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Table 1. Crystal data and structure refinement for 1.

Identification code	1
Empirical formula	C10 H12 B2 Fe O4
Formula weight	273.67
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 7.429(6) A alpha = 90 deg. b = 7.011(4) A beta = 90.62(5) deg. c = 10.031(5) A gamma = 90 deg.
Volume	522.4(6) A^3
Z, Calculated density	2, 1.740 Mg/m^3
Absorption coefficient	1.438 mm^-1
F(000)	280
Crystal size	0.30 x 0.15 x 0.11 mm
Theta range for data collection	3.55 to 26.97 deg.
Limiting indices	-9<=h<=9, -8<=k<=8, 0<=l<=11
Reflections collected / unique	1915 / 944 [R(int) = 0.1326]
Completeness to theta = 26.97	88.3 %
Absorption correction	Psi-scan
Max. and min. transmission	1.0000 and 0.7836
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	944 / 0 / 71
Goodness-of-fit on F^2	0.986
Final R indices [I>2sigma(I)]	R1 = 0.0913, wR2 = 0.2219
R indices (all data)	R1 = 0.1532, wR2 = 0.2598
Extinction coefficient	0.001(7)
Largest diff. peak and hole	1.236 and -0.893 e.A^-3

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

	x	y	z	U(eq)
Fe	0	0	0	17(1)
O(2)	-4068(11)	3243(12)	1042(8)	36(2)
O(1)	-3983(11)	3338(12)	-1294(8)	36(2)
B(1)	-3630(16)	2384(19)	-136(14)	28(3)
C(1)	-2693(10)	369(10)	-208(8)	33(3)
C(2)	-2038(12)	-507(12)	-1383(6)	38(3)
C(3)	-1186(12)	-2244(11)	-1012(8)	45(4)
C(4)	-1315(11)	-2441(10)	393(9)	36(3)
C(5)	-2246(12)	-826(13)	890(6)	48(4)

Table 3. Bond lengths [A] and angles [deg] for 1.

Fe-C(5)#1	1.987(8)
Fe-C(5)	1.987(8)
Fe-C(4)#1	2.011(8)
Fe-C(4)	2.011(8)
Fe-C(1)	2.026(7)
Fe-C(1)#1	2.026(7)
Fe-C(3)#1	2.064(8)
Fe-C(3)	2.064(8)
Fe-C(2)#1	2.073(8)
Fe-C(2)	2.073(8)
O(2)-B(1)	1.369(15)
O(1)-B(1)	1.364(16)
B(1)-C(1)	1.576(14)
C(1)-C(2)	1.4200
C(1)-C(5)	1.4200
C(2)-C(3)	1.4200
C(3)-C(4)	1.4200
C(4)-C(5)	1.4200
C(5)#1-Fe-C(5)	180.0(7)
C(5)#1-Fe-C(4)#1	41.60(15)
C(5)-Fe-C(4)#1	138.4(7)
C(5)#1-Fe-C(4)	138.4(7)
C(5)-Fe-C(4)	41.60(15)
C(4)#1-Fe-C(4)	180.0(10)
C(5)#1-Fe-C(1)	138.6(7)
C(5)-Fe-C(1)	41.43(15)
C(4)#1-Fe-C(1)	110.6(7)
C(4)-Fe-C(1)	69.37(19)
C(5)#1-Fe-C(1)#1	41.4(7)
C(5)-Fe-C(1)#1	138.57(15)
C(4)#1-Fe-C(1)#1	69.4(7)
C(4)-Fe-C(1)#1	110.63(19)
C(1)-Fe-C(1)#1	180.0(4)
C(5)#1-Fe-C(3)#1	69.06(19)
C(5)-Fe-C(3)#1	110.9(8)

C(4)#1-Fe-C(3)#1	40.75(14)
C(4)-Fe-C(3)#1	139.2(8)
C(1)-Fe-C(3)#1	111.7(7)
C(1)#1-Fe-C(3)#1	68.3(7)
C(5)#1-Fe-C(3)	110.9(8)
C(5)-Fe-C(3)	69.06(19)
C(4)#1-Fe-C(3)	139.2(8)
C(4)-Fe-C(3)	40.75(14)
C(1)-Fe-C(3)	68.34(18)
C(1)#1-Fe-C(3)	111.66(18)
C(3)#1-Fe-C(3)	180.0(12)
C(5)#1-Fe-C(2)#1	68.88(18)
C(5)-Fe-C(2)#1	111.1(8)
C(4)#1-Fe-C(2)#1	68.44(19)
C(4)-Fe-C(2)#1	111.6(7)
C(1)-Fe-C(2)#1	139.5(7)
C(1)#1-Fe-C(2)#1	40.5(7)
C(3)#1-Fe-C(2)#1	40.14(15)
C(3)-Fe-C(2)#1	139.9(6)
C(5)#1-Fe-C(2)	111.1(8)
C(5)-Fe-C(2)	68.88(18)
C(4)#1-Fe-C(2)	111.6(7)
C(4)-Fe-C(2)	68.44(19)
C(1)-Fe-C(2)	40.51(14)
C(1)#1-Fe-C(2)	139.49(14)
C(3)#1-Fe-C(2)	139.9(6)
C(3)-Fe-C(2)	40.14(15)
C(2)#1-Fe-C(2)	180.0(9)
O(2)-B(1)-O(1)	118.3(11)
O(2)-B(1)-C(1)	122.9(11)
O(1)-B(1)-C(1)	118.8(10)
C(2)-C(1)-C(5)	108.0
C(2)-C(1)-B(1)	125.5(7)
C(5)-C(1)-B(1)	126.4(7)
C(2)-C(1)-Fe	71.5(3)
C(5)-C(1)-Fe	67.8(3)
B(1)-C(1)-Fe	123.1(6)
C(3)-C(2)-C(1)	108.0
C(3)-C(2)-Fe	69.6(3)
C(1)-C(2)-Fe	68.0(3)
C(4)-C(3)-C(2)	108.0
C(4)-C(3)-Fe	67.6(3)
C(2)-C(3)-Fe	70.3(3)
C(5)-C(4)-C(3)	108.0
C(5)-C(4)-Fe	68.3(3)
C(3)-C(4)-Fe	71.6(3)
C(4)-C(5)-C(1)	108.0
C(4)-C(5)-Fe	70.1(3)
C(1)-C(5)-Fe	70.8(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z

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Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe	16(1)	19(1)	17(1)	-3(1)	-1(1)	3(1)
O(2)	50(5)	30(4)	28(5)	5(4)	-1(4)	8(4)
O(1)	50(5)	34(4)	24(5)	4(4)	-6(4)	18(4)
B(1)	28(6)	30(6)	26(8)	-11(6)	3(6)	-8(5)
C(1)	16(4)	46(8)	38(7)	-11(6)	0(5)	5(5)
C(2)	43(6)	49(8)	22(7)	-20(5)	-6(5)	22(6)
C(3)	50(7)	53(8)	33(8)	-14(7)	-15(7)	10(7)
C(4)	32(5)	18(5)	60(9)	16(6)	20(6)	1(5)
C(5)	52(7)	64(8)	30(8)	23(7)	16(6)	11(7)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(2)	-2148	-27	-2245	45
H(3)	-640	-3101	-1588	55
H(4)	-868	-3450	898	44
H(5)	-2516	-592	1778	58

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Table 6. Crystal data and structure refinement for 2a.

Identification code	2a
Empirical formula	C15 H14 B Fe N O2
Formula weight	306.93
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/a
Unit cell dimensions	a = 8.838(2) A alpha = 90 deg. b = 9.385(4) A beta = 96.400(10) deg. c = 15.937(3) A gamma = 90 deg.
Volume	1313.7(7) A^3
Z, Calculated density	4, 1.552 Mg/m^3
Absorption coefficient	1.146 mm^-1
F(000)	632
Crystal size	0.19 x 0.17 x 0.16 mm
Theta range for data collection	3.33 to 24.96 deg.
Limiting indices	-10<=h<=10, 0<=k<=11, 0<=l<=18
Reflections collected / unique	2393 / 2307 [R(int) = 0.1394]
Completeness to theta = 24.96	99.7 %
Absorption correction	Psi-scan
Max. and min. transmission	1.00 and 0.86
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2307 / 0 / 92
Goodness-of-fit on F^2	0.928
Final R indices [I>2sigma(I)]	R1 = 0.0682, wR2 = 0.1447
R indices (all data)	R1 = 0.2642, wR2 = 0.2228
Largest diff. peak and hole	0.626 and -0.564 e.A^-3

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Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 2a.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	2113(2)	5119(2)	1536(1)	32(1)
C(1)	1444(8)	3931(8)	2506(3)	33(3)
C(2)	226(7)	4797(7)	2143(4)	35(2)
C(3)	-76(7)	4429(8)	1276(4)	41(3)
C(4)	956(9)	3336(8)	1104(3)	46(3)
C(5)	1896(8)	3028(7)	1864(5)	37(3)
C(6)	3878(8)	6448(8)	1988(3)	37(3)
C(7)	2653(8)	7243(7)	1568(4)	38(3)
C(8)	2386(8)	6739(8)	724(4)	42(3)
C(9)	3446(9)	5632(8)	623(4)	45(3)
C(10)	4369(8)	5453(7)	1404(4)	40(3)
B(1)	4504(13)	6595(15)	2935(8)	36(3)
O(1)	3777(9)	7434(9)	3489(5)	53(2)
O(2)	5835(8)	6020(9)	3214(5)	48(2)
C(11)	2142(12)	3980(11)	3414(6)	33(3)
C(12)	1485(12)	4769(13)	3992(6)	44(3)
C(13)	2116(13)	4770(14)	4820(7)	56(3)
N(1)	3369(11)	4012(11)	5098(6)	51(3)
C(14)	4012(15)	3271(14)	4526(8)	56(4)
C(15)	3435(13)	3241(13)	3689(7)	47(3)

Table 8. Bond lengths [A] and angles [deg] for 2a.

Fe(1)-C(9)	2.029(7)
Fe(1)-C(8)	2.027(7)
Fe(1)-C(4)	2.041(8)
Fe(1)-C(3)	2.038(7)
Fe(1)-C(5)	2.045(7)
Fe(1)-C(2)	2.042(7)
Fe(1)-C(1)	2.046(7)
Fe(1)-C(10)	2.052(7)
Fe(1)-C(7)	2.049(7)
Fe(1)-C(6)	2.064(7)
C(1)-C(2)	1.4200
C(1)-C(5)	1.4200
C(1)-C(11)	1.509(11)
C(2)-C(3)	1.4200
C(2)-H(2)	0.9300
C(3)-C(4)	1.4200
C(3)-H(3)	0.9300
C(4)-C(5)	1.4200
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
C(6)-C(7)	1.4200
C(6)-C(10)	1.4200
C(6)-B(1)	1.554(13)
C(7)-C(8)	1.4200
C(7)-H(7)	0.9300
C(8)-C(9)	1.4200

C(8)-H(8)	0.9300
C(9)-C(10)	1.4200
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
B(1)-O(2)	1.325(14)
B(1)-O(1)	1.393(14)
O(2)-H(200)	1.33(13)
C(11)-C(12)	1.361(13)
C(11)-C(15)	1.366(14)
C(12)-C(13)	1.373(14)
C(12)-H(12)	0.9300
C(13)-N(1)	1.349(14)
C(13)-H(13)	0.9300
N(1)-C(14)	1.324(15)
C(14)-C(15)	1.374(15)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300

C(9)-Fe(1)-C(8)	40.98(13)
C(9)-Fe(1)-C(4)	105.2(3)
C(8)-Fe(1)-C(4)	119.4(3)
C(9)-Fe(1)-C(3)	122.9(3)
C(8)-Fe(1)-C(3)	106.6(3)
C(4)-Fe(1)-C(3)	40.74(13)
C(9)-Fe(1)-C(5)	119.3(3)
C(8)-Fe(1)-C(5)	154.6(3)
C(4)-Fe(1)-C(5)	40.67(14)
C(3)-Fe(1)-C(5)	68.47(18)
C(9)-Fe(1)-C(2)	160.9(3)
C(8)-Fe(1)-C(2)	125.1(3)
C(4)-Fe(1)-C(2)	68.50(17)
C(3)-Fe(1)-C(2)	40.73(12)
C(5)-Fe(1)-C(2)	68.40(17)
C(9)-Fe(1)-C(1)	155.6(3)
C(8)-Fe(1)-C(1)	162.8(3)
C(4)-Fe(1)-C(1)	68.41(17)
C(3)-Fe(1)-C(1)	68.45(16)
C(5)-Fe(1)-C(1)	40.61(13)
C(2)-Fe(1)-C(1)	40.65(12)
C(9)-Fe(1)-C(10)	40.72(13)
C(8)-Fe(1)-C(10)	68.56(17)
C(4)-Fe(1)-C(10)	123.1(3)
C(3)-Fe(1)-C(10)	159.8(3)
C(5)-Fe(1)-C(10)	107.0(3)
C(2)-Fe(1)-C(10)	157.7(3)
C(1)-Fe(1)-C(10)	121.7(3)
C(9)-Fe(1)-C(7)	68.58(17)
C(8)-Fe(1)-C(7)	40.77(14)
C(4)-Fe(1)-C(7)	155.9(3)
C(3)-Fe(1)-C(7)	121.8(3)
C(5)-Fe(1)-C(7)	162.8(3)
C(2)-Fe(1)-C(7)	109.4(3)
C(1)-Fe(1)-C(7)	126.7(3)
C(10)-Fe(1)-C(7)	68.16(16)
C(9)-Fe(1)-C(6)	68.29(17)
C(8)-Fe(1)-C(6)	68.33(17)
C(4)-Fe(1)-C(6)	160.8(3)
C(3)-Fe(1)-C(6)	157.9(3)
C(5)-Fe(1)-C(6)	125.4(3)
C(2)-Fe(1)-C(6)	123.3(3)
C(1)-Fe(1)-C(6)	109.6(2)
C(10)-Fe(1)-C(6)	40.37(13)
C(7)-Fe(1)-C(6)	40.40(13)

