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Synthetic and reaction chemistry of heteroatom stabilized boryl and cationic borylene complexes

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Supporting Information

Contents

1. Characterizing data for 11a,b and 12a,b[a-d]

11a: ^{1}H NMR (400 MHz, CD_2Cl_2) δ 5.05 (s, 5H, Cp), 7.22 (m, 9H, *ortho*- and *para*-CH of PPh_3), 7.50 (s, 4H, *para*-CH of $BAr^{f}_{4}^{-}$), 7.56 (m, 6H, *meta*-CH of PPh_3), 7.70 (s, 8H, *ortho*-CH of $BAr^{f}_{4}^{-}$). ^{13}C NMR (76 MHz, C_6D_6) δ 87.9 (Cp), 117.4 (*para*-CH of $BAr^{f}_{4}^{-}$), 124.6 (q, $^{1}J_{CF}$ = 272 Hz, CF_3 of $BAr^{f}_{4}^{-}$), 128.9 (q, $^{2}J_{CF}$ = 34 Hz, *meta*-C of $BAr^{f}_{4}^{-}$), 129.7 (d, J = 11.1 Hz, *meta*-CH of PPh_3), 131.6 (d, J = 52.2 Hz, *ipso*-C of PPh_3), 132.7 (d, J = 2.8 Hz, *para*-CH of PPh_3), 133.4 (d, J = 10.3 Hz, *ortho*-CH of PPh_3), 134.8 (*ortho*-CH of $BAr^{f}_{4}^{-}$), 161.8 (q, $^{1}J_{CB}$ = 49 Hz, *ipso*-C of $BAr^{f}_{4}^{-}$), 209.1 (d, J = 24.8 Hz, CO). ^{11}B NMR (96 MHz, CD_2Cl_2) δ –7.7 ($BAr^{f}_{4}^{-}$). ^{19}F NMR (283 MHz, CD_2Cl_2) δ –62.7 (CF_3). IR (CD_2Cl_2 soln, cm^{-1}) ν(CO) 2059, 2017.

12a: ^{1}H NMR (400 MHz, CD_2Cl_2) δ 1.20 (d, J = 6.8 Hz, 24H, CH_3 of ^{i}Pr), 3.62 (sept, J = 6.8 Hz, 4H, CH of ^{i}Pr). ^{13}C NMR (76 MHz, C_6D_6) δ 22.9 (CH_3 of ^{i}Pr), 48.2 (CH of ^{i}Pr). ^{11}B NMR (96 MHz, CD_2Cl_2) δ 35.6. Mass spec. (EI): 286.2 (15 %) $[M]^+$, 271.2 (100 %) $[M - Me]^+$; exact mass: calc. for $[M]^+$ 286.1875, meas. 286.1873.
Data reported for **11a** by Nöth and W. Rattay[a]: ^{1}H NMR δ 1.13 (d, J = 6.8 Hz), 3.56 (sept, J = 6.8 Hz). ^{13}C NMR δ 23.1, 48.4. ^{11}B NMR δ 37.3.
Data reported for **11a** by Maringgele and Meller[b]: ^{1}H NMR δ 1.26 (d, J = 6.8 Hz), 3.68 (sept, J = 6.8 Hz). ^{13}C NMR δ 23.2, 48.2. ^{11}B NMR δ 36.3. Mass spec. (EI): 286 (20 %) $[M]^+$, 271 (100 %) $[M - Me]^+$.

11b: ^{1}H NMR (400 MHz, CD_2Cl_2) δ 5.13 (s, 5H, Cp), 7.29 (m, 9H, *ortho*- and *para*-CH of PPh_3), 7.52 (s, 4H, *para*-CH of $BAr^{f}_{4}^{-}$), 7.59 (m, 6H, *meta*-CH of PPh_3), 7.68 (s, 8H, *ortho*-CH of $BAr^{f}_{4}^{-}$). ^{13}C NMR (76 MHz, C_6D_6) δ 86.5 (Cp), 117.5 (*para*-CH of $BAr^{f}_{4}^{-}$), 124.6 (q, $^{1}J_{CF}$ = 273 Hz, CF_3 of $BAr^{f}_{4}^{-}$), 128.9 (q, $^{2}J_{CF}$ = 34 Hz, *meta*-C of $BAr^{f}_{4}^{-}$), 130.4 (*meta*-CH of $AsPh_3$), 131.8 (*ipso*-C of $AsPh_3$), 132.4 (*para*-CH of $AsPh_3$), 133.7 (*ortho*-CH of $AsPh_3$), 134.7 (*ortho*-CH of $BAr^{f}_{4}^{-}$), 161.8 (q, $^{1}J_{CB}$ = 49 Hz, *ipso*-C of $BAr^{f}_{4}^{-}$), 208.6 (CO). ^{11}B NMR (96 MHz, CD_2Cl_2) δ –7.7 ($BAr^{f}_{4}^{-}$). ^{19}F NMR (283 MHz, CD_2Cl_2) δ –62.7 (CF_3). IR (CD_2Cl_2 soln, cm^{-1}) ν(CO) 2057, 2014.

12b: ^{1}H NMR (400 MHz, CD_2Cl_2) δ 1.16 (d, J = 6.7 Hz, 36H, CH_3 of ^{i}Pr), 3.53 (sept, J = 6.7 Hz, 4H, CH of ^{i}Pr). ^{13}C NMR (76 MHz, C_6D_6) δ 22.7 (CH_3 of ^{i}Pr), 43.7 (CH of ^{i}Pr). ^{11}B NMR (96 MHz, CD_2Cl_2) δ 20.2. Mass spec. (EI): 381.1 (22 %) $[M]^+$.
Data reported for **11b** by Meller *et al.*[d]: ^{1}H NMR δ 1.16 (d, J = 7 Hz), 3.57 (sept, J = 7 Hz). ^{11}B NMR δ 20.5. Mass spec. (EI): M^+ 381 (40 %).

(a) H. Nöth and W. Rattay, *J. Organomet. Chem.*, 1986, **312**, 139. (b) W. Maringgele and A. Meller, *Z. Anorg. Allg. Chem.*, 1989, **572**, 140. (c) H. Schumann and L. Eguren, *J. Organomet. Chem.*, 1991, **403**, 183. (d) W. Maringgele, M. Noltemeyer and A. Meller, *Organometallics*, 1997, **16**, 2276-2284.

2. Details of the crystal structure of (η^5-C_5H_5)Fe(CO)$_2$B(OMes)Cl (2a)

Table 2.1 Crystal data and structure refinement for **2a**

Empirical formula	C16 H16 B1 Cl1 Fe O3	
Formula weight	358.40	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.8325(3) Å	α= 81.631(2)°.
	b = 8.0671(3) Å	β= 81.424(2)°.
	c = 13.6886(6) Å	γ = 75.958(2)°.
Volume	824.29(6) Å^3	
Z	2	
Density (calculated)	1.444 Mg/m^3	
Absorption coefficient	1.084 mm^{-1}	
F(000)	368	
Crystal size	0.23 x 0.23 x 0.05 mm^3	
Theta range for data collection	2.93 to 27.49°.	
Index ranges	-9<=h<=10, -10<=k<=10, -16<=l<=17	
Reflections collected	13020	
Independent reflections	3685 [R(int) = 0.0678]	
Completeness to theta = 27.49°	97.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9478 and 0.7887	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3685 / 0 / 202	
Goodness-of-fit on F^2	1.160	
Final R indices [I>2sigma(I)]	R1 = 0.0516, wR2 = 0.1113	
R indices (all data)	R1 = 0.0913, wR2 = 0.1359	
Largest diff. peak and hole	0.518 and -0.588 e.Å^{-3}	

Table 2.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2a**

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	496(5)	-4373(4)	1178(2)	36(1)
C(2)	3403(5)	-6728(5)	885(3)	41(1)
C(3)	4293(5)	-5755(5)	2762(3)	43(1)
C(4)	2618(5)	-5010(5)	3238(3)	42(1)
C(5)	2013(5)	-3384(4)	2703(3)	42(1)
C(6)	3343(6)	-3126(5)	1905(3)	49(1)
C(7)	4722(5)	-4584(5)	1950(3)	50(1)
C(8)	-1401(4)	-8425(4)	2861(2)	31(1)
C(9)	-1813(4)	-9340(4)	2181(2)	35(1)
C(10)	-2646(4)	-10672(4)	2549(3)	38(1)
C(11)	-3066(4)	-11098(4)	3567(3)	36(1)
C(12)	-2673(4)	-10101(4)	4215(3)	36(1)
C(13)	-1842(4)	-8747(4)	3878(2)	33(1)
C(14)	-1332(5)	-8911(5)	1081(3)	51(1)
C(15)	-3920(5)	-12598(5)	3944(3)	51(1)
C(16)	-1431(5)	-7690(5)	4603(3)	43(1)
B(1)	1193(5)	-7177(5)	2386(3)	29(1)
Cl(1)	2506(1)	-9224(1)	2879(1)	42(1)
Fe(1)	2392(1)	-5319(1)	1777(1)	31(1)
O(1)	-771(4)	-3746(3)	817(2)	49(1)
O(2)	4086(4)	-7678(4)	328(2)	61(1)
O(3)	-574(3)	-7053(3)	2489(2)	34(1)

Table 2.3 Bond lengths [Å] and angles [°] for **2a**

C(1)-O(1)	1.147(4)
C(1)-Fe(1)	1.758(4)
C(2)-O(2)	1.141(4)
C(2)-Fe(1)	1.757(4)
C(3)-C(7)	1.406(5)
C(3)-C(4)	1.409(5)
C(3)-Fe(1)	2.089(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.415(5)
C(4)-Fe(1)	2.089(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.421(5)
C(5)-Fe(1)	2.090(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.392(5)
C(6)-Fe(1)	2.118(3)
C(6)-H(6)	0.9500
C(7)-Fe(1)	2.106(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.386(5)
C(8)-C(13)	1.386(5)
C(8)-O(3)	1.410(4)
C(9)-C(10)	1.385(5)
C(9)-C(14)	1.507(5)
C(10)-C(11)	1.396(5)
C(10)-H(10)	0.9500
C(11)-C(12)	1.392(5)
C(11)-C(15)	1.512(5)
C(12)-C(13)	1.392(5)
C(12)-H(12)	0.9500
C(13)-C(16)	1.514(5)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
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
B(1)-O(3)	1.350(4)
B(1)-Cl(1)	1.816(4)
B(1)-Fe(1)	1.977(4)
O(1)-C(1)-Fe(1)	177.8(3)
O(2)-C(2)-Fe(1)	177.8(3)
C(7)-C(3)-C(4)	107.8(3)
C(7)-C(3)-Fe(1)	71.1(2)
C(4)-C(3)-Fe(1)	70.31(19)
C(7)-C(3)-H(3)	126.1
C(4)-C(3)-H(3)	126.1
Fe(1)-C(3)-H(3)	124.2
C(3)-C(4)-C(5)	107.6(3)
C(3)-C(4)-Fe(1)	70.3(2)
C(5)-C(4)-Fe(1)	70.25(19)
C(3)-C(4)-H(4)	126.2

C(5)-C(4)-H(4)	126.2
Fe(1)-C(4)-H(4)	124.9
C(4)-C(5)-C(6)	107.9(3)
C(4)-C(5)-Fe(1)	70.17(19)
C(6)-C(5)-Fe(1)	71.3(2)
C(4)-C(5)-H(5)	126.0
C(6)-C(5)-H(5)	126.0
Fe(1)-C(5)-H(5)	124.1
C(7)-C(6)-C(5)	107.4(3)
C(7)-C(6)-Fe(1)	70.3(2)
C(5)-C(6)-Fe(1)	69.23(19)
C(7)-C(6)-H(6)	126.3
C(5)-C(6)-H(6)	126.3
Fe(1)-C(6)-H(6)	125.8
C(6)-C(7)-C(3)	109.2(3)
C(6)-C(7)-Fe(1)	71.2(2)
C(3)-C(7)-Fe(1)	69.8(2)
C(6)-C(7)-H(7)	125.4
C(3)-C(7)-H(7)	125.4
Fe(1)-C(7)-H(7)	125.2
C(9)-C(8)-C(13)	122.9(3)
C(9)-C(8)-O(3)	118.0(3)
C(13)-C(8)-O(3)	119.0(3)
C(10)-C(9)-C(8)	117.8(3)
C(10)-C(9)-C(14)	121.6(3)
C(8)-C(9)-C(14)	120.6(3)
C(9)-C(10)-C(11)	121.9(3)
C(9)-C(10)-H(10)	119.0
C(11)-C(10)-H(10)	119.0
C(12)-C(11)-C(10)	117.8(3)
C(12)-C(11)-C(15)	121.6(3)
C(10)-C(11)-C(15)	120.5(3)
C(11)-C(12)-C(13)	122.1(3)
C(11)-C(12)-H(12)	118.9
C(13)-C(12)-H(12)	118.9
C(8)-C(13)-C(12)	117.4(3)
C(8)-C(13)-C(16)	121.9(3)
C(12)-C(13)-C(16)	120.7(3)
C(9)-C(14)-H(14A)	109.5
C(9)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(9)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(11)-C(15)-H(15A)	109.5
C(11)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(11)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(13)-C(16)-H(16A)	109.5
C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(13)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
O(3)-B(1)-Cl(1)	115.5(3)
O(3)-B(1)-Fe(1)	125.2(3)
Cl(1)-B(1)-Fe(1)	119.4(2)

