Models of the iron-only hydrogenase: A comparison of chelate and bridge isomers of $Fe_2(CO)_4\{Ph_2PN(R)PPh_2\}(\mu\text{-pdt})$ as proton-reduction catalysts

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Supporting Information

Table 1. Crystal data and structure refinement for **2a**

Identification code	str0459	
Chemical formula	$C_{34}H_{31}Fe_2NO_4P_2S_2$	
Formula weight	755.36	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, P21/n	
Unit cell parameters	a = 9.8036(6) Å	α = 90°
	b = 17.9672(12) Å	β = 100.9190(10)°
	c = 18.4965(12) Å	γ = 90°
Cell volume	3199.0(4) $Å^3$	
Z	4	
Calculated density	1.568 g/cm^3	
Absorption coefficient μ	1.178 mm^{-1}	
F(000)	1552	
Crystal colour and size	red, 0.18 × 0.16 × 0.04 mm^3	
Data collection method	Bruker SMART APEX diffractometer	
	ω rotation with narrow frames	
θ range for data collection	1.59 to 28.29°	
Index ranges	h −12 to 12, k −23 to 23, l −24 to 23	
Completeness to θ = 26.00°	99.8 %	
Reflections collected	27778	
Independent reflections	7641 (R_{int} = 0.0281)	
Reflections with $F^2>2\sigma$	6556	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.8159 and 0.9544	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0451, 1.2266	
Data / restraints / parameters	7641 / 0 / 406	
Final R indices [$F^2>2\sigma$]	R1 = 0.0330, wR2 = 0.0813	
R indices (all data)	R1 = 0.0401, wR2 = 0.0843	
Goodness-of-fit on F^2	1.057	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	0.746 and −0.352 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for str0459. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Fe(1)	0.65872(3)	0.678835(14)	0.215303(14)	0.01544(7)
Fe(2)	0.54249(3)	0.614895(15)	0.092700(14)	0.01765(7)
P(1)	0.87033(5)	0.63464(3)	0.25595(2)	0.01520(10)
P(2)	0.65150(5)	0.60552(3)	0.31093(2)	0.01530(10)
S(1)	0.43198(5)	0.67838(3)	0.17030(3)	0.02083(11)
S(2)	0.68892(5)	0.71357(3)	0.10416(3)	0.02077(10)
N(1)	0.82373(15)	0.58311(8)	0.32540(8)	0.0167(3)
O(1)	0.67460(19)	0.83051(8)	0.26881(9)	0.0364(4)
O(2)	0.32712(17)	0.62616(9)	–0.04110(8)	0.0354(4)
O(3)	0.74895(16)	0.53793(10)	0.02516(9)	0.0374(4)
O(4)	0.4524(2)	0.46845(9)	0.13421(9)	0.0448(5)
C(1)	0.6728(2)	0.76839(11)	0.25248(10)	0.0234(4)
C(2)	0.4128(2)	0.62311(11)	0.01039(11)	0.0238(4)
C(3)	0.6710(2)	0.56772(11)	0.05337(11)	0.0243(4)
C(4)	0.4871(2)	0.52699(12)	0.12230(11)	0.0269(4)
C(5)	0.3799(2)	0.77099(12)	0.13309(12)	0.0309(5)
C(6)	0.4371(2)	0.79567(12)	0.06620(12)	0.0312(5)
C(7)	0.5940(2)	0.79988(11)	0.07695(12)	0.0297(5)
C(8)	0.9092(2)	0.56109(11)	0.39669(10)	0.0225(4)
C(9)	1.0264(2)	0.51031(13)	0.39082(11)	0.0301(5)
C(10)	1.1563(3)	0.52407(17)	0.42118(13)	0.0465(7)
C(11)	0.95009(18)	0.57279(10)	0.19785(10)	0.0175(4)
C(12)	1.0222(2)	0.60296(11)	0.14641(11)	0.0256(4)
C(13)	1.0793(2)	0.55693(13)	0.10000(12)	0.0304(5)
C(14)	1.0635(2)	0.48107(13)	0.10306(12)	0.0302(5)
C(15)	0.9880(2)	0.45061(12)	0.15150(12)	0.0288(4)
C(16)	0.9308(2)	0.49641(11)	0.19860(11)	0.0229(4)
C(17)	1.01622(19)	0.69144(10)	0.30270(10)	0.0183(4)
C(18)	1.1532(2)	0.68114(12)	0.29400(14)	0.0336(5)
C(19)	1.2597(2)	0.72415(14)	0.33339(15)	0.0404(6)
C(20)	1.2313(2)	0.77651(12)	0.38289(12)	0.0318(5)
C(21)	1.0963(2)	0.78825(12)	0.39107(12)	0.0291(5)
C(22)	0.9895(2)	0.74636(12)	0.35085(11)	0.0271(4)
C(23)	0.61247(19)	0.64100(10)	0.39814(10)	0.0183(4)
C(24)	0.6223(2)	0.71694(11)	0.41415(11)	0.0229(4)
C(25)	0.5815(2)	0.74529(12)	0.47611(11)	0.0255(4)
C(26)	0.5302(2)	0.69884(12)	0.52399(11)	0.0276(4)
C(27)	0.5249(3)	0.62334(13)	0.51090(12)	0.0352(5)
C(28)	0.5646(3)	0.59464(12)	0.44808(11)	0.0308(5)
C(29)	0.55785(19)	0.51755(10)	0.30414(10)	0.0182(4)
C(30)	0.6243(2)	0.44875(11)	0.30741(10)	0.0219(4)
C(31)	0.5479(2)	0.38329(11)	0.29942(11)	0.0276(4)
C(32)	0.4042(2)	0.38577(12)	0.28721(11)	0.0300(5)
C(33)	0.3368(2)	0.45377(13)	0.28369(12)	0.0309(5)
C(34)	0.4132(2)	0.51938(12)	0.29250(11)	0.0255(4)

Table 3. Bond lengths [Å] and angles [°] for str0459.

Fe(1)–C(1)	1.745(2)	Fe(1)–P(1)	2.2156(5)
Fe(1)–P(2)	2.2172(5)	Fe(1)–S(1)	2.2211(5)
Fe(1)–S(2)	2.2212(5)	Fe(1)–Fe(2)	2.6042(4)
Fe(2)–C(3)	1.784(2)	Fe(2)–C(4)	1.789(2)
Fe(2)–C(2)	1.795(2)	Fe(2)–S(1)	2.2637(5)
Fe(2)–S(2)	2.2657(5)	P(1)–N(1)	1.7143(15)
P(1)–C(11)	1.8218(18)	P(1)–C(17)	1.8348(19)
P(1)–P(2)	2.5956(7)	P(2)–N(1)	1.7069(15)
P(2)–C(29)	1.8202(19)	P(2)–C(23)	1.8408(18)
S(1)–C(5)	1.836(2)	S(2)–C(7)	1.830(2)
N(1)–C(8)	1.476(2)	O(1)–C(1)	1.156(2)
O(2)–C(2)	1.146(2)	O(3)–C(3)	1.137(2)
O(4)–C(4)	1.140(3)	C(5)–C(6)	1.518(3)
C(6)–C(7)	1.514(3)	C(8)–C(9)	1.487(3)
C(9)–C(10)	1.315(3)	C(11)–C(16)	1.386(3)
C(11)–C(12)	1.398(3)	C(12)–C(13)	1.384(3)
C(13)–C(14)	1.374(3)	C(14)–C(15)	1.379(3)
C(15)–C(16)	1.391(3)	C(17)–C(22)	1.387(3)
C(17)–C(18)	1.394(3)	C(18)–C(19)	1.390(3)
C(19)–C(20)	1.378(3)	C(20)–C(21)	1.376(3)
C(21)–C(22)	1.386(3)	C(23)–C(28)	1.390(3)
C(23)–C(24)	1.396(3)	C(24)–C(25)	1.381(3)
C(25)–C(26)	1.379(3)	C(26)–C(27)	1.377(3)
C(27)–C(28)	1.392(3)	C(29)–C(30)	1.393(3)
C(29)–C(34)	1.394(3)	C(30)–C(31)	1.387(3)
C(31)–C(32)	1.385(3)	C(32)–C(33)	1.384(3)
C(33)–C(34)	1.389(3)		

C(1)–Fe(1)–P(1)	101.41(7)	C(1)–Fe(1)–P(2)	104.21(6)
P(1)–Fe(1)–P(2)	71.683(18)	C(1)–Fe(1)–S(1)	98.62(7)
P(1)–Fe(1)–S(1)	158.77(2)	P(2)–Fe(1)–S(1)	96.65(2)
C(1)–Fe(1)–S(2)	95.24(7)	P(1)–Fe(1)–S(2)	97.72(2)
P(2)–Fe(1)–S(2)	159.26(2)	S(1)–Fe(1)–S(2)	87.34(2)
C(1)–Fe(1)–Fe(2)	137.63(6)	P(1)–Fe(1)–Fe(2)	111.375(16)
P(2)–Fe(1)–Fe(2)	110.960(17)	S(1)–Fe(1)–Fe(2)	55.269(14)
S(2)–Fe(1)–Fe(2)	55.323(15)	C(3)–Fe(2)–C(4)	89.09(9)
C(3)–Fe(2)–C(2)	97.74(9)	C(4)–Fe(2)–C(2)	97.17(9)
C(3)–Fe(2)–S(1)	163.30(6)	C(4)–Fe(2)–S(1)	92.37(7)
C(2)–Fe(2)–S(1)	98.58(7)	C(3)–Fe(2)–S(2)	85.75(7)
C(4)–Fe(2)–S(2)	152.33(7)	C(2)–Fe(2)–S(2)	110.45(7)
S(1)–Fe(2)–S(2)	85.25(2)	C(3)–Fe(2)–Fe(1)	109.78(6)
C(4)–Fe(2)–Fe(1)	103.36(6)	C(2)–Fe(2)–Fe(1)	145.59(6)
S(1)–Fe(2)–Fe(1)	53.742(15)	S(2)–Fe(2)–Fe(1)	53.728(14)
N(1)–P(1)–C(11)	108.52(8)	N(1)–P(1)–C(17)	103.99(8)
C(11)–P(1)–C(17)	103.53(9)	N(1)–P(1)–Fe(1)	94.73(5)
C(11)–P(1)–Fe(1)	119.83(6)	C(17)–P(1)–Fe(1)	123.83(6)
N(1)–P(1)–P(2)	40.55(5)	C(11)–P(1)–P(2)	125.95(6)
C(17)–P(1)–P(2)	123.77(6)	Fe(1)–P(1)–P(2)	54.188(16)
N(1)–P(2)–C(29)	106.08(8)	N(1)–P(2)–C(23)	107.93(8)
C(29)–P(2)–C(23)	100.10(8)	N(1)–P(2)–Fe(1)	94.89(5)
C(29)–P(2)–Fe(1)	123.56(6)	C(23)–P(2)–Fe(1)	122.45(6)
N(1)–P(2)–P(1)	40.76(5)	C(29)–P(2)–P(1)	126.26(6)
C(23)–P(2)–P(1)	126.72(6)	Fe(1)–P(2)–P(1)	54.129(16)

C(5)–S(1)–Fe(1)	108.95(8)	C(5)–S(1)–Fe(2)	110.58(7)
Fe(1)–S(1)–Fe(2)	70.989(17)	C(7)–S(2)–Fe(1)	110.04(8)
C(7)–S(2)–Fe(2)	110.92(7)	Fe(1)–S(2)–Fe(2)	70.949(17)
C(8)–N(1)–P(2)	125.49(12)	C(8)–N(1)–P(1)	128.87(13)
P(2)–N(1)–P(1)	98.70(8)	O(1)–C(1)–Fe(1)	171.82(18)
O(2)–C(2)–Fe(2)	177.29(19)	O(3)–C(3)–Fe(2)	176.78(18)
O(4)–C(4)–Fe(2)	173.09(18)	C(6)–C(5)–S(1)	116.78(15)
C(7)–C(6)–C(5)	115.50(17)	C(6)–C(7)–S(2)	116.42(15)
N(1)–C(8)–C(9)	114.51(16)	C(10)–C(9)–C(8)	123.6(2)
C(16)–C(11)–C(12)	118.57(17)	C(16)–C(11)–P(1)	121.58(14)
C(12)–C(11)–P(1)	119.60(15)	C(13)–C(12)–C(11)	120.44(19)
C(14)–C(13)–C(12)	120.33(19)	C(13)–C(14)–C(15)	119.93(19)
C(14)–C(15)–C(16)	120.1(2)	C(11)–C(16)–C(15)	120.51(18)
C(22)–C(17)–C(18)	118.15(18)	C(22)–C(17)–P(1)	118.22(15)
C(18)–C(17)–P(1)	123.60(15)	C(19)–C(18)–C(17)	120.7(2)
C(20)–C(19)–C(18)	120.1(2)	C(21)–C(20)–C(19)	119.8(2)
C(20)–C(21)–C(22)	120.15(19)	C(21)–C(22)–C(17)	121.01(19)
C(28)–C(23)–C(24)	117.60(17)	C(28)–C(23)–P(2)	121.83(15)
C(24)–C(23)–P(2)	120.46(14)	C(25)–C(24)–C(23)	121.15(18)
C(26)–C(25)–C(24)	120.53(19)	C(27)–C(26)–C(25)	119.30(19)
C(26)–C(27)–C(28)	120.3(2)	C(23)–C(28)–C(27)	121.05(19)
C(30)–C(29)–C(34)	118.76(18)	C(30)–C(29)–P(2)	122.82(14)
C(34)–C(29)–P(2)	118.38(15)	C(31)–C(30)–C(29)	120.63(19)
C(32)–C(31)–C(30)	120.1(2)	C(33)–C(32)–C(31)	119.82(19)
C(32)–C(33)–C(34)	120.1(2)	C(33)–C(34)–C(29)	120.53(19)

Table 4. Anisotropic displacement parameters ($Å^2$) for str0459. 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)	0.01582(14)	0.01547(13)	0.01419(13)	–0.00013(9)	0.00073(10)	0.00192(9)
Fe(2)	0.01809(14)	0.01946(14)	0.01535(13)	–0.00074(10)	0.00300(10)	0.00024(10)
P(1)	0.0145(2)	0.0157(2)	0.0149(2)	–0.00003(17)	0.00173(16)	0.00069(17)
P(2)	0.0153(2)	0.0168(2)	0.0138(2)	–0.00076(17)	0.00263(17)	0.00238(17)
S(1)	0.0160(2)	0.0269(2)	0.0192(2)	–0.00088(18)	0.00228(17)	0.00450(18)
S(2)	0.0235(2)	0.0204(2)	0.0178(2)	0.00299(18)	0.00219(17)	–0.00137(18)
N(1)	0.0151(7)	0.0196(7)	0.0151(7)	0.0026(6)	0.0021(6)	0.0028(6)
O(1)	0.0563(11)	0.0196(7)	0.0333(9)	–0.0031(6)	0.0088(8)	0.0025(7)
O(2)	0.0342(9)	0.0388(9)	0.0282(8)	–0.0022(7)	–0.0069(7)	0.0012(7)
O(3)	0.0292(8)	0.0494(10)	0.0351(9)	–0.0131(8)	0.0100(7)	0.0063(7)
O(4)	0.0799(14)	0.0290(9)	0.0281(9)	–0.0025(7)	0.0165(9)	–0.0158(9)
C(1)	0.0277(10)	0.0229(10)	0.0187(9)	0.0019(7)	0.0023(8)	0.0036(8)
C(2)	0.0253(10)	0.0234(10)	0.0229(10)	–0.0017(8)	0.0050(8)	–0.0002(8)
C(3)	0.0249(10)	0.0268(10)	0.0201(9)	–0.0031(8)	0.0016(8)	–0.0015(8)
C(4)	0.0367(12)	0.0278(11)	0.0173(9)	–0.0033(8)	0.0077(8)	–0.0010(9)
C(5)	0.0282(11)	0.0316(11)	0.0292(11)	–0.0022(9)	–0.0035(9)	0.0157(9)
C(6)	0.0382(12)	0.0223(10)	0.0279(11)	0.0027(8)	–0.0069(9)	0.0080(9)
C(7)	0.0385(12)	0.0198(9)	0.0273(11)	0.0071(8)	–0.0023(9)	0.0002(9)
C(8)	0.0209(9)	0.0306(10)	0.0153(9)	0.0041(8)	0.0017(7)	0.0040(8)
C(9)	0.0346(12)	0.0325(11)	0.0219(10)	0.0055(9)	0.0023(9)	0.0144(9)
C(10)	0.0280(12)	0.077(2)	0.0336(13)	0.0062(13)	0.0043(10)	0.0212(13)
C(11)	0.0141(8)	0.0213(9)	0.0167(8)	–0.0009(7)	0.0020(7)	0.0017(7)
C(12)	0.0253(10)	0.0246(10)	0.0291(10)	0.0031(8)	0.0104(8)	–0.0013(8)
C(13)	0.0289(11)	0.0369(12)	0.0297(11)	0.0036(9)	0.0166(9)	0.0006(9)
C(14)	0.0297(11)	0.0362(12)	0.0274(11)	–0.0068(9)	0.0121(9)	0.0044(9)
C(15)	0.0375(12)	0.0227(10)	0.0287(11)	–0.0044(8)	0.0124(9)	–0.0007(9)
C(16)	0.0268(10)	0.0229(9)	0.0211(9)	–0.0013(8)	0.0097(8)	–0.0026(8)
C(17)	0.0169(9)	0.0174(8)	0.0187(9)	0.0015(7)	–0.0012(7)	0.0001(7)
C(18)	0.0203(10)	0.0307(11)	0.0467(14)	–0.0151(10)	–0.0018(9)	0.0052(8)
C(19)	0.0160(10)	0.0438(14)	0.0578(16)	–0.0159(12)	–0.0020(10)	0.0028(9)
C(20)	0.0258(11)	0.0292(11)	0.0355(12)	–0.0062(9)	–0.0066(9)	–0.0031(9)
C(21)	0.0301(11)	0.0297(11)	0.0269(11)	–0.0105(9)	0.0034(9)	–0.0015(9)
C(22)	0.0198(10)	0.0348(11)	0.0275(10)	–0.0079(9)	0.0067(8)	–0.0007(8)
C(23)	0.0171(9)	0.0224(9)	0.0152(8)	–0.0028(7)	0.0026(7)	0.0018(7)
C(24)	0.0236(10)	0.0241(10)	0.0213(9)	–0.0027(8)	0.0049(8)	–0.0028(8)
C(25)	0.0257(10)	0.0264(10)	0.0241(10)	–0.0078(8)	0.0044(8)	–0.0011(8)
C(26)	0.0289(11)	0.0359(11)	0.0190(9)	–0.0087(8)	0.0067(8)	–0.0020(9)
C(27)	0.0538(15)	0.0347(12)	0.0215(11)	–0.0024(9)	0.0184(10)	–0.0083(11)
C(28)	0.0505(14)	0.0220(10)	0.0220(10)	–0.0018(8)	0.0122(9)	–0.0013(9)
C(29)	0.0208(9)	0.0214(9)	0.0130(8)	–0.0005(7)	0.0051(7)	–0.0008(7)
C(30)	0.0221(10)	0.0225(9)	0.0227(10)	–0.0001(8)	0.0085(8)	0.0010(8)
C(31)	0.0383(12)	0.0214(10)	0.0259(10)	–0.0017(8)	0.0131(9)	–0.0030(9)
C(32)	0.0380(13)	0.0327(11)	0.0213(10)	–0.0045(8)	0.0105(9)	–0.0158(9)
C(33)	0.0219(10)	0.0436(13)	0.0272(11)	–0.0021(9)	0.0047(8)	–0.0088(9)
C(34)	0.0211(10)	0.0298(11)	0.0255(10)	–0.0008(8)	0.0039(8)	0.0000(8)

Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for str0459.

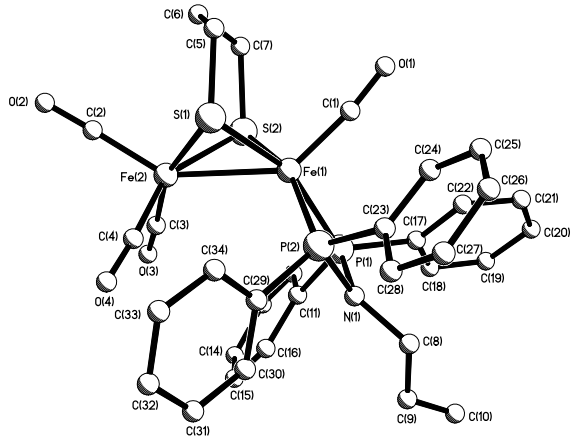
	x	y	z	U
H(5A)	0.2793	0.7723	0.1203	0.037
H(5B)	0.4080	0.8072	0.1719	0.037
H(6A)	0.4041	0.7615	0.0261	0.037
H(6B)	0.3994	0.8444	0.0513	0.037
H(7A)	0.6260	0.8373	0.1141	0.036
H(7B)	0.6182	0.8170	0.0313	0.036
H(8A)	0.8498	0.5369	0.4260	0.027
H(8B)	0.9464	0.6057	0.4228	0.027
H(9A)	1.0067	0.4664	0.3642	0.036
H(10A)	1.1790	0.5675	0.4481	0.056
H(10B)	1.2257	0.4903	0.4158	0.056
H(12A)	1.0319	0.6543	0.1433	0.031
H(13A)	1.1287	0.5775	0.0666	0.036
H(14A)	1.1037	0.4503	0.0725	0.036
H(15A)	0.9753	0.3994	0.1527	0.035
H(16A)	0.8793	0.4756	0.2308	0.028
H(18A)	1.1734	0.6451	0.2615	0.040
H(19A)	1.3504	0.7176	0.3263	0.048
H(20A)	1.3031	0.8039	0.4107	0.038
H(21A)	1.0767	0.8244	0.4236	0.035
H(22A)	0.8984	0.7552	0.3562	0.032
H(24A)	0.6570	0.7490	0.3825	0.028
H(25A)	0.5887	0.7961	0.4856	0.031
H(26A)	0.4995	0.7183	0.5647	0.033
H(27A)	0.4946	0.5914	0.5442	0.042
H(28A)	0.5590	0.5436	0.4394	0.037
H(30A)	0.7207	0.4467	0.3150	0.026
H(31A)	0.5933	0.3376	0.3023	0.033
H(32A)	0.3530	0.3419	0.2814	0.036
H(33A)	0.2403	0.4555	0.2754	0.037
H(34A)	0.3674	0.5649	0.2906	0.031

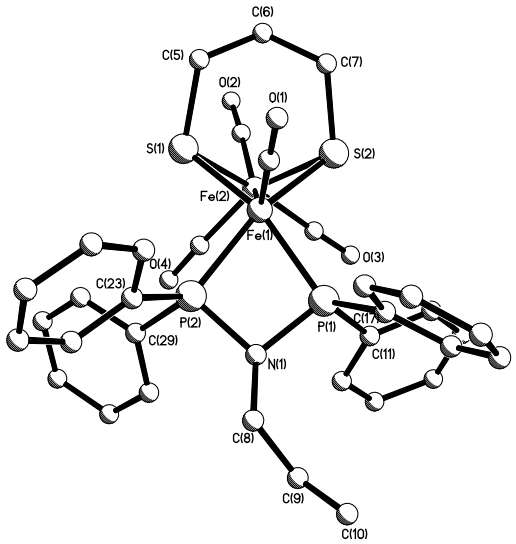
Table 6. Torsion angles [°] for str0459.

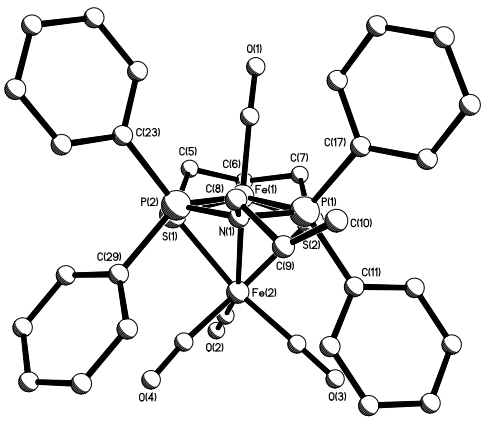
C(1)–Fe(1)–Fe(2)–C(3)	122.38(12)	P(1)–Fe(1)–Fe(2)–C(3)	−15.72(7)
P(2)–Fe(1)–Fe(2)–C(3)	−93.51(7)	S(1)–Fe(1)–Fe(2)–C(3)	−176.92(7)
S(2)–Fe(1)–Fe(2)–C(3)	68.81(7)	C(1)–Fe(1)–Fe(2)–C(4)	−143.71(12)
P(1)–Fe(1)–Fe(2)–C(4)	78.19(7)	P(2)–Fe(1)–Fe(2)–C(4)	0.40(7)
S(1)–Fe(1)–Fe(2)–C(4)	−83.02(7)	S(2)–Fe(1)–Fe(2)–C(4)	162.71(8)
C(1)–Fe(1)–Fe(2)–C(2)	−18.71(16)	P(1)–Fe(1)–Fe(2)–C(2)	−156.81(12)
P(2)–Fe(1)–Fe(2)–C(2)	125.40(12)	S(1)–Fe(1)–Fe(2)–C(2)	41.98(12)
S(2)–Fe(1)–Fe(2)–C(2)	−72.28(12)	C(1)–Fe(1)–Fe(2)–S(1)	−60.69(10)
P(1)–Fe(1)–Fe(2)–S(1)	161.21(2)	P(2)–Fe(1)–Fe(2)–S(1)	83.42(2)
S(2)–Fe(1)–Fe(2)–S(1)	−114.26(2)	C(1)–Fe(1)–Fe(2)–S(2)	53.57(10)
P(1)–Fe(1)–Fe(2)–S(2)	−84.53(2)	P(2)–Fe(1)–Fe(2)–S(2)	−162.32(2)
S(1)–Fe(1)–Fe(2)–S(2)	114.26(2)	C(1)–Fe(1)–P(1)–N(1)	101.73(8)
P(2)–Fe(1)–P(1)–N(1)	0.37(5)	S(1)–Fe(1)–P(1)–N(1)	−58.61(8)
S(2)–Fe(1)–P(1)–N(1)	−161.30(5)	Fe(2)–Fe(1)–P(1)–N(1)	−105.60(5)
C(1)–Fe(1)–P(1)–C(11)	−143.75(10)	P(2)–Fe(1)–P(1)–C(11)	114.88(7)
S(1)–Fe(1)–P(1)–C(11)	55.91(10)	S(2)–Fe(1)–P(1)–C(11)	−46.78(7)
Fe(2)–Fe(1)–P(1)–C(11)	8.92(7)	C(1)–Fe(1)–P(1)–C(17)	−8.60(10)
P(2)–Fe(1)–P(1)–C(17)	−109.97(8)	S(1)–Fe(1)–P(1)–C(17)	−168.95(8)
S(2)–Fe(1)–P(1)–C(17)	88.36(8)	Fe(2)–Fe(1)–P(1)–C(17)	144.07(7)
C(1)–Fe(1)–P(1)–P(2)	101.37(7)	S(1)–Fe(1)–P(1)–P(2)	−58.98(6)
S(2)–Fe(1)–P(1)–P(2)	−161.67(2)	Fe(2)–Fe(1)–P(1)–P(2)	−105.966(19)
C(1)–Fe(1)–P(2)–N(1)	−97.90(9)	P(1)–Fe(1)–P(2)–N(1)	−0.37(5)
S(1)–Fe(1)–P(2)–N(1)	161.43(5)	S(2)–Fe(1)–P(2)–N(1)	61.29(8)
Fe(2)–Fe(1)–P(2)–N(1)	106.15(5)	C(1)–Fe(1)–P(2)–C(29)	149.12(10)
P(1)–Fe(1)–P(2)–C(29)	−113.35(8)	S(1)–Fe(1)–P(2)–C(29)	48.45(8)
S(2)–Fe(1)–P(2)–C(29)	−51.69(10)	Fe(2)–Fe(1)–P(2)–C(29)	−6.83(8)
C(1)–Fe(1)–P(2)–C(23)	16.96(10)	P(1)–Fe(1)–P(2)–C(23)	114.49(7)
S(1)–Fe(1)–P(2)–C(23)	−83.71(7)	S(2)–Fe(1)–P(2)–C(23)	176.15(8)
Fe(2)–Fe(1)–P(2)–C(23)	−138.99(7)	C(1)–Fe(1)–P(2)–P(1)	−97.53(7)
S(1)–Fe(1)–P(2)–P(1)	161.80(2)	S(2)–Fe(1)–P(2)–P(1)	61.66(6)
Fe(2)–Fe(1)–P(2)–P(1)	106.518(18)	C(11)–P(1)–P(2)–N(1)	75.88(11)
C(17)–P(1)–P(2)–N(1)	−70.48(11)	Fe(1)–P(1)–P(2)–N(1)	179.43(8)
N(1)–P(1)–P(2)–C(29)	−71.04(11)	C(11)–P(1)–P(2)–C(29)	4.84(11)
C(17)–P(1)–P(2)–C(29)	−141.52(10)	Fe(1)–P(1)–P(2)–C(29)	108.39(8)
N(1)–P(1)–P(2)–C(23)	73.90(11)	C(11)–P(1)–P(2)–C(23)	149.78(10)
C(17)–P(1)–P(2)–C(23)	3.42(11)	Fe(1)–P(1)–P(2)–C(23)	−106.66(8)
N(1)–P(1)–P(2)–Fe(1)	−179.43(8)	C(11)–P(1)–P(2)–Fe(1)	−103.56(7)
C(17)–P(1)–P(2)–Fe(1)	110.09(7)	C(1)–Fe(1)–S(1)–C(5)	37.58(10)
P(1)–Fe(1)–S(1)–C(5)	−161.90(9)	P(2)–Fe(1)–S(1)–C(5)	143.11(7)
S(2)–Fe(1)–S(1)–C(5)	−57.32(8)	Fe(2)–Fe(1)–S(1)–C(5)	−105.95(8)
C(1)–Fe(1)–S(1)–Fe(2)	143.53(7)	P(1)–Fe(1)–S(1)–Fe(2)	−55.95(6)
P(2)–Fe(1)–S(1)–Fe(2)	−110.939(19)	S(2)–Fe(1)–S(1)–Fe(2)	48.637(17)
C(3)–Fe(2)–S(1)–C(5)	113.9(2)	C(4)–Fe(2)–S(1)–C(5)	−151.40(10)
C(2)–Fe(2)–S(1)–C(5)	−53.78(10)	S(2)–Fe(2)–S(1)–C(5)	56.22(8)
Fe(1)–Fe(2)–S(1)–C(5)	103.74(8)	C(3)–Fe(2)–S(1)–Fe(1)	10.1(2)
C(4)–Fe(2)–S(1)–Fe(1)	104.86(7)	C(2)–Fe(2)–S(1)–Fe(1)	−157.52(7)
S(2)–Fe(2)–S(1)–Fe(1)	−47.521(17)	C(1)–Fe(1)–S(2)–C(7)	−40.98(10)
P(1)–Fe(1)–S(2)–C(7)	−143.27(8)	P(2)–Fe(1)–S(2)–C(7)	159.25(9)
S(1)–Fe(1)–S(2)–C(7)	57.44(8)	Fe(2)–Fe(1)–S(2)–C(7)	106.03(8)
C(1)–Fe(1)–S(2)–Fe(2)	−147.01(7)	P(1)–Fe(1)–S(2)–Fe(2)	110.700(18)