C(2)-C(1)-C(5)	108.0
C(2)-C(1)-C(11)	125.7(6)
C(5)-C(1)-C(11)	126.3(6)
C(2)-C(1)-Fe(1)	69.5(3)
C(5)-C(1)-Fe(1)	69.7(3)
C(11)-C(1)-Fe(1)	125.9(6)
C(3)-C(2)-C(1)	108.0
C(3)-C(2)-Fe(1)	69.5(3)
C(1)-C(2)-Fe(1)	69.8(3)
C(3)-C(2)-H(2)	126.0
C(1)-C(2)-H(2)	126.0
Fe(1)-C(2)-H(2)	126.2
C(2)-C(3)-C(4)	108.0
C(2)-C(3)-Fe(1)	69.8(3)
C(4)-C(3)-Fe(1)	69.7(3)
C(2)-C(3)-H(3)	126.0
C(4)-C(3)-H(3)	126.0
Fe(1)-C(3)-H(3)	126.1
C(5)-C(4)-C(3)	108.0
C(5)-C(4)-Fe(1)	69.8(3)
C(3)-C(4)-Fe(1)	69.5(3)
C(5)-C(4)-H(4)	126.0
C(3)-C(4)-H(4)	126.0
Fe(1)-C(4)-H(4)	126.2
C(4)-C(5)-C(1)	108.0
C(4)-C(5)-Fe(1)	69.5(3)
C(1)-C(5)-Fe(1)	69.7(3)
C(4)-C(5)-H(5)	126.0
C(1)-C(5)-H(5)	126.0
Fe(1)-C(5)-H(5)	126.4
C(7)-C(6)-C(10)	108.0
C(7)-C(6)-B(1)	125.6(7)
C(10)-C(6)-B(1)	126.4(7)
C(7)-C(6)-Fe(1)	69.2(3)
C(10)-C(6)-Fe(1)	69.4(3)
B(1)-C(6)-Fe(1)	124.5(6)
C(8)-C(7)-C(6)	108.0
C(8)-C(7)-Fe(1)	68.8(3)
C(6)-C(7)-Fe(1)	70.4(3)
C(8)-C(7)-H(7)	126.0
C(6)-C(7)-H(7)	126.0
Fe(1)-C(7)-H(7)	126.4
C(7)-C(8)-C(9)	108.0
C(7)-C(8)-Fe(1)	70.4(3)
C(9)-C(8)-Fe(1)	69.6(3)
C(7)-C(8)-H(8)	126.0
C(9)-C(8)-H(8)	126.0
Fe(1)-C(8)-H(8)	125.6
C(10)-C(9)-C(8)	108.0
C(10)-C(9)-Fe(1)	70.5(3)
C(8)-C(9)-Fe(1)	69.4(3)
C(10)-C(9)-H(9)	126.0
C(8)-C(9)-H(9)	126.0
Fe(1)-C(9)-H(9)	125.7
C(9)-C(10)-C(6)	108.0
C(9)-C(10)-Fe(1)	68.8(3)
C(6)-C(10)-Fe(1)	70.3(3)
C(9)-C(10)-H(10)	126.0
C(6)-C(10)-H(10)	126.0
Fe(1)-C(10)-H(10)	126.5
O(2)-B(1)-O(1)	118.2(10)
O(2)-B(1)-C(6)	119.7(10)
O(1)-B(1)-C(6)	121.7(10)

B(1)-O(2)-H(200)	120(5)
C(12)-C(11)-C(15)	117.6(10)
C(12)-C(11)-C(1)	120.4(9)
C(15)-C(11)-C(1)	122.0(10)
C(11)-C(12)-C(13)	119.5(11)
C(11)-C(12)-H(12)	120.3
C(13)-C(12)-H(12)	120.3
N(1)-C(13)-C(12)	123.1(12)
N(1)-C(13)-H(13)	118.5
C(12)-C(13)-H(13)	118.5
C(14)-N(1)-C(13)	116.8(11)
N(1)-C(14)-C(15)	122.5(13)
N(1)-C(14)-H(14)	118.7
C(15)-C(14)-H(14)	118.7
C(11)-C(15)-C(14)	120.5(12)
C(11)-C(15)-H(15)	119.7
C(14)-C(15)-H(15)	119.7

Table 9. Anisotropic displacement parameters (A^2 x 10^3) for 2a. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe(1)	32(1)	35(1)	29(1)	-1(1)	2(1)	-3(1)
B(1)	16(6)	47(9)	46(8)	-5(7)	6(6)	-11(6)
O(1)	45(5)	71(6)	42(5)	-17(5)	3(4)	-6(5)
O(2)	33(5)	68(6)	43(5)	8(4)	-4(4)	1(4)
N(1)	47(6)	62(7)	45(6)	8(6)	2(5)	-6(6)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 2a.

	x	y	z	U(eq)
H(2)	-285	5484	2424	42
H(3)	-819	4834	890	49
H(4)	1007	2898	584	55
H(5)	2671	2353	1929	44
H(7)	2119	7967	1804	45
H(8)	1646	7074	311	50
H(9)	3523	5116	132	54
H(10)	5156	4798	1514	48
H(200)	6260(140)	5960(130)	4040(80)	80(40)
H(12)	616	5303	3828	53
H(13)	1658	5319	5206	68
H(14)	4887	2750	4697	67
H(15)	3928	2714	3307	56

Table 11. Crystal data and structure refinement for 2b.

Identification code	2b
Empirical formula	C15 H15 B Fe N O2.50
Formula weight	315.94
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 17.330(3) A alpha = 90 deg. b = 13.121(3) A beta = 131.08(2) deg. c = 15.996(3) A gamma = 90 deg.
Volume	2741.8(9) A^3
Z, Calculated density	8, 1.536 Mg/m^3
Absorption coefficient	1.103 mm^-1
F(000)	1304
Crystal size	0.19 x 0.17 x 0.16 mm
Theta range for data collection	3.06 to 24.98 deg.
Limiting indices	-20<=h<=15, 0<=k<=15, 0<=l<=18
Reflections collected / unique	2503 / 2411 [R(int) = 0.0265]
Completeness to theta = 24.98	99.8 %
Absorption correction	Psi-scan
Max. and min. transmission	1.0000 and 0.4638
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2411 / 0 / 194
Goodness-of-fit on F^2	0.769
Final R indices [I>2sigma(I)]	R1 = 0.0378, wR2 = 0.0947
R indices (all data)	R1 = 0.0835, wR2 = 0.1245
Largest diff. peak and hole	0.410 and -0.445 e.A^-3

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 2b.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	3636(1)	3250(1)	2887(1)	38(1)
C(1)	4068(3)	4065(3)	4223(3)	40(1)
C(2)	4897(3)	3471(3)	4504(4)	48(1)
C(3)	5097(3)	3768(4)	3810(4)	52(1)
C(4)	4400(3)	4536(3)	3097(4)	51(1)
C(5)	3776(3)	4724(3)	3352(4)	44(1)
C(6)	3319(3)	1736(3)	2679(3)	45(1)
C(7)	3440(4)	2082(3)	1920(4)	52(1)
C(8)	2709(4)	2852(4)	1259(4)	60(1)
C(9)	2128(4)	3000(4)	1566(4)	56(1)
C(10)	2492(4)	2315(3)	2432(4)	49(1)
B(1)	4050(4)	993(4)	3663(4)	47(1)
O(1)	3919(3)	727(3)	4391(3)	59(1)
O(2)	4839(3)	576(3)	3801(3)	66(1)
C(11)	3596(3)	3998(3)	4711(3)	40(1)
C(12)	2779(4)	4616(4)	4347(4)	60(1)
C(13)	2341(4)	4536(4)	4815(5)	65(1)
N(1)	2645(3)	3894(3)	5619(3)	57(1)
C(14)	3440(4)	3313(4)	5975(4)	63(1)
C(15)	3931(4)	3339(4)	5561(4)	54(1)
O(3)	0	3933(11)	2500	257(7)

Table 13. Bond lengths [A] and angles [deg] for 2b.

Fe(1)-C(10)	2.017(5)
Fe(1)-C(8)	2.034(5)
Fe(1)-C(4)	2.031(5)
Fe(1)-C(5)	2.028(4)
Fe(1)-C(2)	2.030(4)
Fe(1)-C(6)	2.030(4)
Fe(1)-C(7)	2.042(5)
Fe(1)-C(3)	2.033(4)
Fe(1)-C(9)	2.036(4)
Fe(1)-C(1)	2.042(4)
C(1)-C(5)	1.419(6)
C(1)-C(2)	1.424(6)
C(1)-C(11)	1.458(6)
C(2)-C(3)	1.417(6)
C(3)-C(4)	1.402(7)
C(4)-C(5)	1.406(6)
C(6)-C(7)	1.435(6)
C(6)-C(10)	1.428(6)
C(6)-B(1)	1.553(7)
C(7)-C(8)	1.408(7)
C(8)-C(9)	1.393(7)
C(9)-C(10)	1.406(6)
B(1)-O(2)	1.350(6)
B(1)-O(1)	1.370(6)
C(11)-C(15)	1.377(6)
C(11)-C(12)	1.385(6)

C(12)-C(13)	1.376(7)
C(13)-N(1)	1.323(6)
N(1)-C(14)	1.331(6)
C(14)-C(15)	1.379(7)
C(10)-Fe(1)-C(8)	67.6(2)
C(10)-Fe(1)-C(4)	160.73(19)
C(8)-Fe(1)-C(4)	107.8(2)
C(10)-Fe(1)-C(5)	124.35(19)
C(8)-Fe(1)-C(5)	121.2(2)
C(4)-Fe(1)-C(5)	40.54(17)
C(10)-Fe(1)-C(2)	121.75(19)
C(8)-Fe(1)-C(2)	162.0(2)
C(4)-Fe(1)-C(2)	68.41(19)
C(5)-Fe(1)-C(2)	68.15(18)
C(10)-Fe(1)-C(6)	41.33(18)
C(8)-Fe(1)-C(6)	68.75(19)
C(4)-Fe(1)-C(6)	156.49(19)
C(5)-Fe(1)-C(6)	161.31(18)
C(2)-Fe(1)-C(6)	107.28(18)
C(10)-Fe(1)-C(7)	68.6(2)
C(8)-Fe(1)-C(7)	40.4(2)
C(4)-Fe(1)-C(7)	121.01(19)
C(5)-Fe(1)-C(7)	156.10(18)
C(2)-Fe(1)-C(7)	125.18(19)
C(6)-Fe(1)-C(7)	41.27(17)
C(10)-Fe(1)-C(3)	157.5(2)
C(8)-Fe(1)-C(3)	125.1(2)
C(4)-Fe(1)-C(3)	40.35(19)
C(5)-Fe(1)-C(3)	67.92(18)
C(2)-Fe(1)-C(3)	40.81(18)
C(6)-Fe(1)-C(3)	121.31(19)
C(7)-Fe(1)-C(3)	108.0(2)
C(10)-Fe(1)-C(9)	40.58(18)
C(8)-Fe(1)-C(9)	40.0(2)
C(4)-Fe(1)-C(9)	123.9(2)
C(5)-Fe(1)-C(9)	107.28(19)
C(2)-Fe(1)-C(9)	156.7(2)
C(6)-Fe(1)-C(9)	69.32(19)
C(7)-Fe(1)-C(9)	68.4(2)
C(3)-Fe(1)-C(9)	160.7(2)
C(10)-Fe(1)-C(1)	107.09(18)
C(8)-Fe(1)-C(1)	155.9(2)
C(4)-Fe(1)-C(1)	68.94(18)
C(5)-Fe(1)-C(1)	40.82(17)
C(2)-Fe(1)-C(1)	40.93(16)
C(6)-Fe(1)-C(1)	123.90(17)
C(7)-Fe(1)-C(1)	161.88(17)
C(3)-Fe(1)-C(1)	68.88(17)
C(9)-Fe(1)-C(1)	120.58(19)
C(5)-C(1)-C(2)	106.2(4)
C(5)-C(1)-C(11)	126.7(4)
C(2)-C(1)-C(11)	127.1(4)
C(5)-C(1)-Fe(1)	69.1(2)
C(2)-C(1)-Fe(1)	69.1(2)
C(11)-C(1)-Fe(1)	125.4(3)
C(3)-C(2)-C(1)	108.5(4)
C(3)-C(2)-Fe(1)	69.7(3)
C(1)-C(2)-Fe(1)	70.0(2)
C(2)-C(3)-C(4)	108.2(4)
C(2)-C(3)-Fe(1)	69.5(2)
C(4)-C(3)-Fe(1)	69.7(3)
C(3)-C(4)-C(5)	107.8(4)

