Supplementary Material (ESI) for Chemical Communications

Molecular N_2 complexes of iron stabilised by N-heterocyclic 'pincer' dicarbene ligands

Andreas A. Danopoulos, Joseph A. Wright and William B. Motherwell

Department of Chemistry, University of Southampton, Highfield, Southampton, SO17 1BJ, UK; e-mail: ad1@soton.ac.uk

Christopher Ingold Laboratories, University College London, 20 Gordon Str., London, UK, WC1H 0AJ

Supporting Information

Synthetic methodology

All manipulations were carried out under nitrogen using standard Schlenk techniques. All solvents were dried over the usual drying agents and distilled under N_2 prior to use.

Complex **1**

A Fisher-Porter bottle equipped with an efficient stir bar was charged in the glove box with 0.5 g (0.6mmol) of Fe(C-N-C)Br_2.thf and 20g Na/Hg (0.4%w/w, 3.5mmol, excess). After it was taken out, 20cm^3 thf were added at room temperature, it was pressurised with N_2 (80psi), and stirred vigorously at room temperature for 3-4h. During the first few minutes the colour of the solution changed from red-purple to dark green-brown. The solution was decanted from the Hg pool, the thf evaporated under reduced pressure, the residue was dissolved in pentane (50cm^3) and filtered. Concentration of the pentane solution to ca 10cm^3 and slow cooling to -35ºC gave dark green-brown plates of **1** as pentane solvate. Yield: 0.15g, ca 36% based on iron. Alternatively the pentane solution can be evaporated to dryness by passing a slow stream of N_2 over it.

Found: C, 66.45; H, 6.92; N, 18.11. Calculated for $C_{40}H_{53}FeN_9$ requires C, 67.12; H, 7.46; N, 17.61%.

NMR (C_6D_6): ^{1}H, δ 1.09 and 1.25 [d, 12H each, J=6.82Hz, $(CH_3)_2CH$], 3.13(sep., 4H, J=6.82Hz, $(CH_3)_2CH$], 6.71 and 7.44 [s, br, 2H each, imidazol-2-yliden backbone], 6.92 [d, 2H, J=7.60Hz, 3-py], 7.20-7.35[m, 7H, aromatic].

$^{13}C\{^1H\}$, δ, 23.23 and 25.82 [$(CH_3)_2CH$], 28.48[$(CH_3)_2CH$], 99.97, 111.13, 114.98,123.90, 125.53, 129.70, 137.34, 142.24 and 147.58 aromatic carbons, 203.87 (carbene).

IR(Nujol, cm^{-1}): 2109, 2031 and 2044(sh).

Complex **2**.

This was prepared by bubbling a slow steam of CO to a thf solution of complex **1** (50mg), for 5min. The formation of **2** is very fast and accompanied by a change of the colour of the solution from green brown to purple. After evaporation of the volatiles the residue was crystallised by dissolving in ether/light petroleum and cooling to –35°C. X-ray quality crystals were obtained by slow evaporation of benzene solutions. In this case there is one benzene molecule incorporated in the lattice. Yield: 0.050mg.The same product could be obtained by reduction of $Fe(C\text{-}N\text{-}C)Br_2$.thf by Na(Hg) in the presence of CO.

Found: C, 72.50; H, 6.32; N, 8.85. Calculated for $C_{37}H_{45}FeN_7$ requires C, 72.62; H, 6.62; N, 9.20%).

NMR (C_6D_6): ^{1}H, δ 1.19 and 1.48 [d, 12H each, J=6.55Hz, $(CH_3)_2CH$], 3.15(sep., 4H, J=6.55Hz, $(CH_3)_2CH$], 6.80 and 7.45 [s, br, 2H each, imidazol-2-yliden backbone], 7.00 [d, 2H, J=7.60Hz, 3-py], 7.20-7.35[m, 7H, aromatic].

$^{13}C\{^1H\}$, δ, 22.76 and 26.24 [$(CH_3)_2CH$], 28.32[$(CH_3)_2CH$], 99.54, 111.18, 119.15,124.10, 125.54, 129.92, 137.10, 142.59 and 147.40 aromatic carbons, 210.43 (carbene), 215.57(CO).

IR(Nujol, cm^{-1}): 1928, 1865.

Complex **3**.

A solution of **1** (0.05g, 0.08mmol) in thf (20cm^3) in a Fisher Porter bottle was pressurised with ethene (80 psi) and the solution was stirred at room temperature for 12h. It was re-pressurised periodically if necessary. After the end of the reaction the

solution was transferred to a Schlenk tube and the volatiles were removed under reduced pressure. The solid residue was extracted into light petroleum ($50cm^3$) , filtered, concentrated to ca $10cm^3$ and left for crystallisation at room temperature. The product appears as red-brown air sensitive blocks after a few days. Additional crop can be obtained by cooling the supernatant at 1° C. Yield: 0.040g, ca 77%.

Found: C, 68.75; H, 6.95; N, 15.55. Calculated for $C_{37}H_{45}FeN_7$ requires C, 69.04; H, 7.05; N, 15.23%).

NMR (C_6D_6): ^{1}H, δ 1.15, 1.20, 1.50 and 1.55 [d, 6H each, J=6.50Hz, $(CH_3)_2CH$], 3.05 and 3.38 (sept., 2H, J=6.55Hz, $(CH_3)_2CH$], 1.85(s, 4H, C_2H_4), 6.80 and 7.50 [s, br, 2H each, imidazol-2-yliden backbone], 7.10 [d, 2H, J=7.60Hz, 3-py], 7.20-7.35[m, 7H, aromatic].

$^{13}C\{^1H\}$, δ, 21.80, 22.00, 26.24, 26.82, $[(CH_3)_2CH]$, 28.15 and 28.79 $[(CH_3)_2CH]$, 36.84$[C_2H_4]$, 99.10, 111.05, 123.09, 124.03, 126.11, 137.10, 145.17, 146.88, 147.66 aromatic carbons, 210.78 (carbene).

IR(Nujol, cm^{-1}): 2056.

Complex **4a**.

To a solution of **1** (0.050g, 0.08mmol) in thf ($20cm^3$) was added PMe_3 ($0.1cm^3$, excess) and the mixture was stirred at room temperature for 2 h. Removal of the volatiles under reduced pressure, extraction of the residue to ether ($10cm^3$), concentration of the ether extracts to *ca* $1cm^3$, and cooling to –35° C gave **4a** as green brown air sensitive blocks. There is one molecule of ether incorporated in the crystal lattice.

The same product can be obtained by reduction of Fe(C-N-C)Br_2.thf with Na(Hg) in thf in the presence of excess of PMe_3. The yield is comparable to the previous variant of the method.

Found: C, 65.34; H, 7.10; N, 12.25. Calculated for $C_{42}H_{60}FeN_7OP$ requires C, 65.87; H, 7.89; N, 12.80%).

NMR (C_6D_6): ^{1}H, δ 0.25 (d, 9H, P(C*H*$_3$)$_3$], 0.95, 1.00, 1.20 and 1.30[d, 6H each, J=6.50Hz, (C*H*$_3$)$_2$CH], 3.05 and 3.38 (sept., 2H, J=6.50Hz, (CH$_3$)$_2$C*H*], 6.80 and 7.40 [d, 2H each, imidazol-2-yliden backbone], 7.10 [d, 2H, J=7.60Hz, 3-py], 7.20-7.35[m, 7H, aromatic].

^{13}C{^{1}H}, δ, 20.78 [d, P(*C*H$_3$)$_3$], 22.74, 23.27, 24.31, 25.39, [(*C*H$_3$)$_2$CH], 28.15 and 28.29 [(CH$_3$)$_2$*C*H], 97.48, 97.53, 109.34, 112.32, 112.40, 123.12, 124.26, 126.17, 138.46, 139.69, 145.97, 148.94 aromatic carbons, 208.56 (carbene).

^{31}P{^{1}H}, δ 20.07.

IR(Nujol, cm^{-1}): 2032.

Complex **4b**

This was prepared by a method analogous to **4a** using PCy_3 instead of PMe_3. Crystallisation was carried out from light petroleum.

NMR (C_6D_6): ^{1}H, δ 0.95, 1.00, 1.20 and 1.30[d, 6H each, (C*H*$_3$)$_2$CH], 3.05 and 3.38 (sept., 2H, (CH$_3$)$_2$C*H*], 1.5-1.8 (m, *ca*. 33H, C_6H_{11}), 6.80 and 7.40 [d, 2H each, imidazol-2-yliden backbone], 7.10 [d, 2H, J=7.60Hz, 3-py], 7.20-7.35[m, 7H, aromatic].

^{31}P{^{1}H}, δ 53.80.

IR(Nujol, cm^{-1}): 2012.

Structural data for 1

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

Identification code	Complex **1**	
Empirical formula	C40 H53 Fe N9	
Formula weight	715.76	
Temperature	120(2) K	
Wavelength	0.71073 ≈	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.7070(17) ≈	α= 73.78(2)∞.
	b = 15.226(3) ≈	β= 79.44(2)∞.
	c = 15.788(5) ≈	γ = 76.978(16)∞.
Volume	1941.8(8) ≈^{3}	
Z	2	
Density (calculated)	1.224 Mg/m^3	
Absorption coefficient	0.428 mm^{-1}	
F(000)	764	
Crystal size	0.60 x 0.25 x 0.01 mm^3	
Theta range for data collection	3.02 to 27.66∞.	
Index ranges	-11<=h<=11, -19<=k<=19, -20<=l<=20	
Reflections collected	34076	
Independent reflections	8972 [R(int) = 0.0698]	
Completeness to theta = 27.66∞	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9957 and 0.7412	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8972 / 0 / 461	
Goodness-of-fit on F^2	1.016	
Final R indices [I>2sigma(I)]	R1 = 0.0583, wR2 = 0.1081	
R indices (all data)	R1 = 0.1035, wR2 = 0.1221	
Largest diff. peak and hole	1.058 and -0.615 e.≈$^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (≈^{2}x 10^3) for **1.** U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8124(3)	573(2)	3335(2)	21(1)
C(2)	9230(3)	1550(2)	2037(2)	17(1)
C(3)	8342(3)	1078(2)	991(2)	23(1)
C(4)	7823(3)	554(2)	1778(2)	24(1)
C(5)	9849(3)	2392(2)	464(2)	17(1)
C(6)	11468(3)	2234(2)	153(2)	20(1)
C(7)	12059(3)	2941(2)	-500(2)	27(1)
C(8)	11072(3)	3773(2)	-828(2)	30(1)
C(9)	9475(3)	3916(2)	-504(2)	27(1)
C(10)	8829(3)	3224(2)	150(2)	22(1)
C(11)	7074(3)	3403(2)	502(2)	25(1)
C(12)	6062(3)	3506(2)	-224(2)	39(1)
C(13)	6632(4)	4251(2)	890(2)	41(1)
C(14)	12524(3)	1305(2)	492(2)	24(1)
C(15)	12583(4)	660(2)	-106(2)	36(1)
C(16)	14201(3)	1398(2)	569(2)	34(1)
C(17)	7285(3)	-81(2)	3886(2)	27(1)
C(18)	7144(3)	-187(2)	4803(2)	29(1)
C(19)	7812(3)	373(2)	5136(2)	25(1)
C(20)	8615(3)	1017(2)	4543(2)	20(1)
C(21)	9961(3)	2276(2)	3972(2)	19(1)
C(22)	9996(3)	2670(2)	5264(2)	27(1)
C(23)	9314(3)	1916(2)	5496(2)	27(1)
C(24)	10954(3)	3719(2)	3826(2)	20(1)
C(25)	12562(3)	3660(2)	3483(2)	21(1)
C(26)	13051(3)	4480(2)	2969(2)	24(1)
C(27)	11983(3)	5311(2)	2807(2)	28(1)
C(28)	10394(3)	5347(2)	3149(2)	25(1)
C(29)	9839(3)	4549(2)	3666(2)	21(1)
C(30)	8084(3)	4596(2)	4019(2)	25(1)
C(31)	7069(3)	4910(3)	3261(2)	42(1)
C(32)	7544(3)	5237(3)	4647(2)	44(1)
C(33)	13726(3)	2747(2)	3666(2)	25(1)

