Biomimics of [FeFe]-hydrogenases incorporating redox-active ligands: Synthesis, redox and spectroelectrochemistry of diiron-dithiolate complexes with ferrocenyl-diphosphines as Fe_4S_4 surrogates

Georgia Orton[a], Shishir Ghosh[a,b], Lucy Alker[b], Jagodish C. Sarker[a], David Pugh[a], Michael G. Richmond[c], František Hartl[d] and Graeme Hogarth[a]*,

[a]*Department of Chemistry, King's College London, 7 Trinity Street, London, SE1 1DB, U.K.*

[b]*Department of Chemistry, University College London, 20 Gordon Street, London, WC1H 0AJ, U.K.*

[c] *Department of Chemistry, University of North Texas, 1155 Union Circle, Box 305070, Denton, Texas 76203, USA*

[d] *Department of Chemistry, University of Reading, Whiteknights, Reading RG6 6AD, U.K.*

Electronic supplementary information

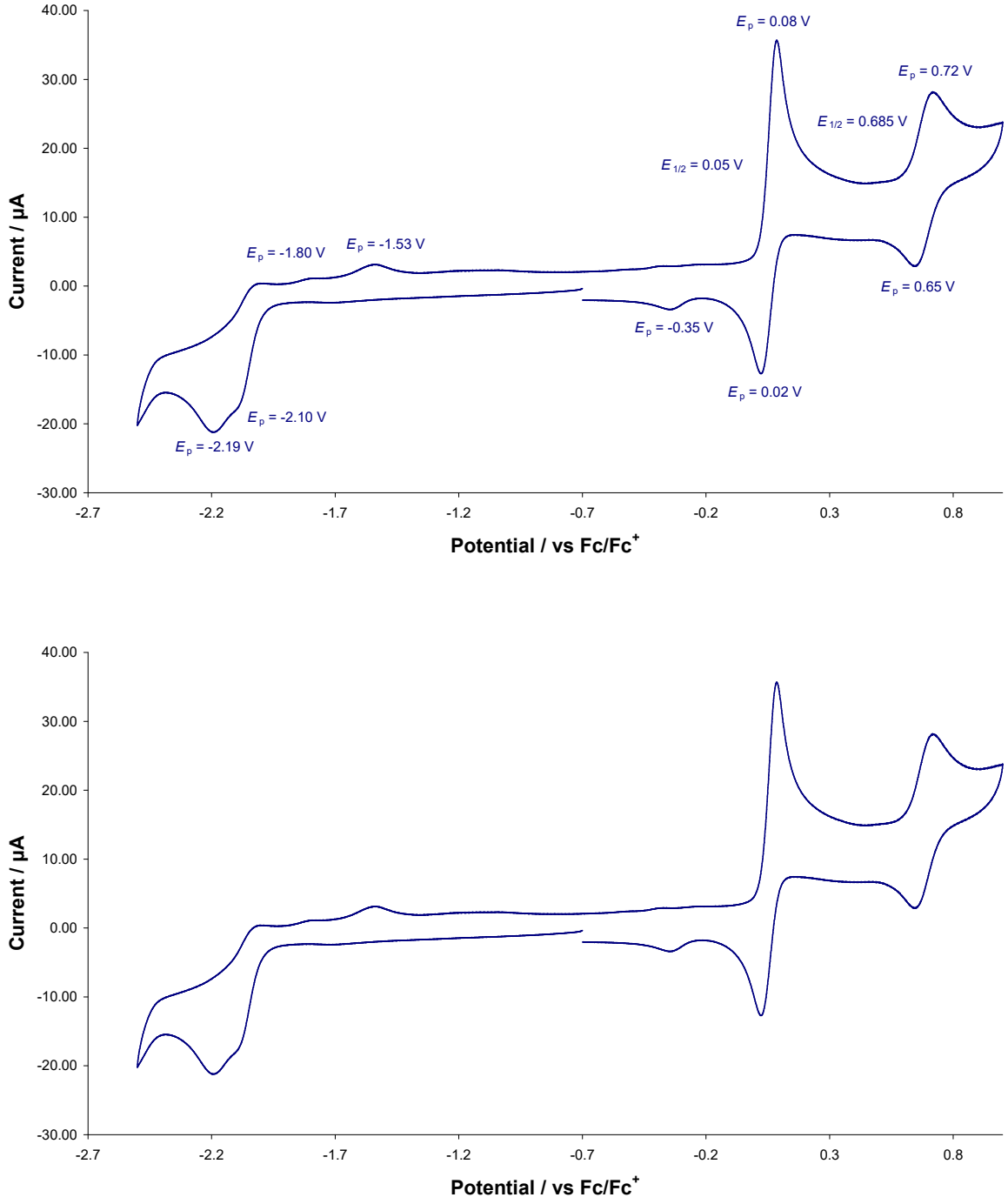
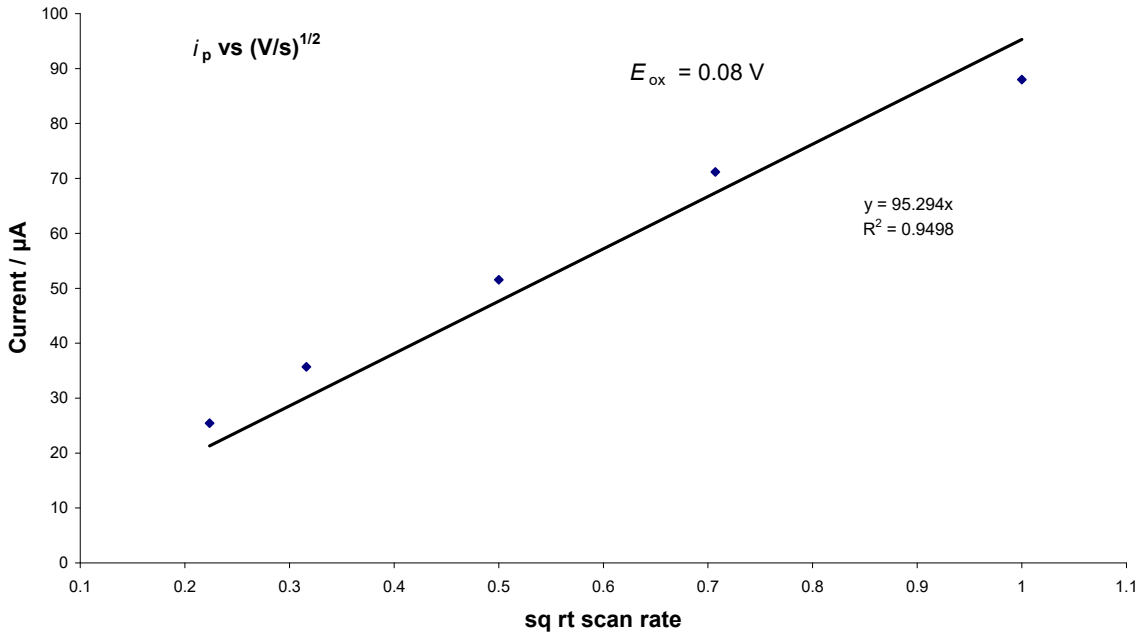


Fig. S1 CV of **1** in MeCN (1 mM solution, supporting electrolyte $[NBu_4][PF_6]$, scan rate 0.1 Vs^{-1}, glassy carbon electrode, potential vs Fc^+/Fc) – CV showing peak potentials on the figure (Top); CV without showing peak potentials (Bottom)



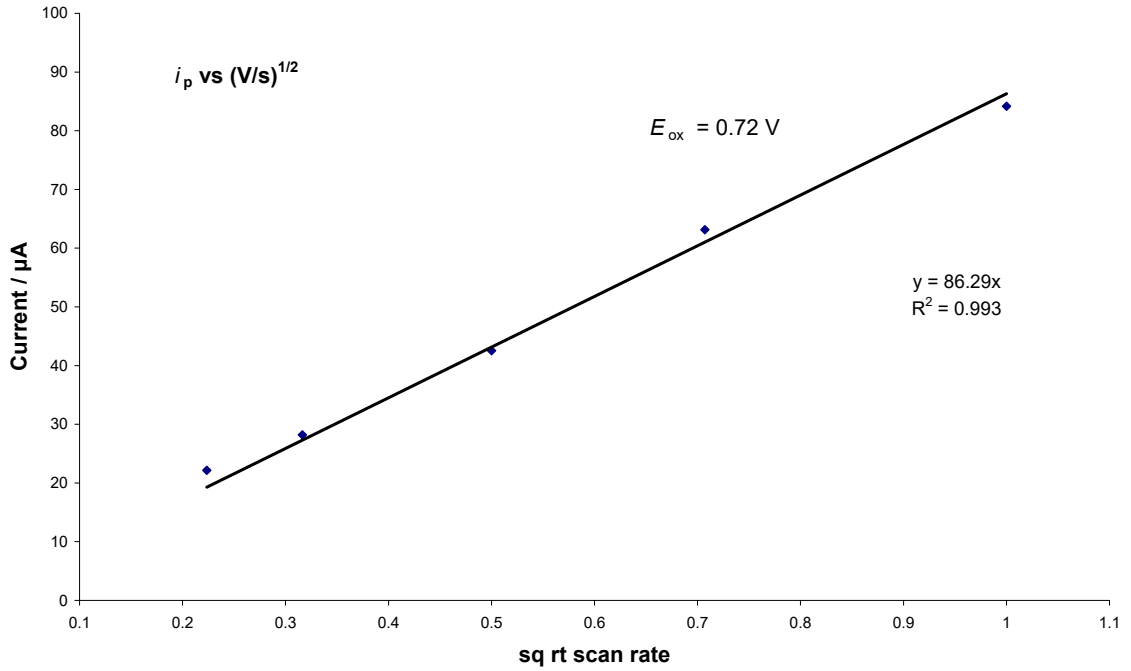


Fig. S2 Scan rate dependence of the oxidation features [at 0.08 V (a) and at 0.72 V (b)] features in the cyclic voltamograms of **1** in MeCN (1 mM solution, supporting electrolyte $[NBu_4][PF_6]$, glassy carbon electrode, potential vs Fc^+/Fc)

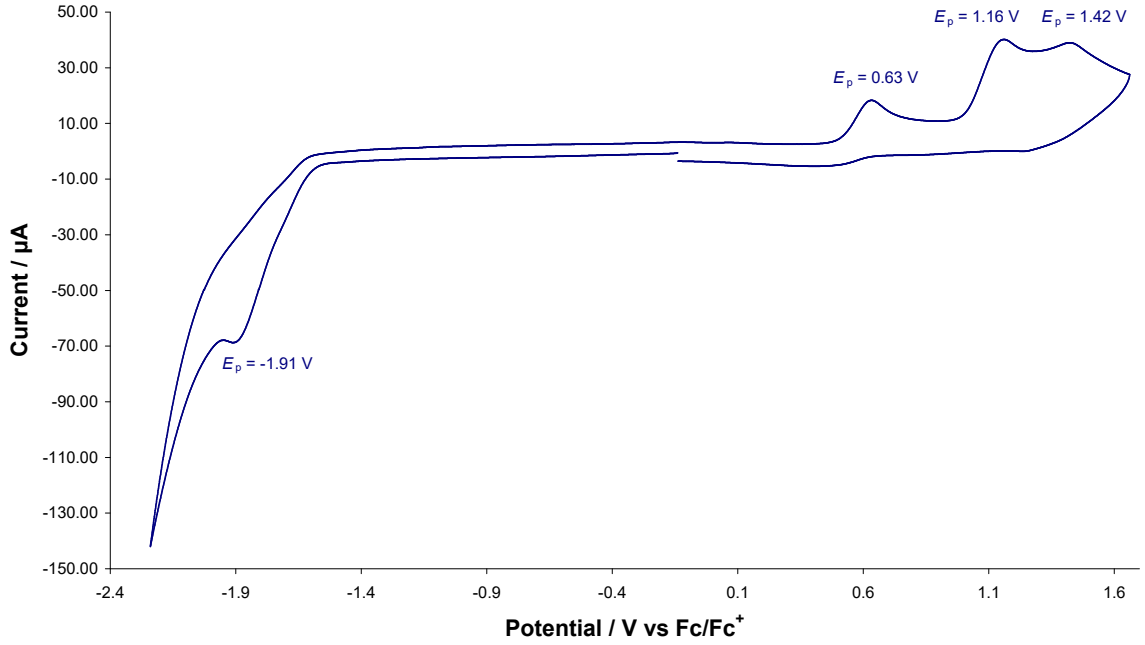


Fig. S3 CV of **1** in CH_2Cl_2 at scan rate 0.1 V/s (1mM solution, supporting electrolyte $[NBu_4][PF_6]$, glassy carbon electrode, potential *vs* Fc^+/Fc).

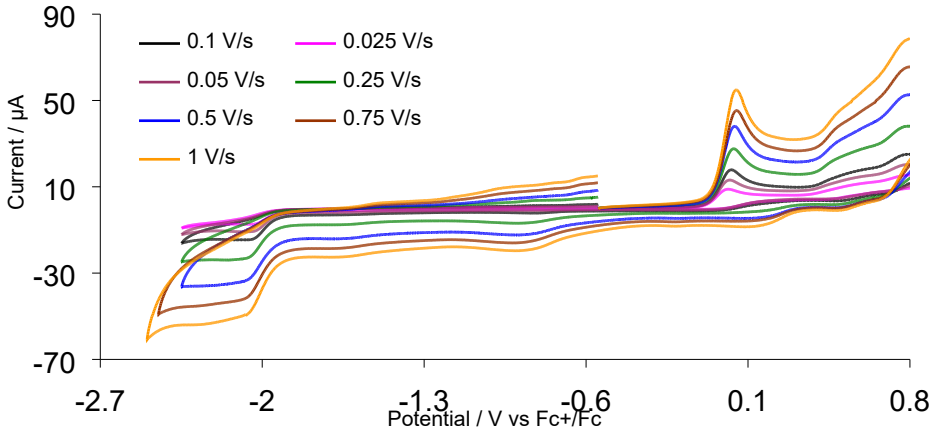


Fig. S4. CVs of **4c** in MeCN at various scan rates (1mM solution, supporting electrolyte $[NBu_4][PF_6]$, glassy carbon electrode, potential *vs* Fc^+/Fc).

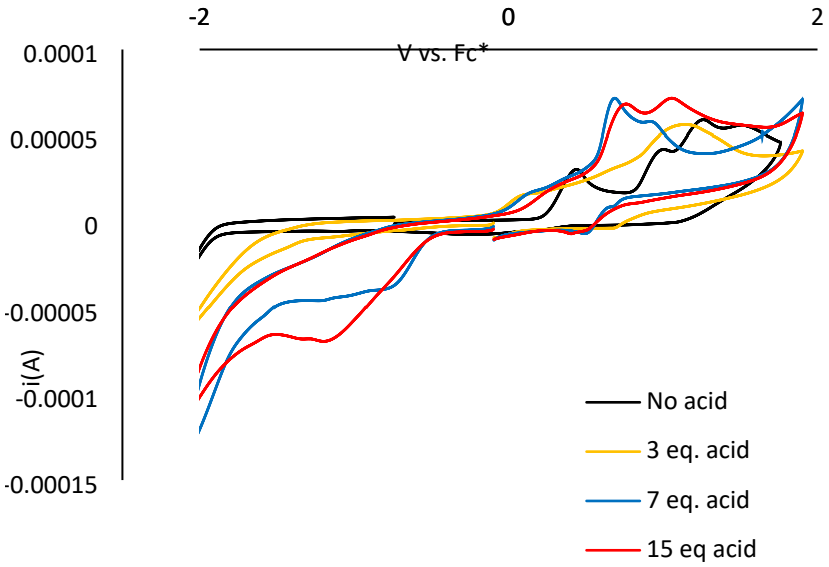


Fig. S5 CVs of **2** in the absence and presence of varying molar equivalents of CF_3CO_2H (1 mM solution in CH_2Cl_2, supporting electrolyte $[NBu_4][PF_6]$, scan rate 0.1 V s^{-1}, glassy carbon electrode, potential vs. $Fc^{*+/0}$)

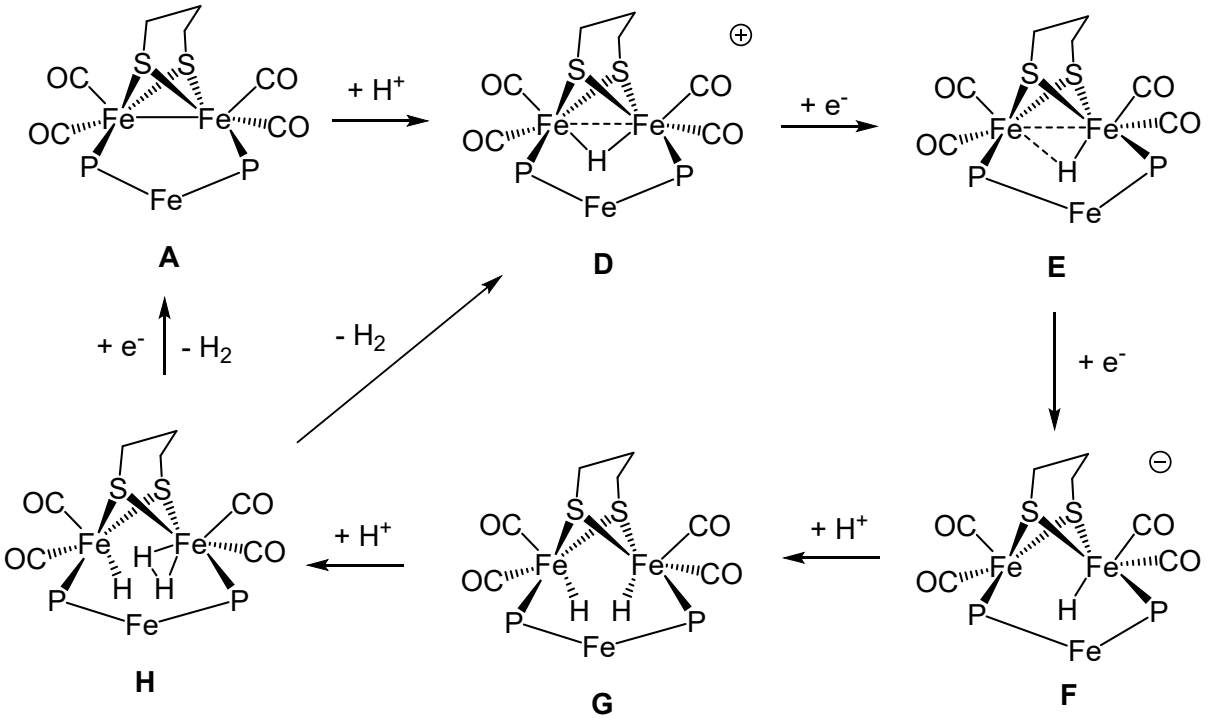


Fig. S6. Alternative reaction pathway for proton-reduction catalysis by **1**

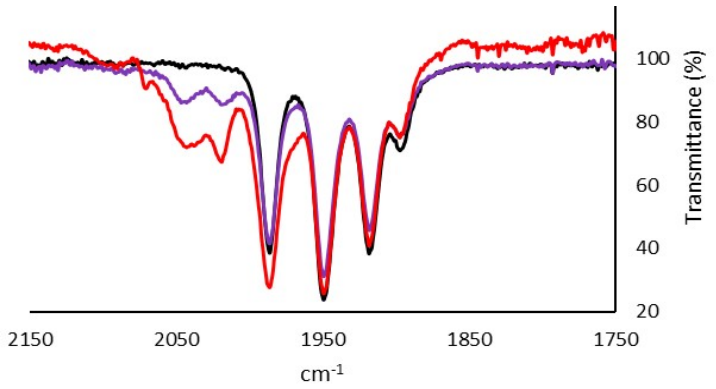


Fig. S7 spectrum in CH_2Cl_2 of **1** (black), after addition of excess [TA][PF_6] (purple), followed by addition of H_2 (red)