C(3)-C(4)-Fe(1)	69.9(3)
C(5)-C(4)-Fe(1)	69.6(2)
C(4)-C(5)-C(1)	109.3(4)
C(4)-C(5)-Fe(1)	69.9(3)
C(1)-C(5)-Fe(1)	70.1(2)
C(7)-C(6)-C(10)	106.0(4)
C(7)-C(6)-B(1)	125.5(4)
C(10)-C(6)-B(1)	128.0(4)
C(7)-C(6)-Fe(1)	69.8(2)
C(10)-C(6)-Fe(1)	68.9(2)
B(1)-C(6)-Fe(1)	119.7(3)
C(8)-C(7)-C(6)	107.6(5)
C(8)-C(7)-Fe(1)	69.5(3)
C(6)-C(7)-Fe(1)	68.9(2)
C(9)-C(8)-C(7)	109.7(4)
C(9)-C(8)-Fe(1)	70.0(3)
C(7)-C(8)-Fe(1)	70.1(3)
C(8)-C(9)-C(10)	107.3(4)
C(8)-C(9)-Fe(1)	69.9(3)
C(10)-C(9)-Fe(1)	69.0(3)
C(9)-C(10)-C(6)	109.4(4)
C(9)-C(10)-Fe(1)	70.4(3)
C(6)-C(10)-Fe(1)	69.8(3)
O(2)-B(1)-O(1)	118.2(5)
O(2)-B(1)-C(6)	119.0(4)
O(1)-B(1)-C(6)	122.8(5)
C(15)-C(11)-C(12)	115.6(4)
C(15)-C(11)-C(1)	123.1(4)
C(12)-C(11)-C(1)	121.2(4)
C(13)-C(12)-C(11)	120.3(5)
N(1)-C(13)-C(12)	124.6(5)
C(14)-N(1)-C(13)	114.8(4)
N(1)-C(14)-C(15)	124.8(5)
C(11)-C(15)-C(14)	119.9(5)

Table 14. Anisotropic displacement parameters (A^2 x 10^3) for 2b.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe(1)	37(1)	37(1)	37(1)	-3(1)	24(1)	-3(1)
C(1)	33(2)	43(2)	39(2)	-7(2)	22(2)	-2(2)
C(2)	37(2)	49(3)	46(2)	-5(2)	23(2)	2(2)
C(3)	41(2)	62(3)	60(3)	-13(2)	37(2)	-6(2)
C(4)	54(3)	49(3)	66(3)	-8(2)	45(3)	-8(2)
C(5)	41(2)	40(2)	55(3)	-4(2)	33(2)	-4(2)
C(6)	50(2)	40(2)	46(2)	-6(2)	32(2)	-7(2)
C(7)	67(3)	47(3)	48(3)	-7(2)	41(2)	-8(2)
C(8)	68(3)	56(3)	43(3)	-4(2)	31(3)	-15(3)
C(9)	41(2)	52(3)	46(2)	-1(2)	15(2)	-6(2)
C(10)	50(3)	48(3)	47(2)	-4(2)	30(2)	-10(2)
B(1)	55(3)	42(3)	54(3)	-2(2)	39(3)	-2(2)
O(1)	68(2)	65(2)	64(2)	18(2)	52(2)	17(2)
O(2)	77(3)	74(2)	72(2)	20(2)	60(2)	24(2)
C(11)	39(2)	43(2)	41(2)	-8(2)	27(2)	-6(2)
C(12)	63(3)	64(3)	73(3)	18(3)	53(3)	22(3)

C(13)	67(3)	63(3)	86(4)	9(3)	60(3)	17(3)
N(1)	66(3)	60(3)	64(3)	-3(2)	50(2)	-1(2)
C(14)	75(3)	72(3)	55(3)	12(3)	49(3)	10(3)
C(15)	56(3)	56(3)	54(3)	8(2)	39(2)	10(2)
O(3)	235(14)	233(14)	169(11)	0	75(10)	0

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 2b.

	x	y	z	U(eq)
H(2)	5249	2971	5051	57
H(3)	5602	3499	3825	62
H(4)	4358	4863	2553	62
H(5)	3253	5204	3005	53
H(7)	3915	1841	1873	62
H(8)	2626	3208	702	72
H(9)	1598	3465	1256	67
H(10)	2236	2249	2789	59
H(100)	3420(50)	930(50)	4270(60)	110(30)
H(200)	5190(50)	200(50)	4300(60)	110(30)
H(12)	2525	5087	3785	72
H(13)	1794	4963	4548	78
H(14)	3682	2855	6544	76
H(15)	4486	2914	5856	65

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Table 16. Crystal data and structure refinement for 2c.

Identification code	2c
Empirical formula	C15 H14 B Fe N O2
Formula weight	306.93
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 9.3704(10) A alpha = 101.61(2) deg. b = 11.583(2) A beta = 101.84(2) deg. c = 13.076(4) A gamma = 96.835(10) deg.
Volume	1341.5(5) A^3
Z, Calculated density	4, 1.520 Mg/m^3
Absorption coefficient	1.122 mm^-1
F(000)	632
Crystal size	0.27 x 0.20 x 0.18 mm
Theta range for data collection	3.05 to 24.97 deg.
Limiting indices	-11<=h<=10, -13<=k<=13, 0<=l<=15
Reflections collected / unique	4930 / 4707 [R(int) = 0.0320]
Completeness to theta = 24.97	99.8 %
Absorption correction	Psi-scan
Max. and min. transmission	1.00 and 0.95
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4707 / 0 / 341
Goodness-of-fit on F^2	0.988
Final R indices [I>2sigma(I)]	R1 = 0.0423, wR2 = 0.1051
R indices (all data)	R1 = 0.0948, wR2 = 0.1252
Largest diff. peak and hole	0.625 and -0.687 e.A^-3

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Table 17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 2c.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	52(1)	6577(1)	1994(1)	33(1)
Fe(2)	4583(1)	3006(1)	3224(1)	30(1)
O(1)	3456(4)	8607(3)	4157(3)	44(1)
O(2)	4424(3)	7353(3)	3011(3)	44(1)
O(3)	5538(4)	3767(3)	470(2)	41(1)
O(4)	4664(3)	5388(3)	1378(3)	38(1)
C(1)	1829(2)	6565(2)	3182(2)	34(1)
C(2)	563(3)	6686(2)	3608(2)	38(1)
C(3)	-537(2)	5670(3)	3078(3)	49(1)
C(4)	49(3)	4922(2)	2325(2)	48(1)
C(5)	1511(3)	5474(2)	2389(2)	39(1)
C(6)	-843(3)	8053(2)	1792(2)	37(1)
C(7)	-1820(3)	7000(3)	1170(3)	45(1)
C(8)	-1078(4)	6378(2)	446(2)	53(1)
C(9)	358(3)	7046(3)	619(2)	54(1)
C(10)	503(3)	8081(2)	1452(2)	42(1)
C(11)	-1148(4)	8927(3)	2682(3)	33(1)
C(12)	-323(5)	10066(4)	3063(4)	48(1)
C(13)	-655(5)	10836(4)	3898(4)	53(1)
C(14)	-2530(5)	9477(4)	3997(4)	42(1)
C(15)	-2270(4)	8647(4)	3169(4)	40(1)
C(16)	5779(3)	4044(2)	2500(2)	31(1)
C(17)	6476(3)	3054(2)	2677(2)	34(1)
C(18)	6814(3)	3118(2)	3799(2)	41(1)
C(19)	6326(3)	4146(3)	4315(2)	41(1)
C(20)	5686(3)	4719(2)	3512(2)	33(1)
C(21)	3211(3)	1441(2)	2421(2)	34(1)
C(22)	3636(3)	1482(2)	3536(2)	38(1)
C(23)	3155(3)	2488(2)	4099(2)	42(1)
C(24)	2434(3)	3068(2)	3332(2)	43(1)
C(25)	2468(3)	2421(2)	2295(2)	40(1)
C(26)	3454(4)	496(3)	1562(3)	34(1)
C(27)	2695(5)	289(4)	505(4)	46(1)
C(28)	2863(6)	-703(4)	-238(4)	54(1)
C(29)	4501(6)	-1249(4)	1021(4)	52(1)
C(30)	4391(5)	-291(4)	1805(4)	45(1)
B(1)	3262(5)	7531(4)	3459(4)	31(1)
B(2)	5295(5)	4386(4)	1406(4)	32(1)
N(1)	-1733(4)	10580(3)	4374(3)	46(1)
N(2)	3742(4)	-1482(3)	10(3)	46(1)

Table 18. Bond lengths [A] and angles [deg] for 2c.

Fe(1)-C(7)	2.029(3)
Fe(1)-C(6)	2.031(3)
Fe(1)-C(1)	2.035(3)
Fe(1)-C(8)	2.037(3)
Fe(1)-C(10)	2.040(3)
Fe(1)-C(5)	2.040(3)
Fe(1)-C(2)	2.040(3)

Fe(1)-C(9)	2.043(3)
Fe(1)-C(4)	2.049(3)
Fe(1)-C(3)	2.049(3)
Fe(2)-C(22)	2.033(3)
Fe(2)-C(21)	2.040(3)
Fe(2)-C(16)	2.042(3)
Fe(2)-C(17)	2.043(3)
Fe(2)-C(23)	2.043(3)
Fe(2)-C(20)	2.049(3)
Fe(2)-C(18)	2.050(3)
Fe(2)-C(19)	2.054(3)
Fe(2)-C(25)	2.054(3)
Fe(2)-C(24)	2.056(3)
O(1)-B(1)	1.356(5)
O(1)-H(200)	0.80(5)
O(2)-B(1)	1.357(6)
O(2)-H(100)	0.70(6)
O(3)-B(2)	1.365(5)
O(3)-H(300)	0.69(5)
O(4)-B(2)	1.367(5)
O(4)-H(400)	0.82(5)
C(1)-C(2)	1.4200
C(1)-C(5)	1.4200
C(1)-B(1)	1.570(5)
C(2)-C(3)	1.4200
C(2)-H(2B)	0.9800
C(3)-C(4)	1.4200
C(3)-H(3B)	0.9800
C(4)-C(5)	1.4200
C(4)-H(4B)	0.9800
C(5)-H(5A)	0.9800
C(6)-C(10)	1.4200
C(6)-C(7)	1.4200
C(6)-C(11)	1.480(4)
C(7)-C(8)	1.4200
C(7)-H(7A)	0.9800
C(8)-C(9)	1.4200
C(8)-H(8A)	0.9800
C(9)-C(10)	1.4200
C(9)-H(9A)	0.9800
C(10)-H(10A)	0.9800
C(11)-C(15)	1.376(6)
C(11)-C(12)	1.386(6)
C(12)-C(13)	1.378(6)
C(12)-H(12A)	0.9300
C(13)-N(1)	1.325(6)
C(13)-H(13A)	0.9300
C(14)-N(1)	1.342(5)
C(14)-C(15)	1.379(6)
C(14)-H(14A)	0.9300
C(15)-H(15A)	0.9300
C(16)-C(17)	1.4200
C(16)-C(20)	1.4200
C(16)-B(2)	1.554(5)
C(17)-C(18)	1.4200
C(17)-H(17A)	0.9800
C(18)-C(19)	1.4200
C(18)-H(18A)	0.9800
C(19)-C(20)	1.4200
C(19)-H(19A)	0.9800
C(20)-H(20A)	0.9800
C(21)-C(22)	1.4200
C(21)-C(25)	1.4200