P(2)–Fe(1)–S(2)–Fe(2)	53.22(6)	S(1)–Fe(1)–S(2)–Fe(2)	−48.594(17)
C(3)–Fe(2)–S(2)–C(7)	136.78(10)	C(4)–Fe(2)–S(2)–C(7)	−143.34(17)
C(2)–Fe(2)–S(2)–C(7)	40.09(11)	S(1)–Fe(2)–S(2)–C(7)	−57.30(8)
Fe(1)–Fe(2)–S(2)–C(7)	−104.84(8)	C(3)–Fe(2)–S(2)–Fe(1)	−118.38(6)
C(4)–Fe(2)–S(2)–Fe(1)	−38.51(15)	C(2)–Fe(2)–S(2)–Fe(1)	144.93(7)
S(1)–Fe(2)–S(2)–Fe(1)	47.532(17)	C(29)–P(2)–N(1)–C(8)	−79.81(16)
C(23)–P(2)–N(1)–C(8)	26.76(17)	Fe(1)–P(2)–N(1)–C(8)	153.18(15)
P(1)–P(2)–N(1)–C(8)	152.72(19)	C(29)–P(2)–N(1)–P(1)	127.48(8)
C(23)–P(2)–N(1)–P(1)	−125.96(8)	Fe(1)–P(2)–N(1)–P(1)	0.46(7)
C(11)–P(1)–N(1)–C(8)	84.54(17)	C(17)–P(1)–N(1)–C(8)	−25.20(17)
Fe(1)–P(1)–N(1)–C(8)	−151.82(15)	P(2)–P(1)–N(1)–C(8)	−151.4(2)
C(11)–P(1)–N(1)–P(2)	−124.11(8)	C(17)–P(1)–N(1)–P(2)	126.15(8)
Fe(1)–P(1)–N(1)–P(2)	−0.46(7)	P(1)–Fe(1)–C(1)–O(1)	132.7(14)
P(2)–Fe(1)–C(1)–O(1)	−153.6(14)	S(1)–Fe(1)–C(1)–O(1)	−54.4(14)
S(2)–Fe(1)–C(1)–O(1)	33.7(14)	Fe(2)–Fe(1)–C(1)–O(1)	−7.9(14)
C(3)–Fe(2)–C(2)–O(2)	105(4)	C(4)–Fe(2)–C(2)–O(2)	15(4)
S(1)–Fe(2)–C(2)–O(2)	−78(4)	S(2)–Fe(2)–C(2)–O(2)	−166(4)
Fe(1)–Fe(2)–C(2)–O(2)	−111(4)	C(4)–Fe(2)–C(3)–O(3)	100(3)
C(2)–Fe(2)–C(3)–O(3)	3(3)	S(1)–Fe(2)–C(3)–O(3)	−164(3)
S(2)–Fe(2)–C(3)–O(3)	−107(3)	Fe(1)–Fe(2)–C(3)–O(3)	−156(3)
C(3)–Fe(2)–C(4)–O(4)	−45.8(18)	C(2)–Fe(2)–C(4)–O(4)	51.9(18)
S(1)–Fe(2)–C(4)–O(4)	150.8(18)	S(2)–Fe(2)–C(4)–O(4)	−124.9(17)
Fe(1)–Fe(2)–C(4)–O(4)	−155.9(18)	Fe(1)–S(1)–C(5)–C(6)	66.23(17)
Fe(2)–S(1)–C(5)–C(6)	−9.95(19)	S(1)–C(5)–C(6)–C(7)	−60.1(2)
C(5)–C(6)–C(7)–S(2)	59.0(2)	Fe(1)–S(2)–C(7)–C(6)	−65.04(17)
Fe(2)–S(2)–C(7)–C(6)	11.51(19)	P(2)–N(1)–C(8)–C(9)	150.91(15)
P(1)–N(1)–C(8)–C(9)	−64.7(2)	N(1)–C(8)–C(9)–C(10)	125.6(2)
N(1)–P(1)–C(11)–C(16)	18.77(18)	C(17)–P(1)–C(11)–C(16)	128.82(16)
Fe(1)–P(1)–C(11)–C(16)	−88.23(16)	P(2)–P(1)–C(11)–C(16)	−22.90(19)
N(1)–P(1)–C(11)–C(12)	−167.09(15)	C(17)–P(1)–C(11)–C(12)	−57.03(17)
Fe(1)–P(1)–C(11)–C(12)	85.91(16)	P(2)–P(1)–C(11)–C(12)	151.24(13)
C(16)–C(11)–C(12)–C(13)	−3.4(3)	P(1)–C(11)–C(12)–C(13)	−177.73(16)
C(11)–C(12)–C(13)–C(14)	1.2(3)	C(12)–C(13)–C(14)–C(15)	1.3(3)
C(13)–C(14)–C(15)–C(16)	−1.7(3)	C(12)–C(11)–C(16)–C(15)	3.1(3)
P(1)–C(11)–C(16)–C(15)	177.29(16)	C(14)–C(15)–C(16)–C(11)	−0.6(3)
N(1)–P(1)–C(17)–C(22)	−67.94(17)	C(11)–P(1)–C(17)–C(22)	178.68(16)
Fe(1)–P(1)–C(17)–C(22)	37.68(18)	P(2)–P(1)–C(17)–C(22)	−28.79(18)
N(1)–P(1)–C(17)–C(18)	110.28(18)	C(11)–P(1)–C(17)–C(18)	−3.1(2)
Fe(1)–P(1)–C(17)–C(18)	−144.09(16)	P(2)–P(1)–C(17)–C(18)	149.44(16)
C(22)–C(17)–C(18)–C(19)	0.9(3)	P(1)–C(17)–C(18)–C(19)	−177.34(19)
C(17)–C(18)–C(19)–C(20)	1.5(4)	C(18)–C(19)–C(20)–C(21)	−2.6(4)
C(19)–C(20)–C(21)–C(22)	1.5(4)	C(20)–C(21)–C(22)–C(17)	0.9(3)
C(18)–C(17)–C(22)–C(21)	−2.1(3)	P(1)–C(17)–C(22)–C(21)	176.25(17)
N(1)–P(2)–C(23)–C(28)	−92.89(18)	C(29)–P(2)–C(23)–C(28)	17.81(19)
Fe(1)–P(2)–C(23)–C(28)	158.94(15)	P(1)–P(2)–C(23)–C(28)	−134.13(16)
N(1)–P(2)–C(23)–C(24)	91.02(16)	C(29)–P(2)–C(23)–C(24)	−158.29(16)
Fe(1)–P(2)–C(23)–C(24)	−17.15(18)	P(1)–P(2)–C(23)–C(24)	49.77(18)
C(28)–C(23)–C(24)–C(25)	−2.1(3)	P(2)–C(23)–C(24)–C(25)	174.11(16)
C(23)–C(24)–C(25)–C(26)	0.2(3)	C(24)–C(25)–C(26)–C(27)	2.4(3)
C(25)–C(26)–C(27)–C(28)	−3.1(4)	C(24)–C(23)–C(28)–C(27)	1.5(3)
P(2)–C(23)–C(28)–C(27)	−174.72(19)	C(26)–C(27)–C(28)–C(23)	1.1(4)
N(1)–P(2)–C(29)–C(30)	−2.68(17)	C(23)–P(2)–C(29)–C(30)	−114.81(16)

Fe(1)–P(2)–C(29)–C(30)	104.64(15)	P(1)–P(2)–C(29)–C(30)	37.31(18)
N(1)–P(2)–C(29)–C(34)	179.71(14)	C(23)–P(2)–C(29)–C(34)	67.58(16)
Fe(1)–P(2)–C(29)–C(34)	–72.98(16)	P(1)–P(2)–C(29)–C(34)	–140.31(13)
C(34)–C(29)–C(30)–C(31)	–0.2(3)	P(2)–C(29)–C(30)–C(31)	–177.76(15)
C(29)–C(30)–C(31)–C(32)	0.7(3)	C(30)–C(31)–C(32)–C(33)	–0.6(3)
C(31)–C(32)–C(33)–C(34)	–0.1(3)	C(32)–C(33)–C(34)–C(29)	0.7(3)
C(30)–C(29)–C(34)–C(33)	–0.6(3)	P(2)–C(29)–C(34)–C(33)	177.14(15)







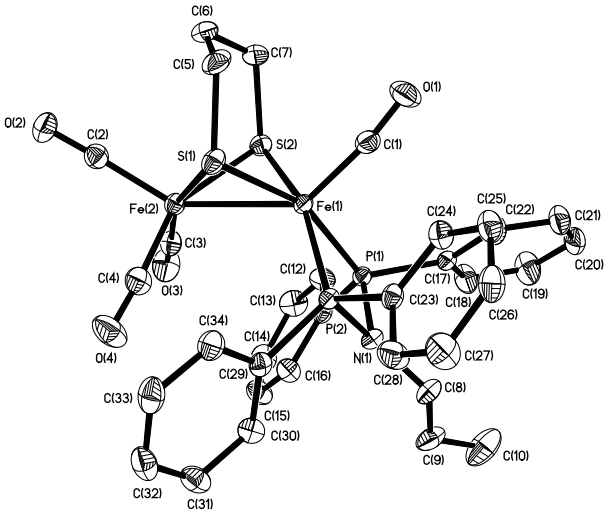


Table 1. Crystal data and structure refinement for **2b**.

Identification code	str0540	
Chemical formula	$C_{34}H_{33}Fe_2NO_4P_2S_2$	
Formula weight	757.37	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, P1bar	
Unit cell parameters	a = 9.7227(10) Å	α = 84.913(2)°
	b = 10.3859(11) Å	β = 80.645(2)°
	c = 18.5263(19) Å	γ = 63.569(2)°
Cell volume	1652.7(3) $Å^3$	
Z	2	
Calculated density	1.522 g/cm^3	
Absorption coefficient μ	1.141 mm^{-1}	
F(000)	780	
Crystal colour and size	brown, 0.24 × 0.16 × 0.14 mm^3	
Data collection method	Bruker SMART APEX diffractometer	
	ω rotation with narrow frames	
θ range for data collection	2.75 to 28.31°	
Index ranges	h −12 to 12, k −13 to 13, l −24 to 23	
Completeness to θ = 26.00°	98.0 %	
Reflections collected	14333	
Independent reflections	7563 (R_{int} = 0.0250)	
Reflections with $F^2>2\sigma$	6917	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.7714 and 0.8566	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0557, 2.8501	
Data / restraints / parameters	7563 / 0 / 406	
Final R indices [$F^2>2\sigma$]	R1 = 0.0421, wR2 = 0.1095	
R indices (all data)	R1 = 0.0453, wR2 = 0.1122	
Goodness-of-fit on F^2	1.030	
Largest and mean shift/su	0.000 and 0.000	
Largest diff. peak and hole	2.451 and −0.726 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for str0540. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Fe(1)	0.51744(4)	0.36202(3)	0.272386(17)	0.01089(9)
Fe(2)	0.44438(4)	0.27286(4)	0.403438(18)	0.01320(9)
P(1)	0.77021(7)	0.29495(6)	0.24932(3)	0.01170(12)
P(2)	0.62387(7)	0.17397(6)	0.19995(3)	0.01232(13)
S(1)	0.29936(7)	0.34150(6)	0.31094(3)	0.01587(13)
S(2)	0.47348(7)	0.47571(6)	0.37575(3)	0.01588(13)
N(1)	0.8103(2)	0.1518(2)	0.19667(11)	0.0148(4)
O(1)	0.3750(2)	0.6158(2)	0.18172(10)	0.0232(4)
O(2)	0.2227(2)	0.3484(2)	0.53867(11)	0.0288(4)
O(3)	0.7204(3)	0.1534(3)	0.47764(13)	0.0345(5)
O(4)	0.4666(3)	–0.0185(2)	0.40865(11)	0.0270(4)
C(1)	0.4404(3)	0.5110(3)	0.21455(13)	0.0146(4)
C(2)	0.3075(3)	0.3215(3)	0.48557(13)	0.0178(5)
C(3)	0.6167(3)	0.2016(3)	0.44650(14)	0.0212(5)
C(4)	0.4596(3)	0.0941(3)	0.40197(13)	0.0174(5)
C(5)	0.1388(3)	0.5205(3)	0.3247(2)	0.0318(7)
C(6)	0.1392(4)	0.6052(4)	0.3825(2)	0.0379(7)
C(7)	0.2825(3)	0.6322(3)	0.38309(17)	0.0287(6)
C(8)	0.9547(3)	0.0757(3)	0.14429(15)	0.0287(6)
C(9)	0.9512(3)	0.1483(3)	0.06958(14)	0.0222(5)
C(10)	1.0131(4)	–0.0809(4)	0.1419(2)	0.0435(8)
C(11)	0.8607(3)	0.3998(3)	0.19396(13)	0.0152(4)
C(12)	1.0157(3)	0.3696(3)	0.19598(15)	0.0228(5)
C(13)	1.0862(3)	0.4415(4)	0.14912(16)	0.0307(7)
C(14)	1.0040(4)	0.5451(4)	0.10003(16)	0.0303(6)
C(15)	0.8503(4)	0.5766(3)	0.09744(16)	0.0276(6)
C(16)	0.7800(3)	0.5044(3)	0.14412(14)	0.0208(5)
C(17)	0.8908(3)	0.2296(3)	0.32218(13)	0.0146(4)
C(18)	0.9848(4)	0.0857(3)	0.33491(17)	0.0285(6)
C(19)	1.0729(4)	0.0444(3)	0.39202(18)	0.0335(7)
C(20)	1.0675(3)	0.1466(3)	0.43731(15)	0.0226(5)
C(21)	0.9739(3)	0.2904(3)	0.42483(13)	0.0171(5)
C(22)	0.8852(3)	0.3326(3)	0.36783(13)	0.0147(4)
C(23)	0.5890(3)	0.1809(3)	0.10479(13)	0.0155(5)
C(24)	0.6396(3)	0.0560(3)	0.06480(14)	0.0195(5)
C(25)	0.6225(3)	0.0646(3)	–0.00891(14)	0.0220(5)
C(26)	0.5525(4)	0.1969(3)	–0.04319(14)	0.0258(6)
C(27)	0.4997(4)	0.3210(3)	–0.00392(15)	0.0278(6)
C(28)	0.5178(3)	0.3137(3)	0.06962(14)	0.0211(5)
C(29)	0.6148(3)	0.0063(3)	0.23047(13)	0.0160(5)
C(30)	0.4810(3)	–0.0069(3)	0.22290(14)	0.0204(5)
C(31)	0.4654(4)	–0.1306(3)	0.24701(15)	0.0250(6)
C(32)	0.5835(4)	–0.2424(3)	0.27833(16)	0.0268(6)
C(33)	0.7155(3)	–0.2293(3)	0.28700(17)	0.0299(6)
C(34)	0.7304(3)	–0.1047(3)	0.26377(15)	0.0235(5)

Table 3. Bond lengths [Å] and angles [°] for str0540.

Fe(1)–C(1)	1.743(2)	Fe(1)–P(1)	2.2124(7)
Fe(1)–P(2)	2.2137(7)	Fe(1)–S(2)	2.2203(7)
Fe(1)–S(1)	2.2214(7)	Fe(1)–Fe(2)	2.6236(5)
Fe(2)–C(3)	1.793(3)	Fe(2)–C(2)	1.794(3)
Fe(2)–C(4)	1.798(3)	Fe(2)–S(2)	2.2524(7)
Fe(2)–S(1)	2.2598(7)	P(1)–N(1)	1.712(2)
P(1)–C(17)	1.817(2)	P(1)–C(11)	1.837(2)
P(1)–P(2)	2.5803(8)	P(2)–N(1)	1.714(2)
P(2)–C(29)	1.818(2)	P(2)–C(23)	1.838(2)
S(1)–C(5)	1.825(3)	S(2)–C(7)	1.838(3)
N(1)–C(8)	1.498(3)	O(1)–C(1)	1.163(3)
O(2)–C(2)	1.143(3)	O(3)–C(3)	1.136(3)
O(4)–C(4)	1.138(3)	C(5)–C(6)	1.446(5)
C(6)–C(7)	1.540(5)	C(8)–C(10)	1.466(5)
C(8)–C(9)	1.514(4)	C(11)–C(16)	1.395(3)
C(11)–C(12)	1.401(3)	C(12)–C(13)	1.389(4)
C(13)–C(14)	1.386(4)	C(14)–C(15)	1.389(4)
C(15)–C(16)	1.388(4)	C(17)–C(18)	1.384(4)
C(17)–C(22)	1.399(3)	C(18)–C(19)	1.388(4)
C(19)–C(20)	1.389(4)	C(20)–C(21)	1.382(4)
C(21)–C(22)	1.388(3)	C(23)–C(28)	1.394(3)
C(23)–C(24)	1.399(3)	C(24)–C(25)	1.393(4)
C(25)–C(26)	1.381(4)	C(26)–C(27)	1.382(4)
C(27)–C(28)	1.393(4)	C(29)–C(34)	1.386(4)
C(29)–C(30)	1.397(4)	C(30)–C(31)	1.388(4)
C(31)–C(32)	1.383(4)	C(32)–C(33)	1.385(4)
C(33)–C(34)	1.388(4)		

C(1)–Fe(1)–P(1)	103.57(8)	C(1)–Fe(1)–P(2)	105.18(8)
P(1)–Fe(1)–P(2)	71.32(2)	C(1)–Fe(1)–S(2)	98.94(8)
P(1)–Fe(1)–S(2)	97.43(2)	P(2)–Fe(1)–S(2)	155.14(3)
C(1)–Fe(1)–S(1)	97.35(8)	P(1)–Fe(1)–S(1)	157.69(3)
P(2)–Fe(1)–S(1)	95.92(3)	S(2)–Fe(1)–S(1)	86.77(3)
C(1)–Fe(1)–Fe(2)	138.66(8)	P(1)–Fe(1)–Fe(2)	110.44(2)
P(2)–Fe(1)–Fe(2)	107.44(2)	S(2)–Fe(1)–Fe(2)	54.656(19)
S(1)–Fe(1)–Fe(2)	54.848(18)	C(3)–Fe(2)–C(2)	97.06(12)
C(3)–Fe(2)–C(4)	89.11(12)	C(2)–Fe(2)–C(4)	94.50(11)
C(3)–Fe(2)–S(2)	89.11(8)	C(2)–Fe(2)–S(2)	101.91(8)
C(4)–Fe(2)–S(2)	163.59(8)	C(3)–Fe(2)–S(1)	157.61(9)
C(2)–Fe(2)–S(1)	105.29(8)	C(4)–Fe(2)–S(1)	90.40(8)
S(2)–Fe(2)–S(1)	85.09(2)	C(3)–Fe(2)–Fe(1)	106.30(8)
C(2)–Fe(2)–Fe(1)	144.71(8)	C(4)–Fe(2)–Fe(1)	111.62(8)
S(2)–Fe(2)–Fe(1)	53.519(18)	S(1)–Fe(2)–Fe(1)	53.488(18)
N(1)–P(1)–C(17)	108.07(11)	N(1)–P(1)–C(11)	105.35(10)
C(17)–P(1)–C(11)	100.33(11)	N(1)–P(1)–Fe(1)	95.50(7)
C(17)–P(1)–Fe(1)	121.02(8)	C(11)–P(1)–Fe(1)	124.68(8)
N(1)–P(1)–P(2)	41.16(7)	C(17)–P(1)–P(2)	127.57(8)
C(11)–P(1)–P(2)	125.21(8)	Fe(1)–P(1)–P(2)	54.36(2)
N(1)–P(2)–C(29)	109.20(11)	N(1)–P(2)–C(23)	106.81(10)
C(29)–P(2)–C(23)	99.69(11)	N(1)–P(2)–Fe(1)	95.40(7)
C(29)–P(2)–Fe(1)	120.60(8)	C(23)–P(2)–Fe(1)	124.02(8)
N(1)–P(2)–P(1)	41.10(7)	C(29)–P(2)–P(1)	128.33(8)
C(23)–P(2)–P(1)	126.14(8)	Fe(1)–P(2)–P(1)	54.32(2)

C(5)–S(1)–Fe(1)	109.21(10)	C(5)–S(1)–Fe(2)	111.89(12)
Fe(1)–S(1)–Fe(2)	71.66(2)	C(7)–S(2)–Fe(1)	109.92(11)
C(7)–S(2)–Fe(2)	109.84(9)	Fe(1)–S(2)–Fe(2)	71.83(2)
C(8)–N(1)–P(1)	126.24(19)	C(8)–N(1)–P(2)	132.32(19)
P(1)–N(1)–P(2)	97.74(10)	O(1)–C(1)–Fe(1)	172.6(2)
O(2)–C(2)–Fe(2)	177.9(2)	O(3)–C(3)–Fe(2)	175.3(2)
O(4)–C(4)–Fe(2)	173.0(2)	C(6)–C(5)–S(1)	117.5(2)
C(5)–C(6)–C(7)	119.0(3)	C(6)–C(7)–S(2)	117.8(2)
C(10)–C(8)–N(1)	115.7(3)	C(10)–C(8)–C(9)	113.9(3)
N(1)–C(8)–C(9)	113.5(2)	C(16)–C(11)–C(12)	118.1(2)
C(16)–C(11)–P(1)	120.32(18)	C(12)–C(11)–P(1)	121.3(2)
C(13)–C(12)–C(11)	120.5(3)	C(14)–C(13)–C(12)	120.5(3)
C(13)–C(14)–C(15)	119.7(3)	C(16)–C(15)–C(14)	119.8(3)
C(15)–C(16)–C(11)	121.4(2)	C(18)–C(17)–C(22)	119.2(2)
C(18)–C(17)–P(1)	123.82(19)	C(22)–C(17)–P(1)	116.99(18)
C(17)–C(18)–C(19)	120.4(3)	C(18)–C(19)–C(20)	120.5(3)
C(21)–C(20)–C(19)	119.4(2)	C(20)–C(21)–C(22)	120.5(2)
C(21)–C(22)–C(17)	120.1(2)	C(28)–C(23)–C(24)	118.5(2)
C(28)–C(23)–P(2)	119.63(19)	C(24)–C(23)–P(2)	121.82(19)
C(25)–C(24)–C(23)	120.6(2)	C(26)–C(25)–C(24)	120.3(2)
C(25)–C(26)–C(27)	119.6(2)	C(26)–C(27)–C(28)	120.6(3)
C(27)–C(28)–C(23)	120.4(2)	C(34)–C(29)–C(30)	119.1(2)
C(34)–C(29)–P(2)	123.0(2)	C(30)–C(29)–P(2)	117.81(19)
C(31)–C(30)–C(29)	120.5(3)	C(32)–C(31)–C(30)	119.9(3)
C(31)–C(32)–C(33)	119.9(3)	C(32)–C(33)–C(34)	120.3(3)
C(29)–C(34)–C(33)	120.3(3)		

Table 4. Anisotropic displacement parameters ($Å^2$) for str0540. 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)	0.01041(16)	0.01068(16)	0.01018(16)	0.00089(11)	–0.00100(12)	–0.00368(13)
Fe(2)	0.01536(17)	0.01292(17)	0.01098(17)	0.00079(12)	–0.00041(12)	–0.00654(14)
P(1)	0.0107(3)	0.0125(3)	0.0105(3)	–0.0007(2)	–0.0011(2)	–0.0038(2)
P(2)	0.0139(3)	0.0121(3)	0.0110(3)	0.0002(2)	–0.0024(2)	–0.0055(2)
S(1)	0.0113(3)	0.0157(3)	0.0191(3)	0.0035(2)	–0.0024(2)	–0.0051(2)
S(2)	0.0195(3)	0.0136(3)	0.0139(3)	–0.0026(2)	0.0025(2)	–0.0079(2)
N(1)	0.0143(9)	0.0142(9)	0.0134(9)	–0.0031(7)	–0.0002(7)	–0.0041(8)
O(1)	0.0250(10)	0.0168(9)	0.0234(10)	0.0056(7)	–0.0064(8)	–0.0054(8)
O(2)	0.0281(11)	0.0318(11)	0.0188(10)	–0.0004(8)	0.0038(8)	–0.0087(9)
O(3)	0.0322(11)	0.0435(13)	0.0381(12)	0.0191(10)	–0.0175(10)	–0.0251(10)
O(4)	0.0393(12)	0.0197(10)	0.0230(10)	0.0003(7)	0.0004(8)	–0.0154(9)
C(1)	0.0139(11)	0.0144(11)	0.0143(11)	–0.0013(8)	–0.0014(8)	–0.0053(9)
C(2)	0.0199(12)	0.0164(11)	0.0152(11)	0.0009(9)	–0.0022(9)	–0.0067(10)
C(3)	0.0258(13)	0.0239(13)	0.0191(12)	0.0058(10)	–0.0045(10)	–0.0163(11)
C(4)	0.0187(12)	0.0198(12)	0.0127(11)	–0.0005(9)	–0.0005(9)	–0.0080(10)
C(5)	0.0112(12)	0.0193(13)	0.057(2)	0.0061(13)	–0.0018(12)	–0.0016(10)
C(6)	0.0307(16)	0.0303(16)	0.0410(18)	–0.0075(13)	–0.0082(14)	–0.0005(13)
C(7)	0.0261(14)	0.0122(12)	0.0383(16)	–0.0062(11)	0.0126(12)	–0.0046(11)
C(8)	0.0229(14)	0.0267(14)	0.0192(13)	–0.0046(10)	0.0059(11)	0.0023(11)
C(9)	0.0213(13)	0.0253(13)	0.0185(12)	–0.0065(10)	0.0059(10)	–0.0108(11)
C(10)	0.0384(19)	0.0377(19)	0.044(2)	–0.0084(15)	0.0050(15)	–0.0095(16)
C(11)	0.0164(11)	0.0194(12)	0.0114(10)	–0.0013(8)	0.0000(8)	–0.0096(10)
C(12)	0.0197(12)	0.0322(15)	0.0191(12)	0.0028(10)	–0.0037(10)	–0.0139(11)
C(13)	0.0225(14)	0.0492(19)	0.0270(15)	0.0048(13)	–0.0026(11)	–0.0229(14)
C(14)	0.0332(16)	0.0440(18)	0.0221(14)	0.0063(12)	0.0002(12)	–0.0270(14)
C(15)	0.0293(15)	0.0323(15)	0.0216(13)	0.0075(11)	–0.0032(11)	–0.0153(13)
C(16)	0.0179(12)	0.0252(13)	0.0195(12)	0.0036(10)	–0.0032(10)	–0.0100(10)
C(17)	0.0140(11)	0.0164(11)	0.0126(10)	0.0001(8)	–0.0029(8)	–0.0056(9)
C(18)	0.0346(16)	0.0159(13)	0.0338(16)	–0.0031(11)	–0.0188(13)	–0.0049(12)
C(19)	0.0409(18)	0.0169(13)	0.0403(17)	0.0035(12)	–0.0268(14)	–0.0042(12)
C(20)	0.0238(13)	0.0243(13)	0.0210(13)	0.0035(10)	–0.0107(10)	–0.0099(11)
C(21)	0.0176(11)	0.0217(12)	0.0147(11)	–0.0018(9)	–0.0013(9)	–0.0112(10)
C(22)	0.0143(11)	0.0141(11)	0.0142(11)	–0.0004(8)	0.0003(8)	–0.0055(9)
C(23)	0.0168(11)	0.0216(12)	0.0109(10)	0.0000(9)	–0.0027(8)	–0.0107(10)
C(24)	0.0210(12)	0.0213(12)	0.0172(12)	–0.0012(9)	–0.0029(9)	–0.0100(10)
C(25)	0.0221(13)	0.0297(14)	0.0181(12)	–0.0053(10)	–0.0021(10)	–0.0141(11)
C(26)	0.0349(15)	0.0378(16)	0.0135(12)	0.0025(10)	–0.0059(11)	–0.0233(13)
C(27)	0.0422(17)	0.0265(14)	0.0185(13)	0.0067(10)	–0.0123(12)	–0.0171(13)
C(28)	0.0294(14)	0.0197(12)	0.0168(12)	0.0013(9)	–0.0066(10)	–0.0123(11)
C(29)	0.0216(12)	0.0123(11)	0.0148(11)	–0.0006(8)	0.0000(9)	–0.0089(9)
C(30)	0.0267(13)	0.0200(12)	0.0181(12)	0.0015(9)	–0.0063(10)	–0.0129(11)
C(31)	0.0341(15)	0.0260(14)	0.0216(13)	–0.0048(10)	0.0005(11)	–0.0197(12)
C(32)	0.0348(15)	0.0167(12)	0.0268(14)	–0.0011(10)	0.0076(12)	–0.0133(12)
C(33)	0.0254(14)	0.0163(13)	0.0377(16)	0.0094(11)	0.0002(12)	–0.0033(11)
C(34)	0.0177(12)	0.0196(13)	0.0293(14)	0.0047(10)	0.0000(10)	–0.0067(10)

Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for str0540.

