

Synthesis

Fe(DMF)Cl(Cl₄-cat)₂Mo₂Fe₂S₄(PEt₃)ClFe₄S₄(PEt₃)₃(CO)₆Cl (III). A solution of **I** (1g, 0.50mmol) in 40mL of CH₂Cl₂ with 0.1ml of DMF was introduced 500 psi of CO. The reaction mixture was stirred for three days and the reddish black solution was dried under nitrogen stream. The residue was loaded on top of silica gel column and the products were separated with hexane/CH₂Cl₂ gradient eluents by flash column chromatography. The compound **III** was separated from 10% CH₂Cl₂ fraction and crystallized as black sea urchin shape crystals. (10mg, 4.4μmol, 0.9% yield) IR(KBr, cm⁻¹) ν(PEt₃) 2968(w), 2937(w), 2878(w), 2868(w). ν(CO) 2019(s), 2003(vs), 1975(s), 1970(s, sh). ν(CO of DMF) 1618(m). ν(Cl₄-cat) 1455(m), 1437(m), 1405(m), 1385(m). Microprobe measurement showed one of Mo, three and half of Fe, four of S, six of Cl and two of P atoms in the crystal. UV(CH₂Cl₂) 310nm. FAB⁺-MS(NBA, *m/z*) 2119([M]-SPEt₃)⁺. ¹H-NMR(300MHz, Benzene-*d*⁶) The spectrum showed *S* ≠ 0 signals due to non-diamagnetic sample. 4.22(Fe-PCH₂, 12H), 3.54(Fe-PCH₂, 6H), 1.38(Mo-PCH₂, 4H), 1.19(Mo-PCH₂CH₃, 18H), 0.83(Fe-CH₂CH₃, 27H), 0.92(d, DMF-Me, 6H), 0.56(Mo-PCH₂, 8H).

Fe₄S₄Cl(PEt₃)₃(CO)₆ (IV) was isolated from the reaction mixture of **I** by eluting pentane though the silica gel flash column in a 22% yield (100mg, 0.11mmol). Anal. Calcd for C₂₄H₄₅ClFe₄O₆P₃S₄ (MW. 909.628): C, 31.69; H, 4.99. Found: C, 30.87, H, 4.34. Mid-IR(KBr, cm⁻¹) ν(PEt₃) 2972(w), 2938(w), 2907(w), 2880(w). ν(CO) 2023(s), 1995(vs), 1959(s), 1948(s). 1457(w), 1421(w), 1413(w), 1379(w), 1034(m), 758(m), 724(m), 616(m), 575(m), 410(w), 386(s), 368(s), 337(w), 324(m). FAB⁺-MS (NBA, *m/z*) 909.8([M]⁺), 817.9([M-FeCl]⁺), 740.9([M-FeCl(CO)₂]⁺). ¹H-NMR(300MHz, CDCl₃) showed *S* ≠ 0 signals. 5.29(Fe-PCH₂, 12H), 3.74(Fe-PCH₂, 6H), 0.88(Fe-PCH₂CH₃, 27H). UV(CH₂Cl₂, nm) 315(3700), 380(2000), 490(1000). Cyclic voltammetry (1,2-dichloroethane, vs. SCE, V) -1.32(irr), -1.73(irr). (DMF, vs. SCE, V) -0.92(irr), -1.37(irr). EPR(CH₂Cl₂, 25K, g) 6.8, 6.6, 5.9, 4.7, 4.3, 3.25, 1.98. At 15K, g = 4.7, 4.3, 3.25 signals increase and those signal was saturated easily by strong power. Mössbauer (125K, vs Fe foil at room temperature with ⁵⁷Co in Rh matrix) δ = 0.077 mm/s and ΔE_Q = 0.368 mm/s.

$(\text{Cl}_4\text{-cat})_2\text{Mo}_2\text{Fe}_2\text{S}_4(\text{PEt}_3)_4$ (V) was isolated from the MeCN eluent after the mixture was eluted by hexanes/ CH_2Cl_2 eluents. The solvent removal under vacuum left black powder. (200mg, 0.14mmol, 28% yield) Analysis, Cald. $[\text{M}\cdot\text{MeCN}]$ MW. 1437.26. C, 31.76; H, 4.42; N, 0.97. Obsd. C, 31.27; H, 4.95; N, 0.89. Mössbauer (Boronic acid, 125K) $\delta = 0.398$ mm/s, $\Delta E_Q = 0.934$ mm/s. The oxidation state of metal atoms in the $(\text{Cl}_4\text{-cat})_2\text{Mo}_2\text{Fe}_2\text{S}_4(\text{PEt}_3)_4$ (V) cluster was also assigned as $\text{Mo}^{\text{IV}}_2\text{Fe}^{\text{II}}_2$ based on the Mössbauer measurement.

Table 1. Crystal data and structure refinement for III.

Empirical formula	C52 H84 Cl13 Fe7 Mo2 N O11 P5 S8
Formula weight	2354.21
Temperature	158(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/m
Unit cell dimensions	a = 11.2718(19) Å alpha = 90 deg. b = 23.256(4) Å beta = 98.109(3) deg. c = 17.637(3) Å gamma = 90 deg.
Volume	4577.1(13) Å ³
Z, Calculated density	2, 1.708 Mg/m ³
Absorption coefficient	2.035 mm ⁻¹
F(000)	2362
Crystal size	0.32 x 0.18 x 0.04 mm
Theta range for data collection	1.17 to 23.33 deg.
Limiting indices	-12<=h<=12, -25<=k<=25, -19<=l<=19
Reflections collected / unique	34704 / 6817 [R(int) = 0.0697]
Completeness to theta = 23.33	99.8 %
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6817 / 30 / 478
Goodness-of-fit on F ²	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0650, wR2 = 0.1851
R indices (all data)	R1 = 0.1055, wR2 = 0.2090
Largest diff. peak and hole	0.964 and -0.850 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **III**.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mo(1)	2007(1)	6902(1)	3082(1)	46(1)
Fe(1)	3558(2)	7500	2352(1)	54(1)
Fe(2)	1227(2)	7500	1821(1)	48(1)
Fe(3)	1570(2)	7500	4912(1)	61(1)
Fe(4)	337(2)	7500	-438(1)	69(1)
Fe(5)	-1574(1)	6741(1)	626(1)	67(1)
Fe(6)	-2346(2)	7500	-759(1)	83(1)
S(1)	3589(3)	7500	3628(2)	56(1)
S(2)	2465(2)	6748(1)	1843(1)	55(1)
S(3)	308(3)	7500	2848(2)	47(1)
S(4)	-2976(3)	7500	400(3)	81(1)
S(5)	-1101(3)	6750(1)	-637(2)	78(1)
S(6)	-212(3)	7500	786(2)	53(1)
Cl(1)	-1044(3)	5301(1)	2717(2)	99(1)
Cl(2)	-2097(3)	4988(1)	4231(2)	116(1)
Cl(3)	-1132(3)	5628(2)	5753(2)	109(1)
Cl(4)	945(3)	6523(1)	5762(2)	85(1)
Cl(5)	5393(3)	7500	2089(2)	80(1)
Cl(6)	3399(4)	7500	5662(2)	91(1)
Cl(7)	-3691(7)	7500	-1802(4)	168(3)
P(1)	3475(3)	6062(1)	3483(2)	84(1)
P(2)	632(5)	7500	-1680(3)	98(2)
P(3)	-2984(4)	6056(2)	313(2)	115(1)
O(1)	769(5)	6222(2)	2935(3)	52(2)
O(2)	1560(5)	6779(2)	4214(3)	53(2)
O(3)	-2080(6)	6739(4)	2203(5)	87(2)
O(4)	311(8)	5882(4)	962(5)	104(3)
O(5)	2060(8)	6565(5)	-103(5)	109(3)
C(1)	307(9)	6084(4)	3541(6)	57(2)
C(2)	-565(9)	5657(4)	3555(6)	68(3)
C(3)	-1031(10)	5513(4)	4240(7)	77(3)
C(4)	-558(11)	5779(5)	4903(7)	75(3)
C(5)	324(9)	6212(4)	4920(6)	64(3)
C(6)	733(8)	6358(4)	4237(6)	55(2)
C(7)	2892(14)	5355(6)	3206(11)	133(6)
C(8)	2550(15)	5244(6)	2377(9)	129(6)
C(9)	3980(20)	6046(10)	4580(14)	209(15)
C(10)	4420(30)	5657(15)	4829(16)	320(20)
C(11)	4922(11)	6088(6)	3103(9)	110(5)
C(12A)	5920(20)	6419(11)	3649(14)	97(8)
C(12B)	5690(30)	5630(13)	3143(17)	112(9)
C(13)	20(20)	6915(8)	-2245(8)	164(8)
C(14)	626(19)	6328(8)	-2065(10)	170(8)
C(15)	2248(17)	7500	-1745(10)	121(7)
C(16)	2640(30)	7500	-2544(13)	201(14)
C(17)	-4470(20)	6219(13)	864(15)	148(10)
C(18)	-3970(30)	6214(14)	-695(13)	171(12)

C(19)	-2420 (40)	5232 (10)	330 (20)	226 (17)
C(17')	-4730 (20)	6290 (30)	80 (30)	140 (20)
C(18')	-2680 (30)	5610 (14)	-619 (15)	92 (13)
C(19')	-2550 (40)	5363 (15)	990 (20)	114 (16)
C(20)	-4900 (40)	5724 (17)	990 (30)	280 (20)
C(20')	-5090 (50)	6590 (20)	-520 (30)	128 (19)
C(21)	-4270 (100)	5840 (40)	-230 (60)	620 (80)
C(21')	-1930 (20)	5248 (11)	-279 (16)	213 (10)
C(22')	-3390 (40)	4980 (20)	910 (30)	132 (19)
C(23)	-1893 (9)	6738 (5)	1570 (8)	78 (3)
C(24)	-440 (11)	6215 (5)	829 (6)	76 (3)
C(25)	1372 (11)	6956 (6)	-255 (6)	87 (4)
O(6)	-253 (10)	7500	4671 (6)	68 (3)
C(26)	-1120 (20)	7500	4970 (12)	107 (6)
N(1)	-2140 (19)	7500	4737 (11)	169 (10)
C(27)	-3200 (20)	7500	5190 (20)	248 (19)
C(28)	-2460 (30)	7081 (12)	3955 (16)	120 (10)
Cl(11)	3524 (6)	3753 (3)	3292 (5)	244 (4)
Cl(12)	5775 (10)	4086 (4)	2856 (6)	319 (5)
C(41)	4948 (16)	3493 (9)	3034 (12)	175 (8)

Table 3. Bond lengths [Å] and angles [deg] for **III**.

Mo(1)-O(1)	2.100(6)	P(1)-C(9)	1.94(3)
Mo(1)-O(2)	2.146(5)	P(2)-C(13)	1.768(16)
Mo(1)-S(2)	2.342(2)	P(2)-C(13)#1	1.768(16)
Mo(1)-S(3)	2.356(3)	P(2)-C(15)	1.842(19)
Mo(1)-S(1)	2.358(3)	P(3)-C(21)	1.70(11)
Mo(1)-P(1)	2.593(3)	P(3)-C(18)	1.99(2)
Mo(1)-Fe(2)	2.6648(17)	P(3)-C(17')	2.02(2)
Mo(1)-Fe(1)	2.6990(17)	P(3)-C(18')	2.02(2)
Mo(1)-Mo(1)#1	2.7825(16)	P(3)-C(19)	2.02(2)
Fe(1)-Cl(5)	2.183(4)	P(3)-C(19')	2.03(2)
Fe(1)-S(1)	2.246(4)	P(3)-C(17)	2.090(19)
Fe(1)-S(2)	2.252(3)	O(1)-C(1)	1.294(11)
Fe(1)-S(2)#1	2.252(3)	O(2)-C(6)	1.357(10)
Fe(1)-Fe(2)	2.662(3)	O(3)-C(23)	1.165(13)
Fe(1)-Mo(1)#1	2.6990(17)	O(4)-C(24)	1.146(13)
Fe(2)-S(3)	2.209(3)	O(5)-C(25)	1.200(14)
Fe(2)-S(2)	2.235(3)	C(1)-C(2)	1.400(13)
Fe(2)-S(2)#1	2.235(3)	C(1)-C(6)	1.406(13)
Fe(2)-S(6)	2.265(4)	C(2)-C(3)	1.422(14)
Fe(2)-Mo(1)#1	2.6648(17)	C(3)-C(4)	1.363(15)
Fe(3)-O(6)	2.039(11)	C(4)-C(5)	1.412(15)
Fe(3)-O(2)	2.079(6)	C(5)-C(6)	1.391(13)
Fe(3)-O(2)#1	2.079(6)	C(7)-C(8)	1.480(19)
Fe(3)-Cl(6)	2.288(5)	C(9)-C(10)	1.09(4)
Fe(4)-C(25)	1.721(14)	C(11)-C(12B)	1.37(3)
Fe(4)-C(25)#1	1.721(14)	C(11)-C(12A)	1.57(3)
Fe(4)-P(2)	2.261(5)	C(12A)-C(12B)	2.04(4)
Fe(4)-S(6)	2.328(4)	C(13)-C(14)	1.54(2)
Fe(4)-S(5)	2.373(3)	C(15)-C(16)	1.54(3)
Fe(4)-S(5)#1	2.373(3)	C(17)-C(20)	1.28(3)
Fe(4)-Fe(6)	2.998(3)	C(17)-C(17')	1.38(5)
Fe(4)-Fe(5)	3.524(2)	C(18)-C(21)	1.27(3)
Fe(5)-C(23)	1.752(13)	C(18)-C(17')	1.72(6)
Fe(5)-C(24)	1.770(14)	C(18)-C(20')	1.59(6)
Fe(5)-P(3)	2.262(4)	C(18)-C(18')	2.01(4)
Fe(5)-S(6)	2.330(3)	C(19)-C(19')	1.23(5)
Fe(5)-S(5)	2.363(3)	C(19)-C(21')	1.28(3)
Fe(5)-S(4)	2.365(3)	C(19)-C(22')	1.71(6)
Fe(5)-Fe(6)	3.040(2)	C(19)-C(18')	1.88(5)
Fe(5)-Fe(5)#1	3.530(3)	C(17')-C(20')	1.28(3)
Fe(6)-Cl(7)	2.212(5)	C(17')-C(21)	1.33(12)
Fe(6)-S(5)	2.231(4)	C(18')-C(21')	1.28(3)
Fe(6)-S(5)#1	2.231(3)	C(19')-C(22')	1.29(3)
Fe(6)-S(4)	2.257(5)	O(6)-C(26)	1.17(2)
S(1)-Mo(1)#1	2.358(3)	C(26)-N(1)	1.17(2)
S(3)-Mo(1)#1	2.356(3)	N(1)-C(27)	1.53(3)
S(4)-Fe(5)#1	2.365(3)	N(1)-C(28)	1.68(3)
S(6)-Fe(5)#1	2.330(3)	N(1)-C(28)#1	1.68(3)
Cl(1)-C(2)	1.713(11)	Cl(11)-C(41)	1.831(18)
Cl(2)-C(3)	1.712(11)	Cl(12)-C(41)	1.72(2)
Cl(3)-C(4)	1.750(10)		
Cl(4)-C(5)	1.710(11)	O(1)-Mo(1)-O(2)	77.0(2)
P(1)-C(7)	1.812(16)	O(1)-Mo(1)-S(2)	89.99(17)
P(1)-C(11)	1.849(12)	O(2)-Mo(1)-S(2)	163.53(17)

