Table 32. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 5.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	543(2)	1698(3)	3403(1)	29(1)
C(1)	-710(8)	1624(11)	4024(4)	24(4)
C(2)	-687(9)	2859(9)	3540(5)	31(4)
C(3)	-594(9)	2381(11)	2767(4)	32(4)
C(4)	-560(9)	850(11)	2772(4)	39(4)
C(5)	-631(9)	382(9)	3549(5)	31(4)
C(6)	1718(8)	1921(12)	4105(5)	26(4)
C(7)	1692(9)	3047(9)	3550(6)	38(5)
C(8)	1726(9)	2410(12)	2807(5)	42(5)
C(9)	1773(9)	890(12)	2902(5)	37(5)
C(10)	1769(9)	588(9)	3704(6)	33(5)
C(11)	-737(10)	1616(18)	4861(8)	28(4)
C(12)	-778(12)	2933(18)	5262(9)	36(5)
C(13)	-818(11)	2927(18)	6054(9)	33(5)
N(1)	-855(9)	1686(19)	6449(9)	47(4)
C(14)	-839(14)	410(20)	6072(11)	47(6)
C(15)	-771(13)	358(19)	5284(10)	38(5)
C(16)	1705(11)	2091(15)	4937(9)	23(4)
C(17)	1720(13)	910(20)	5423(11)	44(5)
C(18)	1776(14)	1120(20)	6216(12)	49(6)
N(2)	1809(11)	2406(19)	6500(9)	49(4)
C(19)	1768(12)	3590(20)	6078(10)	40(5)
C(20)	1718(11)	3440(20)	5290(9)	32(4)
O(1)	2745(10)	2988(17)	497(9)	76(5)
O(2)	5806(10)	3682(15)	1023(7)	70(5)
O(3)	2061(9)	2715(15)	8025(7)	54(4)
O(4)	-1525(8)	1690(16)	930(7)	56(4)
Cl(1)	4081(4)	2420(8)	1885(3)	75(2)
Cl(2)	729(4)	1578(5)	782(3)	54(1)

Table 33. Bond lengths [A] and angles [deg] for 5.

Fe(1)-C(3)	2.021(11)
Fe(1)-C(2)	2.025(11)
Fe(1)-C(4)	2.033(12)
Fe(1)-C(7)	2.036(12)
Fe(1)-C(1)	2.040(10)
Fe(1)-C(6)	2.040(11)
Fe(1)-C(8)	2.043(11)
Fe(1)-C(5)	2.045(12)
Fe(1)-C(10)	2.049(12)
Fe(1)-C(9)	2.051(11)
C(1)-C(2)	1.4200
C(1)-C(5)	1.4200
C(1)-C(11)	1.455(15)
C(2)-C(3)	1.4200
C(3)-C(4)	1.4200
C(4)-C(5)	1.4200
C(6)-C(7)	1.4200
C(6)-C(10)	1.4200

C(6)-C(16)	1.454(17)
C(7)-C(8)	1.4200
C(8)-C(9)	1.4200
C(9)-C(10)	1.4200
C(11)-C(15)	1.38(2)
C(11)-C(12)	1.41(2)
C(12)-C(13)	1.38(2)
C(13)-N(1)	1.34(2)
N(1)-C(14)	1.35(2)
C(14)-C(15)	1.37(2)
C(16)-C(17)	1.38(2)
C(16)-C(20)	1.40(2)
C(17)-C(18)	1.39(3)
C(18)-N(2)	1.29(2)
N(2)-C(19)	1.32(2)
C(19)-C(20)	1.38(2)
C(3)-Fe(1)-C(2)	41.1(2)
C(3)-Fe(1)-C(4)	41.0(2)
C(2)-Fe(1)-C(4)	69.0(3)
C(3)-Fe(1)-C(7)	118.8(4)
C(2)-Fe(1)-C(7)	108.2(4)
C(4)-Fe(1)-C(7)	152.7(4)
C(3)-Fe(1)-C(1)	68.9(2)
C(2)-Fe(1)-C(1)	40.90(19)
C(4)-Fe(1)-C(1)	68.7(3)
C(7)-Fe(1)-C(1)	127.9(4)
C(3)-Fe(1)-C(6)	155.9(4)
C(2)-Fe(1)-C(6)	122.9(4)
C(4)-Fe(1)-C(6)	163.0(4)
C(7)-Fe(1)-C(6)	40.8(2)
C(1)-Fe(1)-C(6)	111.3(3)
C(3)-Fe(1)-C(8)	104.1(4)
C(2)-Fe(1)-C(8)	124.0(4)
C(4)-Fe(1)-C(8)	116.8(4)
C(7)-Fe(1)-C(8)	40.7(2)
C(1)-Fe(1)-C(8)	163.1(4)
C(6)-Fe(1)-C(8)	68.5(3)
C(3)-Fe(1)-C(5)	68.8(3)
C(2)-Fe(1)-C(5)	68.7(2)
C(4)-Fe(1)-C(5)	40.8(2)
C(7)-Fe(1)-C(5)	165.6(4)
C(1)-Fe(1)-C(5)	40.69(19)
C(6)-Fe(1)-C(5)	128.1(4)
C(8)-Fe(1)-C(5)	152.8(4)
C(3)-Fe(1)-C(10)	159.8(4)
C(2)-Fe(1)-C(10)	158.4(4)
C(4)-Fe(1)-C(10)	124.2(4)
C(7)-Fe(1)-C(10)	68.4(2)
C(1)-Fe(1)-C(10)	123.3(4)
C(6)-Fe(1)-C(10)	40.6(2)
C(8)-Fe(1)-C(10)	68.3(3)
C(5)-Fe(1)-C(10)	108.9(4)
C(3)-Fe(1)-C(9)	121.8(4)
C(2)-Fe(1)-C(9)	159.9(4)
C(4)-Fe(1)-C(9)	104.5(4)
C(7)-Fe(1)-C(9)	68.4(3)
C(1)-Fe(1)-C(9)	156.2(4)
C(6)-Fe(1)-C(9)	68.3(3)
C(8)-Fe(1)-C(9)	40.6(2)
C(5)-Fe(1)-C(9)	119.5(4)
C(10)-Fe(1)-C(9)	40.5(2)
C(2)-C(1)-C(5)	108.0