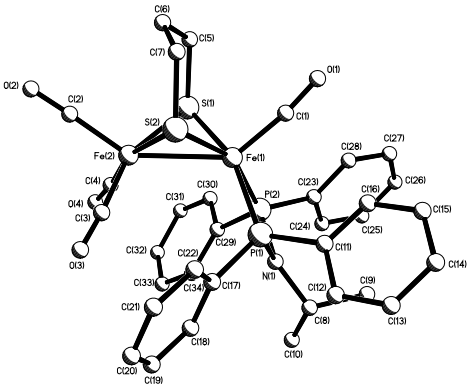
	x	y	z	U
H(5A)	0.1364	0.5759	0.2782	0.038
H(5B)	0.0411	0.5098	0.3345	0.038
H(6A)	0.1224	0.5580	0.4296	0.045
H(6B)	0.0484	0.7002	0.3811	0.045
H(7A)	0.2677	0.6816	0.4290	0.034
H(7B)	0.2849	0.6996	0.3422	0.034
H(8A)	1.0362	0.0888	0.1651	0.034
H(9A)	1.0488	0.0939	0.0381	0.033
H(9B)	0.9381	0.2464	0.0746	0.033
H(9C)	0.8645	0.1517	0.0476	0.033
H(10A)	1.0128	–0.1205	0.1919	0.065
H(10B)	1.1192	–0.1229	0.1160	0.065
H(10C)	0.9464	–0.1038	0.1163	0.065
H(12A)	1.0729	0.2993	0.2297	0.027
H(13A)	1.1915	0.4194	0.1507	0.037
H(14A)	1.0526	0.5944	0.0683	0.036
H(15A)	0.7934	0.6473	0.0638	0.033
H(16A)	0.6747	0.5266	0.1421	0.025
H(18A)	0.9889	0.0149	0.3044	0.034
H(19A)	1.1375	–0.0546	0.4002	0.040
H(20A)	1.1277	0.1180	0.4765	0.027
H(21A)	0.9701	0.3608	0.4555	0.020
H(22A)	0.8207	0.4317	0.3598	0.018
H(24A)	0.6860	–0.0355	0.0881	0.023
H(25A)	0.6591	–0.0210	–0.0357	0.026
H(26A)	0.5407	0.2025	–0.0934	0.031
H(27A)	0.4507	0.4121	–0.0273	0.033
H(28A)	0.4813	0.3998	0.0960	0.025
H(30A)	0.4001	0.0695	0.2011	0.024
H(31A)	0.3738	–0.1386	0.2420	0.030
H(32A)	0.5741	–0.3282	0.2939	0.032
H(33A)	0.7961	–0.3057	0.3089	0.036
H(34A)	0.8203	–0.0956	0.2707	0.028

Table 6. Torsion angles [°] for str0540.

C(1)–Fe(1)–Fe(2)–C(3)	−135.15(15)	P(1)–Fe(1)–Fe(2)–C(3)	8.22(9)
P(2)–Fe(1)–Fe(2)–C(3)	84.26(9)	S(2)–Fe(1)–Fe(2)–C(3)	−76.33(9)
S(1)–Fe(1)–Fe(2)–C(3)	169.15(9)	C(1)–Fe(1)–Fe(2)–C(2)	−5.74(19)
P(1)–Fe(1)–Fe(2)–C(2)	137.64(15)	P(2)–Fe(1)–Fe(2)–C(2)	−146.32(15)
S(2)–Fe(1)–Fe(2)–C(2)	53.09(15)	S(1)–Fe(1)–Fe(2)–C(2)	−61.43(15)
C(1)–Fe(1)–Fe(2)–C(4)	129.20(15)	P(1)–Fe(1)–Fe(2)–C(4)	−87.43(9)
P(2)–Fe(1)–Fe(2)–C(4)	−11.39(9)	S(2)–Fe(1)–Fe(2)–C(4)	−171.98(9)
S(1)–Fe(1)–Fe(2)–C(4)	73.50(9)	C(1)–Fe(1)–Fe(2)–S(2)	−58.82(12)
P(1)–Fe(1)–Fe(2)–S(2)	84.55(3)	P(2)–Fe(1)–Fe(2)–S(2)	160.59(3)
S(1)–Fe(1)–Fe(2)–S(2)	−114.52(3)	C(1)–Fe(1)–Fe(2)–S(1)	55.70(12)
P(1)–Fe(1)–Fe(2)–S(1)	−160.93(3)	P(2)–Fe(1)–Fe(2)–S(1)	−84.89(3)
S(2)–Fe(1)–Fe(2)–S(1)	114.52(3)	C(1)–Fe(1)–P(1)–N(1)	−103.15(11)
P(2)–Fe(1)–P(1)–N(1)	−1.45(7)	S(2)–Fe(1)–P(1)–N(1)	155.74(7)
S(1)–Fe(1)–P(1)–N(1)	56.04(10)	Fe(2)–Fe(1)–P(1)–N(1)	100.76(7)
C(1)–Fe(1)–P(1)–C(17)	141.92(12)	P(2)–Fe(1)–P(1)–C(17)	−116.38(10)
S(2)–Fe(1)–P(1)–C(17)	40.81(10)	S(1)–Fe(1)–P(1)–C(17)	−58.89(12)
Fe(2)–Fe(1)–P(1)–C(17)	−14.16(10)	C(1)–Fe(1)–P(1)–C(11)	9.81(13)
P(2)–Fe(1)–P(1)–C(11)	111.51(10)	S(2)–Fe(1)–P(1)–C(11)	−91.30(10)
S(1)–Fe(1)–P(1)–C(11)	169.00(10)	Fe(2)–Fe(1)–P(1)–C(11)	−146.28(9)
C(1)–Fe(1)–P(1)–P(2)	−101.70(8)	S(2)–Fe(1)–P(1)–P(2)	157.19(3)
S(1)–Fe(1)–P(1)–P(2)	57.49(7)	Fe(2)–Fe(1)–P(1)–P(2)	102.22(2)
C(1)–Fe(1)–P(2)–N(1)	100.94(11)	P(1)–Fe(1)–P(2)–N(1)	1.45(7)
S(2)–Fe(1)–P(2)–N(1)	−64.67(10)	S(1)–Fe(1)–P(2)–N(1)	−159.77(7)
Fe(2)–Fe(1)–P(2)–N(1)	−104.82(7)	C(1)–Fe(1)–P(2)–C(29)	−142.98(13)
P(1)–Fe(1)–P(2)–C(29)	117.54(10)	S(2)–Fe(1)–P(2)–C(29)	51.42(12)
S(1)–Fe(1)–P(2)–C(29)	−43.69(10)	Fe(2)–Fe(1)–P(2)–C(29)	11.27(10)
C(1)–Fe(1)–P(2)–C(23)	−13.54(13)	P(1)–Fe(1)–P(2)–C(23)	−113.03(10)
S(2)–Fe(1)–P(2)–C(23)	−179.15(10)	S(1)–Fe(1)–P(2)–C(23)	85.74(10)
Fe(2)–Fe(1)–P(2)–C(23)	140.70(9)	C(1)–Fe(1)–P(2)–P(1)	99.49(8)
S(2)–Fe(1)–P(2)–P(1)	−66.12(6)	S(1)–Fe(1)–P(2)–P(1)	−161.23(3)
Fe(2)–Fe(1)–P(2)–P(1)	−106.27(2)	C(17)–P(1)–P(2)–N(1)	−73.41(14)
C(11)–P(1)–P(2)–N(1)	71.65(14)	Fe(1)–P(1)–P(2)–N(1)	−177.80(11)
N(1)–P(1)–P(2)–C(29)	74.43(15)	C(17)–P(1)–P(2)–C(29)	1.02(15)
C(11)–P(1)–P(2)–C(29)	146.08(14)	Fe(1)–P(1)–P(2)–C(29)	−103.37(10)
N(1)–P(1)–P(2)–C(23)	−73.01(15)	C(17)–P(1)–P(2)–C(23)	−146.43(14)
C(11)–P(1)–P(2)–C(23)	−1.36(15)	Fe(1)–P(1)–P(2)–C(23)	109.18(10)
N(1)–P(1)–P(2)–Fe(1)	177.80(11)	C(17)–P(1)–P(2)–Fe(1)	104.39(10)
C(11)–P(1)–P(2)–Fe(1)	−110.55(10)	C(1)–Fe(1)–S(1)–C(5)	−39.13(15)
P(1)–Fe(1)–S(1)–C(5)	161.25(13)	P(2)–Fe(1)–S(1)–C(5)	−145.32(12)
S(2)–Fe(1)–S(1)–C(5)	59.48(12)	Fe(2)–Fe(1)–S(1)–C(5)	107.49(12)
C(1)–Fe(1)–S(1)–Fe(2)	−146.62(8)	P(1)–Fe(1)–S(1)–Fe(2)	53.76(7)
P(2)–Fe(1)–S(1)–Fe(2)	107.19(2)	S(2)–Fe(1)–S(1)–Fe(2)	−48.01(2)
C(3)–Fe(2)–S(1)–C(5)	−132.2(2)	C(2)–Fe(2)–S(1)–C(5)	44.36(13)
C(4)–Fe(2)–S(1)–C(5)	139.14(13)	S(2)–Fe(2)–S(1)–C(5)	−56.66(11)
Fe(1)–Fe(2)–S(1)–C(5)	−103.91(11)	C(3)–Fe(2)–S(1)–Fe(1)	−28.3(2)
C(2)–Fe(2)–S(1)–Fe(1)	148.27(8)	C(4)–Fe(2)–S(1)–Fe(1)	−116.95(8)
S(2)–Fe(2)–S(1)–Fe(1)	47.24(2)	C(1)–Fe(1)–S(2)–C(7)	39.98(13)
P(1)–Fe(1)–S(2)–C(7)	145.05(10)	P(2)–Fe(1)–S(2)–C(7)	−154.08(11)
S(1)–Fe(1)–S(2)–C(7)	−56.96(10)	Fe(2)–Fe(1)–S(2)–C(7)	−105.13(10)
C(1)–Fe(1)–S(2)–Fe(2)	145.11(8)	P(1)–Fe(1)–S(2)–Fe(2)	−109.82(2)

P(2)–Fe(1)–S(2)–Fe(2)	−48.95(7)	S(1)–Fe(1)–S(2)–Fe(2)	48.17(2)
C(3)–Fe(2)–S(2)–C(7)	−143.63(14)	C(2)–Fe(2)–S(2)–C(7)	−46.60(14)
C(4)–Fe(2)–S(2)–C(7)	132.6(3)	S(1)–Fe(2)–S(2)–C(7)	58.02(11)
Fe(1)–Fe(2)–S(2)–C(7)	105.24(11)	C(3)–Fe(2)–S(2)–Fe(1)	111.13(9)
C(2)–Fe(2)–S(2)–Fe(1)	−151.83(8)	C(4)–Fe(2)–S(2)–Fe(1)	27.3(3)
S(1)–Fe(2)–S(2)–Fe(1)	−47.22(2)	C(17)–P(1)–N(1)–C(8)	−72.7(2)
C(11)–P(1)–N(1)–C(8)	33.9(2)	Fe(1)–P(1)–N(1)–C(8)	162.2(2)
P(2)–P(1)–N(1)–C(8)	160.4(3)	C(17)–P(1)–N(1)–P(2)	126.96(11)
C(11)–P(1)–N(1)–P(2)	−126.46(11)	Fe(1)–P(1)–N(1)–P(2)	1.79(9)
C(29)–P(2)–N(1)–C(8)	74.6(2)	C(23)–P(2)–N(1)–C(8)	−32.3(3)
Fe(1)–P(2)–N(1)–C(8)	−160.3(2)	P(1)–P(2)–N(1)–C(8)	−158.5(3)
C(29)–P(2)–N(1)–P(1)	−126.85(11)	C(23)–P(2)–N(1)–P(1)	126.21(11)
Fe(1)–P(2)–N(1)–P(1)	−1.79(9)	P(1)–Fe(1)–C(1)–O(1)	−149.4(17)
P(2)–Fe(1)–C(1)–O(1)	136.7(17)	S(2)–Fe(1)–C(1)–O(1)	−49.4(17)
S(1)–Fe(1)–C(1)–O(1)	38.4(17)	Fe(2)–Fe(1)–C(1)–O(1)	−4.5(18)
C(3)–Fe(2)–C(2)–O(2)	−53(7)	C(4)–Fe(2)–C(2)–O(2)	37(7)
S(2)–Fe(2)–C(2)–O(2)	−143(7)	S(1)–Fe(2)–C(2)–O(2)	129(7)
Fe(1)–Fe(2)–C(2)–O(2)	176(100)	C(2)–Fe(2)–C(3)–O(3)	34(3)
C(4)–Fe(2)–C(3)–O(3)	−61(3)	S(2)–Fe(2)–C(3)–O(3)	135(3)
S(1)–Fe(2)–C(3)–O(3)	−150(3)	Fe(1)–Fe(2)–C(3)–O(3)	−173(3)
C(3)–Fe(2)–C(4)–O(4)	65.6(19)	C(2)–Fe(2)–C(4)–O(4)	−31.4(19)
S(2)–Fe(2)–C(4)–O(4)	149.4(17)	S(1)–Fe(2)–C(4)–O(4)	−136.8(19)
Fe(1)–Fe(2)–C(4)–O(4)	172.8(19)	Fe(1)–S(1)–C(5)–C(6)	−66.2(3)
Fe(2)–S(1)–C(5)–C(6)	11.1(3)	S(1)–C(5)–C(6)–C(7)	54.7(4)
C(5)–C(6)–C(7)–S(2)	−51.2(4)	Fe(1)–S(2)–C(7)–C(6)	59.1(3)
Fe(2)–S(2)–C(7)–C(6)	−18.1(3)	P(1)–N(1)–C(8)–C(10)	141.7(3)
P(2)–N(1)–C(8)–C(10)	−65.0(4)	P(1)–N(1)–C(8)–C(9)	−83.8(3)
P(2)–N(1)–C(8)–C(9)	69.5(3)	N(1)–P(1)–C(11)–C(16)	87.1(2)
C(17)–P(1)–C(11)–C(16)	−160.8(2)	Fe(1)–P(1)–C(11)–C(16)	−21.0(2)
P(2)–P(1)–C(11)–C(16)	46.7(2)	N(1)–P(1)–C(11)–C(12)	−87.6(2)
C(17)–P(1)–C(11)–C(12)	24.5(2)	Fe(1)–P(1)–C(11)–C(12)	164.28(18)
P(2)–P(1)–C(11)–C(12)	−127.98(19)	C(16)–C(11)–C(12)–C(13)	−0.5(4)
P(1)–C(11)–C(12)–C(13)	174.3(2)	C(11)–C(12)–C(13)–C(14)	0.5(5)
C(12)–C(13)–C(14)–C(15)	−0.4(5)	C(13)–C(14)–C(15)–C(16)	0.2(5)
C(14)–C(15)–C(16)–C(11)	−0.1(4)	C(12)–C(11)–C(16)–C(15)	0.3(4)
P(1)–C(11)–C(16)–C(15)	−174.6(2)	N(1)–P(1)–C(17)–C(18)	−6.1(3)
C(11)–P(1)–C(17)–C(18)	−116.1(2)	Fe(1)–P(1)–C(17)–C(18)	102.2(2)
P(2)–P(1)–C(17)–C(18)	35.5(3)	N(1)–P(1)–C(17)–C(22)	174.62(18)
C(11)–P(1)–C(17)–C(22)	64.6(2)	Fe(1)–P(1)–C(17)–C(22)	−77.1(2)
P(2)–P(1)–C(17)–C(22)	−143.81(15)	C(22)–C(17)–C(18)–C(19)	−0.4(4)
P(1)–C(17)–C(18)–C(19)	−179.7(3)	C(17)–C(18)–C(19)–C(20)	0.3(5)
C(18)–C(19)–C(20)–C(21)	−0.3(5)	C(19)–C(20)–C(21)–C(22)	0.3(4)
C(20)–C(21)–C(22)–C(17)	−0.4(4)	C(18)–C(17)–C(22)–C(21)	0.4(4)
P(1)–C(17)–C(22)–C(21)	179.74(18)	N(1)–P(2)–C(23)–C(28)	−95.4(2)
C(29)–P(2)–C(23)–C(28)	151.0(2)	Fe(1)–P(2)–C(23)–C(28)	13.4(2)
P(1)–P(2)–C(23)–C(28)	−54.3(2)	N(1)–P(2)–C(23)–C(24)	81.1(2)
C(29)–P(2)–C(23)–C(24)	−32.5(2)	Fe(1)–P(2)–C(23)–C(24)	−170.09(17)
P(1)–P(2)–C(23)–C(24)	122.15(19)	C(28)–C(23)–C(24)–C(25)	1.6(4)
P(2)–C(23)–C(24)–C(25)	−174.9(2)	C(23)–C(24)–C(25)–C(26)	−1.3(4)
C(24)–C(25)–C(26)–C(27)	0.2(4)	C(25)–C(26)–C(27)–C(28)	0.6(5)
C(26)–C(27)–C(28)–C(23)	−0.2(4)	C(24)–C(23)–C(28)–C(27)	−0.9(4)
P(2)–C(23)–C(28)–C(27)	175.7(2)	N(1)–P(2)–C(29)–C(34)	15.7(2)

C(23)–P(2)–C(29)–C(34)	127.5(2)	Fe(1)–P(2)–C(29)–C(34)	–93.0(2)
P(1)–P(2)–C(29)–C(34)	–26.4(3)	N(1)–P(2)–C(29)–C(30)	–167.48(19)
C(23)–P(2)–C(29)–C(30)	–55.8(2)	Fe(1)–P(2)–C(29)–C(30)	83.7(2)
P(1)–P(2)–C(29)–C(30)	150.40(16)	C(34)–C(29)–C(30)–C(31)	–1.3(4)
P(2)–C(29)–C(30)–C(31)	–178.2(2)	C(29)–C(30)–C(31)–C(32)	–0.5(4)
C(30)–C(31)–C(32)–C(33)	1.4(4)	C(31)–C(32)–C(33)–C(34)	–0.6(5)
C(30)–C(29)–C(34)–C(33)	2.2(4)	P(2)–C(29)–C(34)–C(33)	178.9(2)
C(32)–C(33)–C(34)–C(29)	–1.2(4)		



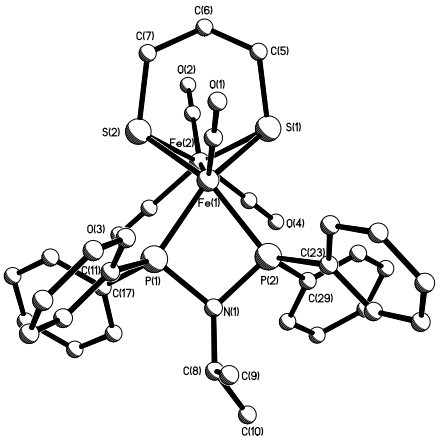


Table 1. Crystal data and structure refinement for **3a**.

Identification code	str0463	
Chemical formula	$C_{34}H_{31}Fe_2NO_4P_2S_2$	
Formula weight	755.36	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, P1bar	
Unit cell parameters	a = 8.8977(5) Å	α = 89.0140(10)°
	b = 10.2309(6) Å	β = 79.5570(10)°
	c = 19.2787(11) Å	γ = 75.4280(10)°
Cell volume	1669.64(17) $Å^3$	
Z	2	
Calculated density	1.502 g/cm^3	
Absorption coefficient μ	1.129 mm^{-1}	
F(000)	776	
Crystal colour and size	red, 0.24 × 0.22 × 0.14 mm^3	
Data collection method	Bruker SMART APEX diffractometer	
	ω rotation with narrow frames	
θ range for data collection	2.06 to 28.25°	
Index ranges	h –11 to 11, k –13 to 13, l –25 to 25	
Completeness to θ = 26.00°	98.7 %	
Reflections collected	14741	
Independent reflections	7671 (R_{int} = 0.0127)	
Reflections with $F^2>2\sigma$	7151	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.7734 and 0.8580	
Structure solution	Patterson synthesis	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0380, 0.8205	
Data / restraints / parameters	7671 / 0 / 406	
Final R indices [$F^2>2\sigma$]	R1 = 0.0263, wR2 = 0.0689	
R indices (all data)	R1 = 0.0284, wR2 = 0.0701	
Goodness-of-fit on F^2	1.029	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	0.539 and –0.269 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for str0463. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Fe(1)	0.98468(2)	0.59488(2)	0.208605(10)	0.01725(6)
Fe(2)	0.87880(2)	0.68785(2)	0.330736(10)	0.01638(6)
P(1)	0.76343(4)	0.68615(4)	0.169791(18)	0.01594(8)
P(2)	0.64051(4)	0.79684(4)	0.315263(18)	0.01473(8)
S(1)	0.83299(4)	0.49817(4)	0.289308(18)	0.01810(8)
S(2)	1.13583(4)	0.58508(4)	0.29153(2)	0.02214(8)
N(1)	0.60977(14)	0.77575(12)	0.23172(6)	0.0161(2)
O(1)	1.17996(15)	0.76043(14)	0.13304(7)	0.0357(3)
O(2)	1.12334(19)	0.36209(15)	0.11194(8)	0.0478(4)
O(3)	0.98132(16)	0.93806(14)	0.31716(8)	0.0407(3)
O(4)	0.80975(16)	0.67651(16)	0.48436(6)	0.0408(3)
C(1)	1.09759(18)	0.69959(17)	0.16260(8)	0.0241(3)
C(2)	1.0679(2)	0.45373(17)	0.14935(9)	0.0273(3)
C(3)	0.93887(18)	0.84070(17)	0.32277(9)	0.0250(3)
C(4)	0.83730(18)	0.68002(17)	0.42409(8)	0.0239(3)
C(5)	0.9491(2)	0.34171(16)	0.32073(9)	0.0283(3)
C(6)	1.0676(2)	0.35745(18)	0.36434(10)	0.0321(4)
C(7)	1.19772(19)	0.41568(18)	0.32513(9)	0.0299(4)
C(8)	0.45228(17)	0.82835(15)	0.21080(8)	0.0198(3)
C(9)	0.41278(19)	0.97313(16)	0.18990(8)	0.0248(3)
C(10)	0.2749(2)	1.05868(19)	0.21066(10)	0.0353(4)
C(11)	0.68309(18)	0.55811(15)	0.13511(8)	0.0204(3)
C(12)	0.55574(19)	0.51598(16)	0.17311(9)	0.0237(3)
C(13)	0.5011(2)	0.41590(18)	0.14489(10)	0.0330(4)
C(14)	0.5741(3)	0.35671(19)	0.07998(11)	0.0396(4)
C(15)	0.7034(3)	0.3948(2)	0.04265(10)	0.0390(4)
C(16)	0.7584(2)	0.49460(17)	0.07002(9)	0.0290(3)
C(17)	0.76663(18)	0.80778(15)	0.09921(8)	0.0216(3)
C(18)	0.6942(2)	0.80627(18)	0.04112(9)	0.0308(4)
C(19)	0.6934(3)	0.9081(2)	–0.00785(10)	0.0426(5)
C(20)	0.7597(3)	1.0125(2)	0.00159(11)	0.0457(5)
C(21)	0.8298(2)	1.01650(19)	0.05961(11)	0.0399(5)
C(22)	0.83467(19)	0.91424(17)	0.10787(9)	0.0286(3)
C(23)	0.46876(17)	0.76115(15)	0.37343(7)	0.0181(3)
C(24)	0.32361(18)	0.85797(17)	0.38851(8)	0.0248(3)
C(25)	0.19698(19)	0.8295(2)	0.43441(9)	0.0306(4)
C(26)	0.2123(2)	0.7048(2)	0.46504(9)	0.0316(4)
C(27)	0.3540(2)	0.60814(18)	0.45062(9)	0.0278(3)
C(28)	0.48211(18)	0.63647(16)	0.40533(8)	0.0220(3)
C(29)	0.60538(17)	0.97824(14)	0.33229(8)	0.0189(3)
C(30)	0.5716(2)	1.02540(17)	0.40214(9)	0.0279(3)
C(31)	0.5610(2)	1.15934(18)	0.41829(10)	0.0346(4)
C(32)	0.5847(2)	1.24686(17)	0.36459(11)	0.0341(4)
C(33)	0.6221(2)	1.20131(17)	0.29537(10)	0.0323(4)
C(34)	0.63283(19)	1.06665(16)	0.27908(9)	0.0250(3)

Table 3. Bond lengths [Å] and angles [°] for str0463.