O(1)-Mo(1)-S(3)	85.02(17)	S(3)-Fe(2)-S(6)	107.20(14)
O(2)-Mo(1)-S(3)	87.14(17)	S(2)-Fe(2)-S(6)	112.85(9)
S(2)-Mo(1)-S(3)	101.96(10)	S(2)#1-Fe(2)-S(6)	112.85(9)
O(1)-Mo(1)-S(1)	161.01(18)	S(3)-Fe(2)-Fe(1)	105.42(11)
O(2)-Mo(1)-S(1)	87.82(18)	S(2)-Fe(2)-Fe(1)	53.90(7)
S(2)-Mo(1)-S(1)	102.58(11)	S(2)#1-Fe(2)-Fe(1)	53.90(7)
S(3)-Mo(1)-S(1)	105.83(8)	S(6)-Fe(2)-Fe(1)	147.38(12)
O(1)-Mo(1)-P(1)	81.59(18)	S(3)-Fe(2)-Mo(1)#1	56.91(8)
O(2)-Mo(1)-P(1)	82.56(17)	S(2)-Fe(2)-Mo(1)#1	105.21(9)
S(2)-Mo(1)-P(1)	85.58(10)	S(2)#1-Fe(2)-Mo(1)#1	56.29(7)
S(3)-Mo(1)-P(1)	164.64(10)	S(6)-Fe(2)-Mo(1)#1	141.94(7)
S(1)-Mo(1)-P(1)	85.20(10)	Fe(1)-Fe(2)-Mo(1)#1	60.89(5)
O(1)-Mo(1)-Fe(2)	98.90(17)	S(3)-Fe(2)-Mo(1)	56.91(7)
O(2)-Mo(1)-Fe(2)	138.82(16)	S(2)-Fe(2)-Mo(1)	56.29(7)
S(2)-Mo(1)-Fe(2)	52.54(7)	S(2)#1-Fe(2)-Mo(1)	105.21(9)
S(3)-Mo(1)-Fe(2)	51.75(8)	S(6)-Fe(2)-Mo(1)	141.94(7)
S(1)-Mo(1)-Fe(2)	100.05(8)	Fe(1)-Fe(2)-Mo(1)	60.89(5)
P(1)-Mo(1)-Fe(2)	138.04(9)	Mo(1)#1-Fe(2)-Mo(1)	62.94(5)
O(1)-Mo(1)-Fe(1)	142.45(16)	O(6)-Fe(3)-O(2)	87.5(2)
O(2)-Mo(1)-Fe(1)	139.95(17)	O(6)-Fe(3)-O(2)#1	87.5(2)
S(2)-Mo(1)-Fe(1)	52.48(7)	O(2)-Fe(3)-O(2)#1	107.6(3)
S(3)-Mo(1)-Fe(1)	100.20(7)	O(6)-Fe(3)-Cl(6)	156.9(3)
S(1)-Mo(1)-Fe(1)	52.22(9)	O(2)-Fe(3)-Cl(6)	105.77(19)
P(1)-Mo(1)-Fe(1)	95.00(8)	O(2)#1-Fe(3)-Cl(6)	105.77(19)
Fe(2)-Mo(1)-Fe(1)	59.50(6)	C(25)-Fe(4)-C(25)#1	94.8(9)
O(1)-Mo(1)-Mo(1)#1	138.82(16)	C(25)-Fe(4)-P(2)	89.6(4)
O(2)-Mo(1)-Mo(1)#1	97.66(16)	C(25)#1-Fe(4)-P(2)	89.6(4)
S(2)-Mo(1)-Mo(1)#1	98.80(6)	C(25)-Fe(4)-S(6)	95.0(4)
S(3)-Mo(1)-Mo(1)#1	53.81(5)	C(25)#1-Fe(4)-S(6)	95.0(4)
S(1)-Mo(1)-Mo(1)#1	53.84(5)	P(2)-Fe(4)-S(6)	173.11(18)
P(1)-Mo(1)-Mo(1)#1	138.89(8)	C(25)-Fe(4)-S(5)	85.3(4)
Fe(2)-Mo(1)-Mo(1)#1	58.53(3)	C(25)#1-Fe(4)-S(5)	177.7(4)
Fe(1)-Mo(1)-Mo(1)#1	58.97(3)	P(2)-Fe(4)-S(5)	92.71(13)
Cl(5)-Fe(1)-S(1)	109.35(17)	S(6)-Fe(4)-S(5)	82.64(10)
Cl(5)-Fe(1)-S(2)	113.39(10)	C(25)-Fe(4)-S(5)#1	177.7(4)
S(1)-Fe(1)-S(2)	109.25(10)	C(25)#1-Fe(4)-S(5)#1	85.3(4)
Cl(5)-Fe(1)-S(2)#1	113.39(10)	P(2)-Fe(4)-S(5)#1	92.71(13)
S(1)-Fe(1)-S(2)#1	109.25(10)	S(6)-Fe(4)-S(5)#1	82.64(10)
S(2)-Fe(1)-S(2)#1	101.96(15)	S(5)-Fe(4)-S(5)#1	94.62(17)
Cl(5)-Fe(1)-Fe(2)	147.49(15)	C(25)-Fe(4)-Fe(6)	132.4(4)
S(1)-Fe(1)-Fe(2)	103.16(11)	C(25)#1-Fe(4)-Fe(6)	132.4(4)
S(2)-Fe(1)-Fe(2)	53.32(7)	P(2)-Fe(4)-Fe(6)	95.70(15)
S(2)#1-Fe(1)-Fe(2)	53.32(7)	S(6)-Fe(4)-Fe(6)	77.41(11)
Cl(5)-Fe(1)-Mo(1)	142.97(8)	S(5)-Fe(4)-Fe(6)	47.33(9)
S(1)-Fe(1)-Mo(1)	56.06(8)	S(5)#1-Fe(4)-Fe(6)	47.33(9)
S(2)-Fe(1)-Mo(1)	55.59(7)	C(25)-Fe(4)-Fe(5)	88.9(4)
S(2)#1-Fe(1)-Mo(1)	103.64(9)	C(25)#1-Fe(4)-Fe(5)	135.8(4)
Fe(2)-Fe(1)-Mo(1)	59.61(5)	P(2)-Fe(4)-Fe(5)	134.45(11)
Cl(5)-Fe(1)-Mo(1)#1	142.97(8)	S(6)-Fe(4)-Fe(5)	40.86(6)
S(1)-Fe(1)-Mo(1)#1	56.06(8)	S(5)-Fe(4)-Fe(5)	41.81(8)
S(2)-Fe(1)-Mo(1)#1	103.64(9)	S(5)#1-Fe(4)-Fe(5)	89.48(10)
S(2)#1-Fe(1)-Mo(1)#1	55.59(7)	Fe(6)-Fe(4)-Fe(5)	54.85(5)
Fe(2)-Fe(1)-Mo(1)#1	59.61(5)	C(23)-Fe(5)-C(24)	92.5(5)
Mo(1)-Fe(1)-Mo(1)#1	62.06(5)	C(23)-Fe(5)-P(3)	89.9(4)
S(3)-Fe(2)-S(2)	110.47(9)	C(24)-Fe(5)-P(3)	91.4(4)
S(3)-Fe(2)-S(2)#1	110.47(9)	C(23)-Fe(5)-S(6)	96.2(4)
S(2)-Fe(2)-S(2)#1	103.03(14)	C(24)-Fe(5)-S(6)	93.1(4)

P(3)-Fe(5)-S(6)	172.25(14)	Fe(5)#1-S(4)-Fe(5)	96.55(15)
C(23)-Fe(5)-S(5)	178.8(4)	Fe(6)-S(5)-Fe(5)	82.81(12)
C(24)-Fe(5)-S(5)	86.8(4)	Fe(6)-S(5)-Fe(4)	81.19(12)
P(3)-Fe(5)-S(5)	91.19(14)	Fe(5)-S(5)-Fe(4)	96.16(11)
S(6)-Fe(5)-S(5)	82.81(11)	Fe(2)-S(6)-Fe(4)	119.61(15)
C(23)-Fe(5)-S(4)	86.6(4)	Fe(2)-S(6)-Fe(5)	118.82(10)
C(24)-Fe(5)-S(4)	175.3(3)	Fe(4)-S(6)-Fe(5)	98.32(11)
P(3)-Fe(5)-S(4)	93.15(15)	Fe(2)-S(6)-Fe(5)#1	118.82(10)
S(6)-Fe(5)-S(4)	82.43(11)	Fe(4)-S(6)-Fe(5)#1	98.32(11)
S(5)-Fe(5)-S(4)	93.95(14)	Fe(5)-S(6)-Fe(5)#1	98.48(14)
C(23)-Fe(5)-Fe(6)	133.8(4)	C(7)-P(1)-C(11)	103.7(7)
C(24)-Fe(5)-Fe(6)	132.9(4)	C(7)-P(1)-C(9)	107.2(10)
P(3)-Fe(5)-Fe(6)	95.82(11)	C(11)-P(1)-C(9)	102.2(9)
S(6)-Fe(5)-Fe(6)	76.50(9)	C(7)-P(1)-Mo(1)	114.6(5)
S(5)-Fe(5)-Fe(6)	46.72(9)	C(11)-P(1)-Mo(1)	115.9(5)
S(4)-Fe(5)-Fe(6)	47.35(11)	C(9)-P(1)-Mo(1)	111.9(5)
C(23)-Fe(5)-Fe(4)	137.0(4)	C(13)-P(2)-C(13)#1	100.7(13)
C(24)-Fe(5)-Fe(4)	88.6(4)	C(13)-P(2)-C(15)	105.9(9)
P(3)-Fe(5)-Fe(4)	133.15(13)	C(13)#1-P(2)-C(15)	105.9(9)
S(6)-Fe(5)-Fe(4)	40.82(8)	C(13)-P(2)-Fe(4)	116.6(6)
S(5)-Fe(5)-Fe(4)	42.03(8)	C(13)#1-P(2)-Fe(4)	116.6(6)
S(4)-Fe(5)-Fe(4)	88.88(10)	C(15)-P(2)-Fe(4)	110.0(6)
Fe(6)-Fe(5)-Fe(4)	53.73(6)	C(21)-P(3)-C(18)	39.3(11)
C(23)-Fe(5)-Fe(5)#1	90.2(4)	C(21)-P(3)-C(17')	41(4)
C(24)-Fe(5)-Fe(5)#1	133.7(3)	C(18)-P(3)-C(17')	50.7(19)
P(3)-Fe(5)-Fe(5)#1	134.75(12)	C(21)-P(3)-C(18')	67(4)
S(6)-Fe(5)-Fe(5)#1	40.76(7)	C(18)-P(3)-C(18')	60.3(13)
S(5)-Fe(5)-Fe(5)#1	89.50(8)	C(17')-P(3)-C(18')	104(2)
S(4)-Fe(5)-Fe(5)#1	41.72(8)	C(21)-P(3)-C(19)	88(3)
Fe(6)-Fe(5)-Fe(5)#1	54.51(4)	C(18)-P(3)-C(19)	108.9(15)
Fe(4)-Fe(5)-Fe(5)#1	59.95(3)	C(17')-P(3)-C(19)	124(2)
Cl(7)-Fe(6)-S(5)	115.36(15)	C(18')-P(3)-C(19)	55.5(16)
Cl(7)-Fe(6)-S(5)#1	115.36(15)	C(21)-P(3)-C(19')	102(2)
S(5)-Fe(6)-S(5)#1	102.89(18)	C(18)-P(3)-C(19')	137.0(16)
Cl(7)-Fe(6)-S(4)	119.2(3)	C(17')-P(3)-C(19')	119(2)
S(5)-Fe(6)-S(4)	100.76(12)	C(18')-P(3)-C(19')	91.0(18)
S(5)#1-Fe(6)-S(4)	100.76(12)	C(19)-P(3)-C(19')	35.5(15)
Cl(7)-Fe(6)-Fe(4)	135.4(3)	C(21)-P(3)-C(17)	69(4)
S(5)-Fe(6)-Fe(4)	51.47(9)	C(18)-P(3)-C(17)	89.9(13)
S(5)#1-Fe(6)-Fe(4)	51.47(9)	C(17')-P(3)-C(17)	39.2(15)
S(4)-Fe(6)-Fe(4)	105.46(13)	C(18')-P(3)-C(17)	135.5(14)
Cl(7)-Fe(6)-Fe(5)	138.86(13)	C(19)-P(3)-C(17)	116.0(14)
S(5)-Fe(6)-Fe(5)	50.47(9)	C(19')-P(3)-C(17)	90.8(17)
S(5)#1-Fe(6)-Fe(5)	105.76(11)	C(21)-P(3)-Fe(5)	150(2)
S(4)-Fe(6)-Fe(5)	50.42(8)	C(18)-P(3)-Fe(5)	111.8(10)
Fe(4)-Fe(6)-Fe(5)	71.42(6)	C(17')-P(3)-Fe(5)	119.3(18)
Fe(1)-S(1)-Mo(1)	71.72(10)	C(18')-P(3)-Fe(5)	111.5(12)
Fe(1)-S(1)-Mo(1)#1	71.72(10)	C(19)-P(3)-Fe(5)	117.0(12)
Mo(1)-S(1)-Mo(1)#1	72.31(10)	C(19')-P(3)-Fe(5)	108.3(13)
Fe(2)-S(2)-Fe(1)	72.78(9)	C(17)-P(3)-Fe(5)	110.0(8)
Fe(2)-S(2)-Mo(1)	71.17(8)	C(1)-O(1)-Mo(1)	115.0(6)
Fe(1)-S(2)-Mo(1)	71.93(9)	C(6)-O(2)-Fe(3)	120.7(5)
Fe(2)-S(3)-Mo(1)#1	71.34(9)	C(6)-O(2)-Mo(1)	112.1(5)
Fe(2)-S(3)-Mo(1)	71.34(9)	Fe(3)-O(2)-Mo(1)	117.4(3)
Mo(1)#1-S(3)-Mo(1)	72.37(10)	O(1)-C(1)-C(2)	123.8(9)
Fe(6)-S(4)-Fe(5)#1	82.23(13)	O(1)-C(1)-C(6)	118.8(8)
Fe(6)-S(4)-Fe(5)	82.23(13)	C(2)-C(1)-C(6)	117.4(9)

