Table 1. Crystal data and structure refinement for **4**.

Identification code	**4**
Empirical formula	C20 H19 B Fe2
Formula weight	381.86
Temperature	149(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 7.5664(9) A alpha = 90 deg.
	b = 10.3258(12) A beta = 105.299(5) deg.
	c = 10.4377(15) A gamma = 90 deg.
Volume	786.59(17) A^3
Z, Calculated density	2, 1.612 Mg/m^3
Absorption coefficient	1.838 mm^-1
F(000)	392
Crystal size	0.36 x 0.22 x 0.16 mm
Theta range for data collection	2.79 to 32.13 deg.
Limiting indices	-11<=h<=10, -15<=k<=15, -14<=l<=15
Reflections collected / unique	13317 / 2534 [R(int) = 0.0348]
Completeness to theta = 32.13	91.6 %
Absorption correction	Empirical, SADABS (Sheldrick, 2000)
Max. and min. transmission	1.000 and 0.860
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2534 / 0 / 109
Goodness-of-fit on F^2	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0356, wR2 = 0.0742
R indices (all data)	R1 = 0.0533, wR2 = 0.0807
Largest diff. peak and hole	0.547 and -0.502 e.A^-3

Table 2. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters (A^2 x 10^4) for **4**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	23923(3)	6200(3)	24342(3)	203(1)
C(1)	45330(30)	15812(19)	36690(20)	273(4)
C(2)	32300(30)	24764(18)	29300(20)	282(4)
C(3)	30570(30)	22578(19)	15600(20)	289(4)
C(4)	42490(30)	12270(20)	14540(20)	297(4)
C(5)	51580(20)	8027(19)	27500(20)	275(4)
C(13)	12440(30)	-5320(20)	35990(20)	324(4)
C(12)	16440(70)	-12280(50)	24850(50)	271(11)
C(14)	1050(60)	4320(40)	32160(50)	263(8)
C(15)	-4090(50)	4480(40)	18150(40)	221(7)
B(1)	8760(50)	-7420(40)	-490(50)	232(8)
C(11)	5330(50)	-5750(40)	13210(40)	215(7)
C(22)	1350(50)	-2860(40)	-26040(50)	219(7)
C(21)	440(50)	840(40)	-12970(40)	200(7)
C(25)	-13020(50)	11080(40)	-14760(40)	214(7)
C(24)	-20040(60)	13240(40)	-28590(50)	244(10)

Table 3. Bond lengths [A] and angles [deg] for **4**.

Fe(1)-C(12)	1.995(5)
Fe(1)-C(11)	1.997(4)
Fe(1)-C(5)	2.0395(18)
Fe(1)-C(1)	2.0415(19)
Fe(1)-C(4)	2.0423(19)
Fe(1)-C(2)	2.0424(19)
Fe(1)-C(3)	2.0466(19)
Fe(1)-C(13)	2.051(2)
Fe(1)-C(15)	2.054(4)
Fe(1)-C(14)	2.108(4)
C(1)-C(2)	1.421(3)
C(1)-C(5)	1.424(3)
C(1)-H(1)	0.9500
C(2)-C(3)	1.420(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.418(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.416(3)
C(4)-H(4)	0.9500
C(5)-H(5)	0.9500
C(13)-C(14)	1.309(4)
C(13)-C(12)	1.465(5)
C(13)-H(13)	0.9500
C(12)-C(11)	1.448(7)
C(12)-H(12)	0.9500
C(14)-C(15)	1.410(6)
C(14)-H(14)	0.9500
C(15)-C(11)	1.443(5)
C(15)-H(15)	0.9500
B(1)-C(11)	1.530(6)
B(1)-C(21)	1.545(6)
B(1)-H(1B)	1.12(4)
C(22)-C(21)	1.436(6)
C(22)-C(13)#1	1.520(5)
C(22)-Fe(1)#1	1.997(4)
C(22)-H(22)	0.9500
C(21)-C(25)	1.446(5)
C(21)-Fe(1)#1	2.045(4)
C(25)-C(24)	1.418(6)
C(25)-Fe(1)#1	2.104(4)
C(25)-H(25)	0.9500
C(24)-C(13)#1	1.352(5)
C(24)-Fe(1)#1	2.093(5)
C(24)-H(24)	0.9500
C(12)-Fe(1)-C(11)	42.54(19)
C(12)-Fe(1)-C(5)	111.75(15)
C(11)-Fe(1)-C(5)	133.36(13)
C(12)-Fe(1)-C(1)	129.19(17)
C(11)-Fe(1)-C(1)	170.87(13)
C(5)-Fe(1)-C(1)	40.85(8)
C(12)-Fe(1)-C(4)	122.97(15)
C(11)-Fe(1)-C(4)	111.72(12)
C(5)-Fe(1)-C(4)	40.60(9)
C(1)-Fe(1)-C(4)	68.35(8)
C(12)-Fe(1)-C(2)	164.20(16)
C(11)-Fe(1)-C(2)	148.34(14)
C(5)-Fe(1)-C(2)	68.63(8)
C(1)-Fe(1)-C(2)	40.73(8)
C(4)-Fe(1)-C(2)	68.33(8)
C(12)-Fe(1)-C(3)	155.09(16)

