)	C(154)	C(155)	119.5(7)
C(102)	C(103)	C(104)	108.3(5)	C(154)	C(155)	C(156)	119.4(8)
Fe(1)	C(104)	C(100)	69.5(4)	C(151)	C(156)	C(155)	122.5(5)
Fe(1)	C(104)	C(103)	70.1(5)	Fe(2)	C(200)	C(201)	70.3(5)
C(100)	C(104)	C(103)	106.6(7)	Fe(2)	C(200)	C(204)	70.3(5)
P(1)	C(111)	C(112)	109.1(5)	C(201)	C(200)	C(204)	107.7(7)
P(2)	C(112)	C(111)	110.9(5)	Fe(2)	C(201)	C(200)	69.9(5)
P(1)	C(121)	C(122)	124.1(6)	Fe(2)	C(201)	C(202)	70.9(5)
P(1)	C(121)	C(126)	118.1(6)	C(200)	C(201)	C(202)	107.1(8)
C(122)	C(121)	C(126)	117.8(8)	Fe(2)	C(202)	C(201)	69.9(4)
C(121)	C(122)	C(123)	120.2(7)	Fe(2)	C(202)	C(203)	70.4(3)
C(122)	C(123)	C(124)	119.1(8)	C(201)	C(202)	C(203)	107.7(7)
C(123)	C(124)	C(125)	122(1)	Fe(2)	C(203)	C(202)	70.9(3)
C(124)	C(125)	C(126)	120(1)	Fe(2)	C(203)	C(204)	69.6(3)
C(121)	C(126)	C(125)	121.2(9)	C(202)	C(203)	C(204)	108.1(7)
P(1)	C(131)	C(132)	119.9(5)	Fe(2)	C(204)	C(200)	71.3(5)
P(1)	C(131)	C(136)	122.6(5)	Fe(2)	C(204)	C(203)	71.5(4)
C(132)	C(131)	C(136)	117.3(5)	C(200)	C(204)	C(203)	109.3(8)
C(131)	C(132)	C(133)	121.2(7)	P(3)	C(211)	C(212)	110.7(4)
C(132)	C(133)	C(134)	120.2(9)	P(4)	C(212)	C(211)	111.5(3)
C(133)	C(134)	C(135)	119.0(6)	P(3)	C(221)	C(222)	121.5(4)
C(134)	C(135)	C(136)	121.1(7)	P(3)	C(221)	C(226)	120.3(6)

Table S2. Interatomic distances (Å) and bond angles (deg) for **1**. (cont'd)

ATOM	ATOM	ATOM	ANGLE	DIHEDRAL ANGLES	
C(222)	C(221)	C(226)	118.1(7)	C12-C11-C1-C2	62
C(221)	C(222)	C(223)	120.9(5)	C22-C21-C2-C3	129.1
C(222)	C(223)	C(224)	118.9(8)	C32-C31-C3-C4	113.1
C(223)	C(224)	C(225)	121(1)	C42-C41-C4-C5	118.1
C(224)	C(225)	C(226)	120.8(6)	C52-C51-C5-C6	112.4
C(221)	C(226)	C(225)	120.6(7)	C62-C61-C6-C1	119.1
P(3)	C(231)	C(232)	122.6(6)		
P(3)	C(231)	C(236)	119.2(4)		
C(232)	C(231)	C(236)	118.2(7)		
C(231)	C(232)	C(233)	119.7(7)		
C(232)	C(233)	C(234)	122.1(6)		
C(233)	C(234)	C(235)	118.5(9)		
C(234)	C(235)	C(236)	120.6(8)		
C(231)	C(236)	C(235)	120.9(6)		
P(4)	C(241)	C(242)	120.6(5)		
P(4)	C(241)	C(246)	121.5(5)		
C(242)	C(241)	C(246)	117.9(8)		
C(241)	C(242)	C(243)	120.6(6)		
C(242)	C(243)	C(244)	120.7(7)		
C(243)	C(244)	C(245)	119.1(9)		
C(244)	C(245)	C(246)	120.4(6)		
C(241)	C(246)	C(245)	121.0(6)		
P(4)	C(251)	C(252)	124.0(6)		
P(4)	C(251)	C(256)	118.2(6)		
C(252)	C(251)	C(256)	117.6(7)		
C(251)	C(252)	C(253)	120.1(9)		
C(252)	C(253)	C(254)	122(1)		
C(253)	C(254)	C(255)	118.3(9)		
C(254)	C(255)	C(256)	121.0(9)		
C(251)	C(256)	C(255)	121.3(9)		
Cl(1)	C(301)	Cl(2)	107.6(8)		
Cl(3)	C(302)	Cl(4)	129(2)		
Cl(5)	C(303)	Cl(6)	110(2)		

Table S2. Interatomic distances (Å) and bond angles (deg) for **2**.