C(1)-C(2)-C(3)	121.7(10)	C(22')-C(19)-C(18')	131(3)
C(1)-C(2)-Cl(1)	117.6(8)	C(19')-C(19)-P(3)	72.6(12)
C(3)-C(2)-Cl(1)	120.7(8)	C(21')-C(19)-P(3)	98(2)
C(4)-C(3)-C(2)	118.4(10)	C(22')-C(19)-P(3)	96(2)
C(4)-C(3)-Cl(2)	121.4(9)	C(18')-C(19)-P(3)	62.1(10)
C(2)-C(3)-Cl(2)	120.1(10)	C(20')-C(17')-C(21)	100(6)
C(3)-C(4)-C(5)	122.1(9)	C(20')-C(17')-C(17)	152(6)
C(3)-C(4)-Cl(3)	119.8(9)	C(21)-C(17')-C(17)	107(5)
C(5)-C(4)-Cl(3)	117.9(10)	C(20')-C(17')-C(18)	62(4)
C(6)-C(5)-C(4)	118.2(10)	C(21)-C(17')-C(18)	47(2)
C(6)-C(5)-Cl(4)	120.2(8)	C(17)-C(17')-C(18)	136.8(14)
C(4)-C(5)-Cl(4)	121.4(8)	C(20')-C(17')-P(3)	120(4)
O(2)-C(6)-C(5)	121.0(9)	C(21)-C(17')-P(3)	56(5)
O(2)-C(6)-C(1)	116.9(8)	C(17)-C(17')-P(3)	73.1(12)
C(5)-C(6)-C(1)	122.1(9)	C(18)-C(17')-P(3)	63.8(11)
C(8)-C(7)-P(1)	117.3(12)	C(21')-C(18')-C(19)	42.7(15)
C(10)-C(9)-P(1)	118(3)	C(21')-C(18')-P(3)	98(2)
C(12B)-C(11)-C(12A)	87.4(17)	C(19)-C(18')-P(3)	62.4(10)
C(12B)-C(11)-P(1)	122.8(16)	C(21')-C(18')-C(18)	156(2)
C(12A)-C(11)-P(1)	112.6(13)	C(19)-C(18')-C(18)	114.0(15)
C(11)-C(12A)-C(12B)	42.2(11)	P(3)-C(18')-C(18)	59.3(8)
C(11)-C(12B)-C(12A)	50.4(13)	C(19)-C(19')-C(22')	85(4)
C(14)-C(13)-P(2)	116.2(14)	C(19)-C(19')-P(3)	72.0(11)
C(16)-C(15)-P(2)	118.4(16)	C(22')-C(19')-P(3)	111(3)
C(20)-C(17)-C(17')	104(4)	C(17')-C(20')-C(18)	73(4)
C(20)-C(17)-P(3)	105(3)	C(18)-C(21)-C(17')	83(6)
C(17')-C(17)-P(3)	67.8(10)	C(18)-C(21)-P(3)	83(5)
C(21)-C(18)-C(17')	50(5)	C(17')-C(21)-P(3)	83(6)
C(21)-C(18)-C(20')	88(6)	C(19)-C(21')-C(18')	95(3)
C(17')-C(18)-C(20')	45.3(15)	C(19')-C(22')-C(19)	46(3)
C(21)-C(18)-P(3)	58(5)	O(3)-C(23)-Fe(5)	178.6(10)
C(17')-C(18)-P(3)	65.5(11)	O(4)-C(24)-Fe(5)	178.7(11)
C(20')-C(18)-P(3)	106(2)	O(5)-C(25)-Fe(4)	176.9(11)
C(21)-C(18)-C(18')	74(6)	C(26)-O(6)-Fe(3)	141.6(14)
C(17')-C(18)-C(18')	116.9(19)	N(1)-C(26)-O(6)	133(2)
C(20')-C(18)-C(18')	162(3)	C(26)-N(1)-C(27)	128(3)
P(3)-C(18)-C(18')	60.4(8)	C(26)-N(1)-C(28)	111.8(17)
C(19')-C(19)-C(21')	156(5)	C(27)-N(1)-C(28)	109.8(19)
C(19')-C(19)-C(22')	49(2)	C(26)-N(1)-C(28)#1	111.8(17)
C(21')-C(19)-C(22')	155(4)	C(27)-N(1)-C(28)#1	109.8(19)
C(19')-C(19)-C(18')	134.6(15)	C(28)-N(1)-C(28)#1	71(2)
C(21')-C(19)-C(18')	42.8(15)	Cl(12)-C(41)-Cl(11)	107.3(11)

Symmetry transformations used to generate equivalent atoms: #1 x, -y+3/2, z

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for III. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Mo(1)	46(1)	44(1)	50(1)	1(1)	12(1)	2(1)
Fe(1)	43(1)	59(1)	62(1)	0	17(1)	0
Fe(2)	46(1)	54(1)	45(1)	0	10(1)	0
Fe(3)	72(1)	60(1)	51(1)	0	11(1)	0
Fe(4)	65(1)	93(2)	51(1)	0	12(1)	0
Fe(5)	60(1)	71(1)	68(1)	-2(1)	1(1)	-12(1)
Fe(6)	74(2)	101(2)	68(2)	0	-10(1)	0
S(1)	47(2)	55(2)	65(2)	0	7(2)	0
S(2)	52(1)	56(2)	59(2)	-7(1)	18(1)	3(1)
S(3)	48(2)	47(2)	48(2)	0	11(1)	0
S(4)	52(2)	100(3)	89(3)	0	6(2)	0
S(5)	83(2)	89(2)	60(2)	-12(2)	2(1)	-7(2)
S(6)	47(2)	66(2)	47(2)	0	7(2)	0
Cl(1)	108(2)	69(2)	124(3)	-22(2)	35(2)	-39(2)
Cl(2)	109(3)	75(2)	178(4)	14(2)	66(3)	-29(2)
Cl(3)	124(3)	97(2)	121(3)	40(2)	73(2)	3(2)
Cl(4)	121(2)	80(2)	57(2)	15(1)	26(2)	3(2)
Cl(5)	50(2)	89(3)	108(3)	0	33(2)	0
Cl(6)	99(3)	90(3)	75(3)	0	-13(2)	0
Cl(7)	169(6)	178(6)	126(5)	0	-79(4)	0
P(1)	74(2)	64(2)	120(3)	22(2)	28(2)	24(2)
P(2)	96(4)	141(5)	61(3)	0	21(2)	0
P(3)	107(3)	107(3)	117(3)	12(2)	-26(2)	-54(2)
O(1)	62(4)	46(4)	51(4)	-2(3)	19(3)	-6(3)
O(2)	59(4)	52(4)	49(4)	7(3)	16(3)	-1(3)
O(3)	56(5)	126(7)	82(6)	23(5)	15(4)	10(4)
O(4)	104(7)	72(6)	127(8)	-14(5)	-19(6)	13(5)
O(5)	105(7)	148(9)	73(5)	-15(5)	15(5)	50(7)
C(1)	58(6)	47(6)	67(7)	-1(5)	14(5)	2(5)
C(2)	75(7)	44(6)	89(8)	2(5)	28(6)	-7(5)
C(3)	83(8)	52(7)	104(10)	16(6)	39(7)	-14(6)
C(4)	90(8)	58(7)	88(8)	29(6)	45(7)	18(7)
C(5)	74(7)	45(6)	76(7)	19(5)	28(6)	7(5)
C(6)	56(6)	42(6)	70(7)	12(5)	21(5)	11(5)
C(7)	122(13)	76(10)	211(19)	25(11)	66(13)	27(9)
C(8)	181(17)	79(10)	132(14)	-8(10)	30(12)	41(10)
C(9)	240(20)	210(20)	200(20)	154(19)	142(18)	180(20)
C(10)	340(50)	430(60)	200(30)	0(40)	90(30)	-230(50)
C(11)	68(8)	92(10)	181(15)	-18(9)	53(9)	6(7)
C(13)	260(20)	149(16)	69(10)	-25(10)	20(12)	-41(16)
C(14)	270(30)	144(17)	132(15)	-44(13)	91(16)	-10(17)
C(15)	113(16)	180(20)	70(12)	0	36(11)	0
C(16)	230(30)	260(40)	110(20)	0	50(20)	0
C(23)	42(6)	96(9)	98(9)	12(7)	17(6)	-15(6)
C(24)	86(9)	57(7)	79(8)	-14(6)	-9(6)	-16(6)
C(25)	85(9)	126(11)	54(7)	-23(7)	28(6)	9(8)
O(6)	76(7)	57(6)	81(7)	0	48(6)	0
C(26)	130(20)	101(15)	81(14)	0	8(15)	0

N(1)	87(14)	320(30)	101(15)	0	27(11)	0
C(27)	120(20)	350(50)	310(40)	0	150(30)	0
Cl(11)	195(6)	151(5)	367(10)	-41(6)	-17(6)	54(5)
Cl(12)	405(15)	227(9)	336(12)	-57(8)	106(10)	-109(10)
C(41)	144(17)	140(17)	230(20)	-29(15)	-15(15)	57(14)

Table 1. Crystal data and structure refinement for IV.

Empirical formula	C ₂₄ H ₄₅ Cl Fe ₄ O ₆ P ₃ S ₄
Formula weight	909.60
Temperature	158(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 32.992(6) Å alpha = 90 deg. b = 12.609(2) Å beta = 110.069(3) deg. c = 39.048(7) Å gamma = 90 deg.
Volume	15257(5) Å ³
Z, Calculated density	16, 1.584 Mg/m ³
Absorption coefficient	1.940 mm ⁻¹
F(000)	7472
Crystal size	0.36 x 0.22 x 0.16 mm
Theta range for data collection	0.66 to 26.43 deg.
Limiting indices	-41<=h<=41, -15<=k<=15, -48<=l<=48
Reflections collected / unique	184935 / 31295 [R(int) = 0.0587]
Completeness to theta = 26.43	99.7 %
Refinement method	Full-matrix-block least-squares on F ²
Data / restraints / parameters	31295 / 0 / 1513
Goodness-of-fit on F ²	1.125
Final R indices [I>2sigma(I)]	R1 = 0.0611, wR2 = 0.1195
R indices (all data)	R1 = 0.0909, wR2 = 0.1285
Largest diff. peak and hole	0.851 and -0.914 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for IV. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	1088(1)	4756(1)	2640(1)	18(1)
Fe(2)	530(1)	2358(1)	2405(1)	19(1)
Fe(3)	492(1)	4195(1)	1730(1)	19(1)
Fe(4)	1290(1)	3024(1)	2198(1)	19(1)
Fe(5)	1419(1)	9962(1)	-109(1)	19(1)
Fe(6)	2011(1)	9411(1)	807(1)	21(1)
Fe(7)	1204(1)	8241(1)	332(1)	21(1)
Fe(8)	1986(1)	7589(1)	132(1)	20(1)
S(1)	654(1)	2358(1)	1838(1)	20(1)
S(2)	1197(1)	4759(1)	2071(1)	19(1)
S(3)	1234(1)	2926(1)	2751(1)	19(1)
S(4)	396(1)	4168(1)	2292(1)	19(1)
S(5)	1847(1)	7591(1)	688(1)	21(1)
S(6)	1275(1)	8132(1)	-219(1)	20(1)
S(7)	2109(1)	9402(1)	242(1)	20(1)
S(8)	1300(1)	9970(1)	460(1)	22(1)
Cl(1)	1899(1)	2344(1)	2165(1)	35(1)
Cl(2)	595(1)	7556(1)	365(1)	34(1)
P(1)	655(1)	4100(1)	1210(1)	24(1)
P(2)	739(1)	633(1)	2530(1)	24(1)
P(3)	1786(1)	5224(1)	2948(1)	23(1)
P(4)	1796(1)	5846(1)	38(1)	23(1)
P(5)	725(1)	10425(1)	-431(1)	24(1)
P(6)	1906(1)	9205(1)	1349(1)	26(1)
O(1)	290(2)	6451(3)	1633(1)	48(1)
O(2)	-416(1)	3606(4)	1402(1)	42(1)
O(3)	-356(1)	1780(4)	1969(1)	42(1)
O(4)	318(1)	2604(3)	3068(1)	40(1)
O(5)	812(1)	6944(3)	2466(1)	39(1)
O(6)	887(1)	4699(3)	3311(1)	39(1)
O(7)	2877(1)	7098(4)	578(1)	42(1)
O(8)	2189(1)	7735(3)	-535(1)	39(1)
O(9)	1641(1)	9893(3)	-770(1)	38(1)
O(10)	1710(1)	12142(3)	65(1)	39(1)
O(11)	2181(2)	11669(3)	940(1)	45(1)
O(12)	2939(1)	9023(4)	1119(1)	52(1)
C(1)	365(2)	5563(5)	1668(2)	31(1)
C(2)	-58(2)	3816(4)	1522(2)	28(1)
C(3)	-7(2)	2002(4)	2140(2)	26(1)
C(4)	406(2)	2489(4)	2813(2)	25(1)
C(5)	925(2)	6085(4)	2537(1)	26(1)
C(6)	966(2)	4723(4)	3051(2)	24(1)
C(7)	2527(2)	7276(4)	404(2)	26(1)
C(8)	2110(2)	7682(4)	-277(2)	25(1)
C(9)	1552(2)	9922(4)	-514(2)	25(1)
C(10)	1586(2)	11298(4)	-7(2)	26(1)
C(11)	2112(2)	10787(5)	884(2)	28(1)
C(12)	2571(2)	9125(5)	1007(2)	31(1)
C(25)	690(2)	5357(5)	987(2)	43(2)
C(26)	1080(2)	6042(5)	1204(2)	50(2)