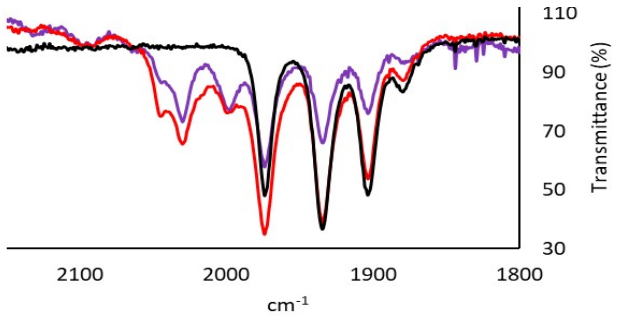


Fig. S8 IR spectrum in CH_2Cl_2 of **2** (black), after addition of excess [TA][PF_6] (purple), followed by addition of H_2 (red)

Crystal data and structure refinement for **1**

Identification code	str0562	
Chemical formula	$C_{41.50}H_{35}ClFe_3O_4P_2S_2$	
Formula weight	926.75	
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 $F^2>2\sigma$	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 [$F^2>2\sigma$]	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}	

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)

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

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)

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)

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

Crystal data and structure refinement for 3

Identification code	2021NCS0348r1
Empirical formula	$C_{40}H_{32}Fe_3O_4P_2S_2$
Formula weight	870.26
Temperature/K	100.00(11)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	15.4691(8)
b/Å	11.0407(4)
c/Å	22.8109(10)
α/°	90
β/°	106.043(4)
γ/°	90
Volume/Å^3	3744.1(3)
Z	4
ρ_{calc}g/cm^3	1.544
μ/mm^{-1}	11.381
F(000)	1776.0
Crystal size/mm^3	0.152 × 0.081 × 0.023
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.192 to 140.546
Index ranges	-18 ≤ h ≤ 17, -13 ≤ k ≤ 13, -22 ≤ l ≤ 27
Reflections collected	21109
Independent reflections	6780 [R_{int} = 0.0755, R_{sigma} = 0.0756]
Data/restraints/parameters	6780/0/460
Goodness-of-fit on F^2	1.029
Final R indexes [I>=2σ (I)]	R_1 = 0.0722, wR_2 = 0.1740
Final R indexes [all data]	R_1 = 0.0941, wR_2 = 0.1864
Largest diff. peak/hole / e Å^{-3}	1.35/-0.73

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 2021NCS0348r1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Fe1	2265.5(6)	1320.6(8)	6362.9(4)	20.5(2)
Fe2	3969.5(6)	1879.3(8)	6830.0(4)	22.3(2)
Fe3	2854.9(7)	4983.9(8)	5574.8(4)	27.7(3)
S1	3231.8(11)	362.3(13)	7134.3(7)	28.5(4)
S2	3388.6(11)	946.8(13)	5938.0(6)	25.3(3)
P1	1433.7(10)	2690.5(13)	5712.9(6)	20.7(3)
P2	4643.5(11)	3219.1(14)	6350.0(7)	25.8(4)
O1	1078(4)	-697(4)	5828(2)	42.3(13)
O2	1396(3)	2054(5)	7291(2)	41.0(12)

O3	3525(3)	3364(4)	7767.5(19)	33.9(11)
O4	5669(3)	820(5)	7538(2)	46.1(13)
C1	1546(5)	100(6)	6041(3)	30.0(15)
C2	1744(4)	1811(6)	6927(3)	27.4(14)
C3	3715(4)	2834(6)	7393(3)	25.3(13)
C4	5030(5)	1280(6)	7247(3)	34.0(16)
C5	3543(6)	-964(6)	6765(3)	41.6(18)
C6	3667(5)	-644(6)	6142(3)	36.9(16)
C7	313(4)	2816(5)	5842(3)	23.3(12)
C8	124(5)	3743(5)	6203(3)	29.0(14)
C9	-717(5)	3802(6)	6315(3)	35.6(16)
C10	-1366(5)	2945(7)	6063(3)	37.1(16)
C11	-1178(5)	2020(6)	5710(3)	34.5(16)
C12	-344(4)	1946(6)	5604(3)	29.6(14)
C13	1117(4)	2397(5)	4887(3)	22.4(12)
C14	453(4)	3071(5)	4491(3)	25.4(13)
C15	237(4)	2872(6)	3865(3)	29.2(14)
C16	672(5)	1993(6)	3633(3)	32.8(15)
C17	1316(5)	1285(6)	4021(3)	31.5(15)
C18	1548(4)	1496(5)	4646(3)	27.4(14)
C19	1788(4)	4260(5)	5792(2)	21.6(12)
C20	1513(5)	5264(5)	5380(3)	29.5(14)
C21	1969(5)	6318(6)	5663(3)	36.7(17)
C22	2535(5)	5990(6)	6251(3)	33.4(16)
C23	2420(4)	4733(5)	6335(3)	26.9(14)
C24	4037(4)	4070(6)	5688(3)	27.6(13)
C25	3367(5)	3617(6)	5172(3)	31.2(15)
C26	3055(5)	4577(7)	4747(3)	37.9(17)
C27	3542(6)	5646(7)	4997(3)	46(2)
C28	4145(5)	5341(6)	5569(3)	39.2(17)
C29	5446(5)	2358(6)	6045(3)	31.5(14)
C30	6251(5)	1946(7)	6430(4)	43.3(18)
C31	6787(5)	1150(8)	6222(4)	49(2)
C32	6513(6)	724(8)	5632(4)	50(2)
C33	5742(5)	1136(7)	5248(4)	45.5(19)
C34	5201(5)	1941(6)	5445(3)	35.5(16)
C35	5337(5)	4443(6)	6785(3)	33.1(15)
C36	6105(6)	4838(8)	6645(4)	57(2)
C37	6599(7)	5858(9)	6939(5)	67(3)
C38	6289(6)	6474(8)	7369(4)	53(2)
C39	5530(5)	6095(7)	7515(3)	43.1(18)
C40	5041(5)	5085(6)	7217(3)	32.8(15)

Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 2021NCS0348r1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe1	29.7(5)	14.1(4)	16.2(4)	0.8(3)	3.8(4)	-2.1(4)
Fe2	30.5(5)	19.3(5)	15.6(4)	0.4(3)	3.7(4)	-0.3(4)
Fe3	40.5(6)	15.0(5)	22.6(5)	2.8(4)	0.2(4)	-7.0(4)
S1	40.4(9)	20.3(7)	23.4(7)	6.0(6)	6.6(6)	-0.5(6)
S2	35.4(8)	20.1(7)	19.8(7)	-1.9(5)	6.8(6)	-2.1(6)
P1	31.7(8)	13.6(7)	15.3(7)	-1.2(5)	3.9(6)	-2.3(6)
P2	33.8(9)	21.0(8)	20.9(7)	-4.1(6)	4.7(6)	-4.4(6)
O1	62(3)	22(2)	34(3)	1(2)	-1(2)	-15(2)
O2	47(3)	54(3)	24(2)	-2(2)	13(2)	7(2)
O3	42(3)	35(3)	22(2)	-7(2)	4(2)	3(2)
O4	42(3)	52(3)	42(3)	15(3)	6(2)	19(3)
C1	45(4)	19(3)	19(3)	6(2)	-3(3)	-3(3)
C2	26(3)	25(3)	28(3)	7(3)	3(3)	3(3)
C3	28(3)	24(3)	21(3)	4(3)	0(2)	-2(2)
C4	49(4)	19(3)	38(4)	5(3)	19(3)	2(3)
C5	61(5)	18(3)	42(4)	6(3)	8(3)	10(3)
C6	56(5)	15(3)	43(4)	0(3)	19(3)	9(3)
C7	27(3)	20(3)	24(3)	3(2)	8(2)	1(2)
C8	46(4)	18(3)	20(3)	-1(2)	6(3)	2(3)
C9	54(5)	25(3)	30(3)	3(3)	15(3)	12(3)
C10	38(4)	38(4)	38(4)	16(3)	15(3)	7(3)
C11	39(4)	25(3)	35(4)	3(3)	3(3)	-1(3)
C12	41(4)	22(3)	23(3)	3(2)	4(3)	0(3)
C13	31(3)	14(3)	20(3)	-1(2)	4(2)	-4(2)
C14	35(3)	16(3)	25(3)	-6(2)	6(3)	0(3)
C15	33(3)	22(3)	26(3)	1(2)	-3(3)	2(3)
C16	48(4)	30(3)	15(3)	-4(3)	-1(3)	-4(3)
C17	48(4)	20(3)	21(3)	-5(2)	2(3)	7(3)
C18	38(4)	20(3)	18(3)	-1(2)	-1(3)	5(3)
C19	27(3)	18(3)	20(3)	-4(2)	7(2)	-7(2)
C20	39(4)	17(3)	27(3)	0(2)	1(3)	-1(3)
C21	55(5)	12(3)	35(4)	2(3)	-1(3)	2(3)
C22	47(4)	16(3)	29(3)	-9(3)	-4(3)	-7(3)
C23	43(4)	18(3)	18(3)	2(2)	5(3)	5(3)
C24	27(3)	28(3)	29(3)	4(3)	11(3)	-6(3)
C25	47(4)	25(3)	22(3)	1(3)	11(3)	-8(3)
C26	54(5)	38(4)	21(3)	10(3)	9(3)	-3(3)
C27	68(5)	30(4)	38(4)	19(3)	12(4)	-13(4)
C28	50(4)	28(4)	38(4)	5(3)	10(3)	-17(3)
C29	41(4)	25(3)	33(3)	-6(3)	17(3)	-3(3)
C30	42(4)	45(4)	45(4)	-6(3)	15(3)	-4(4)
C31	40(4)	54(5)	54(5)	-7(4)	16(4)	3(4)

Anisotropic Displacement Parameters ($Å^2×10^3$) for 2021NCS0348r1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C32	46(5)	44(5)	65(5)	-12(4)	21(4)	0(4)
C33	53(5)	42(4)	48(4)	-18(4)	25(4)	-15(4)
C34	40(4)	35(4)	37(4)	-6(3)	19(3)	-11(3)
C35	36(4)	31(4)	30(3)	-7(3)	4(3)	-7(3)
C36	71(6)	50(5)	53(5)	-22(4)	24(4)	-24(4)
C37	73(6)	60(6)	75(6)	-23(5)	34(5)	-37(5)
C38	63(6)	39(4)	49(5)	-16(4)	3(4)	-18(4)
C39	56(5)	32(4)	37(4)	-15(3)	7(3)	-5(4)
C40	39(4)	26(3)	31(3)	-4(3)	6(3)	-3(3)

Bond Lengths for 2021NCS0348r1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	Fe2	2.6289(13)	C7	C8	1.394(9)
Fe1	S1	2.2353(17)	C7	C12	1.394(8)
Fe1	S2	2.2491(19)	C8	C9	1.394(10)
Fe1	P1	2.2556(17)	C9	C10	1.384(10)
Fe1	C1	1.772(6)	C10	C11	1.381(10)
Fe1	C2	1.780(7)	C11	C12	1.379(10)
Fe2	S1	2.2421(18)	C13	C14	1.383(8)
Fe2	S2	2.2354(16)	C13	C18	1.393(9)
Fe2	P2	2.2595(19)	C14	C15	1.392(8)
Fe2	C3	1.788(7)	C15	C16	1.368(9)
Fe2	C4	1.781(7)	C16	C17	1.378(9)
Fe3	C19	2.014(6)	C17	C18	1.390(8)
Fe3	C20	2.023(7)	C19	C20	1.439(8)
Fe3	C21	2.059(7)	C19	C23	1.447(8)
Fe3	C22	2.070(7)	C20	C21	1.419(9)
Fe3	C23	2.046(6)	C21	C22	1.432(9)
Fe3	C24	2.042(7)	C22	C23	1.419(9)
Fe3	C25	2.037(7)	C24	C25	1.427(9)
Fe3	C26	2.045(7)	C24	C28	1.448(9)
Fe3	C27	2.042(7)	C25	C26	1.427(9)
Fe3	C28	2.037(8)	C26	C27	1.431(10)
S1	C5	1.820(7)	C27	C28	1.419(10)
S2	C6	1.838(6)	C29	C30	1.387(10)
P1	C7	1.843(6)	C29	C34	1.393(9)
P1	C13	1.839(6)	C30	C31	1.379(11)
P1	C19	1.812(6)	C31	C32	1.378(11)
P2	C24	1.805(6)	C32	C33	1.348(12)
P2	C29	1.845(7)	C33	C34	1.380(10)

Bond Lengths for 2021NCS0348r1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P2	C35	1.837(7)	C35	C36	1.383(11)
O1	C1	1.158(8)	C35	C40	1.390(10)
O2	C2	1.140(8)	C36	C37	1.421(11)
O3	C3	1.138(8)	C37	C38	1.383(13)
O4	C4	1.146(8)	C38	C39	1.371(12)
C5	C6	1.526(10)	C39	C40	1.412(9)

Bond Angles for 2021NCS0348r1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
S1	Fe1	Fe2	54.16(5)	C19	P1	Fe1	118.29(19)
S1	Fe1	S2	79.88(6)	C19	P1	C7	100.6(3)
S1	Fe1	P1	166.12(7)	C19	P1	C13	105.0(3)
S2	Fe1	Fe2	53.87(5)	C24	P2	Fe2	122.9(2)
S2	Fe1	P1	102.01(6)	C24	P2	C29	101.6(3)
P1	Fe1	Fe2	115.79(6)	C24	P2	C35	99.2(3)
C1	Fe1	Fe2	142.2(2)	C29	P2	Fe2	107.1(2)
C1	Fe1	S1	99.96(19)	C35	P2	Fe2	119.9(2)
C1	Fe1	S2	98.8(2)	C35	P2	C29	103.2(3)
C1	Fe1	P1	93.4(2)	O1	C1	Fe1	179.6(7)
C1	Fe1	C2	99.9(3)	O2	C2	Fe1	175.8(6)
C2	Fe1	Fe2	103.8(2)	O3	C3	Fe2	174.6(6)
C2	Fe1	S1	85.01(19)	O4	C4	Fe2	173.7(6)
C2	Fe1	S2	157.7(2)	C6	C5	S1	111.3(4)
C2	Fe1	P1	88.91(19)	C5	C6	S2	112.1(5)
S1	Fe2	Fe1	53.92(5)	C8	C7	P1	120.7(5)
S1	Fe2	P2	168.99(7)	C12	C7	P1	120.1(5)
S2	Fe2	Fe1	54.35(5)	C12	C7	C8	119.1(6)
S2	Fe2	S1	80.03(6)	C9	C8	C7	120.1(6)
S2	Fe2	P2	89.06(6)	C10	C9	C8	119.9(6)
P2	Fe2	Fe1	120.16(6)	C11	C10	C9	120.1(7)
C3	Fe2	Fe1	92.00(19)	C12	C11	C10	120.3(6)
C3	Fe2	S1	89.2(2)	C11	C12	C7	120.5(6)
C3	Fe2	S2	144.4(2)	C14	C13	P1	120.9(5)
C3	Fe2	P2	100.6(2)	C14	C13	C18	118.5(5)
C4	Fe2	Fe1	143.3(2)	C18	C13	P1	120.6(4)
C4	Fe2	S1	91.7(2)	C13	C14	C15	120.6(6)
C4	Fe2	S2	113.2(2)	C16	C15	C14	120.4(6)
C4	Fe2	P2	91.2(2)	C15	C16	C17	119.9(6)
C4	Fe2	C3	100.9(3)	C16	C17	C18	120.0(6)
C19	Fe3	C20	41.8(2)	C17	C18	C13	120.6(6)
C19	Fe3	C21	69.3(3)	P1	C19	Fe3	126.9(3)