Fe(1)–C(1)	1.7689(16)	Fe(1)–C(2)	1.7751(17)
Fe(1)–P(1)	2.2119(4)	Fe(1)–S(1)	2.2537(4)
Fe(1)–S(2)	2.2540(4)	Fe(1)–Fe(2)	2.4816(3)
Fe(2)–C(3)	1.7712(17)	Fe(2)–C(4)	1.7750(16)
Fe(2)–P(2)	2.2036(4)	Fe(2)–S(2)	2.2579(4)
Fe(2)–S(1)	2.2671(4)	P(1)–N(1)	1.7177(12)
P(1)–C(17)	1.8293(15)	P(1)–C(11)	1.8300(15)
P(2)–N(1)	1.7078(12)	P(2)–C(29)	1.8280(15)
P(2)–C(23)	1.8362(15)	S(1)–C(5)	1.8326(16)
S(2)–C(7)	1.8267(18)	N(1)–C(8)	1.4946(18)
O(1)–C(1)	1.147(2)	O(2)–C(2)	1.142(2)
O(3)–C(3)	1.148(2)	O(4)–C(4)	1.145(2)
C(5)–C(6)	1.501(2)	C(6)–C(7)	1.511(3)
C(8)–C(9)	1.500(2)	C(9)–C(10)	1.313(2)
C(11)–C(12)	1.393(2)	C(11)–C(16)	1.396(2)
C(12)–C(13)	1.395(2)	C(13)–C(14)	1.374(3)
C(14)–C(15)	1.382(3)	C(15)–C(16)	1.387(2)
C(17)–C(18)	1.392(2)	C(17)–C(22)	1.398(2)
C(18)–C(19)	1.393(2)	C(19)–C(20)	1.373(3)
C(20)–C(21)	1.382(3)	C(21)–C(22)	1.386(2)
C(23)–C(28)	1.394(2)	C(23)–C(24)	1.401(2)
C(24)–C(25)	1.390(2)	C(25)–C(26)	1.382(3)
C(26)–C(27)	1.379(3)	C(27)–C(28)	1.393(2)
C(29)–C(34)	1.385(2)	C(29)–C(30)	1.393(2)
C(30)–C(31)	1.387(2)	C(31)–C(32)	1.379(3)
C(32)–C(33)	1.375(3)	C(33)–C(34)	1.394(2)

C(1)–Fe(1)–C(2)	95.14(8)	C(1)–Fe(1)–P(1)	96.70(5)
C(2)–Fe(1)–P(1)	101.09(6)	C(1)–Fe(1)–S(1)	165.84(5)
C(2)–Fe(1)–S(1)	98.23(6)	P(1)–Fe(1)–S(1)	85.310(15)
C(1)–Fe(1)–S(2)	86.13(5)	C(2)–Fe(1)–S(2)	108.88(6)
P(1)–Fe(1)–S(2)	149.547(17)	S(1)–Fe(1)–S(2)	85.159(15)
C(1)–Fe(1)–Fe(2)	108.87(5)	C(2)–Fe(1)–Fe(2)	149.81(6)
P(1)–Fe(1)–Fe(2)	94.161(13)	S(1)–Fe(1)–Fe(2)	56.965(11)
S(2)–Fe(1)–Fe(2)	56.707(12)	C(3)–Fe(2)–C(4)	99.56(8)
C(3)–Fe(2)–P(2)	90.13(5)	C(4)–Fe(2)–P(2)	97.95(5)
C(3)–Fe(2)–S(2)	85.72(5)	C(4)–Fe(2)–S(2)	108.99(5)
P(2)–Fe(2)–S(2)	153.064(17)	C(3)–Fe(2)–S(1)	154.81(6)
C(4)–Fe(2)–S(1)	105.59(5)	P(2)–Fe(2)–S(1)	87.899(15)
S(2)–Fe(2)–S(1)	84.759(15)	C(3)–Fe(2)–Fe(1)	99.09(5)
C(4)–Fe(2)–Fe(1)	155.28(5)	P(2)–Fe(2)–Fe(1)	98.098(13)
S(2)–Fe(2)–Fe(1)	56.558(11)	S(1)–Fe(2)–Fe(1)	56.450(11)
N(1)–P(1)–C(17)	100.95(6)	N(1)–P(1)–C(11)	104.04(7)
C(17)–P(1)–C(11)	103.56(7)	N(1)–P(1)–Fe(1)	115.67(4)
C(17)–P(1)–Fe(1)	118.94(5)	C(11)–P(1)–Fe(1)	111.86(5)
N(1)–P(2)–C(29)	107.37(6)	N(1)–P(2)–C(23)	104.87(6)
C(29)–P(2)–C(23)	100.95(7)	N(1)–P(2)–Fe(2)	112.86(4)
C(29)–P(2)–Fe(2)	111.01(5)	C(23)–P(2)–Fe(2)	118.64(5)
C(5)–S(1)–Fe(1)	111.42(6)	C(5)–S(1)–Fe(2)	113.67(6)
Fe(1)–S(1)–Fe(2)	66.585(13)	C(7)–S(2)–Fe(1)	113.14(6)
C(7)–S(2)–Fe(2)	113.63(6)	Fe(1)–S(2)–Fe(2)	66.735(13)
C(8)–N(1)–P(2)	122.50(9)	C(8)–N(1)–P(1)	118.39(9)
P(2)–N(1)–P(1)	119.07(7)	O(1)–C(1)–Fe(1)	175.24(15)

O(2)–C(2)–Fe(1)	178.82(16)	O(3)–C(3)–Fe(2)	178.43(15)
O(4)–C(4)–Fe(2)	179.23(17)	C(6)–C(5)–S(1)	116.08(12)
C(5)–C(6)–C(7)	114.05(15)	C(6)–C(7)–S(2)	116.17(11)
N(1)–C(8)–C(9)	116.40(12)	C(10)–C(9)–C(8)	123.95(16)
C(12)–C(11)–C(16)	118.84(15)	C(12)–C(11)–P(1)	122.41(11)
C(16)–C(11)–P(1)	118.62(13)	C(11)–C(12)–C(13)	120.16(15)
C(14)–C(13)–C(12)	120.24(18)	C(13)–C(14)–C(15)	120.17(16)
C(14)–C(15)–C(16)	120.12(17)	C(15)–C(16)–C(11)	120.41(17)
C(18)–C(17)–C(22)	118.75(15)	C(18)–C(17)–P(1)	123.74(13)
C(22)–C(17)–P(1)	117.28(12)	C(17)–C(18)–C(19)	119.99(18)
C(20)–C(19)–C(18)	120.61(19)	C(19)–C(20)–C(21)	120.05(17)
C(20)–C(21)–C(22)	119.91(19)	C(21)–C(22)–C(17)	120.66(18)
C(28)–C(23)–C(24)	118.35(14)	C(28)–C(23)–P(2)	119.98(11)
C(24)–C(23)–P(2)	121.65(12)	C(25)–C(24)–C(23)	120.37(16)
C(26)–C(25)–C(24)	120.37(16)	C(27)–C(26)–C(25)	120.05(15)
C(26)–C(27)–C(28)	119.92(16)	C(27)–C(28)–C(23)	120.92(15)
C(34)–C(29)–C(30)	118.80(14)	C(34)–C(29)–P(2)	122.31(12)
C(30)–C(29)–P(2)	118.25(12)	C(31)–C(30)–C(29)	120.77(16)
C(32)–C(31)–C(30)	119.66(17)	C(33)–C(32)–C(31)	120.38(15)
C(32)–C(33)–C(34)	119.99(17)	C(29)–C(34)–C(33)	120.35(16)

Table 4. Anisotropic displacement parameters ($Å^2$) for str0463. 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)	0.01578(10)	0.02042(11)	0.01408(10)	0.00037(8)	–0.00139(7)	–0.00282(8)
Fe(2)	0.01558(10)	0.01987(11)	0.01390(10)	0.00037(8)	–0.00293(7)	–0.00468(8)
P(1)	0.01746(17)	0.01706(17)	0.01274(16)	0.00016(13)	–0.00224(13)	–0.00368(13)
P(2)	0.01596(17)	0.01512(16)	0.01295(16)	–0.00035(12)	–0.00187(12)	–0.00411(13)
S(1)	0.01838(16)	0.01757(16)	0.01755(16)	0.00147(13)	–0.00303(13)	–0.00330(13)
S(2)	0.01596(17)	0.0300(2)	0.01986(17)	0.00189(14)	–0.00394(13)	–0.00438(14)
N(1)	0.0157(5)	0.0190(6)	0.0127(5)	–0.0016(4)	–0.0031(4)	–0.0023(4)
O(1)	0.0294(6)	0.0486(8)	0.0338(7)	0.0150(6)	–0.0065(5)	–0.0189(6)
O(2)	0.0534(9)	0.0382(8)	0.0398(8)	–0.0151(6)	–0.0049(7)	0.0090(7)
O(3)	0.0327(7)	0.0332(7)	0.0641(10)	0.0103(6)	–0.0161(6)	–0.0182(6)
O(4)	0.0384(7)	0.0656(10)	0.0182(6)	0.0032(6)	–0.0050(5)	–0.0127(7)
C(1)	0.0208(7)	0.0324(8)	0.0185(7)	0.0032(6)	–0.0049(6)	–0.0052(6)
C(2)	0.0259(8)	0.0295(8)	0.0227(8)	–0.0006(6)	–0.0038(6)	–0.0006(6)
C(3)	0.0185(7)	0.0292(8)	0.0281(8)	0.0032(6)	–0.0067(6)	–0.0063(6)
C(4)	0.0198(7)	0.0311(8)	0.0212(7)	–0.0002(6)	–0.0057(6)	–0.0060(6)
C(5)	0.0287(8)	0.0201(7)	0.0341(9)	0.0082(6)	–0.0069(7)	–0.0022(6)
C(6)	0.0314(9)	0.0307(9)	0.0311(9)	0.0075(7)	–0.0090(7)	0.0002(7)
C(7)	0.0211(8)	0.0337(9)	0.0315(9)	0.0049(7)	–0.0090(6)	0.0023(7)
C(8)	0.0173(7)	0.0233(7)	0.0185(7)	–0.0004(5)	–0.0054(5)	–0.0031(5)
C(9)	0.0255(8)	0.0262(8)	0.0227(7)	0.0027(6)	–0.0080(6)	–0.0040(6)
C(10)	0.0317(9)	0.0286(9)	0.0391(10)	0.0034(7)	–0.0028(7)	0.0012(7)
C(11)	0.0239(7)	0.0194(7)	0.0180(7)	–0.0011(5)	–0.0073(6)	–0.0033(6)
C(12)	0.0258(8)	0.0216(7)	0.0246(8)	0.0008(6)	–0.0071(6)	–0.0062(6)
C(13)	0.0340(9)	0.0281(8)	0.0422(10)	0.0021(7)	–0.0135(8)	–0.0134(7)
C(14)	0.0504(12)	0.0297(9)	0.0459(11)	–0.0078(8)	–0.0217(9)	–0.0135(8)
C(15)	0.0530(12)	0.0337(10)	0.0298(9)	–0.0128(8)	–0.0093(8)	–0.0079(9)
C(16)	0.0335(9)	0.0290(8)	0.0223(8)	–0.0055(6)	–0.0031(6)	–0.0052(7)
C(17)	0.0213(7)	0.0220(7)	0.0165(7)	0.0039(5)	0.0018(5)	–0.0002(6)
C(18)	0.0367(9)	0.0311(9)	0.0193(7)	0.0025(6)	–0.0040(7)	0.0003(7)
C(19)	0.0535(12)	0.0421(11)	0.0203(8)	0.0089(8)	–0.0040(8)	0.0073(9)
C(20)	0.0480(12)	0.0385(11)	0.0346(10)	0.0214(8)	0.0090(9)	0.0053(9)
C(21)	0.0326(9)	0.0278(9)	0.0509(12)	0.0133(8)	0.0079(8)	–0.0043(7)
C(22)	0.0226(8)	0.0265(8)	0.0325(9)	0.0061(7)	0.0016(6)	–0.0037(6)
C(23)	0.0188(7)	0.0227(7)	0.0137(6)	–0.0021(5)	–0.0016(5)	–0.0079(6)
C(24)	0.0208(7)	0.0299(8)	0.0219(7)	0.0017(6)	–0.0030(6)	–0.0037(6)
C(25)	0.0186(7)	0.0441(10)	0.0261(8)	–0.0015(7)	–0.0009(6)	–0.0046(7)
C(26)	0.0232(8)	0.0531(11)	0.0220(8)	0.0017(7)	–0.0003(6)	–0.0185(8)
C(27)	0.0330(9)	0.0323(9)	0.0226(8)	0.0047(6)	–0.0037(6)	–0.0175(7)
C(28)	0.0233(7)	0.0233(7)	0.0202(7)	–0.0003(6)	–0.0020(6)	–0.0084(6)
C(29)	0.0181(7)	0.0169(6)	0.0215(7)	–0.0020(5)	–0.0039(5)	–0.0039(5)
C(30)	0.0349(9)	0.0261(8)	0.0227(8)	–0.0047(6)	–0.0001(6)	–0.0109(7)
C(31)	0.0372(10)	0.0296(9)	0.0359(10)	–0.0150(7)	0.0008(8)	–0.0105(7)
C(32)	0.0300(9)	0.0185(7)	0.0544(12)	–0.0083(7)	–0.0098(8)	–0.0053(7)
C(33)	0.0361(9)	0.0211(8)	0.0450(10)	0.0091(7)	–0.0160(8)	–0.0110(7)
C(34)	0.0288(8)	0.0221(7)	0.0261(8)	0.0024(6)	–0.0086(6)	–0.0079(6)

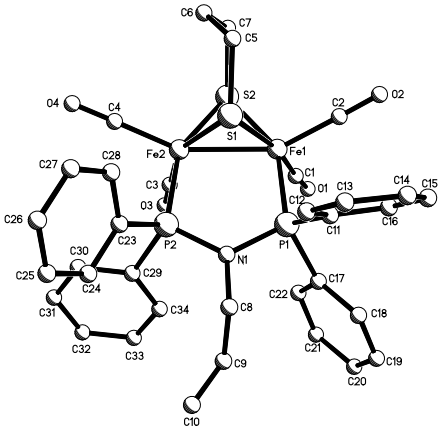
Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for str0463.

	x	y	z	U
H(5A)	0.8767	0.2958	0.3485	0.034
H(5B)	1.0047	0.2836	0.2801	0.034
H(6A)	1.1146	0.2697	0.3814	0.039
H(6B)	1.0128	0.4157	0.4051	0.039
H(7A)	1.2547	0.3550	0.2856	0.036
H(7B)	1.2712	0.4175	0.3564	0.036
H(8A)	0.3715	0.8172	0.2500	0.024
H(8B)	0.4469	0.7726	0.1716	0.024
H(9A)	0.4906	1.0042	0.1605	0.030
H(10A)	0.1947	1.0306	0.2401	0.042
H(10B)	0.2574	1.1474	0.1959	0.042
H(12A)	0.5070	0.5547	0.2174	0.028
H(13A)	0.4149	0.3892	0.1701	0.040
H(14A)	0.5364	0.2908	0.0611	0.048
H(15A)	0.7537	0.3534	–0.0009	0.047
H(16A)	0.8460	0.5194	0.0449	0.035
H(18A)	0.6464	0.7373	0.0350	0.037
H(19A)	0.6475	0.9053	–0.0473	0.051
H(20A)	0.7574	1.0806	–0.0311	0.055
H(21A)	0.8737	1.0877	0.0663	0.048
H(22A)	0.8837	0.9164	0.1464	0.034
H(24A)	0.3119	0.9417	0.3677	0.030
H(25A)	0.1014	0.8947	0.4446	0.037
H(26A)	0.1268	0.6861	0.4954	0.038
H(27A)	0.3642	0.5241	0.4711	0.033
H(28A)	0.5778	0.5713	0.3963	0.026
H(30A)	0.5559	0.9664	0.4384	0.033
H(31A)	0.5381	1.1900	0.4651	0.042
H(32A)	0.5753	1.3372	0.3752	0.041
H(33A)	0.6403	1.2603	0.2594	0.039
H(34A)	0.6585	1.0360	0.2322	0.030

Table 6. Torsion angles [°] for str0463.

C(1)–Fe(1)–Fe(2)–C(3)	6.73(7)	C(2)–Fe(1)–Fe(2)–C(3)	147.64(12)
P(1)–Fe(1)–Fe(2)–C(3)	−91.80(5)	S(1)–Fe(1)–Fe(2)–C(3)	−173.46(5)
S(2)–Fe(1)–Fe(2)–C(3)	78.69(5)	C(1)–Fe(1)–Fe(2)–C(4)	−131.82(13)
C(2)–Fe(1)–Fe(2)–C(4)	9.08(17)	P(1)–Fe(1)–Fe(2)–C(4)	129.65(12)
S(1)–Fe(1)–Fe(2)–C(4)	47.99(12)	S(2)–Fe(1)–Fe(2)–C(4)	−59.87(12)
C(1)–Fe(1)–Fe(2)–P(2)	98.17(5)	C(2)–Fe(1)–Fe(2)–P(2)	−120.93(11)
P(1)–Fe(1)–Fe(2)–P(2)	−0.365(16)	S(1)–Fe(1)–Fe(2)–P(2)	−82.022(16)
S(2)–Fe(1)–Fe(2)–P(2)	170.124(18)	C(1)–Fe(1)–Fe(2)–S(2)	−71.95(5)
C(2)–Fe(1)–Fe(2)–S(2)	68.95(11)	P(1)–Fe(1)–Fe(2)–S(2)	−170.489(18)
S(1)–Fe(1)–Fe(2)–S(2)	107.854(18)	C(1)–Fe(1)–Fe(2)–S(1)	−179.81(5)
C(2)–Fe(1)–Fe(2)–S(1)	−38.90(11)	P(1)–Fe(1)–Fe(2)–S(1)	81.656(16)
S(2)–Fe(1)–Fe(2)–S(1)	−107.854(18)	C(1)–Fe(1)–P(1)–N(1)	−111.31(7)
C(2)–Fe(1)–P(1)–N(1)	152.08(8)	S(1)–Fe(1)–P(1)–N(1)	54.60(5)
S(2)–Fe(1)–P(1)–N(1)	−17.55(6)	Fe(2)–Fe(1)–P(1)–N(1)	−1.73(5)
C(1)–Fe(1)–P(1)–C(17)	9.13(8)	C(2)–Fe(1)–P(1)–C(17)	−87.47(8)
S(1)–Fe(1)–P(1)–C(17)	175.04(6)	S(2)–Fe(1)–P(1)–C(17)	102.89(6)
Fe(2)–Fe(1)–P(1)–C(17)	118.71(6)	C(1)–Fe(1)–P(1)–C(11)	129.82(8)
C(2)–Fe(1)–P(1)–C(11)	33.22(8)	S(1)–Fe(1)–P(1)–C(11)	−64.27(5)
S(2)–Fe(1)–P(1)–C(11)	−136.41(6)	Fe(2)–Fe(1)–P(1)–C(11)	−120.60(5)
C(3)–Fe(2)–P(2)–N(1)	101.62(7)	C(4)–Fe(2)–P(2)–N(1)	−158.71(7)
S(2)–Fe(2)–P(2)–N(1)	20.84(6)	S(1)–Fe(2)–P(2)–N(1)	−53.26(5)
Fe(1)–Fe(2)–P(2)–N(1)	2.42(5)	C(3)–Fe(2)–P(2)–C(29)	−18.98(8)
C(4)–Fe(2)–P(2)–C(29)	80.69(8)	S(2)–Fe(2)–P(2)–C(29)	−99.76(6)
S(1)–Fe(2)–P(2)–C(29)	−173.86(5)	Fe(1)–Fe(2)–P(2)–C(29)	−118.18(5)
C(3)–Fe(2)–P(2)–C(23)	−135.18(7)	C(4)–Fe(2)–P(2)–C(23)	−35.51(8)
S(2)–Fe(2)–P(2)–C(23)	144.04(6)	S(1)–Fe(2)–P(2)–C(23)	69.94(5)
Fe(1)–Fe(2)–P(2)–C(23)	125.62(5)	C(1)–Fe(1)–S(1)–C(5)	−106.7(2)
C(2)–Fe(1)–S(1)–C(5)	53.92(8)	P(1)–Fe(1)–S(1)–C(5)	154.47(6)
S(2)–Fe(1)–S(1)–C(5)	−54.48(6)	Fe(2)–Fe(1)–S(1)–C(5)	−107.47(6)
C(1)–Fe(1)–S(1)–Fe(2)	0.7(2)	C(2)–Fe(1)–S(1)–Fe(2)	161.39(6)
P(1)–Fe(1)–S(1)–Fe(2)	−98.059(14)	S(2)–Fe(1)–S(1)–Fe(2)	52.984(13)
C(3)–Fe(2)–S(1)–C(5)	119.48(14)	C(4)–Fe(2)–S(1)–C(5)	−57.02(8)
P(2)–Fe(2)–S(1)–C(5)	−154.69(6)	S(2)–Fe(2)–S(1)–C(5)	51.26(6)
Fe(1)–Fe(2)–S(1)–C(5)	104.16(6)	C(3)–Fe(2)–S(1)–Fe(1)	15.32(12)
C(4)–Fe(2)–S(1)–Fe(1)	−161.18(5)	P(2)–Fe(2)–S(1)–Fe(1)	101.156(14)
S(2)–Fe(2)–S(1)–Fe(1)	−52.901(13)	C(1)–Fe(1)–S(2)–C(7)	−137.49(8)
C(2)–Fe(1)–S(2)–C(7)	−43.37(9)	P(1)–Fe(1)–S(2)–C(7)	125.87(7)
S(1)–Fe(1)–S(2)–C(7)	53.69(6)	Fe(2)–Fe(1)–S(2)–C(7)	106.90(6)
C(1)–Fe(1)–S(2)–Fe(2)	115.61(5)	C(2)–Fe(1)–S(2)–Fe(2)	−150.27(6)
P(1)–Fe(1)–S(2)–Fe(2)	18.97(3)	S(1)–Fe(1)–S(2)–Fe(2)	−53.208(13)
C(3)–Fe(2)–S(2)–C(7)	149.96(8)	C(4)–Fe(2)–S(2)–C(7)	51.31(9)
P(2)–Fe(2)–S(2)–C(7)	−128.21(7)	S(1)–Fe(2)–S(2)–C(7)	−53.39(7)
Fe(1)–Fe(2)–S(2)–C(7)	−106.20(7)	C(3)–Fe(2)–S(2)–Fe(1)	−103.85(5)
C(4)–Fe(2)–S(2)–Fe(1)	157.51(6)	P(2)–Fe(2)–S(2)–Fe(1)	−22.02(4)
S(1)–Fe(2)–S(2)–Fe(1)	52.806(13)	C(29)–P(2)–N(1)–C(8)	−63.66(12)
C(23)–P(2)–N(1)–C(8)	43.13(12)	Fe(2)–P(2)–N(1)–C(8)	173.69(10)
C(29)–P(2)–N(1)–P(1)	118.47(8)	C(23)–P(2)–N(1)–P(1)	−134.73(8)
Fe(2)–P(2)–N(1)–P(1)	−4.18(9)	C(17)–P(1)–N(1)–C(8)	56.22(12)
C(11)–P(1)–N(1)–C(8)	−50.91(12)	Fe(1)–P(1)–N(1)–C(8)	−174.00(9)
C(17)–P(1)–N(1)–P(2)	−125.83(9)	C(11)–P(1)–N(1)–P(2)	127.04(8)

Fe(1)–P(1)–N(1)–P(2)	3.96(9)	C(2)–Fe(1)–C(1)–O(1)	–53.4(18)
P(1)–Fe(1)–C(1)–O(1)	–155.3(18)	S(1)–Fe(1)–C(1)–O(1)	107.3(18)
S(2)–Fe(1)–C(1)–O(1)	55.2(18)	Fe(2)–Fe(1)–C(1)–O(1)	108.0(18)
C(1)–Fe(1)–C(2)–O(2)	93(9)	P(1)–Fe(1)–C(2)–O(2)	–169(9)
S(1)–Fe(1)–C(2)–O(2)	–83(9)	S(2)–Fe(1)–C(2)–O(2)	5(9)
Fe(2)–Fe(1)–C(2)–O(2)	–50(9)	C(4)–Fe(2)–C(3)–O(3)	105(6)
P(2)–Fe(2)–C(3)–O(3)	–156(6)	S(2)–Fe(2)–C(3)–O(3)	–3(6)
S(1)–Fe(2)–C(3)–O(3)	–71(6)	Fe(1)–Fe(2)–C(3)–O(3)	–58(6)
C(3)–Fe(2)–C(4)–O(4)	41(11)	P(2)–Fe(2)–C(4)–O(4)	–51(11)
S(2)–Fe(2)–C(4)–O(4)	129(11)	S(1)–Fe(2)–C(4)–O(4)	–141(11)
Fe(1)–Fe(2)–C(4)–O(4)	179(100)	Fe(1)–S(1)–C(5)–C(6)	68.17(14)
Fe(2)–S(1)–C(5)–C(6)	–4.73(15)	S(1)–C(5)–C(6)–C(7)	–63.60(18)
C(5)–C(6)–C(7)–S(2)	61.11(19)	Fe(1)–S(2)–C(7)–C(6)	–64.24(14)
Fe(2)–S(2)–C(7)–C(6)	9.38(16)	P(2)–N(1)–C(8)–C(9)	84.48(15)
P(1)–N(1)–C(8)–C(9)	–97.64(14)	N(1)–C(8)–C(9)–C(10)	–136.17(17)
N(1)–P(1)–C(11)–C(12)	–23.06(14)	C(17)–P(1)–C(11)–C(12)	–128.24(13)
Fe(1)–P(1)–C(11)–C(12)	102.49(13)	N(1)–P(1)–C(11)–C(16)	160.93(13)
C(17)–P(1)–C(11)–C(16)	55.76(14)	Fe(1)–P(1)–C(11)–C(16)	–73.52(13)
C(16)–C(11)–C(12)–C(13)	–2.6(2)	P(1)–C(11)–C(12)–C(13)	–178.64(13)
C(11)–C(12)–C(13)–C(14)	1.1(3)	C(12)–C(13)–C(14)–C(15)	0.8(3)
C(13)–C(14)–C(15)–C(16)	–1.1(3)	C(14)–C(15)–C(16)–C(11)	–0.5(3)
C(12)–C(11)–C(16)–C(15)	2.4(2)	P(1)–C(11)–C(16)–C(15)	178.51(14)
N(1)–P(1)–C(17)–C(18)	–97.11(14)	C(11)–P(1)–C(17)–C(18)	10.40(15)
Fe(1)–P(1)–C(17)–C(18)	135.22(12)	N(1)–P(1)–C(17)–C(22)	77.36(13)
C(11)–P(1)–C(17)–C(22)	–175.14(12)	Fe(1)–P(1)–C(17)–C(22)	–50.32(13)
C(22)–C(17)–C(18)–C(19)	1.3(2)	P(1)–C(17)–C(18)–C(19)	175.72(14)
C(17)–C(18)–C(19)–C(20)	–1.8(3)	C(18)–C(19)–C(20)–C(21)	0.8(3)
C(19)–C(20)–C(21)–C(22)	0.7(3)	C(20)–C(21)–C(22)–C(17)	–1.2(3)
C(18)–C(17)–C(22)–C(21)	0.1(2)	P(1)–C(17)–C(22)–C(21)	–174.61(13)
N(1)–P(2)–C(23)–C(28)	101.38(12)	C(29)–P(2)–C(23)–C(28)	–147.15(12)
Fe(2)–P(2)–C(23)–C(28)	–25.70(13)	N(1)–P(2)–C(23)–C(24)	–80.37(13)
C(29)–P(2)–C(23)–C(24)	31.10(14)	Fe(2)–P(2)–C(23)–C(24)	152.55(11)
C(28)–C(23)–C(24)–C(25)	0.2(2)	P(2)–C(23)–C(24)–C(25)	–178.06(13)
C(23)–C(24)–C(25)–C(26)	–0.8(3)	C(24)–C(25)–C(26)–C(27)	0.5(3)
C(25)–C(26)–C(27)–C(28)	0.2(3)	C(26)–C(27)–C(28)–C(23)	–0.8(2)
C(24)–C(23)–C(28)–C(27)	0.6(2)	P(2)–C(23)–C(28)–C(27)	178.87(12)
N(1)–P(2)–C(29)–C(34)	–30.11(15)	C(23)–P(2)–C(29)–C(34)	–139.65(13)
Fe(2)–P(2)–C(29)–C(34)	93.68(13)	N(1)–P(2)–C(29)–C(30)	159.17(12)
C(23)–P(2)–C(29)–C(30)	49.64(14)	Fe(2)–P(2)–C(29)–C(30)	–77.03(13)
C(34)–C(29)–C(30)–C(31)	1.8(3)	P(2)–C(29)–C(30)–C(31)	172.87(14)
C(29)–C(30)–C(31)–C(32)	–0.2(3)	C(30)–C(31)–C(32)–C(33)	–1.5(3)
C(31)–C(32)–C(33)–C(34)	1.5(3)	C(30)–C(29)–C(34)–C(33)	–1.8(2)
P(2)–C(29)–C(34)–C(33)	–172.51(13)	C(32)–C(33)–C(34)–C(29)	0.2(3)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C23
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P1
N1
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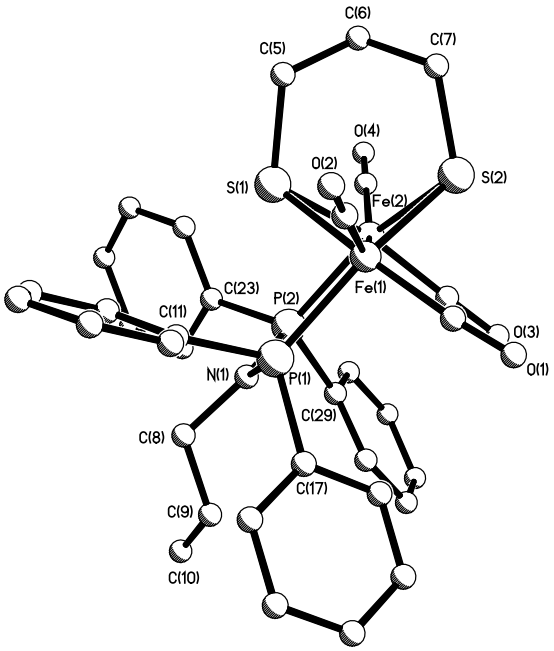
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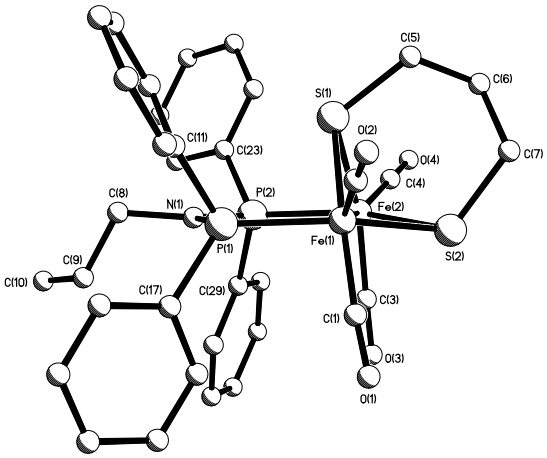
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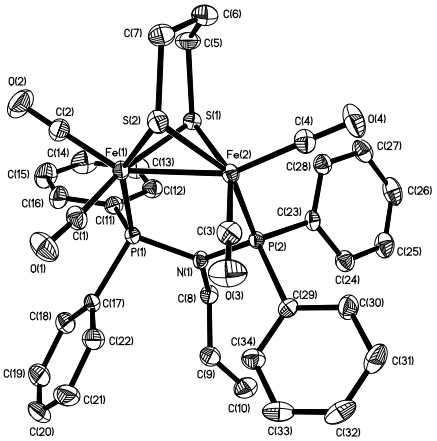
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C(32)

Table 1. Crystal data and structure refinement for **3b**.