C(27)	281(2)	3305(6)	844(2)	47(2)
C(28)	-141(2)	3876(7)	629(2)	65(2)
C(29)	1179(2)	3469(5)	1280(2)	35(1)
C(30)	1323(2)	3404(6)	953(2)	51(2)
C(31)	762(2)	179(5)	2984(2)	36(1)
C(32)	1111(2)	693(5)	3305(2)	46(2)
C(33)	1277(2)	347(4)	2516(2)	39(2)
C(34)	1441(2)	-791(5)	2614(2)	55(2)
C(35)	393(2)	-385(4)	2239(2)	31(1)
C(36)	388(2)	-427(5)	1850(2)	49(2)
C(37)	1830(2)	6354(5)	3251(2)	40(2)
C(38)	2286(2)	6786(5)	3443(2)	50(2)
C(39)	2132(2)	4199(5)	3237(2)	33(1)
C(40)	2007(2)	3816(5)	3557(2)	39(2)
C(41)	2110(2)	5611(4)	2670(2)	29(1)
C(42)	1965(2)	6646(5)	2460(2)	35(1)
C(43)	1272(2)	5549(4)	88(2)	30(1)
C(44)	1107(2)	4424(5)	3(2)	46(2)
C(45)	2171(2)	4877(4)	333(2)	31(1)
C(46)	2253(2)	4956(5)	737(2)	36(1)
C(47)	1754(2)	5330(5)	-409(2)	34(1)
C(48)	1394(2)	5797(5)	-731(2)	43(2)
C(49)	388(2)	10810(5)	-158(2)	45(2)
C(50)	525(2)	11858(6)	48(2)	55(2)
C(51)	380(2)	9406(5)	-717(2)	45(2)
C(52)	515(2)	9049(6)	-1045(2)	50(2)
C(53)	695(2)	11535(6)	-726(2)	57(2)
C(54)	242(3)	11963(7)	-937(2)	77(3)
C(55)	1354(2)	9355(5)	1346(2)	42(2)
C(56)	1199(2)	10485(5)	1319(2)	46(2)
C(57)	2047(2)	7890(5)	1562(2)	37(2)
C(58)	2519(2)	7582(5)	1652(2)	54(2)
C(59)	2239(2)	10094(5)	1709(2)	36(1)
C(60)	2260(2)	9838(5)	2098(2)	42(2)
Fe(9)	4466(1)	5283(1)	3291(1)	20(1)
Fe(10)	3665(1)	6337(1)	2772(1)	20(1)
Fe(11)	4443(1)	6903(1)	2561(1)	19(1)
Fe(12)	3914(1)	4465(1)	2396(1)	18(1)
Fe(13)	3055(1)	2523(1)	-68(1)	18(1)
Fe(14)	3851(1)	3217(1)	-240(1)	18(1)
Fe(15)	3059(1)	4428(1)	-713(1)	18(1)
Fe(16)	3614(1)	4895(1)	212(1)	17(1)
S(9)	3741(1)	6261(1)	2221(1)	20(1)
S(10)	4588(1)	5140(1)	2741(1)	21(1)
S(11)	3766(1)	4633(1)	2946(1)	20(1)
S(12)	4294(1)	7073(1)	3114(1)	20(1)
S(13)	3770(1)	4972(1)	-342(1)	18(1)
S(14)	2933(1)	4342(1)	-163(1)	18(1)
S(15)	3760(1)	3059(1)	302(1)	18(1)
S(16)	3211(1)	2589(1)	-619(1)	19(1)
Cl(3)	3084(1)	7162(1)	2813(1)	33(1)
Cl(4)	4461(1)	2498(1)	-264(1)	30(1)
P(7)	4305(1)	5555(1)	3810(1)	23(1)
P(8)	4237(1)	8608(1)	2397(1)	24(1)
P(9)	3231(1)	3908(1)	2070(1)	21(1)
P(10)	3220(1)	4297(1)	-1234(1)	22(1)
P(11)	4305(1)	5337(1)	563(1)	19(1)
P(12)	3248(1)	777(1)	25(1)	20(1)
O(13)	4725(1)	3081(3)	3474(1)	41(1)
O(14)	5350(1)	6020(4)	3636(1)	44(1)
O(15)	4684(1)	6584(3)	1915(1)	39(1)

O(16)	5333(1)	7465(3)	2979(1)	39(1)
O(17)	4176(2)	4488(3)	1754(1)	40(1)
O(18)	4211(1)	2321(3)	2632(1)	36(1)
O(19)	2149(1)	3898(4)	-1052(1)	40(1)
O(20)	2881(2)	6698(3)	-809(1)	43(1)
O(21)	3327(1)	7078(3)	26(1)	34(1)
O(22)	3363(1)	4812(3)	857(1)	35(1)
O(23)	2817(1)	2630(3)	584(1)	35(1)
O(24)	2168(1)	2020(3)	-520(1)	37(1)
C(13)	4617(2)	3935(5)	3401(2)	29(1)
C(14)	5001(2)	5743(4)	3506(2)	29(1)
C(15)	4583(2)	6703(4)	2164(2)	27(1)
C(16)	4982(2)	7270(4)	2819(2)	25(1)
C(17)	4071(2)	4454(4)	2003(2)	26(1)
C(18)	4086(2)	3152(4)	2537(1)	23(1)
C(19)	2508(2)	4089(4)	-931(1)	26(1)
C(20)	2952(2)	5812(5)	-770(1)	25(1)
C(21)	3444(2)	6229(4)	104(1)	21(1)
C(22)	3460(2)	4839(4)	607(2)	23(1)
C(23)	2914(2)	2578(4)	332(1)	23(1)
C(24)	2516(2)	2210(4)	-345(1)	24(1)
C(61)	4520(2)	6820(5)	4032(2)	36(1)
C(62)	4473(2)	7046(5)	4403(2)	47(2)
C(63)	4523(2)	4582(5)	4173(2)	34(1)
C(64)	5012(2)	4551(6)	4336(2)	45(2)
C(65)	3728(2)	5601(5)	3756(2)	34(1)
C(66)	3523(2)	4504(5)	3746(2)	38(2)
C(67)	3692(2)	8909(4)	2388(2)	33(1)
C(68)	3532(2)	10033(5)	2271(2)	52(2)
C(69)	4570(2)	9668(4)	2677(2)	27(1)
C(70)	4539(2)	9797(5)	3052(2)	43(2)
C(71)	4244(2)	9002(5)	1943(2)	39(2)
C(72)	3914(2)	8448(6)	1628(2)	49(2)
C(73)	3146(2)	3655(6)	1591(2)	43(2)
C(74)	3390(2)	2690(6)	1519(2)	56(2)
C(75)	3046(2)	2642(4)	2198(2)	35(1)
C(76)	3029(2)	2587(6)	2580(2)	58(2)
C(77)	2807(2)	4844(5)	2064(2)	40(2)
C(78)	2352(2)	4638(5)	1806(2)	38(2)
C(79)	3749(2)	3706(5)	-1158(2)	29(1)
C(80)	3904(2)	3627(6)	-1484(2)	47(2)
C(81)	2852(2)	3434(5)	-1582(2)	32(1)
C(82)	2430(2)	3958(6)	-1824(2)	50(2)
C(83)	3230(2)	5523(5)	-1482(2)	38(1)
C(84)	3605(2)	6258(5)	-1281(2)	46(2)
C(85)	4408(2)	6767(4)	606(2)	27(1)
C(86)	4198(2)	7333(5)	845(2)	38(2)
C(87)	4491(2)	4934(4)	1044(1)	27(1)
C(88)	4542(2)	3743(4)	1116(2)	34(1)
C(89)	4722(2)	4834(5)	396(2)	30(1)
C(90)	5191(2)	5012(5)	646(2)	35(1)
C(91)	2867(2)	-186(4)	-265(1)	25(1)
C(92)	2820(2)	-169(5)	-666(2)	33(1)
C(93)	3305(2)	238(4)	473(1)	28(1)
C(94)	3673(2)	688(5)	796(2)	38(2)
C(95)	3761(2)	471(4)	-40(2)	27(1)
C(96)	3894(2)	-693(5)	2(2)	38(2)

Table 3. Bond lengths [Å] and angles [deg] for IV.

Fe(1)-C(5)	1.764(6)	P(1)-C(27)	1.831(6)
Fe(1)-C(6)	1.786(6)	P(1)-C(29)	1.836(6)
Fe(1)-P(3)	2.2786(16)	P(2)-C(33)	1.829(6)
Fe(1)-S(4)	2.3420(15)	P(2)-C(35)	1.830(6)
Fe(1)-S(3)	2.3662(14)	P(2)-C(31)	1.843(6)
Fe(1)-S(2)	2.3707(15)	P(3)-C(37)	1.826(6)
Fe(1)-Fe(4)	2.9981(11)	P(3)-C(41)	1.833(5)
Fe(1)-Fe(3)	3.4940(12)	P(3)-C(39)	1.834(6)
Fe(1)-Fe(2)	3.4948(11)	P(4)-C(47)	1.823(5)
Fe(2)-C(3)	1.776(6)	P(4)-C(45)	1.838(5)
Fe(2)-C(4)	1.784(6)	P(4)-C(43)	1.843(5)
Fe(2)-P(2)	2.2838(16)	P(5)-C(53)	1.793(7)
Fe(2)-S(4)	2.3372(15)	P(5)-C(51)	1.822(6)
Fe(2)-S(3)	2.3619(15)	P(5)-C(49)	1.853(7)
Fe(2)-S(1)	2.3855(15)	P(6)-C(55)	1.826(6)
Fe(2)-Fe(4)	3.0068(11)	P(6)-C(59)	1.838(6)
Fe(2)-Fe(3)	3.4790(11)	P(6)-C(57)	1.841(6)
Fe(3)-C(1)	1.772(6)	O(1)-C(1)	1.145(7)
Fe(3)-C(2)	1.779(6)	O(2)-C(2)	1.144(7)
Fe(3)-P(1)	2.2748(16)	O(3)-C(3)	1.148(7)
Fe(3)-S(4)	2.3236(15)	O(4)-C(4)	1.140(6)
Fe(3)-S(2)	2.3584(15)	O(5)-C(5)	1.148(6)
Fe(3)-S(1)	2.3820(15)	O(6)-C(6)	1.130(6)
Fe(3)-Fe(4)	3.0250(11)	O(7)-C(7)	1.145(6)
Fe(4)-Cl(1)	2.2277(16)	O(8)-C(8)	1.128(6)
Fe(4)-S(3)	2.2360(15)	O(9)-C(9)	1.134(6)
Fe(4)-S(2)	2.2410(14)	O(10)-C(10)	1.139(6)
Fe(4)-S(1)	2.2498(15)	O(11)-C(11)	1.141(7)
Fe(5)-C(10)	1.775(6)	O(12)-C(12)	1.149(7)
Fe(5)-C(9)	1.780(6)	C(25)-C(26)	1.539(9)
Fe(5)-P(5)	2.2777(16)	C(27)-C(28)	1.535(10)
Fe(5)-S(7)	2.3274(15)	C(29)-C(30)	1.513(8)
Fe(5)-S(6)	2.3656(15)	C(31)-C(32)	1.525(8)
Fe(5)-S(8)	2.3851(15)	C(33)-C(34)	1.535(8)
Fe(5)-Fe(7)	3.0036(11)	C(35)-C(36)	1.515(8)
Fe(5)-Fe(8)	3.4831(11)	C(37)-C(38)	1.532(8)
Fe(5)-Fe(6)	3.5076(12)	C(39)-C(40)	1.522(8)
Fe(6)-C(11)	1.773(6)	C(41)-C(42)	1.528(8)
Fe(6)-C(12)	1.779(6)	C(43)-C(44)	1.515(8)
Fe(6)-P(6)	2.2759(16)	C(45)-C(46)	1.511(8)
Fe(6)-S(7)	2.3348(15)	C(47)-C(48)	1.521(8)
Fe(6)-S(5)	2.3683(15)	C(49)-C(50)	1.532(9)
Fe(6)-S(8)	2.3773(15)	C(51)-C(52)	1.561(9)
Fe(6)-Fe(7)	3.0529(11)	C(53)-C(54)	1.535(10)
Fe(6)-Fe(8)	3.4758(11)	C(55)-C(56)	1.505(9)
Fe(7)-Cl(2)	2.2319(16)	C(57)-C(58)	1.524(9)
Fe(7)-S(8)	2.2344(15)	C(59)-C(60)	1.530(8)
Fe(7)-S(6)	2.2474(15)	Fe(9)-C(14)	1.773(6)
Fe(7)-S(5)	2.2535(15)	Fe(9)-C(13)	1.782(6)
Fe(7)-Fe(8)	3.0525(11)	Fe(9)-P(7)	2.2882(16)
Fe(8)-C(7)	1.780(6)	Fe(9)-S(10)	2.3283(15)
Fe(8)-C(8)	1.784(6)	Fe(9)-S(12)	2.3712(15)
Fe(8)-P(4)	2.2793(16)	Fe(9)-S(11)	2.3828(15)
Fe(8)-S(7)	2.3369(15)	Fe(9)-Fe(10)	3.0297(11)
Fe(8)-S(5)	2.3654(15)	Fe(9)-Fe(11)	3.4876(11)
Fe(8)-S(6)	2.3761(15)	Fe(9)-Fe(12)	3.4960(12)
P(1)-C(25)	1.831(6)	Fe(10)-Cl(3)	2.2328(15)

Fe(10) -S(11)	2.2433 (15)	P(10) -C(81)	1.837 (6)
Fe(10) -S(12)	2.2463 (15)	P(11) -C(89)	1.825 (5)
Fe(10) -S(9)	2.2535 (15)	P(11) -C(85)	1.831 (5)
Fe(10) -Fe(12)	3.0378 (11)	P(11) -C(87)	1.839 (5)
Fe(10) -Fe(11)	3.0385 (11)	P(12) -C(93)	1.826 (5)
Fe(11) -C(16)	1.778 (6)	P(12) -C(91)	1.833 (5)
Fe(11) -C(15)	1.780 (6)	P(12) -C(95)	1.834 (5)
Fe(11) -P(8)	2.2799 (16)	O(13) -C(13)	1.139 (7)
Fe(11) -S(10)	2.3310 (15)	O(14) -C(14)	1.143 (6)
Fe(11) -S(9)	2.3805 (15)	O(15) -C(15)	1.140 (6)
Fe(11) -S(12)	2.3823 (15)	O(16) -C(16)	1.139 (6)
Fe(11) -Fe(12)	3.4833 (11)	O(17) -C(17)	1.137 (6)
Fe(12) -C(18)	1.775 (6)	O(18) -C(18)	1.140 (6)
Fe(12) -C(17)	1.783 (6)	O(19) -C(19)	1.142 (6)
Fe(12) -P(9)	2.2860 (16)	O(20) -C(20)	1.141 (6)
Fe(12) -S(10)	2.3295 (15)	O(21) -C(21)	1.144 (6)
Fe(12) -S(11)	2.3692 (15)	O(22) -C(22)	1.127 (6)
Fe(12) -S(9)	2.3780 (14)	O(23) -C(23)	1.138 (6)
Fe(13) -C(23)	1.779 (5)	O(24) -C(24)	1.141 (6)
Fe(13) -C(24)	1.780 (6)	C(61) -C(62)	1.535 (8)
Fe(13) -P(12)	2.2853 (15)	C(63) -C(64)	1.520 (8)
Fe(13) -S(14)	2.3357 (15)	C(65) -C(66)	1.534 (8)
Fe(13) -S(16)	2.3765 (15)	C(67) -C(68)	1.527 (8)
Fe(13) -S(15)	2.3769 (14)	C(69) -C(70)	1.511 (8)
Fe(13) -Fe(14)	3.0505 (11)	C(71) -C(72)	1.506 (9)
Fe(13) -Fe(15)	3.4828 (11)	C(73) -C(74)	1.537 (9)
Fe(13) -Fe(16)	3.4872 (11)	C(75) -C(76)	1.512 (8)
Fe(14) -Cl(4)	2.2393 (15)	C(77) -C(78)	1.515 (8)
Fe(14) -S(15)	2.2425 (15)	C(79) -C(80)	1.529 (7)
Fe(14) -S(13)	2.2483 (14)	C(81) -C(82)	1.537 (8)
Fe(14) -S(16)	2.2627 (14)	C(83) -C(84)	1.529 (8)
Fe(14) -Fe(16)	3.0256 (10)	C(85) -C(86)	1.521 (8)
Fe(14) -Fe(15)	3.0424 (11)	C(87) -C(88)	1.525 (7)
Fe(15) -C(19)	1.774 (6)	C(89) -C(90)	1.538 (7)
Fe(15) -C(20)	1.779 (6)	C(91) -C(92)	1.519 (7)
Fe(15) -P(10)	2.2757 (16)	C(93) -C(94)	1.527 (7)
Fe(15) -S(14)	2.3258 (15)	C(95) -C(96)	1.525 (7)
Fe(15) -S(16)	2.3754 (15)		
Fe(15) -S(13)	2.3962 (15)	C(5) -Fe(1) -C(6)	94.6 (2)
Fe(15) -Fe(16)	3.4948 (11)	C(5) -Fe(1) -P(3)	92.73 (17)
Fe(16) -C(21)	1.776 (5)	C(6) -Fe(1) -P(3)	91.75 (18)
Fe(16) -C(22)	1.783 (5)	C(5) -Fe(1) -S(4)	90.47 (17)
Fe(16) -P(11)	2.2895 (15)	C(6) -Fe(1) -S(4)	92.19 (17)
Fe(16) -S(14)	2.3273 (14)	P(3) -Fe(1) -S(4)	174.71 (6)
Fe(16) -S(15)	2.3666 (14)	C(5) -Fe(1) -S(3)	174.31 (17)
Fe(16) -S(13)	2.3935 (14)	C(6) -Fe(1) -S(3)	84.67 (16)
P(7) -C(63)	1.825 (6)	P(3) -Fe(1) -S(3)	92.94 (5)
P(7) -C(61)	1.838 (6)	S(4) -Fe(1) -S(3)	83.92 (5)
P(7) -C(65)	1.841 (6)	C(5) -Fe(1) -S(2)	85.26 (18)
P(8) -C(67)	1.823 (5)	C(6) -Fe(1) -S(2)	175.72 (18)
P(8) -C(69)	1.834 (5)	P(3) -Fe(1) -S(2)	92.53 (5)
P(8) -C(71)	1.848 (6)	S(4) -Fe(1) -S(2)	83.53 (5)
P(9) -C(73)	1.823 (6)	S(3) -Fe(1) -S(2)	95.00 (5)
P(9) -C(77)	1.825 (6)	C(5) -Fe(1) -Fe(4)	132.19 (18)
P(9) -C(75)	1.839 (6)	C(6) -Fe(1) -Fe(4)	131.70 (16)
P(10) -C(79)	1.827 (5)	P(3) -Fe(1) -Fe(4)	96.26 (5)
P(10) -C(83)	1.832 (6)	S(4) -Fe(1) -Fe(4)	78.47 (4)

