Electronic Supplementary Material (ESI) for Chemical Communications

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Hydrogenase biomimetics: $Fe_2(CO)_4$(μ-dppf)(μ-pdt) (dppf = 1,1'-bis(diphenylphosphino)ferrocene)) both a proton-reduction and hydrogen oxidation catalyst[#]

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Cyclic voltammetry. Electrochemistry was carried out in deoxygenated acetonitrile solution with 0.1 M $TBAPF_6$ as supporting electrolyte. The working electrode was a 3 mm diameter glassy carbon electrode which was polished with 0.3 μm alumina slurry prior to each scan. The counter electrode was a Pt wire and the quasi-reference electrode was a silver wire. All CVs were referenced to the Fc^+/Fc redox couple. An Autolab potentiostat (EcoChemie, Netherlands) was used for all electrochemical measurements. Catalysis studies were carried out by adding equivalents of $HBF_4.Et_2O$ (purchased from Sigma- Aldrich).

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Chemical oxidation of 2 with $FcPF_6$

2 was treated with 1 molar equivalent of $FcPF_6$ and the resulting changes to the IR spectrum monitored. As **2** first undergoes oxidation reversibly at $E_{1/2}$ = 0.05 V vs. Fc^+/Fc, addition of Fc^+ does not result in stoichiometric oxidation of the complex as the oxidation potential of **2** is not sufficiently negative relative to the Fc^+/Fc couple. However the potentials are similar enough to allow the following equilibrium to be established:

$$Fc^+ + \mathbf{2} = Fc + \mathbf{2}^+$$

Thus conversion of some of **2** to $\mathbf{2}^+$ can be observed in the IR spectrum. The 60 cm^{-1} shift of the first ν_{CO} band to higher energy is indicative of oxidation of the diiron centre, allowing assignment of the couple at 0.05 V vs. Fc^+/Fc to this process rather than oxidation of the dppf ligand.

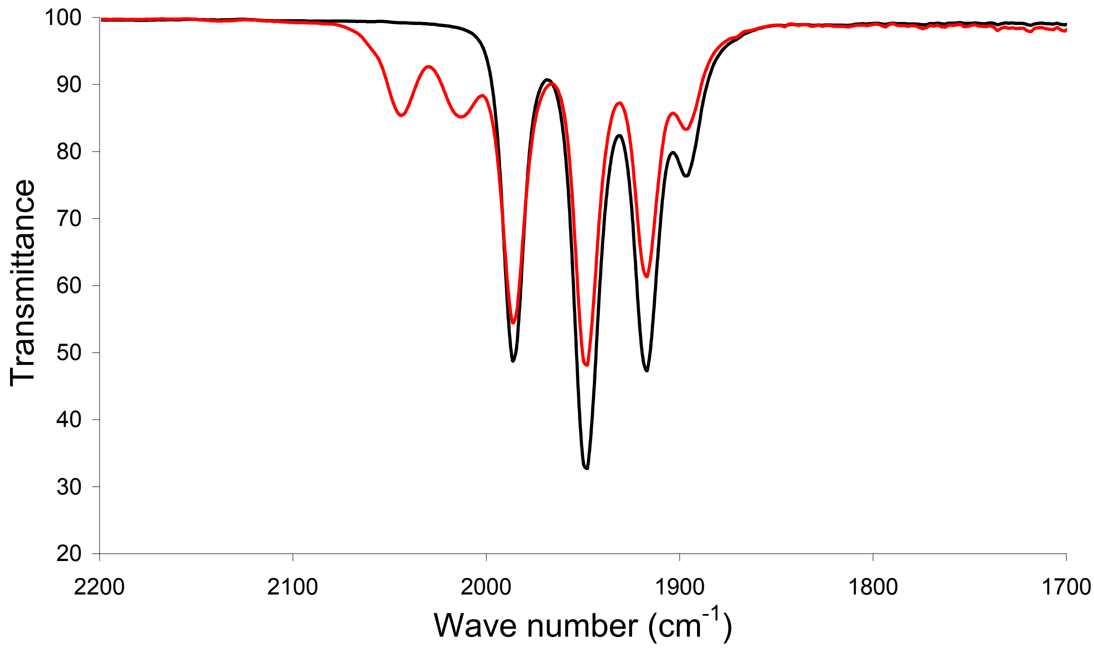


Fig. S1. IR spectra of $Fe_2(CO)_4$(μ-dppf)(μ-pdt) (**2**) (black) and **2** + 1 equiv. $FcPF_6$ (red) in CH_2CL_2.

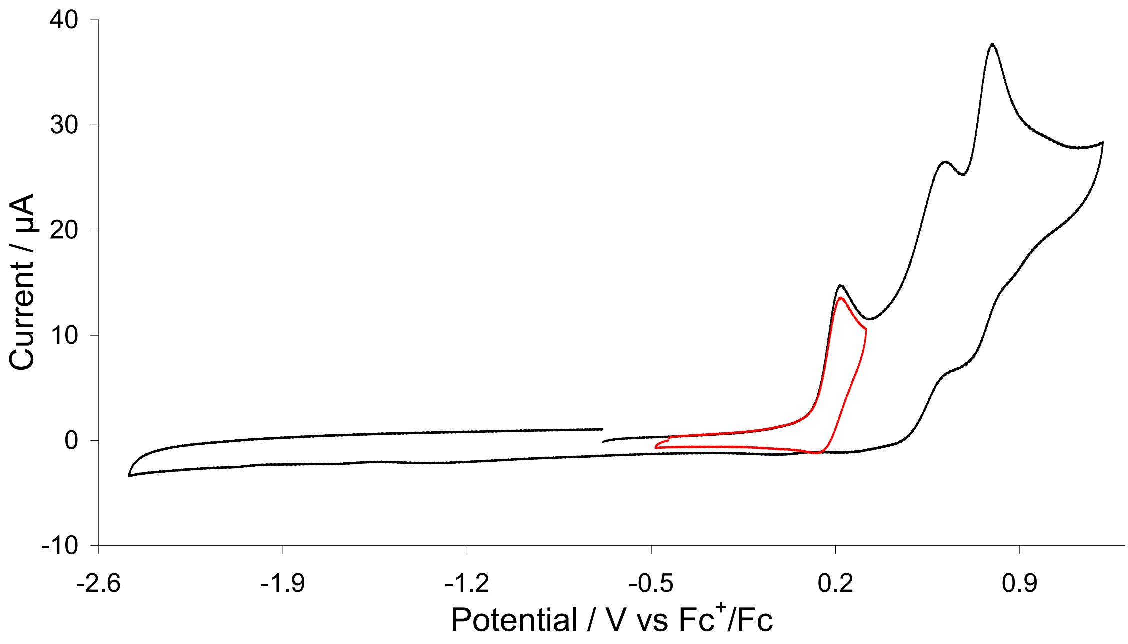


Fig. S2. CV of dppf (black) cycling to 1.2 V vs. Fc/Fc^+ and CV of dppf (red) cycling to 0.3 V vs. Fc/Fc^+ (1 mM solution in acetonitrile, supporting electrolyte $[NBu_4][PF_6]$, scan rate 0.1 Vs^{-1}, glassy carbon electrode, potential vs Fc^+/Fc)

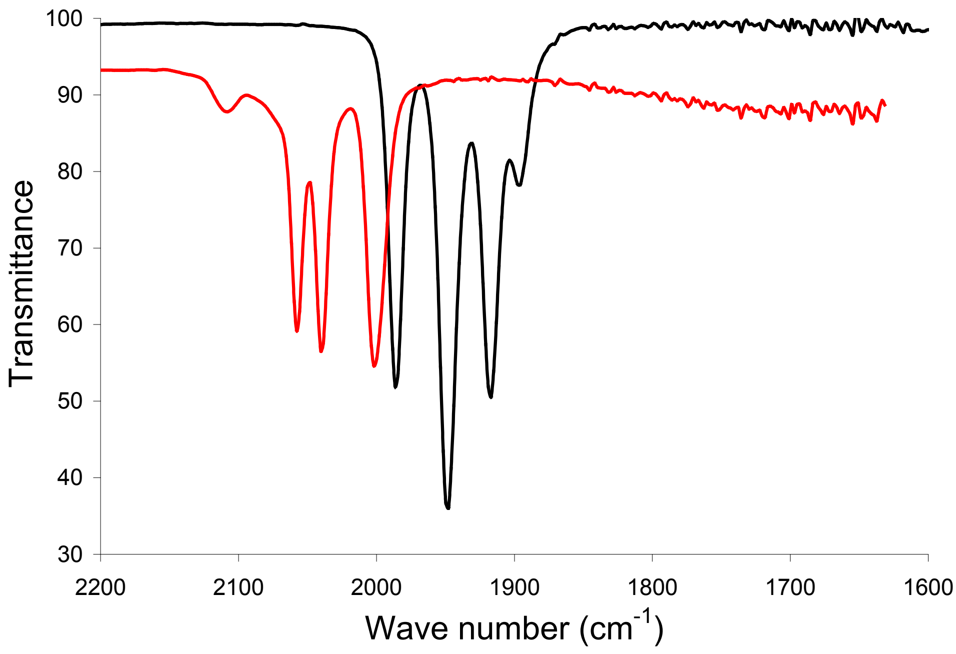


Fig. S4. IR spectra of $Fe_2(CO)_4$(μ-dppf)(μ-pdt) (**2**) (black), **2** + one equiv. HBF_4 (red) in CH_2Cl_2.

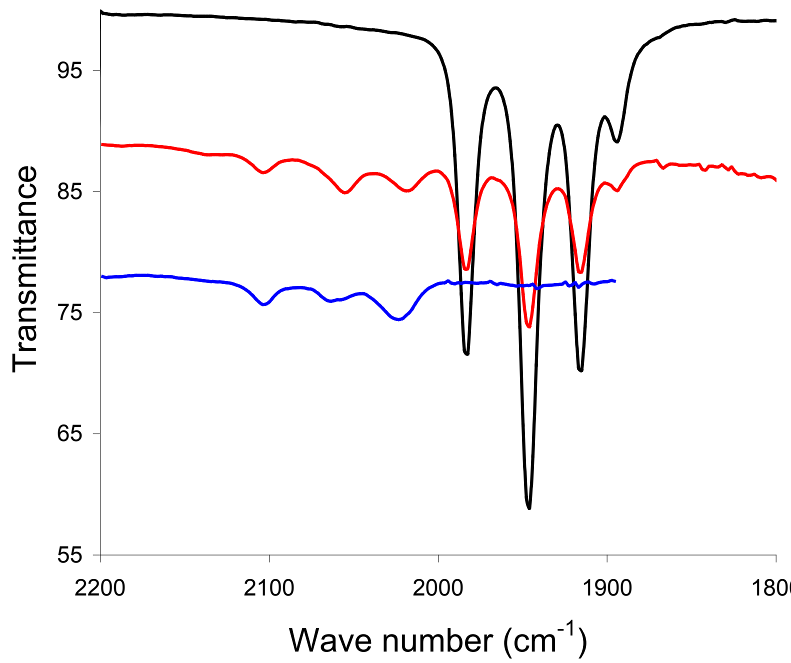


Fig. S5. IR spectra of $Fe_2(CO)_4$(μ-dppf)(μ-pdt) (**2**) (black), **2** + one equiv. HBF_4 (red) and **2** + two equiv. HBF_4 (blue) in MeCN.