ATOM	ATOM	DISTANCE	ATOM	ATOM	DISTANCE
Fe1	P1	2.175(2)	C2	C21	1.494(9)
Fe1	P2	2.175(2)	C2	C1	1.402(8)
Fe1	C14	1.996(6)	C2	C3	1.405(7)
Fe1	C100	2.090(7)	C3	C31	1.508(9)
Fe1	C101	2.090(8)	C3	C4	1.422(9)
Fe1	C102	2.082(8)	C4	C41	1.497(7)
Fe1	C103	2.089(8)	C4	C5	1.406(9)
Fe1	C104	2.101(7)	C5	C51	1.498(10)
Fe2	P3	2.1521(19)	C5	C6	1.396(7)
Fe2	P4	2.164(2)	C6	C1	1.420(9)
Fe2	C24	1.985(6)	C6	C61	1.488(9)
Fe2	C200	2.091(8)	C1	C11	1.490(7)
Fe2	C201	2.072(8)	C11	C12	1.355(8)
Fe2	C202	2.096(8)	C12	C15	1.514(9)
Fe2	C203	2.102(6)	C12	C13	1.439(8)
Fe2	C204	2.098(8)	C13	C14	1.371(9)
Cl	C900	1.972(12)	C21	C22	1.358(9)
Cl2	C900	1.613(13)	C22	C23	1.440(9)
S1	C11	1.731(6)	C22	C25	1.489(8)
S1	C14	1.743(5)	C23	C24	1.370(8)
S2	C21	1.748(6)	C31	C36	1.395(9)
S2	C24	1.765(7)	C31	C32	1.365(10)
P1	C121	1.841(7)	C32	C33	1.386(10)
P1	C111	1.852(7)	C33	C34	1.386(11)
P1	C131	1.834(6)	C34	C35	1.352(12)
P2	C141	1.832(6)	C35	C36	1.392(11)
P2	C112	1.827(6)	C41	C42	1.367(10)
P2	C151	1.846(8)	C41	C46	1.385(9)
P3	C221	1.828(8)	C42	C43	1.400(11)
P3	C231	1.843(7)	C43	C44	1.388(12)
P3	C211	1.827(6)	C44	C45	1.360(14)
P4	C251	1.851(7)	C45	C46	1.383(11)
P4	C212	1.862(6)	C51	C56	1.374(10)
P4	C241	1.836(8)	C51	C52	1.361(11)
O1	C912	1.494(15)	C52	C53	1.391(14)
O2	C911	1.455(13)	C53	C54	1.360(17)

Table S3. Interatomic distances (Å) and bond angles (deg) for **2**. (cont'd.)

ATOM	ATOM	DISTANCE	ATOM	ATOM	DISTANCE
C54	C55	1.357(17)	C155	C156	1.390(14)
C55	C56	1.421(13)	C200	C201	1.396(12)
C61	C66	1.384(9)	C141	C142	1.368(9)
C61	C62	1.387(9)	C201	C202	1.406(11)
C62	C63	1.395(10)	C202	C203	1.413(10)
C63	C64	1.368(11)	C203	C204	1.409(12)
C64	C65	1.379(11)	C211	C212	1.542(8)
C65	C66	1.384(10)	C221	C226	1.393(11)
C100	C104	1.392(11)	C221	C222	1.387(11)
C100	C101	1.415(11)	C222	C223	1.375(12)
C101	C102	1.401(11)	C223	C224	1.380(13)
C102	C103	1.410(11)	C224	C225	1.360(17)
C103	C104	1.424(10)	C225	C226	1.377(13)
C111	C112	1.547(9)	C231	C232	1.387(9)
C121	C126	1.389(11)	C231	C236	1.382(9)
C121	C122	1.379(12)	C232	C233	1.385(10)
C122	C123	1.401(12)	C200	C204	1.386(12)
C123	C124	1.357(14)	C233	C234	1.351(10)
C124	C125	1.380(13)	C234	C235	1.368(11)
C125	C126	1.383(11)	C235	C236	1.375(11)
C131	C136	1.397(10)	C241	C242	1.358(11)
C131	C132	1.377(9)	C241	C246	1.377(10)
C132	C133	1.373(11)	C242	C243	1.422(12)
C133	C134	1.370(12)	C243	C244	1.353(15)
C134	C135	1.387(11)	C244	C245	1.356(14)
C135	C136	1.391(10)	C245	C246	1.406(12)
C141	C146	1.381(9)	C251	C256	1.377(10)
C142	C143	1.353(13)	C251	C252	1.363(9)
C143	C144	1.365(12)	C252	C253	1.404(11)
C144	C145	1.372(11)	C253	C254	1.373(11)
C145	C146	1.371(10)	C254	C255	1.366(11)
C151	C152	1.367(11)	C255	C256	1.384(11)
C151	C156	1.384(11)			
C152	C153	1.372(13)	C11	C21	2.9460(3)
C153	C154	1.403(14)	C11	C61	2.8919(3)
C154	C155	1.341(15)	C21	C31	2.9244(2)
C31	C41	2.8893(3)			
C41	C51	2.9088(3)			
C51	C61	2.8951(2)			
Fe1	Fe2	6.794(1)			