C(21)-C(26)	1.477(4)
C(22)-C(23)	1.4200
C(22)-H(22A)	0.9800
C(23)-C(24)	1.4200
C(23)-H(23A)	0.9800
C(24)-C(25)	1.4200
C(24)-H(24A)	0.9800
C(25)-H(25A)	0.9800
C(26)-C(30)	1.377(6)
C(26)-C(27)	1.378(6)
C(27)-C(28)	1.394(6)
C(27)-H(27A)	0.9300
C(28)-N(2)	1.335(6)
C(28)-H(28A)	0.9300
C(29)-N(2)	1.323(6)
C(29)-C(30)	1.380(6)
C(29)-H(29A)	0.9300
C(30)-H(30A)	0.9300

C(7)-Fe(1)-C(6)	40.94(6)
C(7)-Fe(1)-C(1)	162.18(11)
C(6)-Fe(1)-C(1)	124.64(11)
C(7)-Fe(1)-C(8)	40.88(6)
C(6)-Fe(1)-C(8)	68.78(7)
C(1)-Fe(1)-C(8)	155.30(12)
C(7)-Fe(1)-C(10)	68.76(7)
C(6)-Fe(1)-C(10)	40.83(5)
C(1)-Fe(1)-C(10)	106.89(11)
C(8)-Fe(1)-C(10)	68.61(8)
C(7)-Fe(1)-C(5)	155.50(11)
C(6)-Fe(1)-C(5)	162.64(11)
C(1)-Fe(1)-C(5)	40.79(5)
C(8)-Fe(1)-C(5)	120.94(11)
C(10)-Fe(1)-C(5)	125.91(11)
C(7)-Fe(1)-C(2)	124.92(12)
C(6)-Fe(1)-C(2)	106.25(11)
C(1)-Fe(1)-C(2)	40.78(5)
C(8)-Fe(1)-C(2)	163.01(12)
C(10)-Fe(1)-C(2)	118.97(11)
C(5)-Fe(1)-C(2)	68.54(7)
C(7)-Fe(1)-C(9)	68.69(8)
C(6)-Fe(1)-C(9)	68.65(7)
C(1)-Fe(1)-C(9)	120.04(12)
C(8)-Fe(1)-C(9)	40.73(6)
C(10)-Fe(1)-C(9)	40.70(6)
C(5)-Fe(1)-C(9)	108.41(11)
C(2)-Fe(1)-C(9)	154.26(12)
C(7)-Fe(1)-C(4)	120.41(11)
C(6)-Fe(1)-C(4)	154.55(12)
C(1)-Fe(1)-C(4)	68.48(7)
C(8)-Fe(1)-C(4)	108.72(11)
C(10)-Fe(1)-C(4)	163.82(12)
C(5)-Fe(1)-C(4)	40.64(5)
C(2)-Fe(1)-C(4)	68.37(8)
C(9)-Fe(1)-C(4)	126.99(12)
C(7)-Fe(1)-C(3)	107.37(11)
C(6)-Fe(1)-C(3)	119.20(11)
C(1)-Fe(1)-C(3)	68.47(7)
C(8)-Fe(1)-C(3)	126.37(12)
C(10)-Fe(1)-C(3)	153.83(12)
C(5)-Fe(1)-C(3)	68.37(7)
C(2)-Fe(1)-C(3)	40.63(6)
C(9)-Fe(1)-C(3)	164.07(13)

C(4)-Fe(1)-C(3)	40.55(6)
C(22)-Fe(2)-C(21)	40.8
C(22)-Fe(2)-C(16)	157.71(11)
C(21)-Fe(2)-C(16)	123.50(10)
C(22)-Fe(2)-C(17)	120.76(10)
C(21)-Fe(2)-C(17)	108.11(10)
C(16)-Fe(2)-C(17)	40.69(5)
C(22)-Fe(2)-C(23)	40.77(5)
C(21)-Fe(2)-C(23)	68.48(7)
C(16)-Fe(2)-C(23)	161.10(11)
C(17)-Fe(2)-C(23)	155.62(11)
C(22)-Fe(2)-C(20)	158.83(11)
C(21)-Fe(2)-C(20)	159.44(11)
C(16)-Fe(2)-C(20)	40.6
C(17)-Fe(2)-C(20)	68.32(7)
C(23)-Fe(2)-C(20)	123.38(10)
C(22)-Fe(2)-C(18)	105.39(10)
C(21)-Fe(2)-C(18)	123.20(11)
C(16)-Fe(2)-C(18)	68.32(7)
C(17)-Fe(2)-C(18)	40.60(5)
C(23)-Fe(2)-C(18)	119.58(11)
C(20)-Fe(2)-C(18)	68.18(7)
C(22)-Fe(2)-C(19)	121.70(11)
C(21)-Fe(2)-C(19)	158.84(11)
C(16)-Fe(2)-C(19)	68.24(7)
C(17)-Fe(2)-C(19)	68.23(7)
C(23)-Fe(2)-C(19)	105.79(10)
C(20)-Fe(2)-C(19)	40.5
C(18)-Fe(2)-C(19)	40.48(5)
C(22)-Fe(2)-C(25)	68.40(7)
C(21)-Fe(2)-C(25)	40.58(5)
C(16)-Fe(2)-C(25)	110.24(10)
C(17)-Fe(2)-C(25)	125.89(11)
C(23)-Fe(2)-C(25)	68.21(7)
C(20)-Fe(2)-C(25)	123.94(10)
C(18)-Fe(2)-C(25)	161.01(11)
C(19)-Fe(2)-C(25)	158.08(11)
C(22)-Fe(2)-C(24)	68.36(7)
C(21)-Fe(2)-C(24)	68.23(7)
C(16)-Fe(2)-C(24)	126.03(11)
C(17)-Fe(2)-C(24)	162.64(12)
C(23)-Fe(2)-C(24)	40.53(5)
C(20)-Fe(2)-C(24)	108.76(10)
C(18)-Fe(2)-C(24)	155.81(12)
C(19)-Fe(2)-C(24)	121.48(11)
C(25)-Fe(2)-C(24)	40.42(5)
B(1)-O(1)-H(200)	110(4)
B(1)-O(2)-H(100)	123(6)
B(2)-O(3)-H(300)	115(4)
B(2)-O(4)-H(400)	116(3)
C(2)-C(1)-C(5)	108.0
C(2)-C(1)-B(1)	125.6(2)
C(5)-C(1)-B(1)	126.1(2)
C(2)-C(1)-Fe(1)	69.82(12)
C(5)-C(1)-Fe(1)	69.80(12)
B(1)-C(1)-Fe(1)	121.3(2)
C(3)-C(2)-C(1)	108.0
C(3)-C(2)-Fe(1)	70.01(12)
C(1)-C(2)-Fe(1)	69.39(11)
C(3)-C(2)-H(2B)	126.0
C(1)-C(2)-H(2B)	126.0
Fe(1)-C(2)-H(2B)	126.0
C(2)-C(3)-C(4)	108.0

C(2)-C(3)-Fe(1)	69.36(11)
C(4)-C(3)-Fe(1)	69.71(11)
C(2)-C(3)-H(3B)	126.0
C(4)-C(3)-H(3B)	126.0
Fe(1)-C(3)-H(3B)	126.0
C(5)-C(4)-C(3)	108.0
C(5)-C(4)-Fe(1)	69.34(11)
C(3)-C(4)-Fe(1)	69.74(11)
C(5)-C(4)-H(4B)	126.0
C(3)-C(4)-H(4B)	126.0
Fe(1)-C(4)-H(4B)	126.0
C(4)-C(5)-C(1)	108.0
C(4)-C(5)-Fe(1)	70.01(12)
C(1)-C(5)-Fe(1)	69.41(11)
C(4)-C(5)-H(5A)	126.0
C(1)-C(5)-H(5A)	126.0
Fe(1)-C(5)-H(5A)	126.0
C(10)-C(6)-C(7)	108.0
C(10)-C(6)-C(11)	126.2(2)
C(7)-C(6)-C(11)	125.7(2)
C(10)-C(6)-Fe(1)	69.92(12)
C(7)-C(6)-Fe(1)	69.46(12)
C(11)-C(6)-Fe(1)	123.5(2)
C(8)-C(7)-C(6)	108.0
C(8)-C(7)-Fe(1)	69.85(12)
C(6)-C(7)-Fe(1)	69.59(12)
C(8)-C(7)-H(7A)	126.0
C(6)-C(7)-H(7A)	126.0
Fe(1)-C(7)-H(7A)	126.0
C(7)-C(8)-C(9)	108.0
C(7)-C(8)-Fe(1)	69.27(12)
C(9)-C(8)-Fe(1)	69.88(12)
C(7)-C(8)-H(8A)	126.0
C(9)-C(8)-H(8A)	126.0
Fe(1)-C(8)-H(8A)	126.0
C(10)-C(9)-C(8)	108.0
C(10)-C(9)-Fe(1)	69.51(12)
C(8)-C(9)-Fe(1)	69.39(12)
C(10)-C(9)-H(9A)	126.0
C(8)-C(9)-H(9A)	126.0
Fe(1)-C(9)-H(9A)	126.0
C(9)-C(10)-C(6)	108.0
C(9)-C(10)-Fe(1)	69.79(12)
C(6)-C(10)-Fe(1)	69.25(12)
C(9)-C(10)-H(10A)	126.0
C(6)-C(10)-H(10A)	126.0
Fe(1)-C(10)-H(10A)	126.0
C(15)-C(11)-C(12)	116.8(4)
C(15)-C(11)-C(6)	121.4(3)
C(12)-C(11)-C(6)	121.8(4)
C(13)-C(12)-C(11)	119.0(4)
C(13)-C(12)-H(12A)	120.5
C(11)-C(12)-H(12A)	120.5
N(1)-C(13)-C(12)	124.9(4)
N(1)-C(13)-H(13A)	117.5
C(12)-C(13)-H(13A)	117.5
N(1)-C(14)-C(15)	123.3(4)
N(1)-C(14)-H(14A)	118.4
C(15)-C(14)-H(14A)	118.4
C(11)-C(15)-C(14)	120.3(4)
C(11)-C(15)-H(15A)	119.8
C(14)-C(15)-H(15A)	119.8
C(17)-C(16)-C(20)	108.0

C(17)-C(16)-B(2)	126.4(2)
C(20)-C(16)-B(2)	125.5(2)
C(17)-C(16)-Fe(2)	69.68(10)
C(20)-C(16)-Fe(2)	69.96(11)
B(2)-C(16)-Fe(2)	129.0(2)
C(18)-C(17)-C(16)	108.0
C(18)-C(17)-Fe(2)	69.99(11)
C(16)-C(17)-Fe(2)	69.63(11)
C(18)-C(17)-H(17A)	126.0
C(16)-C(17)-H(17A)	126.0
Fe(2)-C(17)-H(17A)	126.0
C(19)-C(18)-C(17)	108.0
C(19)-C(18)-Fe(2)	69.91(10)
C(17)-C(18)-Fe(2)	69.41(11)
C(19)-C(18)-H(18A)	126.0
C(17)-C(18)-H(18A)	126.0
Fe(2)-C(18)-H(18A)	126.0
C(18)-C(19)-C(20)	108.0
C(18)-C(19)-Fe(2)	69.61(10)
C(20)-C(19)-Fe(2)	69.56(11)
C(18)-C(19)-H(19A)	126.0
C(20)-C(19)-H(19A)	126.0
Fe(2)-C(19)-H(19A)	126.0
C(19)-C(20)-C(16)	108.0
C(19)-C(20)-Fe(2)	69.95(11)
C(16)-C(20)-Fe(2)	69.42(11)
C(19)-C(20)-H(20A)	126.0
C(16)-C(20)-H(20A)	126.0
Fe(2)-C(20)-H(20A)	126.0
C(22)-C(21)-C(25)	108.0
C(22)-C(21)-C(26)	124.7(2)
C(25)-C(21)-C(26)	127.3(2)
C(22)-C(21)-Fe(2)	69.34(11)
C(25)-C(21)-Fe(2)	70.25(11)
C(26)-C(21)-Fe(2)	128.2(2)
C(23)-C(22)-C(21)	108.0
C(23)-C(22)-Fe(2)	69.99(11)
C(21)-C(22)-Fe(2)	69.86(11)
C(23)-C(22)-H(22A)	126.0
C(21)-C(22)-H(22A)	126.0
Fe(2)-C(22)-H(22A)	126.0
C(24)-C(23)-C(22)	108.0
C(24)-C(23)-Fe(2)	70.23(11)
C(22)-C(23)-Fe(2)	69.24(11)
C(24)-C(23)-H(23A)	126.0
C(22)-C(23)-H(23A)	126.0
Fe(2)-C(23)-H(23A)	126.0
C(23)-C(24)-C(25)	108.0
C(23)-C(24)-Fe(2)	69.24(11)
C(25)-C(24)-Fe(2)	69.72(11)
C(23)-C(24)-H(24A)	126.0
C(25)-C(24)-H(24A)	126.0
Fe(2)-C(24)-H(24A)	126.0
C(24)-C(25)-C(21)	108.0
C(24)-C(25)-Fe(2)	69.86(11)
C(21)-C(25)-Fe(2)	69.17(11)
C(24)-C(25)-H(25A)	126.0
C(21)-C(25)-H(25A)	126.0
Fe(2)-C(25)-H(25A)	126.0
C(30)-C(26)-C(27)	116.3(4)
C(30)-C(26)-C(21)	120.5(4)
C(27)-C(26)-C(21)	123.0(4)
C(26)-C(27)-C(28)	119.6(4)