Bond Angles for 2021NCS0348r1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C19	Fe3	C22	69.4(2)	C20	C19	Fe3	69.4(4)
C19	Fe3	C23	41.8(2)	C20	C19	P1	130.2(4)
C19	Fe3	C24	122.6(2)	C20	C19	C23	106.8(5)
C19	Fe3	C25	105.3(3)	C23	C19	Fe3	70.3(3)
C19	Fe3	C26	118.9(3)	C23	C19	P1	123.0(4)
C19	Fe3	C27	155.2(3)	C19	C20	Fe3	68.8(4)
C19	Fe3	C28	161.5(3)	C21	C20	Fe3	71.0(4)
C20	Fe3	C21	40.7(2)	C21	C20	C19	108.3(5)
C20	Fe3	C22	68.8(3)	C20	C21	Fe3	68.3(4)
C20	Fe3	C23	69.4(3)	C20	C21	C22	108.5(5)
C20	Fe3	C24	158.8(3)	C22	C21	Fe3	70.1(4)
C20	Fe3	C25	121.2(3)	C21	C22	Fe3	69.3(4)
C20	Fe3	C26	103.8(3)	C23	C22	Fe3	68.9(4)
C20	Fe3	C27	119.3(3)	C23	C22	C21	107.9(5)
C20	Fe3	C28	156.4(3)	C19	C23	Fe3	68.0(3)
C21	Fe3	C22	40.6(3)	C22	C23	Fe3	70.8(4)
C23	Fe3	C21	68.3(3)	C22	C23	C19	108.5(5)
C23	Fe3	C22	40.3(2)	P2	C24	Fe3	127.1(3)
C24	Fe3	C21	159.8(3)	C25	C24	Fe3	69.4(4)
C24	Fe3	C22	124.1(3)	C25	C24	P2	126.8(5)
C24	Fe3	C23	108.6(2)	C25	C24	C28	106.3(6)
C24	Fe3	C26	69.5(3)	C28	C24	Fe3	69.0(4)
C24	Fe3	C27	69.6(3)	C28	C24	P2	127.0(5)
C25	Fe3	C21	157.8(3)	C24	C25	Fe3	69.7(4)
C25	Fe3	C22	159.5(3)	C24	C25	C26	109.4(6)
C25	Fe3	C23	122.8(2)	C26	C25	Fe3	69.8(4)
C25	Fe3	C24	40.9(3)	C25	C26	Fe3	69.2(4)
C25	Fe3	C26	40.9(3)	C25	C26	C27	107.4(6)
C25	Fe3	C27	68.8(3)	C27	C26	Fe3	69.4(4)
C26	Fe3	C21	121.4(3)	C26	C27	Fe3	69.6(4)
C26	Fe3	C22	159.2(3)	C28	C27	Fe3	69.4(4)
C26	Fe3	C23	157.2(3)	C28	C27	C26	108.1(6)
C27	Fe3	C21	106.6(3)	C24	C28	Fe3	69.4(4)
C27	Fe3	C22	124.3(3)	C27	C28	Fe3	69.9(4)
C27	Fe3	C23	161.3(3)	C27	C28	C24	108.8(6)
C27	Fe3	C26	41.0(3)	C30	C29	P2	120.6(5)
C28	Fe3	C21	122.8(3)	C30	C29	C34	117.8(7)
C28	Fe3	C22	109.7(3)	C34	C29	P2	120.8(5)
C28	Fe3	C23	125.7(3)	C31	C30	C29	120.7(7)
C28	Fe3	C24	41.6(3)	C32	C31	C30	120.1(8)
C28	Fe3	C25	68.7(3)	C33	C32	C31	119.8(8)
C28	Fe3	C26	68.8(3)	C32	C33	C34	120.9(7)
C28	Fe3	C27	40.7(3)	C33	C34	C29	120.5(7)

Bond Angles for 2021NCS0348r1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Fe1	S1	Fe2	71.91(5)	C36	C35	P2	121.2(6)
C5	S1	Fe1	102.8(2)	C36	C35	C40	118.4(6)
C5	S1	Fe2	103.6(3)	C40	C35	P2	120.0(5)
Fe2	S2	Fe1	71.78(5)	C35	C36	C37	121.6(8)
C6	S2	Fe1	102.8(2)	C38	C37	C36	118.5(8)
C6	S2	Fe2	101.7(2)	C39	C38	C37	120.7(7)
C7	P1	Fe1	109.65(19)	C38	C39	C40	120.3(7)
C13	P1	Fe1	119.8(2)	C35	C40	C39	120.4(7)
C13	P1	C7	100.4(3)				

Torsion Angles for 2021NCS0348r1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Fe1	S1	C5	C6	40.2(6)	C13	P1	C19	C20	28.9(7)
Fe1	S2	C6	C5	-33.6(6)	C13	P1	C19	C23	-153.6(5)
Fe1	P1	C7	C8	97.6(5)	C13	C14	C15	C16	0.9(10)
Fe1	P1	C7	C12	-79.2(5)	C14	C13	C18	C17	0.2(9)
Fe1	P1	C13	C14	165.5(4)	C14	C15	C16	C17	1.2(10)
Fe1	P1	C13	C18	-15.1(6)	C15	C16	C17	C18	-2.5(10)
Fe1	P1	C19	Fe3	72.3(4)	C16	C17	C18	C13	1.8(10)
Fe1	P1	C19	C20	165.7(5)	C18	C13	C14	C15	-1.5(9)
Fe1	P1	C19	C23	-16.9(6)	C19	P1	C7	C8	-27.8(5)
Fe2	S1	C5	C6	-33.9(6)	C19	P1	C7	C12	155.4(5)
Fe2	S2	C6	C5	40.1(6)	C19	P1	C13	C14	-58.5(6)
Fe2	P2	C24	Fe3	46.6(5)	C19	P1	C13	C18	120.8(5)
Fe2	P2	C24	C25	-44.2(7)	C19	C20	C21	Fe3	58.9(5)
Fe2	P2	C24	C28	137.0(6)	C19	C20	C21	C22	0.2(8)
Fe2	P2	C29	C30	-74.6(6)	C20	C19	C23	Fe3	-60.1(4)
Fe2	P2	C29	C34	95.1(6)	C20	C19	C23	C22	-0.8(7)
Fe2	P2	C35	C36	144.1(6)	C20	C21	C22	Fe3	57.6(5)
Fe2	P2	C35	C40	-43.4(6)	C20	C21	C22	C23	-0.7(9)
Fe3	C19	C20	C21	-60.3(5)	C21	C22	C23	Fe3	58.5(5)
Fe3	C19	C23	C22	59.3(5)	C21	C22	C23	C19	0.9(8)
Fe3	C20	C21	C22	-58.7(5)	C23	C19	C20	Fe3	60.7(4)
Fe3	C21	C22	C23	-58.3(5)	C23	C19	C20	C21	0.4(8)
Fe3	C22	C23	C19	-57.6(4)	C24	P2	C29	C30	155.3(6)
Fe3	C24	C25	C26	58.7(5)	C24	P2	C29	C34	-35.0(6)
Fe3	C24	C28	C27	-58.9(6)	C24	P2	C35	C36	-79.1(7)
Fe3	C25	C26	C27	59.1(5)	C24	P2	C35	C40	93.3(6)
Fe3	C26	C27	C28	59.0(6)	C24	C25	C26	Fe3	-58.6(5)
Fe3	C27	C28	C24	58.6(5)	C24	C25	C26	C27	0.5(8)
S1	C5	C6	S2	-3.9(8)	C25	C24	C28	Fe3	59.7(5)

Torsion Angles for 2021NCS0348r1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
P1	C7	C8	C9	-177.7(5)	C25	C24	C28	C27	0.8(8)
P1	C7	C12	C11	178.6(5)	C25	C26	C27	Fe3	-59.0(5)
P1	C13	C14	C15	177.8(5)	C25	C26	C27	C28	0.0(9)
P1	C13	C18	C17	-179.2(5)	C26	C27	C28	Fe3	-59.1(6)
P1	C19	C20	Fe3	-121.6(6)	C26	C27	C28	C24	-0.5(9)
P1	C19	C20	C21	178.2(5)	C28	C24	C25	Fe3	-59.4(5)
P1	C19	C23	Fe3	121.9(5)	C28	C24	C25	C26	-0.8(8)
P1	C19	C23	C22	-178.8(5)	C29	P2	C24	Fe3	165.9(4)
P2	C24	C25	Fe3	121.6(5)	C29	P2	C24	C25	75.2(6)
P2	C24	C25	C26	-179.8(5)	C29	P2	C24	C28	-103.6(7)
P2	C24	C28	Fe3	-121.4(6)	C29	P2	C35	C36	25.2(7)
P2	C24	C28	C27	179.8(6)	C29	P2	C35	C40	-162.3(5)
P2	C29	C30	C31	170.0(6)	C29	C30	C31	C32	-2.1(13)
P2	C29	C34	C33	-169.4(6)	C30	C29	C34	C33	0.6(10)
P2	C35	C36	C37	173.9(8)	C30	C31	C32	C33	3.5(13)
P2	C35	C40	C39	-174.4(5)	C31	C32	C33	C34	-2.9(13)
C7	P1	C13	C14	45.6(5)	C32	C33	C34	C29	0.9(12)
C7	P1	C13	C18	-135.1(5)	C34	C29	C30	C31	0.0(11)
C7	P1	C19	Fe3	-168.4(4)	C35	P2	C24	Fe3	-88.4(4)
C7	P1	C19	C20	-75.0(6)	C35	P2	C24	C25	-179.1(6)
C7	P1	C19	C23	102.5(5)	C35	P2	C24	C28	2.1(7)
C7	C8	C9	C10	-0.6(9)	C35	P2	C29	C30	52.8(7)
C8	C7	C12	C11	1.7(9)	C35	P2	C29	C34	-137.5(6)
C8	C9	C10	C11	1.2(10)	C35	C36	C37	C38	-1.0(15)
C9	C10	C11	C12	-0.4(10)	C36	C35	C40	C39	-1.8(11)
C10	C11	C12	C7	-1.1(9)	C36	C37	C38	C39	1.0(15)
C12	C7	C8	C9	-0.9(9)	C37	C38	C39	C40	-1.5(13)
C13	P1	C7	C8	-135.4(5)	C38	C39	C40	C35	1.9(11)
C13	P1	C7	C12	47.8(5)	C40	C35	C36	C37	1.3(13)
C13	P1	C19	Fe3	-64.5(4)					

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 2021NCS0348r1.

Atom	*x*	*y*	*z*	U(eq)
H5A	4110.63	-1306.09	7026.65	50
H5B	3069.19	-1588.02	6713.97	50
H6A	3277.94	-1174.81	5828.28	44
H6B	4299.5	-798.7	6146.52	44
H8	568.02	4334.36	6373.37	35
H9	-843.7	4429.3	6564.24	43
H10	-1943.13	2994.32	6132.45	45

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 2021NCS0348r1.

Atom	*x*	*y*	*z*	U(eq)
H11	-1624.41	1430.95	5539.67	41
H12	-215.59	1298.66	5366.67	35
H14	141.15	3676.33	4648.34	31
H15	-214.67	3348.49	3597.14	35
H16	530.19	1869.9	3204.37	39
H17	1601.52	653.64	3861.53	38
H18	2005.27	1021.81	4910.88	33
H20	1096.94	5228.22	4986.61	35
H21	1908.36	7107.35	5490.43	44
H22	2918.76	6520.28	6535.25	40
H23	2709.44	4278.61	6688.76	32
H25	3160.96	2802.78	5119.94	37
H26	2606.21	4516.65	4368.18	45
H27	3473.1	6424.13	4812.46	55
H28	4551.63	5882.24	5831.36	47
H30	6434.57	2215.23	6841.82	52
H31	7345.71	895.31	6486.7	59
H32	6866.24	141.65	5495.95	61
H33	5570.32	868.16	4836.4	55
H34	4655.8	2213.41	5169.99	43
H36	6307.29	4416.53	6344.35	68
H37	7130.86	6111.8	6842.72	80
H38	6605.42	7165.84	7565.25	64
H39	5332.74	6514.55	7817.71	52
H40	4505.56	4843.78	7311.42	39

Crystal data and structure refinement for 4a

Identification code	xstr0167
Empirical formula	$C_{50}H_{38}Fe_3O_4P_2S_2$
Formula weight	996.41
Temperature/K	150.0(1)
Crystal system	triclinic
Space group	P-1
a/Å	11.7727(4)
b/Å	12.3881(3)
c/Å	18.5833(3)
α/°	76.2386(18)
β/°	79.887(2)
γ/°	82.837(3)
Volume/Å^3	2581.75(12)
Z	2
ρ_{calc}g/cm^3	1.282
μ/mm^{-1}	1.013
F(000)	1020.0
Crystal size/mm^3	0.2326 × 0.1938 × 0.1221
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.57 to 51.994
Index ranges	-14 ≤ h ≤ 12, -15 ≤ k ≤ 11, -22 ≤ l ≤ 17
Reflections collected	16058
Independent reflections	10055 [R_{int} = 0.0238, R_{sigma} = 0.0463]
Data/restraints/parameters	10055/0/550
Goodness-of-fit on F^2	1.053
Final R indexes [I>=2σ (I)]	R_1 = 0.0759, wR_2 = 0.2279
Final R indexes [all data]	R_1 = 0.0883, wR_2 = 0.2472
Largest diff. peak/hole / e Å^{-3}	4.31/-0.55

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for xstr0167. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Fe1	6959.7(6)	7036.2(6)	8538.5(4)	15.3(2)
Fe2	6626.8(6)	9020.7(6)	7671.0(4)	15.2(2)
Fe3	9445.2(7)	7046.3(6)	6346.1(4)	19.3(2)
S1	5836.2(11)	8490.6(10)	8892.6(7)	16.8(3)
S2	5773.2(11)	7472.2(10)	7662.3(7)	16.3(3)
P1	7870.2(12)	5636.9(11)	8024.3(7)	18.2(3)
P2	7597.4(12)	9366.2(11)	6489.2(7)	17.4(3)
O1	9025(4)	7665(4)	8954(2)	30.8(9)

O2	6343(4)	5460(4)	9960(2)	36.8(11)
O3	8438(4)	10120(4)	8043(2)	31.8(10)
O4	4814(4)	10835(3)	7360(2)	30.5(9)
C0AA	8227(5)	7406(5)	8770(3)	21.3(11)
C2	6552(5)	6054(5)	9385(3)	22.7(11)
C3	7733(5)	9687(5)	7897(3)	21.3(11)
C4	5538(5)	10143(4)	7457(3)	21.0(11)
C5	6394(5)	9091(5)	9527(3)	20.5(11)
C6	6724(6)	8409(5)	10178(3)	31.2(13)
C7	7026(7)	8904(7)	10717(4)	45.8(18)
C8	6983(7)	10034(7)	10605(4)	46.0(18)
C9	6660(6)	10703(6)	9964(4)	36.1(15)
C10	6357(5)	10231(5)	9422(3)	28.0(12)
C11	4262(5)	7665(4)	8026(3)	20.2(11)
C12	3786(5)	7048(5)	8721(3)	24.3(12)
C13	2594(5)	7174(6)	8950(3)	31.6(13)
C14	1881(5)	7915(6)	8506(4)	37.0(15)
C15	2367(5)	8530(6)	7815(4)	33.9(14)
C16	3540(5)	8393(5)	7581(3)	24.0(11)
C17	8521(5)	5815(4)	7047(3)	19.8(10)
C18	9633(5)	5358(5)	6735(3)	25.3(12)
C19	9711(6)	5622(5)	5939(3)	28.6(13)
C20	8665(5)	6222(5)	5755(3)	26.2(12)
C21	7928(5)	6346(4)	6425(3)	20.8(11)
C22	9044(5)	8695(4)	6341(3)	19.4(10)
C23	9720(5)	8178(5)	6929(3)	21.4(11)
C24	10785(5)	7737(5)	6605(4)	27.6(12)
C25	10815(5)	7953(5)	5820(3)	27.4(12)
C26	9758(5)	8541(5)	5647(3)	22.4(11)
C27	6981(5)	9249(4)	5670(3)	20.8(11)
C28	6043(5)	8639(5)	5741(3)	23.6(11)
C29	5635(6)	8524(6)	5105(3)	33.3(14)
C30	6171(6)	9016(6)	4402(4)	37.7(15)
C31	7082(6)	9638(6)	4324(3)	34.7(15)
C32	7489(6)	9772(5)	4952(3)	27.8(12)
C33	7865(5)	10849(4)	6217(3)	23.5(12)
C34	8905(6)	11224(5)	6288(3)	30.5(13)
C35	9034(7)	12370(6)	6113(4)	44.0(19)
C36	8133(8)	13137(6)	5887(4)	46(2)
C37	7117(7)	12778(5)	5813(4)	42.7(18)
C38	6966(6)	11650(5)	5976(3)	30.9(13)
C39	9061(5)	4914(5)	8512(3)	27.1(12)
C40	8955(7)	3878(6)	9023(4)	44.4(18)
C41	9831(8)	3406(8)	9419(4)	58(2)
C42	10861(7)	3912(8)	9313(4)	58(2)

C43	10994(7)	4919(7)	8799(4)	45.1(18)
C44	10091(6)	5418(6)	8406(4)	33.4(14)
C45	6945(5)	4517(4)	8068(3)	22.8(11)
C46	5794(6)	4561(5)	8408(4)	30.9(13)
C47	5107(6)	3720(5)	8431(4)	37.0(15)
C48	5552(7)	2835(5)	8096(4)	38.6(16)
C49	6677(7)	2788(5)	7758(4)	41.4(17)
C50	7391(6)	3622(5)	7739(4)	34.1(14)