Identification code	str0541	
Chemical formula	$C_{34}H_{33}Fe_2NO_4P_2S_2$	
Formula weight	757.37	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, P1bar	
Unit cell parameters	a = 10.4283(11) Å	α = 84.906(2)°
	b = 11.7343(13) Å	β = 73.720(2)°
	c = 14.6476(16) Å	γ = 74.371(2)°
Cell volume	1656.8(3) $Å^3$	
Z	2	
Calculated density	1.518 g/cm^3	
Absorption coefficient μ	1.138 mm^{-1}	
F(000)	780	
Crystal colour and size	orange, 0.12 × 0.11 × 0.06 mm^3	
Data collection method	Bruker SMART APEX diffractometer	
	ω rotation with narrow frames	
θ range for data collection	2.48 to 28.25°	
Index ranges	h −13 to 13, k −14 to 15, l −18 to 18	
Completeness to θ = 26.00°	97.9 %	
Reflections collected	14313	
Independent reflections	7555 (R_{int} = 0.0286)	
Reflections with $F^2>2\sigma$	6538	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.8755 and 0.9349	
Structure solution	Patterson synthesis	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0610, 0.9132	
Data / restraints / parameters	7555 / 0 / 406	
Final R indices [$F^2>2\sigma$]	R1 = 0.0398, wR2 = 0.1046	
R indices (all data)	R1 = 0.0466, wR2 = 0.1091	
Goodness-of-fit on F^2	1.035	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	1.825 and −0.458 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for str0541. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Fe(1)	0.55757(3)	0.27560(3)	0.26357(2)	0.01304(9)
Fe(2)	0.69934(3)	0.14796(3)	0.36097(2)	0.01195(9)
P(1)	0.70498(6)	0.38115(5)	0.19101(4)	0.01314(12)
P(2)	0.87564(6)	0.22797(5)	0.30454(4)	0.01147(12)
S(1)	0.49780(6)	0.12122(5)	0.35217(4)	0.01621(13)
S(2)	0.57836(6)	0.33599(5)	0.39975(4)	0.01320(12)
N(1)	0.84207(19)	0.35785(16)	0.24007(13)	0.0130(4)
O(1)	0.6461(2)	0.11117(18)	0.10654(13)	0.0298(4)
O(2)	0.2996(2)	0.42513(19)	0.23278(16)	0.0363(5)
O(3)	0.82935(19)	–0.08447(15)	0.27402(13)	0.0245(4)
O(4)	0.72433(19)	0.08203(16)	0.55371(12)	0.0228(4)
C(1)	0.6118(3)	0.1783(2)	0.16648(17)	0.0191(5)
C(2)	0.4018(3)	0.3686(2)	0.24438(18)	0.0211(5)
C(3)	0.7808(2)	0.0083(2)	0.30603(17)	0.0165(5)
C(4)	0.7167(2)	0.1051(2)	0.47730(16)	0.0154(4)
C(5)	0.3588(3)	0.1658(2)	0.46008(19)	0.0246(5)
C(6)	0.3172(3)	0.2936(3)	0.4847(2)	0.0345(7)
C(7)	0.4276(2)	0.3420(2)	0.50109(17)	0.0199(5)
C(8)	0.9444(3)	0.4324(2)	0.22623(17)	0.0182(5)
C(9)	1.0386(3)	0.4319(2)	0.12585(18)	0.0239(5)
C(10)	0.8792(3)	0.5594(2)	0.26174(19)	0.0230(5)
C(11)	0.7676(3)	0.3485(2)	0.06383(16)	0.0167(5)
C(12)	0.8992(3)	0.2821(2)	0.01919(17)	0.0191(5)
C(13)	0.9313(3)	0.2472(2)	–0.07494(18)	0.0261(6)
C(14)	0.8313(3)	0.2779(3)	–0.12412(18)	0.0311(7)
C(15)	0.6993(3)	0.3439(3)	–0.08048(19)	0.0288(6)
C(16)	0.6678(3)	0.3790(2)	0.01273(18)	0.0233(5)
C(17)	0.6354(3)	0.5422(2)	0.18726(18)	0.0197(5)
C(18)	0.5299(3)	0.5986(2)	0.26294(19)	0.0241(5)
C(19)	0.4794(4)	0.7209(3)	0.2623(2)	0.0365(7)
C(20)	0.5341(4)	0.7872(3)	0.1856(2)	0.0442(9)
C(21)	0.6350(4)	0.7328(3)	0.1090(2)	0.0382(7)
C(22)	0.6862(3)	0.6100(2)	0.1086(2)	0.0274(6)
C(23)	0.9233(2)	0.2612(2)	0.40848(16)	0.0142(4)
C(24)	0.9963(2)	0.1648(2)	0.45257(17)	0.0183(5)
C(25)	1.0104(3)	0.1759(2)	0.54254(18)	0.0211(5)
C(26)	0.9544(3)	0.2829(2)	0.58889(18)	0.0243(5)
C(27)	0.8841(3)	0.3789(2)	0.54563(18)	0.0260(6)
C(28)	0.8673(3)	0.3683(2)	0.45580(17)	0.0192(5)
C(29)	1.0398(2)	0.1438(2)	0.22955(16)	0.0146(4)
C(30)	1.0362(2)	0.0759(2)	0.15675(17)	0.0172(5)
C(31)	1.1575(3)	0.0208(2)	0.09091(17)	0.0205(5)
C(32)	1.2833(3)	0.0316(2)	0.09737(18)	0.0230(5)
C(33)	1.2886(3)	0.0970(2)	0.16963(19)	0.0240(5)
C(34)	1.1678(2)	0.1534(2)	0.23488(17)	0.0191(5)

Table 3. Bond lengths [Å] and angles [°] for str0541.

Fe(1)–C(1)	1.770(2)	Fe(1)–C(2)	1.776(3)
Fe(1)–P(1)	2.2142(7)	Fe(1)–S(1)	2.2565(7)
Fe(1)–S(2)	2.2594(6)	Fe(1)–Fe(2)	2.4646(5)
Fe(2)–C(3)	1.776(2)	Fe(2)–C(4)	1.778(2)
Fe(2)–P(2)	2.2102(7)	Fe(2)–S(1)	2.2464(7)
Fe(2)–S(2)	2.2591(7)	P(1)–N(1)	1.722(2)
P(1)–C(11)	1.831(2)	P(1)–C(17)	1.835(2)
P(2)–N(1)	1.7261(19)	P(2)–C(29)	1.827(2)
P(2)–C(23)	1.831(2)	S(1)–C(5)	1.824(3)
S(2)–C(7)	1.825(2)	N(1)–C(8)	1.515(3)
O(1)–C(1)	1.147(3)	O(2)–C(2)	1.143(3)
O(3)–C(3)	1.150(3)	O(4)–C(4)	1.148(3)
C(5)–C(6)	1.492(4)	C(6)–C(7)	1.496(4)
C(8)–C(9)	1.522(3)	C(8)–C(10)	1.532(3)
C(11)–C(12)	1.389(3)	C(11)–C(16)	1.400(3)
C(12)–C(13)	1.396(3)	C(13)–C(14)	1.381(4)
C(14)–C(15)	1.387(4)	C(15)–C(16)	1.385(4)
C(17)–C(18)	1.390(4)	C(17)–C(22)	1.401(4)
C(18)–C(19)	1.390(4)	C(19)–C(20)	1.385(5)
C(20)–C(21)	1.370(5)	C(21)–C(22)	1.395(4)
C(23)–C(28)	1.391(3)	C(23)–C(24)	1.399(3)
C(24)–C(25)	1.388(3)	C(25)–C(26)	1.383(4)
C(26)–C(27)	1.377(4)	C(27)–C(28)	1.395(3)
C(29)–C(34)	1.394(3)	C(29)–C(30)	1.401(3)
C(30)–C(31)	1.391(3)	C(31)–C(32)	1.382(4)
C(32)–C(33)	1.383(4)	C(33)–C(34)	1.388(3)

C(1)–Fe(1)–C(2)	101.08(12)	C(1)–Fe(1)–P(1)	92.15(8)
C(2)–Fe(1)–P(1)	100.36(8)	C(1)–Fe(1)–S(1)	85.17(8)
C(2)–Fe(1)–S(1)	105.80(8)	P(1)–Fe(1)–S(1)	153.74(3)
C(1)–Fe(1)–S(2)	152.37(9)	C(2)–Fe(1)–S(2)	106.44(8)
P(1)–Fe(1)–S(2)	85.36(2)	S(1)–Fe(1)–S(2)	85.09(2)
C(1)–Fe(1)–Fe(2)	96.39(8)	C(2)–Fe(1)–Fe(2)	154.09(8)
P(1)–Fe(1)–Fe(2)	97.93(2)	S(1)–Fe(1)–Fe(2)	56.619(19)
S(2)–Fe(1)–Fe(2)	56.939(18)	C(3)–Fe(2)–C(4)	97.93(11)
C(3)–Fe(2)–P(2)	96.82(8)	C(4)–Fe(2)–P(2)	100.80(8)
C(3)–Fe(2)–S(1)	87.52(8)	C(4)–Fe(2)–S(1)	107.85(8)
P(2)–Fe(2)–S(1)	150.15(3)	C(3)–Fe(2)–S(2)	166.56(8)
C(4)–Fe(2)–S(2)	95.09(7)	P(2)–Fe(2)–S(2)	83.94(2)
S(1)–Fe(2)–S(2)	85.33(2)	C(3)–Fe(2)–Fe(1)	109.66(8)
C(4)–Fe(2)–Fe(1)	146.79(7)	P(2)–Fe(2)–Fe(1)	94.07(2)
S(1)–Fe(2)–Fe(1)	57.012(19)	S(2)–Fe(2)–Fe(1)	56.950(18)
N(1)–P(1)–C(11)	110.22(10)	N(1)–P(1)–C(17)	105.76(10)
C(11)–P(1)–C(17)	100.80(11)	N(1)–P(1)–Fe(1)	112.31(7)
C(11)–P(1)–Fe(1)	110.25(8)	C(17)–P(1)–Fe(1)	116.82(9)
N(1)–P(2)–C(29)	102.49(10)	N(1)–P(2)–C(23)	107.66(10)
C(29)–P(2)–C(23)	103.01(11)	N(1)–P(2)–Fe(2)	115.43(7)
C(29)–P(2)–Fe(2)	121.15(8)	C(23)–P(2)–Fe(2)	105.90(7)
C(5)–S(1)–Fe(2)	112.64(9)	C(5)–S(1)–Fe(1)	113.32(9)
Fe(2)–S(1)–Fe(1)	66.369(19)	C(7)–S(2)–Fe(2)	111.99(9)
C(7)–S(2)–Fe(1)	114.23(8)	Fe(2)–S(2)–Fe(1)	66.111(19)
C(8)–N(1)–P(1)	127.65(15)	C(8)–N(1)–P(2)	115.92(15)
P(1)–N(1)–P(2)	116.19(11)	O(1)–C(1)–Fe(1)	176.9(2)

O(2)–C(2)–Fe(1)	177.6(2)	O(3)–C(3)–Fe(2)	176.6(2)
O(4)–C(4)–Fe(2)	177.1(2)	C(6)–C(5)–S(1)	116.74(19)
C(5)–C(6)–C(7)	115.9(3)	C(6)–C(7)–S(2)	115.67(18)
N(1)–C(8)–C(9)	114.63(19)	N(1)–C(8)–C(10)	114.1(2)
C(9)–C(8)–C(10)	110.5(2)	C(12)–C(11)–C(16)	118.7(2)
C(12)–C(11)–P(1)	124.73(19)	C(16)–C(11)–P(1)	115.92(19)
C(11)–C(12)–C(13)	120.6(2)	C(14)–C(13)–C(12)	119.9(3)
C(13)–C(14)–C(15)	120.3(2)	C(16)–C(15)–C(14)	119.8(3)
C(15)–C(16)–C(11)	120.8(3)	C(18)–C(17)–C(22)	119.0(2)
C(18)–C(17)–P(1)	119.93(19)	C(22)–C(17)–P(1)	121.1(2)
C(17)–C(18)–C(19)	120.5(3)	C(20)–C(19)–C(18)	119.8(3)
C(21)–C(20)–C(19)	120.5(3)	C(20)–C(21)–C(22)	120.2(3)
C(21)–C(22)–C(17)	119.9(3)	C(28)–C(23)–C(24)	118.8(2)
C(28)–C(23)–P(2)	123.45(18)	C(24)–C(23)–P(2)	116.28(17)
C(25)–C(24)–C(23)	120.3(2)	C(26)–C(25)–C(24)	120.3(2)
C(27)–C(26)–C(25)	119.9(2)	C(26)–C(27)–C(28)	120.4(2)
C(23)–C(28)–C(27)	120.3(2)	C(34)–C(29)–C(30)	118.3(2)
C(34)–C(29)–P(2)	123.19(18)	C(30)–C(29)–P(2)	118.15(17)
C(31)–C(30)–C(29)	120.6(2)	C(32)–C(31)–C(30)	120.1(2)
C(31)–C(32)–C(33)	119.9(2)	C(32)–C(33)–C(34)	120.3(2)
C(33)–C(34)–C(29)	120.7(2)		

Table 4. Anisotropic displacement parameters ($Å^2$) for str0541. 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)	0.01164(16)	0.01492(17)	0.01291(17)	–0.00198(12)	–0.00401(12)	–0.00265(12)
Fe(2)	0.01119(16)	0.01154(16)	0.01301(16)	–0.00027(12)	–0.00307(12)	–0.00290(12)
P(1)	0.0149(3)	0.0125(3)	0.0117(3)	–0.0002(2)	–0.0048(2)	–0.0018(2)
P(2)	0.0108(3)	0.0123(3)	0.0117(3)	–0.0011(2)	–0.0040(2)	–0.0024(2)
S(1)	0.0135(3)	0.0171(3)	0.0189(3)	–0.0027(2)	–0.0027(2)	–0.0062(2)
S(2)	0.0123(3)	0.0138(3)	0.0128(3)	–0.00203(19)	–0.0025(2)	–0.0025(2)
N(1)	0.0139(9)	0.0133(9)	0.0136(9)	0.0014(7)	–0.0055(7)	–0.0054(7)
O(1)	0.0340(11)	0.0324(11)	0.0239(10)	–0.0123(8)	0.0013(8)	–0.0157(9)
O(2)	0.0240(10)	0.0387(12)	0.0461(13)	0.0061(10)	–0.0181(10)	–0.0007(9)
O(3)	0.0286(10)	0.0157(9)	0.0268(10)	–0.0048(7)	–0.0046(8)	–0.0033(7)
O(4)	0.0276(10)	0.0234(9)	0.0172(9)	0.0014(7)	–0.0058(7)	–0.0070(8)
C(1)	0.0172(11)	0.0233(12)	0.0176(11)	–0.0017(9)	–0.0011(9)	–0.0099(10)
C(2)	0.0210(12)	0.0222(12)	0.0205(12)	–0.0001(9)	–0.0069(10)	–0.0047(10)
C(3)	0.0144(11)	0.0188(12)	0.0174(11)	0.0023(9)	–0.0039(9)	–0.0071(9)
C(4)	0.0138(10)	0.0132(11)	0.0185(12)	–0.0019(8)	–0.0037(9)	–0.0022(8)
C(5)	0.0163(12)	0.0294(14)	0.0248(13)	–0.0038(10)	0.0039(10)	–0.0090(10)
C(6)	0.0291(15)	0.0363(17)	0.0340(16)	–0.0041(13)	–0.0005(13)	–0.0090(13)
C(7)	0.0155(11)	0.0247(13)	0.0159(11)	–0.0061(9)	0.0023(9)	–0.0042(10)
C(8)	0.0193(11)	0.0201(12)	0.0187(11)	0.0002(9)	–0.0053(9)	–0.0105(9)
C(9)	0.0224(13)	0.0273(14)	0.0248(13)	0.0039(10)	–0.0049(11)	–0.0138(11)
C(10)	0.0311(14)	0.0180(12)	0.0248(13)	–0.0014(10)	–0.0093(11)	–0.0121(10)
C(11)	0.0250(12)	0.0151(11)	0.0118(10)	0.0011(8)	–0.0052(9)	–0.0082(9)
C(12)	0.0233(12)	0.0170(12)	0.0167(11)	–0.0001(9)	–0.0021(10)	–0.0081(10)
C(13)	0.0352(15)	0.0216(13)	0.0191(12)	–0.0037(10)	0.0029(11)	–0.0129(11)
C(14)	0.057(2)	0.0304(15)	0.0120(11)	0.0004(10)	–0.0067(12)	–0.0238(14)
C(15)	0.0438(17)	0.0325(15)	0.0193(13)	0.0058(11)	–0.0164(12)	–0.0185(13)
C(16)	0.0274(13)	0.0257(13)	0.0187(12)	0.0026(10)	–0.0098(10)	–0.0070(11)
C(17)	0.0257(13)	0.0123(11)	0.0229(12)	0.0004(9)	–0.0131(10)	–0.0011(9)
C(18)	0.0325(14)	0.0186(12)	0.0215(12)	–0.0030(9)	–0.0145(11)	0.0014(10)
C(19)	0.0505(19)	0.0232(14)	0.0344(16)	–0.0100(12)	–0.0252(15)	0.0103(13)
C(20)	0.072(2)	0.0141(13)	0.050(2)	–0.0008(13)	–0.0384(19)	0.0051(14)
C(21)	0.057(2)	0.0181(14)	0.0429(18)	0.0113(12)	–0.0232(16)	–0.0088(14)
C(22)	0.0358(15)	0.0198(13)	0.0273(14)	0.0046(10)	–0.0128(12)	–0.0055(11)
C(23)	0.0120(10)	0.0194(11)	0.0122(10)	–0.0019(8)	–0.0032(8)	–0.0053(9)
C(24)	0.0156(11)	0.0206(12)	0.0202(12)	0.0003(9)	–0.0066(9)	–0.0054(9)
C(25)	0.0184(12)	0.0286(14)	0.0197(12)	0.0058(10)	–0.0101(10)	–0.0084(10)
C(26)	0.0253(13)	0.0362(15)	0.0159(12)	–0.0012(10)	–0.0068(10)	–0.0139(11)
C(27)	0.0336(15)	0.0254(14)	0.0202(13)	–0.0083(10)	–0.0063(11)	–0.0079(11)
C(28)	0.0219(12)	0.0182(12)	0.0174(11)	–0.0023(9)	–0.0052(10)	–0.0045(10)
C(29)	0.0123(10)	0.0134(11)	0.0155(11)	–0.0002(8)	–0.0017(9)	–0.0011(8)
C(30)	0.0168(11)	0.0171(11)	0.0170(11)	–0.0024(9)	–0.0023(9)	–0.0046(9)
C(31)	0.0240(13)	0.0175(12)	0.0181(12)	–0.0033(9)	–0.0020(10)	–0.0049(10)
C(32)	0.0174(12)	0.0230(13)	0.0220(13)	–0.0026(10)	0.0007(10)	0.0005(10)
C(33)	0.0122(11)	0.0288(14)	0.0286(14)	–0.0030(11)	–0.0024(10)	–0.0034(10)
C(34)	0.0162(11)	0.0212(12)	0.0195(12)	–0.0024(9)	–0.0037(9)	–0.0042(9)

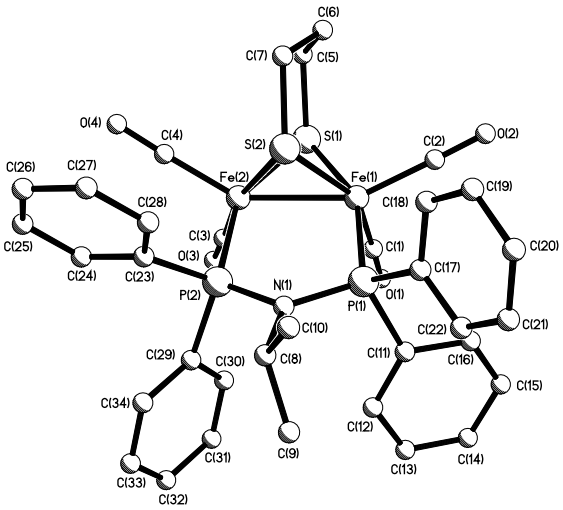
Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for str0541.

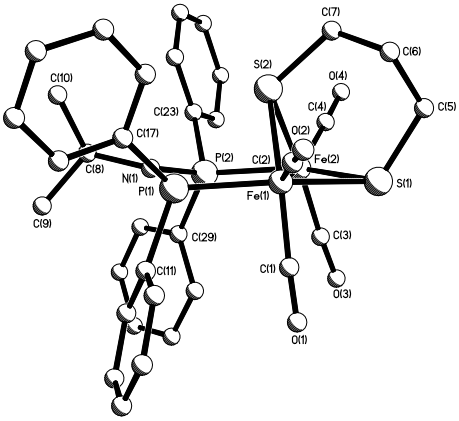
	x	y	z	U
H(5A)	0.2764	0.1439	0.4538	0.030
H(5B)	0.3870	0.1191	0.5141	0.030
H(6A)	0.2391	0.3060	0.5429	0.041
H(6B)	0.2830	0.3402	0.4327	0.041
H(7A)	0.4592	0.2977	0.5549	0.024
H(7B)	0.3865	0.4256	0.5204	0.024
H(8A)	1.0068	0.3945	0.2674	0.022
H(9A)	1.0799	0.3501	0.1044	0.036
H(9B)	1.1119	0.4696	0.1255	0.036
H(9C)	0.9846	0.4757	0.0830	0.036
H(10A)	0.8193	0.5581	0.3265	0.034
H(10B)	0.8243	0.6041	0.2197	0.034
H(10C)	0.9522	0.5973	0.2617	0.034
H(12A)	0.9679	0.2601	0.0530	0.023
H(13A)	1.0217	0.2023	–0.1051	0.031
H(14A)	0.8531	0.2539	–0.1881	0.037
H(15A)	0.6307	0.3649	–0.1144	0.035
H(16A)	0.5773	0.4243	0.0424	0.028
H(18A)	0.4921	0.5531	0.3155	0.029
H(19A)	0.4075	0.7590	0.3144	0.044
H(20A)	0.5013	0.8710	0.1860	0.053
H(21A)	0.6703	0.7789	0.0560	0.046
H(22A)	0.7554	0.5724	0.0551	0.033
H(24A)	1.0364	0.0914	0.4207	0.022
H(25A)	1.0588	0.1097	0.5724	0.025
H(26A)	0.9644	0.2902	0.6504	0.029
H(27A)	0.8467	0.4526	0.5771	0.031
H(28A)	0.8175	0.4346	0.4268	0.023
H(30A)	0.9500	0.0675	0.1523	0.021
H(31A)	1.1538	–0.0244	0.0414	0.025
H(32A)	1.3661	–0.0059	0.0522	0.028
H(33A)	1.3753	0.1033	0.1746	0.029
H(34A)	1.1725	0.1990	0.2837	0.023

Table 6. Torsion angles [°] for str0541.

C(1)–Fe(1)–Fe(2)–C(3)	−6.56(11)	C(2)–Fe(1)–Fe(2)–C(3)	125.7(2)
P(1)–Fe(1)–Fe(2)–C(3)	−99.64(8)	S(1)–Fe(1)–Fe(2)–C(3)	73.34(8)
S(2)–Fe(1)–Fe(2)–C(3)	−178.80(8)	C(1)–Fe(1)–Fe(2)–C(4)	−150.98(16)
C(2)–Fe(1)–Fe(2)–C(4)	−18.7(2)	P(1)–Fe(1)–Fe(2)–C(4)	115.94(14)
S(1)–Fe(1)–Fe(2)–C(4)	−71.07(14)	S(2)–Fe(1)–Fe(2)–C(4)	36.78(14)
C(1)–Fe(1)–Fe(2)–P(2)	92.17(8)	C(2)–Fe(1)–Fe(2)–P(2)	−135.52(19)
P(1)–Fe(1)–Fe(2)–P(2)	−0.91(2)	S(1)–Fe(1)–Fe(2)–P(2)	172.08(3)
S(2)–Fe(1)–Fe(2)–P(2)	−80.07(2)	C(1)–Fe(1)–Fe(2)–S(1)	−79.90(8)
C(2)–Fe(1)–Fe(2)–S(1)	52.40(19)	P(1)–Fe(1)–Fe(2)–S(1)	−172.98(3)
S(2)–Fe(1)–Fe(2)–S(1)	107.85(3)	C(1)–Fe(1)–Fe(2)–S(2)	172.24(8)
C(2)–Fe(1)–Fe(2)–S(2)	−55.45(19)	P(1)–Fe(1)–Fe(2)–S(2)	79.16(3)
S(1)–Fe(1)–Fe(2)–S(2)	−107.85(3)	C(1)–Fe(1)–P(1)–N(1)	−107.22(11)
C(2)–Fe(1)–P(1)–N(1)	151.11(11)	S(1)–Fe(1)–P(1)–N(1)	−23.78(10)
S(2)–Fe(1)–P(1)–N(1)	45.22(7)	Fe(2)–Fe(1)–P(1)–N(1)	−10.46(7)
C(1)–Fe(1)–P(1)–C(11)	16.13(12)	C(2)–Fe(1)–P(1)–C(11)	−85.55(12)
S(1)–Fe(1)–P(1)–C(11)	99.56(10)	S(2)–Fe(1)–P(1)–C(11)	168.56(9)
Fe(2)–Fe(1)–P(1)–C(11)	112.89(9)	C(1)–Fe(1)–P(1)–C(17)	130.35(12)
C(2)–Fe(1)–P(1)–C(17)	28.67(12)	S(1)–Fe(1)–P(1)–C(17)	−146.22(10)
S(2)–Fe(1)–P(1)–C(17)	−77.22(9)	Fe(2)–Fe(1)–P(1)–C(17)	−132.89(9)
C(3)–Fe(2)–P(2)–N(1)	122.88(11)	C(4)–Fe(2)–P(2)–N(1)	−137.67(10)
S(1)–Fe(2)–P(2)–N(1)	25.93(10)	S(2)–Fe(2)–P(2)–N(1)	−43.62(8)
Fe(1)–Fe(2)–P(2)–N(1)	12.50(8)	C(3)–Fe(2)–P(2)–C(29)	−1.68(12)
C(4)–Fe(2)–P(2)–C(29)	97.78(12)	S(1)–Fe(2)–P(2)–C(29)	−98.62(10)
S(2)–Fe(2)–P(2)–C(29)	−168.17(9)	Fe(1)–Fe(2)–P(2)–C(29)	−112.05(9)
C(3)–Fe(2)–P(2)–C(23)	−118.14(11)	C(4)–Fe(2)–P(2)–C(23)	−18.68(11)
S(1)–Fe(2)–P(2)–C(23)	144.92(9)	S(2)–Fe(2)–P(2)–C(23)	75.36(8)
Fe(1)–Fe(2)–P(2)–C(23)	131.49(8)	C(3)–Fe(2)–S(1)–C(5)	137.96(12)
C(4)–Fe(2)–S(1)–C(5)	40.42(13)	P(2)–Fe(2)–S(1)–C(5)	−122.64(11)
S(2)–Fe(2)–S(1)–C(5)	−53.43(10)	Fe(1)–Fe(2)–S(1)–C(5)	−106.60(10)
C(3)–Fe(2)–S(1)–Fe(1)	−115.44(8)	C(4)–Fe(2)–S(1)–Fe(1)	147.03(8)
P(2)–Fe(2)–S(1)–Fe(1)	−16.03(5)	S(2)–Fe(2)–S(1)–Fe(1)	53.18(2)
C(1)–Fe(1)–S(1)–C(5)	−153.48(13)	C(2)–Fe(1)–S(1)–C(5)	−53.31(13)
P(1)–Fe(1)–S(1)–C(5)	121.47(11)	S(2)–Fe(1)–S(1)–C(5)	52.41(10)
Fe(2)–Fe(1)–S(1)–C(5)	105.60(10)	C(1)–Fe(1)–S(1)–Fe(2)	100.92(8)
C(2)–Fe(1)–S(1)–Fe(2)	−158.91(9)	P(1)–Fe(1)–S(1)–Fe(2)	15.87(6)
S(2)–Fe(1)–S(1)–Fe(2)	−53.194(19)	C(3)–Fe(2)–S(2)–C(7)	112.6(3)
C(4)–Fe(2)–S(2)–C(7)	−53.01(12)	P(2)–Fe(2)–S(2)–C(7)	−153.36(9)
S(1)–Fe(2)–S(2)–C(7)	54.54(9)	Fe(1)–Fe(2)–S(2)–C(7)	107.77(9)
C(3)–Fe(2)–S(2)–Fe(1)	4.9(3)	C(4)–Fe(2)–S(2)–Fe(1)	−160.78(8)
P(2)–Fe(2)–S(2)–Fe(1)	98.87(2)	S(1)–Fe(2)–S(2)–Fe(1)	−53.23(2)
C(1)–Fe(1)–S(2)–C(7)	−121.27(19)	C(2)–Fe(1)–S(2)–C(7)	53.50(13)
P(1)–Fe(1)–S(2)–C(7)	152.95(10)	S(1)–Fe(1)–S(2)–C(7)	−51.54(10)
Fe(2)–Fe(1)–S(2)–C(7)	−104.46(10)	C(1)–Fe(1)–S(2)–Fe(2)	−16.82(17)
C(2)–Fe(1)–S(2)–Fe(2)	157.96(9)	P(1)–Fe(1)–S(2)–Fe(2)	−102.59(2)
S(1)–Fe(1)–S(2)–Fe(2)	52.91(2)	C(11)–P(1)–N(1)–C(8)	72.0(2)
C(17)–P(1)–N(1)–C(8)	−36.2(2)	Fe(1)–P(1)–N(1)–C(8)	−164.65(17)
C(11)–P(1)–N(1)–P(2)	−102.13(13)	C(17)–P(1)–N(1)–P(2)	149.72(12)
Fe(1)–P(1)–N(1)–P(2)	21.23(13)	C(29)–P(2)–N(1)–C(8)	−63.81(18)
C(23)–P(2)–N(1)–C(8)	44.40(18)	Fe(2)–P(2)–N(1)–C(8)	162.40(13)
C(29)–P(2)–N(1)–P(1)	111.02(13)	C(23)–P(2)–N(1)–P(1)	−140.77(12)