C(34)	14971(3)	2632(2)	2865(2)	38(1)
C(35)	14522(4)	2626(2)	4486(2)	46(1)
C(36)	3229(6)	7959(3)	2338(3)	84(2)
C(37)	1641(7)	8592(3)	1901(3)	99(2)
C(38)	372(5)	8048(3)	1988(3)	78(1)
C(39)	4296(9)	8489(4)	2455(4)	130(3)
C(40)	5769(7)	7883(4)	2817(4)	100(2)
Fe(1)	10064(1)	1962(1)	2869(1)	17(1)
N(1)	12127(3)	1311(2)	2774(1)	21(1)
N(2)	13332(3)	865(2)	2759(2)	29(1)
N(3)	10391(3)	3082(2)	2141(1)	22(1)
N(4)	10608(3)	3764(2)	1697(2)	35(1)
N(5)	8828(2)	1118(1)	3645(1)	18(1)
N(6)	8373(2)	827(1)	2420(1)	19(1)
N(7)	9203(2)	1671(1)	1146(1)	17(1)
N(8)	9286(2)	1680(2)	4716(1)	20(1)
N(9)	10395(2)	2886(2)	4346(1)	21(1)

Table 3. Bond lengths [≈] and angles [∞] for **1**.

C(1)-N(5)	1.367(3)
C(1)-C(17)	1.376(3)
C(1)-N(6)	1.377(3)
C(2)-N(7)	1.370(3)
C(2)-N(6)	1.402(3)
C(2)-Fe(1)	1.915(3)
C(3)-C(4)	1.338(4)
C(3)-N(7)	1.390(3)
C(3)-H(3)	0.9500
C(4)-N(6)	1.390(3)
C(4)-H(4)	0.9500
C(5)-C(10)	1.394(4)
C(5)-C(6)	1.395(3)
C(5)-N(7)	1.440(3)
C(6)-C(7)	1.387(4)
C(6)-C(14)	1.517(4)
C(7)-C(8)	1.385(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.381(4)
C(8)-H(8)	0.9500
C(9)-C(10)	1.392(4)
C(9)-H(9)	0.9500
C(10)-C(11)	1.518(4)
C(11)-C(12)	1.523(4)
C(11)-C(13)	1.524(4)
C(11)-H(11)	1.0000
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(16)	1.528(4)
C(14)-C(15)	1.529(4)
C(14)-H(14)	1.0000
C(15)-H(15A)	0.9800

C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(18)	1.396(4)
C(17)-H(17)	0.9500
C(18)-C(19)	1.388(4)
C(18)-H(18)	0.9500
C(19)-C(20)	1.373(3)
C(19)-H(19)	0.9500
C(20)-N(5)	1.364(3)
C(20)-N(8)	1.383(3)
C(21)-N(9)	1.379(3)
C(21)-N(8)	1.394(3)
C(21)-Fe(1)	1.912(3)
C(22)-C(23)	1.340(4)
C(22)-N(9)	1.389(3)
C(22)-H(22)	0.9500
C(23)-N(8)	1.382(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.398(3)
C(24)-C(29)	1.400(4)
C(24)-N(9)	1.438(3)
C(25)-C(26)	1.394(4)
C(25)-C(33)	1.513(4)
C(26)-C(27)	1.381(4)
C(26)-H(26)	0.9500
C(27)-C(28)	1.385(4)
C(27)-H(27)	0.9500
C(28)-C(29)	1.394(4)
C(28)-H(28)	0.9500
C(29)-C(30)	1.521(3)
C(30)-C(31)	1.522(4)
C(30)-C(32)	1.523(4)
C(30)-H(30)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800

C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(35)	1.526(4)
C(33)-C(34)	1.529(4)
C(33)-H(33)	1.0000
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-C(39)	1.426(7)
C(36)-C(37)	1.641(7)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-C(38)	1.489(6)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-C(40)	1.505(8)
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
Fe(1)-N(3)	1.820(2)
Fe(1)-N(1)	1.847(2)
Fe(1)-N(5)	1.890(2)
N(1)-N(2)	1.115(3)
N(3)-N(4)	1.113(3)

N(5)-C(1)-C(17)	123.0(2)
N(5)-C(1)-N(6)	108.1(2)
C(17)-C(1)-N(6)	128.9(2)

N(7)-C(2)-N(6)	102.3(2)
N(7)-C(2)-Fe(1)	142.92(18)
N(6)-C(2)-Fe(1)	114.66(17)
C(4)-C(3)-N(7)	108.0(2)
C(4)-C(3)-H(3)	126.0
N(7)-C(3)-H(3)	126.0
C(3)-C(4)-N(6)	106.4(2)
C(3)-C(4)-H(4)	126.8
N(6)-C(4)-H(4)	126.8
C(10)-C(5)-C(6)	122.7(2)
C(10)-C(5)-N(7)	118.5(2)
C(6)-C(5)-N(7)	118.8(2)
C(7)-C(6)-C(5)	117.6(2)
C(7)-C(6)-C(14)	121.4(2)
C(5)-C(6)-C(14)	121.0(2)
C(8)-C(7)-C(6)	121.0(2)
C(8)-C(7)-H(7)	119.5
C(6)-C(7)-H(7)	119.5
C(9)-C(8)-C(7)	120.4(3)
C(9)-C(8)-H(8)	119.8
C(7)-C(8)-H(8)	119.8
C(8)-C(9)-C(10)	120.7(3)
C(8)-C(9)-H(9)	119.7
C(10)-C(9)-H(9)	119.7
C(9)-C(10)-C(5)	117.7(2)
C(9)-C(10)-C(11)	119.6(2)
C(5)-C(10)-C(11)	122.7(2)
C(10)-C(11)-C(12)	110.5(2)
C(10)-C(11)-C(13)	111.5(2)
C(12)-C(11)-C(13)	111.0(2)
C(10)-C(11)-H(11)	107.9
C(12)-C(11)-H(11)	107.9
C(13)-C(11)-H(11)	107.9
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5

H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(6)-C(14)-C(16)	113.1(2)
C(6)-C(14)-C(15)	109.7(2)
C(16)-C(14)-C(15)	110.6(2)
C(6)-C(14)-H(14)	107.8
C(16)-C(14)-H(14)	107.8
C(15)-C(14)-H(14)	107.8
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(1)-C(17)-C(18)	118.2(3)
C(1)-C(17)-H(17)	120.9
C(18)-C(17)-H(17)	120.9
C(19)-C(18)-C(17)	120.1(2)
C(19)-C(18)-H(18)	120.0
C(17)-C(18)-H(18)	120.0
C(20)-C(19)-C(18)	118.2(3)
C(20)-C(19)-H(19)	120.9
C(18)-C(19)-H(19)	120.9
N(5)-C(20)-C(19)	123.4(2)
N(5)-C(20)-N(8)	108.3(2)
C(19)-C(20)-N(8)	128.2(2)
N(9)-C(21)-N(8)	102.0(2)

N(9)-C(21)-Fe(1)	142.84(19)
N(8)-C(21)-Fe(1)	115.05(18)
C(23)-C(22)-N(9)	107.9(2)
C(23)-C(22)-H(22)	126.1
N(9)-C(22)-H(22)	126.1
C(22)-C(23)-N(8)	106.3(2)
C(22)-C(23)-H(23)	126.8
N(8)-C(23)-H(23)	126.8
C(25)-C(24)-C(29)	123.2(2)
C(25)-C(24)-N(9)	118.9(2)
C(29)-C(24)-N(9)	117.9(2)
C(26)-C(25)-C(24)	117.1(2)
C(26)-C(25)-C(33)	121.4(2)
C(24)-C(25)-C(33)	121.5(2)
C(27)-C(26)-C(25)	121.1(2)
C(27)-C(26)-H(26)	119.5
C(25)-C(26)-H(26)	119.5
C(26)-C(27)-C(28)	120.6(3)
C(26)-C(27)-H(27)	119.7
C(28)-C(27)-H(27)	119.7
C(27)-C(28)-C(29)	120.8(3)
C(27)-C(28)-H(28)	119.6
C(29)-C(28)-H(28)	119.6
C(28)-C(29)-C(24)	117.2(2)
C(28)-C(29)-C(30)	120.2(2)
C(24)-C(29)-C(30)	122.6(2)
C(29)-C(30)-C(31)	111.1(2)
C(29)-C(30)-C(32)	111.4(2)
C(31)-C(30)-C(32)	110.2(2)
C(29)-C(30)-H(30)	108.0
C(31)-C(30)-H(30)	108.0
C(32)-C(30)-H(30)	108.0
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5

C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(25)-C(33)-C(35)	111.1(2)
C(25)-C(33)-C(34)	112.8(2)
C(35)-C(33)-C(34)	110.7(2)
C(25)-C(33)-H(33)	107.3
C(35)-C(33)-H(33)	107.3
C(34)-C(33)-H(33)	107.3
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(39)-C(36)-C(37)	114.1(5)
C(39)-C(36)-H(36A)	108.7
C(37)-C(36)-H(36A)	108.7
C(39)-C(36)-H(36B)	108.7
C(37)-C(36)-H(36B)	108.7
H(36A)-C(36)-H(36B)	107.6
C(38)-C(37)-C(36)	113.0(3)
C(38)-C(37)-H(37A)	109.0
C(36)-C(37)-H(37A)	109.0
C(38)-C(37)-H(37B)	109.0
C(36)-C(37)-H(37B)	109.0
H(37A)-C(37)-H(37B)	107.8
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5