Anisotropic Displacement Parameters ($Å^2×10^3$) for xstr0167. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe1	16.5(4)	15.8(4)	13.1(4)	-3.3(3)	-0.7(3)	-0.8(3)
Fe2	17.0(4)	15.5(4)	13.1(4)	-3.6(3)	-0.7(3)	-2.4(3)
Fe3	21.0(4)	19.7(4)	16.6(4)	-5.8(3)	2.4(3)	-3.7(3)
S1	18.4(6)	18.1(6)	14.1(6)	-5.3(5)	-0.2(5)	-1.7(5)
S2	17.6(6)	16.9(6)	14.5(6)	-4.0(4)	-1.1(5)	-3.0(5)
P1	20.3(7)	16.5(6)	16.1(6)	-3.1(5)	-0.7(5)	1.6(5)
P2	21.9(7)	15.7(6)	14.3(6)	-3.1(5)	0.1(5)	-5.2(5)
O1	22(2)	42(3)	32(2)	-11.0(19)	-7.6(17)	-6.4(18)
O2	52(3)	29(2)	23(2)	2.7(18)	3(2)	-9(2)
O3	31(2)	42(3)	29(2)	-14.5(19)	-2.6(18)	-17(2)
O4	29(2)	27(2)	36(2)	-9.3(18)	−10.7(18)	6.6(18)
C0AA	21(3)	25(3)	16(2)	-6(2)	1(2)	2(2)
C2	27(3)	22(3)	19(3)	-5(2)	-3(2)	0(2)
C3	22(3)	26(3)	13(2)	-2(2)	1(2)	-3(2)
C4	24(3)	19(3)	20(3)	-5(2)	-1(2)	-3(2)
C5	18(3)	26(3)	19(3)	-13(2)	3(2)	-1(2)
C6	41(4)	32(3)	24(3)	-13(2)	-8(3)	1(3)
C7	51(5)	61(5)	36(4)	-23(3)	-23(3)	1(4)
C8	45(4)	64(5)	44(4)	-38(4)	-8(3)	-8(4)
C9	37(4)	38(4)	39(4)	-24(3)	5(3)	-6(3)
C10	31(3)	26(3)	28(3)	-12(2)	-2(2)	-3(2)
C11	21(3)	23(3)	18(3)	-7(2)	1(2)	-7(2)
C12	23(3)	26(3)	23(3)	-4(2)	0(2)	-6(2)
C13	25(3)	42(4)	26(3)	-7(3)	6(2)	-11(3)
C14	18(3)	56(4)	39(4)	-16(3)	1(3)	-10(3)
C15	18(3)	49(4)	38(3)	-11(3)	-12(2)	-1(3)
C16	24(3)	30(3)	20(3)	-6(2)	-5(2)	-3(2)
C17	24(3)	16(2)	18(3)	-5.0(19)	0(2)	0(2)
C18	27(3)	20(3)	26(3)	-7(2)	3(2)	2(2)
C19	35(3)	25(3)	26(3)	-12(2)	7(2)	-6(2)
C20	37(3)	26(3)	18(3)	-7(2)	-1(2)	-12(2)
C21	25(3)	21(3)	16(2)	-3(2)	0(2)	-5(2)

C22	23(3)	18(2)	18(2)	-6.3(19)	2(2)	-7(2)
C23	22(3)	23(3)	19(3)	-6(2)	-1(2)	-6(2)
C24	21(3)	28(3)	37(3)	-14(2)	0(2)	-6(2)
C25	25(3)	28(3)	28(3)	-9(2)	8(2)	-11(2)
C26	27(3)	22(3)	17(3)	-5(2)	5(2)	-8(2)
C27	26(3)	16(2)	19(3)	-3(2)	-3(2)	1(2)
C28	27(3)	28(3)	16(3)	-2(2)	-6(2)	-3(2)
C29	37(4)	39(3)	29(3)	-8(3)	-17(3)	-5(3)
C30	44(4)	47(4)	25(3)	-11(3)	-13(3)	4(3)
C31	48(4)	38(3)	14(3)	-2(2)	-4(2)	4(3)
C32	34(3)	26(3)	22(3)	-3(2)	-4(2)	-4(2)
C33	35(3)	17(3)	16(3)	-4(2)	6(2)	-9(2)
C34	39(4)	32(3)	22(3)	-9(2)	5(2)	-15(3)
C35	64(5)	45(4)	29(3)	-15(3)	11(3)	-38(4)
C36	80(6)	20(3)	35(4)	-9(3)	16(4)	-19(3)
C37	64(5)	17(3)	37(4)	-4(3)	14(3)	-1(3)
C38	41(4)	21(3)	27(3)	-4(2)	4(3)	-3(2)
C39	27(3)	33(3)	17(3)	-5(2)	-3(2)	11(2)
C40	38(4)	48(4)	34(4)	10(3)	-1(3)	4(3)
C41	51(5)	64(5)	38(4)	15(4)	-5(4)	15(4)
C42	43(5)	82(6)	38(4)	-1(4)	-13(3)	28(4)
C43	35(4)	59(5)	43(4)	-15(3)	-15(3)	12(3)
C44	31(3)	37(3)	31(3)	-7(3)	-9(3)	6(3)
C45	31(3)	14(2)	20(3)	0(2)	0(2)	-1(2)
C46	36(3)	22(3)	35(3)	-10(2)	2(3)	-5(2)
C47	37(4)	29(3)	44(4)	-10(3)	4(3)	-10(3)
C48	59(5)	26(3)	34(3)	-9(3)	3(3)	-22(3)
C49	64(5)	20(3)	38(4)	-13(3)	10(3)	-9(3)
C50	46(4)	24(3)	29(3)	-8(2)	9(3)	-7(3)

Bond Lengths for xstr0167.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	Fe2	2.6253(10)	C11	C16	1.386(8)
Fe1	S1	2.2568(14)	C12	C13	1.393(8)
Fe1	S2	2.2552(14)	C13	C14	1.386(10)
Fe1	P1	2.2431(15)	C14	C15	1.393(10)
Fe1	C0AA	1.764(6)	C15	C16	1.375(8)
Fe1	C2	1.777(5)	C17	C18	1.440(8)
Fe2	S1	2.2700(14)	C17	C21	1.437(8)
Fe2	S2	2.2783(14)	C18	C19	1.426(8)
Fe2	P2	2.2595(14)	C19	C20	1.409(9)
Fe2	C3	1.782(6)	C20	C21	1.416(8)
Fe2	C4	1.790(6)	C22	C23	1.443(8)
Fe3	C17	2.044(5)	C22	C26	1.450(7)
Fe3	C18	2.042(6)	C23	C24	1.398(8)

Fe3	C19	2.048(6)	C24	C25	1.415(9)
Fe3	C20	2.053(6)	C25	C26	1.409(9)
Fe3	C21	2.049(6)	C27	C28	1.385(8)
Fe3	C22	2.036(5)	C27	C32	1.401(8)
Fe3	C23	2.050(5)	C28	C29	1.395(8)
Fe3	C24	2.062(6)	C29	C30	1.380(10)
Fe3	C25	2.048(6)	C30	C31	1.365(10)
Fe3	C26	2.027(5)	C31	C32	1.387(9)
S1	C5	1.784(5)	C33	C34	1.399(9)
S2	C11	1.796(6)	C33	C38	1.413(9)
P1	C17	1.816(5)	C34	C35	1.400(9)
P1	C39	1.826(6)	C35	C36	1.386(12)
P1	C45	1.846(6)	C36	C37	1.366(12)
P2	C22	1.805(6)	C37	C38	1.384(9)
P2	C27	1.840(6)	C39	C40	1.408(9)
P2	C33	1.838(5)	C39	C44	1.395(9)
O1	C0AA	1.158(7)	C40	C41	1.363(11)
O2	C2	1.150(7)	C41	C42	1.396(14)
O3	C3	1.144(7)	C42	C43	1.386(12)
O4	C4	1.137(7)	C43	C44	1.392(9)
C5	C6	1.388(8)	C45	C46	1.391(9)
C5	C10	1.375(8)	C45	C50	1.394(8)
C6	C7	1.406(9)	C46	C47	1.385(9)
C7	C8	1.360(12)	C47	C48	1.389(10)
C8	C9	1.366(11)	C48	C49	1.363(11)
C9	C10	1.392(9)	C49	C50	1.401(9)
C11	C12	1.395(8)			

Bond Angles for xstr0167.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
S1	Fe1	Fe2	54.79(4)	C33	P2	Fe2	108.24(17)
S2	Fe1	Fe2	55.03(4)	C33	P2	C27	99.6(3)
S2	Fe1	S1	79.25(5)	O1	C0AA	Fe1	176.6(5)
P1	Fe1	Fe2	119.05(5)	O2	C2	Fe1	174.4(5)
P1	Fe1	S1	169.55(6)	O3	C3	Fe2	179.6(5)
P1	Fe1	S2	90.31(5)	O4	C4	Fe2	176.2(5)
C0AA	Fe1	Fe2	91.16(18)	C6	C5	S1	119.4(4)
C0AA	Fe1	S1	93.96(18)	C10	C5	S1	120.2(4)
C0AA	Fe1	S2	142.87(18)	C10	C5	C6	119.8(5)
C0AA	Fe1	P1	94.63(18)	C5	C6	C7	118.9(6)
C0AA	Fe1	C2	97.8(3)	C8	C7	C6	120.6(7)
C2	Fe1	Fe2	149.35(18)	C7	C8	C9	120.4(6)
C2	Fe1	S1	95.22(18)	C8	C9	C10	120.0(6)

C2	Fe1	S2	119.04(19)	C5	C10	C9	120.3(6)
C2	Fe1	P1	89.49(18)	C12	C11	S2	121.8(4)
S1	Fe2	Fe1	54.32(4)	C16	C11	S2	118.8(4)
S1	Fe2	S2	78.49(5)	C16	C11	C12	119.3(5)
S2	Fe2	Fe1	54.20(4)	C13	C12	C11	119.3(5)
P2	Fe2	Fe1	118.75(5)	C14	C13	C12	121.1(6)
P2	Fe2	S1	172.49(6)	C13	C14	C15	119.1(6)
P2	Fe2	S2	99.80(5)	C16	C15	C14	120.0(6)
C3	Fe2	Fe1	99.00(17)	C15	C16	C11	121.2(5)
C3	Fe2	S1	92.45(17)	P1	C17	Fe3	131.5(3)
C3	Fe2	S2	151.99(18)	C18	C17	Fe3	69.3(3)
C3	Fe2	P2	85.72(17)	C18	C17	P1	128.5(4)
C3	Fe2	C4	103.0(3)	C21	C17	Fe3	69.7(3)
C4	Fe2	Fe1	142.43(18)	C21	C17	P1	124.4(4)
C4	Fe2	S1	94.40(17)	C21	C17	C18	106.6(5)
C4	Fe2	S2	104.07(18)	C17	C18	Fe3	69.4(3)
C4	Fe2	P2	93.11(18)	C19	C18	Fe3	69.8(3)
C17	Fe3	C19	69.2(2)	C19	C18	C17	108.2(5)
C17	Fe3	C20	68.8(2)	C18	C19	Fe3	69.4(3)
C17	Fe3	C21	41.1(2)	C20	C19	Fe3	70.1(3)
C17	Fe3	C23	109.9(2)	C20	C19	C18	108.0(5)
C17	Fe3	C24	125.6(2)	C19	C20	Fe3	69.7(3)
C17	Fe3	C25	160.4(2)	C19	C20	C21	108.8(5)
C18	Fe3	C17	41.3(2)	C21	C20	Fe3	69.7(3)
C18	Fe3	C19	40.8(2)	C17	C21	Fe3	69.2(3)
C18	Fe3	C20	68.1(2)	C20	C21	Fe3	70.0(3)
C18	Fe3	C21	68.6(2)	C20	C21	C17	108.3(5)
C18	Fe3	C23	124.0(2)	P2	C22	Fe3	125.4(3)
C18	Fe3	C24	108.8(3)	C23	C22	Fe3	69.8(3)
C18	Fe3	C25	122.4(2)	C23	C22	P2	124.7(4)
C19	Fe3	C20	40.2(3)	C23	C22	C26	106.0(5)
C19	Fe3	C21	68.2(2)	C26	C22	Fe3	68.8(3)
C19	Fe3	C23	158.2(3)	C26	C22	P2	129.3(4)
C19	Fe3	C24	121.9(3)	C22	C23	Fe3	68.8(3)
C19	Fe3	C25	105.3(2)	C24	C23	Fe3	70.6(3)
C20	Fe3	C24	156.2(2)	C24	C23	C22	108.6(5)
C21	Fe3	C20	40.4(2)	C23	C24	Fe3	69.7(3)
C21	Fe3	C23	126.3(2)	C23	C24	C25	108.9(5)
C21	Fe3	C24	162.6(2)	C25	C24	Fe3	69.3(3)
C22	Fe3	C17	123.1(2)	C24	C25	Fe3	70.4(3)
C22	Fe3	C18	160.1(2)	C26	C25	Fe3	69.0(3)
C22	Fe3	C19	157.8(2)	C26	C25	C24	108.3(5)
C22	Fe3	C20	122.6(2)	C22	C26	Fe3	69.4(3)
C22	Fe3	C21	107.7(2)	C25	C26	Fe3	70.6(3)
C22	Fe3	C23	41.4(2)	C25	C26	C22	108.2(5)

C22	Fe3	C24	68.5(2)	C28	C27	P2	121.9(4)
C22	Fe3	C25	69.1(2)	C28	C27	C32	118.9(5)
C23	Fe3	C20	161.3(2)	C32	C27	P2	119.2(4)
C23	Fe3	C24	39.7(2)	C27	C28	C29	120.2(5)
C25	Fe3	C20	119.9(2)	C30	C29	C28	119.9(6)
C25	Fe3	C21	156.0(2)	C31	C30	C29	120.4(6)
C25	Fe3	C23	67.9(2)	C30	C31	C32	120.4(6)
C25	Fe3	C24	40.3(2)	C31	C32	C27	120.1(6)
C26	Fe3	C17	158.7(2)	C34	C33	P2	122.2(5)
C26	Fe3	C18	157.2(2)	C34	C33	C38	118.5(5)
C26	Fe3	C19	120.2(2)	C38	C33	P2	119.2(5)
C26	Fe3	C20	105.2(2)	C33	C34	C35	119.6(7)
C26	Fe3	C21	121.3(2)	C36	C35	C34	120.6(7)
C26	Fe3	C22	41.8(2)	C37	C36	C35	120.0(6)
C26	Fe3	C23	69.0(2)	C36	C37	C38	120.7(7)
C26	Fe3	C24	68.1(2)	C37	C38	C33	120.5(7)
C26	Fe3	C25	40.5(2)	C40	C39	P1	121.9(5)
Fe1	S1	Fe2	70.89(4)	C44	C39	P1	119.6(5)
C5	S1	Fe1	114.91(18)	C44	C39	C40	118.4(6)
C5	S1	Fe2	115.17(18)	C41	C40	C39	120.2(8)
Fe1	S2	Fe2	70.77(4)	C40	C41	C42	121.3(7)
C11	S2	Fe1	114.63(18)	C43	C42	C41	119.4(7)
C11	S2	Fe2	108.39(18)	C42	C43	C44	119.5(8)
C17	P1	Fe1	123.80(18)	C43	C44	C39	121.2(7)
C17	P1	C39	102.3(3)	C46	C45	P1	121.3(4)
C17	P1	C45	98.4(2)	C46	C45	C50	118.9(5)
C39	P1	Fe1	111.97(19)	C50	C45	P1	119.9(5)
C39	P1	C45	103.7(3)	C47	C46	C45	120.6(6)
C45	P1	Fe1	114.06(19)	C46	C47	C48	120.3(6)
C22	P2	Fe2	117.15(18)	C49	C48	C47	119.5(6)
C22	P2	C27	103.2(2)	C48	C49	C50	121.0(6)
C22	P2	C33	101.9(3)	C45	C50	C49	119.7(6)
C27	P2	Fe2	123.40(19)				

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for xstr0167.

Atom	*x*	*y*	*z*	U(eq)
H6	6745.1	7637.27	10256.45	37
H7	7257.83	8456.25	11152.64	55
H8	7174.63	10351.88	10968.94	55
H9	6641.66	11474.46	9888.07	43
H10	6129.5	10688.87	8987.87	34
H12	4258.86	6558.09	9027.04	29

H13	2272.43	6753.81	9407.95	38
H14	1087.6	8001.53	8666.79	44
H15	1898.83	9032.97	7512.96	41
H16	3855.3	8796.6	7114.92	29
H18	10201.98	4958.22	7006.59	30
H19	10342.38	5432.56	5601.25	34
H20	8488.31	6492.01	5272.08	31
H21	7185.98	6709.58	6456.52	25
H23	9486.18	8144.7	7438.09	26
H24	11377.87	7361.48	6864.29	33
H25	11427.53	7743.81	5476.43	33
H26	9553.03	8788.02	5170.26	27
H28	5682.94	8305.33	6214.89	28
H29	5003.28	8115.53	5154.39	40
H30	5909.31	8923.34	3978.02	45
H31	7430.86	9974.61	3848.18	42
H32	8099.9	10208.88	4895.44	33
H34	9507.62	10714.1	6449.57	37
H35	9731.76	12618.26	6147.83	53
H36	8218.83	13896.92	5786.21	55
H37	6520.96	13295.83	5651.61	51
H38	6268.29	11417.92	5926.26	37
H40	8285.21	3516.06	9091.89	53
H41	9741.52	2732.59	9765.62	69
H42	11452.9	3576.78	9584.39	70
H43	11680.48	5258.36	8717	54
H44	10176.26	6099.47	8067.81	40
H46	5483.04	5159.51	8622.72	37
H47	4344.13	3748.47	8670.21	44
H48	5086.57	2277.5	8103.55	46
H49	6975.97	2193.88	7535.9	50
H50	8157.68	3579.12	7508.73	41

Crystal data and structure refinement for 4c

Identification code	xstr0193
Empirical formula	$C_{50}H_{40}Fe_3N_2O_4P_2S_2$
Formula weight	1026.45
Temperature/K	132(2)
Crystal system	triclinic
Space group	P-1
a/Å	12.2873(6)
b/Å	12.6980(6)
c/Å	18.6853(9)
α/°	79.137(4)
β/°	74.698(4)
γ/°	83.481(4)
Volume/Å^3	2755.3(2)
Z	2
ρ_{calc}g/cm^3	1.237
μ/mm^{-1}	0.953
F(000)	1052.0
Crystal size/mm^3	0.2165 × 0.1939 × 0.1504
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.7 to 51.998
Index ranges	-14 ≤ h ≤ 15, -12 ≤ k ≤ 15, -23 ≤ l ≤ 21
Reflections collected	16932
Independent reflections	10695 [R_{int} = 0.0330, R_{sigma} = 0.0620]
Data/restraints/parameters	10695/0/570
Goodness-of-fit on F^2	1.080
Final R indexes [I>=2σ (I)]	R_1 = 0.0677, wR_2 = 0.1939
Final R indexes [all data]	R_1 = 0.0857, wR_2 = 0.2132
Largest diff. peak/hole / e Å^{-3}	2.09/-0.53