Table S3. Interatomic distances (Å) and bond angles (deg) for **2**. (cont'd)

ATOM	ATOM	ATOM	ANGLE	ATOM	ATOM	ATOM	ANGLE
P1	Fe1	P2	84.30(8)	P4	Fe2	C200	130.0(2)
P1	Fe1	C14	96.66(18)	P4	Fe2	C201	165.3(2)
P1	Fe1	C100	126.9(2)	P4	Fe2	C202	133.7(2)
P1	Fe1	C101	162.5(2)	P4	Fe2	C203	101.39(19)
P1	Fe1	C102	133.0(2)	P4	Fe2	C204	100.1(2)
P1	Fe1	C103	99.1(2)	C24	Fe2	C200	86.7(3)
P1	Fe1	C104	96.7(2)	C24	Fe2	C201	94.6(3)
P2	Fe1	C14	86.4(2)	C24	Fe2	C202	132.0(3)
P2	Fe1	C100	148.7(2)	C24	Fe2	C203	152.1(3)
P2	Fe1	C101	110.5(2)	C24	Fe2	C204	115.5(3)
P2	Fe1	C102	96.0(2)	C200	Fe2	C201	39.2(3)
P2	Fe1	C103	116.6(2)	C200	Fe2	C202	65.7(3)
P2	Fe1	C104	156.3(2)	C200	Fe2	C203	65.5(3)
C14	Fe1	C100	87.1(3)	C200	Fe2	C204	38.6(3)
C14	Fe1	C101	93.6(3)	C201	Fe2	C202	39.4(3)
C14	Fe1	C102	130.3(3)	C201	Fe2	C203	66.0(3)
C14	Fe1	C103	153.1(3)	C201	Fe2	C204	65.5(3)
C14	Fe1	C104	116.8(3)	C202	Fe2	C203	39.3(3)
C100	Fe1	C101	39.6(3)	C202	Fe2	C204	65.6(3)
C100	Fe1	C102	65.8(3)	C203	Fe2	C204	39.2(3)
C100	Fe1	C103	66.0(3)	C11	S1	C14	95.1(3)
C100	Fe1	C104	38.8(3)	C21	S2	C24	94.8(3)
C101	Fe1	C102	39.2(3)	Fe1	P1	C111	110.6(2)
C101	Fe1	C103	66.4(3)	Fe1	P1	C121	114.0(2)
C101	Fe1	C104	66.0(3)	Fe1	P1	C131	126.5(2)
C102	Fe1	C103	39.5(3)	C111	P1	C121	105.4(4)
C102	Fe1	C104	66.1(3)	C111	P1	C131	101.2(3)
C103	Fe1	C104	39.8(3)	C121	P1	C131	96.8(3)
P3	Fe2	P4	84.30(8)	Fe1	P2	C112	106.7(2)
P3	Fe2	C24	85.92(18)	Fe1	P2	C141	121.6(2)
P3	Fe2	C200	145.4(2)	Fe1	P2	C151	120.7(3)
P3	Fe2	C201	108.0(2)	C112	P2	C141	103.5(3)
P3	Fe2	C202	95.3(2)	C112	P2	C151	102.1(3)
P3	Fe2	C203	118.4(2)	C141	P2	C151	99.6(3)
P3	Fe2	C204	157.5(2)	Fe2	P3	C211	107.3(2)
P4	Fe2	C24	94.25(19)	Fe2	P3	C221	119.4(3)

Table S3. Interatomic distances (Å) and bond angles (deg) for **2**. (cont'd.)