C(26)-C(27)-H(27A)	120.2
C(28)-C(27)-H(27A)	120.2
N(2)-C(28)-C(27)	123.7(4)
N(2)-C(28)-H(28A)	118.1
C(27)-C(28)-H(28A)	118.1
N(2)-C(29)-C(30)	123.9(4)
N(2)-C(29)-H(29A)	118.1
C(30)-C(29)-H(29A)	118.1
C(26)-C(30)-C(29)	120.5(4)
C(26)-C(30)-H(30A)	119.8
C(29)-C(30)-H(30A)	119.8
O(1)-B(1)-O(2)	114.0(4)
O(1)-B(1)-C(1)	123.8(4)
O(2)-B(1)-C(1)	122.2(4)
O(3)-B(2)-O(4)	117.8(4)
O(3)-B(2)-C(16)	123.1(4)
O(4)-B(2)-C(16)	119.1(4)
C(13)-N(1)-C(14)	115.7(4)
C(29)-N(2)-C(28)	115.9(4)

Table 19. Anisotropic displacement parameters (A^2 x 10^3) for 2c.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe(1)	28(1)	35(1)	33(1)	4(1)	5(1)	4(1)
Fe(2)	36(1)	27(1)	30(1)	10(1)	10(1)	7(1)
O(1)	43(2)	37(2)	48(2)	-1(1)	14(2)	3(1)
O(2)	37(2)	44(2)	52(2)	7(2)	20(2)	5(1)
O(3)	65(2)	34(2)	29(2)	8(1)	15(2)	21(2)
O(4)	51(2)	38(2)	33(2)	13(1)	16(1)	19(1)
C(1)	34(2)	33(2)	35(2)	11(2)	5(2)	9(2)
C(2)	33(2)	49(3)	34(2)	8(2)	12(2)	6(2)
C(3)	37(2)	57(3)	55(3)	20(2)	16(2)	-1(2)
C(4)	44(3)	34(2)	58(3)	9(2)	3(2)	-2(2)
C(5)	44(2)	33(2)	39(2)	6(2)	9(2)	7(2)
C(6)	32(2)	41(2)	37(2)	10(2)	5(2)	11(2)
C(7)	35(2)	43(3)	47(3)	5(2)	-4(2)	4(2)
C(8)	62(3)	50(3)	38(3)	2(2)	-2(2)	16(2)
C(9)	68(3)	63(3)	35(3)	13(2)	19(2)	18(3)
C(10)	43(2)	47(3)	41(3)	17(2)	16(2)	10(2)
C(11)	29(2)	34(2)	37(2)	11(2)	5(2)	9(2)
C(12)	45(3)	42(3)	58(3)	7(2)	23(2)	3(2)
C(13)	52(3)	36(2)	71(4)	5(2)	22(3)	4(2)
C(14)	38(2)	43(2)	50(3)	15(2)	17(2)	10(2)
C(15)	32(2)	37(2)	47(3)	7(2)	5(2)	2(2)
C(16)	34(2)	29(2)	29(2)	7(2)	8(2)	2(2)
C(17)	37(2)	35(2)	32(2)	7(2)	11(2)	9(2)
C(18)	43(3)	46(3)	37(2)	19(2)	6(2)	13(2)
C(19)	48(3)	44(2)	27(2)	6(2)	6(2)	7(2)
C(20)	40(2)	27(2)	30(2)	8(2)	9(2)	3(2)
C(21)	36(2)	28(2)	41(2)	14(2)	11(2)	4(2)
C(22)	46(2)	30(2)	43(3)	15(2)	18(2)	7(2)
C(23)	51(3)	37(2)	44(3)	10(2)	23(2)	4(2)
C(24)	39(2)	36(2)	57(3)	8(2)	20(2)	10(2)
C(25)	34(2)	35(2)	52(3)	14(2)	9(2)	7(2)

C(26)	38(2)	27(2)	37(2)	9(2)	12(2)	1(2)
C(27)	57(3)	41(2)	44(3)	17(2)	10(2)	18(2)
C(28)	70(3)	53(3)	34(3)	7(2)	5(2)	11(3)
C(29)	61(3)	42(3)	52(3)	6(2)	10(3)	20(2)
C(30)	49(3)	42(3)	42(3)	6(2)	1(2)	15(2)
B(1)	30(2)	30(2)	32(2)	12(2)	3(2)	5(2)
B(2)	31(2)	33(2)	33(3)	10(2)	9(2)	4(2)
N(1)	44(2)	42(2)	54(2)	6(2)	16(2)	14(2)
N(2)	60(2)	36(2)	42(2)	6(2)	14(2)	10(2)

Table 20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 2c.

	x	y	z	U(eq)
H(2B)	465	7355	4168	46
H(3B)	-1530	5518	3205	59
H(4B)	-468	4161	1840	57
H(5A)	2182	5160	1959	46
H(7A)	-2828	6747	1232	54
H(8A)	-1482	5617	-78	63
H(9A)	1120	6825	239	64
H(10A)	1382	8701	1746	50
H(12A)	444	10306	2760	58
H(13A)	-79	11592	4147	63
H(14A)	-3297	9261	4311	50
H(15A)	-2856	7894	2938	48
H(17A)	6687	2436	2123	41
H(18A)	7294	2549	4154	49
H(19A)	6408	4411	5088	49
H(20A)	5253	5449	3635	39
H(22A)	4162	914	3860	45
H(23A)	3298	2738	4880	51
H(24A)	2000	3793	3491	52
H(25A)	2062	2622	1613	48
H(27A)	2073	807	287	55
H(28A)	2334	-829	-946	64
H(29A)	5147	-1761	1215	63
H(30A)	4955	-176	2502	54
H(400)	4530(50)	5590(40)	800(40)	43(14)
H(200)	2760(60)	8660(50)	4410(40)	65(19)
H(300)	5770(60)	3230(40)	490(40)	50(17)
H(100)	4440(70)	6820(60)	2650(50)	100(30)

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Table 21. Crystal data and structure refinement for 3a.

Identification code	3
Empirical formula	C15 H15 B Fe N2 O5
Formula weight	369.95
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/a
Unit cell dimensions	a = 14.080(5) A alpha = 90 deg. b = 8.443(5) A beta = 116.15(2) deg. c = 14.343(5) A gamma = 90 deg.
Volume	1530.5(12) A^3
Z, Calculated density	4, 1.605 Mg/m^3
Absorption coefficient	1.014 mm^-1
F(000)	760
Crystal size	0.19 x 0.17 x 0.11 mm
Theta range for data collection	3.16 to 24.97 deg.
Limiting indices	-16<=h<=15, 0<=k<=10, 0<=l<=17
Reflections collected / unique	2797 / 2685 [R(int) = 0.0552]
Completeness to theta = 24.97	99.7 %
Absorption correction	Psi-scan
Max. and min. transmission	1.00 and 0.83
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2685 / 0 / 196
Goodness-of-fit on F^2	0.859
Final R indices [I>2sigma(I)]	R1 = 0.0598, wR2 = 0.1526
R indices (all data)	R1 = 0.1790, wR2 = 0.2265
Largest diff. peak and hole	0.517 and -0.869 e.A^-3

Table 22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 3a.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	5796(1)	3281(1)	3674(1)	39(1)
C(1)	5990(4)	892(6)	3809(4)	42(2)
C(2)	6842(4)	1610(8)	3689(4)	48(2)
C(3)	7351(4)	2684(7)	4525(5)	66(3)
C(4)	6814(6)	2630(7)	5162(4)	67(3)
C(5)	5973(5)	1523(8)	4720(4)	58(3)
C(6)	5251(4)	4407(7)	2299(4)	39(2)
C(7)	5755(4)	5512(6)	3117(4)	48(2)
C(8)	5217(5)	5492(7)	3753(4)	61(3)
C(9)	4381(5)	4374(8)	3329(5)	55(2)
C(10)	4401(4)	3704(7)	2430(4)	50(2)
C(11)	5623(7)	3970(10)	1524(6)	43(2)
C(12)	6523(4)	4662(5)	1557(3)	61(3)
C(13)	6872(4)	4241(5)	792(3)	65(3)
N(1)	6312(4)	3200(5)	71(3)	69(2)
C(14)	5457(4)	2497(5)	14(3)	75(3)
C(15)	5068(4)	2824(5)	759(3)	59(3)
B(1)	5133(8)	-206(13)	2995(8)	46(2)
O(1)	4286(6)	-621(8)	3128(6)	69(2)
O(2)	5221(5)	-741(8)	2125(5)	62(2)
N(2)	7385(6)	-1394(9)	1454(6)	52(2)
O(3)	7160(6)	-1416(9)	2194(5)	74(2)
O(4)	8049(6)	-2381(8)	1447(5)	66(2)
O(5)	6980(7)	-442(10)	744(7)	91(3)

Table 23. Bond lengths [A] and angles [deg] for 3a.

Fe(1)-C(6)	2.013(5)
Fe(1)-C(10)	2.020(6)
Fe(1)-C(1)	2.033(6)
Fe(1)-C(2)	2.033(5)
Fe(1)-C(7)	2.037(6)
Fe(1)-C(5)	2.045(6)
Fe(1)-C(3)	2.046(6)
Fe(1)-C(9)	2.049(6)
Fe(1)-C(4)	2.053(6)
Fe(1)-C(8)	2.060(6)
C(1)-C(2)	1.4200
C(1)-C(5)	1.4200
C(1)-B(1)	1.561(12)
C(2)-C(3)	1.4200
C(2)-H(2)	0.9300
C(3)-C(4)	1.4200
C(3)-H(3)	0.9300
C(4)-C(5)	1.4200
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
C(6)-C(7)	1.4200
C(6)-C(10)	1.4200
C(6)-C(11)	1.470(9)

C(7)-C(8)	1.4200
C(7)-H(7)	0.9300
C(8)-C(9)	1.4200
C(8)-H(8)	0.9300
C(9)-C(10)	1.4200
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-C(12)	1.376(10)
C(11)-C(15)	1.413(9)
C(12)-C(13)	1.4307
C(12)-H(12)	0.9300
C(13)-N(1)	1.3208
C(13)-H(13)	0.9300
N(1)-C(14)	1.3128
N(1)-H(1)	0.8888
C(14)-C(15)	1.4255
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
B(1)-O(1)	1.334(12)
B(1)-O(2)	1.383(11)
O(1)-H(100)	1.01(8)
O(2)-H(200)	1.22(8)
N(2)-O(5)	1.223(9)
N(2)-O(3)	1.233(9)
N(2)-O(4)	1.256(9)

C(6)-Fe(1)-C(10)	41.24(10)
C(6)-Fe(1)-C(1)	122.7(2)
C(10)-Fe(1)-C(1)	107.3(2)
C(6)-Fe(1)-C(2)	107.5(2)
C(10)-Fe(1)-C(2)	123.4(2)
C(1)-Fe(1)-C(2)	40.89(10)
C(6)-Fe(1)-C(7)	41.04(10)
C(10)-Fe(1)-C(7)	68.98(13)
C(1)-Fe(1)-C(7)	159.1(2)
C(2)-Fe(1)-C(7)	122.7(2)
C(6)-Fe(1)-C(5)	158.8(2)
C(10)-Fe(1)-C(5)	122.2(2)
C(1)-Fe(1)-C(5)	40.75(11)
C(2)-Fe(1)-C(5)	68.58(13)
C(7)-Fe(1)-C(5)	158.7(2)
C(6)-Fe(1)-C(3)	123.1(2)
C(10)-Fe(1)-C(3)	159.9(3)
C(1)-Fe(1)-C(3)	68.58(12)
C(2)-Fe(1)-C(3)	40.75(10)
C(7)-Fe(1)-C(3)	107.4(2)
C(5)-Fe(1)-C(3)	68.34(13)
C(6)-Fe(1)-C(9)	68.90(13)
C(10)-Fe(1)-C(9)	40.85(11)
C(1)-Fe(1)-C(9)	123.1(2)
C(2)-Fe(1)-C(9)	159.8(3)
C(7)-Fe(1)-C(9)	68.42(13)
C(5)-Fe(1)-C(9)	107.2(2)
C(3)-Fe(1)-C(9)	157.9(3)
C(6)-Fe(1)-C(4)	159.3(3)
C(10)-Fe(1)-C(4)	158.1(3)
C(1)-Fe(1)-C(4)	68.43(13)
C(2)-Fe(1)-C(4)	68.43(13)
C(7)-Fe(1)-C(4)	122.8(2)
C(5)-Fe(1)-C(4)	40.54(10)
C(3)-Fe(1)-C(4)	40.54(10)
C(9)-Fe(1)-C(4)	122.1(2)
C(6)-Fe(1)-C(8)	68.68(13)