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for xstr0193. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Fe1	1055.0(6)	3411.7(5)	2399.0(4)	16.81(18)
Fe2	3076.4(6)	3136.8(5)	1508.8(4)	16.36(18)
Fe3	2990.5(6)	682.0(5)	3657.8(4)	20.16(19)
S1	2639.1(10)	4165.0(9)	2416.6(6)	17.5(3)
S2	1631.7(10)	4202.2(9)	1175.8(6)	17.9(3)
P1	679.1(10)	2439.0(10)	3571.6(7)	18.7(3)
P2	4480.5(10)	2280.5(10)	2002.5(7)	18.7(3)
O1	-732(3)	5112(3)	2749(2)	30.8(9)
O2	-131(3)	1819(3)	2002(2)	31.2(9)

O3	4643(3)	3803(3)	57(2)	37.2(9)
O4	2462(3)	1264(3)	1054(2)	29.7(8)
N1	2542(5)	8962(4)	1524(3)	35.8(11)
N2	-393(6)	3049(4)	-1133(3)	50.1(15)
C1	-49(4)	4419(4)	2641(3)	21.7(10)
C2	338(4)	2432(4)	2154(3)	22.5(10)
C3	4074(4)	3564(4)	649(3)	23.4(10)
C4	2709(4)	1985(4)	1251(3)	20.6(10)
C5	2539(4)	5584(4)	2094(3)	18.2(9)
C6	3200(4)	6072(4)	1410(3)	22.8(10)
C7	3193(5)	7177(4)	1217(3)	26.3(11)
C8	2512(5)	7854(4)	1696(3)	26.9(11)
C9	1831(5)	7362(4)	2375(3)	28.5(12)
C10	1844(4)	6245(4)	2572(3)	23.8(11)
C11	1036(4)	3714(4)	537(3)	19.6(10)
C12	1721(5)	3371(4)	-106(3)	26.3(11)
C13	1244(5)	3158(5)	-660(3)	32.8(13)
C14	93(5)	3269(4)	-575(3)	30.7(12)
C15	-603(5)	3576(4)	91(3)	30.2(12)
C16	-132(5)	3816(4)	632(3)	25.7(11)
C17	1337(4)	1079(4)	3685(3)	20.0(10)
C18	1445(4)	345(4)	4357(3)	24.3(11)
C19	2035(5)	-608(4)	4147(3)	27.4(11)
C20	2287(5)	-506(4)	3345(3)	25.4(11)
C21	1857(4)	524(4)	3063(3)	22.1(10)
C22	4261(4)	1578(4)	2970(3)	21.5(10)
C23	4704(4)	523(4)	3251(3)	25.3(11)
C24	4431(4)	388(4)	4043(3)	26.6(11)
C25	3819(5)	1336(4)	4271(3)	29.0(12)
C26	3726(4)	2074(4)	3617(3)	22.6(10)
C27	-837(4)	2176(4)	3868(3)	23.1(10)
C28	-1230(5)	1251(5)	3774(3)	31.2(12)
C29	-2379(5)	1109(5)	3952(3)	39.8(15)
C30	-3159(5)	1933(6)	4213(3)	46.6(17)
C31	-2780(5)	2864(6)	4313(3)	39.9(14)
C32	-1630(5)	2992(5)	4142(3)	33.7(13)
C33	809(4)	2968(4)	4397(3)	24.6(11)
C34	308(5)	2455(5)	5123(3)	31.1(12)
C35	436(6)	2830(6)	5747(3)	44.3(16)
C36	1034(6)	3721(6)	5654(3)	47.0(17)
C37	1497(6)	4256(5)	4943(3)	41.0(15)
C38	1399(5)	3874(5)	4317(3)	30.0(12)
C39	5282(4)	1266(4)	1459(3)	25.1(11)
C40	6322(5)	1465(5)	946(3)	34.4(13)
C41	6901(6)	699(6)	520(4)	48.7(18)

C42	6436(6)	-283(6)	600(4)	49.5(18)
C43	5411(6)	-479(5)	1095(3)	40.9(15)
C44	4823(5)	285(4)	1520(3)	32.9(13)
C45	5584(4)	3155(4)	1997(3)	24.0(11)
C46	5580(5)	4217(5)	1640(3)	31.9(12)
C47	6415(5)	4876(5)	1642(3)	36.7(13)
C48	7248(5)	4475(5)	2006(3)	35.7(13)
C49	7264(5)	3415(5)	2359(3)	37.4(14)
C50	6444(5)	2758(5)	2352(3)	30.3(12)

Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for xstr0193. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe1	17.7(4)	17.0(3)	16.1(3)	-4.4(3)	-3.9(3)	-0.4(3)
Fe2	17.4(4)	16.5(3)	15.1(3)	-4.0(3)	-3.5(3)	0.3(3)
Fe3	21.5(4)	20.6(4)	18.3(4)	-0.7(3)	-6.3(3)	-2.4(3)
S1	19.3(6)	17.8(6)	16.1(5)	-5.0(4)	-3.8(4)	-1.2(4)
S2	20.2(6)	16.8(6)	17.2(6)	-4.0(4)	-5.3(5)	0.6(4)
P1	18.0(6)	22.0(6)	16.6(6)	-4.4(5)	-4.0(5)	-2.6(5)
P2	18.4(6)	19.4(6)	17.6(6)	-3.5(5)	-4.3(5)	1.5(5)
O1	25(2)	29(2)	42(2)	-17.3(17)	-10.2(17)	10.7(16)
O2	39(2)	31(2)	29(2)	-6.6(16)	-12.4(17)	-12.9(18)
O3	33(2)	45(2)	25(2)	-1.7(17)	5.5(17)	-6.4(18)
O4	42(2)	18.9(18)	31(2)	-9.0(15)	-11.7(17)	0.0(16)
N1	51(3)	20(2)	37(3)	-7.3(19)	-9(2)	-4(2)
N2	71(4)	40(3)	57(4)	-19(3)	-42(3)	4(3)
C1	26(3)	22(2)	20(2)	-5.5(19)	-8(2)	-6(2)
C2	27(3)	23(3)	16(2)	1.5(19)	-6(2)	1(2)
C3	24(3)	22(2)	23(3)	-3(2)	-5(2)	2(2)
C4	18(2)	24(3)	19(2)	-3.4(19)	-5.1(19)	2.3(19)
C5	21(2)	17(2)	19(2)	-6.6(18)	-6.3(19)	0.7(18)
C6	24(3)	23(3)	21(2)	-6(2)	-3(2)	-2(2)
C7	30(3)	26(3)	21(2)	-5(2)	-1(2)	-5(2)
C8	34(3)	20(2)	31(3)	-5(2)	-13(2)	-3(2)
C9	36(3)	23(3)	28(3)	-14(2)	-5(2)	4(2)
C10	28(3)	22(2)	21(2)	-7(2)	-1(2)	-6(2)
C11	25(3)	15(2)	21(2)	-0.2(18)	-9(2)	-3.7(19)
C12	32(3)	26(3)	23(3)	-7(2)	-8(2)	1(2)
C13	39(3)	35(3)	28(3)	-14(2)	-12(2)	6(3)
C14	46(3)	20(3)	34(3)	-4(2)	-25(3)	0(2)
C15	29(3)	28(3)	39(3)	3(2)	-21(3)	-6(2)
C16	31(3)	25(3)	21(3)	0(2)	-10(2)	-3(2)
C17	21(2)	23(2)	18(2)	-2.0(19)	-6.9(19)	-6.3(19)

C18	24(3)	29(3)	19(2)	-1(2)	-5(2)	-3(2)
C19	28(3)	25(3)	30(3)	4(2)	-13(2)	-8(2)
C20	28(3)	19(2)	31(3)	-3(2)	-11(2)	-5(2)
C21	24(3)	22(2)	22(2)	-3.7(19)	-9(2)	-2(2)
C22	21(2)	23(2)	21(2)	-2.5(19)	-5(2)	-4(2)
C23	17(2)	26(3)	30(3)	-1(2)	-5(2)	0(2)
C24	22(3)	30(3)	30(3)	4(2)	-15(2)	-3(2)
C25	30(3)	39(3)	21(3)	-3(2)	-10(2)	-10(2)
C26	19(2)	23(3)	27(3)	-4(2)	-5(2)	-6(2)
C27	16(2)	34(3)	17(2)	-1(2)	-0.6(19)	-8(2)
C28	29(3)	41(3)	25(3)	-1(2)	-10(2)	-11(2)
C29	37(3)	54(4)	31(3)	8(3)	-15(3)	-26(3)
C30	20(3)	82(5)	32(3)	14(3)	-9(2)	-14(3)
C31	22(3)	57(4)	34(3)	2(3)	-2(2)	-2(3)
C32	24(3)	38(3)	33(3)	0(2)	-1(2)	1(2)
C33	22(3)	34(3)	19(2)	-11(2)	-4(2)	1(2)
C34	27(3)	42(3)	23(3)	-7(2)	-2(2)	-4(2)
C35	46(4)	65(4)	18(3)	-14(3)	2(3)	-6(3)
C36	50(4)	67(5)	29(3)	-27(3)	-5(3)	-7(3)
C37	46(4)	50(4)	32(3)	-25(3)	-3(3)	-10(3)
C38	30(3)	36(3)	26(3)	-13(2)	-4(2)	-3(2)
C39	25(3)	30(3)	20(2)	-5(2)	-8(2)	10(2)
C40	32(3)	43(3)	27(3)	-8(2)	-6(2)	5(3)
C41	41(4)	68(5)	32(3)	-19(3)	0(3)	17(3)
C42	52(4)	57(4)	40(4)	-30(3)	-8(3)	25(3)
C43	47(4)	38(3)	41(3)	-19(3)	-17(3)	15(3)
C44	34(3)	30(3)	33(3)	-14(2)	-6(2)	10(2)
C45	19(2)	32(3)	21(2)	-6(2)	-1(2)	-4(2)
C46	22(3)	34(3)	40(3)	0(2)	-11(2)	-8(2)
C47	38(3)	30(3)	43(3)	4(3)	-14(3)	-12(3)
C48	24(3)	45(3)	41(3)	-5(3)	-11(3)	-12(3)
C49	23(3)	54(4)	36(3)	1(3)	-13(2)	-7(3)
C50	26(3)	37(3)	28(3)	1(2)	-11(2)	-4(2)

Bond Lengths for xstr0193.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	Fe2	2.6266(9)	C11	C12	1.386(7)
Fe1	S1	2.2745(13)	C11	C16	1.393(7)
Fe1	S2	2.2750(13)	C12	C13	1.395(7)
Fe1	P1	2.2616(14)	C13	C14	1.375(8)
Fe1	C1	1.784(5)	C14	C15	1.407(8)
Fe1	C2	1.792(5)	C15	C16	1.382(7)
Fe2	S1	2.2506(12)	C17	C18	1.444(7)

Fe2	S2	2.2558(13)	C17	C21	1.438(7)
Fe2	P2	2.2463(13)	C18	C19	1.404(7)
Fe2	C3	1.778(5)	C19	C20	1.432(7)
Fe2	C4	1.762(5)	C20	C21	1.413(7)
Fe3	C17	2.027(5)	C22	C23	1.445(7)
Fe3	C18	2.040(5)	C22	C26	1.438(7)
Fe3	C19	2.050(5)	C23	C24	1.411(7)
Fe3	C20	2.064(5)	C24	C25	1.418(8)
Fe3	C21	2.044(5)	C25	C26	1.415(7)
Fe3	C22	2.044(5)	C27	C28	1.377(8)
Fe3	C23	2.042(5)	C27	C32	1.411(8)
Fe3	C24	2.052(5)	C28	C29	1.388(8)
Fe3	C25	2.050(5)	C29	C30	1.403(10)
Fe3	C26	2.055(5)	C30	C31	1.380(10)
S1	C5	1.790(5)	C31	C32	1.385(8)
S2	C11	1.786(5)	C33	C34	1.400(7)
P1	C17	1.821(5)	C33	C38	1.393(8)
P1	C27	1.848(5)	C34	C35	1.392(8)
P1	C33	1.844(5)	C35	C36	1.377(9)
P2	C22	1.823(5)	C36	C37	1.378(9)
P2	C39	1.827(5)	C37	C38	1.384(7)
P2	C45	1.845(5)	C39	C40	1.398(8)
O1	C1	1.153(6)	C39	C44	1.398(8)
O2	C2	1.136(6)	C40	C41	1.386(8)
O3	C3	1.148(6)	C41	C42	1.396(11)
O4	C4	1.147(6)	C42	C43	1.368(10)
N1	C8	1.385(7)	C43	C44	1.387(8)
N2	C14	1.412(7)	C45	C46	1.387(8)
C5	C6	1.395(7)	C45	C50	1.391(7)
C5	C10	1.395(6)	C46	C47	1.396(8)
C6	C7	1.380(7)	C47	C48	1.375(8)
C7	C8	1.405(7)	C48	C49	1.384(9)
C8	C9	1.400(8)	C49	C50	1.383(8)
C9	C10	1.396(7)			

Bond Angles for xstr0193.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
S1	Fe1	Fe2	54.09(3)	O1	C1	Fe1	175.2(5)
S1	Fe1	S2	78.98(5)	O2	C2	Fe1	178.9(5)
S2	Fe1	Fe2	54.23(3)	O3	C3	Fe2	172.7(5)
P1	Fe1	Fe2	118.22(4)	O4	C4	Fe2	176.9(4)
P1	Fe1	S1	99.20(5)	C6	C5	S1	122.8(4)
P1	Fe1	S2	171.76(5)	C6	C5	C10	118.0(4)

C1	Fe1	Fe2	142.03(16)	C10	C5	S1	118.9(4)
C1	Fe1	S1	103.64(16)	C7	C6	C5	121.2(5)
C1	Fe1	S2	94.62(16)	C6	C7	C8	121.5(5)
C1	Fe1	P1	93.62(16)	N1	C8	C7	121.9(5)
C1	Fe1	C2	102.6(2)	N1	C8	C9	120.9(5)
C2	Fe1	Fe2	99.79(16)	C9	C8	C7	117.2(5)
C2	Fe1	S1	152.75(17)	C10	C9	C8	121.2(5)
C2	Fe1	S2	91.84(15)	C5	C10	C9	120.8(5)
C2	Fe1	P1	86.21(15)	C12	C11	S2	120.9(4)
S1	Fe2	Fe1	54.94(4)	C12	C11	C16	119.2(4)
S1	Fe2	S2	79.88(5)	C16	C11	S2	119.3(4)
S2	Fe2	Fe1	54.91(4)	C11	C12	C13	120.2(5)
P2	Fe2	Fe1	119.25(4)	C14	C13	C12	121.0(5)
P2	Fe2	S1	89.31(5)	C13	C14	N2	121.1(6)
P2	Fe2	S2	169.12(5)	C13	C14	C15	118.7(5)
C3	Fe2	Fe1	148.39(16)	C15	C14	N2	120.2(6)
C3	Fe2	S1	119.51(17)	C16	C15	C14	120.4(5)
C3	Fe2	S2	94.10(16)	C15	C16	C11	120.4(5)
C3	Fe2	P2	90.14(16)	P1	C17	Fe3	125.8(3)
C4	Fe2	Fe1	92.09(16)	C18	C17	Fe3	69.7(3)
C4	Fe2	S1	143.35(16)	C18	C17	P1	130.3(4)
C4	Fe2	S2	94.39(15)	C21	C17	Fe3	70.0(3)
C4	Fe2	P2	95.04(15)	C21	C17	P1	123.3(4)
C4	Fe2	C3	96.9(2)	C21	C17	C18	106.4(4)
C17	Fe3	C18	41.60(19)	C17	C18	Fe3	68.7(3)
C17	Fe3	C19	69.1(2)	C19	C18	Fe3	70.3(3)
C17	Fe3	C20	69.0(2)	C19	C18	C17	108.6(4)
C17	Fe3	C21	41.37(19)	C18	C19	Fe3	69.5(3)
C17	Fe3	C22	122.68(19)	C18	C19	C20	108.4(4)
C17	Fe3	C23	160.0(2)	C20	C19	Fe3	70.1(3)
C17	Fe3	C24	158.1(2)	C19	C20	Fe3	69.1(3)
C17	Fe3	C25	122.1(2)	C21	C20	Fe3	69.1(3)
C17	Fe3	C26	107.3(2)	C21	C20	C19	107.8(5)
C18	Fe3	C19	40.2(2)	C17	C21	Fe3	68.7(3)
C18	Fe3	C20	68.2(2)	C20	C21	Fe3	70.6(3)
C18	Fe3	C21	68.8(2)	C20	C21	C17	108.8(4)
C18	Fe3	C22	158.8(2)	P2	C22	Fe3	132.4(3)
C18	Fe3	C23	157.4(2)	C23	C22	Fe3	69.2(3)
C18	Fe3	C24	121.2(2)	C23	C22	P2	129.1(4)
C18	Fe3	C25	105.7(2)	C26	C22	Fe3	69.9(3)
C18	Fe3	C26	121.8(2)	C26	C22	P2	123.9(4)
C19	Fe3	C20	40.7(2)	C26	C22	C23	106.5(4)
C19	Fe3	C24	106.1(2)	C22	C23	Fe3	69.4(3)
C19	Fe3	C25	120.4(2)	C24	C23	Fe3	70.2(3)
C19	Fe3	C26	156.4(2)	C24	C23	C22	108.3(4)