C(2)-C(1)-C(11)	126.6(9)
C(5)-C(1)-C(11)	125.3(9)
C(2)-C(1)-Fe(1)	69.0(5)
C(5)-C(1)-Fe(1)	69.9(5)
C(11)-C(1)-Fe(1)	123.4(8)
C(3)-C(2)-C(1)	108.0
C(3)-C(2)-Fe(1)	69.3(4)
C(1)-C(2)-Fe(1)	70.1(4)
C(4)-C(3)-C(2)	108.0
C(4)-C(3)-Fe(1)	70.0(5)
C(2)-C(3)-Fe(1)	69.6(4)
C(5)-C(4)-C(3)	108.0
C(5)-C(4)-Fe(1)	70.1(4)
C(3)-C(4)-Fe(1)	69.0(5)
C(4)-C(5)-C(1)	108.0
C(4)-C(5)-Fe(1)	69.2(4)
C(1)-C(5)-Fe(1)	69.5(4)
C(7)-C(6)-C(10)	108.0
C(7)-C(6)-C(16)	126.4(9)
C(10)-C(6)-C(16)	125.6(9)
C(7)-C(6)-Fe(1)	69.5(5)
C(10)-C(6)-Fe(1)	70.0(5)
C(16)-C(6)-Fe(1)	126.5(9)
C(6)-C(7)-C(8)	108.0
C(6)-C(7)-Fe(1)	69.8(4)
C(8)-C(7)-Fe(1)	69.9(4)
C(9)-C(8)-C(7)	108.0
C(9)-C(8)-Fe(1)	70.0(5)
C(7)-C(8)-Fe(1)	69.4(4)
C(10)-C(9)-C(8)	108.0
C(10)-C(9)-Fe(1)	69.7(4)
C(8)-C(9)-Fe(1)	69.4(5)
C(9)-C(10)-C(6)	108.0
C(9)-C(10)-Fe(1)	69.8(4)
C(6)-C(10)-Fe(1)	69.3(4)
C(15)-C(11)-C(12)	118.0(13)
C(15)-C(11)-C(1)	122.5(14)
C(12)-C(11)-C(1)	119.4(13)
C(13)-C(12)-C(11)	119.5(15)
N(1)-C(13)-C(12)	121.1(16)
C(13)-N(1)-C(14)	120.2(15)
N(1)-C(14)-C(15)	120.9(18)
C(11)-C(15)-C(14)	120.2(17)
C(17)-C(16)-C(20)	116.4(15)
C(17)-C(16)-C(6)	121.4(13)
C(20)-C(16)-C(6)	122.2(13)
C(16)-C(17)-C(18)	119.8(18)
N(2)-C(18)-C(17)	120(2)
C(18)-N(2)-C(19)	123.8(17)
N(2)-C(19)-C(20)	118.1(18)
C(19)-C(20)-C(16)	121.7(17)

Table 34. Anisotropic displacement parameters (A^2 x 10^3) for 5.
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)	25(1)	35(1)	26(1)	-1(1)	2(1)	1(1)
N(1)	29(8)	55(9)	56(11)	9(10)	1(7)	3(9)
N(2)	38(10)	80(12)	30(10)	10(11)	-6(8)	-10(8)
O(1)	50(9)	92(12)	86(10)	15(9)	-3(8)	-5(8)
O(2)	63(10)	91(12)	58(9)	18(8)	-7(7)	-21(8)
O(3)	44(8)	87(10)	32(7)	9(7)	-11(6)	9(7)
O(4)	48(8)	70(9)	51(8)	-13(9)	10(6)	0(9)
Cl(1)	56(4)	136(5)	32(3)	-16(3)	2(2)	-24(3)
Cl(2)	58(3)	43(3)	62(3)	3(3)	3(3)	-3(3)

Table 35. Hydrogen coordinates (x 10^4) and isotropic
displacement parameters (A^2 x 10^3) for 5.

	x	y	z	U(eq)
H(2)	-726	3814	3702	37
H(3)	-562	2967	2333	39
H(4)	-501	258	2342	46
H(5)	-627	-570	3717	37
H(7)	1658	4030	3656	45
H(8)	1718	2902	2340	50
H(9)	1802	212	2508	44
H(10)	1794	-323	3927	39
H(12)	-777	3801	4994	43
H(13)	-820	3798	6320	39
H(100)	-990(90)	2050(140)	7160(80)	30(40)
H(14)	-873	-446	6351	57
H(15)	-749	-529	5034	46
H(17)	1692	-16	5220	53
H(18)	1789	322	6544	59
H(200)	1920(80)	2720(120)	7090(80)	10(30)
H(19)	1773	4497	6307	48
H(20)	1692	4267	4984	38

Table 36. Crystal data and structure refinement for 6.

Identification code	6
Empirical formula	C32 H24 Fe N2
Formula weight	492.38
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 8.0675(10) A alpha = 90 deg. b = 8.033(3) A beta = 98.415(10) deg. c = 17.907(3) A gamma = 90 deg.
Volume	1148.0(5) A^3
Z, Calculated density	2, 1.424 Mg/m^3
Absorption coefficient	0.682 mm^-1
F(000)	512
Crystal size	0.20 x 0.18 x 0.16 mm
Theta range for data collection	3.42 to 24.98 deg.
Limiting indices	-9<=h<=9, 0<=k<=9, 0<=l<=21
Reflections collected / unique	3334 / 2015 [R(int) = 0.0035]
Completeness to theta = 24.98	99.6 %
Absorption correction	Psi-scan
Max. and min. transmission	1.00 and 0.79
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2015 / 0 / 161
Goodness-of-fit on F^2	1.071
Final R indices [I>2sigma(I)]	R1 = 0.0479, wR2 = 0.1057
R indices (all data)	R1 = 0.1150, wR2 = 0.1309
Extinction coefficient	0.0019(16)
Largest diff. peak and hole	0.322 and -0.224 e.A^-3

Table 37. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 6.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	5000	0	0	47(1)
N(1)	14698(4)	1426(5)	4138(2)	63(1)
C(1)	5627(4)	1479(5)	929(2)	47(1)
C(2)	4121(5)	604(6)	977(3)	57(1)
C(3)	2938(5)	1050(7)	343(3)	67(1)
C(4)	3691(5)	2176(7)	-91(3)	66(1)
C(5)	5357(5)	2464(6)	262(2)	56(1)
C(6)	7199(4)	1409(5)	1473(2)	42(1)
C(7)	8679(5)	2049(6)	1300(2)	57(1)
C(8)	10131(5)	2032(6)	1814(2)	55(1)
C(9)	10163(4)	1371(5)	2530(2)	43(1)
C(10)	8693(5)	707(6)	2703(2)	51(1)
C(11)	7235(5)	715(6)	2183(2)	53(1)
C(12)	11736(4)	1376(5)	3078(2)	43(1)
C(13)	13064(5)	2405(6)	3003(3)	59(1)
C(14)	14488(5)	2392(6)	3528(3)	68(1)
C(15)	13431(5)	416(5)	4206(2)	57(1)
C(16)	11954(5)	342(5)	3708(2)	50(1)

Table 38. Bond lengths [A] and angles [deg] for 6.