C(11)-Fe(1)-C(3)	117.99(13)
C(5)-Fe(1)-C(3)	68.49(8)
C(1)-Fe(1)-C(3)	68.43(8)
C(4)-Fe(1)-C(3)	40.59(8)
C(2)-Fe(1)-C(3)	40.64(8)
C(12)-Fe(1)-C(13)	42.43(15)
C(11)-Fe(1)-C(13)	69.08(12)
C(5)-Fe(1)-C(13)	122.33(9)
C(1)-Fe(1)-C(13)	107.30(9)
C(4)-Fe(1)-C(13)	158.42(9)
C(2)-Fe(1)-C(13)	123.08(9)
C(3)-Fe(1)-C(13)	159.42(9)
C(12)-Fe(1)-C(15)	69.46(18)
C(11)-Fe(1)-C(15)	41.72(15)
C(5)-Fe(1)-C(15)	171.31(13)
C(1)-Fe(1)-C(15)	145.24(12)
C(4)-Fe(1)-C(15)	131.14(14)
C(2)-Fe(1)-C(15)	112.72(12)
C(3)-Fe(1)-C(15)	106.60(12)
C(13)-Fe(1)-C(15)	64.73(13)
C(12)-Fe(1)-C(14)	68.53(18)
C(11)-Fe(1)-C(14)	69.15(17)
C(5)-Fe(1)-C(14)	149.10(15)
C(1)-Fe(1)-C(14)	113.33(15)
C(4)-Fe(1)-C(14)	164.92(13)
C(2)-Fe(1)-C(14)	102.69(13)
C(3)-Fe(1)-C(14)	124.89(12)
C(13)-Fe(1)-C(14)	36.66(12)
C(15)-Fe(1)-C(14)	39.59(15)
C(2)-C(1)-C(5)	107.96(18)
C(2)-C(1)-Fe(1)	69.67(11)
C(5)-C(1)-Fe(1)	69.50(11)
C(2)-C(1)-H(1)	126.0
C(5)-C(1)-H(1)	126.0
Fe(1)-C(1)-H(1)	126.4
C(3)-C(2)-C(1)	108.02(17)
C(3)-C(2)-Fe(1)	69.84(11)
C(1)-C(2)-Fe(1)	69.60(11)
C(3)-C(2)-H(2)	126.0
C(1)-C(2)-H(2)	126.0
Fe(1)-C(2)-H(2)	126.1
C(4)-C(3)-C(2)	107.83(18)
C(4)-C(3)-Fe(1)	69.54(11)
C(2)-C(3)-Fe(1)	69.52(11)
C(4)-C(3)-H(3)	126.1
C(2)-C(3)-H(3)	126.1
Fe(1)-C(3)-H(3)	126.4
C(5)-C(4)-C(3)	108.44(18)
C(5)-C(4)-Fe(1)	69.59(11)
C(3)-C(4)-Fe(1)	69.87(11)
C(5)-C(4)-H(4)	125.8
C(3)-C(4)-H(4)	125.8
Fe(1)-C(4)-H(4)	126.3
C(4)-C(5)-C(1)	107.75(17)
C(4)-C(5)-Fe(1)	69.81(11)
C(1)-C(5)-Fe(1)	69.65(11)
C(4)-C(5)-H(5)	126.1
C(1)-C(5)-H(5)	126.1
Fe(1)-C(5)-H(5)	126.0
C(14)-C(13)-C(12)	112.8(3)
C(14)-C(13)-Fe(1)	74.0(2)
C(12)-C(13)-Fe(1)	66.7(2)
C(14)-C(13)-H(13)	123.6