S(3) - Fe(1) - Fe(4)	47.49(4)	C(2) - Fe(3) - S(4)	88.76(18)
S(2) - Fe(1) - Fe(4)	47.59(4)	P(1) - Fe(3) - S(4)	173.31(6)
C(5) - Fe(1) - Fe(3)	86.53(17)	C(1) - Fe(3) - S(2)	85.61(18)
C(6) - Fe(1) - Fe(3)	133.49(17)	C(2) - Fe(3) - S(2)	172.64(18)
P(3) - Fe(1) - Fe(3)	134.70(5)	P(1) - Fe(3) - S(2)	91.77(5)
S(4) - Fe(1) - Fe(3)	41.31(3)	S(4) - Fe(3) - S(2)	84.20(5)
S(3) - Fe(1) - Fe(3)	89.84(4)	C(1) - Fe(3) - S(1)	177.3(2)
S(2) - Fe(1) - Fe(3)	42.23(4)	C(2) - Fe(3) - S(1)	87.18(18)
Fe(4) - Fe(1) - Fe(3)	54.90(2)	P(1) - Fe(3) - S(1)	89.97(5)
C(5) - Fe(1) - Fe(2)	132.08(17)	S(4) - Fe(3) - S(1)	85.02(5)
C(6) - Fe(1) - Fe(2)	87.43(17)	S(2) - Fe(3) - S(1)	94.33(5)
P(3) - Fe(1) - Fe(2)	135.13(4)	C(1) - Fe(3) - Fe(4)	132.28(18)
S(4) - Fe(1) - Fe(2)	41.63(3)	C(2) - Fe(3) - Fe(4)	133.15(18)
S(3) - Fe(1) - Fe(2)	42.29(4)	P(1) - Fe(3) - Fe(4)	95.18(5)
S(2) - Fe(1) - Fe(2)	89.46(4)	S(4) - Fe(3) - Fe(4)	78.16(4)
Fe(4) - Fe(1) - Fe(2)	54.53(2)	S(2) - Fe(3) - Fe(4)	47.22(4)
Fe(3) - Fe(1) - Fe(2)	59.71(2)	S(1) - Fe(3) - Fe(4)	47.36(4)
C(3) - Fe(2) - C(4)	93.1(2)	C(1) - Fe(3) - Fe(2)	134.15(19)
C(3) - Fe(2) - P(2)	92.95(18)	C(2) - Fe(3) - Fe(2)	86.13(17)
C(4) - Fe(2) - P(2)	92.46(17)	P(1) - Fe(3) - Fe(2)	133.09(5)
C(3) - Fe(2) - S(4)	92.91(17)	S(4) - Fe(3) - Fe(2)	41.87(3)
C(4) - Fe(2) - S(4)	89.51(17)	S(2) - Fe(3) - Fe(2)	90.04(4)
P(2) - Fe(2) - S(4)	173.71(6)	S(1) - Fe(3) - Fe(2)	43.18(4)
C(3) - Fe(2) - S(3)	177.01(18)	Fe(4) - Fe(3) - Fe(2)	54.53(2)
C(4) - Fe(2) - S(3)	86.69(18)	C(1) - Fe(3) - Fe(1)	87.99(17)
P(2) - Fe(2) - S(3)	90.03(5)	C(2) - Fe(3) - Fe(1)	130.39(18)
S(4) - Fe(2) - S(3)	84.12(5)	P(1) - Fe(3) - Fe(1)	134.12(5)
C(3) - Fe(2) - S(1)	85.12(17)	S(4) - Fe(3) - Fe(1)	41.71(4)
C(4) - Fe(2) - S(1)	173.78(17)	S(2) - Fe(3) - Fe(1)	42.50(3)
P(2) - Fe(2) - S(1)	93.58(5)	S(1) - Fe(3) - Fe(1)	90.16(4)
S(4) - Fe(2) - S(1)	84.64(5)	Fe(4) - Fe(3) - Fe(1)	54.18(2)
S(3) - Fe(2) - S(1)	94.81(5)	Fe(2) - Fe(3) - Fe(1)	60.16(2)
C(3) - Fe(2) - Fe(4)	132.25(17)	Cl(1) - Fe(4) - S(3)	114.20(6)
C(4) - Fe(2) - Fe(4)	133.07(17)	Cl(1) - Fe(4) - S(2)	114.92(6)
P(2) - Fe(2) - Fe(4)	95.98(4)	S(3) - Fe(4) - S(2)	102.54(5)
S(4) - Fe(2) - Fe(4)	78.36(4)	Cl(1) - Fe(4) - S(1)	119.12(6)
S(3) - Fe(2) - Fe(4)	47.37(4)	S(3) - Fe(4) - S(1)	102.35(5)
S(1) - Fe(2) - Fe(4)	47.62(4)	S(2) - Fe(4) - S(1)	101.45(5)
C(3) - Fe(2) - Fe(3)	87.63(17)	Cl(1) - Fe(4) - Fe(1)	134.17(5)
C(4) - Fe(2) - Fe(3)	130.97(17)	S(3) - Fe(4) - Fe(1)	51.27(4)
P(2) - Fe(2) - Fe(3)	136.51(5)	S(2) - Fe(4) - Fe(1)	51.36(4)
S(4) - Fe(2) - Fe(3)	41.57(4)	S(1) - Fe(4) - Fe(1)	106.71(4)
S(3) - Fe(2) - Fe(3)	90.28(4)	Cl(1) - Fe(4) - Fe(2)	139.42(5)
S(1) - Fe(2) - Fe(3)	43.10(3)	S(3) - Fe(4) - Fe(2)	51.00(4)
Fe(4) - Fe(2) - Fe(3)	55.02(2)	S(2) - Fe(4) - Fe(2)	105.56(4)
C(3) - Fe(2) - Fe(1)	134.63(17)	S(1) - Fe(4) - Fe(2)	51.56(4)
C(4) - Fe(2) - Fe(1)	86.96(17)	Fe(1) - Fe(4) - Fe(2)	71.18(3)
P(2) - Fe(2) - Fe(1)	132.40(5)	Cl(1) - Fe(4) - Fe(3)	140.21(5)
S(4) - Fe(2) - Fe(1)	41.73(4)	S(3) - Fe(4) - Fe(3)	105.49(4)
S(3) - Fe(2) - Fe(1)	42.39(3)	S(2) - Fe(4) - Fe(3)	50.57(4)
S(1) - Fe(2) - Fe(1)	90.09(4)	S(1) - Fe(4) - Fe(3)	51.15(4)
Fe(4) - Fe(2) - Fe(1)	54.29(2)	Fe(1) - Fe(4) - Fe(3)	70.91(3)
Fe(3) - Fe(2) - Fe(1)	60.14(2)	Fe(2) - Fe(4) - Fe(3)	70.45(3)
C(1) - Fe(3) - C(2)	92.5(2)	C(10) - Fe(5) - C(9)	94.4(2)
C(1) - Fe(3) - P(1)	92.71(19)	C(10) - Fe(5) - P(5)	93.28(17)
C(2) - Fe(3) - P(1)	95.43(18)	C(9) - Fe(5) - P(5)	91.41(18)
C(1) - Fe(3) - S(4)	92.31(19)	C(10) - Fe(5) - S(7)	89.39(17)

C(9) -Fe(5) -S(7)	91.52(18)	S(5) -Fe(6) -Fe(8)	42.72(4)
P(5) -Fe(5) -S(7)	175.87(6)	S(8) -Fe(6) -Fe(8)	90.05(4)
C(10) -Fe(5) -S(6)	173.91(18)	Fe(7) -Fe(6) -Fe(8)	55.29(2)
C(9) -Fe(5) -S(6)	84.63(17)	C(11) -Fe(6) -Fe(5)	89.16(18)
P(5) -Fe(5) -S(6)	92.75(5)	C(12) -Fe(6) -Fe(5)	128.31(19)
S(7) -Fe(5) -S(6)	84.63(5)	P(6) -Fe(6) -Fe(5)	139.69(5)
C(10) -Fe(5) -S(8)	85.58(18)	S(7) -Fe(6) -Fe(5)	41.13(4)
C(9) -Fe(5) -S(8)	175.28(18)	S(5) -Fe(6) -Fe(5)	88.93(4)
P(5) -Fe(5) -S(8)	93.30(6)	S(8) -Fe(6) -Fe(5)	42.65(3)
S(7) -Fe(5) -S(8)	83.76(5)	Fe(7) -Fe(6) -Fe(5)	53.96(2)
S(6) -Fe(5) -S(8)	94.92(5)	Fe(8) -Fe(6) -Fe(5)	59.83(2)
C(10) -Fe(5) -Fe(7)	132.22(18)	Cl(2) -Fe(7) -S(8)	115.24(6)
C(9) -Fe(5) -Fe(7)	131.85(17)	Cl(2) -Fe(7) -S(6)	115.10(6)
P(5) -Fe(5) -Fe(7)	96.37(5)	S(8) -Fe(7) -S(6)	102.71(5)
S(7) -Fe(5) -Fe(7)	79.51(4)	Cl(2) -Fe(7) -S(5)	119.92(6)
S(6) -Fe(5) -Fe(7)	47.68(4)	S(8) -Fe(7) -S(5)	100.70(6)
S(8) -Fe(5) -Fe(7)	47.29(4)	S(6) -Fe(7) -S(5)	100.54(5)
C(10) -Fe(5) -Fe(8)	131.15(17)	Cl(2) -Fe(7) -Fe(5)	135.08(5)
C(9) -Fe(5) -Fe(8)	86.72(17)	S(8) -Fe(7) -Fe(5)	51.66(4)
P(5) -Fe(5) -Fe(8)	135.56(5)	S(6) -Fe(7) -Fe(5)	51.11(4)
S(7) -Fe(5) -Fe(8)	41.79(4)	S(5) -Fe(7) -Fe(5)	105.00(5)
S(6) -Fe(5) -Fe(8)	42.85(4)	Cl(2) -Fe(7) -Fe(8)	140.11(5)
S(8) -Fe(5) -Fe(8)	89.75(4)	S(8) -Fe(7) -Fe(8)	104.60(4)
Fe(7) -Fe(5) -Fe(8)	55.55(2)	S(6) -Fe(7) -Fe(8)	50.53(4)
C(10) -Fe(5) -Fe(6)	86.33(18)	S(5) -Fe(7) -Fe(8)	50.23(4)
C(9) -Fe(5) -Fe(6)	132.80(18)	Fe(5) -Fe(7) -Fe(8)	70.21(3)
P(5) -Fe(5) -Fe(6)	135.73(5)	Cl(2) -Fe(7) -Fe(6)	140.04(5)
S(7) -Fe(5) -Fe(6)	41.29(3)	S(8) -Fe(7) -Fe(6)	50.59(4)
S(6) -Fe(5) -Fe(6)	89.94(4)	S(6) -Fe(7) -Fe(6)	104.82(4)
S(8) -Fe(5) -Fe(6)	42.48(4)	S(5) -Fe(7) -Fe(6)	50.30(4)
Fe(7) -Fe(5) -Fe(6)	55.27(2)	Fe(5) -Fe(7) -Fe(6)	70.77(3)
Fe(8) -Fe(5) -Fe(6)	59.63(2)	Fe(8) -Fe(7) -Fe(6)	69.40(3)
C(11) -Fe(6) -C(12)	91.1(3)	C(7) -Fe(8) -C(8)	93.2(2)
C(11) -Fe(6) -P(6)	91.91(18)	C(7) -Fe(8) -P(4)	92.66(18)
C(12) -Fe(6) -P(6)	91.97(19)	C(8) -Fe(8) -P(4)	93.05(17)
C(11) -Fe(6) -S(7)	94.95(18)	C(7) -Fe(8) -S(7)	91.80(18)
C(12) -Fe(6) -S(7)	87.45(19)	C(8) -Fe(8) -S(7)	91.23(17)
P(6) -Fe(6) -S(7)	173.12(6)	P(4) -Fe(8) -S(7)	173.63(6)
C(11) -Fe(6) -S(5)	177.6(2)	C(7) -Fe(8) -S(5)	85.59(17)
C(12) -Fe(6) -S(5)	91.31(19)	C(8) -Fe(8) -S(5)	175.64(17)
P(6) -Fe(6) -S(5)	88.57(5)	P(4) -Fe(8) -S(5)	91.19(5)
S(7) -Fe(6) -S(5)	84.60(5)	S(7) -Fe(8) -S(5)	84.62(5)
C(11) -Fe(6) -S(8)	84.12(18)	C(7) -Fe(8) -S(6)	175.98(18)
C(12) -Fe(6) -S(8)	169.57(19)	C(8) -Fe(8) -S(6)	87.11(17)
P(6) -Fe(6) -S(8)	97.41(6)	P(4) -Fe(8) -S(6)	91.32(5)
S(7) -Fe(6) -S(8)	83.78(5)	S(7) -Fe(8) -S(6)	84.19(5)
S(5) -Fe(6) -S(8)	93.46(5)	S(5) -Fe(8) -S(6)	93.77(5)
C(11) -Fe(6) -Fe(7)	130.52(18)	C(7) -Fe(8) -Fe(7)	132.01(17)
C(12) -Fe(6) -Fe(7)	136.63(19)	C(8) -Fe(8) -Fe(7)	133.29(17)
P(6) -Fe(6) -Fe(7)	97.50(5)	P(4) -Fe(8) -Fe(7)	95.30(5)
S(7) -Fe(6) -Fe(7)	78.35(4)	S(7) -Fe(8) -Fe(7)	78.33(4)
S(5) -Fe(6) -Fe(7)	47.06(4)	S(5) -Fe(8) -Fe(7)	47.08(4)
S(8) -Fe(6) -Fe(7)	46.57(4)	S(6) -Fe(8) -Fe(7)	46.89(4)
C(11) -Fe(6) -Fe(8)	136.89(18)	C(7) -Fe(8) -Fe(6)	86.30(17)
C(12) -Fe(6) -Fe(8)	87.17(18)	C(8) -Fe(8) -Fe(6)	132.99(17)
P(6) -Fe(6) -Fe(8)	131.18(5)	P(4) -Fe(8) -Fe(6)	133.95(5)
S(7) -Fe(6) -Fe(8)	41.95(4)	S(7) -Fe(8) -Fe(6)	41.90(4)