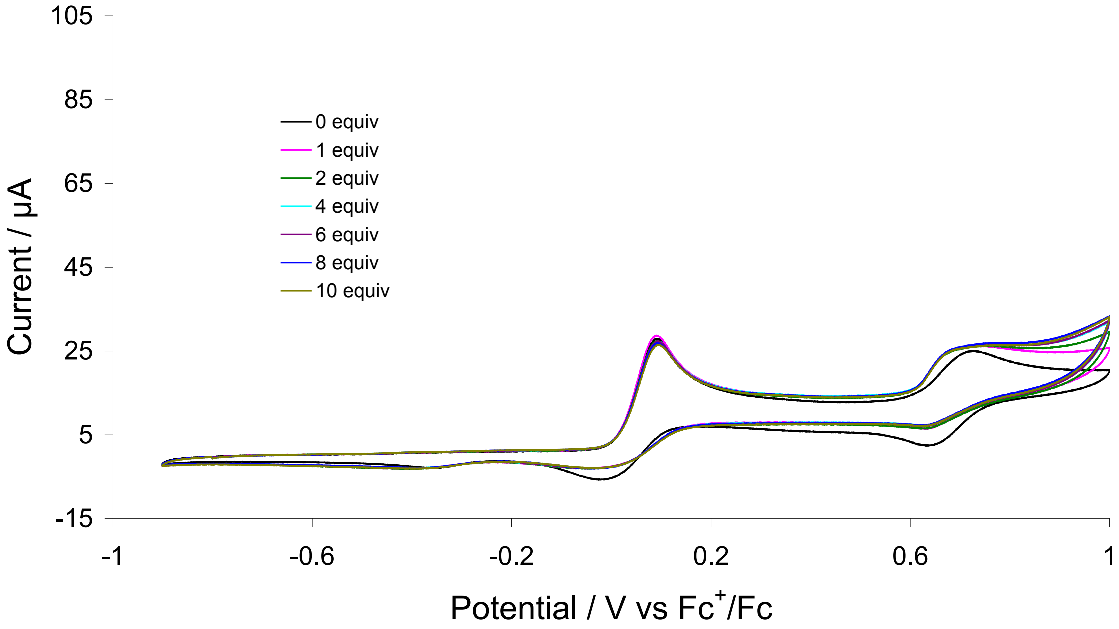


Fig. S6. CVs of $Fe_2(CO)_4$(μ-dppf)(μ-pdt) (**2**) in the absence of pyridine and in the presence of 1, 2, 4, 6, 8 and 10 molar equivalents of pyridine (1 mM solution in acetonitrile, supporting electrolyte $[NBu_4][PF_6]$, scan rate 0.1 Vs^{-1}, glassy carbon electrode, potential vs Fc^+/Fc)

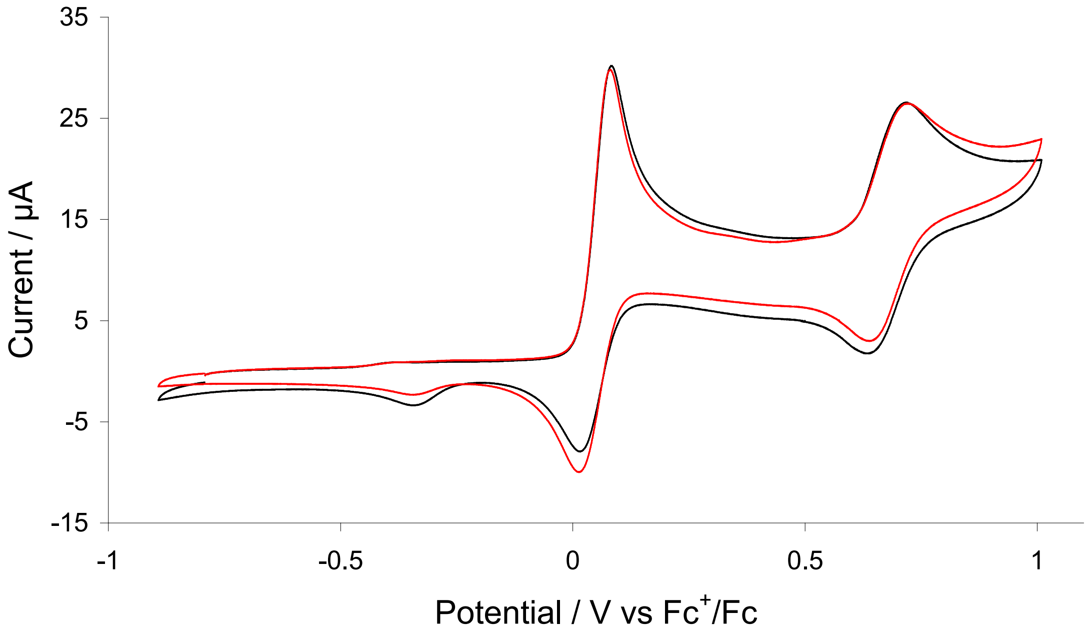


Fig. S7. CVs of $Fe_2(CO)_4$(μ-dppf)(μ-pdt) (**2**) in the absence of H_2 (black) and in the presence of H_2 (red) (1 mM solution in acetonitrile, supporting electrolyte $[NBu_4][PF_6]$, scan rate 0.1 Vs^{-1}, glassy carbon electrode, potential vs Fc^+/Fc)

Table 1. Crystal data and structure refinement for str0562.

Identification code	str0562	
Chemical formula	$C_{41.50}H_{34}ClFe_3O_4P_2S_2$	
Formula weight	925.75	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, P1bar	
Unit cell parameters	a = 9.7365(19) Å	α = 99.609(3)°
	b = 13.149(3) Å	β = 94.376(3)°
	c = 16.654(3) Å	γ = 111.343(3)°
Cell volume	1936.1(7) $Å^3$	
Z	2	
Calculated density	1.588 g/cm^3	
Absorption coefficient μ	1.411 mm^{-1}	
F(000)	944	
Crystal colour and size	red, 0.38 × 0.32 × 0.16 mm^3	
Data collection method	Bruker SMART APEX diffractometer	
	ω rotation with narrow frames	
θ range for data collection	2.59 to 28.35°	
Index ranges	h –12 to 12, k –17 to 17, l –21 to 21	
Completeness to θ = 26.00°	98.8 %	
Reflections collected	16800	
Independent reflections	8886 (R_{int} = 0.0333)	
Reflections with F^2>2σ	8134	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.6161 and 0.8057	
Structure solution	Patterson synthesis	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0471, 0.7689	
Data / restraints / parameters	8886 / 0 / 511	
Final R indices [F^2>2σ]	R1 = 0.0345, wR2 = 0.0911	
R indices (all data)	R1 = 0.0374, wR2 = 0.0929	
Goodness-of-fit on F^2	1.049	
Largest and mean shift/su	0.000 and 0.000	
Largest diff. peak and hole	0.597 and –0.725 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for str0562. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Fe(1)	0.11524(3)	0.11104(2)	0.311588(15)	0.01639(7)
Fe(2)	0.26805(3)	0.32140(2)	0.313764(15)	0.01615(7)
Fe(3)	0.48739(3)	0.11629(2)	0.157848(16)	0.02020(8)
P(1)	0.20980(5)	−0.01647(4)	0.27117(3)	0.01656(10)
P(2)	0.46943(5)	0.36607(4)	0.24689(3)	0.01692(10)
S(1)	0.04314(5)	0.25203(4)	0.35447(3)	0.02003(10)
S(2)	0.32936(5)	0.21971(4)	0.39608(3)	0.01760(10)
O(1)	−0.12940(18)	−0.04843(14)	0.37222(11)	0.0374(4)
O(2)	−0.04810(17)	0.07670(14)	0.14822(9)	0.0313(3)
O(3)	0.35984(18)	0.53477(13)	0.42898(10)	0.0315(3)
O(4)	0.10390(19)	0.35568(16)	0.17251(11)	0.0403(4)
C(1)	−0.0279(2)	0.01244(17)	0.35069(13)	0.0243(4)
C(2)	0.0187(2)	0.09034(16)	0.21182(12)	0.0223(4)
C(3)	0.3301(2)	0.45287(16)	0.38174(12)	0.0212(4)
C(4)	0.1706(2)	0.34277(17)	0.22696(12)	0.0241(4)
C(5)	0.0580(2)	0.28628(18)	0.46661(13)	0.0264(4)
C(6)	0.1378(2)	0.23096(19)	0.51444(13)	0.0266(4)
C(7)	0.2991(2)	0.26117(19)	0.50221(12)	0.0255(4)
C(8)	0.3415(2)	0.17869(17)	0.11067(11)	0.0236(4)
C(9)	0.4724(2)	0.26668(16)	0.15803(11)	0.0210(4)
C(10)	0.5978(2)	0.25979(18)	0.12045(13)	0.0277(4)
C(11)	0.5434(3)	0.16868(19)	0.05136(13)	0.0331(5)
C(12)	0.3867(3)	0.11901(18)	0.04522(12)	0.0300(5)
C(13)	0.6450(2)	0.09935(18)	0.23902(13)	0.0264(4)
C(14)	0.5238(2)	0.10651(16)	0.27831(11)	0.0208(4)
C(15)	0.3893(2)	0.01722(16)	0.23561(11)	0.0187(4)
C(16)	0.4315(2)	−0.04598(17)	0.17020(12)	0.0238(4)
C(17)	0.5883(2)	0.00573(19)	0.17232(13)	0.0279(4)
C(18)	0.2443(2)	−0.09066(16)	0.34981(12)	0.0204(4)
C(19)	0.2807(2)	−0.18371(18)	0.32642(14)	0.0281(4)
C(20)	0.3255(3)	−0.2328(2)	0.38578(15)	0.0350(5)
C(21)	0.3364(2)	−0.1892(2)	0.46843(15)	0.0332(5)
C(22)	0.2988(2)	−0.0980(2)	0.49268(13)	0.0311(5)
C(23)	0.2516(2)	−0.04931(17)	0.43338(12)	0.0244(4)
C(24)	0.0825(2)	−0.12666(16)	0.18788(12)	0.0213(4)
C(25)	0.0867(2)	−0.11364(18)	0.10648(13)	0.0273(4)
C(26)	−0.0182(3)	−0.1913(2)	0.04279(14)	0.0374(5)
C(27)	−0.1306(3)	−0.2814(2)	0.06056(17)	0.0465(7)
C(28)	−0.1383(3)	−0.2942(2)	0.14075(17)	0.0416(6)
C(29)	−0.0319(2)	−0.21772(18)	0.20468(14)	0.0288(4)
C(30)	0.6614(2)	0.41833(16)	0.29947(11)	0.0196(4)
C(31)	0.6957(2)	0.39915(16)	0.37618(11)	0.0204(4)
C(32)	0.8438(2)	0.43491(18)	0.41173(13)	0.0271(4)
C(33)	0.9576(2)	0.49115(19)	0.37176(14)	0.0292(4)
C(34)	0.9251(2)	0.51325(19)	0.29583(14)	0.0304(5)
C(35)	0.7780(2)	0.47710(18)	0.25969(13)	0.0270(4)
C(36)	0.4801(2)	0.48705(16)	0.20207(12)	0.0211(4)
C(37)	0.5239(3)	0.59215(18)	0.25393(14)	0.0307(5)
C(38)	0.5261(3)	0.6840(2)	0.22224(17)	0.0404(6)

C(39)	0.4844(3)	0.6724(2)	0.13899(17)	0.0412(6)
C(40)	0.4420(3)	0.5691(2)	0.08706(15)	0.0368(5)
C(41)	0.4406(2)	0.47723(19)	0.11846(13)	0.0283(4)
Cl(1)	0.87963(11)	0.42452(11)	0.03311(8)	0.0910(4)
C(50)	1.0596(7)	0.5307(8)	0.0565(5)	0.078(3)

Table 3. Bond lengths [Å] and angles [°] for str0562.