Fe(1)-C(4)#1	2.036(4)
Fe(1)-C(4)	2.036(4)
Fe(1)-C(3)	2.039(4)
Fe(1)-C(3)#1	2.039(4)
Fe(1)-C(2)	2.041(4)
Fe(1)-C(2)#1	2.041(4)
Fe(1)-C(1)	2.047(4)
Fe(1)-C(1)#1	2.047(4)
Fe(1)-C(5)	2.045(5)
Fe(1)-C(5)#1	2.045(5)
N(1)-C(15)	1.325(5)
N(1)-C(14)	1.330(6)
C(1)-C(2)	1.418(6)
C(1)-C(5)	1.424(6)
C(1)-C(6)	1.482(5)
C(2)-C(3)	1.418(6)
C(2)-H(2)	0.9300
C(3)-C(4)	1.388(7)
C(3)-H(3)	0.9300
C(4)-C(5)	1.418(6)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
C(6)-C(7)	1.376(5)
C(6)-C(11)	1.384(5)
C(7)-C(8)	1.380(5)
C(7)-H(7)	0.9300
C(8)-C(9)	1.384(5)
C(8)-H(8)	0.9300
C(9)-C(10)	1.377(5)

C(9)-C(12)	1.486(5)
C(10)-C(11)	1.390(5)
C(10)-H(10)	0.9300
C(11)-H(11)	0.9300
C(12)-C(13)	1.374(6)
C(12)-C(16)	1.391(5)
C(13)-C(14)	1.374(5)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-C(16)	1.382(5)
C(15)-H(15)	0.9300
C(16)-H(16)	0.9300
C(4)#1-Fe(1)-C(4)	180.0(2)
C(4)#1-Fe(1)-C(3)	140.16(19)
C(4)-Fe(1)-C(3)	39.84(19)
C(4)#1-Fe(1)-C(3)#1	39.84(19)
C(4)-Fe(1)-C(3)#1	140.16(19)
C(3)-Fe(1)-C(3)#1	180.0(3)
C(4)#1-Fe(1)-C(2)	112.1(2)
C(4)-Fe(1)-C(2)	67.9(2)
C(3)-Fe(1)-C(2)	40.69(17)
C(3)#1-Fe(1)-C(2)	139.31(17)
C(4)#1-Fe(1)-C(2)#1	67.9(2)
C(4)-Fe(1)-C(2)#1	112.1(2)
C(3)-Fe(1)-C(2)#1	139.31(17)
C(3)#1-Fe(1)-C(2)#1	40.69(17)
C(2)-Fe(1)-C(2)#1	180.0(2)
C(4)#1-Fe(1)-C(1)	111.69(17)
C(4)-Fe(1)-C(1)	68.31(17)
C(3)-Fe(1)-C(1)	68.31(16)
C(3)#1-Fe(1)-C(1)	111.69(16)
C(2)-Fe(1)-C(1)	40.58(16)
C(2)#1-Fe(1)-C(1)	139.42(16)
C(4)#1-Fe(1)-C(1)#1	68.31(17)
C(4)-Fe(1)-C(1)#1	111.69(17)
C(3)-Fe(1)-C(1)#1	111.69(16)
C(3)#1-Fe(1)-C(1)#1	68.31(16)
C(2)-Fe(1)-C(1)#1	139.42(16)
C(2)#1-Fe(1)-C(1)#1	40.58(16)
C(1)-Fe(1)-C(1)#1	180.00(14)
C(4)#1-Fe(1)-C(5)	139.34(17)
C(4)-Fe(1)-C(5)	40.66(17)
C(3)-Fe(1)-C(5)	67.9(2)
C(3)#1-Fe(1)-C(5)	112.1(2)
C(2)-Fe(1)-C(5)	68.17(19)
C(2)#1-Fe(1)-C(5)	111.83(19)
C(1)-Fe(1)-C(5)	40.71(16)
C(1)#1-Fe(1)-C(5)	139.29(16)
C(4)#1-Fe(1)-C(5)#1	40.66(17)
C(4)-Fe(1)-C(5)#1	139.34(17)
C(3)-Fe(1)-C(5)#1	112.1(2)
C(3)#1-Fe(1)-C(5)#1	67.9(2)
C(2)-Fe(1)-C(5)#1	111.83(19)
C(2)#1-Fe(1)-C(5)#1	68.17(19)
C(1)-Fe(1)-C(5)#1	139.29(16)
C(1)#1-Fe(1)-C(5)#1	40.71(16)
C(5)-Fe(1)-C(5)#1	180.0(2)
C(15)-N(1)-C(14)	115.2(4)
C(2)-C(1)-C(5)	107.4(3)
C(2)-C(1)-C(6)	126.9(4)
C(5)-C(1)-C(6)	125.7(4)
C(2)-C(1)-Fe(1)	69.5(2)

C(5)-C(1)-Fe(1)	69.6(2)
C(6)-C(1)-Fe(1)	126.7(3)
C(1)-C(2)-C(3)	108.0(4)
C(1)-C(2)-Fe(1)	69.9(2)
C(3)-C(2)-Fe(1)	69.6(3)
C(1)-C(2)-H(2)	126.0
C(3)-C(2)-H(2)	126.0
Fe(1)-C(2)-H(2)	126.1
C(4)-C(3)-C(2)	108.3(4)
C(4)-C(3)-Fe(1)	70.0(3)
C(2)-C(3)-Fe(1)	69.8(2)
C(4)-C(3)-H(3)	125.8
C(2)-C(3)-H(3)	125.8
Fe(1)-C(3)-H(3)	126.0
C(3)-C(4)-C(5)	108.7(4)
C(3)-C(4)-Fe(1)	70.2(3)
C(5)-C(4)-Fe(1)	70.0(2)
C(3)-C(4)-H(4)	125.6
C(5)-C(4)-H(4)	125.6
Fe(1)-C(4)-H(4)	125.8
C(1)-C(5)-C(4)	107.6(4)
C(1)-C(5)-Fe(1)	69.7(3)
C(4)-C(5)-Fe(1)	69.3(3)
C(1)-C(5)-H(5)	126.2
C(4)-C(5)-H(5)	126.2
Fe(1)-C(5)-H(5)	126.3
C(7)-C(6)-C(11)	117.0(3)
C(7)-C(6)-C(1)	121.7(4)
C(11)-C(6)-C(1)	121.2(4)
C(6)-C(7)-C(8)	121.7(4)
C(6)-C(7)-H(7)	119.1
C(8)-C(7)-H(7)	119.1
C(9)-C(8)-C(7)	121.4(4)
C(9)-C(8)-H(8)	119.3
C(7)-C(8)-H(8)	119.3
C(10)-C(9)-C(8)	117.2(3)
C(10)-C(9)-C(12)	122.2(4)
C(8)-C(9)-C(12)	120.5(4)
C(9)-C(10)-C(11)	121.3(4)
C(9)-C(10)-H(10)	119.3
C(11)-C(10)-H(10)	119.3
C(6)-C(11)-C(10)	121.3(4)
C(6)-C(11)-H(11)	119.4
C(10)-C(11)-H(11)	119.4
C(13)-C(12)-C(16)	115.5(4)
C(13)-C(12)-C(9)	122.7(4)
C(16)-C(12)-C(9)	121.8(4)
C(14)-C(13)-C(12)	121.0(4)
C(14)-C(13)-H(13)	119.5
C(12)-C(13)-H(13)	119.5
N(1)-C(14)-C(13)	124.0(4)
N(1)-C(14)-H(14)	118.0
C(13)-C(14)-H(14)	118.0
N(1)-C(15)-C(16)	124.8(4)
N(1)-C(15)-H(15)	117.6
C(16)-C(15)-H(15)	117.6
C(15)-C(16)-C(12)	119.5(4)
C(15)-C(16)-H(16)	120.3
C(12)-C(16)-H(16)	120.3