Fe(2)–P(2)–N(1)–P(1)	−22.77(13)	C(2)–Fe(1)–C(1)–O(1)	−116(4)
P(1)–Fe(1)–C(1)–O(1)	143(4)	S(1)–Fe(1)–C(1)–O(1)	−11(4)
S(2)–Fe(1)–C(1)–O(1)	59(4)	Fe(2)–Fe(1)–C(1)–O(1)	45(4)
C(1)–Fe(1)–C(2)–O(2)	68(6)	P(1)–Fe(1)–C(2)–O(2)	162(6)
S(1)–Fe(1)–C(2)–O(2)	−20(6)	S(2)–Fe(1)–C(2)–O(2)	−109(6)
Fe(2)–Fe(1)–C(2)–O(2)	−63(6)	C(4)–Fe(2)–C(3)–O(3)	51(4)
P(2)–Fe(2)–C(3)–O(3)	153(4)	S(1)–Fe(2)–C(3)–O(3)	−56(4)
S(2)–Fe(2)–C(3)–O(3)	−114(4)	Fe(1)–Fe(2)–C(3)–O(3)	−110(4)
C(3)–Fe(2)–C(4)–O(4)	−171(4)	P(2)–Fe(2)–C(4)–O(4)	90(4)
S(1)–Fe(2)–C(4)–O(4)	−81(4)	S(2)–Fe(2)–C(4)–O(4)	5(4)
Fe(1)–Fe(2)–C(4)–O(4)	−25(4)	Fe(2)–S(1)–C(5)–C(6)	63.7(2)
Fe(1)–S(1)–C(5)–C(6)	−9.2(3)	S(1)–C(5)–C(6)–C(7)	−60.3(3)
C(5)–C(6)–C(7)–S(2)	61.4(3)	Fe(2)–S(2)–C(7)–C(6)	−66.0(2)
Fe(1)–S(2)–C(7)–C(6)	6.7(2)	P(1)–N(1)–C(8)–C(9)	−66.6(3)
P(2)–N(1)–C(8)–C(9)	107.5(2)	P(1)–N(1)–C(8)–C(10)	62.3(3)
P(2)–N(1)–C(8)–C(10)	−123.58(19)	N(1)–P(1)–C(11)–C(12)	18.0(2)
C(17)–P(1)–C(11)–C(12)	129.4(2)	Fe(1)–P(1)–C(11)–C(12)	−106.6(2)
N(1)–P(1)–C(11)–C(16)	−171.76(18)	C(17)–P(1)–C(11)–C(16)	−60.4(2)
Fe(1)–P(1)–C(11)–C(16)	63.7(2)	C(16)–C(11)–C(12)–C(13)	0.5(4)
P(1)–C(11)–C(12)–C(13)	170.52(19)	C(11)–C(12)–C(13)–C(14)	−0.6(4)
C(12)–C(13)–C(14)–C(15)	0.3(4)	C(13)–C(14)–C(15)–C(16)	0.0(4)
C(14)–C(15)–C(16)–C(11)	−0.1(4)	C(12)–C(11)–C(16)–C(15)	−0.1(4)
P(1)–C(11)–C(16)–C(15)	−171.1(2)	N(1)–P(1)–C(17)–C(18)	−91.7(2)
C(11)–P(1)–C(17)–C(18)	153.5(2)	Fe(1)–P(1)–C(17)–C(18)	34.1(2)
N(1)–P(1)–C(17)–C(22)	88.8(2)	C(11)–P(1)–C(17)–C(22)	−26.0(2)
Fe(1)–P(1)–C(17)–C(22)	−145.40(19)	C(22)–C(17)–C(18)–C(19)	−2.6(4)
P(1)–C(17)–C(18)–C(19)	177.9(2)	C(17)–C(18)–C(19)–C(20)	0.3(4)
C(18)–C(19)–C(20)–C(21)	1.8(5)	C(19)–C(20)–C(21)–C(22)	−1.5(5)
C(20)–C(21)–C(22)–C(17)	−0.8(5)	C(18)–C(17)–C(22)–C(21)	2.8(4)
P(1)–C(17)–C(22)–C(21)	−177.7(2)	N(1)–P(2)–C(23)–C(28)	33.9(2)
C(29)–P(2)–C(23)–C(28)	141.8(2)	Fe(2)–P(2)–C(23)–C(28)	−90.1(2)
N(1)–P(2)–C(23)–C(24)	−160.01(17)	C(29)–P(2)–C(23)–C(24)	−52.2(2)
Fe(2)–P(2)–C(23)–C(24)	76.00(18)	C(28)–C(23)–C(24)–C(25)	1.0(4)
P(2)–C(23)–C(24)–C(25)	−165.76(19)	C(23)–C(24)–C(25)–C(26)	−1.0(4)
C(24)–C(25)–C(26)–C(27)	0.1(4)	C(25)–C(26)–C(27)–C(28)	0.9(4)
C(24)–C(23)–C(28)–C(27)	0.0(4)	P(2)–C(23)–C(28)–C(27)	165.7(2)
C(26)–C(27)–C(28)–C(23)	−0.9(4)	N(1)–P(2)–C(29)–C(34)	87.3(2)
C(23)–P(2)–C(29)–C(34)	−24.4(2)	Fe(2)–P(2)–C(29)–C(34)	−142.32(18)
N(1)–P(2)–C(29)–C(30)	−85.88(19)	C(23)–P(2)–C(29)–C(30)	162.41(18)
Fe(2)–P(2)–C(29)–C(30)	44.5(2)	C(34)–C(29)–C(30)–C(31)	−0.8(3)
P(2)–C(29)–C(30)–C(31)	172.77(19)	C(29)–C(30)–C(31)–C(32)	0.6(4)
C(30)–C(31)–C(32)–C(33)	0.2(4)	C(31)–C(32)–C(33)–C(34)	−1.0(4)
C(32)–C(33)–C(34)–C(29)	0.9(4)	C(30)–C(29)–C(34)–C(33)	0.0(4)
P(2)–C(29)–C(34)–C(33)	−173.2(2)		





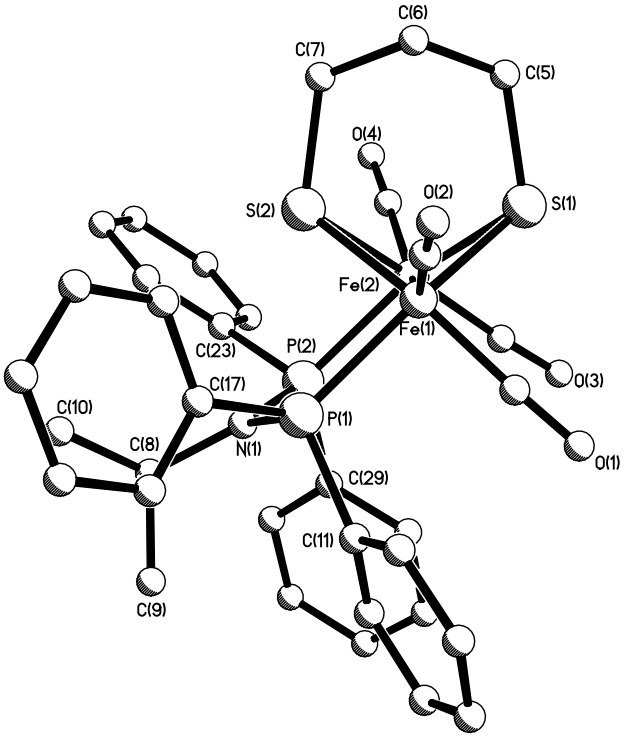


Table 1. Crystal data and structure refinement for **3e**.

Identification code	str0451	
Chemical formula	C_{127} H_{80} Cl_2 Fe_8 N_4 O_{22} P_8 S_8	
Formula weight	3035.97	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	orthorhombic, Pbam	
Unit cell parameters	a = 21.7006(12) Å	α = 90°
	b = 15.3850(9) Å	β = 90°
	c = 20.0483(11) Å	γ = 90°
Cell volume	6693.4(7) $Å^3$	
Z	2	
Calculated density	1.528 g/cm^3	
Absorption coefficient μ	1.170 mm^{-1}	
F(000)	3160	
Crystal colour and size	orange, 0.12 × 0.12 × 0.12 mm^3	
Data collection method	Bruker SMART APEX diffractometer	
	ω rotation with narrow frames	
θ range for data collection	1.62 to 28.31°	
Index ranges	h –28 to 28, k –20 to 20, l –26 to 26	
Completeness to θ = 26.00°	99.7 %	
Reflections collected	57217	
Independent reflections	8411 (R_{int} = 0.0481)	
Reflections with $F^2>2\sigma$	6792	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.8724 and 0.8724	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0847, 15.7626	
Data / restraints / parameters	8411 / 0 / 422	
Final R indices [$F^2>2\sigma$]	R1 = 0.0572, wR2 = 0.1523	
R indices (all data)	R1 = 0.0718, wR2 = 0.1621	
Goodness-of-fit on F^2	1.047	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	1.832 and –2.255 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for str0451. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Fe(1)	0.18079(2)	0.57970(3)	0.43799(2)	0.02234(14)
Fe(2)	0.16844(2)	0.39335(3)	0.06203(2)	0.01716(13)
P(1)	0.19058(4)	0.43810(6)	0.42602(4)	0.02214(19)
P(2)	0.11211(4)	0.27575(5)	0.07336(4)	0.01755(18)
S(1)	0.18288(6)	0.70190(8)	0.5000	0.0280(3)
S(2)	0.09731(6)	0.54520(8)	0.5000	0.0236(2)
S(3)	0.08989(5)	0.44486(7)	0.0000	0.0185(2)
S(4)	0.22664(5)	0.48404(8)	0.0000	0.0233(2)
N(1)	0.2090(2)	0.3906(3)	0.5000	0.0224(8)
N(2)	0.10483(18)	0.2209(3)	0.0000	0.0196(8)
O(1)	0.31149(16)	0.6083(2)	0.41328(19)	0.0525(9)
O(2)	0.13554(19)	0.6340(2)	0.30693(15)	0.0545(9)
O(3)	0.28002(12)	0.2937(2)	0.08851(15)	0.0378(7)
O(4)	0.15496(14)	0.47273(19)	0.19393(13)	0.0360(6)
C(1)	0.2596(2)	0.5960(3)	0.4221(2)	0.0332(8)
C(2)	0.1526(2)	0.6115(2)	0.35822(19)	0.0332(8)
C(3)	0.1084(3)	0.7577(4)	0.5000	0.0518(18)
C(4)	0.0572(4)	0.7156(5)	0.4702(4)	0.0326(16)
C(5)	0.0367(3)	0.6278(4)	0.5000	0.0338(12)
C(6)	0.12431(17)	0.3774(2)	0.39377(19)	0.0297(8)
C(7)	0.08061(19)	0.4183(3)	0.3536(2)	0.0357(9)
C(8)	0.0333(2)	0.3705(3)	0.3249(2)	0.0446(11)
C(9)	0.0288(2)	0.2831(4)	0.3363(3)	0.0558(14)
C(10)	0.0708(3)	0.2426(3)	0.3765(4)	0.0699(18)
C(11)	0.1185(2)	0.2896(3)	0.4060(3)	0.0539(13)
C(12)	0.25233(18)	0.3980(2)	0.37298(17)	0.0275(7)
C(13)	0.2411(2)	0.3644(3)	0.30943(19)	0.0395(10)
C(14)	0.2899(3)	0.3396(3)	0.2687(2)	0.0511(12)
C(15)	0.3492(2)	0.3495(3)	0.2901(2)	0.0500(12)
C(16)	0.3613(2)	0.3835(3)	0.3519(2)	0.0472(11)
C(17)	0.31356(19)	0.4073(3)	0.3937(2)	0.0365(9)
C(18)	0.23568(16)	0.3323(2)	0.07844(17)	0.0239(7)
C(19)	0.15935(15)	0.4418(2)	0.14203(17)	0.0228(7)
C(20)	0.0836(2)	0.5636(3)	0.0000	0.0255(10)
C(21)	0.1382(3)	0.6119(5)	0.0272(4)	0.0291(15)
C(22)	0.1976(3)	0.5954(4)	0.0000	0.0483(18)
C(23)	0.03334(15)	0.2864(2)	0.10574(16)	0.0232(7)
C(24)	–0.0081(2)	0.2182(3)	0.0988(3)	0.0608(16)
C(25)	–0.0667(2)	0.2242(4)	0.1263(4)	0.078(2)
C(26)	–0.08496(19)	0.2969(3)	0.1599(2)	0.0423(10)
C(27)	–0.04452(17)	0.3637(3)	0.16770(17)	0.0299(8)
C(28)	0.01449(16)	0.3589(2)	0.14021(17)	0.0269(7)
C(29)	0.14231(16)	0.1942(2)	0.13015(17)	0.0237(7)
C(30)	0.16985(18)	0.1180(3)	0.10918(19)	0.0318(8)
C(31)	0.1957(2)	0.0603(3)	0.1550(2)	0.0414(10)
C(32)	0.1953(2)	0.0795(3)	0.2216(2)	0.0460(11)
C(33)	0.1675(3)	0.1555(3)	0.2432(2)	0.0614(16)
C(34)	0.1409(3)	0.2121(3)	0.1979(2)	0.0487(13)
C(40)	0.5000	0.5000	0.447(2)	0.165(14)

Cl(1)	0.4380(3)	0.5270(4)	0.5000	0.188(2)
C(41)	0.0987(4)	–0.0410(6)	0.0000	0.069(2)
O(10)	0.0567(3)	0.0332(5)	0.0000	0.090(2)
O(11)	0.5137(4)	0.4665(6)	0.3007(4)	0.074(2)
O(12)	–0.0321(5)	–0.0073(7)	0.1708(6)	0.098(3)

Table 3. Bond lengths [Å] and angles [°] for str0451.

Fe(1)–C(1)	1.758(4)	Fe(1)–C(2)	1.781(4)
Fe(1)–P(1)	2.2020(10)	Fe(1)–S(1)	2.2544(11)
Fe(1)–S(2)	2.2603(11)	Fe(1)–Fe(1A)	2.4866(9)
Fe(2)–C(18)	1.766(4)	Fe(2)–C(19)	1.780(4)
Fe(2)–P(2)	2.1954(9)	Fe(2)–S(3)	2.2540(10)
Fe(2)–S(4)	2.2556(11)	Fe(2)–Fe(2B)	2.4871(9)
P(1)–N(1)	1.701(2)	P(1)–C(12)	1.818(4)
P(1)–C(6)	1.832(4)	P(2)–N(2)	1.703(2)
P(2)–C(29)	1.817(3)	P(2)–C(23)	1.836(3)
S(1)–C(3)	1.830(6)	S(1)–Fe(1A)	2.2544(11)
S(2)–C(5)	1.829(5)	S(2)–Fe(1A)	2.2603(11)
S(3)–C(20)	1.832(5)	S(3)–Fe(2B)	2.2540(10)
S(4)–C(22)	1.825(6)	S(4)–Fe(2B)	2.2556(11)
N(1)–P(1A)	1.701(2)	N(2)–P(2B)	1.703(2)
O(1)–C(1)	1.155(5)	O(2)–C(2)	1.146(5)
O(3)–C(18)	1.149(4)	O(4)–C(19)	1.148(4)
C(3)–C(4A)	1.417(10)	C(3)–C(4)	1.417(10)
C(4)–C(4A)	1.193(16)	C(4)–C(5)	1.542(9)
C(5)–C(4A)	1.542(9)	C(6)–C(11)	1.378(6)
C(6)–C(7)	1.393(5)	C(7)–C(8)	1.387(6)
C(8)–C(9)	1.368(7)	C(9)–C(10)	1.366(8)
C(10)–C(11)	1.395(7)	C(12)–C(13)	1.397(5)
C(12)–C(17)	1.399(6)	C(13)–C(14)	1.391(6)
C(14)–C(15)	1.364(8)	C(15)–C(16)	1.370(7)
C(16)–C(17)	1.381(6)	C(20)–C(21)	1.500(9)
C(20)–C(21B)	1.500(9)	C(21)–C(21B)	1.093(15)
C(21)–C(22)	1.424(9)	C(22)–C(21B)	1.424(9)
C(23)–C(28)	1.374(5)	C(23)–C(24)	1.388(6)
C(24)–C(25)	1.389(6)	C(25)–C(26)	1.365(7)
C(26)–C(27)	1.360(6)	C(27)–C(28)	1.396(5)
C(29)–C(30)	1.382(5)	C(29)–C(34)	1.387(5)
C(30)–C(31)	1.395(5)	C(31)–C(32)	1.366(6)
C(32)–C(33)	1.385(7)	C(33)–C(34)	1.384(6)
C(40)–Cl(1C)	1.77(2)	C(40)–Cl(1)	1.77(2)
Cl(1)–C(40C)	1.77(2)	C(41)–O(10)	1.460(11)
O(11)–O(11D)	1.191(16)	O(12)–O(12E)	1.41(2)

C(1)–Fe(1)–C(2)	97.63(19)	C(1)–Fe(1)–P(1)	91.57(13)
C(2)–Fe(1)–P(1)	101.96(13)	C(1)–Fe(1)–S(1)	87.79(14)
C(2)–Fe(1)–S(1)	105.84(13)	P(1)–Fe(1)–S(1)	152.03(4)
C(1)–Fe(1)–S(2)	155.92(14)	C(2)–Fe(1)–S(2)	106.43(14)
P(1)–Fe(1)–S(2)	84.54(4)	S(1)–Fe(1)–S(2)	84.76(4)
C(1)–Fe(1)–Fe(1A)	100.43(13)	C(2)–Fe(1)–Fe(1A)	153.89(13)
P(1)–Fe(1)–Fe(1A)	96.25(3)	S(1)–Fe(1)–Fe(1A)	56.53(2)
S(2)–Fe(1)–Fe(1A)	56.63(2)	C(18)–Fe(2)–C(19)	98.42(15)
C(18)–Fe(2)–P(2)	90.15(12)	C(19)–Fe(2)–P(2)	100.96(11)
C(18)–Fe(2)–S(3)	156.14(11)	C(19)–Fe(2)–S(3)	105.44(11)
P(2)–Fe(2)–S(3)	85.74(4)	C(18)–Fe(2)–S(4)	88.22(12)
C(19)–Fe(2)–S(4)	107.45(11)	P(2)–Fe(2)–S(4)	151.47(4)
S(3)–Fe(2)–S(4)	84.36(4)	C(18)–Fe(2)–Fe(2B)	100.74(11)
C(19)–Fe(2)–Fe(2B)	154.33(11)	P(2)–Fe(2)–Fe(2B)	95.94(2)
S(3)–Fe(2)–Fe(2B)	56.515(19)	S(4)–Fe(2)–Fe(2B)	56.54(2)
N(1)–P(1)–C(12)	101.02(17)	N(1)–P(1)–C(6)	105.9(2)

C(12)–P(1)–C(6)	101.50(17)	N(1)–P(1)–Fe(1)	110.64(13)
C(12)–P(1)–Fe(1)	118.04(13)	C(6)–P(1)–Fe(1)	117.82(13)
N(2)–P(2)–C(29)	103.46(17)	N(2)–P(2)–C(23)	105.27(17)
C(29)–P(2)–C(23)	100.13(16)	N(2)–P(2)–Fe(2)	111.75(12)
C(29)–P(2)–Fe(2)	115.67(11)	C(23)–P(2)–Fe(2)	118.79(12)
C(3)–S(1)–Fe(1)	111.92(17)	C(3)–S(1)–Fe(1A)	111.92(17)
Fe(1)–S(1)–Fe(1A)	66.94(4)	C(5)–S(2)–Fe(1A)	114.40(16)
C(5)–S(2)–Fe(1)	114.40(16)	Fe(1A)–S(2)–Fe(1)	66.74(4)
C(20)–S(3)–Fe(2)	113.99(14)	C(20)–S(3)–Fe(2B)	113.99(14)
Fe(2)–S(3)–Fe(2B)	66.97(4)	C(22)–S(4)–Fe(2B)	112.81(16)
C(22)–S(4)–Fe(2)	112.81(16)	Fe(2B)–S(4)–Fe(2)	66.92(4)
P(1A)–N(1)–P(1)	121.4(2)	P(2)–N(2)–P(2B)	119.5(2)
O(1)–C(1)–Fe(1)	178.0(4)	O(2)–C(2)–Fe(1)	178.0(4)
C(4A)–C(3)–C(4)	49.8(7)	C(4A)–C(3)–S(1)	118.5(5)
C(4)–C(3)–S(1)	118.5(5)	C(4A)–C(4)–C(3)	65.1(3)
C(4A)–C(4)–C(5)	67.2(3)	C(3)–C(4)–C(5)	117.6(6)
C(4A)–C(5)–C(4)	45.5(6)	C(4A)–C(5)–S(2)	113.7(4)
C(4)–C(5)–S(2)	113.7(4)	C(11)–C(6)–C(7)	118.8(4)
C(11)–C(6)–P(1)	120.5(3)	C(7)–C(6)–P(1)	120.6(3)
C(8)–C(7)–C(6)	120.3(4)	C(9)–C(8)–C(7)	120.3(4)
C(10)–C(9)–C(8)	119.9(4)	C(9)–C(10)–C(11)	120.6(5)
C(6)–C(11)–C(10)	120.1(5)	C(13)–C(12)–C(17)	118.2(4)
C(13)–C(12)–P(1)	122.1(3)	C(17)–C(12)–P(1)	119.5(3)
C(14)–C(13)–C(12)	120.3(4)	C(15)–C(14)–C(13)	120.2(4)
C(14)–C(15)–C(16)	120.4(4)	C(15)–C(16)–C(17)	120.4(5)
C(16)–C(17)–C(12)	120.4(4)	O(3)–C(18)–Fe(2)	178.8(4)
O(4)–C(19)–Fe(2)	178.4(3)	C(21)–C(20)–C(21B)	42.7(6)
C(21)–C(20)–S(3)	115.8(4)	C(21B)–C(20)–S(3)	115.8(4)
C(21B)–C(21)–C(22)	67.4(3)	C(21B)–C(21)–C(20)	68.6(3)
C(22)–C(21)–C(20)	119.1(5)	C(21B)–C(22)–C(21)	45.1(6)
C(21B)–C(22)–S(4)	118.7(4)	C(21)–C(22)–S(4)	118.7(4)
C(28)–C(23)–C(24)	118.1(3)	C(28)–C(23)–P(2)	121.8(3)
C(24)–C(23)–P(2)	120.0(3)	C(23)–C(24)–C(25)	120.2(4)
C(26)–C(25)–C(24)	121.1(4)	C(27)–C(26)–C(25)	119.2(4)
C(26)–C(27)–C(28)	120.4(4)	C(23)–C(28)–C(27)	121.0(3)
C(30)–C(29)–C(34)	118.4(3)	C(30)–C(29)–P(2)	123.5(3)
C(34)–C(29)–P(2)	118.0(3)	C(29)–C(30)–C(31)	120.9(4)
C(32)–C(31)–C(30)	120.3(4)	C(31)–C(32)–C(33)	119.4(4)
C(34)–C(33)–C(32)	120.5(4)	C(33)–C(34)–C(29)	120.6(4)
Cl(1C)–C(40)–Cl(1)	105(2)	C(40C)–Cl(1)–C(40)	75(2)

Symmetry operations for equivalent atoms

A x,y,–z+1 B x,y,–z C –x+1,–y+1,–z+1

D –x+1,–y+1,z E –x,–y,z

Table 4. Anisotropic displacement parameters ($Å^2$) for str0451. 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)	0.0298(3)	0.0215(3)	0.0157(2)	0.00137(17)	0.00068(18)	0.00027(19)
Fe(2)	0.0162(2)	0.0196(2)	0.0157(2)	–0.00070(16)	–0.00119(16)	0.00008(16)
P(1)	0.0275(4)	0.0230(4)	0.0159(4)	–0.0015(3)	–0.0010(3)	0.0018(3)
P(2)	0.0185(4)	0.0204(4)	0.0137(4)	0.0003(3)	–0.0003(3)	0.0001(3)
S(1)	0.0346(7)	0.0206(6)	0.0288(6)	0.000	0.000	–0.0016(5)
S(2)	0.0290(6)	0.0214(6)	0.0203(5)	0.000	0.000	0.0003(5)
S(3)	0.0159(5)	0.0222(5)	0.0174(5)	0.000	0.000	0.0012(4)
S(4)	0.0192(5)	0.0223(6)	0.0282(6)	0.000	0.000	–0.0033(4)
N(1)	0.032(2)	0.0208(19)	0.0150(18)	0.000	0.000	0.0027(16)
N(2)	0.0203(19)	0.025(2)	0.0138(17)	0.000	0.000	–0.0023(15)
O(1)	0.0429(19)	0.0470(19)	0.068(2)	–0.0013(17)	0.0171(17)	–0.0127(15)
O(2)	0.090(3)	0.0457(18)	0.0280(16)	0.0088(14)	–0.0163(16)	0.0004(18)
O(3)	0.0255(14)	0.0443(16)	0.0438(16)	0.0008(13)	–0.0061(12)	0.0104(12)
O(4)	0.0432(16)	0.0426(16)	0.0223(13)	–0.0086(12)	–0.0007(11)	0.0030(13)
C(1)	0.040(2)	0.0293(19)	0.0306(19)	0.0015(15)	0.0077(16)	–0.0046(16)
C(2)	0.048(2)	0.0255(19)	0.0262(19)	0.0020(14)	–0.0036(17)	0.0015(16)
C(3)	0.036(3)	0.023(3)	0.096(6)	0.000	0.000	0.007(2)
C(4)	0.032(4)	0.031(4)	0.035(4)	0.000(3)	0.000(3)	0.008(3)
C(5)	0.033(3)	0.026(3)	0.043(3)	0.000	0.000	0.007(2)
C(6)	0.0297(18)	0.0323(19)	0.0270(18)	–0.0106(15)	–0.0033(14)	0.0003(15)
C(7)	0.038(2)	0.042(2)	0.0273(19)	–0.0005(16)	–0.0076(16)	0.0008(17)
C(8)	0.039(2)	0.063(3)	0.032(2)	–0.011(2)	–0.0115(18)	0.003(2)
C(9)	0.046(3)	0.054(3)	0.067(3)	–0.029(3)	–0.019(2)	–0.002(2)
C(10)	0.062(3)	0.033(3)	0.115(5)	–0.015(3)	–0.034(3)	–0.008(2)
C(11)	0.050(3)	0.032(2)	0.080(4)	–0.008(2)	–0.027(3)	0.001(2)
C(12)	0.0363(19)	0.0261(18)	0.0202(16)	0.0000(13)	0.0025(14)	0.0076(15)
C(13)	0.051(3)	0.046(2)	0.0218(18)	–0.0038(17)	0.0007(17)	0.010(2)
C(14)	0.072(3)	0.056(3)	0.025(2)	–0.0077(19)	0.010(2)	0.013(3)
C(15)	0.058(3)	0.051(3)	0.041(3)	0.004(2)	0.023(2)	0.019(2)
C(16)	0.037(2)	0.059(3)	0.046(3)	0.004(2)	0.012(2)	0.014(2)
C(17)	0.036(2)	0.043(2)	0.030(2)	–0.0023(17)	0.0024(16)	0.0065(17)
C(18)	0.0234(17)	0.0279(17)	0.0205(16)	–0.0024(13)	–0.0022(12)	–0.0005(13)
C(19)	0.0212(16)	0.0240(17)	0.0232(17)	0.0032(13)	–0.0016(13)	0.0002(12)
C(20)	0.028(2)	0.020(2)	0.029(3)	0.000	0.000	0.0039(19)
C(21)	0.032(4)	0.020(3)	0.034(3)	–0.002(3)	–0.002(3)	0.005(3)
C(22)	0.035(3)	0.014(2)	0.096(6)	0.000	0.000	–0.003(2)
C(23)	0.0195(15)	0.0308(17)	0.0193(15)	0.0003(13)	0.0048(12)	–0.0016(13)
C(24)	0.044(3)	0.050(3)	0.089(4)	–0.034(3)	0.038(3)	–0.022(2)
C(25)	0.048(3)	0.067(4)	0.117(5)	–0.042(4)	0.050(3)	–0.034(3)
C(26)	0.028(2)	0.061(3)	0.039(2)	–0.002(2)	0.0156(17)	–0.0043(19)
C(27)	0.0280(18)	0.043(2)	0.0187(16)	0.0004(15)	0.0030(13)	0.0104(16)
C(28)	0.0210(16)	0.0348(19)	0.0250(17)	–0.0025(14)	0.0003(13)	0.0003(14)
C(29)	0.0271(17)	0.0250(17)	0.0190(16)	0.0033(13)	–0.0030(13)	–0.0008(13)
C(30)	0.0337(19)	0.039(2)	0.0231(18)	0.0014(15)	0.0029(15)	0.0134(16)
C(31)	0.049(3)	0.040(2)	0.035(2)	0.0048(18)	0.0017(19)	0.021(2)
C(32)	0.066(3)	0.039(2)	0.033(2)	0.0124(18)	–0.012(2)	0.009(2)
C(33)	0.121(5)	0.043(3)	0.021(2)	0.0004(18)	–0.020(3)	0.021(3)

C(34)	0.095(4)	0.030(2)	0.0209(19)	–0.0027(16)	–0.011(2)	0.019(2)

Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for str0451.

	x	y	z	U
H(7A)	0.0832	0.4791	0.3459	0.043
H(8A)	0.0039	0.3987	0.2972	0.054
H(9A)	–0.0034	0.2505	0.3163	0.067
H(10A)	0.0674	0.1819	0.3845	0.084
H(11A)	0.1471	0.2611	0.4344	0.065
H(13A)	0.2000	0.3584	0.2940	0.047
H(14A)	0.2820	0.3158	0.2258	0.061
H(15A)	0.3824	0.3327	0.2620	0.060
H(16A)	0.4027	0.3908	0.3661	0.057
H(17A)	0.3224	0.4300	0.4367	0.044
H(24A)	0.0037	0.1674	0.0751	0.073
H(25A)	–0.0944	0.1768	0.1218	0.093
H(26A)	–0.1255	0.3009	0.1776	0.051
H(27A)	–0.0565	0.4139	0.1920	0.036
H(28A)	0.0420	0.4064	0.1454	0.032
H(30A)	0.1712	0.1046	0.0629	0.038
H(31A)	0.2137	0.0076	0.1399	0.050
H(32A)	0.2139	0.0410	0.2527	0.055
H(33A)	0.1667	0.1688	0.2894	0.074
H(34A)	0.1215	0.2636	0.2134	0.058

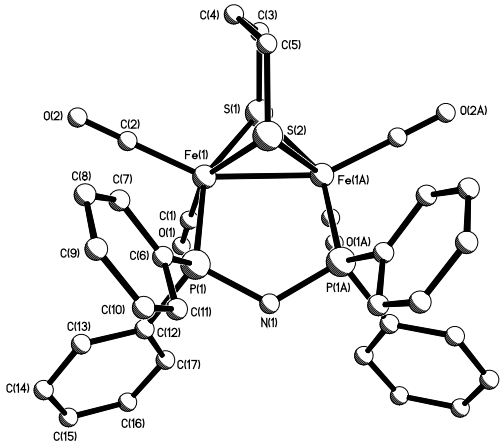
Table 6. Torsion angles [°] for str0451.