Fe(1)–C(2)	1.773(2)	Fe(1)–C(1)	1.775(2)
Fe(1)–P(1)	2.2256(6)	Fe(1)–S(1)	2.2410(6)
Fe(1)–S(2)	2.2540(6)	Fe(1)–Fe(2)	2.6133(6)
Fe(2)–C(3)	1.765(2)	Fe(2)–C(4)	1.786(2)
Fe(2)–S(1)	2.2508(6)	Fe(2)–S(2)	2.2565(6)
Fe(2)–P(2)	2.2679(6)	Fe(3)–C(10)	2.030(2)
Fe(3)–C(15)	2.0330(19)	Fe(3)–C(9)	2.035(2)
Fe(3)–C(14)	2.0440(19)	Fe(3)–C(11)	2.049(2)
Fe(3)–C(8)	2.050(2)	Fe(3)–C(16)	2.052(2)
Fe(3)–C(12)	2.061(2)	Fe(3)–C(17)	2.063(2)
Fe(3)–C(13)	2.065(2)	P(1)–C(15)	1.8116(19)
P(1)–C(24)	1.822(2)	P(1)–C(18)	1.8378(19)
P(2)–C(9)	1.813(2)	P(2)–C(30)	1.8296(19)
P(2)–C(36)	1.840(2)	S(1)–C(5)	1.828(2)
S(2)–C(7)	1.839(2)	O(1)–C(1)	1.149(3)
O(2)–C(2)	1.150(3)	O(3)–C(3)	1.148(2)
O(4)–C(4)	1.147(3)	C(5)–C(6)	1.509(3)
C(6)–C(7)	1.512(3)	C(8)–C(12)	1.427(3)
C(8)–C(9)	1.433(3)	C(9)–C(10)	1.438(3)
C(10)–C(11)	1.423(3)	C(11)–C(12)	1.411(3)
C(13)–C(14)	1.417(3)	C(13)–C(17)	1.418(3)
C(14)–C(15)	1.435(3)	C(15)–C(16)	1.436(3)
C(16)–C(17)	1.422(3)	C(18)–C(23)	1.394(3)
C(18)–C(19)	1.397(3)	C(19)–C(20)	1.391(3)
C(20)–C(21)	1.380(4)	C(21)–C(22)	1.384(3)
C(22)–C(23)	1.397(3)	C(24)–C(29)	1.393(3)
C(24)–C(25)	1.396(3)	C(25)–C(26)	1.387(3)
C(26)–C(27)	1.382(4)	C(27)–C(28)	1.378(4)
C(28)–C(29)	1.391(3)	C(30)–C(31)	1.382(3)
C(30)–C(35)	1.404(3)	C(31)–C(32)	1.391(3)
C(32)–C(33)	1.378(3)	C(33)–C(34)	1.383(3)
C(34)–C(35)	1.385(3)	C(36)–C(41)	1.387(3)
C(36)–C(37)	1.398(3)	C(37)–C(38)	1.391(3)
C(38)–C(39)	1.381(4)	C(39)–C(40)	1.381(4)
C(40)–C(41)	1.391(3)	Cl(1)–C(50A)	1.760(6)
Cl(1)–C(50)	1.762(8)	C(50)–Cl(1A)	1.760(6)
C(50)–C(50A)	2.004(17)		

C(2)–Fe(1)–C(1)	98.41(9)	C(2)–Fe(1)–P(1)	92.92(7)
C(1)–Fe(1)–P(1)	90.64(7)	C(2)–Fe(1)–S(1)	89.39(7)
C(1)–Fe(1)–S(1)	94.15(7)	P(1)–Fe(1)–S(1)	174.34(2)
C(2)–Fe(1)–S(2)	142.40(7)	C(1)–Fe(1)–S(2)	118.96(7)
P(1)–Fe(1)–S(2)	90.77(2)	S(1)–Fe(1)–S(2)	84.26(2)
C(2)–Fe(1)–Fe(2)	91.95(7)	C(1)–Fe(1)–Fe(2)	147.07(7)
P(1)–Fe(1)–Fe(2)	120.10(2)	S(1)–Fe(1)–Fe(2)	54.598(19)
S(2)–Fe(1)–Fe(2)	54.638(15)	C(3)–Fe(2)–C(4)	102.38(9)
C(3)–Fe(2)–S(1)	96.06(6)	C(4)–Fe(2)–S(1)	85.65(7)
C(3)–Fe(2)–S(2)	100.69(7)	C(4)–Fe(2)–S(2)	155.55(7)
S(1)–Fe(2)–S(2)	83.98(2)	C(3)–Fe(2)–P(2)	94.75(6)
C(4)–Fe(2)–P(2)	86.50(7)	S(1)–Fe(2)–P(2)	167.79(2)
S(2)–Fe(2)–P(2)	99.59(2)	C(3)–Fe(2)–Fe(1)	139.61(6)
C(4)–Fe(2)–Fe(1)	101.73(7)	S(1)–Fe(2)–Fe(1)	54.248(14)
S(2)–Fe(2)–Fe(1)	54.549(17)	P(2)–Fe(2)–Fe(1)	118.646(17)

C(10)–Fe(3)–C(15)	157.78(8)	C(10)–Fe(3)–C(9)	41.43(8)
C(15)–Fe(3)–C(9)	122.57(8)	C(10)–Fe(3)–C(14)	120.36(8)
C(15)–Fe(3)–C(14)	41.22(7)	C(9)–Fe(3)–C(14)	106.80(8)
C(10)–Fe(3)–C(11)	40.82(9)	C(15)–Fe(3)–C(11)	160.82(9)
C(9)–Fe(3)–C(11)	69.10(8)	C(14)–Fe(3)–C(11)	155.82(9)
C(10)–Fe(3)–C(8)	68.95(9)	C(15)–Fe(3)–C(8)	109.36(8)
C(9)–Fe(3)–C(8)	41.08(8)	C(14)–Fe(3)–C(8)	125.12(8)
C(11)–Fe(3)–C(8)	68.33(9)	C(10)–Fe(3)–C(16)	157.92(8)
C(15)–Fe(3)–C(16)	41.16(7)	C(9)–Fe(3)–C(16)	160.12(8)
C(14)–Fe(3)–C(16)	68.44(8)	C(11)–Fe(3)–C(16)	123.32(8)
C(8)–Fe(3)–C(16)	124.77(8)	C(10)–Fe(3)–C(12)	68.36(9)
C(15)–Fe(3)–C(12)	125.73(8)	C(9)–Fe(3)–C(12)	68.84(8)
C(14)–Fe(3)–C(12)	162.47(9)	C(11)–Fe(3)–C(12)	40.17(10)
C(8)–Fe(3)–C(12)	40.63(8)	C(16)–Fe(3)–C(12)	109.55(9)
C(10)–Fe(3)–C(17)	120.78(9)	C(15)–Fe(3)–C(17)	68.84(8)
C(9)–Fe(3)–C(17)	157.48(9)	C(14)–Fe(3)–C(17)	67.89(8)
C(11)–Fe(3)–C(17)	106.30(9)	C(8)–Fe(3)–C(17)	159.50(9)
C(16)–Fe(3)–C(17)	40.43(8)	C(12)–Fe(3)–C(17)	122.69(9)
C(10)–Fe(3)–C(13)	104.74(9)	C(15)–Fe(3)–C(13)	68.87(8)
C(9)–Fe(3)–C(13)	121.70(8)	C(14)–Fe(3)–C(13)	40.34(8)
C(11)–Fe(3)–C(13)	120.15(9)	C(8)–Fe(3)–C(13)	159.85(8)
C(16)–Fe(3)–C(13)	68.00(8)	C(12)–Fe(3)–C(13)	156.54(9)
C(17)–Fe(3)–C(13)	40.16(9)	C(15)–P(1)–C(24)	103.61(9)
C(15)–P(1)–C(18)	97.04(9)	C(24)–P(1)–C(18)	104.39(9)
C(15)–P(1)–Fe(1)	123.03(6)	C(24)–P(1)–Fe(1)	110.71(7)
C(18)–P(1)–Fe(1)	115.75(7)	C(9)–P(2)–C(30)	101.97(9)
C(9)–P(2)–C(36)	102.03(9)	C(30)–P(2)–C(36)	98.93(9)
C(9)–P(2)–Fe(2)	118.94(7)	C(30)–P(2)–Fe(2)	123.22(6)
C(36)–P(2)–Fe(2)	108.16(6)	C(5)–S(1)–Fe(1)	112.16(7)
C(5)–S(1)–Fe(2)	111.13(7)	Fe(1)–S(1)–Fe(2)	71.154(19)
C(7)–S(2)–Fe(1)	112.58(7)	C(7)–S(2)–Fe(2)	110.83(8)
Fe(1)–S(2)–Fe(2)	70.81(2)	O(1)–C(1)–Fe(1)	173.81(19)
O(2)–C(2)–Fe(1)	177.76(18)	O(3)–C(3)–Fe(2)	174.21(17)
O(4)–C(4)–Fe(2)	177.68(18)	C(6)–C(5)–S(1)	116.49(15)
C(5)–C(6)–C(7)	113.54(18)	C(6)–C(7)–S(2)	115.34(15)
C(12)–C(8)–C(9)	108.04(19)	C(12)–C(8)–Fe(3)	70.09(13)
C(9)–C(8)–Fe(3)	68.88(11)	C(8)–C(9)–C(10)	107.11(17)
C(8)–C(9)–P(2)	123.85(15)	C(10)–C(9)–P(2)	129.03(16)
C(8)–C(9)–Fe(3)	70.04(11)	C(10)–C(9)–Fe(3)	69.12(12)
P(2)–C(9)–Fe(3)	126.82(10)	C(11)–C(10)–C(9)	108.11(19)
C(11)–C(10)–Fe(3)	70.30(12)	C(9)–C(10)–Fe(3)	69.44(11)
C(12)–C(11)–C(10)	108.38(19)	C(12)–C(11)–Fe(3)	70.37(12)
C(10)–C(11)–Fe(3)	68.88(12)	C(11)–C(12)–C(8)	108.36(19)
C(11)–C(12)–Fe(3)	69.46(13)	C(8)–C(12)–Fe(3)	69.28(11)
C(14)–C(13)–C(17)	108.03(18)	C(14)–C(13)–Fe(3)	69.03(11)
C(17)–C(13)–Fe(3)	69.85(12)	C(13)–C(14)–C(15)	108.69(17)
C(13)–C(14)–Fe(3)	70.63(11)	C(15)–C(14)–Fe(3)	68.98(10)
C(14)–C(15)–C(16)	106.69(16)	C(14)–C(15)–P(1)	124.11(14)
C(16)–C(15)–P(1)	128.53(15)	C(14)–C(15)–Fe(3)	69.80(11)
C(16)–C(15)–Fe(3)	70.12(11)	P(1)–C(15)–Fe(3)	132.15(10)
C(17)–C(16)–C(15)	108.24(18)	C(17)–C(16)–Fe(3)	70.22(12)
C(15)–C(16)–Fe(3)	68.72(11)	C(13)–C(17)–C(16)	108.34(18)
C(13)–C(17)–Fe(3)	69.99(12)	C(16)–C(17)–Fe(3)	69.35(12)
C(23)–C(18)–C(19)	118.76(18)	C(23)–C(18)–P(1)	121.55(15)
C(19)–C(18)–P(1)	119.30(15)	C(20)–C(19)–C(18)	120.4(2)