C(10)-Fe(1)-C(8)	68.55(13)
C(1)-Fe(1)-C(8)	159.0(2)
C(2)-Fe(1)-C(8)	158.5(3)
C(7)-Fe(1)-C(8)	40.55(11)
C(5)-Fe(1)-C(8)	122.7(2)
C(3)-Fe(1)-C(8)	122.4(2)
C(9)-Fe(1)-C(8)	40.44(10)
C(4)-Fe(1)-C(8)	107.3(2)
C(2)-C(1)-C(5)	108.0
C(2)-C(1)-B(1)	125.4(5)
C(5)-C(1)-B(1)	126.1(5)
C(2)-C(1)-Fe(1)	69.6(2)
C(5)-C(1)-Fe(1)	70.1(2)
B(1)-C(1)-Fe(1)	119.4(5)
C(3)-C(2)-C(1)	108.0
C(3)-C(2)-Fe(1)	70.1(2)
C(1)-C(2)-Fe(1)	69.6(2)
C(3)-C(2)-H(2)	126.0
C(1)-C(2)-H(2)	126.0
Fe(1)-C(2)-H(2)	125.9
C(4)-C(3)-C(2)	108.0
C(4)-C(3)-Fe(1)	70.0(2)
C(2)-C(3)-Fe(1)	69.1(2)
C(4)-C(3)-H(3)	126.0
C(2)-C(3)-H(3)	126.0
Fe(1)-C(3)-H(3)	126.4
C(3)-C(4)-C(5)	108.0
C(3)-C(4)-Fe(1)	69.4(2)
C(5)-C(4)-Fe(1)	69.4(2)
C(3)-C(4)-H(4)	126.0
C(5)-C(4)-H(4)	126.0
Fe(1)-C(4)-H(4)	126.7
C(4)-C(5)-C(1)	108.0
C(4)-C(5)-Fe(1)	70.0(2)
C(1)-C(5)-Fe(1)	69.1(2)
C(4)-C(5)-H(5)	126.0
C(1)-C(5)-H(5)	126.0
Fe(1)-C(5)-H(5)	126.4
C(7)-C(6)-C(10)	108.0
C(7)-C(6)-C(11)	125.1(5)
C(10)-C(6)-C(11)	126.7(5)
C(7)-C(6)-Fe(1)	70.4(2)
C(10)-C(6)-Fe(1)	69.6(2)
C(11)-C(6)-Fe(1)	120.9(5)
C(6)-C(7)-C(8)	108.0
C(6)-C(7)-Fe(1)	68.5(2)
C(8)-C(7)-Fe(1)	70.6(2)
C(6)-C(7)-H(7)	126.0
C(8)-C(7)-H(7)	126.0
Fe(1)-C(7)-H(7)	126.5
C(9)-C(8)-C(7)	108.0
C(9)-C(8)-Fe(1)	69.4(2)
C(7)-C(8)-Fe(1)	68.9(2)
C(9)-C(8)-H(8)	126.0
C(7)-C(8)-H(8)	126.0
Fe(1)-C(8)-H(8)	127.3
C(10)-C(9)-C(8)	108.0
C(10)-C(9)-Fe(1)	68.5(2)
C(8)-C(9)-Fe(1)	70.2(2)
C(10)-C(9)-H(9)	126.0
C(8)-C(9)-H(9)	126.0
Fe(1)-C(9)-H(9)	126.9
C(9)-C(10)-C(6)	108.0

C(9)-C(10)-Fe(1)	70.7(2)
C(6)-C(10)-Fe(1)	69.1(2)
C(9)-C(10)-H(10)	126.0
C(6)-C(10)-H(10)	126.0
Fe(1)-C(10)-H(10)	125.8
C(12)-C(11)-C(15)	120.2(6)
C(12)-C(11)-C(6)	119.8(6)
C(15)-C(11)-C(6)	120.0(6)
C(11)-C(12)-C(13)	119.4(4)
C(11)-C(12)-H(12)	120.3
C(13)-C(12)-H(12)	120.3
N(1)-C(13)-C(12)	118.5
N(1)-C(13)-H(13)	120.8
C(12)-C(13)-H(13)	120.8
C(14)-N(1)-C(13)	124.4
C(14)-N(1)-H(1)	124.9
C(13)-N(1)-H(1)	110.6
N(1)-C(14)-C(15)	120.6
N(1)-C(14)-H(14)	119.7
C(15)-C(14)-H(14)	119.7
C(11)-C(15)-C(14)	116.8(4)
C(11)-C(15)-H(15)	121.6
C(14)-C(15)-H(15)	121.6
O(1)-B(1)-O(2)	118.9(9)
O(1)-B(1)-C(1)	119.6(8)
O(2)-B(1)-C(1)	121.4(8)
B(1)-O(1)-H(100)	111(5)
B(1)-O(2)-H(200)	129(5)
O(5)-N(2)-O(3)	121.7(8)
O(5)-N(2)-O(4)	120.2(8)
O(3)-N(2)-O(4)	118.1(8)

Table 24. Anisotropic displacement parameters (A^2 x 10^3) for 3a.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe(1)	44(1)	39(1)	36(1)	0(1)	19(1)	4(1)
C(1)	42(5)	44(5)	37(5)	2(4)	14(4)	11(4)
C(2)	39(4)	51(5)	48(5)	-4(4)	14(4)	19(5)
C(3)	46(5)	61(7)	64(6)	-3(5)	-2(5)	12(5)
C(4)	77(7)	63(7)	35(5)	-7(4)	3(5)	26(6)
C(5)	87(7)	47(6)	38(4)	10(4)	25(5)	6(5)
C(6)	39(5)	42(5)	40(5)	15(4)	22(4)	14(4)
C(7)	66(6)	40(5)	41(5)	-5(4)	26(5)	6(4)
C(8)	90(8)	47(6)	50(6)	8(5)	34(6)	27(6)
C(9)	47(5)	65(7)	60(6)	6(5)	30(5)	16(5)
C(10)	41(5)	61(6)	44(5)	6(4)	15(4)	1(4)
C(11)	47(5)	43(5)	35(4)	-5(4)	15(4)	0(4)
C(12)	78(7)	57(6)	65(6)	-3(5)	47(6)	-11(5)
C(13)	78(7)	63(7)	69(7)	14(5)	46(6)	7(6)
N(1)	91(6)	73(6)	61(5)	11(5)	50(5)	25(6)
C(14)	104(9)	71(7)	40(5)	-14(5)	22(6)	14(7)
C(15)	56(5)	69(7)	51(5)	4(5)	22(5)	3(5)
B(1)	55(6)	46(6)	42(5)	7(5)	25(5)	7(5)
O(1)	87(5)	66(5)	67(5)	-26(4)	48(4)	-20(4)
O(2)	63(4)	74(5)	55(4)	-13(3)	31(4)	-6(4)

N(2)	47(4)	58(5)	52(4)	-8(4)	24(4)	-4(4)
O(3)	72(4)	98(6)	70(4)	-11(4)	48(4)	1(4)
O(4)	83(5)	58(4)	78(5)	13(4)	56(4)	15(4)
O(5)	93(6)	92(6)	84(6)	30(5)	34(5)	39(5)

Table 25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 3a.

	x	y	z	U(eq)
H(2)	7033	1412	3156	57
H(3)	7934	3312	4636	80
H(4)	6984	3217	5764	80
H(5)	5495	1257	4980	70
H(7)	6336	6139	3218	58
H(8)	5384	6103	4345	74
H(9)	3903	4125	3593	66
H(10)	3939	2939	2002	60
H(12)	6899	5397	2071	73
H(13)	7480	4690	803	78
H(1)	6586	3061	-375	160(60)
H(14)	5100	1778	-518	91
H(15)	4478	2307	742	71
H(100)	3780(60)	-1260(100)	2520(60)	50(20)
H(200)	5880(170)	-1600(300)	2080(170)	280(120)

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Table 26. Crystal data and structure refinement for 3b.

Identification code	3b
Empirical formula	C30 H36 B2 Fe2 N2 O11 S
Formula weight	765.99
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 21.954(4) A alpha = 90 deg. b = 7.3620(15) A beta = 111.35(3) deg. c = 20.871(4) A gamma = 90 deg.
Volume	3141.8(11) A^3
Z, Calculated density	4, 1.619 Mg/m^3
Absorption coefficient	1.055 mm^-1
F(000)	1584
Crystal size	0.24 x 0.20 x 0.16 mm
Theta range for data collection	3.00 to 24.98 deg.
Limiting indices	0<=h<=26, -8<=k<=0, -24<=l<=23
Reflections collected / unique	5576 / 5426 [R(int) = 0.0248]
Completeness to theta = 24.98	98.2 %
Absorption correction	Psi-scan
Max. and min. transmission	1.00 and 0.88
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5426 / 0 / 445
Goodness-of-fit on F^2	1.137
Final R indices [I>2sigma(I)]	R1 = 0.0396, wR2 = 0.1049
R indices (all data)	R1 = 0.0603, wR2 = 0.1175
Largest diff. peak and hole	0.452 and -0.686 e.A^-3

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Table 27. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 3b.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	5525(1)	4321(1)	1498(1)	40(1)
Fe(1)	8742(1)	3406(1)	1350(1)	26(1)
Fe(2)	1275(1)	3071(1)	1116(1)	27(1)
O(1)	7346(1)	3780(4)	2211(1)	45(1)
O(2)	7048(2)	5399(4)	1142(2)	50(1)
O(3)	2990(1)	4511(4)	2467(1)	46(1)
O(4)	2740(1)	6366(4)	1448(1)	44(1)
O(5)	5146(2)	5783(4)	1639(2)	82(1)
O(6)	6075(1)	3831(4)	2118(1)	57(1)
O(7)	5770(1)	4873(5)	960(2)	68(1)
O(8)	5099(1)	2727(4)	1255(2)	60(1)
O(9)	4323(2)	4361(6)	3014(2)	79(1)
O(10)	5169(2)	-2010(4)	190(2)	58(1)
O(11)	4016(2)	7205(5)	1723(2)	54(1)
C(1)	8135(1)	1514(3)	717(1)	30(1)
C(2)	8669(1)	669(3)	1239(1)	37(1)
C(3)	9255(1)	1282(3)	1170(1)	42(1)
C(4)	9084(1)	2506(3)	606(1)	40(1)
C(5)	8391(1)	2649(3)	326(1)	33(1)
C(6)	8240(1)	4873(3)	1840(1)	30(1)
C(7)	8765(1)	3906(3)	2328(1)	36(1)
C(8)	9355(1)	4483(3)	2257(1)	42(1)
C(9)	9195(1)	5806(3)	1727(1)	39(1)
C(10)	8506(1)	6048(3)	1469(1)	33(1)
C(11)	7442(2)	1236(4)	590(2)	33(1)
C(12)	7235(2)	331(5)	1061(2)	47(1)
C(13)	6598(2)	-6(7)	912(2)	65(1)
C(14)	6325(2)	1438(7)	-143(2)	63(1)
C(15)	6963(2)	1793(5)	-29(2)	45(1)
C(16)	1823(1)	5074(3)	1755(1)	31(1)
C(17)	1563(1)	3872(3)	2123(1)	39(1)
C(18)	871(1)	3906(3)	1805(1)	43(1)
C(19)	703(1)	5128(3)	1240(1)	42(1)
C(20)	1291(1)	5850(3)	1210(1)	35(1)
C(21)	1854(1)	1622(3)	727(1)	32(1)
C(22)	1313(1)	2366(3)	184(1)	36(1)
C(23)	732(1)	1683(3)	246(1)	41(1)
C(24)	914(1)	517(3)	828(1)	42(1)
C(25)	1607(1)	480(3)	1125(1)	35(1)
C(26)	2547(2)	1956(4)	861(2)	31(1)
C(27)	2751(2)	2954(5)	404(2)	39(1)
C(28)	3402(2)	3231(5)	540(2)	45(1)
C(29)	3681(2)	1615(5)	1565(2)	42(1)
C(30)	3036(2)	1279(5)	1453(2)	37(1)
B(1)	7493(2)	4662(5)	1719(2)	31(1)
B(2)	2570(2)	5357(5)	1905(2)	33(1)
N(1)	6157(2)	532(7)	323(2)	75(1)
N(2)	3849(1)	2564(4)	1112(2)	41(1)

Table 28. Bond lengths [A] and angles [deg] for 3b.