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

Table 39. Anisotropic displacement parameters (A^2 x 10^3) for 6.
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)	33(1)	63(1)	43(1)	-6(1)	-6(1)	7(1)
N(1)	59(2)	63(2)	60(2)	7(2)	-18(2)	-9(2)
C(1)	41(2)	55(3)	44(2)	-3(2)	1(2)	7(2)
C(2)	37(2)	84(3)	51(2)	-11(2)	7(2)	5(2)
C(3)	35(2)	96(4)	66(3)	-21(3)	-5(2)	12(2)
C(4)	56(3)	78(3)	58(3)	-12(3)	-16(2)	30(3)
C(5)	54(2)	55(3)	54(3)	1(2)	-6(2)	7(2)
C(6)	42(2)	46(2)	36(2)	-2(2)	-2(2)	5(2)
C(7)	49(2)	79(3)	40(2)	18(2)	0(2)	-5(2)
C(8)	44(2)	72(3)	45(3)	10(2)	-3(2)	-11(2)
C(9)	45(2)	41(2)	40(2)	-3(2)	-5(2)	1(2)
C(10)	47(2)	66(3)	38(2)	8(2)	-4(2)	-8(2)
C(11)	44(2)	66(3)	46(2)	3(2)	0(2)	-10(2)
C(12)	43(2)	42(2)	40(2)	-5(2)	-3(2)	2(2)
C(13)	56(2)	61(3)	56(3)	13(2)	-9(2)	-11(2)
C(14)	55(3)	69(3)	71(3)	15(3)	-16(2)	-19(2)
C(15)	62(3)	59(3)	44(2)	6(2)	-9(2)	-1(2)
C(16)	53(2)	50(3)	43(2)	1(2)	-4(2)	-8(2)

Table 40. Hydrogen coordinates (x 10^4) and isotropic
displacement parameters (A^2 x 10^3) for 6.

	x	y	z	U(eq)
H(2)	3939	-133	1358	69
H(3)	1845	657	236	80
H(4)	3186	2661	-538	80
H(5)	6132	3169	89	67
H(7)	8702	2504	824	68
H(8)	11109	2475	1677	66
H(10)	8675	243	3178	62
H(11)	6264	246	2314	63
H(13)	12997	3120	2592	71
H(14)	15358	3102	3452	81
H(15)	13544	-295	4620	68
H(16)	11111	-394	3793	59

Table 41. Crystal data and structure refinement for 7.

Identification code	7
Empirical formula	C18 H14 Fe N4
Formula weight	342.18
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 3.5330(14) A alpha = 90 deg. b = 19.178(5) A beta = 96.48(3) deg. c = 10.350(3) A gamma = 90 deg.
Volume	696.8(4) A^3
Z, Calculated density	2, 1.631 Mg/m^3
Absorption coefficient	1.086 mm^-1
F(000)	352
Crystal size	0.22 x 0.20 x 0.16 mm
Theta range for data collection	3.96 to 22.97 deg.
Limiting indices	-3<=h<=3, -20<=k<=20, -11<=l<=0
Reflections collected / unique	1002 / 485 [R(int) = 0.0615]
Completeness to theta = 22.97	99.6 %
Absorption correction	Psi-scan
Max. and min. transmission	1.00 and 0.84
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	485 / 0 / 57
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0650, wR2 = 0.1540
R indices (all data)	R1 = 0.0945, wR2 = 0.1736
Largest diff. peak and hole	0.458 and -0.599 e.A^-3

Table 42. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 7.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	0	3070(1)	7500	28(1)
C(1)	-5000	3693(3)	7500	34(2)
C(2)	-4866(18)	3261(3)	8611(6)	42(2)
C(3)	4928(19)	2559(3)	6827(6)	54(2)
N(1)	-6679(14)	5540(2)	6436(4)	40(1)
C(4)	-5000	4458(3)	7500	29(2)
C(5)	-6656(16)	4844(3)	6458(5)	35(1)
C(6)	-5000	5842(4)	7500	44(2)

Table 43. Bond lengths [A] and angles [deg] for 7.

Fe(1)-C(2)#1	2.068(6)
Fe(1)-C(2)#2	2.068(6)
Fe(1)-C(3)#3	2.092(6)
Fe(1)-C(3)#4	2.092(6)
Fe(1)-C(1)#2	2.132(4)
Fe(1)-C(1)	2.132(4)
Fe(1)-C(3)#5	2.180(7)
Fe(1)-C(3)	2.180(7)
Fe(1)-C(2)	2.204(7)
Fe(1)-C(2)#5	2.204(7)
C(1)-C(2)#1	1.414(6)
C(1)-C(2)	1.414(6)
C(1)-C(4)	1.466(9)
C(1)-Fe(1)#3	2.132(4)
C(2)-C(3)#5	1.421(8)
C(2)-Fe(1)#3	2.068(6)
C(2)-H(2)	0.9300
C(3)-C(3)#4	1.389(13)
C(3)-C(2)#5	1.421(8)
C(3)-Fe(1)#2	2.092(6)
C(3)-H(3)	0.9300
N(1)-C(6)	1.324(5)
N(1)-C(5)	1.334(7)
C(4)-C(5)#1	1.383(6)
C(4)-C(5)	1.383(6)
C(5)-H(5)	0.9300
C(6)-N(1)#1	1.324(5)
C(6)-H(6)	0.9300
C(2)#1-Fe(1)-C(2)#2	159.6(3)
C(2)#1-Fe(1)-C(3)#3	39.9(2)
C(2)#2-Fe(1)-C(3)#3	158.9(2)
C(2)#1-Fe(1)-C(3)#4	158.9(2)
C(2)#2-Fe(1)-C(3)#4	39.9(2)
C(3)#3-Fe(1)-C(3)#4	124.0(3)
C(2)#1-Fe(1)-C(1)#2	125.1(2)
C(2)#2-Fe(1)-C(1)#2	39.31(17)
C(3)#3-Fe(1)-C(1)#2	160.23(19)