C(21)–C(20)–C(19)	120.4(2)	C(20)–C(21)–C(22)	120.0(2)
C(21)–C(22)–C(23)	119.9(2)	C(18)–C(23)–C(22)	120.5(2)
C(29)–C(24)–C(25)	118.81(18)	C(29)–C(24)–P(1)	120.78(16)
C(25)–C(24)–P(1)	119.91(15)	C(26)–C(25)–C(24)	121.0(2)
C(27)–C(26)–C(25)	119.4(2)	C(28)–C(27)–C(26)	120.4(2)
C(27)–C(28)–C(29)	120.5(2)	C(28)–C(29)–C(24)	119.9(2)
C(31)–C(30)–C(35)	118.91(18)	C(31)–C(30)–P(2)	122.09(14)
C(35)–C(30)–P(2)	118.97(15)	C(30)–C(31)–C(32)	120.08(18)
C(33)–C(32)–C(31)	120.62(19)	C(32)–C(33)–C(34)	120.01(19)
C(33)–C(34)–C(35)	119.7(2)	C(34)–C(35)–C(30)	120.62(19)
C(41)–C(36)–C(37)	118.36(19)	C(41)–C(36)–P(2)	122.29(16)
C(37)–C(36)–P(2)	119.31(15)	C(38)–C(37)–C(36)	120.5(2)
C(39)–C(38)–C(37)	120.3(2)	C(40)–C(39)–C(38)	119.6(2)
C(39)–C(40)–C(41)	120.2(2)	C(36)–C(41)–C(40)	120.9(2)
C(50A)–Cl(1)–C(50)	69.3(5)	Cl(1A)–C(50)–Cl(1)	110.7(5)
Cl(1A)–C(50)–C(50A)	55.4(3)	Cl(1)–C(50)–C(50A)	55.3(4)

Symmetry operations for equivalent atoms
A –x+2,–y+1,–z

Table 4. Anisotropic displacement parameters ($Å^2$) for str0562. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	0.01556(13)	0.01632(13)	0.01775(13)	0.00480(10)	0.00340(10)	0.00592(10)
Fe(2)	0.01581(13)	0.01663(13)	0.01639(13)	0.00498(10)	0.00302(9)	0.00589(10)
Fe(3)	0.02229(15)	0.02053(14)	0.01720(14)	0.00341(10)	0.00709(10)	0.00697(11)
P(1)	0.0171(2)	0.0163(2)	0.0164(2)	0.00440(17)	0.00252(16)	0.00610(18)
P(2)	0.0168(2)	0.0178(2)	0.0156(2)	0.00536(17)	0.00276(16)	0.00507(18)
S(1)	0.0173(2)	0.0196(2)	0.0249(2)	0.00539(18)	0.00598(17)	0.00821(18)
S(2)	0.0176(2)	0.0196(2)	0.0162(2)	0.00518(16)	0.00317(15)	0.00718(17)
O(1)	0.0304(8)	0.0342(9)	0.0488(10)	0.0190(8)	0.0174(7)	0.0069(7)
O(2)	0.0280(8)	0.0406(9)	0.0252(7)	0.0077(6)	–0.0016(6)	0.0139(7)
O(3)	0.0357(9)	0.0231(8)	0.0315(8)	0.0010(6)	0.0084(6)	0.0079(7)
O(4)	0.0330(9)	0.0535(11)	0.0381(9)	0.0242(8)	–0.0010(7)	0.0157(8)
C(1)	0.0248(10)	0.0241(10)	0.0265(10)	0.0072(8)	0.0062(8)	0.0110(8)
C(2)	0.0206(9)	0.0221(9)	0.0261(10)	0.0062(8)	0.0068(7)	0.0093(8)
C(3)	0.0190(9)	0.0229(10)	0.0234(9)	0.0086(8)	0.0060(7)	0.0077(7)
C(4)	0.0215(9)	0.0258(10)	0.0258(10)	0.0095(8)	0.0055(7)	0.0078(8)
C(5)	0.0295(11)	0.0258(11)	0.0263(10)	0.0051(8)	0.0139(8)	0.0115(9)
C(6)	0.0301(11)	0.0296(11)	0.0207(10)	0.0061(8)	0.0105(8)	0.0103(9)
C(7)	0.0290(11)	0.0301(11)	0.0160(9)	0.0045(8)	0.0034(7)	0.0099(9)
C(8)	0.0297(10)	0.0230(9)	0.0166(9)	0.0066(7)	0.0019(7)	0.0076(8)
C(9)	0.0262(10)	0.0196(9)	0.0171(8)	0.0062(7)	0.0055(7)	0.0072(8)
C(10)	0.0314(11)	0.0267(10)	0.0269(10)	0.0107(8)	0.0161(8)	0.0086(9)
C(11)	0.0478(14)	0.0311(11)	0.0232(10)	0.0080(9)	0.0184(9)	0.0149(10)
C(12)	0.0462(13)	0.0275(11)	0.0149(9)	0.0051(8)	0.0062(8)	0.0117(10)
C(13)	0.0194(9)	0.0315(11)	0.0291(10)	0.0060(8)	0.0055(8)	0.0105(8)
C(14)	0.0192(9)	0.0238(9)	0.0189(9)	0.0051(7)	0.0030(7)	0.0075(7)
C(15)	0.0199(9)	0.0198(9)	0.0183(8)	0.0053(7)	0.0043(7)	0.0087(7)
C(16)	0.0279(10)	0.0214(9)	0.0236(9)	0.0038(8)	0.0065(8)	0.0111(8)
C(17)	0.0280(11)	0.0318(11)	0.0297(10)	0.0077(9)	0.0116(8)	0.0160(9)
C(18)	0.0178(9)	0.0229(9)	0.0233(9)	0.0108(7)	0.0049(7)	0.0080(7)
C(19)	0.0330(11)	0.0306(11)	0.0289(10)	0.0123(9)	0.0100(8)	0.0178(9)
C(20)	0.0382(13)	0.0387(13)	0.0449(13)	0.0231(11)	0.0152(10)	0.0260(11)
C(21)	0.0278(11)	0.0438(13)	0.0388(12)	0.0278(11)	0.0088(9)	0.0170(10)
C(22)	0.0311(11)	0.0394(12)	0.0251(10)	0.0157(9)	0.0055(8)	0.0119(10)
C(23)	0.0270(10)	0.0249(10)	0.0231(9)	0.0092(8)	0.0054(8)	0.0100(8)
C(24)	0.0206(9)	0.0187(9)	0.0240(9)	0.0033(7)	0.0001(7)	0.0077(7)
C(25)	0.0280(10)	0.0246(10)	0.0248(10)	0.0054(8)	–0.0010(8)	0.0059(8)
C(26)	0.0420(13)	0.0352(13)	0.0254(11)	0.0039(9)	–0.0071(9)	0.0069(10)
C(27)	0.0413(14)	0.0319(13)	0.0441(14)	0.0013(11)	–0.0178(11)	–0.0039(11)
C(28)	0.0296(12)	0.0294(12)	0.0511(15)	0.0110(11)	–0.0069(10)	–0.0044(10)
C(29)	0.0256(10)	0.0251(10)	0.0325(11)	0.0094(9)	0.0008(8)	0.0052(8)
C(30)	0.0172(9)	0.0188(9)	0.0211(9)	0.0039(7)	0.0026(7)	0.0051(7)
C(31)	0.0215(9)	0.0194(9)	0.0196(9)	0.0029(7)	0.0024(7)	0.0079(7)
C(32)	0.0269(10)	0.0301(11)	0.0240(10)	0.0024(8)	–0.0023(8)	0.0133(9)
C(33)	0.0181(9)	0.0311(11)	0.0339(11)	–0.0008(9)	–0.0023(8)	0.0086(8)
C(34)	0.0208(10)	0.0296(11)	0.0367(11)	0.0052(9)	0.0086(8)	0.0050(8)
C(35)	0.0225(10)	0.0299(11)	0.0264(10)	0.0096(8)	0.0047(8)	0.0057(8)
C(36)	0.0181(9)	0.0227(9)	0.0249(9)	0.0109(8)	0.0074(7)	0.0070(7)
C(37)	0.0421(13)	0.0264(11)	0.0281(10)	0.0096(9)	0.0156(9)	0.0145(10)
C(38)	0.0563(16)	0.0271(12)	0.0475(14)	0.0143(10)	0.0265(12)	0.0207(11)

C(39)	0.0488(15)	0.0389(13)	0.0542(15)	0.0290(12)	0.0216(12)	0.0267(12)
C(40)	0.0348(12)	0.0464(14)	0.0376(12)	0.0258(11)	0.0056(10)	0.0178(11)
C(41)	0.0257(10)	0.0300(11)	0.0289(10)	0.0131(9)	0.0025(8)	0.0075(9)
Cl(1)	0.0668(6)	0.1258(9)	0.1232(9)	0.0898(8)	0.0510(6)	0.0513(6)
C(50)	0.040(3)	0.127(7)	0.098(5)	0.090(5)	0.031(3)	0.034(4)