C21	Fe3	C19	68.3(2)	C23	C24	Fe3	69.4(3)
C21	Fe3	C20	40.23(19)	C23	C24	C25	108.5(4)
C21	Fe3	C24	158.5(2)	C25	C24	Fe3	69.7(3)
C21	Fe3	C25	160.4(2)	C24	C25	Fe3	69.9(3)
C21	Fe3	C26	125.4(2)	C26	C25	Fe3	70.0(3)
C22	Fe3	C19	160.4(2)	C26	C25	C24	108.2(5)
C22	Fe3	C20	124.7(2)	C22	C26	Fe3	69.1(3)
C22	Fe3	C21	109.1(2)	C25	C26	Fe3	69.6(3)
C22	Fe3	C24	68.8(2)	C25	C26	C22	108.5(4)
C22	Fe3	C25	68.9(2)	C28	C27	P1	122.4(4)
C22	Fe3	C26	41.06(19)	C28	C27	C32	118.6(5)
C23	Fe3	C19	122.6(2)	C32	C27	P1	118.8(4)
C23	Fe3	C20	108.3(2)	C27	C28	C29	121.2(6)
C23	Fe3	C21	123.9(2)	C28	C29	C30	119.6(6)
C23	Fe3	C22	41.42(19)	C31	C30	C29	119.9(5)
C23	Fe3	C24	40.3(2)	C30	C31	C32	119.9(6)
C23	Fe3	C25	68.3(2)	C31	C32	C27	120.7(6)
C23	Fe3	C26	68.6(2)	C34	C33	P1	119.9(4)
C24	Fe3	C20	122.2(2)	C38	C33	P1	121.4(4)
C24	Fe3	C26	67.9(2)	C38	C33	C34	118.7(5)
C25	Fe3	C20	156.9(2)	C35	C34	C33	120.0(6)
C25	Fe3	C24	40.5(2)	C36	C35	C34	120.2(6)
C25	Fe3	C26	40.3(2)	C35	C36	C37	120.3(5)
C26	Fe3	C20	161.7(2)	C36	C37	C38	120.0(6)
Fe2	S1	Fe1	70.96(4)	C37	C38	C33	120.7(5)
C5	S1	Fe1	110.71(16)	C40	C39	P2	121.7(4)
C5	S1	Fe2	115.37(15)	C40	C39	C44	118.4(5)
Fe2	S2	Fe1	70.86(4)	C44	C39	P2	119.8(4)
C11	S2	Fe1	114.96(16)	C41	C40	C39	120.9(6)
C11	S2	Fe2	114.41(16)	C40	C41	C42	119.6(6)
C17	P1	Fe1	117.14(16)	C43	C42	C41	119.9(6)
C17	P1	C27	101.3(2)	C42	C43	C44	120.9(6)
C17	P1	C33	104.0(2)	C43	C44	C39	120.2(6)
C27	P1	Fe1	108.90(16)	C46	C45	P2	121.2(4)
C33	P1	Fe1	122.51(18)	C46	C45	C50	118.5(5)
C33	P1	C27	99.8(2)	C50	C45	P2	120.3(4)
C22	P2	Fe2	123.54(17)	C45	C46	C47	120.8(5)
C22	P2	C39	102.8(2)	C48	C47	C46	119.9(5)
C22	P2	C45	98.9(2)	C47	C48	C49	119.7(5)
C39	P2	Fe2	112.21(16)	C50	C49	C48	120.5(5)
C39	P2	C45	102.6(2)	C49	C50	C45	120.6(5)
C45	P2	Fe2	114.11(17)				

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for xstr0193.

Atom	*x*	*y*	*z*	U(eq)
H1A	2696.17	9157.11	1043.87	43
H1B	1890.81	9250.5	1722.88	43
H2A	131.09	2797.41	-1478.8	60
H2B	-890.27	2579	-936.78	60
H6	3654.7	5645.59	1078.24	27
H7	3650.19	7478.86	759.41	32
H9	1362.28	7788.09	2701.95	34
H10	1384.25	5937.83	3026.2	29
H12	2500.41	3282.69	-168.81	32
H13	1712.06	2937.48	-1091.85	39
H15	-1384.79	3618.66	168.68	36
H16	-598.31	4045.58	1060.97	31
H18	1169.28	479.53	4847.14	29
H19	2230.21	-1204	4474.21	33
H20	2665.63	-1024.56	3060.43	30
H21	1902.48	797.41	2558.87	27
H23	5101.2	18.64	2959.11	30
H24	4620.18	-219.74	4362.8	32
H25	3529.34	1451.11	4764.36	35
H26	3377.24	2764.44	3608.38	27
H28	-715.72	712.09	3587.25	37
H29	-2631.4	471.2	3899.35	48
H30	-3931.1	1852.38	4317.97	56
H31	-3295.73	3404.75	4495.85	48
H32	-1378.65	3621.77	4207.94	40
H34	-111.6	1863.18	5187.58	37
H35	117.56	2478.69	6228.44	53
H36	1126.19	3962.81	6072.77	56
H37	1874.94	4873.72	4882.97	49
H38	1730.87	4227.14	3838.4	36
H40	6630.8	2120.36	888.96	41
H41	7595.7	837.49	182.56	58
H42	6821.44	-802.3	318.71	59
H43	5103.86	-1133.99	1145.96	49
H44	4120.88	144.12	1846.7	40
H46	5014.68	4493.73	1396.36	38
H47	6407.79	5584.96	1396.39	44
H48	7797.95	4915.18	2016.21	43
H49	7831.25	3141.22	2601.97	45
H50	6466.68	2045.4	2587.91	36

Computational Details

B3LYP geometries and energies for all optimized structures

Species A

HF energy= -2967.84983714
No Imaginary frequency
Zero-point correction= 0.430050 (Hartree/Particle)
Thermal correction to Energy= 0.467039
Thermal correction to Enthalpy= 0.467983
Thermal correction to Gibbs Free Energy= 0.364165
Sum of electronic and zero-point Energies= -2967.419787
Sum of electronic and thermal Energies= -2967.382798
Sum of electronic and thermal Enthalpies= -2967.381854
Sum of electronic and thermal Free Energies= -2967.485672

Coordinates: **A**

Fe	0.15120000	0.28550000	5.06710000
Fe	0.49980000	2.86960000	5.03230000
Fe	4.05930000	0.88780000	2.48230000
P	1.81460000	-1.15040000	4.37060000
P	2.42280000	3.61180000	4.02130000
S	-1.40970000	1.83180000	5.79200000
S	1.62580000	1.43110000	6.42940000
O	-1.30510000	-1.94680000	6.26720000
O	-1.02910000	0.27040000	2.38330000
O	0.24120000	5.25780000	6.69660000
O	-1.02370000	3.69810000	2.65480000
C	-0.67950000	-1.07670000	5.82470000
C	-0.56580000	0.31750000	3.44560000
C	0.36920000	4.32400000	6.02400000
C	-0.42310000	3.35330000	3.57910000
C	-1.49680000	1.90120000	7.64160000
C	-0.42060000	1.14560000	8.42010000
C	1.00980000	1.61680000	8.17000000
C	2.39150000	1.85520000	1.71670000
C	3.12930000	2.73030000	2.58670000
C	4.44930000	2.86580000	2.02500000
C	4.51570000	2.08000000	0.83650000
C	3.24380000	1.45730000	0.64650000
C	5.62420000	0.17620000	3.65940000
C	4.40550000	0.16880000	4.39930000
C	3.45940000	-0.67200000	3.71640000
C	4.12240000	-1.17930000	2.54290000
C	5.44950000	-0.65430000	2.51020000
C	1.23200000	-2.36180000	3.09760000
H	1.96150000	-3.16430000	2.93550000
H	0.29080000	-2.80500000	3.44280000
H	1.03390000	-1.85430000	2.14690000
C	2.35830000	-2.28530000	5.73470000
H	1.49800000	-2.84650000	6.11720000
H	3.12310000	-2.98740000	5.38030000
H	2.77170000	-1.68650000	6.55380000
C	2.21960000	5.31030000	3.29610000
H	3.16490000	5.66950000	2.87080000
H	1.46390000	5.29090000	2.50310000
H	1.88660000	6.00840000	4.07340000
C	3.86550000	3.90210000	5.14110000
H	4.72320000	4.31790000	4.59890000
H	3.55940000	4.61740000	5.91400000

H	4.15770000	2.97320000	5.63690000
H	-2.48600000	1.50000000	7.89600000
H	-1.49750000	2.96570000	7.91050000
H	-0.63820000	1.26260000	9.49490000
H	-0.49280000	0.07280000	8.20400000
H	1.70340000	1.03940000	8.79430000
H	1.12850000	2.67460000	8.43740000
H	1.36980000	1.53520000	1.87280000
H	2.98170000	0.77190000	-0.15160000
H	5.39120000	1.94970000	0.20990000
H	5.26660000	3.44140000	2.44390000
H	3.68380000	-1.82530000	1.79190000
H	6.18140000	-0.82740000	1.72910000
H	6.51480000	0.74320000	3.90680000
H	4.20480000	0.70890000	5.31610000

Species A_alt1
HF energy= -2967.84134425
No imaginary frequency
Zero-point correction= 0.430745 (Hartree/Particle)
Thermal correction to Energy= 0.467441
Thermal correction to Enthalpy= 0.468385
Thermal correction to Gibbs Free Energy= 0.364861
Sum of electronic and zero-point Energies= -2967.410599
Sum of electronic and thermal Energies= -2967.373904
Sum of electronic and thermal Enthalpies= -2967.372959
Sum of electronic and thermal Free Energies= -2967.476483

Coordinates: **A_alt1**

Fe	-0.28298300	1.10074100	5.30968600
Fe	0.28696300	3.62446100	5.24795900
Fe	3.79705000	5.82592000	6.70472700
P	2.36643400	3.80055200	4.21352900
S	-1.79422100	2.78666300	5.88528200
S	1.13662900	2.18201000	6.83815100
O	-1.96736300	-1.08584600	6.31850000
O	1.94205000	-0.71258200	4.69768900
O	-1.02578700	4.58201800	2.81374600
O	-1.13355300	1.21836200	2.50297900
C	-1.28096300	-0.22397900	5.97377300
C	1.08067100	0.02337300	4.91435000
C	-0.49802300	4.20062300	3.77101100
C	-0.79885200	1.22256600	3.60965300
C	-2.13176700	2.66490000	7.70420800
C	-1.14365500	1.87435500	8.56232000
C	0.30602900	2.34539400	8.49185500
C	4.41080200	3.89988700	6.28223600
C	3.80400900	4.49515700	5.12175100
C	4.57887300	5.66375400	4.79400700
C	5.64062200	5.78244300	5.74131900
C	5.53849700	4.69068100	6.65661300
C	2.58094300	7.49925000	6.81425100
C	1.82492300	6.30426000	7.08974200
C	2.43102700	5.68423400	8.23842000
C	3.53375900	6.48709000	8.65887000
C	3.63011500	7.60505300	7.77622400
C	3.14171100	2.24687200	3.56599100
H	4.08300200	2.48208900	3.05346600

H	3.35197600	1.55833600	4.38903400
H	2.45775500	1.75422000	2.86657800
C	2.38414000	4.81937900	2.66282200
H	3.38632300	4.84468900	2.21888000
H	1.69052600	4.37487700	1.94036400
H	2.05234800	5.84539600	2.85517500
H	-3.12517200	2.20408100	7.77503500
H	-2.23053300	3.69101800	8.07675700
H	-1.47853600	1.94594000	9.61098100
H	-1.18748900	0.81225400	8.29806400
H	0.91637500	1.75636100	9.18767900
H	0.38439900	3.39611400	8.79756400
H	4.04168200	3.02233500	6.80008100
H	6.18210600	4.51212800	7.51077200
H	6.37442000	6.57993400	5.77594600
H	4.38079300	6.35433000	3.98282200
H	4.20485400	6.26236000	9.48027500
H	4.38508300	8.38261600	7.80918400
H	2.40605900	8.19076800	5.99896500
P	0.33282300	5.69464600	6.21067200
H	2.13041200	4.74508600	8.68592800
C	0.00941700	7.09309500	5.03347700
H	-0.01562400	8.05853600	5.55301800
H	0.77141300	7.12985000	4.24744900
H	-0.96000200	6.92674000	4.55060900
C	-0.96782400	6.08227600	7.47991100
H	-1.95970800	5.87661500	7.06076700
H	-0.82935200	5.46165700	8.37085800
H	-0.90790700	7.13686700	7.77662300

Species A_alt2
HF energy= -2967.84637819
No Imaginary frequency
Zero-point correction= 0.430714 (Hartree/Particle)
Thermal correction to Energy= 0.467550
Thermal correction to Enthalpy= 0.468495
Thermal correction to Gibbs Free Energy= 0.364049
Sum of electronic and zero-point Energies= -2967.415664
Sum of electronic and thermal Energies= -2967.378828
Sum of electronic and thermal Enthalpies= -2967.377884
Sum of electronic and thermal Free Energies= -2967.482329

Coordinates: **A_alt2**

Fe	-0.39170000	0.77330000	5.58710000
Fe	0.35910000	3.20660000	4.87240000
Fe	1.85860000	5.95460000	1.87220000
P	2.53940000	3.22830000	3.99900000
S	-1.71880000	2.68140000	5.68290000
S	1.13070000	2.11020000	6.72640000
O	-1.50170000	-1.08960000	7.58030000
O	1.89120000	-0.85820000	4.73440000
O	0.42110000	5.89220000	5.96610000
O	-2.02010000	-0.06460000	3.29760000
C	-1.07290000	-0.31550000	6.84020000
C	0.99320000	-0.20330000	5.05520000
C	0.42310000	4.84440000	5.46150000
C	-1.36670000	0.27320000	4.19110000
C	-1.95550000	3.26990000	7.42460000

C	-1.08840000	2.61360000	8.49570000
C	0.41470000	2.78650000	8.29800000
C	3.08860000	6.05060000	3.52630000
C	3.04040000	4.70360000	3.02090000
C	3.53050000	4.74780000	1.66800000
C	3.86840000	6.09850000	1.35080000
C	3.60020000	6.90170000	2.50050000
C	0.40010000	5.31920000	0.54910000
C	-0.04790000	5.17590000	1.91090000
C	-0.03430000	6.49120000	2.49490000
C	0.42030000	7.41880000	1.51030000
C	0.69300000	6.69520000	0.31020000
C	3.90210000	3.23550000	5.25840000
H	4.87180000	3.35780000	4.76060000
H	3.75190000	4.06010000	5.96370000
H	3.89020000	2.30020000	5.82630000
C	3.12910000	1.84780000	2.91040000
H	4.17280000	2.00480000	2.61080000
H	3.05670000	0.90710000	3.46440000
H	2.51010000	1.75360000	2.01340000
H	-3.01560000	3.09430000	7.64640000
H	-1.79940000	4.35650000	7.40620000
H	-1.35780000	3.05270000	9.47070000
H	-1.32920000	1.54690000	8.56200000
H	0.95690000	2.27750000	9.10470000
H	0.69540000	3.84740000	8.33130000
H	2.76380000	6.37250000	4.50880000
H	3.72610000	7.97620000	2.57280000
H	4.23450000	6.45310000	0.39380000
H	3.60920000	3.90560000	0.99090000
H	0.56910000	8.48190000	1.66290000
H	1.08500000	7.11000000	-0.61170000
H	0.52900000	4.51810000	-0.16840000
P	-0.58070000	3.63980000	2.76180000
H	-0.29050000	6.73610000	3.51820000
C	-0.36950000	2.39690000	1.39870000
H	-0.94750000	2.69060000	0.51370000
H	0.68230000	2.30010000	1.11330000
H	-0.72610000	1.42150000	1.74060000
C	-2.42230000	3.86240000	2.69690000
H	-2.92590000	2.93400000	2.98490000
H	-2.73000000	4.64400000	3.39910000
H	-2.72500000	4.14590000	1.68140000

Species B
HF energy= -2967.64235172
No imaginary frequency
Zero-point correction= 0.430492 (Hartree/Particle)
Thermal correction to Energy= 0.467908
Thermal correction to Enthalpy= 0.468852
Thermal correction to Gibbs Free Energy= 0.363181
Sum of electronic and zero-point Energies= -2967.211859
Sum of electronic and thermal Energies= -2967.174444
Sum of electronic and thermal Enthalpies= -2967.173499
Sum of electronic and thermal Free Energies= -2967.279171

Coordinates: **B**

Fe	0.17230000	0.25900000	5.14920000

Fe	0.40100000	2.89110000	5.03310000
Fe	4.07070000	0.82590000	2.60090000
P	1.76360000	-1.26400000	4.43240000
P	2.28200000	3.69370000	3.85000000
S	-1.37360000	1.79520000	6.01750000
S	1.76800000	1.54850000	6.30920000
O	-1.91840000	-1.83750000	5.36680000
O	-0.54850000	0.79180000	2.33690000
O	0.40180000	5.16250000	6.86340000
O	-1.46990000	4.11190000	3.08330000
C	-1.10200000	-1.04090000	5.26890000
C	-0.22690000	0.73080000	3.44490000
C	0.40810000	4.29320000	6.11590000
C	-0.74290000	3.63460000	3.82280000
C	-1.26650000	1.78620000	7.86530000
C	-0.08500000	1.02690000	8.46170000
C	1.28670000	1.59110000	8.10460000
C	2.55890000	1.86390000	1.59860000
C	3.16280000	2.69990000	2.60450000
C	4.56250000	2.80910000	2.27010000
C	4.80080000	2.05540000	1.08570000
C	3.56560000	1.47340000	0.67270000
C	5.59070000	0.00620000	3.77830000
C	4.37050000	0.04060000	4.50930000
C	3.39260000	-0.74640000	3.79980000
C	4.04160000	-1.25000000	2.61470000
C	5.38830000	-0.78670000	2.60920000
C	1.13920000	-2.40630000	3.12460000
H	1.86600000	-3.19890000	2.91340000
H	0.20830000	-2.87400000	3.46430000
H	0.92680000	-1.85710000	2.20070000
C	2.22190000	-2.41950000	5.80250000
H	1.32500000	-2.91870000	6.18920000
H	2.92800000	-3.17800000	5.44370000
H	2.69100000	-1.85900000	6.61850000
C	1.90200000	5.23650000	2.89920000
H	2.82190000	5.65490000	2.47430000
H	1.20960000	5.01750000	2.07900000
H	1.44060000	5.98350000	3.55670000
C	3.61220000	4.26970000	4.99200000
H	4.41150000	4.77280000	4.43650000
H	3.19100000	4.98550000	5.70710000
H	4.02620000	3.42520000	5.55040000
H	-2.21070000	1.33640000	8.19370000
H	-1.27480000	2.83350000	8.19260000
H	-0.18430000	1.05690000	9.55810000
H	-0.13910000	-0.03250000	8.17430000
H	2.07160000	1.01510000	8.60800000
H	1.38590000	2.63210000	8.43570000
H	1.51710000	1.58230000	1.54000000
H	3.42170000	0.81890000	-0.17930000
H	5.76420000	1.91540000	0.60860000
H	5.31630000	3.34870000	2.83050000
H	3.58590000	-1.86060000	1.84480000
H	6.11770000	-0.97380000	1.82950000
H	6.50400000	0.52570000	4.04520000
H	4.20060000	0.57060000	5.43690000