H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(36)-C(39)-C(40)	112.3(5)
C(36)-C(39)-H(39A)	109.1
C(40)-C(39)-H(39A)	109.1
C(36)-C(39)-H(39B)	109.1
C(40)-C(39)-H(39B)	109.1
H(39A)-C(39)-H(39B)	107.9
C(39)-C(40)-H(40A)	109.5
C(39)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(39)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
N(3)-Fe(1)-N(1)	98.88(10)
N(3)-Fe(1)-N(5)	154.90(9)
N(1)-Fe(1)-N(5)	106.22(9)
N(3)-Fe(1)-C(21)	97.10(10)
N(1)-Fe(1)-C(21)	99.93(10)
N(5)-Fe(1)-C(21)	78.82(10)
N(3)-Fe(1)-C(2)	97.02(10)
N(1)-Fe(1)-C(2)	99.77(10)
N(5)-Fe(1)-C(2)	78.94(10)
C(21)-Fe(1)-C(2)	153.61(10)
N(2)-N(1)-Fe(1)	175.0(2)
N(4)-N(3)-Fe(1)	179.2(2)
C(20)-N(5)-C(1)	117.0(2)
C(20)-N(5)-Fe(1)	121.34(17)
C(1)-N(5)-Fe(1)	121.61(17)
C(1)-N(6)-C(4)	132.1(2)
C(1)-N(6)-C(2)	116.1(2)
C(4)-N(6)-C(2)	111.6(2)
C(2)-N(7)-C(3)	111.7(2)
C(2)-N(7)-C(5)	123.7(2)
C(3)-N(7)-C(5)	124.3(2)
C(23)-N(8)-C(20)	131.9(2)

C(23)-N(8)-C(21)	112.3(2)
C(20)-N(8)-C(21)	115.6(2)
C(21)-N(9)-C(22)	111.5(2)
C(21)-N(9)-C(24)	123.0(2)
C(22)-N(9)-C(24)	124.8(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\approx^2$x 10^3)for 04jaw029. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	17(1)	17(1)	27(2)	-2(1)	-3(1)	-3(1)
C(2)	14(1)	15(1)	20(1)	-3(1)	-2(1)	1(1)
C(3)	25(1)	21(1)	27(2)	-9(1)	-8(1)	-6(1)
C(4)	24(1)	20(1)	33(2)	-7(1)	-10(1)	-7(1)
C(5)	23(1)	16(1)	15(1)	-5(1)	-3(1)	-6(1)
C(6)	22(1)	24(1)	16(1)	-8(1)	-3(1)	-4(1)
C(7)	24(1)	35(2)	24(2)	-10(1)	1(1)	-10(1)
C(8)	39(2)	30(2)	22(2)	-1(1)	-2(1)	-16(1)
C(9)	32(2)	21(2)	26(2)	-1(1)	-8(1)	-4(1)
C(10)	26(1)	21(1)	19(1)	-6(1)	-4(1)	-6(1)
C(11)	24(1)	18(1)	28(2)	-2(1)	-4(1)	1(1)
C(12)	27(2)	43(2)	47(2)	-8(2)	-10(1)	-4(1)
C(13)	38(2)	35(2)	47(2)	-17(2)	1(2)	0(1)
C(14)	24(1)	24(2)	23(2)	-7(1)	-3(1)	-1(1)
C(15)	40(2)	31(2)	38(2)	-14(1)	-4(1)	0(1)
C(16)	22(2)	40(2)	36(2)	-9(1)	-4(1)	-1(1)
C(17)	24(1)	21(1)	35(2)	-2(1)	-3(1)	-8(1)
C(18)	23(1)	23(2)	32(2)	4(1)	3(1)	-6(1)
C(19)	22(1)	24(2)	23(2)	2(1)	1(1)	-5(1)
C(20)	17(1)	20(1)	20(1)	-1(1)	-1(1)	-2(1)
C(21)	16(1)	21(1)	19(1)	-3(1)	-1(1)	-3(1)
C(22)	34(2)	33(2)	16(1)	-9(1)	0(1)	-7(1)
C(23)	32(2)	32(2)	14(1)	-4(1)	1(1)	-7(1)
C(24)	24(1)	22(1)	16(1)	-7(1)	-2(1)	-7(1)
C(25)	22(1)	24(1)	20(1)	-9(1)	-5(1)	-4(1)
C(26)	21(1)	31(2)	26(2)	-13(1)	-1(1)	-9(1)
C(27)	31(2)	26(2)	28(2)	-6(1)	-3(1)	-12(1)
C(28)	27(1)	22(1)	27(2)	-7(1)	-8(1)	-1(1)
C(29)	23(1)	26(2)	19(1)	-11(1)	-3(1)	-5(1)
C(30)	21(1)	26(2)	28(2)	-8(1)	-1(1)	-3(1)
C(31)	28(2)	69(2)	38(2)	-23(2)	-5(1)	-12(2)
C(32)	25(2)	70(2)	47(2)	-38(2)	2(1)	-5(2)
C(33)	22(1)	24(2)	30(2)	-9(1)	-2(1)	-4(1)

C(34)	30(2)	33(2)	48(2)	-14(2)	6(1)	-1(1)
C(35)	45(2)	41(2)	55(2)	-16(2)	-26(2)	8(2)
C(36)	139(4)	56(3)	49(3)	-28(2)	41(3)	-29(3)
C(37)	130(5)	38(3)	80(4)	10(2)	20(3)	23(3)
C(38)	81(3)	58(3)	84(3)	-1(2)	-20(3)	-3(3)
C(39)	193(7)	80(4)	111(5)	-53(4)	85(5)	-63(5)
C(40)	134(5)	99(4)	83(4)	-34(3)	-28(4)	-31(4)
Fe(1)	19(1)	17(1)	16(1)	-3(1)	-1(1)	-6(1)
N(1)	25(1)	22(1)	18(1)	-5(1)	-1(1)	-8(1)
N(2)	26(1)	30(1)	29(1)	-8(1)	-3(1)	-1(1)
N(3)	30(1)	22(1)	18(1)	-8(1)	-4(1)	-8(1)
N(4)	58(2)	24(1)	25(1)	-1(1)	-11(1)	-17(1)
N(5)	17(1)	16(1)	20(1)	-3(1)	-1(1)	-3(1)
N(6)	19(1)	17(1)	22(1)	-4(1)	-3(1)	-6(1)
N(7)	20(1)	16(1)	19(1)	-7(1)	-5(1)	-4(1)
N(8)	20(1)	23(1)	16(1)	-2(1)	0(1)	-5(1)
N(9)	23(1)	21(1)	18(1)	-4(1)	0(1)	-6(1)

Structural data for 2

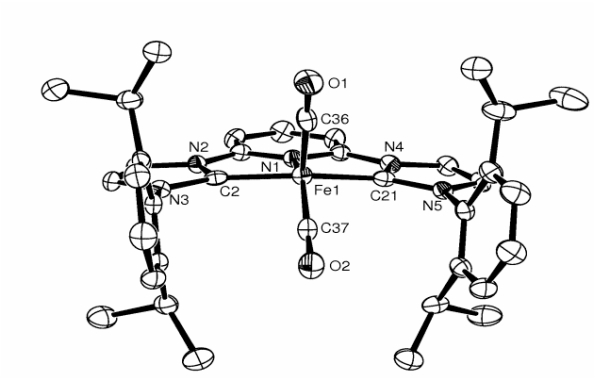

Table 5. Crystal data and structure refinement for **2**.

Identification code	**2**	
Empirical formula	C46 H50 Fe N5 O2	
Formula weight	760.76	
Temperature	120(2) K	
Wavelength	0.71073 ≈	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 17.343(3) ≈	α= 90∞.
	b = 16.989(2) ≈	β= 90∞.
	c = 27.436(4) ≈	γ = 90∞.
Volume	8084(2) ≈^{3}	
Z	8	
Density (calculated)	1.250 Mg/m^3	
Absorption coefficient	0.417 mm^{-1}	
F(000)	3224	
Crystal size	0.10 x 0.04 x 0.01 mm^3	
Theta range for data collection	2.97 to 24.65∞.	
Index ranges	-20<=h<=17, -19<=k<=16, -32<=l<=24	
Reflections collected	23527	
Independent reflections	6816 [R(int) = 0.0761]	
Completeness to theta = 24.65∞	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9958 and 0.4310708662	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6816 / 2 / 495	
Goodness-of-fit on F^2	1.018	
Final R indices [I>2sigma(I)]	R1 = 0.0568, wR2 = 0.1066	
R indices (all data)	R1 = 0.0950, wR2 = 0.1192	
Largest diff. peak and hole	0.356 and -0.451 e.≈$^{-3}$	

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($\approx^2$x 10^3) for 04nts021. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3128(2)	-199(2)	3769(1)	22(1)
C(2)	2483(2)	887(2)	4119(1)	19(1)
C(3)	1783(2)	244(2)	4707(1)	24(1)
C(4)	2183(2)	-311(2)	4473(1)	25(1)
C(5)	1615(2)	1716(2)	4630(1)	19(1)
C(6)	908(2)	1922(2)	4419(1)	21(1)
C(7)	602(2)	2659(2)	4534(1)	25(1)
C(8)	975(2)	3157(2)	4856(1)	29(1)
C(9)	1660(2)	2927(2)	5073(1)	25(1)
C(10)	2001(2)	2207(2)	4967(1)	21(1)
C(11)	2737(2)	1940(2)	5214(1)	26(1)
C(12)	3254(2)	2610(2)	5387(1)	40(1)
C(13)	2545(2)	1404(2)	5647(1)	36(1)
C(14)	469(2)	1344(2)	4098(1)	27(1)
C(15)	-103(2)	866(2)	4410(1)	30(1)
C(16)	31(2)	1737(2)	3681(1)	36(1)
C(17)	3357(2)	-962(2)	3676(1)	27(1)
C(18)	3915(2)	-1083(2)	3321(1)	31(1)
C(19)	4242(2)	-446(2)	3074(1)	27(1)
C(20)	3983(2)	297(2)	3188(1)	22(1)
C(21)	3856(2)	1685(2)	3192(1)	21(1)
C(22)	4818(2)	2002(2)	2652(1)	24(1)
C(23)	4809(2)	1213(2)	2677(1)	26(1)
C(24)	4088(2)	3124(2)	3035(1)	21(1)
C(25)	3617(2)	3508(2)	2699(1)	26(1)
C(26)	3479(2)	4308(2)	2772(1)	32(1)
C(27)	3795(2)	4702(2)	3163(1)	31(1)
C(28)	4259(2)	4304(2)	3489(1)	28(1)
C(29)	4425(2)	3510(2)	3435(1)	23(1)
C(30)	4962(2)	3077(2)	3782(1)	28(1)
C(31)	5771(2)	3018(2)	3568(1)	41(1)
C(32)	5012(2)	3451(2)	4293(1)	34(1)
C(33)	3294(2)	3098(2)	2250(1)	36(1)

C(34)	3760(2)	3325(2)	1796(1)	49(1)
C(35)	2439(2)	3269(2)	2171(1)	42(1)
C(36)	2230(2)	1764(2)	3277(1)	26(1)
C(37)	3140(2)	2328(2)	3986(1)	24(1)
C(38)	2667(2)	900(2)	2099(1)	39(1)
C(39)	3166(2)	499(2)	1796(2)	49(1)
C(40)	2960(3)	328(2)	1326(2)	53(1)
C(41)	2243(3)	554(2)	1157(1)	53(1)
C(42)	1733(3)	949(2)	1461(2)	58(1)
C(43)	1959(3)	1122(2)	1934(1)	45(1)
C(44)	86(4)	13(3)	489(2)	68(2)
C(45)	604(3)	-372(3)	205(3)	68(2)
C(46)	-517(3)	380(2)	287(2)	64(2)
Fe(1)	3027(1)	1476(1)	3636(1)	20(1)
N(1)	3416(2)	431(1)	3523(1)	21(1)
N(2)	2609(2)	74(1)	4115(1)	20(1)
N(3)	1961(2)	972(1)	4496(1)	19(1)
N(4)	4227(2)	1019(1)	3006(1)	21(1)
N(5)	4244(2)	2287(1)	2964(1)	20(1)
O(1)	1697(1)	1984(1)	3060(1)	36(1)
O(2)	3180(1)	2912(1)	4206(1)	35(1)