C(2)-Fe(1)-C(1)	95.82(16)
C(2)-Fe(1)-B(1)	84.87(16)
C(1)-Fe(1)-B(1)	87.76(15)
C(2)-Fe(1)-C(4)	138.69(16)
C(1)-Fe(1)-C(4)	123.73(15)
B(1)-Fe(1)-C(4)	85.25(14)
C(2)-Fe(1)-C(3)	102.88(15)
C(1)-Fe(1)-C(3)	160.90(15)
B(1)-Fe(1)-C(3)	97.63(15)
C(4)-Fe(1)-C(3)	39.40(14)
C(2)-Fe(1)-C(5)	160.29(16)
C(1)-Fe(1)-C(5)	94.88(15)
B(1)-Fe(1)-C(5)	112.08(15)
C(4)-Fe(1)-C(5)	39.58(13)
C(3)-Fe(1)-C(5)	66.10(14)
C(2)-Fe(1)-C(7)	95.55(16)
C(1)-Fe(1)-C(7)	135.68(16)
B(1)-Fe(1)-C(7)	135.89(16)
C(4)-Fe(1)-C(7)	65.65(15)
C(3)-Fe(1)-C(7)	39.16(15)
C(5)-Fe(1)-C(7)	65.42(15)
C(2)-Fe(1)-C(6)	121.77(17)
C(1)-Fe(1)-C(6)	101.16(16)
B(1)-Fe(1)-C(6)	150.23(16)
C(4)-Fe(1)-C(6)	66.08(15)
C(3)-Fe(1)-C(6)	65.64(15)
C(5)-Fe(1)-C(6)	39.47(15)
C(7)-Fe(1)-C(6)	38.48(15)
B(1)-O(3)-C(8)	124.6(3)

Symmetry transformations used to generate equivalent atoms:

Table 2.4 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2a**

The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	47(2)	29(2)	32(2)	-3(1)	-4(2)	-9(2)
C(2)	38(2)	43(2)	41(2)	-2(2)	-9(2)	-8(2)
C(3)	34(2)	41(2)	58(2)	-14(2)	-21(2)	-3(2)
C(4)	43(2)	48(2)	38(2)	-10(2)	-13(2)	-12(2)
C(5)	42(2)	35(2)	52(2)	-17(2)	-14(2)	-3(2)
C(6)	58(3)	39(2)	58(2)	-7(2)	-9(2)	-24(2)
C(7)	34(2)	56(3)	65(3)	-20(2)	-2(2)	-18(2)
C(8)	20(2)	31(2)	38(2)	1(2)	-5(1)	-2(1)
C(9)	24(2)	42(2)	37(2)	-8(2)	-4(1)	-4(2)
C(10)	31(2)	41(2)	43(2)	-13(2)	-10(2)	-5(2)
C(11)	24(2)	32(2)	52(2)	-3(2)	-7(2)	-3(2)
C(12)	29(2)	41(2)	34(2)	4(2)	-7(2)	-4(2)
C(13)	26(2)	33(2)	39(2)	-3(2)	-7(2)	-3(2)
C(14)	52(2)	67(3)	35(2)	-10(2)	3(2)	-15(2)
C(15)	50(2)	36(2)	66(3)	3(2)	-13(2)	-12(2)
C(16)	45(2)	45(2)	39(2)	-5(2)	-7(2)	-11(2)
B(1)	30(2)	29(2)	27(2)	-7(2)	-5(2)	-2(2)
Cl(1)	32(1)	30(1)	60(1)	4(1)	-9(1)	-2(1)
Fe(1)	31(1)	29(1)	33(1)	-5(1)	-5(1)	-7(1)
O(1)	49(2)	49(2)	49(2)	-5(1)	-23(1)	0(1)
O(2)	61(2)	68(2)	50(2)	-28(2)	2(2)	1(2)
O(3)	27(1)	32(1)	41(1)	2(1)	-5(1)	-7(1)

Table 2.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **2a**

	x	y	z	U(eq)
H(3)	5005	-6854	2954	52
H(4)	2005	-5508	3814	50
H(5)	912	-2604	2850	50
H(6)	3298	-2139	1428	59
H(7)	5785	-4760	1504	59
H(10)	-2941	-11314	2095	45
H(12)	-2981	-10352	4909	43
H(14A)	-1897	-7710	880	77
H(14B)	-1744	-9667	714	77
H(14C)	-42	-9076	933	77
H(15A)	-4089	-12729	4673	76
H(15B)	-3152	-13651	3710	76
H(15C)	-5071	-12385	3694	76
H(16A)	-146	-7812	4553	64
H(16B)	-1874	-8096	5281	64
H(16C)	-2007	-6477	4445	64

3. Details of the crystal structure of (η^5-C_5H_5)Fe(CO)$_2$B(OMes)SPh (2d)

Table 3.1 Crystal data and structure refinement for **2d**

Empirical formula	C22 H21 B Fe O3 S	
Formula weight	432.11	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 14.4401(4) Å	α= 90°.
	b = 9.7496(3) Å	β= 91.901(1)°.
	c = 14.5657(6) Å	γ = 90°.
Volume	2049.51(12) Å^3	
Z	4	
Density (calculated)	1.400 Mg/m^3	
Absorption coefficient	0.857 mm^{-1}	
F(000)	896	
Crystal size	0.35 x 0.12 x 0.10 mm^3	
Theta range for data collection	3.49 to 27.43°.	
Index ranges	-18<=h<=18, -9<=k<=12, -18<=l<=18	
Reflections collected	12489	
Independent reflections	4272 [R(int) = 0.0699]	
Completeness to theta = 25.00°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9192 and 0.7535	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4272 / 0 / 253	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0534, wR2 = 0.1088	
R indices (all data)	R1 = 0.1027, wR2 = 0.1295	
Largest diff. peak and hole	0.398 and -0.520 e.Å^{-3}	

Table 3.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2d**

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	33(2)	1272(4)	3843(3)	33(1)
C(2)	1126(3)	1664(4)	2554(2)	31(1)
C(3)	-441(3)	-1300(4)	3106(3)	40(1)
C(4)	526(3)	-1481(3)	3295(3)	34(1)
C(5)	982(3)	-1302(4)	2474(3)	34(1)
C(6)	312(3)	-1012(4)	1767(3)	36(1)
C(7)	-567(3)	-1030(4)	2163(3)	39(1)
C(8)	-1417(2)	3199(4)	3150(2)	28(1)
C(9)	-2156(2)	2533(4)	3539(3)	34(1)
C(10)	-2438(3)	3017(4)	4387(3)	40(1)
C(11)	-2018(3)	4122(4)	4830(3)	40(1)
C(12)	-1283(3)	4748(4)	4408(3)	37(1)
C(13)	-970(2)	4303(4)	3565(3)	32(1)
C(14)	-2634(3)	1340(4)	3067(3)	49(1)
C(15)	-2352(3)	4629(5)	5742(3)	61(1)
C(16)	-160(3)	4986(4)	3122(3)	43(1)
C(17)	-1123(3)	2959(4)	225(2)	33(1)
C(18)	-2068(3)	3022(5)	358(3)	48(1)
C(19)	-2598(3)	3979(6)	-131(3)	62(1)
C(20)	-2208(3)	4841(5)	-751(3)	56(1)
C(21)	-1279(3)	4762(4)	-898(3)	50(1)
C(22)	-741(3)	3822(4)	-415(3)	40(1)
B(1)	-551(3)	1850(4)	2025(3)	28(1)
Fe(1)	245(1)	517(1)	2780(1)	25(1)
O(1)	-44(2)	1684(3)	4577(2)	49(1)
O(2)	1711(2)	2457(3)	2424(2)	50(1)
O(3)	-1163(2)	2819(3)	2268(2)	35(1)
S(1)	-387(1)	1725(1)	775(1)	44(1)

Table 3.3 Bond lengths [Å] and angles [°] for **2d**

C(1)-O(1)	1.151(4)
C(1)-Fe(1)	1.751(4)
C(2)-O(2)	1.165(4)
C(2)-Fe(1)	1.734(4)
C(3)-C(7)	1.406(6)
C(3)-C(4)	1.424(5)
C(3)-Fe(1)	2.092(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.396(5)
C(4)-Fe(1)	2.122(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.418(5)
C(5)-Fe(1)	2.123(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.411(5)
C(6)-Fe(1)	2.102(4)
C(6)-H(6)	0.9500
C(7)-Fe(1)	2.094(4)
C(7)-H(7)	0.9500
C(8)-C(13)	1.383(5)
C(8)-C(9)	1.386(5)
C(8)-O(3)	1.398(4)
C(9)-C(10)	1.395(5)
C(9)-C(14)	1.507(5)
C(10)-C(11)	1.385(6)
C(10)-H(10)	0.9500
C(11)-C(12)	1.386(5)
C(11)-C(15)	1.511(5)
C(12)-C(13)	1.392(5)
C(12)-H(12)	0.9500
C(13)-C(16)	1.510(5)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
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(22)	1.384(5)
C(17)-C(18)	1.385(5)
C(17)-S(1)	1.779(4)
C(18)-C(19)	1.389(6)
C(18)-H(18)	0.9500
C(19)-C(20)	1.368(6)
C(19)-H(19)	0.9500
C(20)-C(21)	1.368(6)
C(20)-H(20)	0.9500
C(21)-C(22)	1.379(5)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500
B(1)-O(3)	1.349(5)
B(1)-S(1)	1.848(4)
B(1)-Fe(1)	2.034(4)

O(1)-C(1)-Fe(1)	173.4(3)
O(2)-C(2)-Fe(1)	178.1(3)
C(7)-C(3)-C(4)	107.9(3)
C(7)-C(3)-Fe(1)	70.5(2)
C(4)-C(3)-Fe(1)	71.4(2)
C(7)-C(3)-H(3)	126.1
C(4)-C(3)-H(3)	126.1
Fe(1)-C(3)-H(3)	123.7
C(5)-C(4)-C(3)	107.8(4)
C(5)-C(4)-Fe(1)	70.9(2)
C(3)-C(4)-Fe(1)	69.1(2)
C(5)-C(4)-H(4)	126.1
C(3)-C(4)-H(4)	126.1
Fe(1)-C(4)-H(4)	125.5
C(4)-C(5)-C(6)	108.5(3)
C(4)-C(5)-Fe(1)	70.7(2)
C(6)-C(5)-Fe(1)	69.6(2)
C(4)-C(5)-H(5)	125.8
C(6)-C(5)-H(5)	125.8
Fe(1)-C(5)-H(5)	125.5
C(7)-C(6)-C(5)	107.6(3)
C(7)-C(6)-Fe(1)	70.1(2)
C(5)-C(6)-Fe(1)	71.2(2)
C(7)-C(6)-H(6)	126.2
C(5)-C(6)-H(6)	126.2
Fe(1)-C(6)-H(6)	124.2
C(3)-C(7)-C(6)	108.2(4)
C(3)-C(7)-Fe(1)	70.3(2)
C(6)-C(7)-Fe(1)	70.6(2)
C(3)-C(7)-H(7)	125.9
C(6)-C(7)-H(7)	125.9
Fe(1)-C(7)-H(7)	124.8
C(13)-C(8)-C(9)	122.7(3)
C(13)-C(8)-O(3)	118.4(3)
C(9)-C(8)-O(3)	118.7(3)
C(8)-C(9)-C(10)	117.1(3)
C(8)-C(9)-C(14)	121.5(3)
C(10)-C(9)-C(14)	121.5(3)
C(11)-C(10)-C(9)	122.6(3)
C(11)-C(10)-H(10)	118.7
C(9)-C(10)-H(10)	118.7
C(10)-C(11)-C(12)	117.8(3)
C(10)-C(11)-C(15)	121.1(4)
C(12)-C(11)-C(15)	121.1(4)
C(11)-C(12)-C(13)	122.0(4)
C(11)-C(12)-H(12)	119.0
C(13)-C(12)-H(12)	119.0
C(8)-C(13)-C(12)	117.8(3)
C(8)-C(13)-C(16)	120.9(3)
C(12)-C(13)-C(16)	121.2(3)
C(9)-C(14)-H(14A)	109.5
C(9)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(9)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(11)-C(15)-H(15A)	109.5
C(11)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5