S(5)-Fe(8)-Fe(6)	42.79(4)	C(45)-P(4)-Fe(8)	116.8(2)
S(6)-Fe(8)-Fe(6)	90.54(4)	C(43)-P(4)-Fe(8)	113.19(18)
Fe(7)-Fe(8)-Fe(6)	55.31(2)	C(53)-P(5)-C(51)	105.8(3)
C(7)-Fe(8)-Fe(5)	133.38(18)	C(53)-P(5)-C(49)	104.7(3)
C(8)-Fe(8)-Fe(5)	88.20(17)	C(51)-P(5)-C(49)	99.5(3)
P(4)-Fe(8)-Fe(5)	133.83(5)	C(53)-P(5)-Fe(5)	112.2(3)
S(7)-Fe(8)-Fe(5)	41.59(4)	C(51)-P(5)-Fe(5)	117.1(2)
S(5)-Fe(8)-Fe(5)	89.57(4)	C(49)-P(5)-Fe(5)	116.0(2)
S(6)-Fe(8)-Fe(5)	42.61(3)	C(55)-P(6)-C(59)	106.0(3)
Fe(7)-Fe(8)-Fe(5)	54.24(2)	C(55)-P(6)-C(57)	101.2(3)
Fe(6)-Fe(8)-Fe(5)	60.54(2)	C(59)-P(6)-C(57)	102.3(3)
Fe(4)-S(1)-Fe(3)	81.49(5)	C(55)-P(6)-Fe(6)	116.8(2)
Fe(4)-S(1)-Fe(2)	80.83(5)	C(59)-P(6)-Fe(6)	113.6(2)
Fe(3)-S(1)-Fe(2)	93.73(5)	C(57)-P(6)-Fe(6)	115.2(2)
Fe(4)-S(2)-Fe(3)	82.21(5)	O(1)-C(1)-Fe(3)	178.9(6)
Fe(4)-S(2)-Fe(1)	81.05(5)	O(2)-C(2)-Fe(3)	176.3(5)
Fe(3)-S(2)-Fe(1)	95.26(5)	O(3)-C(3)-Fe(2)	179.4(6)
Fe(4)-S(3)-Fe(2)	81.63(5)	O(4)-C(4)-Fe(2)	177.5(5)
Fe(4)-S(3)-Fe(1)	81.25(5)	O(5)-C(5)-Fe(1)	178.7(6)
Fe(2)-S(3)-Fe(1)	95.32(5)	O(6)-C(6)-Fe(1)	179.7(6)
Fe(3)-S(4)-Fe(2)	96.57(5)	O(7)-C(7)-Fe(8)	178.5(5)
Fe(3)-S(4)-Fe(1)	96.99(5)	O(8)-C(8)-Fe(8)	179.7(5)
Fe(2)-S(4)-Fe(1)	96.64(5)	O(9)-C(9)-Fe(5)	179.2(5)
Fe(7)-S(5)-Fe(8)	82.69(5)	O(10)-C(10)-Fe(5)	177.3(5)
Fe(7)-S(5)-Fe(6)	82.64(5)	O(11)-C(11)-Fe(6)	178.7(6)
Fe(8)-S(5)-Fe(6)	94.49(5)	O(12)-C(12)-Fe(6)	173.4(6)
Fe(7)-S(6)-Fe(5)	81.21(5)	C(26)-C(25)-P(1)	113.7(4)
Fe(7)-S(6)-Fe(8)	82.58(5)	C(28)-C(27)-P(1)	114.2(5)
Fe(5)-S(6)-Fe(8)	94.54(5)	C(30)-C(29)-P(1)	116.8(4)
Fe(5)-S(7)-Fe(6)	97.59(5)	C(32)-C(31)-P(2)	115.4(4)
Fe(5)-S(7)-Fe(8)	96.62(5)	C(34)-C(33)-P(2)	116.0(4)
Fe(6)-S(7)-Fe(8)	96.15(5)	C(36)-C(35)-P(2)	115.8(4)
Fe(7)-S(8)-Fe(6)	82.84(5)	C(38)-C(37)-P(3)	116.1(5)
Fe(7)-S(8)-Fe(5)	81.04(5)	C(40)-C(39)-P(3)	116.2(4)
Fe(6)-S(8)-Fe(5)	94.87(5)	C(42)-C(41)-P(3)	113.9(4)
C(25)-P(1)-C(27)	103.9(3)	C(44)-C(43)-P(4)	116.5(4)
C(25)-P(1)-C(29)	103.6(3)	C(46)-C(45)-P(4)	116.9(4)
C(27)-P(1)-C(29)	103.1(3)	C(48)-C(47)-P(4)	115.6(4)
C(25)-P(1)-Fe(3)	116.8(2)	C(50)-C(49)-P(5)	113.5(5)
C(27)-P(1)-Fe(3)	115.0(2)	C(52)-C(51)-P(5)	114.3(5)
C(29)-P(1)-Fe(3)	112.80(19)	C(54)-C(53)-P(5)	116.6(6)
C(33)-P(2)-C(35)	104.5(3)	C(56)-C(55)-P(6)	114.3(5)
C(33)-P(2)-C(31)	104.3(3)	C(58)-C(57)-P(6)	114.5(4)
C(35)-P(2)-C(31)	100.9(3)	C(60)-C(59)-P(6)	116.2(4)
C(33)-P(2)-Fe(2)	114.03(18)	C(14)-Fe(9)-C(13)	92.7(3)
C(35)-P(2)-Fe(2)	117.2(2)	C(14)-Fe(9)-P(7)	91.69(19)
C(31)-P(2)-Fe(2)	114.2(2)	C(13)-Fe(9)-P(7)	93.45(18)
C(37)-P(3)-C(41)	104.1(3)	C(14)-Fe(9)-S(10)	90.02(19)
C(37)-P(3)-C(39)	104.9(3)	C(13)-Fe(9)-S(10)	91.48(18)
C(41)-P(3)-C(39)	100.6(3)	P(7)-Fe(9)-S(10)	174.70(6)
C(37)-P(3)-Fe(1)	112.7(2)	C(14)-Fe(9)-S(12)	85.76(18)
C(41)-P(3)-Fe(1)	116.46(19)	C(13)-Fe(9)-S(12)	175.67(19)
C(39)-P(3)-Fe(1)	116.45(19)	P(7)-Fe(9)-S(12)	90.65(5)
C(47)-P(4)-C(45)	100.2(3)	S(10)-Fe(9)-S(12)	84.47(5)
C(47)-P(4)-C(43)	105.3(3)	C(14)-Fe(9)-S(11)	173.83(19)
C(45)-P(4)-C(43)	104.6(3)	C(13)-Fe(9)-S(11)	86.84(18)
C(47)-P(4)-Fe(8)	115.2(2)	P(7)-Fe(9)-S(11)	94.48(5)

S(10)-Fe(9)-S(11)	83.85(5)	S(10)-Fe(11)-S(12)	84.17(5)
S(12)-Fe(9)-S(11)	94.24(5)	S(9)-Fe(11)-S(12)	94.14(5)
C(14)-Fe(9)-Fe(10)	132.16(18)	C(16)-Fe(11)-Fe(10)	132.91(17)
C(13)-Fe(9)-Fe(10)	133.42(18)	C(15)-Fe(11)-Fe(10)	134.38(18)
P(7)-Fe(9)-Fe(10)	96.45(5)	P(8)-Fe(11)-Fe(10)	95.71(5)
S(10)-Fe(9)-Fe(10)	78.71(4)	S(10)-Fe(11)-Fe(10)	78.49(4)
S(12)-Fe(9)-Fe(10)	47.24(4)	S(9)-Fe(11)-Fe(10)	47.24(4)
S(11)-Fe(9)-Fe(10)	47.12(4)	S(12)-Fe(11)-Fe(10)	47.06(4)
C(14)-Fe(9)-Fe(11)	86.14(17)	C(16)-Fe(11)-Fe(12)	132.41(17)
C(13)-Fe(9)-Fe(11)	132.97(18)	C(15)-Fe(11)-Fe(12)	88.75(17)
P(7)-Fe(9)-Fe(11)	133.58(5)	P(8)-Fe(11)-Fe(12)	134.28(5)
S(10)-Fe(9)-Fe(11)	41.57(4)	S(10)-Fe(11)-Fe(12)	41.62(4)
S(12)-Fe(9)-Fe(11)	42.93(4)	S(9)-Fe(11)-Fe(12)	42.92(3)
S(11)-Fe(9)-Fe(11)	89.66(4)	S(12)-Fe(11)-Fe(12)	90.02(4)
Fe(10)-Fe(9)-Fe(11)	55.04(2)	Fe(10)-Fe(11)-Fe(12)	55.01(2)
C(14)-Fe(9)-Fe(12)	131.37(19)	C(16)-Fe(11)-Fe(9)	87.26(16)
C(13)-Fe(9)-Fe(12)	88.07(18)	C(15)-Fe(11)-Fe(9)	133.59(17)
P(7)-Fe(9)-Fe(12)	136.84(5)	P(8)-Fe(11)-Fe(9)	134.65(5)
S(10)-Fe(9)-Fe(12)	41.38(4)	S(10)-Fe(11)-Fe(9)	41.51(4)
S(12)-Fe(9)-Fe(12)	89.90(4)	S(9)-Fe(11)-Fe(9)	90.05(4)
S(11)-Fe(9)-Fe(12)	42.48(3)	S(12)-Fe(11)-Fe(9)	42.68(3)
Fe(10)-Fe(9)-Fe(12)	54.93(2)	Fe(10)-Fe(11)-Fe(9)	54.80(2)
Fe(11)-Fe(9)-Fe(12)	59.84(2)	Fe(12)-Fe(11)-Fe(9)	60.20(2)
Cl(3)-Fe(10)-S(11)	117.82(6)	C(18)-Fe(12)-C(17)	95.8(2)
Cl(3)-Fe(10)-S(12)	113.93(6)	C(18)-Fe(12)-P(9)	92.04(17)
S(11)-Fe(10)-S(12)	101.78(5)	C(17)-Fe(12)-P(9)	92.30(18)
Cl(3)-Fe(10)-S(9)	117.90(6)	C(18)-Fe(12)-S(10)	91.22(17)
S(11)-Fe(10)-S(9)	101.24(5)	C(17)-Fe(12)-S(10)	89.82(18)
S(12)-Fe(10)-S(9)	101.61(5)	P(9)-Fe(12)-S(10)	175.92(6)
Cl(3)-Fe(10)-Fe(9)	136.79(5)	C(18)-Fe(12)-S(11)	86.97(17)
S(11)-Fe(10)-Fe(9)	51.11(4)	C(17)-Fe(12)-S(11)	173.38(18)
S(12)-Fe(10)-Fe(9)	50.80(4)	P(9)-Fe(12)-S(11)	93.60(5)
S(9)-Fe(10)-Fe(9)	105.24(4)	S(10)-Fe(12)-S(11)	84.12(5)
Cl(3)-Fe(10)-Fe(12)	141.03(5)	C(18)-Fe(12)-S(9)	175.52(17)
S(11)-Fe(10)-Fe(12)	50.62(4)	C(17)-Fe(12)-S(9)	82.62(17)
S(12)-Fe(10)-Fe(12)	105.04(4)	P(9)-Fe(12)-S(9)	92.22(5)
S(9)-Fe(10)-Fe(12)	50.81(4)	S(10)-Fe(12)-S(9)	84.59(5)
Fe(9)-Fe(10)-Fe(12)	70.36(3)	S(11)-Fe(12)-S(9)	94.14(5)
Cl(3)-Fe(10)-Fe(11)	137.34(5)	C(18)-Fe(12)-Fe(10)	133.35(17)
S(11)-Fe(10)-Fe(11)	104.78(4)	C(17)-Fe(12)-Fe(10)	129.04(17)
S(12)-Fe(10)-Fe(11)	50.93(4)	P(9)-Fe(12)-Fe(10)	97.45(4)
S(9)-Fe(10)-Fe(11)	50.86(4)	S(10)-Fe(12)-Fe(10)	78.52(4)
Fe(9)-Fe(10)-Fe(11)	70.16(3)	S(11)-Fe(12)-Fe(10)	47.04(4)
Fe(12)-Fe(10)-Fe(11)	69.96(3)	S(9)-Fe(12)-Fe(10)	47.26(4)
C(16)-Fe(11)-C(15)	91.2(2)	C(18)-Fe(12)-Fe(11)	132.77(17)
C(16)-Fe(11)-P(8)	93.30(17)	C(17)-Fe(12)-Fe(11)	83.71(17)
C(15)-Fe(11)-P(8)	91.75(17)	P(9)-Fe(12)-Fe(11)	135.19(4)
C(16)-Fe(11)-S(10)	90.87(17)	S(10)-Fe(12)-Fe(11)	41.65(3)
C(15)-Fe(11)-S(10)	92.20(17)	S(11)-Fe(12)-Fe(11)	89.99(4)
P(8)-Fe(11)-S(10)	174.20(6)	S(9)-Fe(12)-Fe(11)	42.97(4)
C(16)-Fe(11)-S(9)	175.22(18)	Fe(10)-Fe(12)-Fe(11)	55.03(2)
C(15)-Fe(11)-S(9)	87.74(18)	C(18)-Fe(12)-Fe(9)	87.98(16)
P(8)-Fe(11)-S(9)	91.41(5)	C(17)-Fe(12)-Fe(9)	131.15(18)
S(10)-Fe(11)-S(9)	84.50(5)	P(9)-Fe(12)-Fe(9)	136.34(4)
C(16)-Fe(11)-S(12)	86.57(17)	S(10)-Fe(12)-Fe(9)	41.35(4)
C(15)-Fe(11)-S(12)	175.72(18)	S(11)-Fe(12)-Fe(9)	42.79(4)
P(8)-Fe(11)-S(12)	92.04(5)	S(9)-Fe(12)-Fe(9)	89.89(4)