ATOM	ATOM	ATOM	ANGLE	ATOM	ATOM	ATOM	ANGLE
Fe2	P3	C231	121.42(18)	Fe1	C14	C13	126.0(4)
C211	P3	C221	105.8(3)	S1	C14	C13	106.4(4)
C211	P3	C231	103.4(3)	S2	C21	C2	120.9(4)
C221	P3	C231	97.5(3)	S2	C21	C22	110.2(5)
Fe2	P4	C212	109.9(2)	C2	C21	C22	128.9(5)
Fe2	P4	C241	122.8(3)	C21	C22	C23	111.3(5)
Fe2	P4	C251	116.9(2)	C21	C22	C25	125.5(6)
C212	P4	C241	102.2(3)	C23	C22	C25	123.2(5)
C212	P4	C251	104.4(3)	C22	C23	C24	118.4(6)
C241	P4	C251	98.4(3)	Fe2	C24	S2	127.6(3)
C3	C2	C1	119.5(5)	Fe2	C24	C23	127.1(5)
C3	C2	C21	119.5(5)	S2	C24	C23	105.2(5)
C1	C2	C21	121.0(5)	C3	C31	C32	122.1(5)
C2	C3	C4	120.5(6)	C3	C31	C36	118.7(6)
C2	C3	C31	121.3(5)	C32	C31	C36	119.2(6)
C4	C3	C31	118.2(5)	C31	C32	C33	120.5(7)
C3	C4	C5	119.0(5)	C32	C33	C34	120.6(7)
C3	C4	C41	120.3(6)	C33	C34	C35	118.8(7)
C5	C4	C41	120.7(6)	C34	C35	C36	121.6(7)
C4	C5	C6	120.9(6)	C31	C36	C35	119.3(7)
C4	C5	C51	119.4(5)	C4	C41	C42	122.3(6)
C6	C5	C51	119.6(6)	C4	C41	C46	119.4(6)
C5	C6	C1	119.4(6)	C42	C41	C46	118.3(6)
C5	C6	C61	120.1(6)	C41	C42	C43	121.2(7)
C1	C6	C61	120.4(5)	C42	C43	C44	119.4(8)
C2	C1	C6	120.4(5)	C43	C44	C45	119.4(7)
C2	C1	C11	121.2(6)	C44	C45	C46	120.8(8)
C6	C1	C11	118.4(6)	C41	C46	C45	120.9(7)
S1	C11	C1	124.0(4)	C5	C51	C52	119.3(7)
S1	C11	C12	109.8(4)	C5	C51	C56	122.3(7)
C1	C11	C12	126.2(6)	C52	C51	C56	118.3(7)
C11	C12	C13	112.3(5)	C51	C52	C53	122.2(8)
C11	C12	C15	127.1(5)	C52	C53	C54	119.5(10)
C13	C12	C15	120.5(5)	C53	C54	C55	120.1(10)
C12	C13	C14	116.4(5)	C54	C55	C56	120.1(9)
Fe1	C14	S1	127.4(3)	C51	C56	C55	119.8(8)

Table S3. Interatomic distances (Å) and bond angles (deg) for **2**. (cont'd)

ATOM	ATOM	ATOM	ANGLE	ATOM	ATOM	ATOM	ANGLE
C6	C61	C62	121.5(6)	C131	C132	C133	121.9(7)
C6	C61	C66	120.2(5)	C132	C133	C134	119.3(7)
C62	C61	C66	118.2(6)	C134	C135	C136	118.4(7)
C61	C62	C63	119.8(6)	P2	C141	C146	122.1(4)
C62	C63	C64	121.3(7)	C142	C141	C146	116.9(6)
C63	C64	C65	119.3(7)	C141	C142	C143	122.4(7)
C64	C65	C66	119.6(7)	C142	C143	C144	120.4(7)
C61	C66	C65	121.9(6)	C143	C144	C145	118.8(8)
Fe1	C100	C101	70.2(4)	C144	C145	C146	120.2(7)
Fe1	C100	C104	71.0(4)	C141	C146	C145	121.2(7)
C101	C100	C104	108.9(7)	P2	C151	C156	121.5(6)
Fe1	C101	C100	70.2(4)	C152	C151	C156	117.2(7)
Fe1	C101	C102	70.1(5)	P2	C151	C152	121.3(6)
C100	C101	C102	107.2(7)	C151	C152	C153	121.9(8)
Fe1	C102	C101	70.7(4)	C152	C153	C154	120.1(9)
Fe1	C102	C103	70.5(4)	C153	C154	C155	118.4(10)
C101	C102	C103	108.9(7)	C154	C155	C156	121.0(10)
Fe1	C103	C102	70.0(4)	C151	C156	C155	121.3(8)
Fe1	C103	C104	70.6(4)	Fe2	C200	C201	69.7(5)
C102	C103	C104	107.1(7)	Fe2	C200	C204	71.0(5)
Fe1	C104	C100	70.2(4)	C201	C200	C204	108.3(8)
Fe1	C104	C103	69.7(4)	Fe2	C201	C200	71.2(5)
C100	C104	C103	107.9(7)	Fe2	C201	C202	71.2(5)
P1	C111	C112	110.6(5)	C200	C201	C202	108.3(7)
P2	C112	C111	107.6(4)	Fe2	C202	C201	69.4(5)
P1	C121	C126	119.9(6)	Fe2	C202	C203	70.6(4)
C122	C121	C126	117.3(7)	C201	C202	C203	107.5(7)
P1	C121	C122	122.5(6)	Fe2	C203	C204	70.3(4)
C121	C122	C123	121.2(8)	Fe2	C203	C202	70.1(4)
C122	C123	C124	120.5(9)	C202	C203	C204	107.3(7)
C123	C124	C125	119.3(8)	Fe2	C204	C200	70.4(5)
C124	C125	C126	120.4(8)	Fe2	C204	C203	70.6(4)
C121	C126	C125	121.4(8)	C200	C204	C203	108.6(7)
P1	C131	C136	122.7(5)	P3	C211	C212	112.3(4)
C132	C131	C136	118.1(6)	P4	C212	C211	109.9(4)
P1	C131	C132	119.3(5)	P3	C221	C222	118.5(6)