C(11)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(13)-C(16)-H(16A)	109.5
C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(13)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(22)-C(17)-C(18)	118.9(4)
C(22)-C(17)-S(1)	118.0(3)
C(18)-C(17)-S(1)	122.9(3)
C(17)-C(18)-C(19)	119.2(4)
C(17)-C(18)-H(18)	120.4
C(19)-C(18)-H(18)	120.4
C(20)-C(19)-C(18)	121.3(4)
C(20)-C(19)-H(19)	119.4
C(18)-C(19)-H(19)	119.4
C(19)-C(20)-C(21)	119.7(4)
C(19)-C(20)-H(20)	120.1
C(21)-C(20)-H(20)	120.1
C(20)-C(21)-C(22)	119.8(4)
C(20)-C(21)-H(21)	120.1
C(22)-C(21)-H(21)	120.1
C(21)-C(22)-C(17)	121.2(4)
C(21)-C(22)-H(22)	119.4
C(17)-C(22)-H(22)	119.4
O(3)-B(1)-S(1)	114.3(3)
O(3)-B(1)-Fe(1)	132.0(3)
S(1)-B(1)-Fe(1)	113.7(2)
C(2)-Fe(1)-C(1)	92.70(17)
C(2)-Fe(1)-B(1)	83.70(16)
C(1)-Fe(1)-B(1)	95.56(16)
C(2)-Fe(1)-C(3)	160.98(16)
C(1)-Fe(1)-C(3)	93.27(16)
B(1)-Fe(1)-C(3)	113.63(16)
C(2)-Fe(1)-C(7)	141.92(16)
C(1)-Fe(1)-C(7)	124.79(16)
B(1)-Fe(1)-C(7)	85.97(16)
C(3)-Fe(1)-C(7)	39.24(15)
C(2)-Fe(1)-C(6)	105.88(16)
C(1)-Fe(1)-C(6)	158.84(16)
B(1)-Fe(1)-C(6)	96.45(16)
C(3)-Fe(1)-C(6)	65.93(16)
C(7)-Fe(1)-C(6)	39.31(14)
C(2)-Fe(1)-C(4)	121.78(15)
C(1)-Fe(1)-C(4)	96.32(15)
B(1)-Fe(1)-C(4)	151.17(16)
C(3)-Fe(1)-C(4)	39.51(15)
C(7)-Fe(1)-C(4)	65.72(15)
C(6)-Fe(1)-C(4)	65.46(15)
C(2)-Fe(1)-C(5)	97.07(15)
C(1)-Fe(1)-C(5)	129.84(15)
B(1)-Fe(1)-C(5)	134.33(15)
C(3)-Fe(1)-C(5)	65.48(15)
C(7)-Fe(1)-C(5)	65.56(15)
C(6)-Fe(1)-C(5)	39.22(14)
C(4)-Fe(1)-C(5)	38.40(13)
B(1)-O(3)-C(8)	128.4(3)

C(17)-S(1)-B(1)	107.76(18)

Symmetry transformations used to generate equivalent atoms:

Table 3.4 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2d**

The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	37(2)	33(2)	28(2)	6(2)	-3(2)	9(2)
C(2)	34(2)	33(2)	27(2)	-3(2)	-1(2)	7(2)
C(3)	41(2)	29(2)	51(3)	-3(2)	7(2)	-7(2)
C(4)	44(2)	25(2)	33(2)	3(2)	2(2)	2(2)
C(5)	40(2)	28(2)	34(2)	-2(2)	0(2)	8(2)
C(6)	49(2)	29(2)	30(2)	-8(2)	-1(2)	4(2)
C(7)	42(2)	28(2)	46(3)	-5(2)	-10(2)	-2(2)
C(8)	31(2)	31(2)	22(2)	1(2)	-4(2)	11(2)
C(9)	29(2)	38(2)	33(2)	4(2)	-7(2)	5(2)
C(10)	30(2)	49(3)	41(2)	10(2)	6(2)	6(2)
C(11)	37(2)	51(3)	30(2)	2(2)	6(2)	16(2)
C(12)	39(2)	36(2)	34(2)	-9(2)	-3(2)	11(2)
C(13)	32(2)	31(2)	32(2)	7(2)	-1(2)	9(2)
C(14)	40(2)	46(3)	60(3)	-6(2)	-4(2)	0(2)
C(15)	67(3)	78(4)	40(3)	-6(2)	14(2)	18(3)
C(16)	46(2)	36(2)	48(3)	3(2)	7(2)	4(2)
C(17)	42(2)	38(2)	19(2)	-2(2)	-6(2)	6(2)
C(18)	46(2)	69(3)	29(2)	7(2)	-7(2)	-5(2)
C(19)	38(2)	108(4)	39(3)	5(3)	-11(2)	12(3)
C(20)	68(3)	65(3)	33(3)	8(2)	-15(2)	23(3)
C(21)	62(3)	47(3)	42(3)	16(2)	-1(2)	5(2)
C(22)	42(2)	47(2)	32(2)	3(2)	3(2)	3(2)
B(1)	29(2)	29(2)	25(2)	2(2)	-4(2)	1(2)
Fe(1)	29(1)	25(1)	21(1)	0(1)	0(1)	2(1)
O(1)	66(2)	58(2)	22(2)	-4(1)	0(1)	23(2)
O(2)	43(2)	46(2)	60(2)	5(2)	5(1)	-8(2)
O(3)	41(1)	41(2)	22(1)	0(1)	-3(1)	13(1)
S(1)	62(1)	46(1)	22(1)	2(1)	1(1)	20(1)

Table 3.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **2d**

	x	y	z	U(eq)
H(3)	-916	-1353	3541	48
H(4)	809	-1687	3877	41
H(5)	1632	-1364	2401	41
H(6)	433	-838	1140	43
H(7)	-1144	-884	1846	47
H(10)	-2939	2571	4671	48
H(12)	-984	5504	4703	44
H(14A)	-2339	1154	2484	73
H(14B)	-3289	1564	2949	73
H(14C)	-2585	527	3462	73
H(15A)	-1972	5409	5950	92
H(15B)	-2302	3889	6196	92
H(15C)	-3001	4919	5671	92
H(16A)	69	5740	3512	64
H(16B)	-358	5347	2519	64
H(16C)	337	4314	3047	64
H(18)	-2349	2419	778	58
H(19)	-3244	4036	-34	74
H(20)	-2581	5492	-1078	67
H(21)	-1005	5353	-1331	60
H(22)	-97	3765	-524	48

4. Details of the crystal structure of (η^5-C_5Me_5)$Fe(CO)_2B(OMes)Cl$ (3a)

Table 4.1 Crystal data and structure refinement for **3a**

Empirical formula	C21 H26 B1 Cl1 Fe1 O3	
Formula weight	428.53	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.3300(3) Å	α= 75.677(2)°.
	b = 8.7470(3) Å	β= 89.5730(10)°.
	c = 14.5400(5) Å	γ = 88.4810(10)°.
Volume	1026.13(6) $Å^3$	
Z	2	
Density (calculated)	1.387 Mg/m^3	
Absorption coefficient	0.883 mm^{-1}	
F(000)	448	
Crystal size	0.20 x 0.20 x 0.05 mm^3	
Theta range for data collection	3.10 to 27.40°.	
Index ranges	-10<=h<=10, -10<=k<=11, -18<=l<=18	
Reflections collected	15859	
Independent reflections	4575 [R(int) = 0.0912]	
Completeness to theta = 27.40°	98.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9572 and 0.8432	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4575 / 0 / 252	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2sigma(I)]	R1 = 0.0548, wR2 = 0.0987	
R indices (all data)	R1 = 0.1143, wR2 = 0.1185	
Largest diff. peak and hole	0.392 and -0.650 $e.Å^{-3}$	

Table 4.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3a**

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3002(4)	659(4)	-1143(2)	28(1)
C(2)	274(5)	2174(4)	-1034(2)	30(1)
C(3)	3938(4)	3386(4)	-2588(2)	24(1)
C(4)	3875(4)	3920(4)	-1731(2)	28(1)
C(5)	2379(4)	4728(4)	-1718(2)	26(1)
C(6)	1509(4)	4702(4)	-2561(2)	24(1)
C(7)	2500(4)	3887(4)	-3107(2)	24(1)
C(8)	5343(4)	2548(4)	-2924(3)	39(1)
C(9)	5196(5)	3710(4)	-1014(3)	42(1)
C(10)	1834(5)	5560(4)	-968(3)	39(1)
C(11)	-107(4)	5473(4)	-2850(3)	37(1)
C(12)	2210(5)	3826(4)	-4110(2)	34(1)
C(13)	-1652(4)	89(4)	-3010(2)	24(1)
C(14)	-1927(4)	340(4)	-3975(2)	25(1)
C(15)	-2992(4)	-632(4)	-4270(2)	26(1)
C(16)	-3806(4)	-1812(4)	-3633(2)	26(1)
C(17)	-3500(4)	-1996(4)	-2670(2)	29(1)
C(18)	-2437(4)	-1079(4)	-2338(2)	28(1)
C(19)	-1111(4)	1647(4)	-4681(2)	34(1)
C(20)	-4952(4)	-2845(4)	-3967(3)	36(1)
C(21)	-2143(5)	-1292(4)	-1293(2)	38(1)
O(1)	3731(3)	-446(3)	-749(2)	42(1)
O(2)	-847(3)	2109(3)	-567(2)	45(1)
O(3)	-717(3)	1139(3)	-2669(2)	26(1)
B(1)	891(5)	1034(4)	-2477(3)	23(1)
Cl(1)	1982(1)	-469(1)	-2933(1)	32(1)
Fe(1)	1977(1)	2373(1)	-1771(1)	22(1)

Table 4.3 Bond lengths [Å] and angles [°] for **3a**

C(1)-O(1)	1.154(4)
C(1)-Fe(1)	1.754(4)
C(2)-O(2)	1.145(4)
C(2)-Fe(1)	1.757(4)
C(3)-C(7)	1.421(5)
C(3)-C(4)	1.435(5)
C(3)-C(8)	1.506(5)
C(3)-Fe(1)	2.096(3)
C(4)-C(5)	1.419(5)
C(4)-C(9)	1.498(5)
C(4)-Fe(1)	2.118(3)
C(5)-C(6)	1.433(5)
C(5)-C(10)	1.514(4)
C(5)-Fe(1)	2.116(3)
C(6)-C(7)	1.435(4)
C(6)-C(11)	1.505(5)
C(6)-Fe(1)	2.105(3)
C(7)-C(12)	1.495(5)
C(7)-Fe(1)	2.113(3)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.385(4)
C(13)-C(18)	1.399(5)
C(13)-O(3)	1.402(4)
C(14)-C(15)	1.386(4)
C(14)-C(19)	1.508(5)
C(15)-C(16)	1.391(5)
C(15)-H(15)	0.9500
C(16)-C(17)	1.395(5)
C(16)-C(20)	1.494(5)
C(17)-C(18)	1.377(5)
C(17)-H(17)	0.9500
C(18)-C(21)	1.505(5)
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)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
O(3)-B(1)	1.366(4)
B(1)-Cl(1)	1.831(4)
B(1)-Fe(1)	1.977(4)

O(1)-C(1)-Fe(1)	177.3(3)

O(2)-C(2)-Fe(1)	177.3(3)
C(7)-C(3)-C(4)	108.6(3)
C(7)-C(3)-C(8)	125.2(3)
C(4)-C(3)-C(8)	126.0(3)
C(7)-C(3)-Fe(1)	70.93(18)
C(4)-C(3)-Fe(1)	70.94(18)
C(8)-C(3)-Fe(1)	127.7(2)
C(5)-C(4)-C(3)	107.5(3)
C(5)-C(4)-C(9)	127.1(3)
C(3)-C(4)-C(9)	125.3(3)
C(5)-C(4)-Fe(1)	70.32(19)
C(3)-C(4)-Fe(1)	69.26(19)
C(9)-C(4)-Fe(1)	127.7(2)
C(4)-C(5)-C(6)	108.6(3)
C(4)-C(5)-C(10)	125.6(3)
C(6)-C(5)-C(10)	125.7(3)
C(4)-C(5)-Fe(1)	70.53(19)
C(6)-C(5)-Fe(1)	69.74(19)
C(10)-C(5)-Fe(1)	128.3(2)
C(5)-C(6)-C(7)	107.6(3)
C(5)-C(6)-C(11)	126.3(3)
C(7)-C(6)-C(11)	126.0(3)
C(5)-C(6)-Fe(1)	70.56(18)
C(7)-C(6)-Fe(1)	70.43(18)
C(11)-C(6)-Fe(1)	127.1(2)
C(3)-C(7)-C(6)	107.7(3)
C(3)-C(7)-C(12)	125.5(3)
C(6)-C(7)-C(12)	126.0(3)
C(3)-C(7)-Fe(1)	69.63(18)
C(6)-C(7)-Fe(1)	69.79(18)
C(12)-C(7)-Fe(1)	134.0(2)
C(3)-C(8)-H(8A)	109.5
C(3)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(3)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(4)-C(9)-H(9A)	109.5
C(4)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(4)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(6)-C(11)-H(11A)	109.5
C(6)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(6)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(7)-C(12)-H(12A)	109.5
C(7)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(7)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5