C(3)#4-Fe(1)-C(1)#2	65.4(2)
C(2)#1-Fe(1)-C(1)	39.31(17)
C(2)#2-Fe(1)-C(1)	125.1(2)
C(3)#3-Fe(1)-C(1)	65.4(2)
C(3)#4-Fe(1)-C(1)	160.23(19)
C(1)#2-Fe(1)-C(1)	111.9(3)
C(2)#1-Fe(1)-C(3)#5	64.9(2)
C(2)#2-Fe(1)-C(3)#5	125.7(2)
C(3)#3-Fe(1)-C(3)#5	37.9(3)
C(3)#4-Fe(1)-C(3)#5	111.5(3)
C(1)#2-Fe(1)-C(3)#5	160.65(17)
C(1)-Fe(1)-C(3)#5	63.9(2)
C(2)#1-Fe(1)-C(3)	125.7(2)
C(2)#2-Fe(1)-C(3)	64.9(2)
C(3)#3-Fe(1)-C(3)	111.5(3)
C(3)#4-Fe(1)-C(3)	37.9(3)
C(1)#2-Fe(1)-C(3)	63.9(2)
C(1)-Fe(1)-C(3)	160.65(17)
C(3)#5-Fe(1)-C(3)	126.5(3)
C(2)#1-Fe(1)-C(2)	64.8(3)
C(2)#2-Fe(1)-C(2)	111.6(3)
C(3)#3-Fe(1)-C(2)	64.0(2)
C(3)#4-Fe(1)-C(2)	126.4(2)
C(1)#2-Fe(1)-C(2)	127.02(19)
C(1)-Fe(1)-C(2)	38.02(15)
C(3)#5-Fe(1)-C(2)	37.8(2)
C(3)-Fe(1)-C(2)	159.9(2)
C(2)#1-Fe(1)-C(2)#5	111.6(3)
C(2)#2-Fe(1)-C(2)#5	64.8(3)
C(3)#3-Fe(1)-C(2)#5	126.4(2)
C(3)#4-Fe(1)-C(2)#5	64.0(2)
C(1)#2-Fe(1)-C(2)#5	38.02(15)
C(1)-Fe(1)-C(2)#5	127.02(19)
C(3)#5-Fe(1)-C(2)#5	159.9(2)
C(3)-Fe(1)-C(2)#5	37.8(2)
C(2)-Fe(1)-C(2)#5	160.9(3)
C(2)#1-C(1)-C(2)	108.2(6)
C(2)#1-C(1)-C(4)	125.9(3)
C(2)-C(1)-C(4)	125.9(3)
C(2)#1-C(1)-Fe(1)#3	73.7(3)
C(2)-C(1)-Fe(1)#3	67.9(3)
C(4)-C(1)-Fe(1)#3	124.06(15)
C(2)#1-C(1)-Fe(1)	67.9(3)
C(2)-C(1)-Fe(1)	73.7(3)
C(4)-C(1)-Fe(1)	124.06(15)
Fe(1)#3-C(1)-Fe(1)	111.9(3)
C(1)-C(2)-C(3)#5	107.4(5)
C(1)-C(2)-Fe(1)#3	72.8(3)
C(3)#5-C(2)-Fe(1)#3	71.0(3)
C(1)-C(2)-Fe(1)	68.2(3)
C(3)#5-C(2)-Fe(1)	70.2(4)
Fe(1)#3-C(2)-Fe(1)	111.6(3)
C(1)-C(2)-H(2)	126.3
C(3)#5-C(2)-H(2)	126.3
Fe(1)#3-C(2)-H(2)	121.6
Fe(1)-C(2)-H(2)	126.8
C(3)#4-C(3)-C(2)#5	108.5(3)
C(3)#4-C(3)-Fe(1)#2	74.5(5)
C(2)#5-C(3)-Fe(1)#2	69.1(3)
C(3)#4-C(3)-Fe(1)	67.6(5)
C(2)#5-C(3)-Fe(1)	72.0(4)
Fe(1)#2-C(3)-Fe(1)	111.5(3)
C(3)#4-C(3)-H(3)	125.7

C(2)#5-C(3)-H(3)	125.7
Fe(1)#2-C(3)-H(3)	122.3
Fe(1)-C(3)-H(3)	126.2
C(6)-N(1)-C(5)	115.0(5)
C(5)#1-C(4)-C(5)	115.1(6)
C(5)#1-C(4)-C(1)	122.4(3)
C(5)-C(4)-C(1)	122.4(3)
N(1)-C(5)-C(4)	123.4(5)
N(1)-C(5)-H(5)	118.3
C(4)-C(5)-H(5)	118.3
N(1)-C(6)-N(1)#1	128.0(7)
N(1)-C(6)-H(6)	116.0
N(1)#1-C(6)-H(6)	116.0

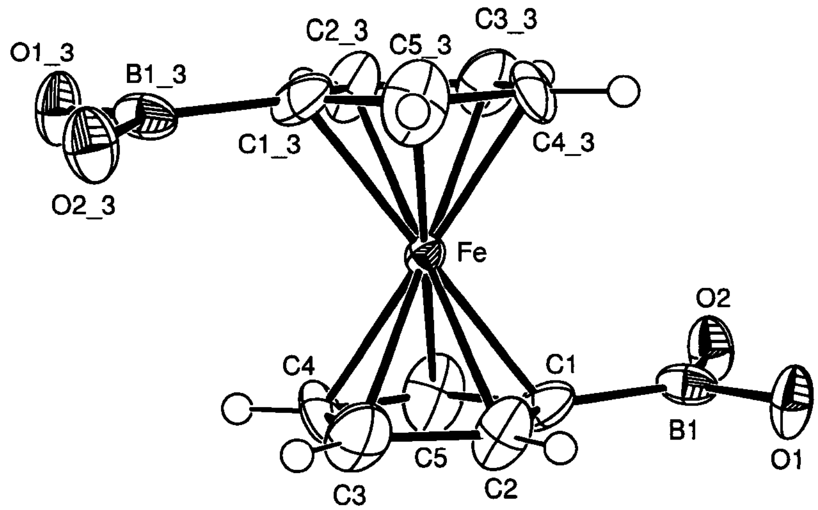
Symmetry transformations used to generate equivalent atoms:
#1 -x-1,y,-z+3/2 #2 x+1,y,z #3 x-1,y,z
#4 -x+1,y,-z+3/2 #5 -x,y,-z+3/2

Table 44. Anisotropic displacement parameters (A^2 x 10^3) for 7.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

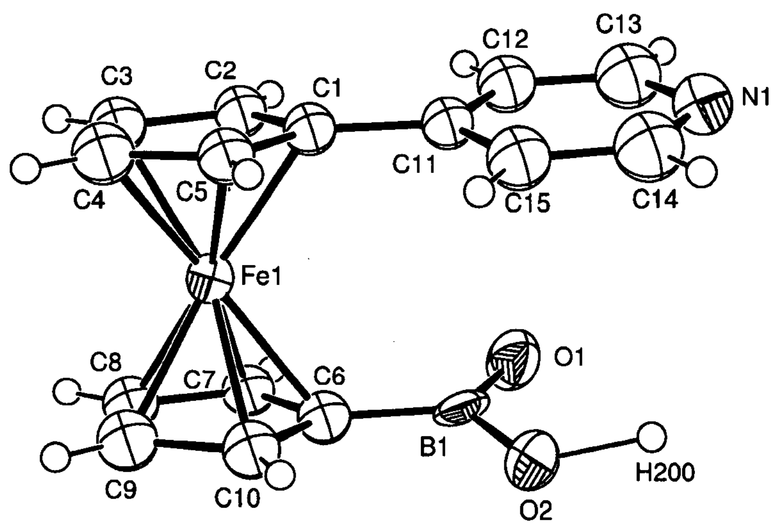
	U11	U22	U33	U23	U13	U12
Fe(1)	34(1)	23(1)	25(1)	0	-7(1)	0
C(1)	38(4)	25(4)	34(4)	0	-14(3)	0
C(2)	47(4)	36(3)	39(3)	3(2)	-15(3)	-2(3)
C(3)	59(4)	30(3)	67(4)	-14(3)	-22(3)	2(3)
N(1)	52(3)	30(2)	38(3)	6(2)	2(2)	0(2)
C(4)	34(4)	25(4)	28(4)	0	-2(3)	0
C(5)	39(3)	34(3)	30(3)	1(2)	0(2)	0(2)
C(6)	53(5)	24(4)	53(5)	0	6(4)	0

Table 45. Hydrogen coordinates (x 10^4) and isotropic
displacement parameters (A^2 x 10^3) for 7.