Table S3. Interatomic distances (Å) and bond angles (deg) for **2**. (cont'd.)

ATOM	ATOM	ATOM	ANGLE	DIHEDRAL ANGLES	
C222	C221	C226	116.9(7)	C12-C11-C1-C1	110.0
P3	C221	C226	124.5(6)	C22-C21-C2-C3	68.2
C221	C222	C223	123.2(8)	C32-C31-C3-C4	117.7
C222	C223	C224	118.2(9)	C42-C31-C4-C5	115.0
C223	C224	C225	120.1(10)	C52-C51-C5-C6	110.1
C224	C225	C226	121.5(8)	C62-C61-C6-C1	119.5
C221	C226	C225	120.1(8)		
P3	C231	C232	121.0(5)		
P3	C231	C236	120.8(5)		
C232	C231	C236	118.2(7)		
C231	C232	C233	119.6(7)		
C232	C233	C234	120.8(7)		
C233	C234	C235	120.7(7)		
C234	C235	C236	118.9(7)		
C231	C236	C235	121.7(7)		
P4	C241	C242	121.6(6)		
P4	C241	C246	121.2(6)		
C242	C241	C246	117.3(7)		
C241	C242	C243	122.2(8)		
C242	C243	C244	119.0(8)		
C243	C244	C245	120.0(9)		
C244	C245	C246	120.6(8)		
C241	C246	C245	120.9(8)		
P4	C251	C252	118.2(5)		
C252	C251	C256	119.2(6)		
P4	C251	C256	122.5(4)		
C251	C252	C253	119.9(7)		
C252	C253	C254	120.7(7)		
C253	C254	C255	118.9(7)		
C254	C255	C256	120.5(8)		
C251	C256	C255	120.8(7)		
Cl	C900	Cl2	103.0(6)		

Table S4. Interatomic distances (Å) and bond angles (deg) for **5**.

ATOM	ATOM	DISTANCE	ATOM	ATOM	DISTANCE
Fe1	P1	2.1637(18)	C123	C124	1.380(9)
Fe1	P2	2.1647(18)	C124	C125	1.351(8)
Fe1	C14	1.997(5)	C125	C126	1.377(8)
Fe1	C101	2.110(6)	C131	C132	1.381(8)
Fe1	C102	2.121(5)	C131	C136	1.377(7)
Fe1	C103	2.111(5)	C132	C133	1.382(10)
Fe1	C104	2.096(6)	C133	C134	1.379(9)
Fe1	C105	2.090(5)	C134	C135	1.381(9)
Cl1	C901	1.897(15)	C135	C136	1.381(9)
Cl2	C901	1.651(15)	C141	C142	1.384(7)
S	C14	1.754(5)	C141	C146	1.386(7)
S	C11	1.725(5)	C142	C143	1.379(8)
P1	C112	1.845(5)	C143	C144	1.381(9)
P1	C121	1.830(5)	C144	C145	1.370(9)
P1	C131	1.852(5)	C145	C146	1.382(7)
P2	C111	1.849(5)	C151	C152	1.390(8)
P2	C151	1.830(5)	C151	C156	1.394(7)
P2	C141	1.840(5)	C152	C153	1.370(8)
C1	C3	1.410(6)	C153	C154	1.372(10)
C1	C11	1.489(7)	C154	C155	1.368(11)
C1	C2	1.400(6)	C155	C156	1.384(9)
C2	C4	1.515(6)			
C2	C3_a	1.403(6)	C4	C11	2.905(8)
C3	C5	1.504(7)	C5	C11	2.892(7)
C11	C12	1.359(7)	C4	C5_a	2.924(8)
C12	C13	1.409(7)	Fe1	Fe2	14.488(5)
C13	C14	1.371(7)			
C101	C102	1.402(7)			
C101	C105	1.421(8)			
C102	C103	1.419(8)			
C103	C104	1.432(7)			
C104	C105	1.409(8)			
C111	C112	1.512(7)			
C121	C126	1.371(8)			
C121	C122	1.380(7)			
C122	C123	1.391(9)			