H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	122.1(3)
C(14)-C(13)-O(3)	120.1(3)
C(18)-C(13)-O(3)	117.3(3)
C(13)-C(14)-C(15)	117.9(3)
C(13)-C(14)-C(19)	121.0(3)
C(15)-C(14)-C(19)	121.1(3)
C(14)-C(15)-C(16)	122.4(3)
C(14)-C(15)-H(15)	118.8
C(16)-C(15)-H(15)	118.8
C(15)-C(16)-C(17)	117.1(3)
C(15)-C(16)-C(20)	121.5(3)
C(17)-C(16)-C(20)	121.4(3)
C(18)-C(17)-C(16)	122.9(3)
C(18)-C(17)-H(17)	118.5
C(16)-C(17)-H(17)	118.5
C(17)-C(18)-C(13)	117.5(3)
C(17)-C(18)-C(21)	121.7(3)
C(13)-C(18)-C(21)	120.8(3)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
B(1)-O(3)-C(13)	128.3(3)
O(3)-B(1)-Cl(1)	114.2(3)
O(3)-B(1)-Fe(1)	123.7(3)
Cl(1)-B(1)-Fe(1)	122.1(2)
C(1)-Fe(1)-C(2)	96.73(16)
C(1)-Fe(1)-B(1)	87.38(15)
C(2)-Fe(1)-B(1)	87.17(15)
C(1)-Fe(1)-C(3)	96.52(14)
C(2)-Fe(1)-C(3)	160.58(14)
B(1)-Fe(1)-C(3)	107.58(14)
C(1)-Fe(1)-C(6)	161.35(14)
C(2)-Fe(1)-C(6)	97.91(14)
B(1)-Fe(1)-C(6)	104.80(14)
C(3)-Fe(1)-C(6)	66.59(12)
C(1)-Fe(1)-C(7)	129.61(14)
C(2)-Fe(1)-C(7)	132.81(14)
B(1)-Fe(1)-C(7)	86.68(14)
C(3)-Fe(1)-C(7)	39.45(12)
C(6)-Fe(1)-C(7)	39.78(12)
C(1)-Fe(1)-C(5)	127.52(15)
C(2)-Fe(1)-C(5)	94.41(14)
B(1)-Fe(1)-C(5)	144.38(14)
C(3)-Fe(1)-C(5)	66.22(12)

C(6)-Fe(1)-C(5)	39.70(13)
C(7)-Fe(1)-C(5)	66.35(12)
C(1)-Fe(1)-C(4)	95.60(14)
C(2)-Fe(1)-C(4)	124.47(15)
B(1)-Fe(1)-C(4)	147.37(15)
C(3)-Fe(1)-C(4)	39.80(13)
C(6)-Fe(1)-C(4)	66.51(13)
C(7)-Fe(1)-C(4)	66.47(13)
C(5)-Fe(1)-C(4)	39.15(13)

Symmetry transformations used to generate equivalent atoms:

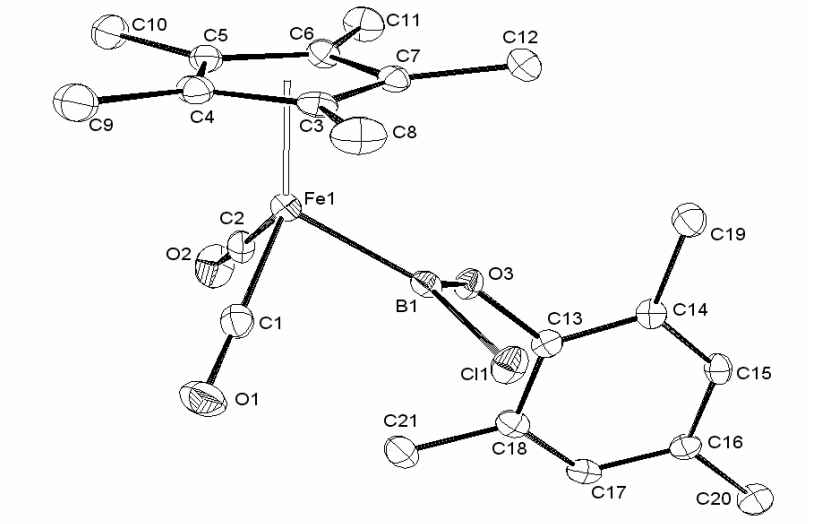
Table 4.4 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3a**

The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	27(2)	33(2)	24(2)	-7(2)	1(2)	-7(2)
C(2)	33(2)	34(2)	24(2)	-9(2)	-4(2)	-2(2)
C(3)	22(2)	16(2)	30(2)	0(1)	4(2)	3(1)
C(4)	26(2)	24(2)	31(2)	-1(2)	-3(2)	-5(2)
C(5)	30(2)	21(2)	25(2)	-5(1)	2(2)	-1(2)
C(6)	23(2)	23(2)	26(2)	-5(1)	0(2)	4(1)
C(7)	26(2)	22(2)	22(2)	-3(1)	5(2)	-5(1)
C(8)	31(2)	30(2)	53(2)	-6(2)	11(2)	4(2)
C(9)	37(2)	38(2)	47(2)	0(2)	-15(2)	-9(2)
C(10)	54(3)	32(2)	33(2)	-14(2)	6(2)	1(2)
C(11)	27(2)	37(2)	44(2)	-5(2)	-4(2)	6(2)
C(12)	47(2)	31(2)	23(2)	-4(2)	4(2)	-6(2)
C(13)	17(2)	25(2)	31(2)	-8(2)	-3(2)	1(1)
C(14)	21(2)	29(2)	27(2)	-8(2)	0(2)	-1(2)
C(15)	23(2)	33(2)	24(2)	-9(2)	-2(2)	2(2)
C(16)	22(2)	23(2)	33(2)	-8(2)	0(2)	1(1)
C(17)	28(2)	22(2)	32(2)	-1(2)	4(2)	1(2)
C(18)	24(2)	27(2)	30(2)	-4(2)	2(2)	7(2)
C(19)	32(2)	39(2)	31(2)	-8(2)	-2(2)	-7(2)
C(20)	30(2)	36(2)	43(2)	-11(2)	2(2)	-6(2)
C(21)	42(2)	39(2)	29(2)	-2(2)	-3(2)	2(2)
O(1)	44(2)	34(2)	41(2)	3(1)	-9(1)	5(1)
O(2)	32(2)	66(2)	41(2)	-22(1)	16(1)	-7(1)
O(3)	23(1)	28(1)	29(1)	-12(1)	-4(1)	2(1)
B(1)	24(2)	22(2)	20(2)	-2(2)	3(2)	3(2)
Cl(1)	27(1)	35(1)	38(1)	-17(1)	-2(1)	6(1)
Fe(1)	20(1)	23(1)	21(1)	-4(1)	0(1)	0(1)

Table 4.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3a**

	x	y	z	U(eq)
H(8A)	4948	1767	-3244	58
H(8B)	6005	2014	-2379	58
H(8C)	5989	3318	-3370	58
H(9A)	5986	4534	-1227	64
H(9B)	5719	2671	-943	64
H(9C)	4747	3789	-402	64
H(10A)	2286	5004	-352	58
H(10B)	659	5566	-929	58
H(10C)	2204	6649	-1138	58
H(11A)	-762	5436	-2283	56
H(11B)	-646	4909	-3260	56
H(11C)	34	6574	-3196	56
H(12A)	2796	4669	-4541	51
H(12B)	1058	3967	-4249	51
H(12C)	2586	2801	-4199	51
H(15)	-3174	-488	-4930	31
H(17)	-4050	-2789	-2223	35
H(19A)	-1502	1689	-5321	51
H(19B)	53	1444	-4656	51
H(19C)	-1353	2657	-4526	51
H(20A)	-5250	-2362	-4628	54
H(20B)	-5917	-2969	-3569	54
H(20C)	-4440	-3883	-3924	54
H(21A)	-2770	-2175	-933	57
H(21B)	-2470	-325	-1109	57
H(21C)	-998	-1516	-1158	57



5. Details of the crystal structure of (η^5-C_5H_5)Fe(CO)$_2$B(N^{i}Pr$_2$)Cl (7a)

Table 5.1 Crystal data and structure refinement for **7a**

Empirical formula	C13 H19 B Cl Fe N O2	
Formula weight	323.40	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 11.7410(4) Å	α= 90°.
	b = 13.9170(4) Å	β= 90°.
	c = 19.0830(7) Å	γ = 90°.
Volume	3118.15(18) Å^3	
Z	8	
Density (calculated)	1.378 Mg/m^3	
Absorption coefficient	1.134 mm^{-1}	
F(000)	1344	
Crystal size	0.25 x 0.10 x 0.10 mm^3	
Theta range for data collection	3.57 to 26.37°.	
Index ranges	-14<=h<=14, -17<=k<=17, -23<=l<=23	
Reflections collected	22231	
Independent reflections	3175 [R(int) = 0.1524]	
Completeness to theta = 26.37°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8950 and 0.7647	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3175 / 0 / 176	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0572, wR2 = 0.1157	
R indices (all data)	R1 = 0.1048, wR2 = 0.1338	
Largest diff. peak and hole	0.505 and -0.537 e.Å^{-3}	

Table 5.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7a**

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1053(4)	1989(3)	413(2)	36(1)
C(2)	1126(3)	428(3)	1039(2)	29(1)
C(3)	1868(4)	-116(3)	-393(2)	33(1)
C(4)	2912(3)	-153(3)	-20(2)	29(1)
C(5)	3482(4)	735(3)	-119(2)	36(1)
C(6)	2784(4)	1311(3)	-548(2)	40(1)
C(7)	1789(4)	784(3)	-715(2)	39(1)
C(8)	3459(3)	55(2)	1785(2)	28(1)
C(9)	2932(4)	-144(3)	2497(2)	48(1)
C(10)	4568(4)	-491(3)	1677(2)	49(1)
C(11)	4423(4)	1559(3)	2149(2)	36(1)
C(12)	3850(5)	2287(3)	2640(3)	62(2)
C(13)	5470(4)	1955(3)	1785(3)	63(2)
B(1)	2980(4)	1552(3)	1119(2)	26(1)
Cl(1)	3238(1)	2847(1)	1000(1)	54(1)
Fe(1)	1911(1)	975(1)	378(1)	23(1)
N(1)	3586(3)	1109(2)	1655(2)	22(1)
O(1)	461(3)	2652(2)	433(2)	60(1)
O(2)	576(2)	81(2)	1476(2)	43(1)

Table 5.3 Bond lengths [Å] and angles [°] for **7a**

C(1)-O(1)	1.155(5)
C(1)-Fe(1)	1.735(4)
C(2)-O(2)	1.160(4)
C(2)-Fe(1)	1.738(4)
C(3)-C(7)	1.398(5)
C(3)-C(4)	1.418(5)
C(3)-Fe(1)	2.115(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.418(5)
C(4)-Fe(1)	2.103(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.407(6)
C(5)-Fe(1)	2.100(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.416(6)
C(6)-Fe(1)	2.096(4)
C(6)-H(6)	0.9500
C(7)-Fe(1)	2.107(4)
C(7)-H(7)	0.9500
C(8)-N(1)	1.496(4)
C(8)-C(9)	1.519(6)
C(8)-C(10)	1.521(6)
C(8)-H(8)	1.0000
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-N(1)	1.499(5)
C(11)-C(13)	1.516(6)
C(11)-C(12)	1.535(6)
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
B(1)-N(1)	1.389(5)
B(1)-Cl(1)	1.841(4)
B(1)-Fe(1)	2.054(4)
O(1)-C(1)-Fe(1)	178.5(4)
O(2)-C(2)-Fe(1)	178.0(4)
C(7)-C(3)-C(4)	108.0(4)
C(7)-C(3)-Fe(1)	70.4(2)
C(4)-C(3)-Fe(1)	69.9(2)
C(7)-C(3)-H(3)	126.0
C(4)-C(3)-H(3)	126.0
Fe(1)-C(3)-H(3)	125.4
C(3)-C(4)-C(5)	108.0(4)
C(3)-C(4)-Fe(1)	70.8(2)
C(5)-C(4)-Fe(1)	70.2(2)
C(3)-C(4)-H(4)	126.0
C(5)-C(4)-H(4)	126.0
Fe(1)-C(4)-H(4)	124.6

C(6)-C(5)-C(4)	107.4(4)
C(6)-C(5)-Fe(1)	70.2(3)
C(4)-C(5)-Fe(1)	70.4(2)
C(6)-C(5)-H(5)	126.3
C(4)-C(5)-H(5)	126.3
Fe(1)-C(5)-H(5)	124.7
C(5)-C(6)-C(7)	108.4(4)
C(5)-C(6)-Fe(1)	70.6(2)
C(7)-C(6)-Fe(1)	70.7(2)
C(5)-C(6)-H(6)	125.8
C(7)-C(6)-H(6)	125.8
Fe(1)-C(6)-H(6)	124.5
C(3)-C(7)-C(6)	108.1(4)
C(3)-C(7)-Fe(1)	71.0(2)
C(6)-C(7)-Fe(1)	69.9(2)
C(3)-C(7)-H(7)	125.9
C(6)-C(7)-H(7)	125.9
Fe(1)-C(7)-H(7)	124.8
N(1)-C(8)-C(9)	111.6(3)
N(1)-C(8)-C(10)	112.4(3)
C(9)-C(8)-C(10)	112.3(3)
N(1)-C(8)-H(8)	106.7
C(9)-C(8)-H(8)	106.7
C(10)-C(8)-H(8)	106.7
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(1)-C(11)-C(13)	113.3(4)
N(1)-C(11)-C(12)	111.9(4)
C(13)-C(11)-C(12)	113.3(4)
N(1)-C(11)-H(11)	105.9
C(13)-C(11)-H(11)	105.9
C(12)-C(11)-H(11)	105.9
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
N(1)-B(1)-Cl(1)	116.1(3)
N(1)-B(1)-Fe(1)	130.2(3)
Cl(1)-B(1)-Fe(1)	113.5(2)
C(1)-Fe(1)-C(2)	91.18(19)
C(1)-Fe(1)-B(1)	90.60(18)
C(2)-Fe(1)-B(1)	89.77(17)