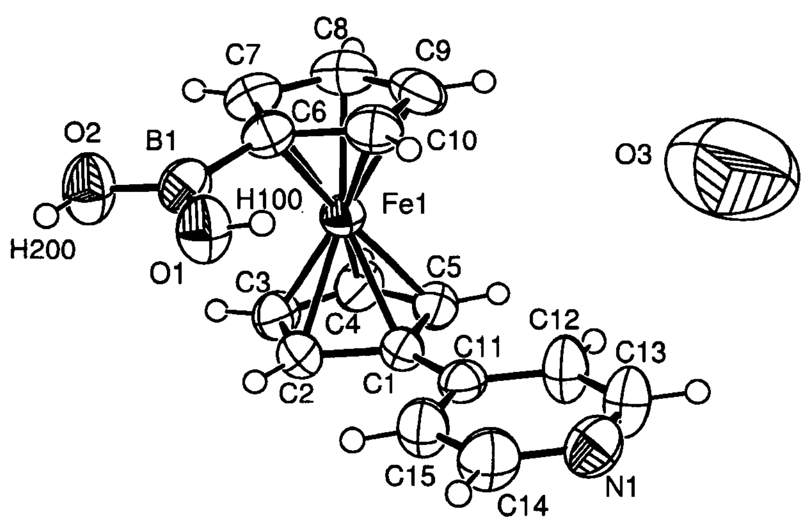
	x	y	z	U(eq)
H(2)	-4758	3409	9470	51
H(3)	4880	2165	6300	65
H(5)	-7814	4607	5735	42
H(6)	-5000	6327	7500	52