Table 7. Bond lengths [≈] and angles [∞] for **2**

C(1)-N(1)	1.359(4)
C(1)-C(17)	1.379(4)
C(1)-N(2)	1.389(4)
C(2)-N(3)	1.384(4)
C(2)-N(2)	1.400(4)
C(2)-Fe(1)	1.910(3)
C(3)-C(4)	1.334(4)
C(3)-N(3)	1.399(4)
C(3)-H(3)	0.9500
C(4)-N(2)	1.393(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.401(4)
C(5)-C(10)	1.414(4)
C(5)-N(3)	1.446(4)
C(6)-C(7)	1.397(4)
C(6)-C(14)	1.523(4)
C(7)-C(8)	1.385(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.384(4)
C(8)-H(8)	0.9500
C(9)-C(10)	1.390(4)
C(9)-H(9)	0.9500
C(10)-C(11)	1.514(4)
C(11)-C(12)	1.525(5)
C(11)-C(13)	1.535(4)
C(11)-H(11)	1.0000
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(16)	1.526(4)
C(14)-C(15)	1.541(4)
C(14)-H(14)	1.0000
C(15)-H(15A)	0.9800

C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(18)	1.389(5)
C(17)-H(17)	0.9500
C(18)-C(19)	1.397(4)
C(18)-H(18)	0.9500
C(19)-C(20)	1.376(4)
C(19)-H(19)	0.9500
C(20)-N(1)	1.366(4)
C(20)-N(4)	1.390(4)
C(21)-N(5)	1.375(4)
C(21)-N(4)	1.398(4)
C(21)-Fe(1)	1.918(3)
C(22)-C(23)	1.342(4)
C(22)-N(5)	1.399(4)
C(22)-H(22)	0.9500
C(23)-N(4)	1.395(4)
C(23)-H(23)	0.9500
C(24)-C(25)	1.394(4)
C(24)-C(29)	1.405(4)
C(24)-N(5)	1.462(4)
C(25)-C(26)	1.395(4)
C(25)-C(33)	1.521(4)
C(26)-C(27)	1.379(5)
C(26)-H(26)	0.9500
C(27)-C(28)	1.380(5)
C(27)-H(27)	0.9500
C(28)-C(29)	1.386(4)
C(28)-H(28)	0.9500
C(29)-C(30)	1.523(4)
C(30)-C(31)	1.525(5)
C(30)-C(32)	1.540(4)
C(30)-H(30)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800

C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(35)	1.527(5)
C(33)-C(34)	1.534(5)
C(33)-H(33)	1.0000
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-O(1)	1.161(4)
C(36)-Fe(1)	1.767(4)
C(37)-O(2)	1.165(4)
C(37)-Fe(1)	1.746(3)
C(38)-C(43)	1.363(5)
C(38)-C(39)	1.381(5)
C(38)-H(38)	0.9500
C(39)-C(40)	1.368(5)
C(39)-H(39)	0.9500
C(40)-C(41)	1.382(6)
C(40)-H(40)	0.9500
C(41)-C(42)	1.389(6)
C(41)-H(41)	0.9500
C(42)-C(43)	1.386(5)
C(42)-H(42)	0.9500
C(43)-H(43)	0.9500
C(44)-C(46)	1.338(7)
C(44)-C(45)	1.357(7)
C(44)-H(44)	0.9500
C(45)-C(46)#1	1.357(7)
C(45)-H(45)	0.9500
C(46)-C(45)#1	1.357(7)
C(46)-H(46)	0.9500
Fe(1)-N(1)	1.925(2)

N(1)-C(1)-C(17)	122.9(3)
N(1)-C(1)-N(2)	108.3(2)
C(17)-C(1)-N(2)	128.7(3)
N(3)-C(2)-N(2)	102.2(2)
N(3)-C(2)-Fe(1)	142.0(2)
N(2)-C(2)-Fe(1)	115.8(2)
C(4)-C(3)-N(3)	108.3(3)
C(4)-C(3)-H(3)	125.9
N(3)-C(3)-H(3)	125.9
C(3)-C(4)-N(2)	106.4(3)
C(3)-C(4)-H(4)	126.8
N(2)-C(4)-H(4)	126.8
C(6)-C(5)-C(10)	122.5(3)
C(6)-C(5)-N(3)	118.4(3)
C(10)-C(5)-N(3)	119.1(3)
C(7)-C(6)-C(5)	117.6(3)
C(7)-C(6)-C(14)	121.3(3)
C(5)-C(6)-C(14)	121.1(3)
C(8)-C(7)-C(6)	121.0(3)
C(8)-C(7)-H(7)	119.5
C(6)-C(7)-H(7)	119.5
C(9)-C(8)-C(7)	120.2(3)
C(9)-C(8)-H(8)	119.9
C(7)-C(8)-H(8)	119.9
C(8)-C(9)-C(10)	121.5(3)
C(8)-C(9)-H(9)	119.2
C(10)-C(9)-H(9)	119.2
C(9)-C(10)-C(5)	117.1(3)
C(9)-C(10)-C(11)	121.9(3)
C(5)-C(10)-C(11)	121.0(3)
C(10)-C(11)-C(12)	114.2(3)
C(10)-C(11)-C(13)	110.0(3)
C(12)-C(11)-C(13)	109.2(3)
C(10)-C(11)-H(11)	107.7
C(12)-C(11)-H(11)	107.7
C(13)-C(11)-H(11)	107.7
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5

H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(6)-C(14)-C(16)	113.6(3)
C(6)-C(14)-C(15)	109.9(3)
C(16)-C(14)-C(15)	109.0(3)
C(6)-C(14)-H(14)	108.1
C(16)-C(14)-H(14)	108.1
C(15)-C(14)-H(14)	108.1
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(1)-C(17)-C(18)	117.9(3)
C(1)-C(17)-H(17)	121.0
C(18)-C(17)-H(17)	121.0
C(17)-C(18)-C(19)	120.6(3)
C(17)-C(18)-H(18)	119.7
C(19)-C(18)-H(18)	119.7
C(20)-C(19)-C(18)	117.9(3)
C(20)-C(19)-H(19)	121.0
C(18)-C(19)-H(19)	121.0
N(1)-C(20)-C(19)	122.8(3)

N(1)-C(20)-N(4)	108.3(2)
C(19)-C(20)-N(4)	128.9(3)
N(5)-C(21)-N(4)	102.2(3)
N(5)-C(21)-Fe(1)	142.6(2)
N(4)-C(21)-Fe(1)	115.2(2)
C(23)-C(22)-N(5)	107.8(3)
C(23)-C(22)-H(22)	126.1
N(5)-C(22)-H(22)	126.1
C(22)-C(23)-N(4)	106.1(3)
C(22)-C(23)-H(23)	126.9
N(4)-C(23)-H(23)	126.9
C(25)-C(24)-C(29)	122.9(3)
C(25)-C(24)-N(5)	118.3(3)
C(29)-C(24)-N(5)	118.8(3)
C(24)-C(25)-C(26)	117.4(3)
C(24)-C(25)-C(33)	122.6(3)
C(26)-C(25)-C(33)	119.9(3)
C(27)-C(26)-C(25)	121.1(3)
C(27)-C(26)-H(26)	119.5
C(25)-C(26)-H(26)	119.5
C(26)-C(27)-C(28)	120.0(3)
C(26)-C(27)-H(27)	120.0
C(28)-C(27)-H(27)	120.0
C(27)-C(28)-C(29)	121.8(3)
C(27)-C(28)-H(28)	119.1
C(29)-C(28)-H(28)	119.1
C(28)-C(29)-C(24)	116.8(3)
C(28)-C(29)-C(30)	122.0(3)
C(24)-C(29)-C(30)	121.2(3)
C(29)-C(30)-C(31)	110.6(3)
C(29)-C(30)-C(32)	113.8(3)
C(31)-C(30)-C(32)	109.0(3)
C(29)-C(30)-H(30)	107.7
C(31)-C(30)-H(30)	107.7
C(32)-C(30)-H(30)	107.7
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5

C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(25)-C(33)-C(35)	112.7(3)
C(25)-C(33)-C(34)	110.4(3)
C(35)-C(33)-C(34)	110.4(3)
C(25)-C(33)-H(33)	107.7
C(35)-C(33)-H(33)	107.7
C(34)-C(33)-H(33)	107.7
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
O(1)-C(36)-Fe(1)	176.2(3)
O(2)-C(37)-Fe(1)	176.3(3)
C(43)-C(38)-C(39)	120.0(4)
C(43)-C(38)-H(38)	120.0
C(39)-C(38)-H(38)	120.0
C(40)-C(39)-C(38)	120.6(4)
C(40)-C(39)-H(39)	119.7
C(38)-C(39)-H(39)	119.7
C(39)-C(40)-C(41)	119.5(4)
C(39)-C(40)-H(40)	120.3
C(41)-C(40)-H(40)	120.3

C(40)-C(41)-C(42)	120.3(4)
C(40)-C(41)-H(41)	119.8
C(42)-C(41)-H(41)	119.8
C(43)-C(42)-C(41)	119.1(4)
C(43)-C(42)-H(42)	120.5
C(41)-C(42)-H(42)	120.5
C(38)-C(43)-C(42)	120.5(4)
C(38)-C(43)-H(43)	119.8
C(42)-C(43)-H(43)	119.8
C(46)-C(44)-C(45)	120.3(4)
C(46)-C(44)-H(44)	119.9
C(45)-C(44)-H(44)	119.9
C(46)#1-C(45)-C(44)	120.1(4)
C(46)#1-C(45)-H(45)	119.9
C(44)-C(45)-H(45)	119.9
C(44)-C(46)-C(45)#1	119.6(4)
C(44)-C(46)-H(46)	120.2
C(45)#1-C(46)-H(46)	120.2
C(37)-Fe(1)-C(36)	99.48(15)
C(37)-Fe(1)-C(2)	96.23(13)
C(36)-Fe(1)-C(2)	98.38(14)
C(37)-Fe(1)-C(21)	96.43(13)
C(36)-Fe(1)-C(21)	100.38(13)
C(2)-Fe(1)-C(21)	155.27(12)
C(37)-Fe(1)-N(1)	144.43(13)
C(36)-Fe(1)-N(1)	116.07(13)
C(2)-Fe(1)-N(1)	78.51(11)
C(21)-Fe(1)-N(1)	78.83(11)
C(1)-N(1)-C(20)	117.8(3)
C(1)-N(1)-Fe(1)	121.2(2)
C(20)-N(1)-Fe(1)	120.9(2)
C(1)-N(2)-C(4)	132.1(2)
C(1)-N(2)-C(2)	115.8(2)
C(4)-N(2)-C(2)	112.0(2)
C(2)-N(3)-C(3)	111.1(2)
C(2)-N(3)-C(5)	123.5(2)
C(3)-N(3)-C(5)	125.3(3)
C(20)-N(4)-C(23)	131.4(3)