C(1)-Fe(1)-C(6)	97.75(19)
C(2)-Fe(1)-C(6)	165.68(17)
B(1)-Fe(1)-C(6)	101.24(18)
C(1)-Fe(1)-C(5)	131.01(18)
C(2)-Fe(1)-C(5)	136.40(17)
B(1)-Fe(1)-C(5)	80.64(17)
C(6)-Fe(1)-C(5)	39.19(17)
C(1)-Fe(1)-C(4)	160.96(17)
C(2)-Fe(1)-C(4)	103.37(16)
B(1)-Fe(1)-C(4)	101.51(17)
C(6)-Fe(1)-C(4)	65.70(16)
C(5)-Fe(1)-C(4)	39.44(15)
C(1)-Fe(1)-C(7)	95.80(18)
C(2)-Fe(1)-C(7)	128.78(17)
B(1)-Fe(1)-C(7)	140.57(18)
C(6)-Fe(1)-C(7)	39.36(16)
C(5)-Fe(1)-C(7)	65.93(17)
C(4)-Fe(1)-C(7)	65.54(16)
C(1)-Fe(1)-C(3)	126.62(18)
C(2)-Fe(1)-C(3)	100.19(17)
B(1)-Fe(1)-C(3)	140.75(17)
C(6)-Fe(1)-C(3)	65.50(16)
C(5)-Fe(1)-C(3)	65.96(16)
C(4)-Fe(1)-C(3)	39.29(14)
C(7)-Fe(1)-C(3)	38.67(15)
B(1)-N(1)-C(8)	120.4(3)
B(1)-N(1)-C(11)	127.8(3)
C(8)-N(1)-C(11)	111.8(3)

Symmetry transformations used to generate equivalent atoms:

Table 5.4 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **7a**

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)	32(3)	35(2)	41(2)	0(2)	-13(2)	5(2)
C(2)	20(2)	36(2)	30(2)	-5(2)	-4(2)	0(2)
C(3)	41(3)	28(2)	30(2)	-8(2)	1(2)	-5(2)
C(4)	33(3)	29(2)	26(2)	-4(2)	7(2)	5(2)
C(5)	35(3)	45(3)	29(2)	-3(2)	11(2)	-6(2)
C(6)	55(3)	36(2)	30(2)	6(2)	10(2)	-6(2)
C(7)	45(3)	47(3)	26(2)	-1(2)	-5(2)	2(2)
C(8)	31(2)	23(2)	29(2)	5(2)	-8(2)	-3(2)
C(9)	53(3)	58(3)	33(2)	8(2)	-11(2)	-22(2)
C(10)	54(3)	33(2)	60(3)	-9(2)	-21(3)	18(2)
C(11)	29(3)	29(2)	50(3)	-1(2)	-19(2)	-4(2)
C(12)	59(4)	52(3)	75(4)	-32(3)	-27(3)	5(3)
C(13)	33(3)	58(3)	98(4)	27(3)	-21(3)	-20(2)
B(1)	24(3)	18(2)	35(3)	-4(2)	2(2)	0(2)
Cl(1)	62(1)	20(1)	80(1)	9(1)	-35(1)	-7(1)
Fe(1)	22(1)	22(1)	26(1)	1(1)	-2(1)	2(1)
N(1)	16(2)	21(2)	29(2)	-3(1)	-7(1)	-2(1)
O(1)	49(2)	44(2)	86(3)	-10(2)	-24(2)	23(2)
O(2)	29(2)	56(2)	45(2)	-2(2)	11(2)	-3(2)

Table 5.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **7a**

	x	y	z	U(eq)
H(3)	1318	-616	-419	39
H(4)	3182	-680	249	35
H(5)	4202	910	69	44
H(6)	2953	1945	-700	48
H(7)	1175	1003	-996	47
H(8)	2911	-192	1426	33
H(9A)	3456	66	2866	72
H(9B)	2787	-834	2546	72
H(9C)	2212	208	2539	72
H(10A)	4902	-310	1225	73
H(10B)	4415	-1183	1681	73
H(10C)	5100	-331	2054	73
H(11)	4701	1027	2456	43
H(12A)	3637	2861	2373	93
H(12B)	4381	2466	3014	93
H(12C)	3166	1999	2846	93
H(13A)	5794	1461	1478	94
H(13B)	6037	2142	2136	94
H(13C)	5258	2518	1505	94

6. Details of the crystal structure of $[(\eta^5\text{-}C_5H_5)Fe(CO)_2\{B(N^iPr_2)(OPPh_3)\}]^+[BAr^f_4]^-$ (13)

Table 6.1 Crystal data and structure refinement for **13**

Empirical formula	C63 H46 B2 F24 Fe N O3 P
Formula weight	1429.45
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 13.0324(2) A alpha = 68.7080(10)deg. b = 13.9949(2) A beta = 83.7430(10)deg. c = 19.1002(3) A gamma = 87.4800(10)deg.
Volume	3226.47(8) A^3
Z, Calculated density	2, 1.471 Mg/m^3
Absorption coefficient	0.373 mm^-1
F(000)	1444
Crystal size	0.38 x 0.25 x 0.20 mm
Theta range for data collection	2.81 to 27.54 deg.
Limiting indices	-16<=h<=16, -17<=k<=18, -24<=l<=24
Reflections collected / unique	51247 / 14704 [R(int) = 0.1118]
Completeness to theta = 27.54	99.0 %
Absorption correction	Sortav (Blessing, 1995)
Max. and min. transmission	0.910 and 0.871
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14704 / 157 / 913
Goodness-of-fit on F^2	1.106
Final R indices [I>2sigma(I)]	R1 = 0.0718, wR2 = 0.1791
R indices (all data)	R1 = 0.1223, wR2 = 0.1992
Extinction coefficient	0.0025(6)
Largest diff. peak and hole	1.086 and -0.608 e.A^-3

Table 6.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **13**

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	762(1)	-627(1)	-2666(1)	26(1)
P(1)	-1423(1)	-2222(1)	-3069(1)	24(1)
F(1)	3615(4)	2004(3)	-4879(2)	54(1)
F(1A)	3224(18)	1760(20)	-4707(14)	67(7)
F(2)	2913(4)	562(4)	-4372(2)	93(2)
F(2A)	3726(13)	200(10)	-4455(8)	37(5)
F(3)	4526(5)	705(5)	-4773(2)	110(2)
F(3A)	4579(19)	1440(20)	-4849(13)	93(8)
F(4)	3688(2)	-1318(2)	-1266(2)	78(1)
F(5)	4564(3)	-1847(2)	-2040(2)	77(1)
F(6)	5293(2)	-1147(2)	-1425(2)	83(1)
F(7)	1360(2)	573(2)	-362(2)	64(1)
F(8)	-116(2)	1272(2)	-524(2)	74(1)
F(9)	1029(3)	1887(3)	-82(2)	81(1)
F(10)	429(4)	4949(3)	-3358(3)	68(2)
F(10A)	-170(12)	4600(12)	-3080(8)	71(4)
F(11)	478(5)	3756(5)	-3795(3)	94(2)
F(11A)	809(8)	4325(9)	-3918(6)	49(3)
F(12)	-662(3)	3814(4)	-2927(3)	94(2)
F(12A)	-349(9)	3327(8)	-3320(6)	52(3)
F(13)	3053(3)	6658(2)	-3552(2)	87(1)
F(14)	4564(3)	7259(2)	-3544(2)	91(1)
F(15)	3989(3)	7342(2)	-4549(2)	94(1)
F(16)	6949(3)	3886(3)	-4778(2)	82(2)
F(16A)	7478(17)	3866(19)	-4213(13)	77(8)
F(17)	7683(3)	4652(5)	-4199(2)	82(2)
F(17A)	7573(14)	5295(14)	-4495(11)	43(5)
F(18)	7006(3)	5489(4)	-5216(2)	89(2)
F(18A)	6886(15)	4908(18)	-5232(12)	57(6)
F(19)	4028(3)	4480(2)	-368(2)	75(1)
F(20)	3524(2)	2977(2)	353(2)	70(1)
F(21)	4973(2)	3507(2)	454(1)	62(1)
F(22)	7624(5)	1480(8)	-1566(5)	117(3)
F(22A)	7254(8)	842(7)	-1101(6)	63(3)
F(23)	8000(3)	2728(5)	-1280(3)	106(3)
F(23A)	7861(8)	2201(9)	-1761(6)	66(4)
F(24)	7538(4)	1383(5)	-390(3)	62(2)
F(24A)	7829(12)	1772(13)	-593(9)	101(6)
O(1)	2571(2)	-1629(2)	-3092(2)	56(1)
O(2)	219(2)	-55(2)	-4199(2)	49(1)
O(3)	-743(2)	-2372(2)	-2426(1)	28(1)
N(1)	559(2)	-2932(2)	-1600(2)	30(1)
C(1)	1009(5)	-372(4)	-1683(3)	60(2)
C(2)	-29(4)	-370(4)	-1746(3)	60(2)
C(3)	-237(3)	410(4)	-2389(3)	52(1)
C(4)	1463(3)	428(4)	-2309(3)	48(1)
C(5)	689(4)	915(3)	-2750(2)	49(1)
C(6)	1862(3)	-1234(3)	-2906(2)	36(1)
C(7)	397(3)	-335(3)	-3578(2)	35(1)

C(8)	15(3)	-3941(3)	-1207(2)	38(1)
C(9)	-1069(3)	-3811(3)	-855(2)	49(1)
C(10)	36(4)	-4582(3)	-1701(3)	48(1)
C(11)	1546(3)	-2906(3)	-1281(2)	42(1)
C(12)	2320(4)	-3691(4)	-1386(3)	59(1)
C(13)	1385(4)	-3002(4)	-456(3)	57(1)
C(14)	-2040(3)	-996(3)	-3319(2)	30(1)
C(15)	-2192(3)	-404(3)	-4052(2)	41(1)
C(16)	-2424(3)	-650(3)	-2736(2)	37(1)
C(17)	-2724(4)	519(3)	-4220(3)	56(1)
C(18)	-2949(3)	274(4)	-2899(3)	49(1)
C(19)	-3097(3)	855(3)	-3645(3)	58(1)
C(20)	-692(3)	-2406(3)	-3853(2)	27(1)
C(21)	-1215(3)	-2479(3)	-4435(2)	36(1)
C(22)	377(3)	-2528(3)	-3887(2)	33(1)
C(23)	909(3)	-2708(3)	-4498(3)	45(1)
C(24)	-678(4)	-2672(3)	-5028(2)	47(1)
C(25)	383(4)	-2778(3)	-5065(2)	48(1)
C(26)	-2385(3)	-3199(3)	-2732(2)	29(1)
C(27)	-2183(3)	-4133(3)	-2836(2)	34(1)
C(28)	-3322(3)	-3061(3)	-2353(2)	38(1)
C(29)	-4040(3)	-3849(3)	-2075(3)	44(1)
C(30)	-2916(3)	-4911(3)	-2553(2)	41(1)
C(31)	-3834(3)	-4762(3)	-2182(2)	42(1)
C(32)	4191(2)	1793(3)	-2723(2)	24(1)
C(33)	4022(3)	1844(3)	-3446(2)	28(1)
C(34)	4016(3)	977(3)	-3637(2)	27(1)
C(35)	4203(3)	10(3)	-3108(2)	30(1)
C(36)	4361(3)	-62(3)	-2385(2)	27(1)
C(37)	4356(3)	816(3)	-2198(2)	27(1)
C(38)	3775(4)	1047(3)	-4398(2)	45(1)
C(39)	4485(3)	-1085(3)	-1790(2)	36(1)
C(40)	2779(3)	2840(2)	-2277(2)	23(1)
C(41)	2329(3)	2204(3)	-1569(2)	27(1)
C(42)	1273(3)	2149(3)	-1377(2)	30(1)
C(43)	608(3)	2722(3)	-1894(2)	32(1)
C(44)	1026(3)	3335(3)	-2604(2)	28(1)
C(45)	2090(3)	3386(3)	-2792(2)	26(1)
C(46)	876(3)	1480(3)	-598(2)	41(1)
C(47)	331(3)	3933(3)	-3178(3)	40(1)
C(48)	4506(3)	3853(3)	-3150(2)	24(1)
C(49)	4090(3)	4818(3)	-3228(2)	29(1)
C(50)	4537(3)	5715(3)	-3750(2)	38(1)
C(51)	5430(3)	5682(3)	-4194(2)	39(1)
C(52)	5868(3)	4740(3)	-4117(2)	32(1)
C(53)	5403(3)	3845(3)	-3609(2)	25(1)
C(54)	4037(4)	6730(4)	-3833(3)	56(1)
C(55)	6878(3)	4690(4)	-4562(2)	44(1)
C(56)	4658(3)	2720(3)	-1761(2)	24(1)
C(57)	5669(3)	2340(3)	-1703(2)	32(1)
C(58)	6237(3)	2319(3)	-1132(2)	41(1)
C(59)	5812(3)	2698(3)	-578(2)	39(1)
C(60)	4829(3)	3094(3)	-620(2)	29(1)
C(61)	4269(3)	3108(3)	-1205(2)	25(1)
C(62)	7320(4)	1905(5)	-1094(3)	79(2)
C(63)	4356(3)	3507(3)	-46(2)	40(1)
B(1)	202(3)	-2099(3)	-2188(2)	25(1)
B(2)	4025(3)	2808(3)	-2479(2)	22(1)