S(1)-O(5)	1.455(3)
S(1)-O(6)	1.457(3)
S(1)-O(7)	1.468(3)
S(1)-O(8)	1.471(3)
Fe(1)-C(2)	2.028(2)
Fe(1)-C(3)	2.040(2)
Fe(1)-C(9)	2.039(2)
Fe(1)-C(8)	2.042(2)
Fe(1)-C(1)	2.044(2)
Fe(1)-C(10)	2.051(2)
Fe(1)-C(7)	2.056(2)
Fe(1)-C(6)	2.062(2)
Fe(1)-C(4)	2.064(2)
Fe(1)-C(5)	2.067(2)
Fe(2)-C(21)	2.040(2)
Fe(2)-C(25)	2.040(2)
Fe(2)-C(18)	2.039(2)
Fe(2)-C(22)	2.045(2)
Fe(2)-C(24)	2.044(2)
Fe(2)-C(19)	2.044(2)
Fe(2)-C(23)	2.047(2)
Fe(2)-C(17)	2.048(2)
Fe(2)-C(20)	2.054(2)
Fe(2)-C(16)	2.057(2)
O(1)-B(1)	1.349(4)
O(1)-H(100)	0.74(5)
O(2)-B(1)	1.356(5)
O(2)-H(200)	0.69(5)
O(3)-B(2)	1.353(4)
O(3)-H(300)	0.80(5)
O(4)-B(2)	1.364(4)
O(4)-H(400)	0.74(6)
O(9)-H(901)	0.86(8)
O(9)-H(902)	0.68(6)
O(10)-H(103)	0.76(6)
O(10)-H(102)	0.82(7)
O(11)-H(111)	0.83(5)
O(11)-H(112)	0.80(5)
C(1)-C(2)	1.4200
C(1)-C(5)	1.4200
C(1)-C(11)	1.460(3)
C(2)-C(3)	1.4200
C(2)-H(2B)	0.9800
C(3)-C(4)	1.4200
C(3)-H(3B)	0.9800
C(4)-C(5)	1.4200
C(4)-H(4B)	0.9800
C(5)-H(5B)	0.9800
C(6)-C(7)	1.4200
C(6)-C(10)	1.4200
C(6)-B(1)	1.575(4)
C(7)-C(8)	1.4200
C(7)-H(7B)	0.9800
C(8)-C(9)	1.4200
C(8)-H(8B)	0.9800
C(9)-C(10)	1.4200
C(9)-H(9A)	0.9800
C(10)-H(10A)	0.9800
C(11)-C(12)	1.394(5)
C(11)-C(15)	1.397(5)

C(12)-C(13)	1.341(5)
C(12)-H(12A)	0.9300
C(13)-N(1)	1.319(6)
C(13)-H(13A)	0.9300
C(14)-N(1)	1.339(6)
C(14)-C(15)	1.358(5)
C(14)-H(14A)	0.9300
C(15)-H(15A)	0.9300
C(16)-C(17)	1.4200
C(16)-C(20)	1.4200
C(16)-B(2)	1.567(4)
C(17)-C(18)	1.4200
C(17)-H(17A)	0.9800
C(18)-C(19)	1.4200
C(18)-H(18A)	0.9800
C(19)-C(20)	1.4200
C(19)-H(19A)	0.9800
C(20)-H(20A)	0.9800
C(21)-C(22)	1.4200
C(21)-C(25)	1.4200
C(21)-C(26)	1.464(4)
C(22)-C(23)	1.4200
C(22)-H(22A)	0.9800
C(23)-C(24)	1.4200
C(23)-H(23A)	0.9800
C(24)-C(25)	1.4200
C(24)-H(24A)	0.9800
C(25)-H(25A)	0.9800
C(26)-C(30)	1.400(5)
C(26)-C(27)	1.402(5)
C(27)-C(28)	1.368(5)
C(27)-H(27A)	0.9300
C(28)-N(2)	1.331(5)
C(28)-H(28A)	0.9300
C(29)-N(2)	1.330(5)
C(29)-C(30)	1.371(5)
C(29)-H(29A)	0.9300
C(30)-H(30A)	0.9300
N(1)-H(101)	0.89(5)
N(2)-H(201)	1.04(4)

O(5)-S(1)-O(6)	110.7(2)
O(5)-S(1)-O(7)	110.3(2)
O(6)-S(1)-O(7)	109.33(16)
O(5)-S(1)-O(8)	108.71(17)
O(6)-S(1)-O(8)	109.03(18)
O(7)-S(1)-O(8)	108.78(19)
C(2)-Fe(1)-C(3)	40.9
C(2)-Fe(1)-C(9)	155.84(9)
C(3)-Fe(1)-C(9)	120.75(9)
C(2)-Fe(1)-C(8)	119.33(9)
C(3)-Fe(1)-C(8)	104.30(8)
C(9)-Fe(1)-C(8)	40.7
C(2)-Fe(1)-C(1)	40.8
C(3)-Fe(1)-C(1)	68.5
C(9)-Fe(1)-C(1)	161.99(9)
C(8)-Fe(1)-C(1)	156.63(9)
C(2)-Fe(1)-C(10)	160.51(9)
C(3)-Fe(1)-C(10)	158.45(9)
C(9)-Fe(1)-C(10)	40.6
C(8)-Fe(1)-C(10)	68.3
C(1)-Fe(1)-C(10)	126.13(8)
C(2)-Fe(1)-C(7)	105.28(8)

C(3)-Fe(1)-C(7)	120.30(9)
C(9)-Fe(1)-C(7)	68.3
C(8)-Fe(1)-C(7)	40.5
C(1)-Fe(1)-C(7)	122.50(8)
C(10)-Fe(1)-C(7)	68.0
C(2)-Fe(1)-C(6)	122.87(8)
C(3)-Fe(1)-C(6)	157.48(9)
C(9)-Fe(1)-C(6)	68.2
C(8)-Fe(1)-C(6)	68.1
C(1)-Fe(1)-C(6)	109.66(8)
C(10)-Fe(1)-C(6)	40.4
C(7)-Fe(1)-C(6)	40.3
C(2)-Fe(1)-C(4)	68.31(5)
C(3)-Fe(1)-C(4)	40.5
C(9)-Fe(1)-C(4)	108.02(8)
C(8)-Fe(1)-C(4)	121.72(8)
C(1)-Fe(1)-C(4)	68.0
C(10)-Fe(1)-C(4)	124.95(8)
C(7)-Fe(1)-C(4)	156.92(9)
C(6)-Fe(1)-C(4)	161.42(9)
C(2)-Fe(1)-C(5)	68.3
C(3)-Fe(1)-C(5)	68.0
C(9)-Fe(1)-C(5)	125.34(8)
C(8)-Fe(1)-C(5)	159.31(9)
C(1)-Fe(1)-C(5)	40.4
C(10)-Fe(1)-C(5)	111.42(8)
C(7)-Fe(1)-C(5)	159.97(9)
C(6)-Fe(1)-C(5)	126.08(8)
C(4)-Fe(1)-C(5)	40.2
C(21)-Fe(2)-C(25)	40.7
C(21)-Fe(2)-C(18)	158.74(10)
C(25)-Fe(2)-C(18)	121.46(9)
C(21)-Fe(2)-C(22)	40.7
C(25)-Fe(2)-C(22)	68.5
C(18)-Fe(2)-C(22)	157.80(9)
C(21)-Fe(2)-C(24)	68.5
C(25)-Fe(2)-C(24)	40.7
C(18)-Fe(2)-C(24)	105.28(8)
C(22)-Fe(2)-C(24)	68.38(5)
C(21)-Fe(2)-C(19)	159.79(9)
C(25)-Fe(2)-C(19)	157.87(9)
C(18)-Fe(2)-C(19)	40.7
C(22)-Fe(2)-C(19)	123.26(9)
C(24)-Fe(2)-C(19)	121.92(8)
C(21)-Fe(2)-C(23)	68.4
C(25)-Fe(2)-C(23)	68.41(5)
C(18)-Fe(2)-C(23)	120.89(9)
C(22)-Fe(2)-C(23)	40.6
C(24)-Fe(2)-C(23)	40.6
C(19)-Fe(2)-C(23)	107.22(8)
C(21)-Fe(2)-C(17)	123.68(9)
C(25)-Fe(2)-C(17)	106.54(8)
C(18)-Fe(2)-C(17)	40.7
C(22)-Fe(2)-C(17)	160.94(9)
C(24)-Fe(2)-C(17)	120.62(8)
C(19)-Fe(2)-C(17)	68.33(5)
C(23)-Fe(2)-C(17)	156.47(9)
C(21)-Fe(2)-C(20)	124.49(8)
C(25)-Fe(2)-C(20)	159.48(9)
C(18)-Fe(2)-C(20)	68.28(5)
C(22)-Fe(2)-C(20)	109.73(8)
C(24)-Fe(2)-C(20)	159.30(9)
C(19)-Fe(2)-C(20)	40.5

C(23)-Fe(2)-C(20)	124.45(8)
C(17)-Fe(2)-C(20)	68.1
C(21)-Fe(2)-C(16)	109.30(8)
C(25)-Fe(2)-C(16)	122.80(8)
C(18)-Fe(2)-C(16)	68.2
C(22)-Fe(2)-C(16)	125.59(8)
C(24)-Fe(2)-C(16)	157.38(9)
C(19)-Fe(2)-C(16)	68.2
C(23)-Fe(2)-C(16)	161.33(9)
C(17)-Fe(2)-C(16)	40.5
C(20)-Fe(2)-C(16)	40.4
B(1)-O(1)-H(100)	115(4)
B(1)-O(2)-H(200)	110(5)
B(2)-O(3)-H(300)	118(3)
B(2)-O(4)-H(400)	113(5)
H(901)-O(9)-H(902)	110(7)
H(103)-O(10)-H(102)	97(6)
H(111)-O(11)-H(112)	104(5)
C(2)-C(1)-C(5)	108.0
C(2)-C(1)-C(11)	126.38(19)
C(5)-C(1)-C(11)	125.60(19)
C(2)-C(1)-Fe(1)	68.96(9)
C(5)-C(1)-Fe(1)	70.64(8)
C(11)-C(1)-Fe(1)	127.21(18)
C(1)-C(2)-C(3)	108.0
C(1)-C(2)-Fe(1)	70.23(8)
C(3)-C(2)-Fe(1)	70.03(8)
C(1)-C(2)-H(2B)	126.0
C(3)-C(2)-H(2B)	126.0
Fe(1)-C(2)-H(2B)	126.0
C(4)-C(3)-C(2)	108.0
C(4)-C(3)-Fe(1)	70.67(8)
C(2)-C(3)-Fe(1)	69.11(8)
C(4)-C(3)-H(3B)	126.0
C(2)-C(3)-H(3B)	126.0
Fe(1)-C(3)-H(3B)	126.0
C(3)-C(4)-C(5)	108.0
C(3)-C(4)-Fe(1)	68.85(8)
C(5)-C(4)-Fe(1)	70.00(8)
C(3)-C(4)-H(4B)	126.0
C(5)-C(4)-H(4B)	126.0
Fe(1)-C(4)-H(4B)	126.0
C(1)-C(5)-C(4)	108.0
C(1)-C(5)-Fe(1)	68.95(8)
C(4)-C(5)-Fe(1)	69.79(9)
C(1)-C(5)-H(5B)	126.0
C(4)-C(5)-H(5B)	126.0
Fe(1)-C(5)-H(5B)	126.0
C(7)-C(6)-C(10)	108.0
C(7)-C(6)-B(1)	126.31(19)
C(10)-C(6)-B(1)	125.68(19)
C(7)-C(6)-Fe(1)	69.61(8)
C(10)-C(6)-Fe(1)	69.40(8)
B(1)-C(6)-Fe(1)	125.66(18)
C(6)-C(7)-C(8)	108.0
C(6)-C(7)-Fe(1)	70.05(8)
C(8)-C(7)-Fe(1)	69.19(8)
C(6)-C(7)-H(7B)	126.0
C(8)-C(7)-H(7B)	126.0
Fe(1)-C(7)-H(7B)	126.0
C(9)-C(8)-C(7)	108.0
C(9)-C(8)-Fe(1)	69.52(8)
C(7)-C(8)-Fe(1)	70.26(8)