Table S4. Interatomic distances (Å) and bond angles (deg) for **5**. (cont'd.)

ATOM	ATOM	ATOM	ANGLE	ATOM	ATOM	ATOM	ANGLE
P1	Fe1	P2	86.51(6)	Fe1	P2	C141	119.34(16)
P1	Fe1	C14	84.90(14)	Fe1	P2	C151	115.23(18)
P1	Fe1	C101	154.60(15)	C111	P2	C141	104.8(2)
P1	Fe1	C102	151.89(16)	C111	P2	C151	103.3(2)
P1	Fe1	C103	113.52(16)	C141	P2	C151	101.4(2)
P1	Fe1	C104	96.91(15)	C2	C1	C3	120.8(4)
P1	Fe1	C105	115.46(16)	C2	C1	C11	120.0(4)
P2	Fe1	C14	91.84(14)	C3	C1	C11	119.2(4)
P2	Fe1	C101	92.62(15)	C1	C2	C4	120.1(4)
P2	Fe1	C102	121.55(16)	C1	C2	C3_a	120.4(4)
P2	Fe1	C103	158.45(16)	C3_a	C2	C4	119.5(4)
P2	Fe1	C104	134.14(15)	C1	C3	C5	120.1(4)
P2	Fe1	C105	98.43(16)	C1	C3	C2_a	118.8(4)
C14	Fe1	C101	120.5(2)	C2_a	C3	C5	121.1(4)
C14	Fe1	C102	91.9(2)	S	C11	C1	122.8(3)
C14	Fe1	C103	97.6(2)	S	C11	C12	108.5(4)
C14	Fe1	C104	134.0(2)	C1	C11	C12	128.6(5)
C14	Fe1	C105	157.6(2)	C11	C12	C13	113.8(5)
C101	Fe1	C102	38.7(2)	C12	C13	C14	116.7(4)
C101	Fe1	C103	65.9(2)	Fe1	C14	S	118.6(3)
C101	Fe1	C104	65.9(2)	Fe1	C14	C13	135.8(4)
C101	Fe1	C105	39.6(2)	S	C14	C13	105.6(4)
C102	Fe1	C103	39.2(2)	Fe1	C101	C102	71.1(3)
C102	Fe1	C104	65.7(2)	Fe1	C101	C105	69.5(3)
C102	Fe1	C105	65.7(2)	C102	C101	C105	108.1(5)
C103	Fe1	C104	39.8(2)	Fe1	C102	C101	70.2(3)
C103	Fe1	C105	66.5(2)	Fe1	C102	C103	70.0(3)
C104	Fe1	C105	39.3(2)	C101	C102	C103	109.0(5)
C11	S	C14	95.4(2)	Fe1	C103	C102	70.8(3)
Fe1	P1	C112	109.85(16)	Fe1	C103	C104	69.5(3)
Fe1	P1	C121	118.18(16)	C102	C103	C104	106.8(5)
Fe1	P1	C131	121.78(17)	Fe1	C104	C103	70.7(3)
C112	P1	C121	103.9(2)	Fe1	C104	C105	70.1(3)
C112	P1	C131	99.4(2)	C103	C104	C105	108.4(5)
C121	P1	C131	100.9(2)	Fe1	C105	C101	71.0(3)
Fe1	P2	C111	111.03(16)	Fe1	C105	C104	70.5(3)

Table S4. Interatomic distances (Å) and bond angles (deg) for **5**. (cont'd)