C(20)-N(4)-C(21)	116.3(3)
C(23)-N(4)-C(21)	112.2(2)
C(21)-N(5)-C(22)	111.7(2)
C(21)-N(5)-C(24)	124.9(3)
C(22)-N(5)-C(24)	123.4(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

Table 8. Anisotropic displacement parameters ($\approx^2$x 10^3)for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	25(2)	18(2)	23(2)	-1(1)	-3(2)	1(2)
C(2)	15(2)	17(2)	24(2)	-4(1)	-7(2)	4(1)
C(3)	24(2)	23(2)	23(2)	4(1)	2(2)	-6(2)
C(4)	26(2)	18(2)	30(2)	2(1)	3(2)	-5(2)
C(5)	19(2)	18(2)	21(2)	3(1)	6(2)	1(1)
C(6)	21(2)	25(2)	16(2)	5(1)	2(1)	-1(2)
C(7)	21(2)	27(2)	28(2)	5(1)	0(2)	7(2)
C(8)	33(2)	20(2)	34(2)	-3(2)	9(2)	6(2)
C(9)	27(2)	22(2)	26(2)	-4(1)	2(2)	-3(2)
C(10)	19(2)	26(2)	19(2)	2(1)	2(2)	-2(2)
C(11)	23(2)	29(2)	24(2)	-7(1)	2(2)	2(2)
C(12)	29(2)	49(2)	42(2)	-2(2)	-9(2)	-5(2)
C(13)	38(2)	38(2)	33(2)	4(2)	-10(2)	2(2)
C(14)	22(2)	32(2)	27(2)	-5(1)	-3(2)	0(2)
C(15)	28(2)	29(2)	34(2)	-2(2)	-1(2)	-2(2)
C(16)	31(2)	48(2)	27(2)	2(2)	-5(2)	-5(2)
C(17)	25(2)	22(2)	35(2)	2(2)	1(2)	-1(2)
C(18)	35(2)	19(2)	40(2)	-6(2)	3(2)	7(2)
C(19)	25(2)	26(2)	32(2)	-4(1)	8(2)	5(2)
C(20)	23(2)	21(2)	22(2)	0(1)	-2(2)	1(2)
C(21)	24(2)	19(2)	20(2)	-1(1)	-5(2)	1(2)
C(22)	24(2)	29(2)	18(2)	1(1)	3(2)	3(2)
C(23)	23(2)	29(2)	24(2)	-2(1)	4(2)	6(2)
C(24)	23(2)	22(2)	19(2)	1(1)	5(2)	1(2)
C(25)	29(2)	26(2)	23(2)	5(1)	-1(2)	3(2)
C(26)	40(2)	26(2)	30(2)	4(2)	-7(2)	8(2)
C(27)	42(2)	20(2)	31(2)	-2(2)	-2(2)	5(2)
C(28)	32(2)	25(2)	28(2)	-6(1)	-2(2)	-1(2)
C(29)	22(2)	27(2)	19(2)	0(1)	2(1)	3(2)
C(30)	27(2)	25(2)	31(2)	-3(1)	-8(2)	-1(2)
C(31)	29(2)	50(2)	44(2)	-11(2)	-12(2)	7(2)
C(32)	37(2)	37(2)	29(2)	1(2)	-8(2)	2(2)
C(33)	48(2)	26(2)	34(2)	-1(2)	-19(2)	6(2)

C(34)	46(3)	73(3)	29(2)	-13(2)	-6(2)	14(2)
C(35)	42(2)	48(2)	37(2)	3(2)	-9(2)	-8(2)
C(36)	29(2)	27(2)	23(2)	2(2)	9(2)	3(2)
C(37)	24(2)	24(2)	25(2)	4(1)	6(2)	0(2)
C(38)	43(3)	40(2)	34(2)	-4(2)	3(2)	-9(2)
C(39)	35(3)	55(3)	58(3)	-12(2)	0(2)	-14(2)
C(40)	55(3)	57(3)	46(3)	-11(2)	13(2)	-17(2)
C(41)	98(4)	29(2)	32(2)	-2(2)	-11(3)	-12(2)
C(42)	74(3)	34(2)	67(3)	-5(2)	-29(3)	8(2)
C(43)	52(3)	37(2)	48(3)	-7(2)	0(2)	4(2)
C(44)	127(5)	37(3)	42(3)	6(2)	-14(3)	-36(3)
C(45)	36(3)	37(3)	129(5)	15(3)	-36(3)	3(2)
C(46)	58(4)	33(2)	102(5)	-15(3)	51(3)	-13(3)
Fe(1)	21(1)	17(1)	21(1)	-1(1)	2(1)	2(1)
N(1)	23(2)	20(1)	20(2)	-2(1)	2(1)	1(1)
N(2)	21(2)	19(1)	20(1)	0(1)	2(1)	0(1)
N(3)	20(2)	18(1)	19(1)	0(1)	-1(1)	1(1)
N(4)	22(2)	21(1)	20(2)	-2(1)	2(1)	4(1)
N(5)	23(2)	18(1)	19(1)	-1(1)	1(1)	1(1)
O(1)	29(2)	44(2)	36(2)	6(1)	-3(1)	9(1)
O(2)	45(2)	22(1)	36(1)	-7(1)	13(1)	-2(1)

Structural data for 3

Table 9. Crystal data and structure refinement for **3**

Identification code	**3**	
Empirical formula	C37 H45 Fe N7	
Formula weight	643.65	
Temperature	120(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 31.84(5) ≈	α= 90∞.
	b = 8.911(12) ≈	β= 92.3(2)∞.
	c = 23.56(5) ≈	γ = 90∞.
Volume	6679(20) ≈^{3}	
Z	8	
Density (calculated)	1.280 Mg/m^3	
Absorption coefficient	0.489 mm^{-1}	
F(000)	2736	
Crystal size	0.24 x 0.20 x 0.04 mm^3	
Theta range for data collection	2.92 to 26.83∞.	
Index ranges	-40<=h<=36, -11<=k<=9, -29<=l<=29	
Reflections collected	32549	
Independent reflections	7073 [R(int) = 0.1619]	
Completeness to theta = 26.83∞	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9807 and 0.7105	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7073 / 0 / 414	
Goodness-of-fit on F^2	1.014	
Final R indices [I>2sigma(I)]	R1 = 0.0797, wR2 = 0.1320	
R indices (all data)	R1 = 0.1771, wR2 = 0.1614	
Largest diff. peak and hole	0.333 and -0.414 e.≈$^{-3}$	

Table 10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($\approx^2$x 10^3) for 04jaw027. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2973(1)	1149(4)	-397(2)	23(1)
C(2)	3587(1)	2623(5)	-470(2)	24(1)
C(3)	3650(1)	2521(5)	-1435(2)	30(1)
C(4)	3316(1)	1673(5)	-1331(2)	29(1)
C(5)	4152(1)	4184(5)	-908(2)	25(1)
C(6)	4038(1)	5701(5)	-918(2)	29(1)
C(7)	4366(2)	6731(5)	-951(2)	37(1)
C(8)	4776(2)	6272(6)	-967(2)	43(1)
C(9)	4876(2)	4772(6)	-946(2)	39(1)
C(10)	4567(1)	3690(5)	-916(2)	29(1)
C(11)	4678(2)	2036(5)	-895(2)	39(1)
C(12)	5082(2)	1707(6)	-541(2)	53(2)
C(13)	4717(2)	1420(6)	-1499(2)	51(2)
C(14)	3581(1)	6193(5)	-909(2)	31(1)
C(15)	3363(2)	6146(6)	-1499(2)	44(1)
C(16)	3532(2)	7758(5)	-649(2)	51(2)
C(17)	2637(1)	236(5)	-555(2)	28(1)
C(18)	2373(1)	-238(5)	-131(2)	30(1)
C(19)	2455(1)	212(5)	431(2)	28(1)
C(20)	2790(1)	1137(5)	548(2)	23(1)
C(21)	3294(1)	2589(4)	1070(2)	22(1)
C(22)	2982(1)	2572(5)	1939(2)	31(1)
C(23)	2738(1)	1734(5)	1594(2)	29(1)
C(24)	3666(1)	3939(5)	1882(2)	26(1)
C(25)	4008(2)	3161(5)	2121(2)	32(1)
C(26)	4335(2)	3994(6)	2373(2)	41(1)
C(27)	4321(2)	5526(6)	2374(2)	42(1)
C(28)	3980(2)	6287(6)	2122(2)	40(1)
C(29)	3638(1)	5509(5)	1875(2)	30(1)
C(30)	3257(2)	6313(5)	1623(2)	34(1)
C(31)	2916(2)	6494(6)	2063(2)	48(2)
C(32)	3354(2)	7857(5)	1377(2)	55(2)
C(33)	4025(2)	1453(5)	2108(2)	35(1)

C(34)	3830(2)	768(5)	2638(2)	44(1)
C(35)	4466(2)	821(6)	2057(2)	53(2)
C(36)	3958(1)	891(5)	475(2)	37(1)
C(37)	4176(2)	2212(6)	570(2)	42(1)
Fe(1)	3555(1)	2710(1)	347(1)	24(1)
N(1)	3735(1)	4638(5)	432(2)	36(1)
N(2)	3874(2)	5788(5)	489(2)	50(1)
N(3)	3056(1)	1619(4)	147(2)	23(1)
N(4)	3273(1)	1748(4)	-744(2)	25(1)
N(5)	3816(1)	3090(4)	-922(2)	25(1)
N(6)	2924(1)	1740(4)	1068(2)	24(1)
N(7)	3322(1)	3089(4)	1632(2)	24(1)

Table11. Bond lengths [≈] and angles [∞] for **3**.