C(12)-C(13)-H(13)	123.6
Fe(1)-C(13)-H(13)	127.3
C(11)-C(12)-C(13)	104.0(4)
C(11)-C(12)-Fe(1)	68.8(2)
C(13)-C(12)-Fe(1)	70.8(2)
C(11)-C(12)-H(12)	128.0
C(13)-C(12)-H(12)	128.0
Fe(1)-C(12)-H(12)	124.1
C(13)-C(14)-C(15)	107.8(4)
C(13)-C(14)-Fe(1)	69.3(2)
C(15)-C(14)-Fe(1)	68.2(2)
C(13)-C(14)-H(14)	126.1
C(15)-C(14)-H(14)	126.1
Fe(1)-C(14)-H(14)	128.0
C(14)-C(15)-C(11)	109.5(3)
C(14)-C(15)-Fe(1)	72.3(2)
C(11)-C(15)-Fe(1)	67.0(2)
C(14)-C(15)-H(15)	125.2
C(11)-C(15)-H(15)	125.2
Fe(1)-C(15)-H(15)	127.1
C(11)-B(1)-C(21)	126.5(3)
C(11)-B(1)-H(1B)	117(2)
C(21)-B(1)-H(1B)	116(2)
C(15)-C(11)-C(12)	105.9(3)
C(15)-C(11)-B(1)	129.7(4)
C(12)-C(11)-B(1)	121.8(4)
C(15)-C(11)-Fe(1)	71.3(2)
C(12)-C(11)-Fe(1)	68.7(2)
B(1)-C(11)-Fe(1)	110.3(2)
C(21)-C(22)-C(13)#1	107.7(3)
C(21)-C(22)-Fe(1)#1	71.0(2)
C(13)#1-C(22)-Fe(1)#1	69.85(17)
C(21)-C(22)-H(22)	126.1
C(13)#1-C(22)-H(22)	126.1
Fe(1)#1-C(22)-H(22)	124.6
C(22)-C(21)-C(25)	106.3(3)
C(22)-C(21)-B(1)	122.9(4)
C(25)-C(21)-B(1)	129.0(3)
C(22)-C(21)-Fe(1)#1	67.4(2)
C(25)-C(21)-Fe(1)#1	71.8(2)
B(1)-C(21)-Fe(1)#1	113.4(2)
C(24)-C(25)-C(21)	107.9(3)
C(24)-C(25)-Fe(1)#1	69.8(2)
C(21)-C(25)-Fe(1)#1	67.4(2)
C(24)-C(25)-H(25)	126.0
C(21)-C(25)-H(25)	126.0
Fe(1)#1-C(25)-H(25)	128.3
C(13)#1-C(24)-C(25)	112.7(4)
C(13)#1-C(24)-Fe(1)#1	69.3(2)
C(25)-C(24)-Fe(1)#1	70.7(2)
C(13)#1-C(24)-H(24)	123.7
C(25)-C(24)-H(24)	123.7
Fe(1)#1-C(24)-H(24)	128.1

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

Table 4. Anisotropic displacement parameters (A^2 x 10^4) for **4**.
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)	152(1)	227(1)	219(2)	32(1)	29(1)	-35(1)
C(1)	217(9)	286(9)	293(11)	-57(8)	29(7)	-40(7)
C(2)	276(10)	217(8)	378(11)	-40(8)	134(8)	-7(7)
C(3)	280(10)	246(9)	344(11)	72(8)	88(8)	-52(7)
C(4)	319(10)	288(10)	341(11)	-49(8)	187(9)	-92(8)
C(5)	157(8)	254(9)	430(12)	-22(8)	102(8)	-7(7)
C(13)	328(10)	373(11)	284(11)	67(9)	103(8)	-100(9)
B(1)	171(17)	190(17)	300(20)	-28(16)	10(15)	-28(14)

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

	x	y	z	U(eq)
H(1)	4919	1514	4609	33
H(2)	2587	3110	3291	34
H(3)	2281	2720	841	35
H(4)	4410	879	649	36
H(5)	6029	121	2969	33
H(13)	1757	-758	4504	39
H(12)	2446	-1942	2518	33
H(14)	-302	1018	3780	32
H(15)	-1247	1041	1279	27
H(1B)	1870(50)	-1520(40)	-160(40)	19(10)
H(22)	918	-928	-2809	26
H(25)	-1655	1557	-788	26
H(24)	-2909	1955	-3226	29