Fe(10) - Fe(12) - Fe(9)	54.71(2)	Fe(16) - Fe(14) - Fe(13)	70.05(3)
Fe(11) - Fe(12) - Fe(9)	59.96(2)	Fe(15) - Fe(14) - Fe(13)	69.72(3)
C(23) - Fe(13) - C(24)	91.9(2)	C(19) - Fe(15) - C(20)	92.8(2)
C(23) - Fe(13) - P(12)	92.29(17)	C(19) - Fe(15) - P(10)	93.89(17)
C(24) - Fe(13) - P(12)	92.79(17)	C(20) - Fe(15) - P(10)	93.28(17)
C(23) - Fe(13) - S(14)	91.00(17)	C(19) - Fe(15) - S(14)	87.38(17)
C(24) - Fe(13) - S(14)	92.29(17)	C(20) - Fe(15) - S(14)	94.06(17)
P(12) - Fe(13) - S(14)	173.85(6)	P(10) - Fe(15) - S(14)	172.48(6)
C(23) - Fe(13) - S(16)	175.07(17)	C(19) - Fe(15) - S(16)	88.08(18)
C(24) - Fe(13) - S(16)	86.63(17)	C(20) - Fe(15) - S(16)	178.35(18)
P(12) - Fe(13) - S(16)	92.47(5)	P(10) - Fe(15) - S(16)	88.02(5)
S(14) - Fe(13) - S(16)	84.37(5)	S(14) - Fe(15) - S(16)	84.61(5)
C(23) - Fe(13) - S(15)	87.27(17)	C(19) - Fe(15) - S(13)	171.24(18)
C(24) - Fe(13) - S(15)	176.21(18)	C(20) - Fe(15) - S(13)	84.63(17)
P(12) - Fe(13) - S(15)	90.93(5)	P(10) - Fe(15) - S(13)	94.62(5)
S(14) - Fe(13) - S(15)	84.05(5)	S(14) - Fe(15) - S(13)	84.44(5)
S(16) - Fe(13) - S(15)	93.94(5)	S(16) - Fe(15) - S(13)	94.25(5)
C(23) - Fe(13) - Fe(14)	133.34(17)	C(19) - Fe(15) - Fe(14)	134.01(17)
C(24) - Fe(13) - Fe(14)	133.36(17)	C(20) - Fe(15) - Fe(14)	131.36(17)
P(12) - Fe(13) - Fe(14)	95.63(4)	P(10) - Fe(15) - Fe(14)	95.22(5)
S(14) - Fe(13) - Fe(14)	78.35(4)	S(14) - Fe(15) - Fe(14)	78.66(4)
S(16) - Fe(13) - Fe(14)	47.30(3)	S(16) - Fe(15) - Fe(14)	47.42(3)
S(15) - Fe(13) - Fe(14)	46.80(4)	S(13) - Fe(15) - Fe(14)	47.00(4)
C(23) - Fe(13) - Fe(15)	132.44(17)	C(19) - Fe(15) - Fe(13)	85.62(17)
C(24) - Fe(13) - Fe(15)	88.02(16)	C(20) - Fe(15) - Fe(13)	135.82(17)
P(12) - Fe(13) - Fe(15)	135.23(5)	P(10) - Fe(15) - Fe(13)	130.90(5)
S(14) - Fe(13) - Fe(15)	41.55(3)	S(14) - Fe(15) - Fe(13)	41.77(4)
S(16) - Fe(13) - Fe(15)	42.86(3)	S(16) - Fe(15) - Fe(13)	42.88(3)
S(15) - Fe(13) - Fe(15)	89.86(4)	S(13) - Fe(15) - Fe(13)	90.35(4)
Fe(14) - Fe(13) - Fe(15)	55.03(2)	Fe(14) - Fe(15) - Fe(13)	55.25(2)
C(23) - Fe(13) - Fe(16)	87.71(17)	C(19) - Fe(15) - Fe(16)	128.59(17)
C(24) - Fe(13) - Fe(16)	133.74(17)	C(20) - Fe(15) - Fe(16)	88.58(16)
P(12) - Fe(13) - Fe(16)	133.47(5)	P(10) - Fe(15) - Fe(16)	137.36(5)
S(14) - Fe(13) - Fe(16)	41.51(3)	S(14) - Fe(15) - Fe(16)	41.33(4)
S(16) - Fe(13) - Fe(16)	89.94(4)	S(16) - Fe(15) - Fe(16)	89.78(4)
S(15) - Fe(13) - Fe(16)	42.57(3)	S(13) - Fe(15) - Fe(16)	43.11(3)
Fe(14) - Fe(13) - Fe(16)	54.64(2)	Fe(14) - Fe(15) - Fe(16)	54.61(2)
Fe(15) - Fe(13) - Fe(16)	60.19(2)	Fe(13) - Fe(15) - Fe(16)	59.97(2)
Cl(4) - Fe(14) - S(15)	114.59(6)	C(21) - Fe(16) - C(22)	94.8(2)
Cl(4) - Fe(14) - S(13)	116.35(6)	C(21) - Fe(16) - P(11)	94.55(16)
S(15) - Fe(14) - S(13)	102.06(5)	C(22) - Fe(16) - P(11)	90.86(17)
Cl(4) - Fe(14) - S(16)	118.70(6)	C(21) - Fe(16) - S(14)	88.69(16)
S(15) - Fe(14) - S(16)	100.93(5)	C(22) - Fe(16) - S(14)	91.83(17)
S(13) - Fe(14) - S(16)	101.64(5)	P(11) - Fe(16) - S(14)	175.60(6)
Cl(4) - Fe(14) - Fe(16)	136.37(5)	C(21) - Fe(16) - S(15)	173.08(17)
S(15) - Fe(14) - Fe(16)	50.77(4)	C(22) - Fe(16) - S(15)	86.46(17)
S(13) - Fe(14) - Fe(16)	51.44(4)	P(11) - Fe(16) - S(15)	92.23(5)
S(16) - Fe(14) - Fe(16)	104.89(4)	S(14) - Fe(16) - S(15)	84.46(5)
Cl(4) - Fe(14) - Fe(15)	140.74(5)	C(21) - Fe(16) - S(13)	83.97(16)
S(15) - Fe(14) - Fe(15)	104.66(4)	C(22) - Fe(16) - S(13)	176.11(17)
S(13) - Fe(14) - Fe(15)	51.21(4)	P(11) - Fe(16) - S(13)	92.91(5)
S(16) - Fe(14) - Fe(15)	50.63(4)	S(14) - Fe(16) - S(13)	84.46(5)
Fe(16) - Fe(14) - Fe(15)	70.33(3)	S(15) - Fe(16) - S(13)	94.36(5)
Cl(4) - Fe(14) - Fe(13)	138.31(5)	C(21) - Fe(16) - Fe(14)	130.30(16)
S(15) - Fe(14) - Fe(13)	50.60(4)	C(22) - Fe(16) - Fe(14)	133.16(17)
S(13) - Fe(14) - Fe(13)	105.27(4)	P(11) - Fe(16) - Fe(14)	96.62(4)
S(16) - Fe(14) - Fe(13)	50.52(4)	S(14) - Fe(16) - Fe(14)	79.00(4)

S(15)-Fe(16)-Fe(14)	47.22(4)	C(73)-P(9)-C(75)	100.3(3)
S(13)-Fe(16)-Fe(14)	47.27(3)	C(77)-P(9)-C(75)	103.9(3)
C(21)-Fe(16)-Fe(13)	130.38(16)	C(73)-P(9)-Fe(12)	113.6(2)
C(22)-Fe(16)-Fe(13)	87.73(16)	C(77)-P(9)-Fe(12)	114.4(2)
P(11)-Fe(16)-Fe(13)	135.02(4)	C(75)-P(9)-Fe(12)	118.07(19)
S(14)-Fe(16)-Fe(13)	41.69(3)	C(79)-P(10)-C(83)	103.8(3)
S(15)-Fe(16)-Fe(13)	42.80(3)	C(79)-P(10)-C(81)	103.3(3)
S(13)-Fe(16)-Fe(13)	90.29(4)	C(83)-P(10)-C(81)	103.6(3)
Fe(14)-Fe(16)-Fe(13)	55.31(2)	C(79)-P(10)-Fe(15)	112.81(18)
C(21)-Fe(16)-Fe(15)	84.45(16)	C(83)-P(10)-Fe(15)	117.7(2)
C(22)-Fe(16)-Fe(15)	133.10(17)	C(81)-P(10)-Fe(15)	114.0(2)
P(11)-Fe(16)-Fe(15)	136.03(4)	C(89)-P(11)-C(85)	103.6(3)
S(14)-Fe(16)-Fe(15)	41.30(3)	C(89)-P(11)-C(87)	104.0(3)
S(15)-Fe(16)-Fe(15)	89.74(4)	C(85)-P(11)-C(87)	101.1(2)
S(13)-Fe(16)-Fe(15)	43.17(4)	C(89)-P(11)-Fe(16)	114.85(19)
Fe(14)-Fe(16)-Fe(15)	55.06(2)	C(85)-P(11)-Fe(16)	114.21(18)
Fe(13)-Fe(16)-Fe(15)	59.84(2)	C(87)-P(11)-Fe(16)	117.23(19)
Fe(10)-S(9)-Fe(12)	81.93(5)	C(93)-P(12)-C(91)	99.7(2)
Fe(10)-S(9)-Fe(11)	81.90(5)	C(93)-P(12)-C(95)	104.9(3)
Fe(12)-S(9)-Fe(11)	94.11(5)	C(91)-P(12)-C(95)	104.2(3)
Fe(9)-S(10)-Fe(12)	97.28(5)	C(93)-P(12)-Fe(13)	116.3(2)
Fe(9)-S(10)-Fe(11)	96.93(5)	C(91)-P(12)-Fe(13)	116.43(18)
Fe(12)-S(10)-Fe(11)	96.73(5)	C(95)-P(12)-Fe(13)	113.59(17)
Fe(10)-S(11)-Fe(12)	82.34(5)	O(13)-C(13)-Fe(9)	178.2(5)
Fe(10)-S(11)-Fe(9)	81.76(5)	O(14)-C(14)-Fe(9)	177.8(6)
Fe(12)-S(11)-Fe(9)	94.73(5)	O(15)-C(15)-Fe(11)	178.2(5)
Fe(10)-S(12)-Fe(9)	81.96(5)	O(16)-C(16)-Fe(11)	176.9(5)
Fe(10)-S(12)-Fe(11)	82.00(5)	O(17)-C(17)-Fe(12)	177.3(5)
Fe(9)-S(12)-Fe(11)	94.39(5)	O(18)-C(18)-Fe(12)	177.6(5)
Fe(14)-S(13)-Fe(16)	81.29(5)	O(19)-C(19)-Fe(15)	175.6(5)
Fe(14)-S(13)-Fe(15)	81.78(5)	O(20)-C(20)-Fe(15)	179.5(7)
Fe(16)-S(13)-Fe(15)	93.71(5)	O(21)-C(21)-Fe(16)	178.1(5)
Fe(15)-S(14)-Fe(16)	97.37(5)	O(22)-C(22)-Fe(16)	179.4(5)
Fe(15)-S(14)-Fe(13)	96.69(5)	O(23)-C(23)-Fe(13)	178.5(5)
Fe(16)-S(14)-Fe(13)	96.81(5)	O(24)-C(24)-Fe(13)	179.1(6)
Fe(14)-S(15)-Fe(16)	82.01(5)	C(62)-C(61)-P(7)	117.3(4)
Fe(14)-S(15)-Fe(13)	82.60(5)	C(64)-C(63)-P(7)	115.0(4)
Fe(16)-S(15)-Fe(13)	94.64(5)	C(66)-C(65)-P(7)	113.9(4)
Fe(14)-S(16)-Fe(15)	81.95(5)	C(68)-C(67)-P(8)	115.9(4)
Fe(14)-S(16)-Fe(13)	82.19(5)	C(70)-C(69)-P(8)	115.5(4)
Fe(15)-S(16)-Fe(13)	94.27(5)	C(72)-C(71)-P(8)	114.5(5)
C(63)-P(7)-C(61)	103.4(3)	C(74)-C(73)-P(9)	114.8(5)
C(63)-P(7)-C(65)	103.1(3)	C(76)-C(75)-P(9)	115.8(4)
C(61)-P(7)-C(65)	104.1(3)	C(78)-C(77)-P(9)	118.5(4)
C(63)-P(7)-Fe(9)	115.9(2)	C(80)-C(79)-P(10)	117.8(4)
C(61)-P(7)-Fe(9)	112.22(19)	C(82)-C(81)-P(10)	115.4(4)
C(65)-P(7)-Fe(9)	116.6(2)	C(84)-C(83)-P(10)	113.5(4)
C(67)-P(8)-C(69)	104.2(3)	C(86)-C(85)-P(11)	114.2(4)
C(67)-P(8)-C(71)	105.2(3)	C(88)-C(87)-P(11)	115.9(4)
C(69)-P(8)-C(71)	99.9(3)	C(90)-C(89)-P(11)	116.1(4)
C(67)-P(8)-Fe(11)	113.48(19)	C(92)-C(91)-P(12)	115.6(4)
C(69)-P(8)-Fe(11)	117.37(19)	C(94)-C(93)-P(12)	116.4(4)
C(71)-P(8)-Fe(11)	114.9(2)	C(96)-C(95)-P(12)	115.8(4)
C(73)-P(9)-C(77)	104.7(3)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for IV.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Fe(1)	19(1)	16(1)	20(1)	-1(1)	7(1)	1(1)
Fe(2)	15(1)	20(1)	22(1)	2(1)	8(1)	-1(1)
Fe(3)	17(1)	20(1)	20(1)	2(1)	6(1)	1(1)
Fe(4)	16(1)	18(1)	24(1)	0(1)	8(1)	-1(1)
Fe(5)	18(1)	19(1)	22(1)	0(1)	9(1)	1(1)
Fe(6)	18(1)	24(1)	21(1)	-1(1)	7(1)	1(1)
Fe(7)	17(1)	23(1)	23(1)	2(1)	9(1)	2(1)
Fe(8)	16(1)	24(1)	22(1)	-1(1)	8(1)	3(1)
S(1)	19(1)	18(1)	23(1)	1(1)	9(1)	-2(1)
S(2)	21(1)	17(1)	21(1)	0(1)	8(1)	-2(1)
S(3)	19(1)	16(1)	22(1)	1(1)	6(1)	0(1)
S(4)	16(1)	19(1)	23(1)	1(1)	8(1)	2(1)
S(5)	17(1)	24(1)	22(1)	1(1)	7(1)	4(1)
S(6)	16(1)	21(1)	22(1)	0(1)	7(1)	2(1)
S(7)	15(1)	25(1)	22(1)	-1(1)	8(1)	0(1)
S(8)	21(1)	22(1)	23(1)	-1(1)	10(1)	4(1)
Cl(1)	25(1)	35(1)	50(1)	2(1)	19(1)	6(1)
Cl(2)	20(1)	37(1)	48(1)	8(1)	16(1)	0(1)
P(1)	24(1)	27(1)	21(1)	2(1)	8(1)	-3(1)
P(2)	21(1)	19(1)	33(1)	5(1)	10(1)	-3(1)
P(3)	22(1)	21(1)	23(1)	-1(1)	5(1)	-3(1)
P(4)	20(1)	24(1)	26(1)	-3(1)	7(1)	4(1)
P(5)	21(1)	24(1)	25(1)	1(1)	6(1)	4(1)
P(6)	27(1)	30(1)	23(1)	0(1)	10(1)	2(1)
O(1)	57(3)	29(2)	55(3)	8(2)	16(2)	17(2)
O(2)	19(2)	58(3)	43(3)	0(2)	5(2)	-4(2)
O(3)	22(2)	58(3)	40(3)	2(2)	6(2)	-11(2)
O(4)	46(3)	52(3)	32(2)	5(2)	26(2)	2(2)
O(5)	48(3)	21(2)	48(3)	2(2)	18(2)	8(2)
O(6)	49(3)	43(3)	34(2)	1(2)	25(2)	6(2)
O(7)	22(2)	54(3)	45(3)	3(2)	7(2)	8(2)
O(8)	45(3)	48(3)	34(2)	-5(2)	26(2)	-2(2)
O(9)	43(3)	43(2)	34(2)	3(2)	22(2)	-5(2)
O(10)	43(3)	25(2)	50(3)	-6(2)	15(2)	-3(2)
O(11)	56(3)	33(3)	50(3)	-9(2)	26(2)	-12(2)
O(12)	18(2)	86(4)	47(3)	9(3)	6(2)	6(2)
C(1)	18(3)	42(4)	25(3)	-5(3)	0(2)	1(3)
C(2)	27(3)	32(3)	26(3)	5(2)	9(2)	4(2)
C(3)	30(3)	27(3)	27(3)	9(2)	15(3)	4(2)
C(4)	23(3)	21(3)	29(3)	6(2)	9(2)	0(2)
C(5)	17(3)	33(3)	25(3)	-9(2)	5(2)	-7(2)
C(6)	24(3)	19(3)	29(3)	-3(2)	10(2)	2(2)
C(7)	20(3)	32(3)	30(3)	-7(2)	14(2)	0(2)
C(8)	19(3)	22(3)	33(3)	-4(2)	8(2)	0(2)
C(9)	27(3)	23(3)	26(3)	3(2)	10(2)	1(2)
C(10)	17(3)	31(3)	32(3)	1(2)	10(2)	2(2)
C(11)	22(3)	33(3)	30(3)	0(2)	12(2)	-3(2)
C(12)	27(3)	38(3)	32(3)	-4(3)	13(3)	0(3)
C(25)	54(4)	45(4)	30(3)	9(3)	16(3)	1(3)
C(26)	65(5)	43(4)	41(4)	9(3)	17(4)	-13(3)
C(27)	40(4)	66(5)	31(3)	-15(3)	8(3)	-17(3)