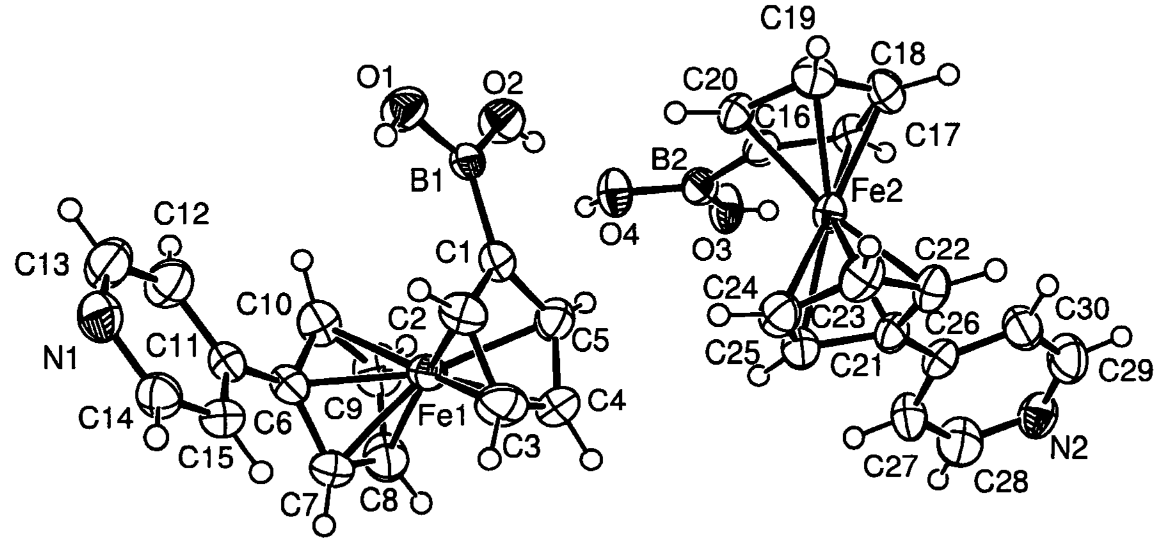
ORTEP drawing of crystalline **1**



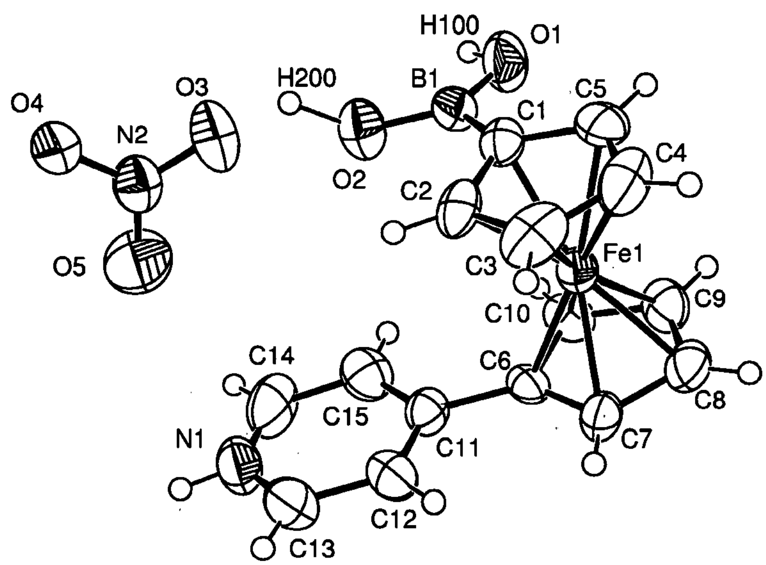
ORTEP drawing of crystalline **2a**



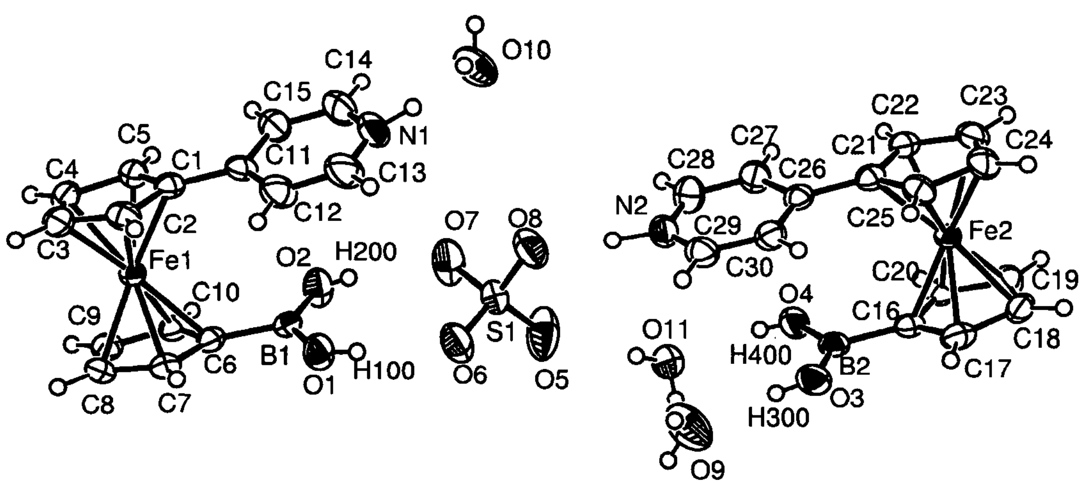
ORTEP drawing of crystalline **2b**



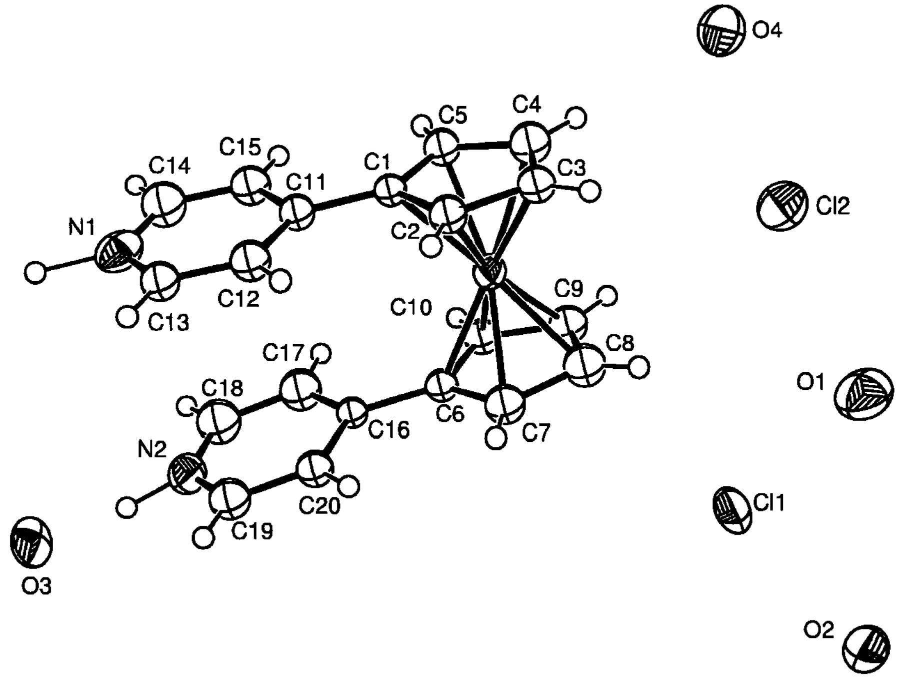
ORTEP drawing of crystalline **2c**



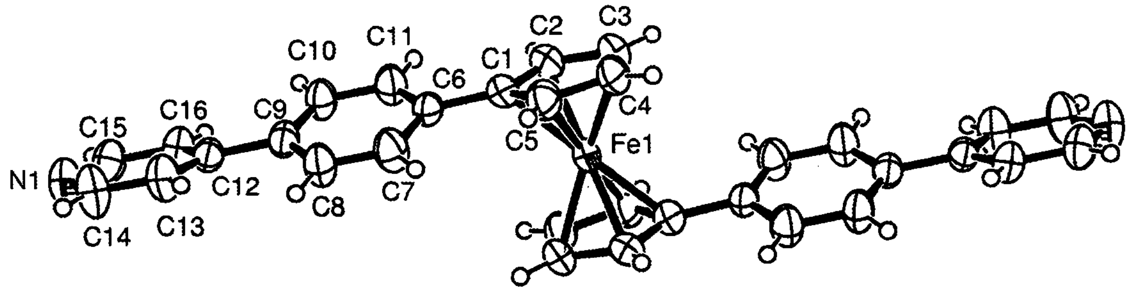
ORTEP drawing of crystalline **3a**



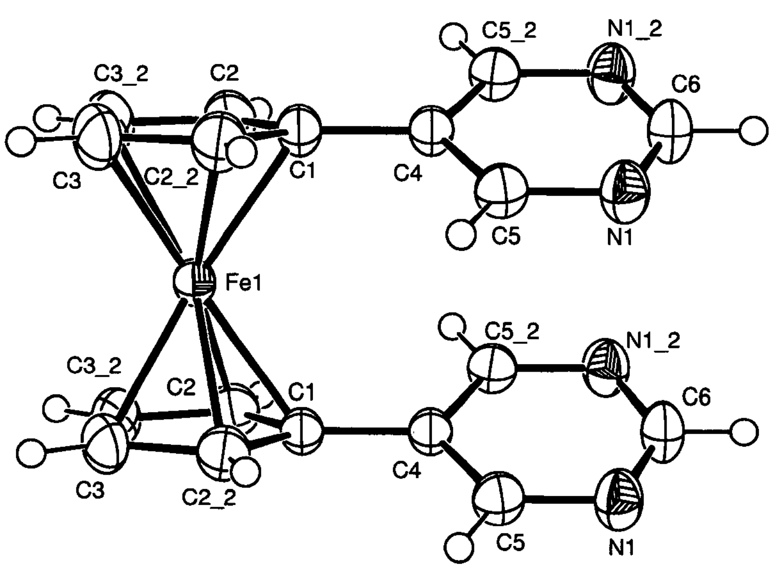