C(1)-N(3)	1.365(6)
C(1)-C(17)	1.382(6)
C(1)-N(4)	1.389(6)
C(2)-N(5)	1.380(6)
C(2)-N(4)	1.403(6)
C(2)-Fe(1)	1.933(6)
C(3)-C(4)	1.334(6)
C(3)-N(5)	1.396(6)
C(3)-H(3)	0.9500
C(4)-N(4)	1.396(6)
C(4)-H(4)	0.9500
C(5)-C(10)	1.394(6)
C(5)-C(6)	1.399(6)
C(5)-N(5)	1.446(5)
C(6)-C(7)	1.396(6)
C(6)-C(14)	1.519(6)
C(7)-C(8)	1.370(7)
C(7)-H(7)	0.9500
C(8)-C(9)	1.375(7)
C(8)-H(8)	0.9500
C(9)-C(10)	1.383(6)
C(9)-H(9)	0.9500
C(10)-C(11)	1.516(7)
C(11)-C(12)	1.533(7)
C(11)-C(13)	1.536(7)
C(11)-H(11)	1.0000
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(15)	1.529(7)
C(14)-C(16)	1.534(6)
C(14)-H(14)	1.0000
C(15)-H(15A)	0.9800

C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(18)	1.398(6)
C(17)-H(17)	0.9500
C(18)-C(19)	1.398(7)
C(18)-H(18)	0.9500
C(19)-C(20)	1.368(6)
C(19)-H(19)	0.9500
C(20)-N(3)	1.363(6)
C(20)-N(6)	1.387(6)
C(21)-N(7)	1.397(6)
C(21)-N(6)	1.401(5)
C(21)-Fe(1)	1.927(6)
C(22)-C(23)	1.330(6)
C(22)-N(7)	1.403(6)
C(22)-H(22)	0.9500
C(23)-N(6)	1.394(6)
C(23)-H(23)	0.9500
C(24)-C(25)	1.393(6)
C(24)-C(29)	1.402(6)
C(24)-N(7)	1.438(6)
C(25)-C(26)	1.393(7)
C(25)-C(33)	1.523(7)
C(26)-C(27)	1.365(7)
C(26)-H(26)	0.9500
C(27)-C(28)	1.393(7)
C(27)-H(27)	0.9500
C(28)-C(29)	1.398(7)
C(28)-H(28)	0.9500
C(29)-C(30)	1.511(7)
C(30)-C(32)	1.529(6)
C(30)-C(31)	1.539(7)
C(30)-H(30)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800

C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(35)	1.523(6)
C(33)-C(34)	1.542(7)
C(33)-H(33)	1.0000
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-C(37)	1.379(6)
C(36)-Fe(1)	2.083(5)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-Fe(1)	2.074(6)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
Fe(1)-N(1)	1.820(5)
Fe(1)-N(3)	1.905(4)
N(1)-N(2)	1.121(5)

N(3)-C(1)-C(17)	123.5(4)
N(3)-C(1)-N(4)	108.8(4)
C(17)-C(1)-N(4)	127.7(4)
N(5)-C(2)-N(4)	101.6(4)
N(5)-C(2)-Fe(1)	143.8(3)
N(4)-C(2)-Fe(1)	114.5(3)
C(4)-C(3)-N(5)	108.9(4)
C(4)-C(3)-H(3)	125.6
N(5)-C(3)-H(3)	125.6
C(3)-C(4)-N(4)	105.4(4)
C(3)-C(4)-H(4)	127.3
N(4)-C(4)-H(4)	127.3
C(10)-C(5)-C(6)	123.4(4)
C(10)-C(5)-N(5)	119.1(4)

C(6)-C(5)-N(5)	117.4(4)
C(5)-C(6)-C(7)	116.2(4)
C(5)-C(6)-C(14)	121.7(4)
C(7)-C(6)-C(14)	122.0(4)
C(8)-C(7)-C(6)	121.4(5)
C(8)-C(7)-H(7)	119.3
C(6)-C(7)-H(7)	119.3
C(7)-C(8)-C(9)	120.6(5)
C(7)-C(8)-H(8)	119.7
C(9)-C(8)-H(8)	119.7
C(8)-C(9)-C(10)	121.0(5)
C(8)-C(9)-H(9)	119.5
C(10)-C(9)-H(9)	119.5
C(9)-C(10)-C(5)	117.3(4)
C(9)-C(10)-C(11)	120.9(4)
C(5)-C(10)-C(11)	121.8(4)
C(10)-C(11)-C(12)	113.2(4)
C(10)-C(11)-C(13)	110.2(4)
C(12)-C(11)-C(13)	109.7(4)
C(10)-C(11)-H(11)	107.9
C(12)-C(11)-H(11)	107.9
C(13)-C(11)-H(11)	107.9
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(6)-C(14)-C(15)	112.3(4)
C(6)-C(14)-C(16)	112.4(4)
C(15)-C(14)-C(16)	109.8(4)
C(6)-C(14)-H(14)	107.4

C(15)-C(14)-H(14)	107.4
C(16)-C(14)-H(14)	107.4
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(1)-C(17)-C(18)	117.9(5)
C(1)-C(17)-H(17)	121.1
C(18)-C(17)-H(17)	121.1
C(19)-C(18)-C(17)	119.7(4)
C(19)-C(18)-H(18)	120.2
C(17)-C(18)-H(18)	120.2
C(20)-C(19)-C(18)	118.7(4)
C(20)-C(19)-H(19)	120.7
C(18)-C(19)-H(19)	120.7
N(3)-C(20)-C(19)	123.4(4)
N(3)-C(20)-N(6)	108.3(4)
C(19)-C(20)-N(6)	128.3(4)
N(7)-C(21)-N(6)	101.3(4)
N(7)-C(21)-Fe(1)	143.8(3)
N(6)-C(21)-Fe(1)	114.8(3)
C(23)-C(22)-N(7)	108.2(4)
C(23)-C(22)-H(22)	125.9
N(7)-C(22)-H(22)	125.9
C(22)-C(23)-N(6)	106.5(4)
C(22)-C(23)-H(23)	126.8
N(6)-C(23)-H(23)	126.8
C(25)-C(24)-C(29)	123.3(4)
C(25)-C(24)-N(7)	118.3(4)
C(29)-C(24)-N(7)	118.3(4)

C(24)-C(25)-C(26)	117.8(5)
C(24)-C(25)-C(33)	121.1(4)
C(26)-C(25)-C(33)	121.0(5)
C(27)-C(26)-C(25)	120.6(5)
C(27)-C(26)-H(26)	119.7
C(25)-C(26)-H(26)	119.7
C(26)-C(27)-C(28)	120.8(5)
C(26)-C(27)-H(27)	119.6
C(28)-C(27)-H(27)	119.6
C(27)-C(28)-C(29)	121.1(5)
C(27)-C(28)-H(28)	119.5
C(29)-C(28)-H(28)	119.5
C(28)-C(29)-C(24)	116.3(4)
C(28)-C(29)-C(30)	121.9(4)
C(24)-C(29)-C(30)	121.8(4)
C(29)-C(30)-C(32)	113.8(4)
C(29)-C(30)-C(31)	111.2(4)
C(32)-C(30)-C(31)	108.7(4)
C(29)-C(30)-H(30)	107.7
C(32)-C(30)-H(30)	107.7
C(31)-C(30)-H(30)	107.7
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(25)-C(33)-C(35)	113.8(4)
C(25)-C(33)-C(34)	111.4(4)
C(35)-C(33)-C(34)	108.7(4)
C(25)-C(33)-H(33)	107.6
C(35)-C(33)-H(33)	107.6

C(34)-C(33)-H(33)	107.6
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(37)-C(36)-Fe(1)	70.3(3)
C(37)-C(36)-H(36A)	116.6
Fe(1)-C(36)-H(36A)	116.6
C(37)-C(36)-H(36B)	116.6
Fe(1)-C(36)-H(36B)	116.6
H(36A)-C(36)-H(36B)	113.6
C(36)-C(37)-Fe(1)	71.0(3)
C(36)-C(37)-H(37A)	116.5
Fe(1)-C(37)-H(37A)	116.5
C(36)-C(37)-H(37B)	116.5
Fe(1)-C(37)-H(37B)	116.5
H(37A)-C(37)-H(37B)	113.5
N(1)-Fe(1)-N(3)	139.96(17)
N(1)-Fe(1)-C(21)	95.79(18)
N(3)-Fe(1)-C(21)	78.8(2)
N(1)-Fe(1)-C(2)	96.81(19)
N(3)-Fe(1)-C(2)	79.1(2)
C(21)-Fe(1)-C(2)	156.84(19)
N(1)-Fe(1)-C(37)	83.1(2)
N(3)-Fe(1)-C(37)	136.9(2)
C(21)-Fe(1)-C(37)	101.8(2)
C(2)-Fe(1)-C(37)	98.9(3)
N(1)-Fe(1)-C(36)	121.9(2)
N(3)-Fe(1)-C(36)	98.2(2)
C(21)-Fe(1)-C(36)	96.5(2)

C(2)-Fe(1)-C(36)	93.2(2)
C(37)-Fe(1)-C(36)	38.75(17)
N(2)-N(1)-Fe(1)	175.3(4)
C(20)-N(3)-C(1)	116.9(4)
C(20)-N(3)-Fe(1)	121.6(3)
C(1)-N(3)-Fe(1)	121.2(3)
C(1)-N(4)-C(4)	131.3(4)
C(1)-N(4)-C(2)	115.9(4)
C(4)-N(4)-C(2)	112.7(4)
C(2)-N(5)-C(3)	111.4(4)
C(2)-N(5)-C(5)	126.8(4)
C(3)-N(5)-C(5)	121.3(4)
C(20)-N(6)-C(23)	131.1(4)
C(20)-N(6)-C(21)	116.1(4)
C(23)-N(6)-C(21)	112.7(4)
C(21)-N(7)-C(22)	111.3(4)
C(21)-N(7)-C(24)	125.0(4)
C(22)-N(7)-C(24)	123.6(4)

Symmetry transformations used to generate equivalent atoms:

Table 12. Anisotropic displacement parameters ($\approx^2$x 10^3)for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	23(3)	24(2)	22(3)	0(2)	0(2)	5(2)
C(2)	22(2)	27(2)	25(3)	-1(2)	2(2)	4(2)
C(3)	34(3)	43(3)	13(2)	0(2)	5(2)	-5(2)
C(4)	33(3)	36(3)	19(3)	-8(2)	4(2)	3(2)
C(5)	27(3)	38(3)	11(2)	1(2)	3(2)	-7(2)
C(6)	29(3)	34(3)	22(3)	3(2)	-1(2)	-4(2)
C(7)	43(3)	38(3)	30(3)	4(2)	-2(2)	-5(3)
C(8)	27(3)	62(4)	42(4)	1(3)	-1(3)	-17(3)
C(9)	23(3)	61(4)	33(3)	-1(3)	4(2)	-1(3)
C(10)	25(3)	41(3)	20(3)	-1(2)	5(2)	0(2)
C(11)	32(3)	51(3)	35(3)	2(3)	9(2)	11(2)
C(12)	48(4)	68(4)	42(4)	8(3)	-4(3)	21(3)
C(13)	47(3)	55(3)	50(4)	-5(3)	-1(3)	16(3)
C(14)	32(3)	30(3)	31(3)	6(2)	3(2)	-1(2)
C(15)	35(3)	54(3)	44(4)	16(3)	-1(3)	3(3)
C(16)	58(4)	39(3)	56(4)	6(3)	12(3)	10(3)
C(17)	29(3)	30(3)	26(3)	-5(2)	-5(2)	0(2)
C(18)	21(3)	32(3)	38(3)	2(2)	-1(2)	-8(2)
C(19)	22(3)	29(3)	31(3)	5(2)	-2(2)	-3(2)
C(20)	20(2)	26(2)	25(3)	0(2)	4(2)	2(2)
C(21)	28(2)	21(2)	18(2)	-1(2)	-2(2)	1(2)
C(22)	28(3)	40(3)	25(3)	6(2)	10(2)	5(2)
C(23)	22(3)	41(3)	24(3)	3(2)	6(2)	-4(2)
C(24)	29(3)	35(3)	14(3)	-2(2)	6(2)	-6(2)
C(25)	33(3)	44(3)	17(3)	-1(2)	1(2)	3(2)
C(26)	29(3)	59(4)	36(3)	-14(3)	-4(2)	4(3)
C(27)	35(3)	54(4)	38(4)	-20(3)	3(3)	-17(3)
C(28)	42(3)	40(3)	38(3)	-15(3)	3(3)	-6(3)
C(29)	34(3)	35(3)	20(3)	-5(2)	8(2)	-1(2)
C(30)	48(3)	32(3)	23(3)	-4(2)	-3(2)	5(2)
C(31)	47(3)	55(3)	42(4)	-2(3)	1(3)	15(3)
C(32)	80(4)	37(3)	48(4)	3(3)	7(3)	12(3)
C(33)	38(3)	37(3)	29(3)	4(2)	3(2)	7(2)