C(28)	40 (4)	104 (7)	43 (4)	-5 (4)	4 (3)	-6 (4)
C(29)	24 (3)	46 (4)	33 (3)	1 (3)	9 (3)	-1 (3)
C(30)	43 (4)	73 (5)	43 (4)	0 (4)	24 (3)	2 (4)
C(31)	29 (3)	34 (3)	39 (3)	16 (3)	5 (3)	-7 (3)
C(32)	42 (4)	48 (4)	36 (4)	17 (3)	-2 (3)	-8 (3)
C(33)	29 (3)	20 (3)	71 (5)	7 (3)	23 (3)	2 (2)
C(34)	39 (4)	28 (3)	108 (7)	14 (4)	36 (4)	7 (3)
C(35)	33 (3)	25 (3)	38 (3)	-1 (2)	15 (3)	-5 (2)
C(36)	71 (5)	36 (4)	42 (4)	-12 (3)	23 (4)	-19 (3)
C(37)	42 (4)	31 (3)	45 (4)	-11 (3)	14 (3)	-6 (3)
C(38)	60 (5)	50 (4)	28 (3)	-7 (3)	0 (3)	-23 (4)
C(39)	26 (3)	32 (3)	33 (3)	5 (3)	1 (3)	-5 (2)
C(40)	41 (4)	41 (4)	26 (3)	8 (3)	3 (3)	-5 (3)
C(41)	23 (3)	34 (3)	31 (3)	2 (2)	11 (2)	-4 (2)
C(42)	29 (3)	37 (3)	38 (3)	8 (3)	8 (3)	-8 (3)
C(43)	19 (3)	24 (3)	46 (4)	-1 (3)	11 (3)	3 (2)
C(44)	43 (4)	30 (3)	63 (5)	-6 (3)	17 (3)	-2 (3)
C(45)	26 (3)	30 (3)	37 (3)	0 (3)	12 (3)	8 (2)
C(46)	30 (3)	38 (3)	42 (4)	10 (3)	14 (3)	10 (3)
C(47)	38 (4)	31 (3)	31 (3)	-10 (3)	11 (3)	8 (3)
C(48)	46 (4)	48 (4)	33 (3)	-12 (3)	10 (3)	4 (3)
C(49)	32 (4)	56 (4)	42 (4)	-6 (3)	7 (3)	9 (3)
C(50)	46 (4)	58 (5)	48 (4)	-22 (4)	-1 (3)	25 (4)
C(51)	34 (4)	42 (4)	49 (4)	-5 (3)	3 (3)	5 (3)
C(52)	60 (5)	50 (4)	26 (3)	-10 (3)	0 (3)	6 (3)
C(53)	56 (5)	54 (5)	53 (5)	24 (4)	10 (4)	9 (4)
C(54)	85 (7)	63 (5)	71 (6)	27 (5)	13 (5)	23 (5)
C(55)	38 (4)	56 (4)	40 (4)	3 (3)	24 (3)	4 (3)
C(56)	41 (4)	59 (4)	41 (4)	-6 (3)	17 (3)	8 (3)
C(57)	57 (4)	31 (3)	23 (3)	5 (2)	13 (3)	0 (3)
C(58)	68 (5)	40 (4)	48 (4)	11 (3)	13 (4)	20 (4)
C(59)	40 (4)	42 (3)	24 (3)	-5 (3)	9 (3)	0 (3)
C(60)	52 (4)	47 (4)	21 (3)	-4 (3)	4 (3)	11 (3)
Fe(9)	15 (1)	21 (1)	22 (1)	5 (1)	5 (1)	0 (1)
Fe(10)	14 (1)	23 (1)	22 (1)	0 (1)	7 (1)	1 (1)
Fe(11)	15 (1)	21 (1)	22 (1)	3 (1)	8 (1)	1 (1)
Fe(12)	16 (1)	20 (1)	20 (1)	2 (1)	8 (1)	3 (1)
Fe(13)	15 (1)	21 (1)	19 (1)	2 (1)	7 (1)	-1 (1)
Fe(14)	16 (1)	19 (1)	21 (1)	0 (1)	8 (1)	1 (1)
Fe(15)	16 (1)	22 (1)	17 (1)	3 (1)	6 (1)	2 (1)
Fe(16)	15 (1)	19 (1)	17 (1)	1 (1)	7 (1)	2 (1)
S(9)	17 (1)	20 (1)	20 (1)	4 (1)	5 (1)	3 (1)
S(10)	15 (1)	23 (1)	25 (1)	5 (1)	9 (1)	3 (1)
S(11)	17 (1)	23 (1)	20 (1)	0 (1)	7 (1)	-2 (1)
S(12)	16 (1)	20 (1)	22 (1)	3 (1)	6 (1)	-1 (1)
S(13)	17 (1)	20 (1)	17 (1)	2 (1)	6 (1)	1 (1)
S(14)	14 (1)	23 (1)	19 (1)	2 (1)	8 (1)	2 (1)
S(15)	15 (1)	20 (1)	19 (1)	2 (1)	6 (1)	0 (1)
S(16)	19 (1)	19 (1)	19 (1)	1 (1)	7 (1)	-1 (1)
Cl(3)	19 (1)	35 (1)	45 (1)	-5 (1)	13 (1)	3 (1)
Cl(4)	22 (1)	30 (1)	41 (1)	-6 (1)	14 (1)	4 (1)
P(7)	23 (1)	24 (1)	21 (1)	3 (1)	6 (1)	-3 (1)
P(8)	23 (1)	23 (1)	26 (1)	3 (1)	9 (1)	1 (1)
P(9)	21 (1)	23 (1)	19 (1)	2 (1)	5 (1)	2 (1)
P(10)	20 (1)	28 (1)	18 (1)	2 (1)	6 (1)	-3 (1)
P(11)	17 (1)	22 (1)	19 (1)	0 (1)	7 (1)	0 (1)
P(12)	18 (1)	21 (1)	22 (1)	3 (1)	6 (1)	-3 (1)
O(13)	40 (3)	25 (2)	50 (3)	10 (2)	7 (2)	7 (2)
O(14)	17 (2)	58 (3)	47 (3)	8 (2)	1 (2)	-7 (2)
O(15)	49 (3)	44 (3)	35 (2)	10 (2)	28 (2)	11 (2)
O(16)	24 (2)	49 (3)	43 (3)	-2 (2)	11 (2)	-12 (2)

O(17)	55(3)	41(2)	40(3)	1(2)	34(2)	5(2)
O(18)	41(3)	22(2)	46(3)	4(2)	15(2)	7(2)
O(19)	19(2)	58(3)	38(2)	1(2)	3(2)	-4(2)
O(20)	52(3)	31(2)	43(3)	6(2)	13(2)	16(2)
O(21)	43(3)	23(2)	39(2)	5(2)	18(2)	8(2)
O(22)	37(2)	48(3)	25(2)	0(2)	19(2)	0(2)
O(23)	35(2)	48(3)	30(2)	3(2)	20(2)	-1(2)
O(24)	21(2)	50(3)	37(2)	2(2)	5(2)	-8(2)
C(13)	30(3)	36(3)	22(3)	2(2)	10(2)	-7(3)
C(14)	25(3)	32(3)	28(3)	10(2)	7(2)	3(2)
C(15)	24(3)	25(3)	31(3)	5(2)	8(2)	1(2)
C(16)	25(3)	28(3)	30(3)	9(2)	18(3)	4(2)
C(17)	26(3)	20(3)	31(3)	1(2)	11(2)	5(2)
C(18)	20(3)	29(3)	21(3)	-2(2)	10(2)	-4(2)
C(19)	23(3)	34(3)	21(3)	9(2)	9(2)	8(2)
C(20)	22(3)	37(3)	14(3)	0(2)	5(2)	2(2)
C(21)	12(2)	33(3)	21(3)	-7(2)	9(2)	-1(2)
C(22)	16(3)	23(3)	29(3)	0(2)	8(2)	1(2)
C(23)	18(3)	23(3)	27(3)	3(2)	7(2)	-1(2)
C(24)	28(3)	25(3)	23(3)	8(2)	13(2)	2(2)
C(61)	43(4)	36(3)	31(3)	-3(3)	15(3)	-12(3)
C(62)	63(5)	47(4)	32(3)	-7(3)	20(3)	-18(3)
C(63)	38(4)	34(3)	28(3)	4(3)	10(3)	-3(3)
C(64)	36(4)	60(4)	33(3)	17(3)	4(3)	5(3)
C(65)	27(3)	42(3)	38(3)	-1(3)	17(3)	-3(3)
C(66)	32(3)	51(4)	34(3)	-5(3)	16(3)	-15(3)
C(67)	20(3)	27(3)	50(4)	-2(3)	11(3)	3(2)
C(68)	28(4)	29(3)	88(6)	7(3)	8(4)	3(3)
C(69)	21(3)	25(3)	40(3)	-1(2)	17(2)	-5(2)
C(70)	49(4)	33(3)	42(4)	-9(3)	11(3)	-14(3)
C(71)	46(4)	35(3)	35(3)	8(3)	13(3)	4(3)
C(72)	49(4)	58(4)	31(3)	7(3)	6(3)	16(3)
C(73)	34(4)	71(5)	24(3)	2(3)	9(3)	3(3)
C(74)	53(5)	75(5)	41(4)	-27(4)	18(3)	-6(4)
C(75)	26(3)	29(3)	40(3)	9(3)	1(3)	-3(2)
C(76)	51(5)	81(5)	33(4)	9(4)	5(3)	-40(4)
C(77)	28(3)	31(3)	56(4)	-4(3)	9(3)	6(3)
C(78)	27(3)	32(3)	52(4)	4(3)	11(3)	4(3)
C(79)	23(3)	37(3)	29(3)	0(2)	13(2)	0(2)
C(80)	42(4)	74(5)	35(4)	-8(3)	25(3)	-3(4)
C(81)	29(3)	42(3)	25(3)	-7(3)	10(2)	-8(3)
C(82)	32(4)	73(5)	33(4)	-5(3)	-3(3)	-7(3)
C(83)	36(4)	44(4)	32(3)	7(3)	10(3)	-2(3)
C(84)	49(4)	35(4)	49(4)	16(3)	12(3)	-12(3)
C(85)	25(3)	26(3)	26(3)	0(2)	6(2)	-2(2)
C(86)	51(4)	33(3)	31(3)	-4(3)	14(3)	0(3)
C(87)	24(3)	33(3)	23(3)	3(2)	8(2)	3(2)
C(88)	36(4)	33(3)	30(3)	6(3)	8(3)	3(3)
C(89)	18(3)	45(3)	30(3)	-3(3)	13(2)	1(2)
C(90)	18(3)	44(4)	42(3)	-4(3)	12(3)	-3(3)
C(91)	23(3)	26(3)	23(3)	3(2)	6(2)	-3(2)
C(92)	35(3)	36(3)	27(3)	-2(3)	9(3)	-9(3)
C(93)	30(3)	27(3)	26(3)	8(2)	8(2)	-5(2)
C(94)	41(4)	38(3)	26(3)	6(3)	0(3)	-8(3)
C(95)	22(3)	24(3)	37(3)	-1(2)	13(2)	-1(2)
C(96)	30(3)	32(3)	52(4)	8(3)	16(3)	9(3)