Table 5. Hydrogen coordinates and isotropic displacement parameters (Å^2) for str0562.

	x	y	z	U
H(8A)	0.2368	0.1615	0.1220	0.028
H(10A)	0.7046	0.3103	0.1395	0.033
H(11A)	0.6056	0.1434	0.0140	0.040
H(12A)	0.3192	0.0522	0.0031	0.036
H(13A)	0.7516	0.1519	0.2550	0.032
H(14A)	0.5307	0.1648	0.3272	0.025
H(16A)	0.3624	−0.1138	0.1295	0.029
H(17A)	0.6481	−0.0191	0.1330	0.034
H(19A)	0.2749	−0.2136	0.2697	0.034
H(20A)	0.3487	−0.2967	0.3693	0.042
H(21A)	0.3698	−0.2218	0.5087	0.040
H(22A)	0.3052	−0.0685	0.5496	0.037
H(23A)	0.2242	0.0125	0.4502	0.029
H(25A)	0.1625	−0.0507	0.0945	0.033
H(26A)	−0.0128	−0.1827	−0.0125	0.045
H(27A)	−0.2030	−0.3347	0.0172	0.056
H(28A)	−0.2169	−0.3557	0.1524	0.050
H(29A)	−0.0372	−0.2276	0.2597	0.035
H(31A)	0.6180	0.3615	0.4046	0.024
H(32A)	0.8668	0.4204	0.4641	0.032
H(33A)	1.0585	0.5148	0.3964	0.035
H(34A)	1.0033	0.5531	0.2686	0.036
H(35A)	0.7557	0.4922	0.2075	0.032
H(37A)	0.5525	0.6009	0.3113	0.037
H(38A)	0.5563	0.7551	0.2580	0.048
H(39A)	0.4850	0.7351	0.1176	0.049
H(40A)	0.4137	0.5608	0.0297	0.044
H(41A)	0.4123	0.4067	0.0822	0.034
H(1)	−0.049(3)	0.261(2)	0.4793(15)	0.026(6)
H(2)	0.103(3)	0.363(2)	0.4787(15)	0.027(6)
H(3)	0.080(3)	0.150(2)	0.4998(13)	0.019(5)
H(4)	0.127(3)	0.249(2)	0.5717(16)	0.032(6)
H(5)	0.344(3)	0.223(2)	0.5353(15)	0.030(6)
H(6)	0.355(3)	0.340(2)	0.5198(15)	0.027(6)

Table 6. Torsion angles [°] for str0562.

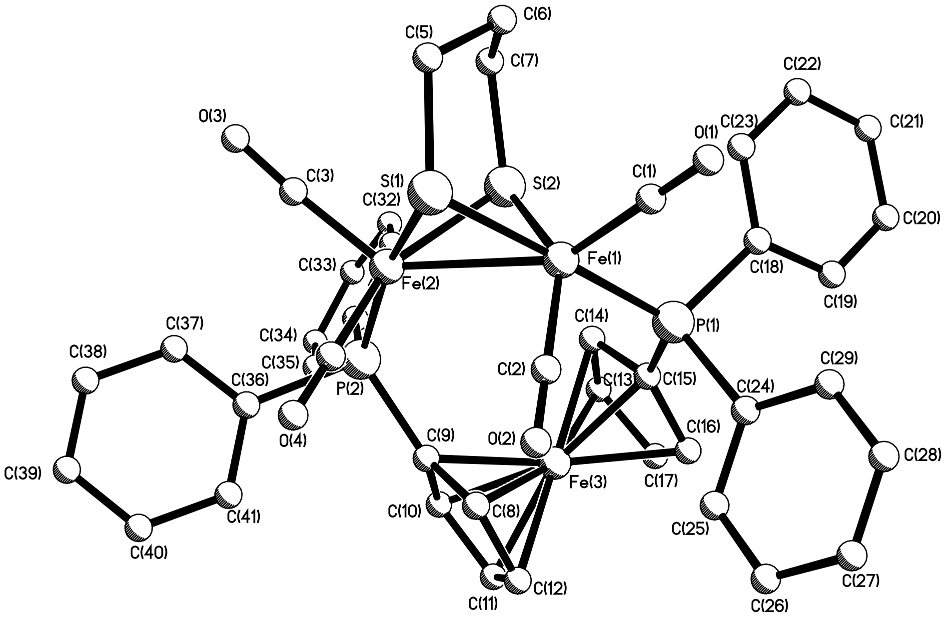
C(2)–Fe(1)–Fe(2)–C(3)	137.64(12)	C(1)–Fe(1)–Fe(2)–C(3)	28.86(16)
P(1)–Fe(1)–Fe(2)–C(3)	−127.85(10)	S(1)–Fe(1)–Fe(2)–C(3)	49.79(10)
S(2)–Fe(1)–Fe(2)–C(3)	−60.95(10)	C(2)–Fe(1)–Fe(2)–C(4)	12.04(9)
C(1)–Fe(1)–Fe(2)–C(4)	−96.74(14)	P(1)–Fe(1)–Fe(2)–C(4)	106.55(7)
S(1)–Fe(1)–Fe(2)–C(4)	−75.82(7)	S(2)–Fe(1)–Fe(2)–C(4)	173.45(7)
C(2)–Fe(1)–Fe(2)–S(1)	87.86(7)	C(1)–Fe(1)–Fe(2)–S(1)	−20.92(12)
P(1)–Fe(1)–Fe(2)–S(1)	−177.64(2)	S(2)–Fe(1)–Fe(2)–S(1)	−110.73(3)
C(2)–Fe(1)–Fe(2)–S(2)	−161.41(6)	C(1)–Fe(1)–Fe(2)–S(2)	89.81(13)
P(1)–Fe(1)–Fe(2)–S(2)	−66.90(3)	S(1)–Fe(1)–Fe(2)–S(2)	110.73(3)
C(2)–Fe(1)–Fe(2)–P(2)	−80.39(7)	C(1)–Fe(1)–Fe(2)–P(2)	170.83(12)
P(1)–Fe(1)–Fe(2)–P(2)	14.12(3)	S(1)–Fe(1)–Fe(2)–P(2)	−168.24(2)
S(2)–Fe(1)–Fe(2)–P(2)	81.02(3)	C(2)–Fe(1)–P(1)–C(15)	91.93(10)
C(1)–Fe(1)–P(1)–C(15)	−169.61(10)	S(1)–Fe(1)–P(1)–C(15)	−21.9(2)
S(2)–Fe(1)–P(1)–C(15)	−50.63(8)	Fe(2)–Fe(1)–P(1)–C(15)	−2.02(8)
C(2)–Fe(1)–P(1)–C(24)	−31.15(9)	C(1)–Fe(1)–P(1)–C(24)	67.31(10)
S(1)–Fe(1)–P(1)–C(24)	−145.0(2)	S(2)–Fe(1)–P(1)–C(24)	−173.71(7)
Fe(2)–Fe(1)–P(1)–C(24)	−125.10(7)	C(2)–Fe(1)–P(1)–C(18)	−149.66(9)
C(1)–Fe(1)–P(1)–C(18)	−51.20(10)	S(1)–Fe(1)–P(1)–C(18)	96.5(2)
S(2)–Fe(1)–P(1)–C(18)	67.78(7)	Fe(2)–Fe(1)–P(1)–C(18)	116.39(7)
C(3)–Fe(2)–P(2)–C(9)	−174.77(10)	C(4)–Fe(2)–P(2)–C(9)	−72.61(10)
S(1)–Fe(2)–P(2)–C(9)	−22.58(13)	S(2)–Fe(2)–P(2)–C(9)	83.54(8)
Fe(1)–Fe(2)–P(2)–C(9)	28.85(8)	C(3)–Fe(2)–P(2)–C(30)	55.04(10)
C(4)–Fe(2)–P(2)–C(30)	157.19(10)	S(1)–Fe(2)–P(2)–C(30)	−152.78(11)
S(2)–Fe(2)–P(2)–C(30)	−46.66(8)	Fe(1)–Fe(2)–P(2)–C(30)	−101.35(8)
C(3)–Fe(2)–P(2)–C(36)	−59.17(9)	C(4)–Fe(2)–P(2)–C(36)	42.98(10)
S(1)–Fe(2)–P(2)–C(36)	93.02(12)	S(2)–Fe(2)–P(2)–C(36)	−160.87(7)
Fe(1)–Fe(2)–P(2)–C(36)	144.45(7)	C(2)–Fe(1)–S(1)–C(5)	161.36(10)
C(1)–Fe(1)–S(1)–C(5)	62.97(10)	P(1)–Fe(1)–S(1)–C(5)	−84.6(2)
S(2)–Fe(1)–S(1)–C(5)	−55.76(8)	Fe(2)–Fe(1)–S(1)–C(5)	−105.81(8)
C(2)–Fe(1)–S(1)–Fe(2)	−92.83(7)	C(1)–Fe(1)–S(1)–Fe(2)	168.77(7)
P(1)–Fe(1)–S(1)–Fe(2)	21.2(2)	S(2)–Fe(1)–S(1)–Fe(2)	50.045(19)
C(3)–Fe(2)–S(1)–C(5)	−42.98(10)	C(4)–Fe(2)–S(1)–C(5)	−145.00(10)
S(2)–Fe(2)–S(1)–C(5)	57.17(8)	P(2)–Fe(2)–S(1)–C(5)	164.90(11)
Fe(1)–Fe(2)–S(1)–C(5)	107.18(8)	C(3)–Fe(2)–S(1)–Fe(1)	−150.16(6)
C(4)–Fe(2)–S(1)–Fe(1)	107.82(7)	S(2)–Fe(2)–S(1)–Fe(1)	−50.004(19)
P(2)–Fe(2)–S(1)–Fe(1)	57.72(10)	C(2)–Fe(1)–S(2)–C(7)	136.73(13)
C(1)–Fe(1)–S(2)–C(7)	−36.33(11)	P(1)–Fe(1)–S(2)–C(7)	−127.49(8)
S(1)–Fe(1)–S(2)–C(7)	55.24(8)	Fe(2)–Fe(1)–S(2)–C(7)	105.25(8)
C(2)–Fe(1)–S(2)–Fe(2)	31.47(11)	C(1)–Fe(1)–S(2)–Fe(2)	−141.58(8)
P(1)–Fe(1)–S(2)–Fe(2)	127.26(2)	S(1)–Fe(1)–S(2)–Fe(2)	−50.010(19)
C(3)–Fe(2)–S(2)–C(7)	37.19(10)	C(4)–Fe(2)–S(2)–C(7)	−123.26(18)
S(1)–Fe(2)–S(2)–C(7)	−57.86(8)	P(2)–Fe(2)–S(2)–C(7)	133.93(8)
Fe(1)–Fe(2)–S(2)–C(7)	−107.61(8)	C(3)–Fe(2)–S(2)–Fe(1)	144.80(6)
C(4)–Fe(2)–S(2)–Fe(1)	−15.65(16)	S(1)–Fe(2)–S(2)–Fe(1)	49.748(18)
P(2)–Fe(2)–S(2)–Fe(1)	−118.46(2)	C(2)–Fe(1)–C(1)–O(1)	−38.2(18)
P(1)–Fe(1)–C(1)–O(1)	−131.2(18)	S(1)–Fe(1)–C(1)–O(1)	51.8(18)
S(2)–Fe(1)–C(1)–O(1)	137.5(18)	Fe(2)–Fe(1)–C(1)–O(1)	68.8(19)
C(1)–Fe(1)–C(2)–O(2)	41(5)	P(1)–Fe(1)–C(2)–O(2)	132(5)
S(1)–Fe(1)–C(2)–O(2)	−53(5)	S(2)–Fe(1)–C(2)–O(2)	−133(5)
Fe(2)–Fe(1)–C(2)–O(2)	−108(5)	C(4)–Fe(2)–C(3)–O(3)	95.3(18)