Table 6.3 Bond lengths [A] and angles [deg] for **13**

Fe(1)-C(6)	1.738(4)
Fe(1)-C(7)	1.754(4)
Fe(1)-B(1)	2.057(4)
Fe(1)-C(2)	2.077(4)
Fe(1)-C(3)	2.079(4)
Fe(1)-C(1)	2.093(4)
Fe(1)-C(5)	2.104(4)
Fe(1)-C(4)	2.114(4)
P(1)-O(3)	1.540(2)
P(1)-C(20)	1.778(4)
P(1)-C(14)	1.785(4)
P(1)-C(26)	1.787(3)
F(1)-C(38)	1.343(6)
F(1A)-C(38)	1.21(2)
F(2)-C(38)	1.324(5)
F(2A)-C(38)	1.234(14)
F(3)-C(38)	1.325(6)
F(3A)-C(38)	1.28(2)
F(4)-C(39)	1.324(5)
F(5)-C(39)	1.313(5)
F(6)-C(39)	1.309(4)
F(7)-C(46)	1.337(5)
F(8)-C(46)	1.319(5)
F(9)-C(46)	1.342(5)
F(10)-C(47)	1.345(6)
F(10A)-C(47)	1.174(13)
F(11)-C(47)	1.284(6)
F(11A)-C(47)	1.402(12)
F(12)-C(47)	1.325(6)
F(12A)-C(47)	1.365(11)
F(13)-C(54)	1.329(6)
F(14)-C(54)	1.322(5)
F(15)-C(54)	1.330(6)
F(16)-C(55)	1.328(6)
F(16A)-C(55)	1.36(2)
F(17)-C(55)	1.308(6)
F(17A)-C(55)	1.312(17)
F(18)-C(55)	1.338(5)
F(18A)-C(55)	1.20(2)
F(19)-C(63)	1.346(5)
F(20)-C(63)	1.337(5)
F(21)-C(63)	1.315(4)
F(22)-C(62)	1.271(7)
F(22A)-C(62)	1.499(10)
F(23)-C(62)	1.400(8)
F(23A)-C(62)	1.319(11)
F(24)-C(62)	1.331(7)
F(24A)-C(62)	1.178(14)
O(1)-C(6)	1.145(5)
O(2)-C(7)	1.152(4)
O(3)-B(1)	1.469(4)
N(1)-B(1)	1.397(5)
N(1)-C(11)	1.490(5)
N(1)-C(8)	1.503(5)
C(1)-C(2)	1.371(7)

C(1)-C(4)	1.401(7)
C(2)-C(3)	1.360(7)
C(3)-C(5)	1.403(6)
C(4)-C(5)	1.378(6)
C(8)-C(10)	1.517(6)
C(8)-C(9)	1.530(6)
C(11)-C(12)	1.512(6)
C(11)-C(13)	1.524(6)
C(14)-C(15)	1.374(5)
C(14)-C(16)	1.406(5)
C(15)-C(17)	1.387(6)
C(16)-C(18)	1.384(6)
C(17)-C(19)	1.380(7)
C(18)-C(19)	1.389(7)
C(20)-C(22)	1.393(5)
C(20)-C(21)	1.402(5)
C(21)-C(24)	1.371(6)
C(22)-C(23)	1.389(5)
C(23)-C(25)	1.377(6)
C(24)-C(25)	1.381(6)
C(26)-C(28)	1.392(5)
C(26)-C(27)	1.402(5)
C(27)-C(30)	1.394(5)
C(28)-C(29)	1.390(5)
C(29)-C(31)	1.376(6)
C(30)-C(31)	1.371(6)
C(32)-C(37)	1.395(5)
C(32)-C(33)	1.399(5)
C(32)-B(2)	1.646(5)
C(33)-C(34)	1.388(5)
C(34)-C(35)	1.394(5)
C(34)-C(38)	1.489(5)
C(35)-C(36)	1.384(5)
C(36)-C(37)	1.398(5)
C(36)-C(39)	1.485(5)
C(40)-C(45)	1.394(5)
C(40)-C(41)	1.402(5)
C(40)-B(2)	1.630(5)
C(41)-C(42)	1.383(5)
C(42)-C(43)	1.386(5)
C(42)-C(46)	1.489(5)
C(43)-C(44)	1.381(5)
C(44)-C(45)	1.393(5)
C(44)-C(47)	1.485(5)
C(48)-C(53)	1.385(5)
C(48)-C(49)	1.395(5)
C(48)-B(2)	1.650(5)
C(49)-C(50)	1.392(5)
C(50)-C(51)	1.373(6)
C(50)-C(54)	1.498(6)
C(51)-C(52)	1.378(6)
C(52)-C(53)	1.391(5)
C(52)-C(55)	1.500(6)
C(56)-C(61)	1.399(5)
C(56)-C(57)	1.399(5)
C(56)-B(2)	1.642(5)
C(57)-C(58)	1.375(5)
C(58)-C(59)	1.400(6)
C(58)-C(62)	1.501(7)
C(59)-C(60)	1.372(5)

C(60)-C(61)	1.393(5)
C(60)-C(63)	1.483(5)
C(6)-Fe(1)-C(7)	89.37(19)
C(6)-Fe(1)-B(1)	83.22(17)
C(7)-Fe(1)-B(1)	98.40(16)
C(6)-Fe(1)-C(2)	141.0(2)
C(7)-Fe(1)-C(2)	129.4(2)
B(1)-Fe(1)-C(2)	86.53(17)
C(6)-Fe(1)-C(3)	163.17(17)
C(7)-Fe(1)-C(3)	96.0(2)
B(1)-Fe(1)-C(3)	111.60(18)
C(2)-Fe(1)-C(3)	38.2(2)
C(6)-Fe(1)-C(1)	106.8(2)
C(7)-Fe(1)-C(1)	157.19(19)
B(1)-Fe(1)-C(1)	99.38(18)
C(2)-Fe(1)-C(1)	38.4(2)
C(3)-Fe(1)-C(1)	64.12(19)
C(6)-Fe(1)-C(5)	124.77(18)
C(7)-Fe(1)-C(5)	93.11(17)
B(1)-Fe(1)-C(5)	149.95(18)
C(2)-Fe(1)-C(5)	64.97(18)
C(3)-Fe(1)-C(5)	39.20(18)
C(1)-Fe(1)-C(5)	64.55(18)
C(6)-Fe(1)-C(4)	99.27(17)
C(7)-Fe(1)-C(4)	124.02(18)
B(1)-Fe(1)-C(4)	137.43(18)
C(2)-Fe(1)-C(4)	64.86(18)
C(3)-Fe(1)-C(4)	64.56(16)
C(1)-Fe(1)-C(4)	38.92(19)
C(5)-Fe(1)-C(4)	38.15(17)
O(3)-P(1)-C(20)	110.94(16)
O(3)-P(1)-C(14)	109.89(15)
C(20)-P(1)-C(14)	112.56(18)
O(3)-P(1)-C(26)	107.77(15)
C(20)-P(1)-C(26)	106.39(17)
C(14)-P(1)-C(26)	109.11(17)
B(1)-O(3)-P(1)	148.0(2)
B(1)-N(1)-C(11)	122.5(3)
B(1)-N(1)-C(8)	125.7(3)
C(11)-N(1)-C(8)	111.8(3)
C(2)-C(1)-C(4)	108.3(4)
C(2)-C(1)-Fe(1)	70.2(3)
C(4)-C(1)-Fe(1)	71.3(2)
C(3)-C(2)-C(1)	108.3(4)
C(3)-C(2)-Fe(1)	71.0(3)
C(1)-C(2)-Fe(1)	71.4(3)
C(2)-C(3)-C(5)	108.7(4)
C(2)-C(3)-Fe(1)	70.8(3)
C(5)-C(3)-Fe(1)	71.4(3)
C(5)-C(4)-C(1)	107.5(4)
C(5)-C(4)-Fe(1)	70.5(2)
C(1)-C(4)-Fe(1)	69.8(2)
C(4)-C(5)-C(3)	107.2(4)
C(4)-C(5)-Fe(1)	71.3(2)
C(3)-C(5)-Fe(1)	69.4(2)
O(1)-C(6)-Fe(1)	177.1(4)
O(2)-C(7)-Fe(1)	173.0(3)
N(1)-C(8)-C(10)	112.7(3)
N(1)-C(8)-C(9)	112.2(3)

C(10)-C(8)-C(9)	113.2(4)
N(1)-C(11)-C(12)	112.7(3)
N(1)-C(11)-C(13)	112.7(4)
C(12)-C(11)-C(13)	110.8(4)
C(15)-C(14)-C(16)	119.2(4)
C(15)-C(14)-P(1)	122.6(3)
C(16)-C(14)-P(1)	118.2(3)
C(14)-C(15)-C(17)	121.0(4)
C(18)-C(16)-C(14)	120.2(4)
C(19)-C(17)-C(15)	119.6(5)
C(16)-C(18)-C(19)	119.4(4)
C(17)-C(19)-C(18)	120.7(4)
C(22)-C(20)-C(21)	119.2(3)
C(22)-C(20)-P(1)	122.0(3)
C(21)-C(20)-P(1)	118.7(3)
C(24)-C(21)-C(20)	120.1(4)
C(23)-C(22)-C(20)	119.8(4)
C(25)-C(23)-C(22)	120.2(4)
C(21)-C(24)-C(25)	120.4(4)
C(23)-C(25)-C(24)	120.2(4)
C(28)-C(26)-C(27)	119.4(3)
C(28)-C(26)-P(1)	121.4(3)
C(27)-C(26)-P(1)	119.2(3)
C(30)-C(27)-C(26)	119.6(4)
C(29)-C(28)-C(26)	120.0(4)
C(31)-C(29)-C(28)	120.2(4)
C(31)-C(30)-C(27)	120.3(4)
C(30)-C(31)-C(29)	120.6(4)
C(37)-C(32)-C(33)	116.1(3)
C(37)-C(32)-B(2)	122.2(3)
C(33)-C(32)-B(2)	121.0(3)
C(34)-C(33)-C(32)	122.4(3)
C(33)-C(34)-C(35)	120.5(3)
C(33)-C(34)-C(38)	121.2(3)
C(35)-C(34)-C(38)	118.2(3)
C(36)-C(35)-C(34)	118.2(3)
C(35)-C(36)-C(37)	120.7(3)
C(35)-C(36)-C(39)	119.8(3)
C(37)-C(36)-C(39)	119.4(3)
C(32)-C(37)-C(36)	122.0(3)
F(1A)-C(38)-F(2A)	122.9(13)
F(1A)-C(38)-F(3A)	93.7(15)
F(2A)-C(38)-F(3A)	102.3(14)
F(1A)-C(38)-F(3)	122.7(12)
F(2A)-C(38)-F(3)	58.5(7)
F(3A)-C(38)-F(3)	44.5(12)
F(1A)-C(38)-F(2)	79.0(12)
F(2A)-C(38)-F(2)	54.5(7)
F(3A)-C(38)-F(2)	140.8(11)
F(3)-C(38)-F(2)	108.5(5)
F(1A)-C(38)-F(1)	27.5(11)
F(2A)-C(38)-F(1)	132.4(7)
F(3A)-C(38)-F(1)	66.9(12)
F(3)-C(38)-F(1)	102.9(4)
F(2)-C(38)-F(1)	103.6(4)
F(1A)-C(38)-C(34)	114.7(12)
F(2A)-C(38)-C(34)	112.9(7)
F(3A)-C(38)-C(34)	105.6(11)
F(3)-C(38)-C(34)	113.7(4)
F(2)-C(38)-C(34)	112.5(4)