C(1)–Fe(1)–P(1)–N(1)	88.8(2)	C(2)–Fe(1)–P(1)–N(1)	−173.0(2)
S(1)–Fe(1)–P(1)–N(1)	0.6(2)	S(2)–Fe(1)–P(1)–N(1)	−67.36(16)
Fe(1A)–Fe(1)–P(1)–N(1)	−11.86(16)	C(1)–Fe(1)–P(1)–C(12)	−26.78(19)
C(2)–Fe(1)–P(1)–C(12)	71.4(2)	S(1)–Fe(1)–P(1)–C(12)	−115.02(16)
S(2)–Fe(1)–P(1)–C(12)	177.04(14)	Fe(1A)–Fe(1)–P(1)–C(12)	−127.45(14)
C(1)–Fe(1)–P(1)–C(6)	−149.23(19)	C(2)–Fe(1)–P(1)–C(6)	−51.1(2)
S(1)–Fe(1)–P(1)–C(6)	122.53(17)	S(2)–Fe(1)–P(1)–C(6)	54.59(14)
Fe(1A)–Fe(1)–P(1)–C(6)	110.10(14)	C(18)–Fe(2)–P(2)–N(2)	−88.35(18)
C(19)–Fe(2)–P(2)–N(2)	173.05(18)	S(3)–Fe(2)–P(2)–N(2)	68.13(14)
S(4)–Fe(2)–P(2)–N(2)	−1.79(18)	Fe(2B)–Fe(2)–P(2)–N(2)	12.46(14)
C(18)–Fe(2)–P(2)–C(29)	29.67(17)	C(19)–Fe(2)–P(2)–C(29)	−68.94(17)
S(3)–Fe(2)–P(2)–C(29)	−173.85(13)	S(4)–Fe(2)–P(2)–C(29)	116.23(15)
Fe(2B)–Fe(2)–P(2)–C(29)	130.48(13)	C(18)–Fe(2)–P(2)–C(23)	148.79(17)
C(19)–Fe(2)–P(2)–C(23)	50.19(17)	S(3)–Fe(2)–P(2)–C(23)	−54.73(13)
S(4)–Fe(2)–P(2)–C(23)	−124.65(15)	Fe(2B)–Fe(2)–P(2)–C(23)	−110.40(13)
C(1)–Fe(1)–S(1)–C(3)	150.52(19)	C(2)–Fe(1)–S(1)–C(3)	53.2(2)
P(1)–Fe(1)–S(1)–C(3)	−120.29(16)	S(2)–Fe(1)–S(1)–C(3)	−52.41(14)
Fe(1A)–Fe(1)–S(1)–C(3)	−105.43(14)	C(1)–Fe(1)–S(1)–Fe(1A)	−104.05(13)
C(2)–Fe(1)–S(1)–Fe(1A)	158.64(15)	P(1)–Fe(1)–S(1)–Fe(1A)	−14.86(12)
S(2)–Fe(1)–S(1)–Fe(1A)	53.02(4)	C(1)–Fe(1)–S(2)–C(5)	127.0(4)
C(2)–Fe(1)–S(2)–C(5)	−50.55(18)	P(1)–Fe(1)–S(2)–C(5)	−151.43(13)
S(1)–Fe(1)–S(2)–C(5)	54.45(13)	Fe(1A)–Fe(1)–S(2)–C(5)	107.38(13)
C(1)–Fe(1)–S(2)–Fe(1A)	19.6(3)	C(2)–Fe(1)–S(2)–Fe(1A)	−157.93(13)
P(1)–Fe(1)–S(2)–Fe(1A)	101.18(3)	S(1)–Fe(1)–S(2)–Fe(1A)	−52.94(4)
C(18)–Fe(2)–S(3)–C(20)	−126.4(3)	C(19)–Fe(2)–S(3)–C(20)	52.67(16)
P(2)–Fe(2)–S(3)–C(20)	152.88(11)	S(4)–Fe(2)–S(3)–C(20)	−53.92(11)
Fe(2B)–Fe(2)–S(3)–C(20)	−107.12(11)	C(18)–Fe(2)–S(3)–Fe(2B)	−19.3(3)
C(19)–Fe(2)–S(3)–Fe(2B)	159.79(11)	P(2)–Fe(2)–S(3)–Fe(2B)	−100.00(3)
S(4)–Fe(2)–S(3)–Fe(2B)	53.21(3)	C(18)–Fe(2)–S(4)–C(22)	−149.75(17)
C(19)–Fe(2)–S(4)–C(22)	−51.48(18)	P(2)–Fe(2)–S(4)–C(22)	123.20(15)
S(3)–Fe(2)–S(4)–C(22)	52.95(13)	Fe(2B)–Fe(2)–S(4)–C(22)	106.13(13)
C(18)–Fe(2)–S(4)–Fe(2B)	104.12(11)	C(19)–Fe(2)–S(4)–Fe(2B)	−157.62(11)
P(2)–Fe(2)–S(4)–Fe(2B)	17.07(10)	S(3)–Fe(2)–S(4)–Fe(2B)	−53.18(3)
C(12)–P(1)–N(1)–P(1A)	150.5(3)	C(6)–P(1)–N(1)–P(1A)	−104.1(3)
Fe(1)–P(1)–N(1)–P(1A)	24.7(3)	C(29)–P(2)–N(2)–P(2B)	−150.3(2)
C(23)–P(2)–N(2)–P(2B)	105.1(2)	Fe(2)–P(2)–N(2)–P(2B)	−25.2(3)
C(2)–Fe(1)–C(1)–O(1)	124(12)	P(1)–Fe(1)–C(1)–O(1)	−134(12)
S(1)–Fe(1)–C(1)–O(1)	18(12)	S(2)–Fe(1)–C(1)–O(1)	−54(12)
Fe(1A)–Fe(1)–C(1)–O(1)	−37(12)	C(1)–Fe(1)–C(2)–O(2)	−44(13)
P(1)–Fe(1)–C(2)–O(2)	−137(13)	S(1)–Fe(1)–C(2)–O(2)	46(13)
S(2)–Fe(1)–C(2)–O(2)	135(13)	Fe(1A)–Fe(1)–C(2)–O(2)	90(13)
Fe(1)–S(1)–C(3)–C(4A)	65.1(4)	Fe(1A)–S(1)–C(3)–C(4A)	−7.8(5)
Fe(1)–S(1)–C(3)–C(4)	7.8(5)	Fe(1A)–S(1)–C(3)–C(4)	−65.1(4)
S(1)–C(3)–C(4)–C(4A)	104.6(4)	C(4A)–C(3)–C(4)–C(5)	−43.6(6)
S(1)–C(3)–C(4)–C(5)	61.0(7)	C(3)–C(4)–C(5)–C(4A)	42.7(6)
C(4A)–C(4)–C(5)–S(2)	−100.6(3)	C(3)–C(4)–C(5)–S(2)	−57.9(6)
Fe(1A)–S(2)–C(5)–C(4A)	12.2(4)	Fe(1)–S(2)–C(5)–C(4A)	−62.1(3)
Fe(1A)–S(2)–C(5)–C(4)	62.1(3)	Fe(1)–S(2)–C(5)–C(4)	−12.2(4)
N(1)–P(1)–C(6)–C(11)	−33.2(4)	C(12)–P(1)–C(6)–C(11)	71.9(4)
Fe(1)–P(1)–C(6)–C(11)	−157.6(4)	N(1)–P(1)–C(6)–C(7)	150.1(3)

C(12)–P(1)–C(6)–C(7)	−104.8(3)	Fe(1)–P(1)–C(6)–C(7)	25.8(4)
C(11)–C(6)–C(7)–C(8)	−1.9(6)	P(1)–C(6)–C(7)–C(8)	174.8(3)
C(6)–C(7)–C(8)–C(9)	0.6(7)	C(7)–C(8)–C(9)–C(10)	0.5(8)
C(8)–C(9)–C(10)–C(11)	−0.3(10)	C(7)–C(6)–C(11)–C(10)	2.1(8)
P(1)–C(6)–C(11)–C(10)	−174.6(5)	C(9)–C(10)–C(11)–C(6)	−1.0(10)
N(1)–P(1)–C(12)–C(13)	133.8(3)	C(6)–P(1)–C(12)–C(13)	24.9(4)
Fe(1)–P(1)–C(12)–C(13)	−105.5(3)	N(1)–P(1)–C(12)–C(17)	−51.5(4)
C(6)–P(1)–C(12)–C(17)	−160.4(3)	Fe(1)–P(1)–C(12)–C(17)	69.2(3)
C(17)–C(12)–C(13)–C(14)	1.0(6)	P(1)–C(12)–C(13)–C(14)	175.8(4)
C(12)–C(13)–C(14)–C(15)	−1.2(7)	C(13)–C(14)–C(15)–C(16)	0.2(8)
C(14)–C(15)–C(16)–C(17)	0.8(8)	C(15)–C(16)–C(17)–C(12)	−0.9(7)
C(13)–C(12)–C(17)–C(16)	0.0(6)	P(1)–C(12)–C(17)–C(16)	−174.9(3)
C(19)–Fe(2)–C(18)–O(3)	−103(17)	P(2)–Fe(2)–C(18)–O(3)	156(17)
S(3)–Fe(2)–C(18)–O(3)	76(17)	S(4)–Fe(2)–C(18)–O(3)	5(17)
Fe(2B)–Fe(2)–C(18)–O(3)	60(17)	C(18)–Fe(2)–C(19)–O(4)	23(11)
P(2)–Fe(2)–C(19)–O(4)	114(11)	S(3)–Fe(2)–C(19)–O(4)	−157(11)
S(4)–Fe(2)–C(19)–O(4)	−68(11)	Fe(2B)–Fe(2)–C(19)–O(4)	−115(11)
Fe(2)–S(3)–C(20)–C(21)	13.3(4)	Fe(2B)–S(3)–C(20)–C(21)	−61.0(3)
Fe(2)–S(3)–C(20)–C(21B)	61.0(3)	Fe(2B)–S(3)–C(20)–C(21B)	−13.3(4)
S(3)–C(20)–C(21)–C(21B)	100.9(2)	C(21B)–C(20)–C(21)–C(22)	−46.4(6)
S(3)–C(20)–C(21)–C(22)	54.5(6)	C(20)–C(21)–C(22)–C(21B)	46.9(6)
C(21B)–C(21)–C(22)–S(4)	−103.1(3)	C(20)–C(21)–C(22)–S(4)	−56.2(6)
Fe(2B)–S(4)–C(22)–C(21B)	10.8(4)	Fe(2)–S(4)–C(22)–C(21B)	−62.6(4)
Fe(2B)–S(4)–C(22)–C(21)	62.6(4)	Fe(2)–S(4)–C(22)–C(21)	−10.8(4)
N(2)–P(2)–C(23)–C(28)	−144.8(3)	C(29)–P(2)–C(23)–C(28)	108.1(3)
Fe(2)–P(2)–C(23)–C(28)	−18.8(3)	N(2)–P(2)–C(23)–C(24)	38.6(4)
C(29)–P(2)–C(23)–C(24)	−68.5(4)	Fe(2)–P(2)–C(23)–C(24)	164.6(4)
C(28)–C(23)–C(24)–C(25)	−0.2(9)	P(2)–C(23)–C(24)–C(25)	176.5(5)
C(23)–C(24)–C(25)–C(26)	0.8(11)	C(24)–C(25)–C(26)–C(27)	−1.6(10)
C(25)–C(26)–C(27)–C(28)	1.7(7)	C(24)–C(23)–C(28)–C(27)	0.3(6)
P(2)–C(23)–C(28)–C(27)	−176.3(3)	C(26)–C(27)–C(28)–C(23)	−1.1(6)
N(2)–P(2)–C(29)–C(30)	18.0(4)	C(23)–P(2)–C(29)–C(30)	126.6(3)
Fe(2)–P(2)–C(29)–C(30)	−104.5(3)	N(2)–P(2)–C(29)–C(34)	−166.0(4)
C(23)–P(2)–C(29)–C(34)	−57.5(4)	Fe(2)–P(2)–C(29)–C(34)	71.5(4)
C(34)–C(29)–C(30)–C(31)	−0.1(6)	P(2)–C(29)–C(30)–C(31)	175.9(3)
C(29)–C(30)–C(31)–C(32)	−1.4(7)	C(30)–C(31)–C(32)–C(33)	1.7(8)
C(31)–C(32)–C(33)–C(34)	−0.6(9)	C(32)–C(33)–C(34)–C(29)	−0.9(9)
C(30)–C(29)–C(34)–C(33)	1.2(7)	P(2)–C(29)–C(34)–C(33)	−175.0(4)
Cl(1C)–C(40)–Cl(1)–C(40C)	0.000(7)		

Symmetry operations for equivalent atoms

A x,y,−z+1 B x,y,−z C −x+1,−y+1,−z+1



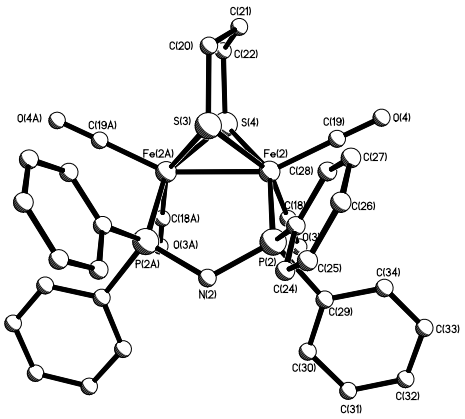


Table 1. Crystal data and structure refinement for **6**.

Identification code	str0954	
Chemical formula	$C_{36}H_{36}BCl_4F_4Fe_2NO_4P_2S_2$	
Formula weight	1013.03	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1/n$	
Unit cell parameters	a = 9.321(3) Å	α = 90°
	b = 31.564(9) Å	β = 100.751(5)°
	c = 13.987(4) Å	γ = 90°
Cell volume	4042.9(19) $Å^3$	
Z	4	
Calculated density	1.664 g/cm^3	
Absorption coefficient μ	1.224 mm^{-1}	
F(000)	2056	
Crystal colour and size	red, 0.40 × 0.20 × 0.20 mm^3	
Data collection method	Bruker SMART 1K CCD diffractometer	
	ω rotation with narrow frames	
θ range for data collection	2.43 to 28.45°	
Index ranges	h −12 to 12, k −41 to 40, l −18 to 18	
Completeness to θ = 26.00°	99.3 %	
Reflections collected	34315	
Independent reflections	9563 (R_{int} = 0.1001)	
Reflections with $F^2>2\sigma$	4650	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.6402 and 0.7918	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0418, 0.0000	
Data / restraints / parameters	9563 / 0 / 509	
Final R indices [$F^2>2\sigma$]	R_1 = 0.0536, wR_2 = 0.0939	
R indices (all data)	R_1 = 0.1164, wR_2 = 0.1019	
Goodness-of-fit on F^2	0.795	
Largest and mean shift/su	0.000 and 0.000	
Largest diff. peak and hole	0.780 and −0.457 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for str0954. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Fe(1)	0.57945(6)	0.129788(17)	0.77916(4)	0.02380(15)
Fe(2)	0.50937(6)	0.052246(17)	0.79004(4)	0.02559(15)
N(1)	0.6885(3)	0.16166(9)	0.6162(2)	0.0224(7)
P(1)	0.77700(11)	0.13938(3)	0.71907(7)	0.0234(2)
P(2)	0.51685(11)	0.15999(3)	0.63756(7)	0.0238(2)
S(1)	0.67680(11)	0.08699(3)	0.89985(7)	0.0257(2)
S(2)	0.36377(11)	0.10786(3)	0.80363(7)	0.0262(2)
C(1)	0.5747(4)	0.17628(13)	0.8426(3)	0.0262(9)
C(2)	0.4330(4)	0.01678(13)	0.8656(3)	0.0284(10)
C(3)	0.6481(5)	0.01557(13)	0.7692(3)	0.0295(10)
C(4)	0.3939(5)	0.03458(12)	0.6791(3)	0.0305(10)
O(1)	0.5607(3)	0.20614(9)	0.8882(2)	0.0390(8)
O(2)	0.3812(3)	–0.00506(9)	0.9129(2)	0.0348(7)
O(3)	0.7291(3)	–0.00877(9)	0.7550(2)	0.0384(8)
O(4)	0.3276(3)	0.02319(9)	0.6086(2)	0.0434(8)
C(5)	0.6110(4)	0.10306(12)	1.0095(3)	0.0290(10)
C(6)	0.4521(4)	0.09612(12)	1.0082(3)	0.0310(10)
C(7)	0.3480(4)	0.11776(12)	0.9293(3)	0.0325(10)
C(8)	0.7352(4)	0.19054(12)	0.5446(3)	0.0269(10)
C(9)	0.8297(5)	0.17199(13)	0.4814(3)	0.0328(10)
C(10)	0.9409(5)	0.19144(14)	0.4599(3)	0.0403(12)
C(11)	0.9233(4)	0.17267(11)	0.7795(3)	0.0233(9)
C(12)	0.9335(4)	0.18084(12)	0.8772(3)	0.0283(10)
C(13)	1.0500(5)	0.20290(13)	0.9283(3)	0.0334(11)
C(14)	1.1557(4)	0.21718(12)	0.8817(3)	0.0291(10)
C(15)	1.1469(4)	0.20965(12)	0.7845(3)	0.0315(10)
C(16)	1.0318(4)	0.18665(12)	0.7337(3)	0.0286(10)
C(17)	0.8710(4)	0.09343(11)	0.6884(3)	0.0239(9)
C(18)	0.9801(4)	0.07583(12)	0.7577(3)	0.0283(10)
C(19)	1.0419(4)	0.03771(13)	0.7407(3)	0.0323(10)
C(20)	0.9990(4)	0.01761(12)	0.6532(3)	0.0317(10)
C(21)	0.8916(4)	0.03401(13)	0.5840(3)	0.0323(10)
C(22)	0.8270(4)	0.07223(12)	0.6015(3)	0.0298(10)
C(23)	0.4536(4)	0.21421(12)	0.6294(3)	0.0232(9)
C(24)	0.3185(4)	0.22672(12)	0.5793(3)	0.0286(10)
C(25)	0.2701(5)	0.26741(13)	0.5874(3)	0.0340(11)
C(26)	0.3559(5)	0.29617(13)	0.6441(3)	0.0354(11)
C(27)	0.4928(5)	0.28510(12)	0.6908(3)	0.0331(11)
C(28)	0.5410(4)	0.24429(12)	0.6838(3)	0.0278(10)
C(29)	0.4010(4)	0.13146(12)	0.5412(3)	0.0241(9)
C(30)	0.2588(4)	0.12399(12)	0.5496(3)	0.0294(10)
C(31)	0.1681(5)	0.10177(12)	0.4800(3)	0.0335(11)
C(32)	0.2192(5)	0.08557(13)	0.4018(3)	0.0385(11)
C(33)	0.3616(5)	0.09219(13)	0.3950(3)	0.0363(11)
C(34)	0.4520(4)	0.11505(11)	0.4636(3)	0.0281(10)
C(40)	0.0247(5)	0.05934(13)	0.0826(3)	0.0438(12)
C(50)	0.9431(8)	0.3204(2)	0.7432(4)	0.093(2)
Cl(1)	0.14573(13)	0.03381(4)	0.01966(9)	0.0478(3)
Cl(2)	0.0698(2)	0.11161(4)	0.10335(12)	0.0898(6)
Cl(3)	0.89189(15)	0.30245(4)	0.62597(9)	0.0560(4)

Cl(4)	0.86910(14)	0.29339(4)	0.82755(9)	0.0536(3)
B(1)	0.7189(6)	0.08011(17)	0.2750(4)	0.0377(13)
F(1)	0.5840(3)	0.06170(9)	0.2494(2)	0.0668(9)
F(2)	0.7669(3)	0.07629(8)	0.37246(18)	0.0650(8)
F(3)	0.8136(3)	0.05972(8)	0.22627(17)	0.0512(7)
F(4)	0.7078(3)	0.12173(8)	0.24931(19)	0.0652(8)

Table 3. Bond lengths [Å] and angles [°] for str0954.

Fe(1)–C(1)	1.720(4)	Fe(1)–P(2)	2.1773(12)
Fe(1)–P(1)	2.1831(13)	Fe(1)–S(2)	2.2124(13)
Fe(1)–S(1)	2.2195(12)	Fe(1)–Fe(2)	2.5451(10)
Fe(2)–C(2)	1.777(5)	Fe(2)–C(3)	1.799(5)
Fe(2)–C(4)	1.805(5)	Fe(2)–S(2)	2.2485(12)
Fe(2)–S(1)	2.2590(12)	N(1)–C(8)	1.479(4)
N(1)–P(1)	1.674(3)	N(1)–P(2)	1.683(3)
P(1)–C(17)	1.788(4)	P(1)–C(11)	1.802(4)
P(1)–P(2)	2.5635(15)	P(2)–C(29)	1.803(4)
P(2)–C(23)	1.807(4)	S(1)–C(5)	1.827(4)
S(2)–C(7)	1.818(4)	C(1)–O(1)	1.159(4)
C(2)–O(2)	1.125(4)	C(3)–O(3)	1.121(4)
C(4)–O(4)	1.120(4)	C(5)–C(6)	1.494(5)
C(6)–C(7)	1.492(5)	C(8)–C(9)	1.479(5)
C(9)–C(10)	1.288(5)	C(11)–C(16)	1.367(5)
C(11)–C(12)	1.377(5)	C(12)–C(13)	1.373(5)
C(13)–C(14)	1.356(5)	C(14)–C(15)	1.366(5)
C(15)–C(16)	1.378(5)	C(17)–C(22)	1.381(5)
C(17)–C(18)	1.384(5)	C(18)–C(19)	1.374(5)
C(19)–C(20)	1.370(5)	C(20)–C(21)	1.358(5)
C(21)–C(22)	1.390(5)	C(23)–C(24)	1.380(5)
C(23)–C(28)	1.383(5)	C(24)–C(25)	1.373(5)
C(25)–C(26)	1.362(6)	C(26)–C(27)	1.366(6)
C(27)–C(28)	1.374(5)	C(29)–C(34)	1.365(5)
C(29)–C(30)	1.372(5)	C(30)–C(31)	1.359(5)
C(31)–C(32)	1.371(5)	C(32)–C(33)	1.365(6)
C(33)–C(34)	1.360(5)	C(40)–Cl(2)	1.714(4)
C(40)–Cl(1)	1.751(4)	C(50)–Cl(4)	1.702(5)
C(50)–Cl(3)	1.716(5)	B(1)–F(2)	1.358(5)
B(1)–F(4)	1.361(6)	B(1)–F(1)	1.371(6)
B(1)–F(3)	1.372(5)		

C(1)–Fe(1)–P(2)	93.88(13)	C(1)–Fe(1)–P(1)	100.68(13)
P(2)–Fe(1)–P(1)	72.02(4)	C(1)–Fe(1)–S(2)	94.32(13)
P(2)–Fe(1)–S(2)	100.40(4)	P(1)–Fe(1)–S(2)	163.53(5)
C(1)–Fe(1)–S(1)	99.96(13)	P(2)–Fe(1)–S(1)	163.83(5)
P(1)–Fe(1)–S(1)	97.05(4)	S(2)–Fe(1)–S(1)	86.92(4)
C(1)–Fe(1)–Fe(2)	139.28(13)	P(2)–Fe(1)–Fe(2)	116.56(4)
P(1)–Fe(1)–Fe(2)	113.62(4)	S(2)–Fe(1)–Fe(2)	55.88(3)
S(1)–Fe(1)–Fe(2)	56.10(3)	C(2)–Fe(2)–C(3)	94.06(18)
C(2)–Fe(2)–C(4)	94.37(18)	C(3)–Fe(2)–C(4)	89.61(17)
C(2)–Fe(2)–S(2)	97.26(13)	C(3)–Fe(2)–S(2)	168.32(13)
C(4)–Fe(2)–S(2)	92.37(13)	C(2)–Fe(2)–S(1)	101.77(13)
C(3)–Fe(2)–S(1)	89.79(12)	C(4)–Fe(2)–S(1)	163.85(13)
S(2)–Fe(2)–S(1)	85.12(4)	C(2)–Fe(2)–Fe(1)	141.00(13)
C(3)–Fe(2)–Fe(1)	114.13(13)	C(4)–Fe(2)–Fe(1)	111.37(12)
S(2)–Fe(2)–Fe(1)	54.55(3)	S(1)–Fe(2)–Fe(1)	54.64(3)
C(8)–N(1)–P(1)	133.0(2)	C(8)–N(1)–P(2)	123.3(2)
P(1)–N(1)–P(2)	99.60(16)	N(1)–P(1)–C(17)	108.63(16)
N(1)–P(1)–C(11)	111.48(17)	C(17)–P(1)–C(11)	102.92(17)
N(1)–P(1)–Fe(1)	94.21(11)	C(17)–P(1)–Fe(1)	117.80(13)
C(11)–P(1)–Fe(1)	121.28(13)	N(1)–P(1)–P(2)	40.33(11)
C(17)–P(1)–P(2)	124.37(13)	C(11)–P(1)–P(2)	129.11(13)

Fe(1)–P(1)–P(2)	53.89(4)	N(1)–P(2)–C(29)	109.87(17)
N(1)–P(2)–C(23)	105.61(16)	C(29)–P(2)–C(23)	106.45(17)
N(1)–P(2)–Fe(1)	94.17(11)	C(29)–P(2)–Fe(1)	118.87(13)
C(23)–P(2)–Fe(1)	120.07(12)	N(1)–P(2)–P(1)	40.07(10)
C(29)–P(2)–P(1)	126.20(13)	C(23)–P(2)–P(1)	122.61(13)
Fe(1)–P(2)–P(1)	54.10(4)	C(5)–S(1)–Fe(1)	108.42(13)
C(5)–S(1)–Fe(2)	114.09(13)	Fe(1)–S(1)–Fe(2)	69.25(4)
C(7)–S(2)–Fe(1)	109.61(14)	C(7)–S(2)–Fe(2)	112.03(13)
Fe(1)–S(2)–Fe(2)	69.57(4)	O(1)–C(1)–Fe(1)	173.9(4)
O(2)–C(2)–Fe(2)	178.1(4)	O(3)–C(3)–Fe(2)	176.5(4)
O(4)–C(4)–Fe(2)	176.9(4)	C(6)–C(5)–S(1)	115.9(3)
C(7)–C(6)–C(5)	116.7(3)	C(6)–C(7)–S(2)	118.5(3)
N(1)–C(8)–C(9)	116.3(3)	C(10)–C(9)–C(8)	123.1(4)
C(16)–C(11)–C(12)	119.0(4)	C(16)–C(11)–P(1)	122.0(3)
C(12)–C(11)–P(1)	118.7(3)	C(13)–C(12)–C(11)	120.8(4)
C(14)–C(13)–C(12)	119.6(4)	C(13)–C(14)–C(15)	120.4(4)
C(14)–C(15)–C(16)	120.1(4)	C(11)–C(16)–C(15)	120.1(4)
C(22)–C(17)–C(18)	118.7(4)	C(22)–C(17)–P(1)	121.7(3)
C(18)–C(17)–P(1)	119.1(3)	C(19)–C(18)–C(17)	120.5(4)
C(20)–C(19)–C(18)	119.8(4)	C(21)–C(20)–C(19)	120.9(4)
C(20)–C(21)–C(22)	119.4(4)	C(17)–C(22)–C(21)	120.5(4)
C(24)–C(23)–C(28)	118.1(4)	C(24)–C(23)–P(2)	124.0(3)
C(28)–C(23)–P(2)	117.6(3)	C(25)–C(24)–C(23)	120.6(4)
C(26)–C(25)–C(24)	120.3(4)	C(25)–C(26)–C(27)	120.2(4)
C(26)–C(27)–C(28)	119.6(4)	C(27)–C(28)–C(23)	121.1(4)
C(34)–C(29)–C(30)	119.2(4)	C(34)–C(29)–P(2)	122.3(3)
C(30)–C(29)–P(2)	118.4(3)	C(31)–C(30)–C(29)	120.6(4)
C(30)–C(31)–C(32)	120.1(4)	C(33)–C(32)–C(31)	119.0(4)
C(34)–C(33)–C(32)	121.0(4)	C(33)–C(34)–C(29)	120.0(4)
Cl(2)–C(40)–Cl(1)	111.6(2)	Cl(4)–C(50)–Cl(3)	114.9(3)
F(2)–B(1)–F(4)	110.2(4)	F(2)–B(1)–F(1)	109.8(4)
F(4)–B(1)–F(1)	108.6(4)	F(2)–B(1)–F(3)	109.6(4)
F(4)–B(1)–F(3)	110.2(4)	F(1)–B(1)–F(3)	108.4(4)