ATOM	ATOM	ATOM	ANGLE	DIHEDRAL ANGLE	
C101	C105	C104	107.8(5)	C2-C1-C11-C12	73.7
P2	C111	C112	112.1(3)		
P1	C112	C111	108.9(4)		
P1	C121	C122	118.1(4)		
P1	C121	C126	124.1(4)		
C122	C121	C126	117.9(5)		
C121	C122	C123	121.2(5)		
C122	C123	C124	119.4(6)		
C123	C124	C125	119.4(6)		
C124	C125	C126	121.2(5)		
C121	C126	C125	121.0(5)		
P1	C131	C132	120.2(4)		
P1	C131	C136	122.0(4)		
C132	C131	C136	117.7(5)		
C131	C132	C133	121.4(5)		
C132	C133	C134	120.2(6)		
C133	C134	C135	119.0(6)		
C134	C135	C136	120.0(5)		
C131	C136	C135	121.7(5)		
P2	C141	C146	122.4(4)		
C142	C141	C146	118.1(5)		
C143	C144	C145	118.3(5)		
C144	C145	C146	120.9(5)		
C141	C146	C145	120.9(5)		
P2	C151	C152	120.9(4)		
C152	C151	C156	117.3(5)		
P2	C151	C156	121.3(4)		
C151	C152	C153	121.6(5)		
C152	C153	C154	120.3(6)		
C153	C154	C155	119.5(6)		
C154	C155	C156	120.6(6)		
C151	C156	C155	120.7(6)		

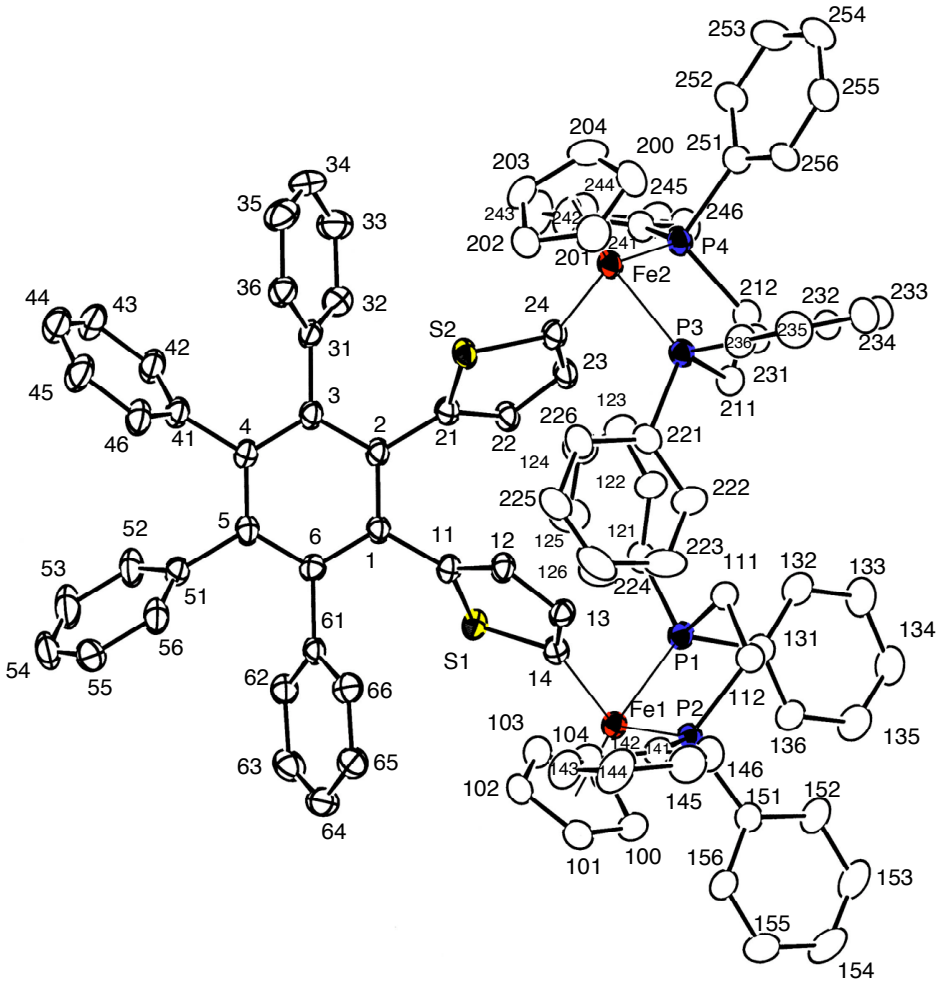

Figure S1. Molecular structure of **1** drawn with thermal ellipsoids at the 30 % probability level. Labels without atom names are for carbon atoms.