Species ^{3}C
HF energy= -2967.31069919
No Imaginary frequency
Zero-point correction= 0.430101 (Hartree/Particle)
Thermal correction to Energy= 0.468001
Thermal correction to Enthalpy= 0.468945
Thermal correction to Gibbs Free Energy= 0.361385
Sum of electronic and zero-point Energies= -2966.880599
Sum of electronic and thermal Energies= -2966.842699
Sum of electronic and thermal Enthalpies= -2966.841754
Sum of electronic and thermal Free Energies= -2966.949315

Coordinates: **^{3}C**

Fe	0.16320000	0.26850000	5.17380000
Fe	0.32970000	2.85750000	5.05590000
Fe	4.13180000	0.77240000	2.70910000
P	1.63680000	-1.35620000	4.43850000
P	2.09190000	3.76240000	3.76240000
S	-1.31270000	1.73290000	6.23910000
S	1.85270000	1.53060000	6.20810000
O	-2.20370000	-1.46900000	4.74370000
O	-0.08410000	1.07580000	2.36530000
O	0.40380000	5.06020000	6.99170000
O	-1.80060000	4.11150000	3.40160000
C	-1.28440000	-0.81070000	4.89380000
C	0.04130000	1.04070000	3.52090000
C	0.38760000	4.22640000	6.21130000
C	-0.97750000	3.63050000	4.02290000
C	-1.00280000	1.75040000	8.06560000
C	0.24620000	1.01490000	8.54090000
C	1.56620000	1.59880000	8.04590000
C	2.79800000	2.01770000	1.50670000
C	3.20530000	2.75620000	2.66710000
C	4.64440000	2.80870000	2.63530000
C	5.09970000	2.13900000	1.45580000
C	3.95200000	1.64810000	0.76340000
C	5.57530000	-0.31910000	3.87580000
C	4.35710000	-0.26870000	4.60430000
C	3.32340000	-0.89790000	3.83030000
C	3.93320000	-1.31450000	2.59300000
C	5.31910000	-0.96370000	2.62930000
C	1.00170000	-2.42940000	3.08120000
H	1.71320000	-3.22340000	2.82680000
H	0.07310000	-2.90470000	3.41790000
H	0.76950000	-1.84010000	2.18660000
C	2.06880000	-2.56090000	5.77260000
H	1.14630000	-3.02740000	6.13970000
H	2.73460000	-3.34650000	5.39590000
H	2.55290000	-2.04680000	6.60990000
C	1.55440000	5.03610000	2.53330000
H	2.41660000	5.49350000	2.03490000
H	0.89620000	4.59360000	1.77710000
H	0.99570000	5.82070000	3.05860000
C	3.30710000	4.68540000	4.79870000
H	4.06420000	5.18470000	4.18330000
H	2.77140000	5.45910000	5.36020000
H	3.79010000	4.01650000	5.51910000
H	-1.90120000	1.28770000	8.48940000
H	-1.00010000	2.80040000	8.38240000
H	0.25850000	1.05410000	9.64080000

H	0.17910000	-0.04830000	8.27000000
H	2.40810000	1.04330000	8.47390000
H	1.67990000	2.64570000	8.35090000
H	1.77900000	1.76560000	1.23990000
H	3.95520000	1.07000000	-0.15470000
H	6.13370000	2.01730000	1.15090000
H	5.28390000	3.29020000	3.36560000
H	3.43960000	-1.82530000	1.77430000
H	6.04180000	-1.14150000	1.84000000
H	6.52450000	0.09710000	4.19700000
H	4.22140000	0.19820000	5.57220000

Species ^{1}C
HF energy= -2967.28336712
No imaginary frequency
Zero-point correction= 0.429825 (Hartree/Particle)
Thermal correction to Energy= 0.467878
Thermal correction to Enthalpy= 0.468822
Thermal correction to Gibbs Free Energy= 0.361563
Sum of electronic and zero-point Energies= -2966.853542
Sum of electronic and thermal Energies= -2966.815489
Sum of electronic and thermal Enthalpies= -2966.814545
Sum of electronic and thermal Free Energies= -2966.921804

Coordinates: **^{1}C**

Fe	0.12140000	0.15700000	5.16790000
Fe	0.42630000	3.05260000	4.99810000
Fe	3.95150000	0.85750000	2.61410000
P	1.78290000	-1.37900000	4.58160000
P	2.34040000	3.89230000	3.88020000
S	-1.37140000	1.85350000	5.85170000
S	1.77470000	1.58290000	6.09110000
O	-2.12030000	-1.80230000	5.11950000
O	-0.38750000	0.62140000	2.32770000
O	0.37170000	5.25840000	6.90760000
O	-1.40850000	4.37320000	3.04770000
C	-1.25980000	-1.06270000	5.10270000
C	-0.14880000	0.48050000	3.43550000
C	0.38740000	4.42030000	6.13460000
C	-0.70460000	3.87750000	3.78850000
C	-1.27140000	1.66440000	7.69780000
C	-0.08640000	0.84030000	8.19520000
C	1.29380000	1.42030000	7.89380000
C	2.52420000	2.05430000	1.63280000
C	3.16830000	2.80760000	2.68210000
C	4.57810000	2.82450000	2.37540000
C	4.77990000	2.10790000	1.16330000
C	3.51510000	1.63290000	0.70690000
C	5.51680000	-0.11630000	3.60970000
C	4.37240000	-0.06160000	4.44840000
C	3.29650000	-0.77000000	3.79170000
C	3.80880000	-1.22410000	2.52010000
C	5.17020000	-0.82720000	2.42210000
C	1.17990000	-2.72900000	3.48570000
H	1.98540000	-3.44830000	3.29840000
H	0.35200000	-3.25880000	3.97100000
H	0.82570000	-2.33690000	2.52550000
C	2.35520000	-2.25800000	6.09860000

H	1.51300000	-2.75970000	6.59120000
H	3.10090000	-3.01300000	5.81940000
H	2.81760000	-1.55630000	6.80050000
C	2.00890000	5.42800000	2.91140000
H	2.94920000	5.81490000	2.50150000
H	1.32860000	5.22170000	2.07790000
H	1.56070000	6.19620000	3.55380000
C	3.65110000	4.41940000	5.06110000
H	4.47180000	4.90460000	4.52050000
H	3.23890000	5.14720000	5.76960000
H	4.04020000	3.56280000	5.61940000
H	-2.21720000	1.18910000	7.98000000
H	-1.27250000	2.67390000	8.12480000
H	-0.17330000	0.74800000	9.28870000
H	-0.16010000	-0.19550000	7.81450000
H	2.07510000	0.78440000	8.32310000
H	1.41090000	2.41980000	8.32770000
H	1.46380000	1.87070000	1.52650000
H	3.34070000	1.03120000	-0.17780000
H	5.73850000	1.92560000	0.69120000
H	5.35870000	3.29030000	2.96500000
H	3.26220000	-1.77830000	1.76640000
H	5.81890000	-1.00770000	1.57270000
H	6.47820000	0.33750000	3.82180000
H	4.32780000	0.40840000	5.42190000

Species D
HF energy= -2968.26442125
No Imaginary frequency
Zero-point correction= 0.440148 (Hartree/Particle)
Thermal correction to Energy= 0.477167
Thermal correction to Enthalpy= 0.478111
Thermal correction to Gibbs Free Energy= 0.374183
Sum of electronic and zero-point Energies= -2967.824273
Sum of electronic and thermal Energies= -2967.787254
Sum of electronic and thermal Enthalpies= -2967.786310
Sum of electronic and thermal Free Energies= -2967.890238

Coordinates: **D**

Fe	0.13110000	0.25010000	5.05920000
Fe	0.51780000	2.86570000	4.95890000
Fe	4.05060000	0.94990000	2.48580000
P	1.83910000	-1.19890000	4.33330000
P	2.48980000	3.68790000	4.03920000
S	-1.43110000	1.85050000	5.70630000
S	1.59020000	1.43190000	6.45390000
O	-0.93670000	-1.88960000	6.76970000
O	-1.59240000	-0.40330000	2.75480000
O	0.33670000	5.17230000	6.76830000
O	-1.04510000	3.96800000	2.70640000
C	-0.49820000	-1.05110000	6.12410000
C	-0.92880000	-0.18300000	3.65860000
C	0.40800000	4.28870000	6.04180000
C	-0.43110000	3.56520000	3.58200000
C	-1.56810000	2.01890000	7.54880000
C	-0.52520000	1.31120000	8.41300000
C	0.93190000	1.69760000	8.16620000
C	2.42300000	1.96880000	1.70280000

C	3.16800000	2.80760000	2.60640000
C	4.50080000	2.92470000	2.06860000
C	4.56540000	2.16550000	0.86540000
C	3.28470000	1.57690000	0.63970000
C	5.61470000	0.18690000	3.64360000
C	4.39800000	0.17520000	4.38350000
C	3.44200000	-0.63570000	3.67490000
C	4.10030000	-1.11850000	2.48580000
C	5.43100000	-0.60840000	2.47280000
C	1.25970000	-2.40200000	3.05780000
H	2.01620000	-3.17390000	2.87580000
H	0.34530000	-2.89170000	3.41220000
H	1.03230000	-1.89450000	2.11360000
C	2.40820000	-2.31970000	5.69300000
H	1.58110000	-2.94100000	6.05480000
H	3.21020000	-2.97160000	5.32800000
H	2.78960000	-1.72200000	6.52800000
C	2.29960000	5.41190000	3.38890000
H	3.25960000	5.78250000	3.01040000
H	1.57440000	5.43290000	2.56790000
H	1.94960000	6.08340000	4.18220000
C	3.88890000	3.89750000	5.22110000
H	4.76760000	4.31890000	4.71960000
H	3.57950000	4.58940000	6.01370000
H	4.15350000	2.94290000	5.68170000
H	-2.56660000	1.63510000	7.78730000
H	-1.58250000	3.09720000	7.74900000
H	-0.75700000	1.55020000	9.46270000
H	-0.63990000	0.22580000	8.32460000
H	1.58420000	1.10870000	8.82120000
H	1.10680000	2.75430000	8.40190000
H	1.38890000	1.67200000	1.82280000
H	3.02140000	0.91990000	-0.18120000
H	5.44750000	2.02960000	0.25010000
H	5.32460000	3.47300000	2.51020000
H	3.66010000	-1.74310000	1.71800000
H	6.16260000	-0.77020000	1.68950000
H	6.51310000	0.73280000	3.90790000
H	4.21700000	0.68160000	5.32320000
H	0.67930000	1.47590000	4.03580000

Species E
HF energy= -2968.43031196
No Imaginary frequency
Zero-point correction= 0.436086 (Hartree/Particle)
Thermal correction to Energy= 0.474011
Thermal correction to Enthalpy= 0.474955
Thermal correction to Gibbs Free Energy= 0.367736
Sum of electronic and zero-point Energies= -2967.994226
Sum of electronic and thermal Energies= -2967.956301
Sum of electronic and thermal Enthalpies= -2967.955357
Sum of electronic and thermal Free Energies= -2968.062576

Coordinates: **E**

Fe	0.13107700	0.25013500	5.05920600
Fe	0.51775900	2.86569200	4.95890400
Fe	4.05064500	0.94991300	2.48582100
P	1.83914700	-1.19893600	4.33329900

P	2.48978000	3.68791900	4.03920000
S	-1.43110500	1.85052800	5.70627100
S	1.59017900	1.43189700	6.45392800
O	-0.93668400	-1.88957600	6.76973900
O	-1.59244600	-0.40328100	2.75482900
O	0.33667000	5.17234700	6.76834700
O	-1.04512700	3.96804800	2.70637600
C	-0.49818900	-1.05105600	6.12405300
C	-0.92883000	-0.18302600	3.65864900
C	0.40804300	4.28871600	6.04176800
C	-0.43107700	3.56524900	3.58197800
C	-1.56807700	2.01891400	7.54876200
C	-0.52519800	1.31119800	8.41296500
C	0.93192100	1.69758100	8.16618000
C	2.42301100	1.96884000	1.70277700
C	3.16801900	2.80761900	2.60643600
C	4.50079700	2.92468400	2.06862400
C	4.56537800	2.16551100	0.86542300
C	3.28471800	1.57687800	0.63970400
C	5.61465000	0.18694500	3.64360700
C	4.39799100	0.17517900	4.38350100
C	3.44202600	-0.63568800	3.67490000
C	4.10033100	-1.11853400	2.48575600
C	5.43096800	-0.60835400	2.47276100
C	1.25974600	-2.40204200	3.05776400
H	2.01615600	-3.17390700	2.87580500
H	0.34528400	-2.89165500	3.41220000
H	1.03232800	-1.89448100	2.11362700
C	2.40821200	-2.31970300	5.69297400
H	1.58108900	-2.94098900	6.05484900
H	3.21017700	-2.97163500	5.32796400
H	2.78955800	-1.72195700	6.52800200
C	2.29955400	5.41192500	3.38887100
H	3.25956800	5.78246100	3.01040100
H	1.57442800	5.43286100	2.56790300
H	1.94959300	6.08337100	4.18221400
C	3.88893200	3.89749500	5.22113000
H	4.76760000	4.31894800	4.71961000
H	3.57950300	4.58938100	6.01367200
H	4.15347300	2.94286000	5.68172900
H	-2.56664000	1.63509600	7.78727800
H	-1.58253500	3.09717500	7.74904900
H	-0.75703400	1.55023300	9.46268600
H	-0.63986000	0.22584600	8.32461000
H	1.58419800	1.10865200	8.82115800
H	1.10679500	2.75429700	8.40189800
H	1.38893500	1.67202600	1.82278200
H	3.02144800	0.91992300	-0.18124600
H	5.44746300	2.02963100	0.25011000
H	5.32464500	3.47302400	2.51016700
H	3.66005700	-1.74307700	1.71803300
H	6.16263800	-0.77016000	1.68951400
H	6.51313900	0.73278800	3.90794600
H	4.21699800	0.68156300	5.32319300
H	0.67927400	1.47590900	4.03584200

Species F
HF energy= -2968.45275120

No Imaginary frequency
Zero-point correction= 0.435001 (Hartree/Particle)
Thermal correction to Energy= 0.472740
Thermal correction to Enthalpy= 0.473684
Thermal correction to Gibbs Free Energy= 0.367536
Sum of electronic and zero-point Energies= -2968.017750
Sum of electronic and thermal Energies= -2967.980011
Sum of electronic and thermal Enthalpies= -2967.979067
Sum of electronic and thermal Free Energies= -2968.085215

Coordinates: **F**

Fe	0.05190000	-0.04080000	4.97090000
Fe	0.48140000	3.26980000	5.03520000
Fe	3.94500000	0.90410000	2.59170000
P	1.75270000	-1.37500000	4.46530000
P	2.41320000	3.87190000	4.06420000
S	-1.33650000	1.84140000	5.52700000
S	1.64570000	1.49740000	6.14720000
O	-1.40560000	-2.21580000	6.26310000
O	-0.86920000	-0.08740000	2.19980000
O	0.56310000	5.23170000	7.25020000
O	-1.27780000	4.80920000	3.28880000
C	-0.77640000	-1.29190000	5.87640000
C	-0.44670000	0.01490000	3.29970000
C	0.52610000	4.41490000	6.42510000
C	-0.56970000	4.22610000	3.99630000
C	-1.47720000	1.88170000	7.37630000
C	-0.37310000	1.16370000	8.16300000
C	1.06970000	1.61340000	7.90740000
C	2.27010000	1.93880000	1.88470000
C	3.06080000	2.81010000	2.70980000
C	4.37010000	2.87580000	2.10990000
C	4.37310000	2.06890000	0.93200000
C	3.07280000	1.48880000	0.79670000
C	5.51350000	0.17110000	3.73150000
C	4.30200000	0.09070000	4.48210000
C	3.37310000	-0.75570000	3.78310000
C	4.03290000	-1.17330000	2.57660000
C	5.34710000	-0.60960000	2.54520000
C	1.38350000	-2.74240000	3.26220000
H	2.23020000	-3.42900000	3.12880000
H	0.52340000	-3.29850000	3.65360000
H	1.09060000	-2.32180000	2.29360000
C	2.46220000	-2.37170000	5.87470000
H	1.66230000	-2.99490000	6.29260000
H	3.30300000	-3.00560000	5.55940000
H	2.80150000	-1.68270000	6.65680000
C	2.38340000	5.50920000	3.17600000
H	3.35760000	5.75160000	2.73140000
H	1.62990000	5.47870000	2.38060000
H	2.10040000	6.29680000	3.88620000
C	3.88110000	4.12030000	5.16720000
H	4.78910000	4.37760000	4.60720000
H	3.65110000	4.93610000	5.86440000
H	4.04450000	3.20810000	5.74910000
H	-2.43960000	1.40870000	7.61850000
H	-1.55050000	2.93840000	7.66840000
H	-0.58500000	1.29320000	9.24050000
H	-0.43880000	0.09190000	7.94750000
H	1.74330000	0.97340000	8.49540000