C(34)	55(4)	40(3)	35(3)	1(2)	7(3)	6(3)
C(35)	49(4)	57(4)	53(4)	16(3)	11(3)	25(3)
C(36)	32(3)	39(3)	40(3)	3(2)	3(3)	8(2)
C(37)	34(3)	68(4)	23(3)	0(3)	2(2)	5(3)
Fe(1)	25(1)	27(1)	19(1)	-1(1)	1(1)	-2(1)
N(1)	44(3)	41(3)	23(3)	-2(2)	10(2)	-5(2)
N(2)	77(4)	42(3)	32(3)	-8(2)	12(2)	-21(3)
N(3)	26(2)	24(2)	20(2)	-2(2)	3(2)	1(2)
N(4)	27(2)	30(2)	17(2)	0(2)	0(2)	1(2)
N(5)	24(2)	31(2)	19(2)	-3(2)	2(2)	1(2)
N(6)	22(2)	31(2)	18(2)	3(2)	1(2)	1(2)
N(7)	21(2)	31(2)	19(2)	2(2)	1(2)	-1(2)

Structural data for 4

Table 13. Crystal data and structure refinement for **4**

Identification code	**4**	
Empirical formula	C42 H60 Fe N7 O P	
Formula weight	765.79	
Temperature	120(2) K	
Wavelength	0.71073 ≈	
Crystal system	Orthorhombic	
Space group	Pna21	
Unit cell dimensions	a = 18.2286(17) ≈	α= 90∞.
	b = 17.4745(18) ≈	β= 90∞.
	c = 13.7220(15) ≈	γ = 90∞.
Volume	4370.9(8) ≈^{3}	
Z	4	
Density (calculated)	1.164 Mg/m^3	
Absorption coefficient	0.420 mm^{-1}	
F(000)	1640	
Crystal size	0.40 x 0.40 x 0.06 mm^3	
Theta range for data collection	2.98 to 27.57∞.	
Index ranges	-23<=h<=14, -20<=k<=22, -17<=l<=17	
Reflections collected	24392	
Independent reflections	9009 [R(int) = 0.0501]	
Completeness to theta = 27.57∞	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9752 and 0.8500	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9009 / 9 / 487	
Goodness-of-fit on F^2	1.017	
Final R indices [I>2sigma(I)]	R1 = 0.0517, wR2 = 0.1146	
R indices (all data)	R1 = 0.0776, wR2 = 0.1249	
Absolute structure parameter	0.036(16)	
Largest diff. peak and hole	0.716 and -0.414 e.≈$^{-3}$	

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($\approx^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2381(2)	5317(2)	2985(3)	45(1)
C(2)	3268(2)	4537(3)	4338(3)	48(1)
C(3)	1746(2)	4280(3)	4258(3)	51(1)
C(4)	1595(2)	4151(2)	1121(3)	25(1)
C(5)	1089(2)	3288(2)	2234(3)	24(1)
C(6)	2076(2)	2691(2)	3022(2)	24(1)
C(7)	1437(2)	1809(2)	3921(3)	30(1)
C(8)	932(2)	2220(2)	3462(3)	29(1)
C(9)	2807(2)	1656(2)	3772(3)	29(1)
C(10)	2979(2)	1126(2)	3052(3)	30(1)
C(11)	2451(2)	925(2)	2224(3)	33(1)
C(12)	2747(2)	1218(3)	1256(3)	45(1)
C(13)	2304(2)	62(2)	2186(3)	41(1)
C(14)	3655(2)	768(2)	3103(3)	34(1)
C(15)	4140(2)	931(2)	3846(3)	39(1)
C(16)	3949(2)	1434(2)	4565(3)	41(1)
C(17)	3283(2)	1821(2)	4533(3)	33(1)
C(18)	3079(3)	2386(2)	5329(3)	48(1)
C(19)	3731(3)	2806(3)	5750(4)	63(1)
C(20)	2661(3)	1977(4)	6139(4)	75(2)
C(21)	385(2)	3479(2)	1934(3)	29(1)
C(22)	309(2)	4029(2)	1221(3)	31(1)
C(23)	921(2)	4379(2)	801(3)	27(1)
C(24)	2497(2)	4843(2)	22(3)	30(1)
C(25)	3226(2)	4797(2)	-16(3)	30(1)
C(26)	2884(2)	4042(2)	1278(3)	23(1)
C(27)	4206(2)	4035(2)	793(3)	26(1)
C(28)	4388(2)	3392(2)	263(3)	34(1)
C(29)	3825(2)	2962(2)	-356(3)	35(1)
C(30)	3935(2)	2104(2)	-317(4)	53(1)
C(31)	3840(3)	3217(3)	-1422(3)	52(1)
C(32)	5102(2)	3119(2)	319(3)	43(1)
C(33)	5616(2)	3485(3)	883(4)	48(1)

C(34)	5423(2)	4113(3)	1419(3)	44(1)
C(35)	4720(2)	4403(2)	1389(3)	38(1)
C(36)	4505(2)	5091(3)	2003(4)	56(1)
C(37)	4928(3)	5133(3)	2971(4)	71(2)
C(38)	4605(4)	5825(3)	1433(5)	92(2)
C(39)	-1836(3)	7299(4)	4203(5)	98(2)
C(40)	-1355(4)	7230(6)	3395(5)	149(4)
C(41)	-354(4)	6508(5)	2349(6)	160(4)
C(42)	214(3)	5924(4)	2472(6)	37(1)
C(43)	-354(4)	6508(5)	2349(6)	160(4)
C(44)	-790(4)	6579(5)	1442(6)	37(1)
Fe(1)	2634(1)	3440(1)	2365(1)	20(1)
N(1)	3469(1)	4327(2)	734(2)	25(1)
N(2)	2285(1)	4387(2)	800(2)	23(1)
N(3)	1699(1)	3629(2)	1840(2)	22(1)
N(4)	1314(1)	2757(2)	2903(2)	24(1)
N(5)	2131(2)	2090(2)	3671(2)	26(1)
N(6)	3528(2)	3084(2)	2626(2)	26(1)
N(7)	4097(2)	2872(2)	2806(2)	37(1)
P(1)	2539(1)	4351(1)	3454(1)	28(1)
O(1)	-845(4)	6616(5)	3233(6)	183(3)

Table 15. Bond lengths [≈] and angles [∞] for **4**.

C(1)-P(1)	1.830(4)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-P(1)	1.828(4)
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
C(3)-P(1)	1.823(4)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-N(3)	1.358(4)
C(4)-C(23)	1.363(5)
C(4)-N(2)	1.396(4)
C(5)-N(4)	1.368(4)
C(5)-N(3)	1.372(4)
C(5)-C(21)	1.387(4)
C(6)-N(5)	1.380(4)
C(6)-N(4)	1.403(4)
C(6)-Fe(1)	1.888(3)
C(7)-C(8)	1.328(5)
C(7)-N(5)	1.400(4)
C(7)-H(7)	0.9500
C(8)-N(4)	1.397(4)
C(8)-H(8)	0.9500
C(9)-C(17)	1.388(5)
C(9)-C(10)	1.391(5)
C(9)-N(5)	1.453(4)
C(10)-C(14)	1.383(5)
C(10)-C(11)	1.529(5)
C(11)-C(12)	1.523(5)
C(11)-C(13)	1.532(5)
C(11)-H(11)	1.0000
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800

C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(15)	1.380(5)
C(14)-H(14)	0.9500
C(15)-C(16)	1.366(6)
C(15)-H(15)	0.9500
C(16)-C(17)	1.390(5)
C(16)-H(16)	0.9500
C(17)-C(18)	1.518(6)
C(18)-C(19)	1.511(6)
C(18)-C(20)	1.526(7)
C(18)-H(18)	1.0000
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.379(5)
C(21)-H(21)	0.9500
C(22)-C(23)	1.396(5)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
C(24)-C(25)	1.331(5)
C(24)-N(2)	1.387(5)
C(24)-H(24)	0.9500
C(25)-N(1)	1.389(4)
C(25)-H(25)	0.9500
C(26)-N(1)	1.394(4)
C(26)-N(2)	1.410(4)
C(26)-Fe(1)	1.881(3)
C(27)-C(28)	1.379(5)
C(27)-C(35)	1.399(5)
C(27)-N(1)	1.441(4)
C(28)-C(32)	1.389(5)
C(28)-C(29)	1.529(5)

C(29)-C(30)	1.513(5)
C(29)-C(31)	1.529(6)
C(29)-H(29)	1.0000
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-C(33)	1.373(6)
C(32)-H(32)	0.9500
C(33)-C(34)	1.367(6)
C(33)-H(33)	0.9500
C(34)-C(35)	1.379(5)
C(34)-H(34)	0.9500
C(35)-C(36)	1.520(6)
C(36)-C(38)	1.514(7)
C(36)-C(37)	1.538(7)
C(36)-H(36)	1.0000
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-C(40)	1.419(6)
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-O(1)	1.436(10)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(41)-C(42)	1.463(7)
C(41)-O(1)	1.520(10)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800

C(42)-H(42C)	0.9800
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
Fe(1)-N(6)	1.779(3)
Fe(1)-N(3)	1.880(3)
Fe(1)-P(1)	2.1898(11)
N(6)-N(7)	1.129(4)

P(1)-C(1)-H(1A)	109.5
P(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
P(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
P(1)-C(2)-H(2A)	109.5
P(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
P(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
P(1)-C(3)-H(3A)	109.5
P(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
P(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
N(3)-C(4)-C(23)	123.8(3)
N(3)-C(4)-N(2)	107.5(3)
C(23)-C(4)-N(2)	128.7(3)
N(4)-C(5)-N(3)	108.3(3)
N(4)-C(5)-C(21)	129.7(3)
N(3)-C(5)-C(21)	121.9(3)
N(5)-C(6)-N(4)	102.2(3)
N(5)-C(6)-Fe(1)	142.7(2)
N(4)-C(6)-Fe(1)	114.9(2)
C(8)-C(7)-N(5)	108.6(3)
C(8)-C(7)-H(7)	125.7