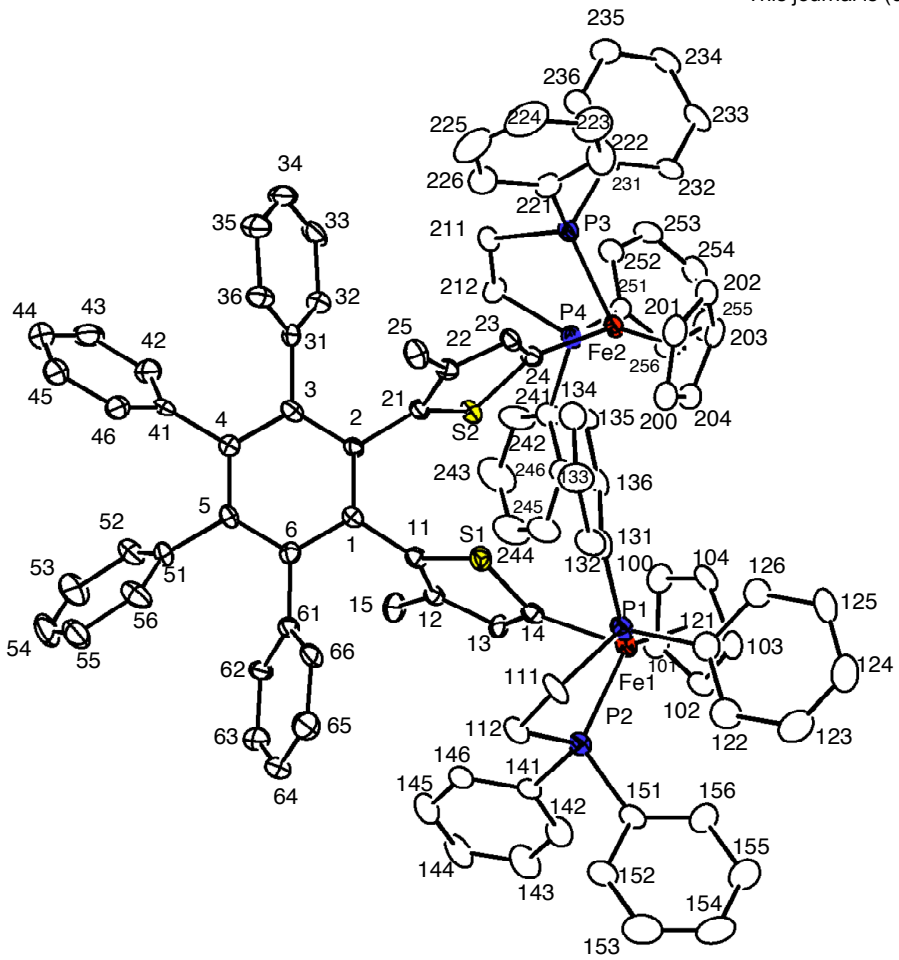

Figure S2. Molecular structure of **2** drawn with thermal ellipsoids at the 30 % probability level. Labels without atom names are for carbon atoms.

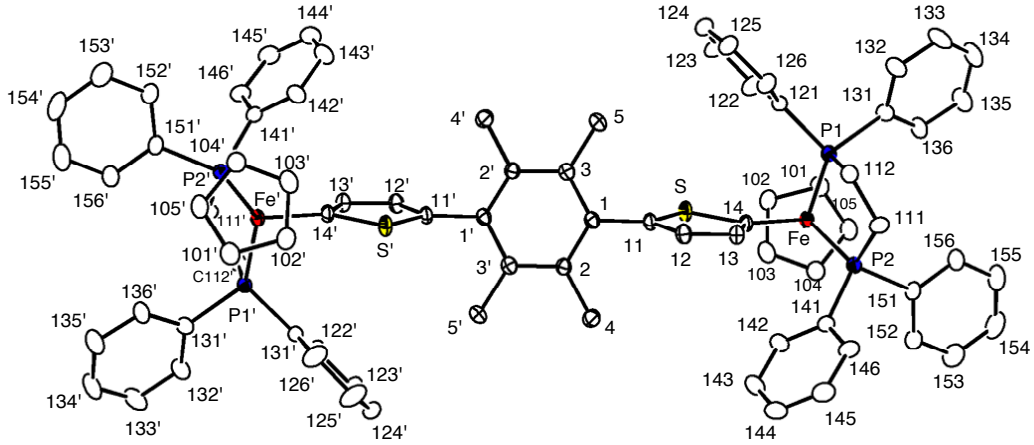

Figure S3. Molecular structure of **5** drawn with thermal ellipsoids at the 30 % probability level. Labels without atom names are for carbon atoms.