H	1.22780000	2.64560000	8.24820000
H	1.25010000	1.64010000	2.08800000
H	2.75730000	0.79260000	0.02740000
H	5.22520000	1.89450000	0.28290000
H	5.21940000	3.43180000	2.49140000
H	3.59830000	-1.79560000	1.80280000
H	6.07170000	-0.72610000	1.74590000
H	6.38900000	0.75550000	3.99520000
H	4.08590000	0.60120000	5.41210000
H	0.46130000	2.34960000	3.83870000

Species G
HF energy= -2968.99671748
No Imaginary frequency
Zero-point correction= 0.446685 (Hartree/Particle)
Thermal correction to Energy= 0.483109
Thermal correction to Enthalpy= 0.484053
Thermal correction to Gibbs Free Energy= 0.382396
Sum of electronic and zero-point Energies= -2968.550033
Sum of electronic and thermal Energies= -2968.513609
Sum of electronic and thermal Enthalpies= -2968.512664
Sum of electronic and thermal Free Energies= -2968.614321

Coordinates: **G**

Fe	1.20130000	-0.10920000	2.55960000
Fe	-0.02960000	2.74070000	3.96010000
Fe	4.46540000	1.83670000	5.40320000
P	3.21010000	-0.88840000	3.29400000
P	1.29750000	3.63770000	5.55030000
S	-0.64110000	1.38040000	2.12300000
S	0.50250000	0.54420000	4.74770000
O	0.13900000	-2.85280000	2.25220000
O	1.95780000	0.13980000	-0.24940000
O	-2.55540000	3.13830000	5.45530000
O	-0.29080000	5.14420000	2.32120000
C	0.45480000	-1.75630000	2.43500000
C	1.66410000	-0.00690000	0.85560000
C	-1.58360000	2.91090000	4.87230000
C	-0.21680000	4.21390000	2.99810000
C	-2.19120000	0.55200000	2.71480000
C	-2.05140000	-0.51060000	3.81730000
C	-1.17000000	-0.20590000	5.04150000
C	3.78780000	3.29660000	4.07140000
C	3.10830000	3.44260000	5.33010000
C	4.12620000	3.66590000	6.32510000
C	5.39930000	3.66910000	5.68210000
C	5.18830000	3.43970000	4.28790000
C	4.66790000	0.40620000	6.90540000
C	3.58950000	0.04750000	6.04660000
C	4.09680000	-0.11510000	4.70920000
C	5.51000000	0.16160000	4.77050000
C	5.85680000	0.47800000	6.11770000
C	4.51160000	-0.89730000	1.97850000
H	5.43980000	-1.36440000	2.32770000
H	4.13800000	-1.46630000	1.11960000
H	4.71980000	0.12480000	1.64250000
C	3.26240000	-2.66100000	3.84810000
H	2.94930000	-3.31390000	3.02450000

H	4.27080000	-2.94440000	4.17400000
H	2.56580000	-2.80370000	4.68220000
C	1.18280000	5.48070000	5.73950000
H	1.84390000	5.84470000	6.53570000
H	1.46350000	5.96750000	4.79860000
H	0.14720000	5.75640000	5.97430000
C	0.99330000	3.08420000	7.28890000
H	1.69270000	3.54420000	7.99730000
H	-0.02740000	3.37120000	7.57030000
H	1.07460000	1.99450000	7.34750000
H	-2.65410000	0.08210000	1.83730000
H	-2.85360000	1.36660000	3.03000000
H	-3.06440000	-0.73240000	4.19240000
H	-1.70460000	-1.44050000	3.36000000
H	-0.99880000	-1.14560000	5.58290000
H	-1.68350000	0.46950000	5.73500000
H	3.30530000	3.08780000	3.12570000
H	5.96000000	3.35040000	3.53150000
H	6.35870000	3.78370000	6.17470000
H	3.96300000	3.79570000	7.38880000
H	6.19790000	0.15840000	3.93400000
H	6.84290000	0.76160000	6.46830000
H	4.58980000	0.62100000	7.96540000
H	2.55260000	-0.06300000	6.33290000
H	1.28290000	2.75640000	3.20890000
H	2.04100000	1.16470000	2.56550000

Species H
HF energy= -2969.37677236
No Imaginary frequency
Zero-point correction= 0.456874 (Hartree/Particle)
Thermal correction to Energy= 0.494682
Thermal correction to Enthalpy= 0.495626
Thermal correction to Gibbs Free Energy= 0.390182
Sum of electronic and zero-point Energies= -2968.919898
Sum of electronic and thermal Energies= -2968.882090
Sum of electronic and thermal Enthalpies= -2968.881146
Sum of electronic and thermal Free Energies= -2968.986590

Coordinates: **H**

Fe	1.23780000	-0.04310000	2.49250000
Fe	-0.00570000	2.74500000	3.91660000
Fe	4.46810000	1.85880000	5.35420000
P	3.26730000	-0.95130000	3.26970000
P	1.28530000	3.66140000	5.56300000
S	-0.65530000	1.39500000	2.05700000
S	0.54110000	0.53190000	4.68570000
O	0.13170000	-2.76020000	2.48020000
O	1.68660000	-0.29270000	-0.43070000
O	-2.52200000	3.04870000	5.45610000
O	-0.42980000	5.21660000	2.39560000
C	0.48810000	-1.67310000	2.51320000
C	1.54450000	-0.21040000	0.69760000
C	-1.55960000	2.86590000	4.85600000
C	-0.29030000	4.26630000	3.02000000
C	-2.19910000	0.56770000	2.66670000
C	-2.05570000	-0.49380000	3.76780000
C	-1.13580000	-0.22640000	4.97240000

C	3.81780000	3.42920000	4.12200000
C	3.09500000	3.46040000	5.36690000
C	4.08040000	3.60710000	6.40740000
C	5.37090000	3.67550000	5.80740000
C	5.20790000	3.56380000	4.39420000
C	4.77810000	0.39090000	6.80720000
C	3.67760000	0.02330000	5.98530000
C	4.14240000	-0.09470000	4.62450000
C	5.54830000	0.23090000	4.63640000
C	5.93150000	0.52130000	5.97670000
C	4.53630000	-1.09230000	1.93720000
H	5.44570000	-1.57720000	2.31030000
H	4.13210000	-1.69790000	1.11780000
H	4.79500000	-0.10450000	1.53860000
C	3.16740000	-2.67800000	3.91720000
H	2.84550000	-3.36510000	3.12620000
H	4.15100000	-2.99050000	4.28620000
H	2.44880000	-2.72890000	4.74220000
C	1.13830000	5.49640000	5.74740000
H	1.77830000	5.86080000	6.55970000
H	1.43670000	5.99230000	4.81700000
H	0.09650000	5.76240000	5.96460000
C	0.93490000	3.07220000	7.27670000
H	1.58440000	3.56130000	8.01170000
H	-0.10590000	3.31110000	7.52620000
H	1.06840000	1.98770000	7.33890000
H	-2.67310000	0.10650000	1.79250000
H	-2.84570000	1.39300000	2.98340000
H	-3.06260000	-0.67790000	4.17330000
H	-1.76630000	-1.43830000	3.30160000
H	-0.95440000	-1.17680000	5.48820000
H	-1.61850000	0.43580000	5.69810000
H	3.37610000	3.34670000	3.13790000
H	6.00350000	3.55610000	3.65790000
H	6.31250000	3.75690000	6.33860000
H	3.88550000	3.64570000	7.47270000
H	6.20750000	0.25820000	3.77730000
H	6.92080000	0.82610000	6.29830000
H	4.73730000	0.57370000	7.87490000
H	2.66220000	-0.14110000	6.31910000
H	1.32280000	2.88070000	3.16870000
H	1.81140000	1.65030000	2.66480000
H	2.37820000	1.18680000	2.31630000

Species I
HF energy= -2968.79481877
No Imaginary frequency
Zero-point correction= 0.446567 (Hartree/Particle)
Thermal correction to Energy= 0.485019
Thermal correction to Enthalpy= 0.485963
Thermal correction to Gibbs Free Energy= 0.378223
Sum of electronic and zero-point Energies= -2968.348252
Sum of electronic and thermal Energies= -2968.309799
Sum of electronic and thermal Enthalpies= -2968.308855
Sum of electronic and thermal Free Energies= -2968.416596

Coordinates: **I**

Fe	-0.24180000	0.44660000	4.43690000

Fe	0.39980000	3.45500000	4.67940000
Fe	4.29490000	0.92650000	3.47930000
P	1.45120000	-1.18350000	4.42510000
P	2.65020000	3.95500000	4.49150000
S	-1.67980000	2.35060000	4.48270000
S	0.81520000	1.65220000	6.20680000
O	-1.86640000	-1.37850000	6.06040000
O	-1.71830000	-0.48910000	2.03650000
O	-0.26400000	5.69850000	6.56040000
O	-0.16320000	4.87580000	2.16100000
C	-1.24660000	-0.61540000	5.47550000
C	-1.13070000	-0.14830000	2.95180000
C	0.00190000	4.85160000	5.82950000
C	0.06700000	4.31860000	3.14140000
C	-2.47860000	2.54230000	6.15020000
C	-1.86620000	1.80850000	7.34550000
C	-0.36740000	1.97570000	7.60710000
C	3.22960000	2.21970000	2.22170000
C	3.68810000	2.92430000	3.39150000
C	5.12440000	2.82160000	3.39310000
C	5.52870000	2.06950000	2.25230000
C	4.35730000	1.69530000	1.52940000
C	5.29960000	-0.01670000	5.04420000
C	3.90950000	0.06000000	5.33790000
C	3.18990000	-0.65240000	4.31140000
C	4.17050000	-1.14930000	3.37700000
C	5.46090000	-0.75910000	3.83540000
C	1.26360000	-2.40910000	3.06030000
H	2.02260000	-3.19640000	3.13460000
H	0.27290000	-2.87380000	3.12700000
H	1.34870000	-1.92150000	2.08240000
C	1.46920000	-2.24230000	5.93700000
H	0.54180000	-2.82150000	6.01070000
H	2.31980000	-2.93230000	5.89300000
H	1.56640000	-1.61300000	6.82820000
C	2.98550000	5.64970000	3.82510000
H	4.06160000	5.86000000	3.82520000
H	2.61120000	5.73700000	2.79950000
H	2.47450000	6.39590000	4.44530000
C	3.57270000	4.00520000	6.09090000
H	4.62170000	4.28670000	5.94140000
H	3.10430000	4.75680000	6.73770000
H	3.52110000	3.03730000	6.59700000
H	-3.51770000	2.21820000	6.02250000
H	-2.49340000	3.62530000	6.31760000
H	-2.38820000	2.17290000	8.24450000
H	-2.11070000	0.74500000	7.28750000
H	-0.06900000	1.30190000	8.41820000
H	-0.13850000	2.99680000	7.93140000
H	2.20220000	2.12960000	1.89190000
H	4.32760000	1.09970000	0.62420000
H	6.54770000	1.79740000	2.00140000
H	5.79290000	3.22380000	4.14540000
H	3.96880000	-1.71850000	2.47740000
H	6.39780000	-0.96070000	3.32910000
H	6.09470000	0.44270000	5.62000000
H	3.46110000	0.55540000	6.18960000
H	0.61680000	1.69980000	3.51180000
H	0.94460000	0.98830000	3.32700000

Species J
HF energy= -2969.37677236
No Imaginary frequency
Zero-point correction= 0.456874 (Hartree/Particle)
Thermal correction to Energy= 0.494682
Thermal correction to Enthalpy= 0.495626
Thermal correction to Gibbs Free Energy= 0.390182
Sum of electronic and zero-point Energies= -2968.919898
Sum of electronic and thermal Energies= -2968.882090
Sum of electronic and thermal Enthalpies= -2968.881146
Sum of electronic and thermal Free Energies= -2968.986590

Coordinates: **J**

Fe	0.14610000	0.08600000	5.32590000
Fe	0.33830000	2.82570000	5.06010000
Fe	4.06400000	0.81550000	2.65560000
P	1.76580000	-1.41980000	4.42720000
P	2.18260000	3.71280000	3.81360000
S	-1.35410000	1.71670000	6.17510000
S	1.77210000	1.53300000	6.26190000
O	-2.23410000	-1.58740000	4.63270000
O	-0.11850000	0.83670000	2.49630000
O	0.30600000	5.18130000	6.78810000
O	-1.63910000	3.99550000	3.15250000
C	-1.31730000	-0.96620000	4.87450000
C	0.06040000	0.73610000	3.62300000
C	0.32420000	4.28310000	6.08510000
C	-0.88080000	3.54650000	3.86930000
C	-1.14390000	1.90900000	8.01440000
C	0.09000000	1.28470000	8.65970000
C	1.45010000	1.69550000	8.09530000
C	2.69960000	1.94920000	1.53980000
C	3.17960000	2.70680000	2.67180000
C	4.61250000	2.81000000	2.52300000
C	4.98830000	2.13710000	1.32780000
C	3.81050000	1.60820000	0.72350000
C	5.55900000	-0.14740000	3.77050000
C	4.35100000	-0.09300000	4.51440000
C	3.32910000	-0.79390000	3.76810000
C	3.94720000	-1.25830000	2.54540000
C	5.31140000	-0.86030000	2.55990000
C	1.06100000	-2.47640000	3.09520000
H	1.79350000	-3.23730000	2.80300000
H	0.16580000	-2.99220000	3.46060000
H	0.79230000	-1.88580000	2.21280000
C	2.28920000	-2.64010000	5.71120000
H	1.42640000	-3.20820000	6.08130000
H	3.00830000	-3.34010000	5.26880000
H	2.77590000	-2.12890000	6.54960000
C	1.68650000	5.14750000	2.76040000
H	2.57990000	5.61040000	2.32480000
H	1.03470000	4.82030000	1.94280000
H	1.15490000	5.89830000	3.35790000
C	3.42210000	4.44970000	4.96140000
H	4.18990000	4.98470000	4.39210000
H	2.93680000	5.17190000	5.62660000
H	3.89570000	3.67260000	5.56970000
H	-2.05360000	1.47650000	8.44480000

H	-1.18700000	2.99000000	8.18980000
H	0.08400000	1.57840000	9.72070000
H	-0.00600000	0.19120000	8.67770000
H	2.24250000	1.10690000	8.57050000
H	1.66170000	2.74950000	8.31030000
H	1.67150000	1.70190000	1.31570000
H	3.76950000	1.01750000	-0.18460000
H	6.00250000	2.01640000	0.96460000
H	5.29750000	3.29910000	3.20450000
H	3.46370000	-1.80850000	1.74730000
H	6.02690000	-1.03640000	1.76500000
H	6.49840000	0.31130000	4.05710000
H	4.22540000	0.38270000	5.47780000
H	0.49660000	-1.00370000	6.57160000
H	-0.06040000	-0.54210000	6.90110000

Species K
HF energy= -2968.46828470
No Imaginary frequency
Zero-point correction= 0.448775 (Hartree/Particle)
Thermal correction to Energy= 0.486935
Thermal correction to Enthalpy= 0.487880
Thermal correction to Gibbs Free Energy= 0.381897
Sum of electronic and zero-point Energies= -2968.019510
Sum of electronic and thermal Energies= -2967.981349
Sum of electronic and thermal Enthalpies= -2967.980405
Sum of electronic and thermal Free Energies= -2968.086388

Coordinates: **K**

Fe	0.19540000	0.25680000	5.03700000
Fe	0.39820000	2.88410000	4.85590000
Fe	4.12470000	0.86530000	2.43550000
P	1.77830000	-1.24190000	4.25420000
P	2.25690000	3.71500000	3.63640000
S	-1.32490000	1.79930000	5.94180000
S	1.79140000	1.57240000	6.09310000
O	-1.99010000	-1.68090000	4.85390000
O	-0.30030000	0.93530000	2.22870000
O	0.41520000	5.17480000	6.66070000
O	-1.54710000	4.09810000	2.97000000
C	-1.13610000	-0.91870000	4.87520000
C	-0.03170000	0.87660000	3.35220000
C	0.41730000	4.29670000	5.92410000
C	-0.79330000	3.62090000	3.68100000
C	-1.13880000	1.90360000	7.78180000
C	0.06440000	1.19320000	8.39290000
C	1.42840000	1.67780000	7.91150000
C	2.67110000	1.92300000	1.36790000
C	3.20800000	2.73660000	2.42980000
C	4.62530000	2.85840000	2.18410000
C	4.93930000	2.13540000	0.99860000
C	3.73460000	1.56020000	0.49640000
C	5.61800000	-0.00680000	3.60870000
C	4.39580000	0.04470000	4.33470000
C	3.40190000	-0.70890000	3.61070000
C	4.04580000	-1.21030000	2.42170000
C	5.40270000	-0.77780000	2.42760000
C	1.13260000	-2.33330000	2.91240000

H	1.85640000	-3.11780000	2.66450000
H	0.20760000	-2.81460000	3.24900000
H	0.90800000	-1.75230000	2.01100000
C	2.27230000	-2.45480000	5.55560000
H	1.38390000	-2.98190000	5.92230000
H	2.98870000	-3.18010000	5.15200000
H	2.73370000	-1.92570000	6.39630000
C	1.81960000	5.21560000	2.64380000
H	2.72330000	5.65860000	2.20930000
H	1.13800000	4.94740000	1.82900000
H	1.32730000	5.96080000	3.28070000
C	3.55130000	4.37160000	4.77680000
H	4.32900000	4.90270000	4.21730000
H	3.09690000	5.07790000	5.48020000
H	4.00220000	3.55420000	5.34750000
H	-2.06680000	1.47300000	8.17520000
H	-1.14700000	2.97140000	8.03220000
H	0.02470000	1.34590000	9.48290000
H	-0.02210000	0.11340000	8.22620000
H	2.22030000	1.08510000	8.38410000
H	1.60020000	2.72500000	8.18940000
H	1.63690000	1.63820000	1.23860000
H	3.64650000	0.92520000	-0.37770000
H	5.93110000	2.01050000	0.57900000
H	5.34150000	3.38590000	2.80180000
H	3.58020000	-1.79950000	1.64120000
H	6.13030000	-0.96890000	1.64710000
H	6.54110000	0.48930000	3.88620000
H	4.23530000	0.56480000	5.26940000
H	0.26420000	-0.60720000	6.28210000