F(1)-C(38)-C(34)	114.7(3)
F(6)-C(39)-F(5)	106.3(4)
F(6)-C(39)-F(4)	105.2(4)
F(5)-C(39)-F(4)	105.2(3)
F(6)-C(39)-C(36)	113.2(3)
F(5)-C(39)-C(36)	114.2(3)
F(4)-C(39)-C(36)	111.9(3)
C(45)-C(40)-C(41)	115.6(3)
C(45)-C(40)-B(2)	124.4(3)
C(41)-C(40)-B(2)	119.6(3)
C(42)-C(41)-C(40)	122.6(3)
C(41)-C(42)-C(43)	120.4(3)
C(41)-C(42)-C(46)	118.4(3)
C(43)-C(42)-C(46)	121.2(3)
C(44)-C(43)-C(42)	118.4(3)
C(43)-C(44)-C(45)	120.8(3)
C(43)-C(44)-C(47)	119.6(3)
C(45)-C(44)-C(47)	119.6(3)
C(44)-C(45)-C(40)	122.1(3)
F(8)-C(46)-F(7)	106.0(3)
F(8)-C(46)-F(9)	107.4(4)
F(7)-C(46)-F(9)	104.0(4)
F(8)-C(46)-C(42)	113.7(4)
F(7)-C(46)-C(42)	112.8(4)
F(9)-C(46)-C(42)	112.3(3)
F(10A)-C(47)-F(11)	126.2(7)
F(10A)-C(47)-F(12)	58.1(8)
F(11)-C(47)-F(12)	109.0(5)
F(10A)-C(47)-F(10)	43.2(8)
F(11)-C(47)-F(10)	107.3(5)
F(12)-C(47)-F(10)	100.5(4)
F(10A)-C(47)-F(12A)	105.3(9)
F(11)-C(47)-F(12A)	60.6(6)
F(12)-C(47)-F(12A)	53.6(5)
F(10)-C(47)-F(12A)	134.7(6)
F(10A)-C(47)-F(11A)	106.9(9)
F(11)-C(47)-F(11A)	37.2(4)
F(12)-C(47)-F(11A)	130.1(6)
F(10)-C(47)-F(11A)	73.1(6)
F(12A)-C(47)-F(11A)	95.3(7)
F(10A)-C(47)-C(44)	119.2(7)
F(11)-C(47)-C(44)	113.6(4)
F(12)-C(47)-C(44)	113.6(4)
F(10)-C(47)-C(44)	111.9(3)
F(12A)-C(47)-C(44)	112.7(6)
F(11A)-C(47)-C(44)	114.5(6)
C(53)-C(48)-C(49)	116.0(3)
C(53)-C(48)-B(2)	122.6(3)
C(49)-C(48)-B(2)	121.0(3)
C(50)-C(49)-C(48)	121.9(4)
C(51)-C(50)-C(49)	120.8(4)
C(51)-C(50)-C(54)	119.4(4)
C(49)-C(50)-C(54)	119.9(4)
C(50)-C(51)-C(52)	118.5(3)
C(51)-C(52)-C(53)	120.4(3)
C(51)-C(52)-C(55)	119.3(3)
C(53)-C(52)-C(55)	120.2(4)
C(48)-C(53)-C(52)	122.4(3)
F(14)-C(54)-F(15)	104.5(4)
F(14)-C(54)-F(13)	110.6(4)

F(15)-C(54)-F(13)	102.5(4)
F(14)-C(54)-C(50)	111.6(4)
F(15)-C(54)-C(50)	113.4(4)
F(13)-C(54)-C(50)	113.6(4)
F(18A)-C(55)-F(17)	126.0(10)
F(18A)-C(55)-F(17A)	104.3(12)
F(17)-C(55)-F(17A)	39.6(8)
F(18A)-C(55)-F(16)	66.0(11)
F(17)-C(55)-F(16)	106.6(5)
F(17A)-C(55)-F(16)	132.6(9)
F(18A)-C(55)-F(18)	38.5(10)
F(17)-C(55)-F(18)	107.4(4)
F(17A)-C(55)-F(18)	72.3(9)
F(16)-C(55)-F(18)	103.4(4)
F(18A)-C(55)-F(16A)	114.8(15)
F(17)-C(55)-F(16A)	51.1(10)
F(17A)-C(55)-F(16A)	89.1(13)
F(16)-C(55)-F(16A)	59.4(11)
F(18)-C(55)-F(16A)	133.7(10)
F(18A)-C(55)-C(52)	118.2(10)
F(17)-C(55)-C(52)	113.7(4)
F(17A)-C(55)-C(52)	112.1(8)
F(16)-C(55)-C(52)	112.9(3)
F(18)-C(55)-C(52)	112.2(4)
F(16A)-C(55)-C(52)	114.0(10)
C(61)-C(56)-C(57)	115.2(3)
C(61)-C(56)-B(2)	122.6(3)
C(57)-C(56)-B(2)	121.9(3)
C(58)-C(57)-C(56)	123.0(4)
C(57)-C(58)-C(59)	120.1(4)
C(57)-C(58)-C(62)	121.1(4)
C(59)-C(58)-C(62)	118.9(4)
C(60)-C(59)-C(58)	118.9(3)
C(59)-C(60)-C(61)	120.0(4)
C(59)-C(60)-C(63)	120.4(3)
C(61)-C(60)-C(63)	119.6(3)
C(60)-C(61)-C(56)	122.9(3)
F(24A)-C(62)-F(22)	117.0(10)
F(24A)-C(62)-F(23A)	113.2(11)
F(22)-C(62)-F(23A)	44.9(5)
F(24A)-C(62)-F(24)	29.2(8)
F(22)-C(62)-F(24)	114.7(7)
F(23A)-C(62)-F(24)	134.4(7)
F(24A)-C(62)-F(23)	70.5(9)
F(22)-C(62)-F(23)	103.6(7)
F(23A)-C(62)-F(23)	61.9(6)
F(24)-C(62)-F(23)	99.5(5)
F(24A)-C(62)-F(22A)	101.8(10)
F(22)-C(62)-F(22A)	45.4(5)
F(23A)-C(62)-F(22A)	90.3(7)
F(24)-C(62)-F(22A)	81.5(6)
F(23)-C(62)-F(22A)	142.2(6)
F(24A)-C(62)-C(58)	125.6(10)
F(22)-C(62)-C(58)	115.8(5)
F(23A)-C(62)-C(58)	112.5(7)
F(24)-C(62)-C(58)	112.8(5)
F(23)-C(62)-C(58)	108.4(5)
F(22A)-C(62)-C(58)	105.7(6)
F(21)-C(63)-F(20)	105.6(3)
F(21)-C(63)-F(19)	106.7(3)

F(20)-C(63)-F(19)	105.7(4)
F(21)-C(63)-C(60)	114.4(4)
F(20)-C(63)-C(60)	112.3(3)
F(19)-C(63)-C(60)	111.5(3)
N(1)-B(1)-O(3)	110.5(3)
N(1)-B(1)-Fe(1)	129.1(3)
O(3)-B(1)-Fe(1)	120.2(3)
C(40)-B(2)-C(56)	112.1(3)
C(40)-B(2)-C(32)	103.1(3)
C(56)-B(2)-C(32)	112.5(3)
C(40)-B(2)-C(48)	114.4(3)
C(56)-B(2)-C(48)	102.9(2)
C(32)-B(2)-C(48)	112.1(3)

Symmetry transformations used to generate equivalent atoms:

Table 6.4 Anisotropic displacement parameters (A^2 x 10^3) for **13**

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)	30(1)	22(1)	28(1)	-10(1)	-3(1)	-3(1)
P(1)	26(1)	22(1)	25(1)	-9(1)	-4(1)	-1(1)
F(1)	85(3)	39(2)	32(2)	-2(2)	-18(2)	-20(2)
F(2)	116(4)	108(3)	44(2)	1(2)	-34(2)	-76(3)
F(3)	152(4)	138(5)	59(3)	-62(3)	-30(3)	89(4)
F(4)	79(2)	48(2)	62(2)	23(1)	22(2)	14(1)
F(5)	136(3)	27(1)	69(2)	-17(1)	-22(2)	16(2)
F(6)	73(2)	49(2)	99(2)	21(2)	-54(2)	-8(2)
F(7)	61(2)	51(2)	53(2)	7(1)	10(1)	-4(1)
F(8)	37(2)	87(2)	70(2)	4(2)	10(1)	-23(2)
F(9)	113(2)	89(2)	42(2)	-30(2)	21(2)	-39(2)
F(10)	86(3)	33(2)	77(3)	2(2)	-50(2)	3(2)
F(11)	123(4)	123(4)	77(3)	-76(3)	-71(3)	80(4)
F(12)	24(2)	109(4)	94(4)	26(3)	-11(2)	10(2)
F(13)	73(2)	48(2)	136(3)	-33(2)	-3(2)	18(2)
F(14)	121(3)	50(2)	126(3)	-50(2)	-64(2)	30(2)
F(15)	114(3)	39(2)	112(3)	-1(2)	-45(2)	16(2)
F(16)	66(2)	84(3)	112(3)	-69(2)	51(2)	-23(2)
F(17)	40(2)	154(5)	62(3)	-51(3)	-5(2)	7(2)
F(18)	88(3)	74(3)	62(2)	12(2)	45(2)	-5(2)
F(19)	128(3)	56(2)	57(2)	-35(2)	-36(2)	41(2)
F(20)	67(2)	93(2)	61(2)	-45(2)	13(2)	-8(2)
F(21)	76(2)	78(2)	48(2)	-39(1)	-26(1)	13(2)
F(22)	81(4)	183(7)	130(5)	-105(5)	-41(4)	63(4)
F(23)	22(2)	145(5)	118(4)	-7(4)	-4(2)	-3(3)
F(24)	40(3)	69(3)	68(3)	-11(3)	-33(2)	24(2)
O(1)	38(2)	40(2)	92(3)	-34(2)	12(2)	-1(1)
O(2)	70(2)	44(2)	29(2)	-6(1)	-10(2)	-17(2)
O(3)	33(1)	23(1)	25(1)	-5(1)	-7(1)	-5(1)
N(1)	32(2)	24(2)	35(2)	-11(1)	-10(1)	-3(1)
C(1)	105(5)	41(3)	51(3)	-31(2)	-42(3)	22(3)
C(2)	80(4)	55(3)	52(3)	-35(3)	30(3)	-28(3)
C(3)	32(2)	56(3)	90(4)	-51(3)	-18(2)	11(2)
C(4)	33(2)	49(3)	85(4)	-51(3)	-5(2)	-4(2)
C(5)	85(4)	23(2)	39(2)	-12(2)	-5(2)	-1(2)
C(6)	33(2)	28(2)	50(3)	-21(2)	1(2)	-8(2)
C(7)	39(2)	26(2)	38(2)	-12(2)	1(2)	-10(2)
C(8)	51(3)	24(2)	36(2)	-2(2)	-15(2)	-1(2)
C(9)	58(3)	45(3)	36(2)	-4(2)	-1(2)	-17(2)
C(10)	69(3)	25(2)	52(3)	-13(2)	-18(2)	6(2)
C(11)	43(2)	33(2)	50(3)	-11(2)	-25(2)	1(2)
C(12)	44(3)	48(3)	83(4)	-18(3)	-18(3)	14(2)
C(13)	76(4)	52(3)	46(3)	-11(2)	-32(3)	-2(3)
C(14)	25(2)	25(2)	41(2)	-12(2)	-7(2)	-2(2)
C(15)	48(3)	32(2)	42(2)	-10(2)	-11(2)	6(2)
C(16)	28(2)	37(2)	51(3)	-24(2)	-1(2)	-2(2)
C(17)	59(3)	31(2)	72(3)	-8(2)	-24(3)	12(2)
C(18)	32(2)	47(3)	81(4)	-40(3)	-5(2)	3(2)
C(19)	38(3)	32(2)	114(5)	-35(3)	-24(3)	10(2)
C(20)	33(2)	20(2)	28(2)	-8(2)	-1(2)	-2(2)