ORTEP drawing of crystalline **3b**



ORTEP drawing of crystalline **5**

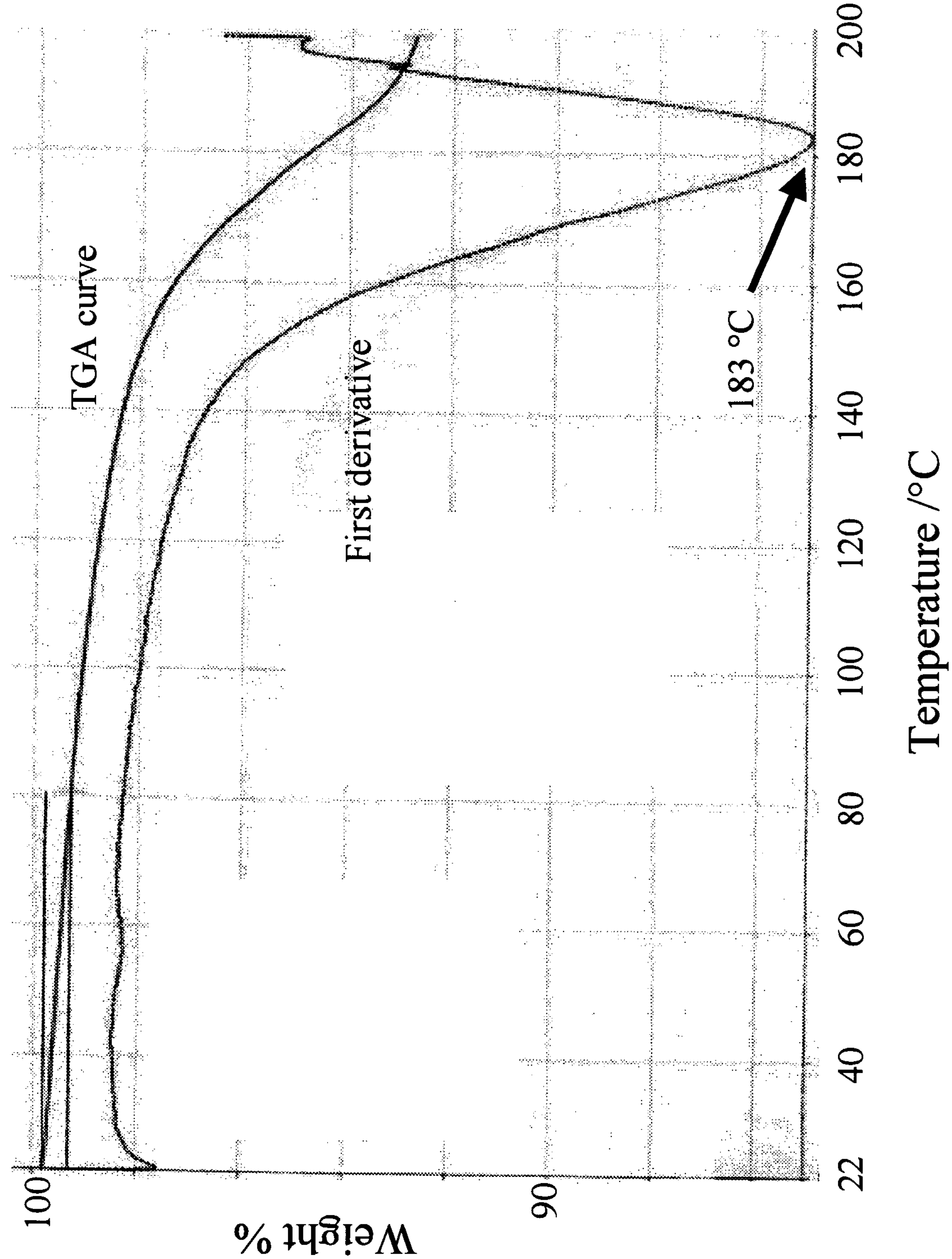


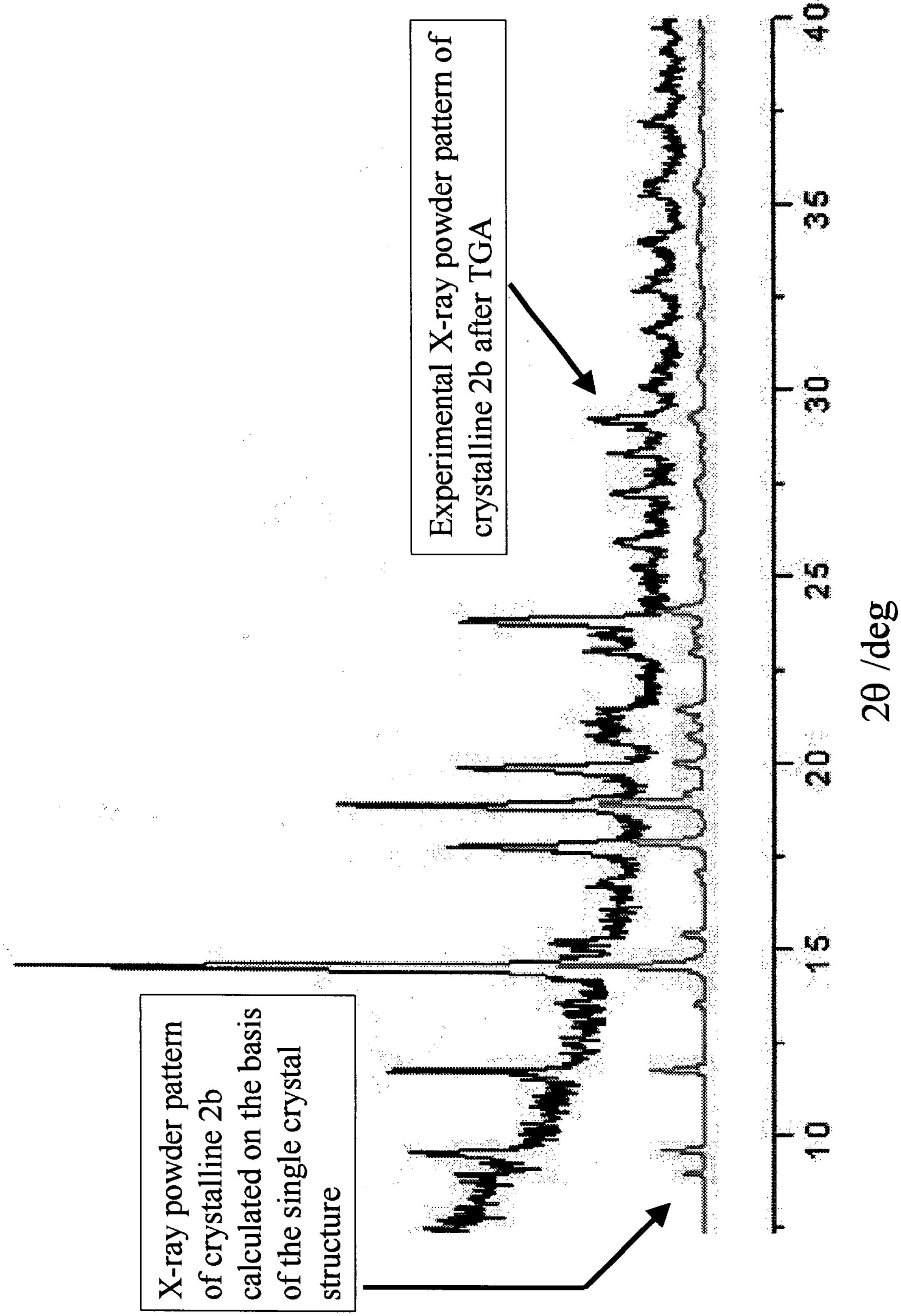
ORTEP drawing of crystalline **6**



ORTEP drawing of crystalline **7**

Thermogravimetric Analysis of crystalline **2b**




Experimental X-ray powder pattern of crystalline 2b after TGA
X-ray powder pattern of crystalline 2b calculated on the basis of the single crystal structure
10
15
20
25
30
35
40
2θ /deg