S(1)–Fe(2)–C(3)–O(3)	8.4(18)	S(2)–Fe(2)–C(3)–O(3)	−76.6(18)
P(2)–Fe(2)–C(3)–O(3)	−177.3(18)	Fe(1)–Fe(2)–C(3)–O(3)	−30.1(18)
C(3)–Fe(2)–C(4)–O(4)	−85(5)	S(1)–Fe(2)–C(4)–O(4)	11(5)
S(2)–Fe(2)–C(4)–O(4)	76(5)	P(2)–Fe(2)–C(4)–O(4)	−179(100)
Fe(1)–Fe(2)–C(4)–O(4)	63(5)	Fe(1)–S(1)–C(5)–C(6)	9.66(19)
Fe(2)–S(1)–C(5)–C(6)	−67.84(17)	S(1)–C(5)–C(6)–C(7)	61.7(2)
C(5)–C(6)–C(7)–S(2)	−62.0(2)	Fe(1)–S(2)–C(7)–C(6)	−8.14(19)
Fe(2)–S(2)–C(7)–C(6)	69.00(17)	C(10)–Fe(3)–C(8)–C(12)	80.89(13)
C(15)–Fe(3)–C(8)–C(12)	−122.75(13)	C(9)–Fe(3)–C(8)–C(12)	119.54(17)
C(14)–Fe(3)–C(8)–C(12)	−166.07(12)	C(11)–Fe(3)–C(8)–C(12)	36.91(13)
C(16)–Fe(3)–C(8)–C(12)	−79.42(14)	C(17)–Fe(3)–C(8)–C(12)	−41.5(3)
C(13)–Fe(3)–C(8)–C(12)	156.0(2)	C(10)–Fe(3)–C(8)–C(9)	−38.65(11)
C(15)–Fe(3)–C(8)–C(9)	117.72(11)	C(14)–Fe(3)–C(8)–C(9)	74.39(13)
C(11)–Fe(3)–C(8)–C(9)	−82.63(13)	C(16)–Fe(3)–C(8)–C(9)	161.04(11)
C(12)–Fe(3)–C(8)–C(9)	−119.54(17)	C(17)–Fe(3)–C(8)–C(9)	−161.1(2)
C(13)–Fe(3)–C(8)–C(9)	36.4(3)	C(12)–C(8)–C(9)–C(10)	0.1(2)
Fe(3)–C(8)–C(9)–C(10)	59.44(14)	C(12)–C(8)–C(9)–P(2)	179.04(14)
Fe(3)–C(8)–C(9)–P(2)	−121.61(15)	C(12)–C(8)–C(9)–Fe(3)	−59.35(14)
C(30)–P(2)–C(9)–C(8)	160.07(16)	C(36)–P(2)–C(9)–C(8)	−97.96(17)
Fe(2)–P(2)–C(9)–C(8)	20.85(19)	C(30)–P(2)–C(9)–C(10)	−21.2(2)
C(36)–P(2)–C(9)–C(10)	80.76(19)	Fe(2)–P(2)–C(9)–C(10)	−160.43(16)
C(30)–P(2)–C(9)–Fe(3)	70.72(14)	C(36)–P(2)–C(9)–Fe(3)	172.69(12)
Fe(2)–P(2)–C(9)–Fe(3)	−68.49(14)	C(10)–Fe(3)–C(9)–C(8)	118.26(16)
C(15)–Fe(3)–C(9)–C(8)	−82.31(13)	C(14)–Fe(3)–C(9)–C(8)	−124.62(11)
C(11)–Fe(3)–C(9)–C(8)	80.58(13)	C(16)–Fe(3)–C(9)–C(8)	−51.7(3)
C(12)–Fe(3)–C(9)–C(8)	37.41(12)	C(17)–Fe(3)–C(9)–C(8)	162.74(19)
C(13)–Fe(3)–C(9)–C(8)	−166.09(11)	C(15)–Fe(3)–C(9)–C(10)	159.43(12)
C(14)–Fe(3)–C(9)–C(10)	117.11(12)	C(11)–Fe(3)–C(9)–C(10)	−37.68(13)
C(8)–Fe(3)–C(9)–C(10)	−118.26(16)	C(16)–Fe(3)–C(9)–C(10)	−170.0(2)
C(12)–Fe(3)–C(9)–C(10)	−80.85(13)	C(17)–Fe(3)–C(9)–C(10)	44.5(3)
C(13)–Fe(3)–C(9)–C(10)	75.65(14)	C(10)–Fe(3)–C(9)–P(2)	−123.81(19)
C(15)–Fe(3)–C(9)–P(2)	35.62(17)	C(14)–Fe(3)–C(9)–P(2)	−6.69(15)
C(11)–Fe(3)–C(9)–P(2)	−161.49(16)	C(8)–Fe(3)–C(9)–P(2)	117.93(18)
C(16)–Fe(3)–C(9)–P(2)	66.2(3)	C(12)–Fe(3)–C(9)–P(2)	155.34(16)
C(17)–Fe(3)–C(9)–P(2)	−79.3(2)	C(13)–Fe(3)–C(9)–P(2)	−48.16(16)
C(8)–C(9)–C(10)–C(11)	−0.1(2)	P(2)–C(9)–C(10)–C(11)	−179.00(16)
Fe(3)–C(9)–C(10)–C(11)	59.91(15)	C(8)–C(9)–C(10)–Fe(3)	−60.02(13)
P(2)–C(9)–C(10)–Fe(3)	121.09(17)	C(15)–Fe(3)–C(10)–C(11)	−170.7(2)
C(9)–Fe(3)–C(10)–C(11)	−119.13(19)	C(14)–Fe(3)–C(10)–C(11)	159.92(13)
C(8)–Fe(3)–C(10)–C(11)	−80.80(15)	C(16)–Fe(3)–C(10)–C(11)	51.8(3)
C(12)–Fe(3)–C(10)–C(11)	−37.03(14)	C(17)–Fe(3)–C(10)–C(11)	79.07(16)
C(13)–Fe(3)–C(10)–C(11)	119.33(14)	C(15)–Fe(3)–C(10)–C(9)	−51.5(3)
C(14)–Fe(3)–C(10)–C(9)	−80.94(14)	C(11)–Fe(3)–C(10)–C(9)	119.13(19)
C(8)–Fe(3)–C(10)–C(9)	38.33(11)	C(16)–Fe(3)–C(10)–C(9)	170.9(2)
C(12)–Fe(3)–C(10)–C(9)	82.10(13)	C(17)–Fe(3)–C(10)–C(9)	−161.80(12)
C(13)–Fe(3)–C(10)–C(9)	−121.53(12)	C(9)–C(10)–C(11)–C(12)	0.1(2)
Fe(3)–C(10)–C(11)–C(12)	59.48(15)	C(9)–C(10)–C(11)–Fe(3)	−59.37(14)
C(10)–Fe(3)–C(11)–C(12)	−119.79(19)	C(15)–Fe(3)–C(11)–C(12)	49.4(3)
C(9)–Fe(3)–C(11)–C(12)	−81.56(14)	C(14)–Fe(3)–C(11)–C(12)	−166.10(19)
C(8)–Fe(3)–C(11)–C(12)	−37.32(13)	C(16)–Fe(3)–C(11)–C(12)	80.92(15)
C(17)–Fe(3)–C(11)–C(12)	121.73(13)	C(13)–Fe(3)–C(11)–C(12)	163.06(13)
C(15)–Fe(3)–C(11)–C(10)	169.2(2)	C(9)–Fe(3)–C(11)–C(10)	38.23(13)