Table 4. Anisotropic displacement parameters ($Å^2$) for str0954. 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)	0.0280(3)	0.0170(3)	0.0259(3)	–0.0005(3)	0.0039(3)	–0.0001(3)
Fe(2)	0.0298(3)	0.0171(3)	0.0293(3)	–0.0007(3)	0.0039(3)	–0.0002(3)
N(1)	0.0261(19)	0.0158(17)	0.0251(19)	0.0003(14)	0.0042(15)	–0.0005(14)
P(1)	0.0270(6)	0.0178(6)	0.0244(6)	–0.0008(4)	0.0022(5)	0.0007(4)
P(2)	0.0277(6)	0.0179(6)	0.0251(6)	0.0000(4)	0.0033(5)	0.0012(5)
S(1)	0.0302(6)	0.0191(5)	0.0267(6)	0.0002(4)	0.0025(5)	0.0003(4)
S(2)	0.0286(6)	0.0201(5)	0.0302(6)	0.0005(5)	0.0059(5)	0.0006(5)
C(1)	0.027(2)	0.025(2)	0.025(2)	0.0105(19)	0.0021(19)	0.0001(19)
C(2)	0.029(3)	0.023(2)	0.030(2)	–0.0027(19)	–0.004(2)	0.0036(19)
C(3)	0.032(3)	0.026(3)	0.027(2)	–0.002(2)	–0.003(2)	–0.007(2)
C(4)	0.038(3)	0.016(2)	0.040(3)	0.004(2)	0.014(2)	0.0024(19)
O(1)	0.054(2)	0.0244(17)	0.0376(18)	–0.0076(14)	0.0067(15)	0.0047(14)
O(2)	0.047(2)	0.0204(17)	0.0381(18)	0.0022(13)	0.0111(15)	–0.0075(14)
O(3)	0.0403(19)	0.0266(18)	0.050(2)	–0.0055(14)	0.0127(16)	0.0046(15)
O(4)	0.050(2)	0.039(2)	0.037(2)	–0.0056(15)	–0.0028(16)	–0.0053(16)
C(5)	0.039(3)	0.022(2)	0.025(2)	–0.0032(18)	0.004(2)	–0.0035(19)
C(6)	0.040(3)	0.025(2)	0.029(2)	0.0004(18)	0.009(2)	0.0011(19)
C(7)	0.037(3)	0.024(2)	0.038(3)	0.0009(19)	0.013(2)	0.0012(19)
C(8)	0.026(2)	0.022(2)	0.030(2)	0.0021(18)	0.0014(19)	–0.0026(18)
C(9)	0.043(3)	0.026(2)	0.030(3)	0.0048(19)	0.011(2)	0.007(2)
C(10)	0.040(3)	0.037(3)	0.047(3)	0.008(2)	0.014(2)	0.006(2)
C(11)	0.026(2)	0.016(2)	0.028(2)	–0.0013(17)	0.0045(19)	0.0043(17)
C(12)	0.030(3)	0.024(2)	0.030(3)	–0.0008(19)	0.002(2)	–0.0054(19)
C(13)	0.042(3)	0.033(3)	0.026(2)	–0.0068(19)	0.005(2)	–0.007(2)
C(14)	0.027(3)	0.023(2)	0.034(3)	–0.0029(19)	–0.003(2)	–0.0059(19)
C(15)	0.029(3)	0.033(3)	0.032(3)	0.003(2)	0.006(2)	–0.007(2)
C(16)	0.033(3)	0.027(2)	0.027(2)	–0.0030(19)	0.008(2)	–0.0013(19)
C(17)	0.023(2)	0.020(2)	0.028(2)	0.0003(18)	0.0037(19)	–0.0045(17)
C(18)	0.033(3)	0.019(2)	0.031(2)	–0.0033(18)	0.000(2)	–0.0030(19)
C(19)	0.027(2)	0.027(2)	0.040(3)	0.003(2)	0.000(2)	0.0042(19)
C(20)	0.030(3)	0.019(2)	0.048(3)	0.001(2)	0.013(2)	0.0032(19)
C(21)	0.040(3)	0.026(2)	0.031(3)	–0.0070(19)	0.008(2)	0.002(2)
C(22)	0.031(3)	0.027(2)	0.030(2)	0.0005(19)	0.003(2)	–0.0016(19)
C(23)	0.027(2)	0.025(2)	0.019(2)	0.0006(17)	0.0068(18)	0.0008(18)
C(24)	0.037(3)	0.026(2)	0.022(2)	0.0024(18)	0.006(2)	–0.001(2)
C(25)	0.037(3)	0.032(3)	0.034(3)	0.012(2)	0.009(2)	0.009(2)
C(26)	0.048(3)	0.027(3)	0.033(3)	0.007(2)	0.012(2)	0.012(2)
C(27)	0.048(3)	0.020(2)	0.035(3)	0.0006(19)	0.016(2)	–0.006(2)
C(28)	0.037(3)	0.025(2)	0.021(2)	0.0045(18)	0.0048(19)	0.000(2)
C(29)	0.028(2)	0.018(2)	0.025(2)	0.0017(17)	0.0008(18)	0.0020(18)
C(30)	0.031(3)	0.029(2)	0.029(2)	–0.0004(19)	0.006(2)	0.003(2)
C(31)	0.029(3)	0.026(2)	0.044(3)	0.003(2)	0.004(2)	–0.001(2)
C(32)	0.042(3)	0.032(3)	0.037(3)	–0.006(2)	–0.004(2)	–0.007(2)
C(33)	0.042(3)	0.034(3)	0.032(3)	–0.007(2)	0.008(2)	0.000(2)
C(34)	0.030(2)	0.018(2)	0.037(3)	0.0001(19)	0.008(2)	–0.0005(18)
C(40)	0.039(3)	0.037(3)	0.057(3)	0.002(2)	0.015(2)	0.007(2)
C(50)	0.138(6)	0.091(5)	0.048(4)	–0.018(3)	0.017(4)	–0.067(4)
Cl(1)	0.0480(8)	0.0434(7)	0.0552(8)	–0.0063(6)	0.0180(6)	–0.0056(6)

Cl(2)	0.1294(14)	0.0358(8)	0.1222(14)	–0.0125(8)	0.0701(12)	–0.0068(8)
Cl(3)	0.0784(10)	0.0400(8)	0.0489(8)	–0.0013(6)	0.0101(7)	–0.0066(7)
Cl(4)	0.0690(9)	0.0417(8)	0.0466(8)	0.0009(6)	0.0017(7)	–0.0064(6)
B(1)	0.049(4)	0.034(3)	0.031(3)	–0.003(2)	0.011(3)	0.002(3)
F(1)	0.061(2)	0.074(2)	0.072(2)	–0.0267(16)	0.0299(17)	–0.0171(16)
F(2)	0.113(2)	0.0512(18)	0.0276(15)	–0.0005(13)	0.0038(15)	0.0042(17)
F(3)	0.0495(17)	0.0540(18)	0.0498(17)	–0.0068(13)	0.0088(14)	0.0183(13)
F(4)	0.100(2)	0.0273(16)	0.069(2)	0.0110(13)	0.0168(17)	0.0104(15)

Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for str0954.

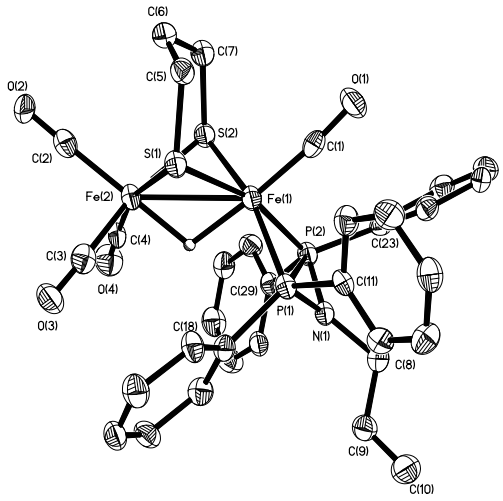
	x	y	z	U
H(1)	0.566(4)	0.0835(12)	0.717(3)	0.051(12)
H(5A)	0.6673	0.0874	1.0655	0.035
H(5B)	0.6324	0.1336	1.0208	0.035
H(6A)	0.4328	0.0653	1.0030	0.037
H(6B)	0.4305	0.1056	1.0715	0.037
H(7A)	0.3578	0.1487	0.9407	0.039
H(7B)	0.2478	0.1098	0.9365	0.039
H(8A)	0.7878	0.2147	0.5804	0.032
H(8B)	0.6466	0.2021	0.5024	0.032
H(9A)	0.8072	0.1444	0.4555	0.039
H(10A)	0.9654	0.2190	0.4850	0.048
H(10B)	0.9983	0.1782	0.4191	0.048
H(12A)	0.8589	0.1711	0.9098	0.034
H(13A)	1.0565	0.2081	0.9958	0.040
H(14A)	1.2364	0.2325	0.9168	0.035
H(15A)	1.2201	0.2203	0.7520	0.038
H(16A)	1.0279	0.1805	0.6668	0.034
H(18A)	1.0125	0.0902	0.8175	0.034
H(19A)	1.1143	0.0253	0.7896	0.039
H(20A)	1.0449	–0.0081	0.6408	0.038
H(21A)	0.8610	0.0195	0.5242	0.039
H(22A)	0.7520	0.0838	0.5533	0.036
H(24A)	0.2584	0.2070	0.5388	0.034
H(25A)	0.1762	0.2755	0.5534	0.041
H(26A)	0.3205	0.3240	0.6512	0.042
H(27A)	0.5544	0.3055	0.7279	0.040
H(28A)	0.6358	0.2366	0.7169	0.033
H(30A)	0.2235	0.1345	0.6045	0.035
H(31A)	0.0691	0.0975	0.4855	0.040
H(32A)	0.1564	0.0700	0.3530	0.046
H(33A)	0.3982	0.0806	0.3416	0.044
H(34A)	0.5507	0.1196	0.4576	0.034
H(40A)	–0.0757	0.0573	0.0443	0.053
H(40B)	0.0264	0.0449	0.1456	0.053
H(50A)	1.0508	0.3188	0.7615	0.111
H(50B)	0.9151	0.3506	0.7453	0.111

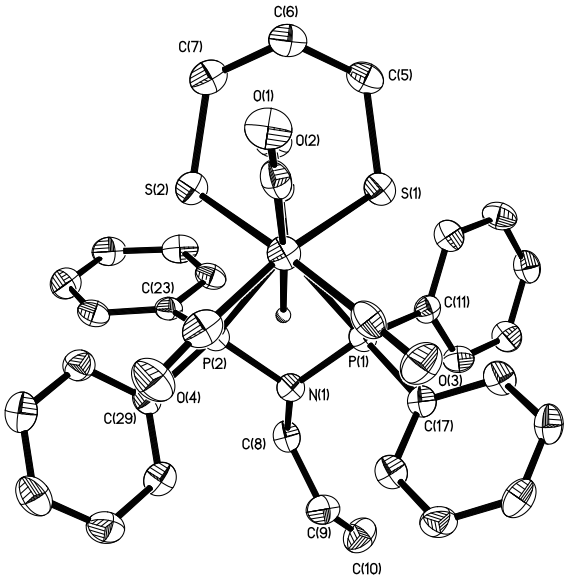
Table 6. Torsion angles [°] for str0954.

C(1)–Fe(1)–Fe(2)–C(2)	−1.1(3)	P(2)–Fe(1)–Fe(2)–C(2)	−135.3(2)
P(1)–Fe(1)–Fe(2)–C(2)	143.8(2)	S(2)–Fe(1)–Fe(2)–C(2)	−50.8(2)
S(1)–Fe(1)–Fe(2)–C(2)	61.4(2)	C(1)–Fe(1)–Fe(2)–C(3)	−133.7(2)
P(2)–Fe(1)–Fe(2)–C(3)	92.12(14)	P(1)–Fe(1)–Fe(2)–C(3)	11.22(14)
S(2)–Fe(1)–Fe(2)–C(3)	176.68(14)	S(1)–Fe(1)–Fe(2)–C(3)	−71.16(14)
C(1)–Fe(1)–Fe(2)–C(4)	126.7(2)	P(2)–Fe(1)–Fe(2)–C(4)	−7.51(15)
P(1)–Fe(1)–Fe(2)–C(4)	−88.41(14)	S(2)–Fe(1)–Fe(2)–C(4)	77.05(14)
S(1)–Fe(1)–Fe(2)–C(4)	−170.80(14)	C(1)–Fe(1)–Fe(2)–S(2)	49.6(2)
P(2)–Fe(1)–Fe(2)–S(2)	−84.56(5)	P(1)–Fe(1)–Fe(2)–S(2)	−165.46(5)
S(1)–Fe(1)–Fe(2)–S(2)	112.15(5)	C(1)–Fe(1)–Fe(2)–S(1)	−62.5(2)
P(2)–Fe(1)–Fe(2)–S(1)	163.29(5)	P(1)–Fe(1)–Fe(2)–S(1)	82.38(5)
S(2)–Fe(1)–Fe(2)–S(1)	−112.15(5)	C(8)–N(1)–P(1)–C(17)	−81.7(3)
P(2)–N(1)–P(1)–C(17)	121.55(17)	C(8)–N(1)–P(1)–C(11)	31.0(4)
P(2)–N(1)–P(1)–C(11)	−125.72(17)	C(8)–N(1)–P(1)–Fe(1)	157.0(3)
P(2)–N(1)–P(1)–Fe(1)	0.33(13)	C(8)–N(1)–P(1)–P(2)	156.7(4)
C(1)–Fe(1)–P(1)–N(1)	−90.90(16)	P(2)–Fe(1)–P(1)–N(1)	−0.26(10)
S(2)–Fe(1)–P(1)–N(1)	64.4(2)	S(1)–Fe(1)–P(1)–N(1)	167.52(11)
Fe(2)–Fe(1)–P(1)–N(1)	111.52(11)	C(1)–Fe(1)–P(1)–C(17)	155.45(19)
P(2)–Fe(1)–P(1)–C(17)	−113.91(15)	S(2)–Fe(1)–P(1)–C(17)	−49.3(2)
S(1)–Fe(1)–P(1)–C(17)	53.88(15)	Fe(2)–Fe(1)–P(1)–C(17)	−2.12(15)
C(1)–Fe(1)–P(1)–C(11)	27.42(19)	P(2)–Fe(1)–P(1)–C(11)	118.06(15)
S(2)–Fe(1)–P(1)–C(11)	−177.30(19)	S(1)–Fe(1)–P(1)–C(11)	−74.16(15)
Fe(2)–Fe(1)–P(1)–C(11)	−130.15(14)	C(1)–Fe(1)–P(1)–P(2)	−90.64(13)
S(2)–Fe(1)–P(1)–P(2)	64.64(16)	S(1)–Fe(1)–P(1)–P(2)	167.78(5)
Fe(2)–Fe(1)–P(1)–P(2)	111.79(4)	C(8)–N(1)–P(2)–C(29)	77.2(3)
P(1)–N(1)–P(2)–C(29)	−123.08(17)	C(8)–N(1)–P(2)–C(23)	−37.3(3)
P(1)–N(1)–P(2)–C(23)	122.49(17)	C(8)–N(1)–P(2)–Fe(1)	−160.1(3)
P(1)–N(1)–P(2)–Fe(1)	−0.33(13)	C(8)–N(1)–P(2)–P(1)	−159.7(4)
C(1)–Fe(1)–P(2)–N(1)	100.24(17)	P(1)–Fe(1)–P(2)–N(1)	0.26(10)
S(2)–Fe(1)–P(2)–N(1)	−164.64(11)	S(1)–Fe(1)–P(2)–N(1)	−48.7(2)
Fe(2)–Fe(1)–P(2)–N(1)	−107.72(11)	C(1)–Fe(1)–P(2)–C(29)	−144.3(2)
P(1)–Fe(1)–P(2)–C(29)	115.69(15)	S(2)–Fe(1)–P(2)–C(29)	−49.21(16)
S(1)–Fe(1)–P(2)–C(29)	66.7(2)	Fe(2)–Fe(1)–P(2)–C(29)	7.71(16)
C(1)–Fe(1)–P(2)–C(23)	−10.5(2)	P(1)–Fe(1)–P(2)–C(23)	−110.46(15)
S(2)–Fe(1)–P(2)–C(23)	84.63(15)	S(1)–Fe(1)–P(2)–C(23)	−159.4(2)
Fe(2)–Fe(1)–P(2)–C(23)	141.56(15)	C(1)–Fe(1)–P(2)–P(1)	99.98(13)
S(2)–Fe(1)–P(2)–P(1)	−164.90(5)	S(1)–Fe(1)–P(2)–P(1)	−48.96(17)
Fe(2)–Fe(1)–P(2)–P(1)	−107.98(4)	C(17)–P(1)–P(2)–N(1)	−78.0(2)
C(11)–P(1)–P(2)–N(1)	76.8(2)	Fe(1)–P(1)–P(2)–N(1)	−179.59(16)
N(1)–P(1)–P(2)–C(29)	77.5(2)	C(17)–P(1)–P(2)–C(29)	−0.5(2)
C(11)–P(1)–P(2)–C(29)	154.4(2)	Fe(1)–P(1)–P(2)–C(29)	−102.04(17)
N(1)–P(1)–P(2)–C(23)	−74.7(2)	C(17)–P(1)–P(2)–C(23)	−152.7(2)
C(11)–P(1)–P(2)–C(23)	2.1(2)	Fe(1)–P(1)–P(2)–C(23)	105.74(15)
N(1)–P(1)–P(2)–Fe(1)	179.59(16)	C(17)–P(1)–P(2)–Fe(1)	101.56(16)
C(11)–P(1)–P(2)–Fe(1)	−103.60(18)	C(1)–Fe(1)–S(1)–C(5)	34.51(19)
P(2)–Fe(1)–S(1)–C(5)	−177.00(19)	P(1)–Fe(1)–S(1)–C(5)	136.71(14)
S(2)–Fe(1)–S(1)–C(5)	−59.34(14)	Fe(2)–Fe(1)–S(1)–C(5)	−109.50(14)
C(1)–Fe(1)–S(1)–Fe(2)	144.01(13)	P(2)–Fe(1)–S(1)–Fe(2)	−67.50(17)
P(1)–Fe(1)–S(1)–Fe(2)	−113.79(4)	S(2)–Fe(1)–S(1)–Fe(2)	50.16(4)
C(2)–Fe(2)–S(1)–C(5)	−44.06(19)	C(3)–Fe(2)–S(1)–C(5)	−138.16(19)

C(4)–Fe(2)–S(1)–C(5)	134.0(5)	S(2)–Fe(2)–S(1)–C(5)	52.36(15)
Fe(1)–Fe(2)–S(1)–C(5)	101.58(15)	C(2)–Fe(2)–S(1)–Fe(1)	−145.64(13)
C(3)–Fe(2)–S(1)–Fe(1)	120.26(13)	C(4)–Fe(2)–S(1)–Fe(1)	32.4(5)
S(2)–Fe(2)–S(1)–Fe(1)	−49.22(4)	C(1)–Fe(1)–S(2)–C(7)	−43.13(18)
P(2)–Fe(1)–S(2)–C(7)	−137.88(14)	P(1)–Fe(1)–S(2)–C(7)	161.21(19)
S(1)–Fe(1)–S(2)–C(7)	56.64(14)	Fe(2)–Fe(1)–S(2)–C(7)	106.98(14)
C(1)–Fe(1)–S(2)–Fe(2)	−150.11(13)	P(2)–Fe(1)–S(2)–Fe(2)	115.14(4)
P(1)–Fe(1)–S(2)–Fe(2)	54.23(16)	S(1)–Fe(1)–S(2)–Fe(2)	−50.34(4)
C(2)–Fe(2)–S(2)–C(7)	46.94(19)	C(3)–Fe(2)–S(2)–C(7)	−118.8(6)
C(4)–Fe(2)–S(2)–C(7)	141.65(19)	S(1)–Fe(2)–S(2)–C(7)	−54.34(15)
Fe(1)–Fe(2)–S(2)–C(7)	−103.63(15)	C(2)–Fe(2)–S(2)–Fe(1)	150.57(13)
C(3)–Fe(2)–S(2)–Fe(1)	−15.1(6)	C(4)–Fe(2)–S(2)–Fe(1)	−114.72(13)
S(1)–Fe(2)–S(2)–Fe(1)	49.30(4)	P(2)–Fe(1)–C(1)–O(1)	111(3)
P(1)–Fe(1)–C(1)–O(1)	−176(3)	S(2)–Fe(1)–C(1)–O(1)	10(3)
S(1)–Fe(1)–C(1)–O(1)	−77(3)	Fe(2)–Fe(1)–C(1)–O(1)	−29(3)
C(3)–Fe(2)–C(2)–O(2)	−159(12)	C(4)–Fe(2)–C(2)–O(2)	−69(12)
S(2)–Fe(2)–C(2)–O(2)	24(12)	S(1)–Fe(2)–C(2)–O(2)	111(12)
Fe(1)–Fe(2)–C(2)–O(2)	64(12)	C(2)–Fe(2)–C(3)–O(3)	50(6)
C(4)–Fe(2)–C(3)–O(3)	−44(6)	S(2)–Fe(2)–C(3)–O(3)	−144(6)
S(1)–Fe(2)–C(3)–O(3)	152(6)	Fe(1)–Fe(2)–C(3)–O(3)	−157(6)
C(2)–Fe(2)–C(4)–O(4)	−122(7)	C(3)–Fe(2)–C(4)–O(4)	−28(7)
S(2)–Fe(2)–C(4)–O(4)	140(7)	S(1)–Fe(2)–C(4)–O(4)	60(7)
Fe(1)–Fe(2)–C(4)–O(4)	88(7)	Fe(1)–S(1)–C(5)–C(6)	67.9(3)
Fe(2)–S(1)–C(5)–C(6)	−7.1(3)	S(1)–C(5)–C(6)–C(7)	−58.9(4)
C(5)–C(6)–C(7)–S(2)	56.3(4)	Fe(1)–S(2)–C(7)–C(6)	−62.1(3)
Fe(2)–S(2)–C(7)–C(6)	13.1(4)	P(1)–N(1)–C(8)–C(9)	71.5(5)
P(2)–N(1)–C(8)–C(9)	−136.3(3)	N(1)–C(8)–C(9)–C(10)	−138.4(4)
N(1)–P(1)–C(11)–C(16)	−55.8(4)	C(17)–P(1)–C(11)–C(16)	60.4(4)
Fe(1)–P(1)–C(11)–C(16)	−165.2(3)	P(2)–P(1)–C(11)–C(16)	−98.5(3)
N(1)–P(1)–C(11)–C(12)	130.5(3)	C(17)–P(1)–C(11)–C(12)	−113.2(3)
Fe(1)–P(1)–C(11)–C(12)	21.2(4)	P(2)–P(1)–C(11)–C(12)	87.9(3)
C(16)–C(11)–C(12)–C(13)	0.4(6)	P(1)–C(11)–C(12)–C(13)	174.3(3)
C(11)–C(12)–C(13)–C(14)	0.6(6)	C(12)–C(13)–C(14)–C(15)	−0.1(6)
C(13)–C(14)–C(15)–C(16)	−1.4(6)	C(12)–C(11)–C(16)–C(15)	−2.0(6)
P(1)–C(11)–C(16)–C(15)	−175.6(3)	C(14)–C(15)–C(16)–C(11)	2.5(6)
N(1)–P(1)–C(17)–C(22)	−23.6(4)	C(11)–P(1)–C(17)–C(22)	−141.9(3)
Fe(1)–P(1)–C(17)–C(22)	81.8(3)	P(2)–P(1)–C(17)–C(22)	18.3(4)
N(1)–P(1)–C(17)–C(18)	163.9(3)	C(11)–P(1)–C(17)–C(18)	45.6(3)
Fe(1)–P(1)–C(17)–C(18)	−90.7(3)	P(2)–P(1)–C(17)–C(18)	−154.2(3)
C(22)–C(17)–C(18)–C(19)	−0.9(6)	P(1)–C(17)–C(18)–C(19)	171.9(3)
C(17)–C(18)–C(19)–C(20)	2.3(6)	C(18)–C(19)–C(20)–C(21)	−2.6(6)
C(19)–C(20)–C(21)–C(22)	1.5(6)	C(18)–C(17)–C(22)–C(21)	−0.2(6)
P(1)–C(17)–C(22)–C(21)	−172.8(3)	C(20)–C(21)–C(22)–C(17)	−0.1(6)
N(1)–P(2)–C(23)–C(24)	134.4(3)	C(29)–P(2)–C(23)–C(24)	17.6(4)
Fe(1)–P(2)–C(23)–C(24)	−121.2(3)	P(1)–P(2)–C(23)–C(24)	174.5(3)
N(1)–P(2)–C(23)–C(28)	−51.6(3)	C(29)–P(2)–C(23)–C(28)	−168.3(3)
Fe(1)–P(2)–C(23)–C(28)	52.9(3)	P(1)–P(2)–C(23)–C(28)	−11.4(4)
C(28)–C(23)–C(24)–C(25)	−3.2(6)	P(2)–C(23)–C(24)–C(25)	170.9(3)
C(23)–C(24)–C(25)–C(26)	1.0(6)	C(24)–C(25)–C(26)–C(27)	2.1(6)
C(25)–C(26)–C(27)–C(28)	−2.9(6)	C(26)–C(27)–C(28)–C(23)	0.6(6)
C(24)–C(23)–C(28)–C(27)	2.3(6)	P(2)–C(23)–C(28)–C(27)	−172.1(3)
N(1)–P(2)–C(29)–C(34)	−1.0(4)	C(23)–P(2)–C(29)–C(34)	112.9(3)

Fe(1)–P(2)–C(29)–C(34)	−107.7(3)	P(1)–P(2)–C(29)–C(34)	−42.9(4)
N(1)–P(2)–C(29)–C(30)	175.2(3)	C(23)–P(2)–C(29)–C(30)	−70.9(3)
Fe(1)–P(2)–C(29)–C(30)	68.5(3)	P(1)–P(2)–C(29)–C(30)	133.2(3)
C(34)–C(29)–C(30)–C(31)	−2.2(6)	P(2)–C(29)–C(30)–C(31)	−178.5(3)
C(29)–C(30)–C(31)–C(32)	1.8(6)	C(30)–C(31)–C(32)–C(33)	−0.2(6)
C(31)–C(32)–C(33)–C(34)	−1.0(6)	C(32)–C(33)–C(34)–C(29)	0.6(6)
C(30)–C(29)–C(34)–C(33)	1.0(6)	P(2)–C(29)–C(34)–C(33)	177.1(3)





Parameters for DigiSim simulation:

The following mechanistic steps were input into DigiSim v3, along with the parameters shown to give the simulated CVs shown is Figures 7 b and c in the main text. K_1, k_2, K_2 and k_2 are given in the main document.

$AH^+ + e = AH$	E = -1.5 V	α = 0.5	k = 0.1 cm s^{-1}
$AH_2^+ + e = AH_2$	E = -1.5 V	α = 0.5	k = 0.1 cm s^{-1}
$AH + e = AH^-$	E = -1.8 V	α = 0.5	k = 0.1 cm s^{-1}
$A + e = A^-$	E = -1.5 V	α = 0.5	k = 0.1 cm s^{-1}

$A + H^+ = AH^+$	$K = K_1$	$k = k_1$
$AH + H^+ = AH_2^+$	$K = K_2$	$k = k_2$
$AH_2 = A + H_2$	$K = 1 \times 10^5$	$k = 1 \times 10^5$
$AH^- + H^+ = AH_2$	$K = 1 \times 10^{10}$	$k = 1 \times 10^{10}$
$A^- + H^+ = AH$	$K = 3 \times 10^{17}$	$k = 1 \times 10^{10}$

Figure SI1: Plots of limiting current for first catalytic peak vs. equivalents of acid added for experimental and simulated data a) for complex **2a**; b) for complex **3a**.