C(9)-C(8)-H(8B)	126.0
C(7)-C(8)-H(8B)	126.0
Fe(1)-C(8)-H(8B)	126.0
C(10)-C(9)-C(8)	108.0
C(10)-C(9)-Fe(1)	70.15(8)
C(8)-C(9)-Fe(1)	69.75(9)
C(10)-C(9)-H(9A)	126.0
C(8)-C(9)-H(9A)	126.0
Fe(1)-C(9)-H(9A)	126.0
C(9)-C(10)-C(6)	108.0
C(9)-C(10)-Fe(1)	69.22(8)
C(6)-C(10)-Fe(1)	70.20(8)
C(9)-C(10)-H(10A)	126.0
C(6)-C(10)-H(10A)	126.0
Fe(1)-C(10)-H(10A)	126.0
C(12)-C(11)-C(15)	117.6(3)
C(12)-C(11)-C(1)	121.6(3)
C(15)-C(11)-C(1)	120.7(3)
C(13)-C(12)-C(11)	120.4(4)
C(13)-C(12)-H(12A)	119.8
C(11)-C(12)-H(12A)	119.8
N(1)-C(13)-C(12)	120.7(4)
N(1)-C(13)-H(13A)	119.7
C(12)-C(13)-H(13A)	119.7
N(1)-C(14)-C(15)	120.6(4)
N(1)-C(14)-H(14A)	119.7
C(15)-C(14)-H(14A)	119.7
C(14)-C(15)-C(11)	119.2(4)
C(14)-C(15)-H(15A)	120.4
C(11)-C(15)-H(15A)	120.4
C(17)-C(16)-C(20)	108.0
C(17)-C(16)-B(2)	124.9(2)
C(20)-C(16)-B(2)	126.9(2)
C(17)-C(16)-Fe(2)	69.41(8)
C(20)-C(16)-Fe(2)	69.70(9)
B(2)-C(16)-Fe(2)	123.16(18)
C(18)-C(17)-C(16)	108.0
C(18)-C(17)-Fe(2)	69.36(9)
C(16)-C(17)-Fe(2)	70.11(8)
C(18)-C(17)-H(17A)	126.0
C(16)-C(17)-H(17A)	126.0
Fe(2)-C(17)-H(17A)	126.0
C(19)-C(18)-C(17)	108.0
C(19)-C(18)-Fe(2)	69.81(8)
C(17)-C(18)-Fe(2)	69.98(8)
C(19)-C(18)-H(18A)	126.0
C(17)-C(18)-H(18A)	126.0
Fe(2)-C(18)-H(18A)	126.0
C(20)-C(19)-C(18)	108.0
C(20)-C(19)-Fe(2)	70.14(8)
C(18)-C(19)-Fe(2)	69.49(8)
C(20)-C(19)-H(19A)	126.0
C(18)-C(19)-H(19A)	126.0
Fe(2)-C(19)-H(19A)	126.0
C(19)-C(20)-C(16)	108.0
C(19)-C(20)-Fe(2)	69.32(8)
C(16)-C(20)-Fe(2)	69.89(8)
C(19)-C(20)-H(20A)	126.0
C(16)-C(20)-H(20A)	126.0
Fe(2)-C(20)-H(20A)	126.0
C(22)-C(21)-C(25)	108.0
C(22)-C(21)-C(26)	126.69(19)
C(25)-C(21)-C(26)	125.31(19)

C(22)-C(21)-Fe(2)	69.82(8)
C(25)-C(21)-Fe(2)	69.62(9)
C(26)-C(21)-Fe(2)	126.20(17)
C(21)-C(22)-C(23)	108.0
C(21)-C(22)-Fe(2)	69.50(8)
C(23)-C(22)-Fe(2)	69.78(9)
C(21)-C(22)-H(22A)	126.0
C(23)-C(22)-H(22A)	126.0
Fe(2)-C(22)-H(22A)	126.0
C(24)-C(23)-C(22)	108.0
C(24)-C(23)-Fe(2)	69.58(9)
C(22)-C(23)-Fe(2)	69.61(8)
C(24)-C(23)-H(23A)	126.0
C(22)-C(23)-H(23A)	126.0
Fe(2)-C(23)-H(23A)	126.0
C(25)-C(24)-C(23)	108.0
C(25)-C(24)-Fe(2)	69.50(8)
C(23)-C(24)-Fe(2)	69.80(9)
C(25)-C(24)-H(24A)	126.0
C(23)-C(24)-H(24A)	126.0
Fe(2)-C(24)-H(24A)	126.0
C(24)-C(25)-C(21)	108.0
C(24)-C(25)-Fe(2)	69.80(8)
C(21)-C(25)-Fe(2)	69.65(8)
C(24)-C(25)-H(25A)	126.0
C(21)-C(25)-H(25A)	126.0
Fe(2)-C(25)-H(25A)	126.0
C(30)-C(26)-C(27)	117.0(3)
C(30)-C(26)-C(21)	121.3(3)
C(27)-C(26)-C(21)	121.7(3)
C(28)-C(27)-C(26)	120.4(3)
C(28)-C(27)-H(27A)	119.8
C(26)-C(27)-H(27A)	119.8
N(2)-C(28)-C(27)	120.2(3)
N(2)-C(28)-H(28A)	119.9
C(27)-C(28)-H(28A)	119.9
N(2)-C(29)-C(30)	120.6(3)
N(2)-C(29)-H(29A)	119.7
C(30)-C(29)-H(29A)	119.7
C(29)-C(30)-C(26)	120.0(3)
C(29)-C(30)-H(30A)	120.0
C(26)-C(30)-H(30A)	120.0
O(1)-B(1)-O(2)	125.0(3)
O(1)-B(1)-C(6)	116.7(3)
O(2)-B(1)-C(6)	118.3(3)
O(3)-B(2)-O(4)	125.7(3)
O(3)-B(2)-C(16)	116.4(3)
O(4)-B(2)-C(16)	117.8(3)
C(13)-N(1)-C(14)	121.6(4)
C(13)-N(1)-H(101)	126(3)
C(14)-N(1)-H(101)	112(3)
C(29)-N(2)-C(28)	121.8(3)
C(29)-N(2)-H(201)	122(2)
C(28)-N(2)-H(201)	116(2)

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Table 29. Anisotropic displacement parameters (A^2 x 10^3) for 3b.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	29(1)	43(1)	47(1)	2(1)	13(1)	-1(1)
Fe(1)	28(1)	25(1)	26(1)	-4(1)	10(1)	-2(1)
Fe(2)	30(1)	24(1)	29(1)	-4(1)	11(1)	-3(1)
O(1)	38(2)	61(2)	40(1)	9(1)	18(1)	-4(1)
O(2)	36(2)	69(2)	46(2)	16(1)	16(1)	6(1)
O(3)	41(2)	52(2)	37(1)	-1(1)	6(1)	4(1)
O(4)	38(2)	55(2)	38(1)	-1(1)	14(1)	-11(1)
O(5)	59(2)	52(2)	151(3)	-15(2)	57(2)	2(2)
O(6)	36(1)	88(2)	42(1)	11(1)	9(1)	-10(1)
O(7)	42(2)	108(3)	53(2)	32(2)	18(1)	7(2)
O(8)	39(2)	53(2)	81(2)	-10(2)	13(2)	-10(1)
O(9)	56(2)	57(2)	96(3)	-3(2)	-5(2)	11(2)
O(10)	53(2)	47(2)	59(2)	9(2)	0(2)	-5(1)
O(11)	41(2)	67(2)	51(2)	-5(2)	14(1)	5(1)
C(1)	36(2)	25(1)	29(2)	-6(1)	12(1)	-5(1)
C(2)	42(2)	29(2)	36(2)	-3(1)	9(2)	0(1)
C(3)	39(2)	39(2)	46(2)	-9(2)	11(2)	10(2)
C(4)	36(2)	46(2)	44(2)	-14(2)	23(2)	-6(2)
C(5)	33(2)	34(2)	33(2)	-4(1)	12(1)	-3(1)
C(6)	35(2)	28(2)	29(2)	-6(1)	15(1)	-2(1)
C(7)	39(2)	43(2)	27(2)	-3(1)	13(1)	0(2)
C(8)	32(2)	52(2)	36(2)	-16(2)	4(2)	-2(2)
C(9)	42(2)	36(2)	44(2)	-17(2)	21(2)	-15(2)
C(10)	41(2)	28(2)	34(2)	-7(1)	18(2)	-3(1)
C(11)	37(2)	28(2)	30(2)	-8(1)	9(1)	-8(1)
C(12)	49(2)	56(2)	37(2)	-4(2)	16(2)	-19(2)
C(13)	58(3)	97(3)	43(2)	-15(2)	23(2)	-36(2)
C(14)	37(2)	105(4)	36(2)	-11(2)	2(2)	-7(2)
C(15)	38(2)	56(2)	38(2)	-3(2)	12(2)	-6(2)
C(16)	40(2)	26(2)	26(2)	-5(1)	13(1)	-3(1)
C(17)	56(2)	35(2)	29(2)	-5(1)	20(2)	-9(2)
C(18)	49(2)	43(2)	50(2)	-15(2)	33(2)	-14(2)
C(19)	35(2)	41(2)	53(2)	-12(2)	18(2)	0(2)
C(20)	42(2)	26(2)	38(2)	-5(1)	18(2)	-1(1)
C(21)	35(2)	28(2)	33(2)	-8(1)	13(1)	1(1)
C(22)	37(2)	38(2)	32(2)	-8(1)	12(2)	0(1)
C(23)	36(2)	41(2)	41(2)	-14(2)	7(2)	-3(1)
C(24)	42(2)	29(2)	55(2)	-13(2)	18(2)	-9(1)
C(25)	38(2)	26(2)	38(2)	-3(1)	10(2)	-4(1)
C(26)	33(2)	27(2)	31(2)	-7(1)	11(1)	4(1)
C(27)	37(2)	44(2)	34(2)	4(2)	11(2)	3(2)
C(28)	43(2)	45(2)	49(2)	6(2)	21(2)	0(2)
C(29)	38(2)	44(2)	39(2)	-3(2)	8(2)	5(2)
C(30)	39(2)	41(2)	33(2)	0(2)	14(2)	3(2)
B(1)	33(2)	33(2)	29(2)	-5(2)	14(2)	-1(2)
B(2)	37(2)	30(2)	30(2)	-10(2)	10(2)	-2(2)
N(1)	39(2)	138(4)	51(2)	-31(2)	21(2)	-36(2)
N(2)	32(2)	42(2)	50(2)	-5(1)	15(1)	-1(1)

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Table 30. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 3b.

	x	y	z	U(eq)
H(2B)	8638	-198	1582	45
H(3B)	9700	920	1459	51
H(4B)	9390	3153	443	48
H(5B)	8135	3414	-63	40
H(7B)	8727	2994	2653	43
H(8B)	9796	4047	2529	51
H(9A)	9505	6446	1568	47
H(10A)	8257	6876	1098	40
H(12A)	7540	-40	1481	56
H(13A)	6466	-626	1228	78
H(14A)	6003	1827	-549	75
H(15A)	7080	2400	-358	54
H(17A)	1817	3146	2525	46
H(18A)	563	3212	1950	52
H(19A)	259	5423	927	51
H(20A)	1325	6723	870	42
H(22A)	1336	3208	-170	43
H(23A)	284	1973	-57	50
H(24A)	614	-140	996	50
H(25A)	1870	-211	1534	42
H(27A)	2442	3430	5	46
H(28A)	3534	3888	233	54
H(29A)	4004	1174	1961	51
H(30A)	2924	602	1769	45
H(101)	5740(30)	180(70)	150(30)	87(16)
H(201)	4330(20)	2770(50)	1166(19)	48(10)
H(100)	7000(20)	3880(70)	2190(30)	76(17)
H(200)	6740(30)	5060(70)	1090(30)	80(20)
H(300)	3370(20)	4720(60)	2580(20)	66(15)
H(400)	3090(30)	6380(80)	1520(30)	100(20)
H(901)	4580(40)	5240(100)	3230(40)	160(30)
H(902)	4480(30)	3550(80)	3090(30)	90(20)
H(103)	5320(30)	-2880(80)	380(30)	100(20)
H(102)	5030(30)	-2430(100)	-200(40)	130(30)
H(111)	4330(20)	6530(60)	1770(20)	63(15)
H(112)	4080(20)	7580(70)	2100(30)	73(17)

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Table 31. Crystal data and structure refinement for 5.

Identification code	5
Empirical formula	C20 H24 Cl2 Fe N2 O4
Formula weight	483.16
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 13.810(9) A alpha = 90 deg. b = 9.270(5) A beta = 90 deg. c = 17.360(5) A gamma = 90 deg.
Volume	2222(2) A^3
Z, Calculated density	4, 1.444 Mg/m^3
Absorption coefficient	0.947 mm^-1
F(000)	1000
Crystal size	0.20 x 0.17 x 0.15 mm
Theta range for data collection	3.18 to 19.99 deg.
Limiting indices	-13<=h<=13, 0<=k<=8, 0<=l<=16
Reflections collected / unique	6858 / 2044 [R(int) = 0.0491]
Completeness to theta = 19.99	99.0 %
Absorption correction	Psi-scan
Max. and min. transmission	1.00 and 0.76
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2044 / 0 / 152
Goodness-of-fit on F^2	1.079
Final R indices [I>2sigma(I)]	R1 = 0.0840, wR2 = 0.1994
R indices (all data)	R1 = 0.1330, wR2 = 0.2414
Absolute structure parameter	0.34(10)
Largest diff. peak and hole	0.732 and -0.760 e.A^-3