C(14)–Fe(3)–C(11)–C(10)	−46.3(3)	C(8)–Fe(3)–C(11)–C(10)	82.46(14)
C(16)–Fe(3)–C(11)–C(10)	−159.30(13)	C(12)–Fe(3)–C(11)–C(10)	119.79(19)
C(17)–Fe(3)–C(11)–C(10)	−118.49(14)	C(13)–Fe(3)–C(11)–C(10)	−77.16(16)
C(10)–C(11)–C(12)–C(8)	−0.1(2)	Fe(3)–C(11)–C(12)–C(8)	58.50(14)
C(10)–C(11)–C(12)–Fe(3)	−58.55(15)	C(9)–C(8)–C(12)–C(11)	0.0(2)
Fe(3)–C(8)–C(12)–C(11)	−58.62(15)	C(9)–C(8)–C(12)–Fe(3)	58.60(14)
C(10)–Fe(3)–C(12)–C(11)	37.62(13)	C(15)–Fe(3)–C(12)–C(11)	−162.09(12)
C(9)–Fe(3)–C(12)–C(11)	82.28(14)	C(14)–Fe(3)–C(12)–C(11)	160.9(3)
C(8)–Fe(3)–C(12)–C(11)	120.09(18)	C(16)–Fe(3)–C(12)–C(11)	−118.88(13)
C(17)–Fe(3)–C(12)–C(11)	−75.93(15)	C(13)–Fe(3)–C(12)–C(11)	−39.3(3)
C(10)–Fe(3)–C(12)–C(8)	−82.47(13)	C(15)–Fe(3)–C(12)–C(8)	77.81(14)
C(9)–Fe(3)–C(12)–C(8)	−37.81(12)	C(14)–Fe(3)–C(12)–C(8)	40.8(3)
C(11)–Fe(3)–C(12)–C(8)	−120.09(18)	C(16)–Fe(3)–C(12)–C(8)	121.03(12)
C(17)–Fe(3)–C(12)–C(8)	163.98(12)	C(13)–Fe(3)–C(12)–C(8)	−159.37(19)
C(10)–Fe(3)–C(13)–C(14)	119.85(12)	C(15)–Fe(3)–C(13)–C(14)	−37.75(12)
C(9)–Fe(3)–C(13)–C(14)	78.32(14)	C(11)–Fe(3)–C(13)–C(14)	161.07(12)
C(8)–Fe(3)–C(13)–C(14)	51.0(3)	C(16)–Fe(3)–C(13)–C(14)	−82.16(13)
C(12)–Fe(3)–C(13)–C(14)	−170.75(19)	C(17)–Fe(3)–C(13)–C(14)	−119.58(18)
C(10)–Fe(3)–C(13)–C(17)	−120.57(13)	C(15)–Fe(3)–C(13)–C(17)	81.83(13)
C(9)–Fe(3)–C(13)–C(17)	−162.10(12)	C(14)–Fe(3)–C(13)–C(17)	119.58(18)
C(11)–Fe(3)–C(13)–C(17)	−79.35(15)	C(8)–Fe(3)–C(13)–C(17)	170.6(2)
C(16)–Fe(3)–C(13)–C(17)	37.42(12)	C(12)–Fe(3)–C(13)–C(17)	−51.2(3)
C(17)–C(13)–C(14)–C(15)	−0.5(2)	Fe(3)–C(13)–C(14)–C(15)	58.65(14)
C(17)–C(13)–C(14)–Fe(3)	−59.16(15)	C(10)–Fe(3)–C(14)–C(13)	−76.45(14)
C(15)–Fe(3)–C(14)–C(13)	119.93(17)	C(9)–Fe(3)–C(14)–C(13)	−119.50(13)
C(11)–Fe(3)–C(14)–C(13)	−43.2(3)	C(8)–Fe(3)–C(14)–C(13)	−160.89(12)
C(16)–Fe(3)–C(14)–C(13)	80.96(13)	C(12)–Fe(3)–C(14)–C(13)	167.7(3)
C(17)–Fe(3)–C(14)–C(13)	37.26(13)	C(10)–Fe(3)–C(14)–C(15)	163.62(11)
C(9)–Fe(3)–C(14)–C(15)	120.57(11)	C(11)–Fe(3)–C(14)–C(15)	−163.15(19)
C(8)–Fe(3)–C(14)–C(15)	79.18(13)	C(16)–Fe(3)–C(14)–C(15)	−38.97(11)
C(12)–Fe(3)–C(14)–C(15)	47.8(3)	C(17)–Fe(3)–C(14)–C(15)	−82.67(12)
C(13)–Fe(3)–C(14)–C(15)	−119.93(17)	C(13)–C(14)–C(15)–C(16)	1.1(2)
Fe(3)–C(14)–C(15)–C(16)	60.75(13)	C(13)–C(14)–C(15)–P(1)	172.42(14)
Fe(3)–C(14)–C(15)–P(1)	−127.91(15)	C(13)–C(14)–C(15)–Fe(3)	−59.67(14)
C(24)–P(1)–C(15)–C(14)	174.97(16)	C(18)–P(1)–C(15)–C(14)	−78.32(18)
Fe(1)–P(1)–C(15)–C(14)	48.72(19)	C(24)–P(1)–C(15)–C(16)	−15.7(2)
C(18)–P(1)–C(15)–C(16)	91.05(19)	Fe(1)–P(1)–C(15)–C(16)	−141.91(15)
C(24)–P(1)–C(15)–Fe(3)	82.08(14)	C(18)–P(1)–C(15)–Fe(3)	−171.22(13)
Fe(1)–P(1)–C(15)–Fe(3)	−44.17(16)	C(10)–Fe(3)–C(15)–C(14)	−40.0(3)
C(9)–Fe(3)–C(15)–C(14)	−77.96(13)	C(11)–Fe(3)–C(15)–C(14)	158.8(3)
C(8)–Fe(3)–C(15)–C(14)	−121.62(12)	C(16)–Fe(3)–C(15)–C(14)	117.29(16)
C(12)–Fe(3)–C(15)–C(14)	−164.05(12)	C(17)–Fe(3)–C(15)–C(14)	80.17(12)
C(13)–Fe(3)–C(15)–C(14)	36.97(11)	C(10)–Fe(3)–C(15)–C(16)	−157.3(2)
C(9)–Fe(3)–C(15)–C(16)	164.75(12)	C(14)–Fe(3)–C(15)–C(16)	−117.29(16)
C(11)–Fe(3)–C(15)–C(16)	41.5(3)	C(8)–Fe(3)–C(15)–C(16)	121.09(12)
C(12)–Fe(3)–C(15)–C(16)	78.66(14)	C(17)–Fe(3)–C(15)–C(16)	−37.12(12)
C(13)–Fe(3)–C(15)–C(16)	−80.32(12)	C(10)–Fe(3)–C(15)–P(1)	78.2(3)
C(9)–Fe(3)–C(15)–P(1)	40.26(17)	C(14)–Fe(3)–C(15)–P(1)	118.22(19)
C(11)–Fe(3)–C(15)–P(1)	−83.0(3)	C(8)–Fe(3)–C(15)–P(1)	−3.39(16)
C(16)–Fe(3)–C(15)–P(1)	−124.49(19)	C(12)–Fe(3)–C(15)–P(1)	−45.83(18)
C(17)–Fe(3)–C(15)–P(1)	−161.60(16)	C(13)–Fe(3)–C(15)–P(1)	155.19(16)
C(14)–C(15)–C(16)–C(17)	−1.3(2)	P(1)–C(15)–C(16)–C(17)	−172.08(15)

Fe(3)–C(15)–C(16)–C(17)	59.29(14)	C(14)–C(15)–C(16)–Fe(3)	–60.54(13)
P(1)–C(15)–C(16)–Fe(3)	128.63(16)	C(10)–Fe(3)–C(16)–C(17)	37.4(3)
C(15)–Fe(3)–C(16)–C(17)	–119.80(17)	C(9)–Fe(3)–C(16)–C(17)	–160.5(2)
C(14)–Fe(3)–C(16)–C(17)	–80.77(13)	C(11)–Fe(3)–C(16)–C(17)	75.31(15)
C(8)–Fe(3)–C(16)–C(17)	160.63(12)	C(12)–Fe(3)–C(16)–C(17)	117.84(13)
C(13)–Fe(3)–C(16)–C(17)	–37.18(12)	C(10)–Fe(3)–C(16)–C(15)	157.2(2)
C(9)–Fe(3)–C(16)–C(15)	–40.7(3)	C(14)–Fe(3)–C(16)–C(15)	39.03(11)
C(11)–Fe(3)–C(16)–C(15)	–164.89(12)	C(8)–Fe(3)–C(16)–C(15)	–79.58(13)
C(12)–Fe(3)–C(16)–C(15)	–122.37(12)	C(17)–Fe(3)–C(16)–C(15)	119.80(17)
C(13)–Fe(3)–C(16)–C(15)	82.61(12)	C(14)–C(13)–C(17)–C(16)	–0.3(2)
Fe(3)–C(13)–C(17)–C(16)	–58.93(15)	C(14)–C(13)–C(17)–Fe(3)	58.65(14)
C(15)–C(16)–C(17)–C(13)	1.0(2)	Fe(3)–C(16)–C(17)–C(13)	59.32(15)
C(15)–C(16)–C(17)–Fe(3)	–58.36(14)	C(10)–Fe(3)–C(17)–C(13)	75.72(14)
C(15)–Fe(3)–C(17)–C(13)	–81.91(13)	C(9)–Fe(3)–C(17)–C(13)	43.1(3)
C(14)–Fe(3)–C(17)–C(13)	–37.42(12)	C(11)–Fe(3)–C(17)–C(13)	117.69(13)
C(8)–Fe(3)–C(17)–C(13)	–170.8(2)	C(16)–Fe(3)–C(17)–C(13)	–119.68(17)
C(12)–Fe(3)–C(17)–C(13)	158.38(12)	C(10)–Fe(3)–C(17)–C(16)	–164.60(12)
C(15)–Fe(3)–C(17)–C(16)	37.77(11)	C(9)–Fe(3)–C(17)–C(16)	162.74(18)
C(14)–Fe(3)–C(17)–C(16)	82.26(12)	C(11)–Fe(3)–C(17)–C(16)	–122.63(13)
C(8)–Fe(3)–C(17)–C(16)	–51.1(3)	C(12)–Fe(3)–C(17)–C(16)	–81.94(14)
C(13)–Fe(3)–C(17)–C(16)	119.68(17)	C(15)–P(1)–C(18)–C(23)	114.53(17)
C(24)–P(1)–C(18)–C(23)	–139.42(16)	Fe(1)–P(1)–C(18)–C(23)	–17.48(18)
C(15)–P(1)–C(18)–C(19)	–58.13(17)	C(24)–P(1)–C(18)–C(19)	47.92(18)
Fe(1)–P(1)–C(18)–C(19)	169.86(14)	C(23)–C(18)–C(19)–C(20)	–0.9(3)
P(1)–C(18)–C(19)–C(20)	171.92(18)	C(18)–C(19)–C(20)–C(21)	–0.9(4)
C(19)–C(20)–C(21)–C(22)	1.8(4)	C(20)–C(21)–C(22)–C(23)	–0.8(3)
C(19)–C(18)–C(23)–C(22)	1.9(3)	P(1)–C(18)–C(23)–C(22)	–170.75(16)
C(21)–C(22)–C(23)–C(18)	–1.1(3)	C(15)–P(1)–C(24)–C(29)	140.41(17)
C(18)–P(1)–C(24)–C(29)	39.32(19)	Fe(1)–P(1)–C(24)–C(29)	–85.88(17)
C(15)–P(1)–C(24)–C(25)	–47.81(19)	C(18)–P(1)–C(24)–C(25)	–148.89(17)
Fe(1)–P(1)–C(24)–C(25)	85.90(17)	C(29)–C(24)–C(25)–C(26)	–1.8(3)
P(1)–C(24)–C(25)–C(26)	–173.79(18)	C(24)–C(25)–C(26)–C(27)	1.6(4)
C(25)–C(26)–C(27)–C(28)	–0.2(4)	C(26)–C(27)–C(28)–C(29)	–1.0(4)
C(27)–C(28)–C(29)–C(24)	0.8(4)	C(25)–C(24)–C(29)–C(28)	0.6(3)
P(1)–C(24)–C(29)–C(28)	172.50(19)	C(9)–P(2)–C(30)–C(31)	–114.53(17)
C(36)–P(2)–C(30)–C(31)	141.05(17)	Fe(2)–P(2)–C(30)–C(31)	22.37(19)
C(9)–P(2)–C(30)–C(35)	63.66(18)	C(36)–P(2)–C(30)–C(35)	–40.76(18)
Fe(2)–P(2)–C(30)–C(35)	–159.44(14)	C(35)–C(30)–C(31)–C(32)	–1.9(3)
P(2)–C(30)–C(31)–C(32)	176.28(15)	C(30)–C(31)–C(32)–C(33)	1.0(3)
C(31)–C(32)–C(33)–C(34)	0.5(3)	C(32)–C(33)–C(34)–C(35)	–1.0(3)
C(33)–C(34)–C(35)–C(30)	0.1(3)	C(31)–C(30)–C(35)–C(34)	1.4(3)
P(2)–C(30)–C(35)–C(34)	–176.89(17)	C(9)–P(2)–C(36)–C(41)	21.04(19)
C(30)–P(2)–C(36)–C(41)	125.41(17)	Fe(2)–P(2)–C(36)–C(41)	–105.16(16)
C(9)–P(2)–C(36)–C(37)	–161.40(17)	C(30)–P(2)–C(36)–C(37)	–57.04(18)
Fe(2)–P(2)–C(36)–C(37)	72.40(17)	C(41)–C(36)–C(37)–C(38)	0.7(3)
P(2)–C(36)–C(37)–C(38)	–176.91(18)	C(36)–C(37)–C(38)–C(39)	0.2(4)
C(37)–C(38)–C(39)–C(40)	–0.7(4)	C(38)–C(39)–C(40)–C(41)	0.2(4)
C(37)–C(36)–C(41)–C(40)	–1.2(3)	P(2)–C(36)–C(41)–C(40)	176.42(17)
C(39)–C(40)–C(41)–C(36)	0.7(4)	C(50A)–Cl(1)–C(50)–Cl(1A)	0.0