N(5)-C(7)-H(7)	125.7
C(7)-C(8)-N(4)	106.2(3)
C(7)-C(8)-H(8)	126.9
N(4)-C(8)-H(8)	126.9
C(17)-C(9)-C(10)	122.1(3)
C(17)-C(9)-N(5)	119.6(3)
C(10)-C(9)-N(5)	118.1(3)
C(14)-C(10)-C(9)	117.8(3)
C(14)-C(10)-C(11)	119.6(3)
C(9)-C(10)-C(11)	122.6(3)
C(12)-C(11)-C(10)	110.4(3)
C(12)-C(11)-C(13)	111.3(3)
C(10)-C(11)-C(13)	111.2(3)
C(12)-C(11)-H(11)	108.0
C(10)-C(11)-H(11)	108.0
C(13)-C(11)-H(11)	108.0
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(10)	121.0(4)
C(15)-C(14)-H(14)	119.5
C(10)-C(14)-H(14)	119.5
C(16)-C(15)-C(14)	120.2(3)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(15)-C(16)-C(17)	120.9(4)
C(15)-C(16)-H(16)	119.6
C(17)-C(16)-H(16)	119.6
C(9)-C(17)-C(16)	118.0(4)

C(9)-C(17)-C(18)	121.5(3)
C(16)-C(17)-C(18)	120.5(4)
C(19)-C(18)-C(17)	113.5(4)
C(19)-C(18)-C(20)	110.0(4)
C(17)-C(18)-C(20)	110.0(4)
C(19)-C(18)-H(18)	107.7
C(17)-C(18)-H(18)	107.7
C(20)-C(18)-H(18)	107.7
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(22)-C(21)-C(5)	118.1(3)
C(22)-C(21)-H(21)	121.0
C(5)-C(21)-H(21)	121.0
C(21)-C(22)-C(23)	121.2(3)
C(21)-C(22)-H(22)	119.4
C(23)-C(22)-H(22)	119.4
C(4)-C(23)-C(22)	117.3(3)
C(4)-C(23)-H(23)	121.3
C(22)-C(23)-H(23)	121.3
C(25)-C(24)-N(2)	105.9(3)
C(25)-C(24)-H(24)	127.0
N(2)-C(24)-H(24)	127.0
C(24)-C(25)-N(1)	108.9(3)
C(24)-C(25)-H(25)	125.5
N(1)-C(25)-H(25)	125.5
N(1)-C(26)-N(2)	100.9(3)
N(1)-C(26)-Fe(1)	144.1(3)
N(2)-C(26)-Fe(1)	114.9(2)

C(28)-C(27)-C(35)	121.5(3)
C(28)-C(27)-N(1)	118.9(3)
C(35)-C(27)-N(1)	119.6(3)
C(27)-C(28)-C(32)	118.4(4)
C(27)-C(28)-C(29)	122.2(3)
C(32)-C(28)-C(29)	119.4(4)
C(30)-C(29)-C(28)	112.3(3)
C(30)-C(29)-C(31)	108.7(4)
C(28)-C(29)-C(31)	112.1(3)
C(30)-C(29)-H(29)	107.8
C(28)-C(29)-H(29)	107.8
C(31)-C(29)-H(29)	107.8
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(29)-C(31)-H(31A)	109.5
C(29)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(29)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(33)-C(32)-C(28)	120.8(4)
C(33)-C(32)-H(32)	119.6
C(28)-C(32)-H(32)	119.6
C(34)-C(33)-C(32)	120.1(4)
C(34)-C(33)-H(33)	120.0
C(32)-C(33)-H(33)	120.0
C(33)-C(34)-C(35)	121.2(4)
C(33)-C(34)-H(34)	119.4
C(35)-C(34)-H(34)	119.4
C(34)-C(35)-C(27)	118.1(4)
C(34)-C(35)-C(36)	120.9(4)
C(27)-C(35)-C(36)	121.0(3)
C(38)-C(36)-C(35)	110.6(4)
C(38)-C(36)-C(37)	110.2(4)

C(35)-C(36)-C(37)	112.8(4)
C(38)-C(36)-H(36)	107.7
C(35)-C(36)-H(36)	107.7
C(37)-C(36)-H(36)	107.7
C(36)-C(37)-H(37A)	109.5
C(36)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(36)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(36)-C(38)-H(38A)	109.5
C(36)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(36)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(40)-C(39)-H(39A)	109.5
C(40)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(40)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(39)-C(40)-O(1)	125.7(9)
C(39)-C(40)-H(40A)	105.9
O(1)-C(40)-H(40A)	105.9
C(39)-C(40)-H(40B)	105.9
O(1)-C(40)-H(40B)	105.9
H(40A)-C(40)-H(40B)	106.2
C(42)-C(41)-O(1)	114.3(7)
C(42)-C(41)-H(41A)	108.7
O(1)-C(41)-H(41A)	108.7
C(42)-C(41)-H(41B)	108.7
O(1)-C(41)-H(41B)	108.7
H(41A)-C(41)-H(41B)	107.6
H(44A)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
N(6)-Fe(1)-N(3)	165.47(13)

N(6)-Fe(1)-C(26)	97.64(14)
N(3)-Fe(1)-C(26)	79.50(13)
N(6)-Fe(1)-C(6)	98.92(13)
N(3)-Fe(1)-C(6)	79.36(13)
C(26)-Fe(1)-C(6)	153.76(15)
N(6)-Fe(1)-P(1)	100.95(10)
N(3)-Fe(1)-P(1)	93.58(9)
C(26)-Fe(1)-P(1)	98.89(11)
C(6)-Fe(1)-P(1)	97.79(11)
C(25)-N(1)-C(26)	111.4(3)
C(25)-N(1)-C(27)	123.3(3)
C(26)-N(1)-C(27)	123.8(3)
C(24)-N(2)-C(4)	131.6(3)
C(24)-N(2)-C(26)	112.8(3)
C(4)-N(2)-C(26)	115.2(3)
C(4)-N(3)-C(5)	117.6(3)
C(4)-N(3)-Fe(1)	121.6(2)
C(5)-N(3)-Fe(1)	120.5(2)
C(5)-N(4)-C(8)	132.4(3)
C(5)-N(4)-C(6)	115.6(3)
C(8)-N(4)-C(6)	111.9(3)
C(6)-N(5)-C(7)	111.1(3)
C(6)-N(5)-C(9)	121.4(3)
C(7)-N(5)-C(9)	124.0(3)
N(7)-N(6)-Fe(1)	178.4(3)
C(3)-P(1)-C(2)	100.8(2)
C(3)-P(1)-C(1)	98.7(2)
C(2)-P(1)-C(1)	100.6(2)
C(3)-P(1)-Fe(1)	115.24(15)
C(2)-P(1)-Fe(1)	121.59(16)
C(1)-P(1)-Fe(1)	116.27(16)
C(40)-O(1)-C(41)	126.7(8)

Symmetry transformations used to generate equivalent atoms:

Table 16. Anisotropic displacement parameters ($\approx^2$x 10^3)for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	53(2)	32(2)	49(3)	-2(2)	2(2)	11(2)
C(2)	57(3)	48(3)	38(2)	-10(2)	-17(2)	1(2)
C(3)	56(3)	46(3)	49(3)	-10(2)	18(2)	-5(2)
C(4)	23(2)	24(2)	27(2)	-1(2)	5(1)	4(1)
C(5)	19(1)	26(2)	26(2)	1(2)	1(1)	0(1)
C(6)	26(2)	24(2)	22(2)	1(2)	1(1)	2(1)
C(7)	25(2)	34(2)	31(2)	13(2)	5(2)	-3(2)
C(8)	25(2)	25(2)	37(2)	7(2)	7(2)	-3(1)
C(9)	20(2)	35(2)	32(2)	15(2)	1(1)	2(1)
C(10)	28(2)	34(2)	28(2)	11(2)	5(2)	2(2)
C(11)	30(2)	46(2)	23(2)	2(2)	-1(2)	9(1)
C(12)	61(3)	47(3)	27(2)	6(2)	1(2)	8(2)
C(13)	43(2)	43(2)	36(3)	6(2)	0(2)	-2(2)
C(14)	27(2)	42(2)	33(2)	13(2)	8(2)	7(2)
C(15)	22(2)	49(3)	46(2)	20(2)	4(2)	2(2)
C(16)	34(2)	47(3)	41(2)	22(2)	-11(2)	-9(2)
C(17)	33(2)	35(2)	32(2)	12(2)	-4(2)	-7(2)
C(18)	58(3)	40(3)	48(3)	3(2)	-18(2)	-3(2)
C(19)	78(4)	56(3)	54(3)	0(3)	-36(3)	-8(3)
C(20)	84(4)	87(4)	53(3)	-16(3)	17(3)	-12(3)
C(21)	18(2)	30(2)	39(2)	-1(2)	2(1)	1(1)
C(22)	20(2)	30(2)	44(2)	2(2)	-3(2)	5(1)
C(23)	27(2)	27(2)	27(2)	6(2)	-2(1)	5(1)
C(24)	37(2)	23(2)	30(2)	9(2)	0(1)	0(2)
C(25)	34(2)	23(2)	33(2)	14(2)	9(2)	-1(2)
C(26)	24(2)	18(2)	26(2)	-2(2)	1(1)	-2(1)
C(27)	23(2)	27(2)	30(2)	9(2)	5(1)	-3(1)
C(28)	26(2)	40(2)	34(2)	7(2)	6(2)	-1(2)
C(29)	28(2)	36(2)	40(2)	-2(2)	4(2)	1(2)
C(30)	40(2)	42(3)	77(3)	-10(3)	5(2)	-7(2)
C(31)	59(3)	50(3)	45(3)	-3(2)	-5(2)	-4(2)
C(32)	29(2)	50(3)	49(3)	-1(2)	7(2)	7(2)
C(33)	25(2)	61(3)	59(3)	5(3)	2(2)	2(2)

C(34)	28(2)	52(3)	52(3)	-2(2)	-1(2)	-6(2)
C(35)	29(2)	37(2)	47(2)	3(2)	9(2)	-6(2)
C(36)	30(2)	55(3)	84(4)	-19(3)	-4(2)	-7(2)
C(37)	60(3)	76(4)	77(4)	-28(3)	0(3)	-19(3)
C(38)	120(5)	44(3)	111(5)	-3(4)	-41(4)	-4(3)
C(39)	58(4)	144(6)	91(5)	-9(5)	-1(3)	-11(4)
C(40)	96(5)	285(13)	68(5)	-43(6)	-27(4)	102(7)
C(41)	121(6)	303(12)	57(4)	-15(6)	27(5)	-110(8)
C(42)	22(2)	51(3)	37(3)	-25(3)	4(2)	-4(2)
C(43)	121(6)	303(12)	57(4)	-15(6)	27(5)	-110(8)
C(44)	22(2)	51(3)	37(3)	-25(3)	4(2)	-4(2)
Fe(1)	17(1)	22(1)	22(1)	3(1)	1(1)	0(1)
N(1)	22(1)	25(2)	29(2)	7(1)	3(1)	-6(1)
N(2)	22(1)	22(2)	26(2)	5(1)	3(1)	3(1)
N(3)	20(1)	22(2)	22(2)	3(1)	1(1)	1(1)
N(4)	19(1)	23(2)	30(2)	4(1)	3(1)	-2(1)
N(5)	21(1)	27(2)	29(2)	4(1)	2(1)	-2(1)
N(6)	25(2)	25(2)	29(2)	7(1)	3(1)	-2(1)
N(7)	20(2)	41(2)	49(2)	16(2)	2(1)	3(1)
P(1)	31(1)	27(1)	27(1)	-2(1)	2(1)	-1(1)
O(1)	131(6)	259(9)	158(7)	-49(6)	20(5)	-56(5)