Symmetry operations for equivalent atoms
A –x+2,–y+1,–z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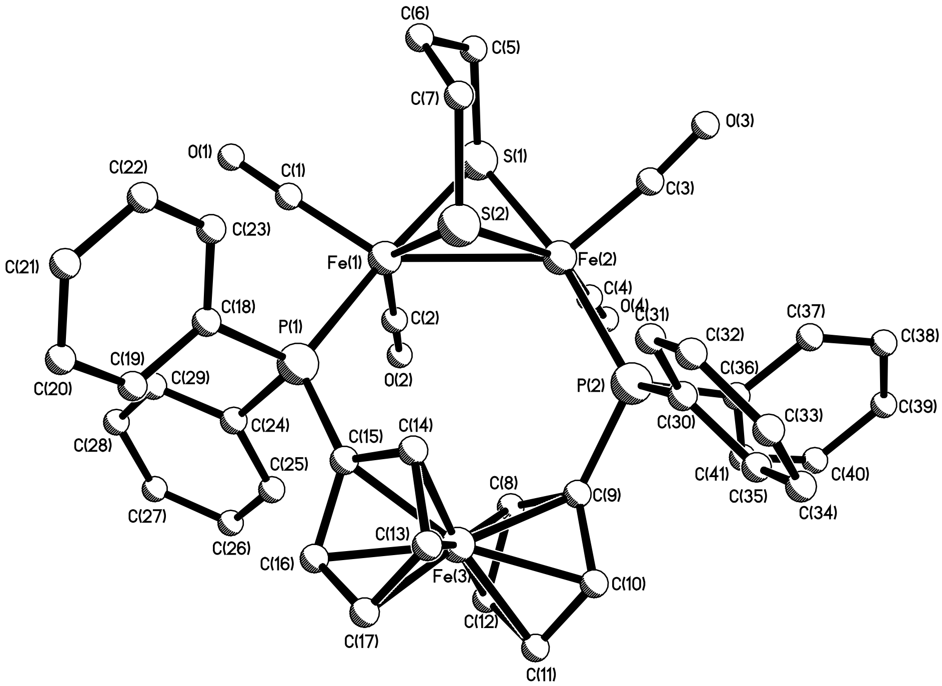
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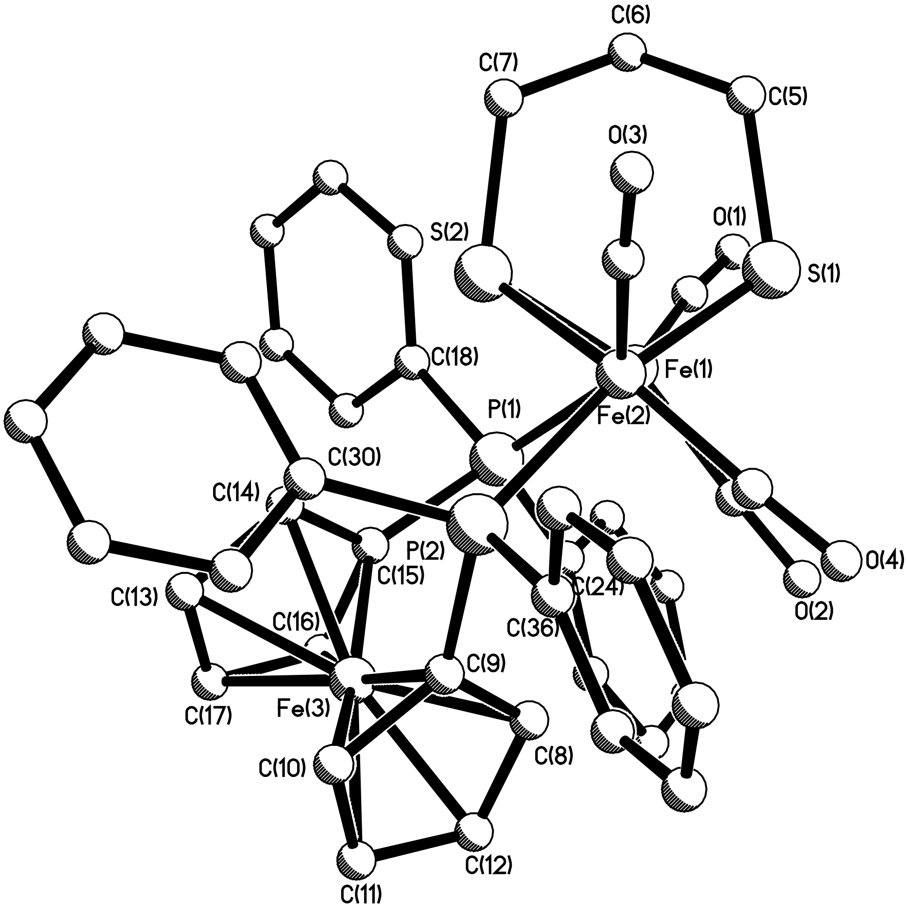
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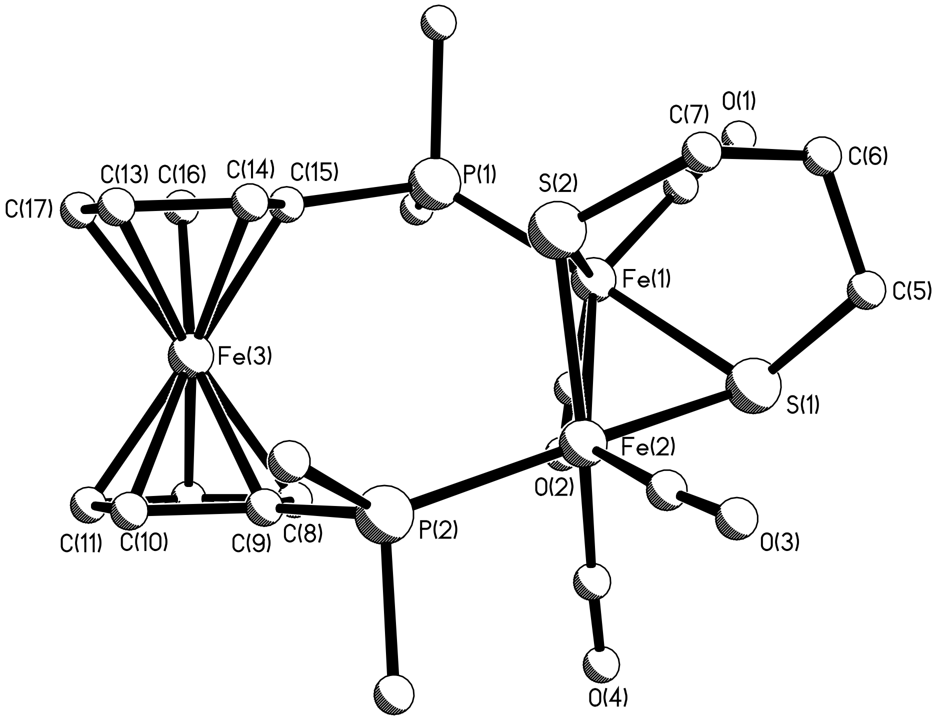
C(24)
C(13)
O(2)
C(36)
C(16)
C(9)
C(17)
Fe(3)
C(8)
C(10)
C(12)
C(11)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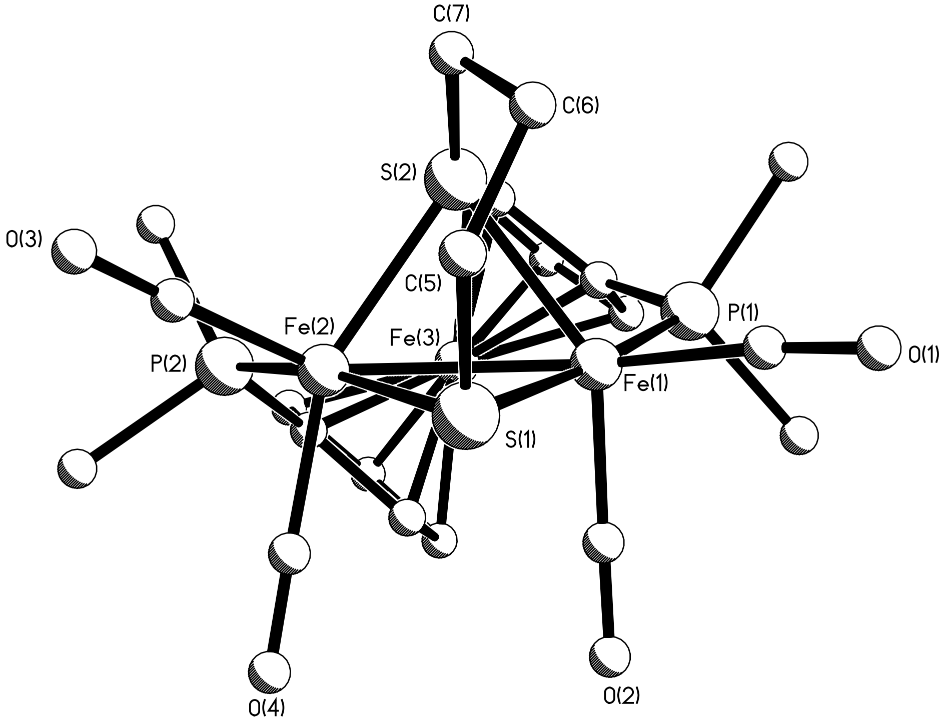
C(6)
C(13)
C(16)
C(14)
C(15)
P(1)
S(2)
C(17)
Fe(1)
C(5)
Fe(3)
S(1)
Fe(2)
O(2)
C(11)
C(10)
C(9)
C(8)
P(2)
O(3)
O(4)


C(7)
C(6)
S(2)
O(3)
C(5)
Fe(2)
Fe(3)
P(1)
P(2)
O(1)
Fe(1)
S(1)
O(4)
O(2)