C(21)	42(2)	38(2)	28(2)	-11(2)	-7(2)	0(2)
C(22)	34(2)	33(2)	37(2)	-17(2)	-2(2)	0(2)
C(23)	38(2)	48(3)	55(3)	-28(2)	9(2)	-4(2)
C(24)	62(3)	51(3)	30(2)	-17(2)	-8(2)	3(2)
C(25)	57(3)	52(3)	39(3)	-23(2)	4(2)	1(2)
C(26)	31(2)	29(2)	23(2)	-7(2)	-4(2)	-4(2)
C(27)	38(2)	30(2)	34(2)	-13(2)	2(2)	-8(2)
C(28)	36(2)	35(2)	46(2)	-20(2)	0(2)	-8(2)
C(29)	34(2)	45(3)	55(3)	-21(2)	7(2)	-10(2)
C(30)	51(3)	29(2)	46(3)	-16(2)	-2(2)	-12(2)
C(31)	44(3)	38(2)	42(2)	-13(2)	2(2)	-20(2)
C(32)	17(2)	25(2)	25(2)	-6(2)	-1(1)	-2(1)
C(33)	27(2)	24(2)	29(2)	-6(2)	-4(2)	-3(2)
C(34)	25(2)	30(2)	28(2)	-13(2)	-2(2)	-2(2)
C(35)	27(2)	24(2)	40(2)	-13(2)	-1(2)	-2(2)
C(36)	20(2)	22(2)	36(2)	-6(2)	-5(2)	3(1)
C(37)	21(2)	25(2)	32(2)	-7(2)	-6(2)	0(1)
C(38)	69(3)	30(2)	38(2)	-13(2)	-9(2)	-7(2)
C(39)	35(2)	28(2)	41(2)	-5(2)	-8(2)	0(2)
C(40)	27(2)	18(2)	24(2)	-8(1)	-4(2)	-4(1)
C(41)	26(2)	25(2)	30(2)	-11(2)	-3(2)	-1(2)
C(42)	27(2)	28(2)	35(2)	-14(2)	4(2)	-9(2)
C(43)	20(2)	33(2)	49(2)	-22(2)	-1(2)	-4(2)
C(44)	25(2)	29(2)	35(2)	-16(2)	-7(2)	3(2)
C(45)	25(2)	23(2)	28(2)	-9(2)	-4(2)	1(2)
C(46)	35(2)	43(3)	40(2)	-11(2)	4(2)	-11(2)
C(47)	30(2)	41(2)	54(3)	-24(2)	-11(2)	13(2)
C(48)	23(2)	22(2)	26(2)	-7(2)	-5(2)	0(1)
C(49)	27(2)	25(2)	33(2)	-9(2)	0(2)	-2(2)
C(50)	43(2)	21(2)	50(3)	-10(2)	-7(2)	-1(2)
C(51)	42(2)	29(2)	35(2)	-2(2)	2(2)	-8(2)
C(52)	34(2)	34(2)	25(2)	-9(2)	1(2)	-3(2)
C(53)	28(2)	25(2)	23(2)	-8(2)	-2(2)	0(2)
C(54)	57(3)	34(3)	74(4)	-16(3)	3(3)	-11(2)
C(55)	42(3)	56(3)	28(2)	-9(2)	6(2)	-14(2)
C(56)	22(2)	22(2)	24(2)	-4(2)	0(1)	-5(1)
C(57)	28(2)	38(2)	31(2)	-14(2)	-6(2)	3(2)
C(58)	29(2)	57(3)	39(2)	-18(2)	-13(2)	6(2)
C(59)	34(2)	50(3)	36(2)	-16(2)	-19(2)	0(2)
C(60)	34(2)	27(2)	26(2)	-9(2)	-5(2)	-5(2)
C(61)	23(2)	22(2)	27(2)	-5(2)	-2(2)	-3(1)
C(62)	63(3)	130(5)	71(4)	-63(4)	-31(3)	32(3)
C(63)	54(3)	37(2)	34(2)	-16(2)	-14(2)	6(2)
B(1)	24(2)	28(2)	27(2)	-14(2)	-3(2)	-1(2)
B(2)	23(2)	20(2)	22(2)	-5(2)	-3(2)	-1(2)

Table 6.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **13**

	x	y	z	U(eq)
H(1)	1361	-836	-1285	72
H(2)	-520	-835	-1398	72
H(3)	-899	585	-2566	62
H(4)	2174	603	-2410	58
H(5)	767	1485	-3212	59
H(8)	420	-4336	-776	46
H(9A)	-1041	-3355	-571	73
H(9B)	-1335	-4481	-514	73
H(9C)	-1527	-3512	-1256	73
H(10A)	-356	-4231	-2134	72
H(10B)	-274	-5252	-1407	72
H(10C)	752	-4677	-1882	72
H(11)	1857	-2217	-1572	50
H(12A)	2047	-4382	-1107	89
H(12B)	2968	-3614	-1196	89
H(12C)	2448	-3587	-1924	89
H(13A)	859	-2508	-396	86
H(13B)	2036	-2861	-299	86
H(13C)	1157	-3699	-141	86
H(15)	-1929	-632	-4449	50
H(16)	-2323	-1053	-2227	44
H(17)	-2831	919	-4728	67
H(18)	-3206	510	-2506	59
H(19)	-3459	1489	-3759	70
H(21)	-1944	-2395	-4418	44
H(22)	741	-2487	-3494	40
H(23)	1639	-2782	-4526	54
H(24)	-1038	-2734	-5416	56
H(25)	750	-2901	-5482	58
H(27)	-1550	-4235	-3098	41
H(28)	-3470	-2427	-2286	45
H(29)	-4674	-3757	-1810	53
H(30)	-2778	-5548	-2617	50
H(31)	-4333	-5294	-1997	50
H(33)	3907	2496	-3821	33
H(35)	4221	-583	-3240	36
H(37)	4469	745	-1699	32
H(41)	2767	1795	-1206	32
H(43)	-117	2693	-1764	39
H(45)	2355	3805	-3288	31
H(49)	3484	4863	-2917	34
H(51)	5738	6295	-4547	46
H(53)	5713	3204	-3575	30
H(57)	5977	2086	-2075	38
H(59)	6198	2681	-179	47
H(61)	3593	3393	-1227	30

7. Details of the crystal structure of $[H_2N^iPr_2]^+[BAr^f_4]^-$ (10)

Table 7.1 Crystal data and structure refinement for **10**

Empirical formula	C152 H112 B4 F96 N4	
Formula weight	3861.70	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 22.3190(4) Å	α= 90°.
	b = 16.0297(5) Å	β= 133.2110(10)°.
	c = 15.4055(5) Å	γ = 90°.
Volume	4017.04(19) Å^3	
Z	1	
Density (calculated)	1.596 Mg/m^3	
Absorption coefficient	0.171 mm^{-1}	
F(000)	1936	
Crystal size	0.25 x 0.23 x 0.23 mm^3	
Theta range for data collection	3.11 to 27.48°.	
Index ranges	-28<=h<=26, -20<=k<=20, -19<=l<=19	
Reflections collected	15523	
Independent reflections	4562 [R(int) = 0.0874]	
Completeness to theta = 27.48°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9617 and 0.9585	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4562 / 18 / 292	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0714, wR2 = 0.1763	
R indices (all data)	R1 = 0.0964, wR2 = 0.1917	
Largest diff. peak and hole	0.569 and -0.362 e.Å^{-3}	
CSD deposit number	282084	

Table 7.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **10**

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	10000	3552(3)	2500	52(1)
C(17)	10638(2)	3981(2)	3623(4)	58(1)
C(19)	11058(3)	3395(3)	4668(4)	71(1)
C(18)	11230(3)	4370(4)	3570(5)	93(2)
C(1)	9317(1)	1780(2)	6311(2)	24(1)
C(2)	8499(2)	1525(2)	5398(2)	24(1)
C(3)	7934(2)	1978(2)	4347(2)	27(1)
C(4)	8158(2)	2713(2)	4164(2)	31(1)
C(5)	8965(2)	2987(2)	5059(2)	30(1)
C(6)	9525(2)	2535(2)	6104(2)	27(1)
C(7)	7077(2)	1647(2)	3393(2)	32(1)
C(8)	9214(2)	3773(2)	4856(3)	45(1)
C(9)	10485(1)	631(2)	7256(2)	23(1)
C(10)	10662(2)	938(2)	6597(2)	25(1)
C(11)	11116(2)	481(2)	6441(2)	27(1)
C(12)	11386(2)	-319(2)	6897(2)	32(1)
C(13)	11216(2)	-640(2)	7541(2)	30(1)
C(14)	10795(2)	-165(2)	7740(2)	27(1)
C(15)	11316(2)	874(2)	5783(2)	31(1)
C(16)	11458(2)	-1511(2)	8008(3)	40(1)
B(1)	10000	1204(3)	7500	23(1)
F(1)	7040(1)	984(2)	2839(2)	65(1)
F(2)	6743(1)	1402(2)	3803(2)	57(1)
F(3)	6560(1)	2204(2)	2545(2)	74(1)
F(4)	9918(1)	4083(2)	5814(2)	83(1)
F(5)	9292(2)	3668(2)	4073(3)	94(1)
F(6)	8668(2)	4380(1)	4386(3)	82(1)
F(7)	11866(1)	1480(2)	6392(2)	70(1)
F(8)	11608(2)	335(1)	5496(2)	65(1)
F(9)	10665(1)	1222(2)	4757(2)	56(1)
F(10)	11926(2)	-1879(1)	7886(2)	67(1)
F(11)	11862(2)	-1568(1)	9161(2)	62(1)
F(12)	10797(1)	-2010(1)	7462(2)	81(1)

Table7.3 Bond lengths [Å] and angles [°] for **10**

N(1)-C(17)#1	1.455(4)
N(1)-C(17)	1.455(4)
N(1)-H(1A)	0.9200
N(1)-H(1B)	0.9200
C(17)-C(19)	1.512(6)
C(17)-C(18)	1.513(6)
C(17)-H(17)	1.0000
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(1)-C(2)	1.400(3)
C(1)-C(6)	1.409(4)
C(1)-B(1)	1.645(3)
C(2)-C(3)	1.395(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.381(4)
C(3)-C(7)	1.500(4)
C(4)-C(5)	1.392(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.387(4)
C(5)-C(8)	1.494(4)
C(6)-H(6)	0.9500
C(7)-F(2)	1.324(3)
C(7)-F(1)	1.329(3)
C(7)-F(3)	1.331(3)
C(8)-F(4)	1.311(4)
C(8)-F(6)	1.321(4)
C(8)-F(5)	1.341(4)
C(9)-C(14)	1.398(4)
C(9)-C(10)	1.407(3)
C(9)-B(1)	1.647(3)
C(10)-C(11)	1.396(3)
C(10)-H(10)	0.9500
C(11)-C(12)	1.387(4)
C(11)-C(15)	1.498(4)
C(12)-C(13)	1.382(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.396(4)
C(13)-C(16)	1.493(4)
C(14)-H(14)	0.9500
C(15)-F(7)	1.324(3)
C(15)-F(8)	1.327(3)
C(15)-F(9)	1.332(3)
C(16)-F(10)	1.321(4)
C(16)-F(11)	1.334(4)
C(16)-F(12)	1.351(4)
B(1)-C(1)#2	1.645(3)
B(1)-C(9)#2	1.647(3)
C(17)#1-N(1)-C(17)	123.7(4)
C(17)#1-N(1)-H(1A)	106.4
C(17)-N(1)-H(1A)	106.4
C(17)#1-N(1)-H(1B)	106.4
C(17)-N(1)-H(1B)	106.4

H(1A)-N(1)-H(1B)	106.5
N(1)-C(17)-C(19)	111.2(3)
N(1)-C(17)-C(18)	108.1(3)
C(19)-C(17)-C(18)	112.7(4)
N(1)-C(17)-H(17)	108.2
C(19)-C(17)-H(17)	108.2
C(18)-C(17)-H(17)	108.2
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(2)-C(1)-C(6)	115.3(2)
C(2)-C(1)-B(1)	122.2(2)
C(6)-C(1)-B(1)	122.4(2)
C(3)-C(2)-C(1)	122.4(2)
C(3)-C(2)-H(2)	118.8
C(1)-C(2)-H(2)	118.8
C(4)-C(3)-C(2)	121.0(2)
C(4)-C(3)-C(7)	119.9(2)
C(2)-C(3)-C(7)	119.0(2)
C(3)-C(4)-C(5)	118.1(2)
C(3)-C(4)-H(4)	121.0
C(5)-C(4)-H(4)	121.0
C(6)-C(5)-C(4)	120.7(3)
C(6)-C(5)-C(8)	121.0(3)
C(4)-C(5)-C(8)	118.3(3)
C(5)-C(6)-C(1)	122.5(2)
C(5)-C(6)-H(6)	118.7
C(1)-C(6)-H(6)	118.7
F(2)-C(7)-F(1)	105.1(3)
F(2)-C(7)-F(3)	105.8(2)
F(1)-C(7)-F(3)	106.0(2)
F(2)-C(7)-C(3)	113.2(2)
F(1)-C(7)-C(3)	112.9(2)
F(3)-C(7)-C(3)	113.0(2)
F(4)-C(8)-F(6)	106.4(3)
F(4)-C(8)-F(5)	105.6(3)
F(6)-C(8)-F(5)	103.8(3)
F(4)-C(8)-C(5)	114.5(3)
F(6)-C(8)-C(5)	113.5(3)
F(5)-C(8)-C(5)	112.2(3)
C(14)-C(9)-C(10)	114.9(2)
C(14)-C(9)-B(1)	123.4(2)
C(10)-C(9)-B(1)	121.5(2)
C(11)-C(10)-C(9)	122.4(2)
C(11)-C(10)-H(10)	118.8
C(9)-C(10)-H(10)	118.8
C(12)-C(11)-C(10)	120.9(2)
C(12)-C(11)-C(15)	120.2(2)
C(10)-C(11)-C(15)	118.9(2)
C(13)-C(12)-C(11)	118.0(2)
C(13)-C(12)-H(12)	121.0

C(11)-C(12)-H(12)	121.0
C(12)-C(13)-C(14)	120.7(3)
C(12)-C(13)-C(16)	120.6(2)
C(14)-C(13)-C(16)	118.7(2)
C(13)-C(14)-C(9)	122.9(2)
C(13)-C(14)-H(14)	118.5
C(9)-C(14)-H(14)	118.5
F(7)-C(15)-F(8)	106.5(2)
F(7)-C(15)-F(9)	105.2(3)
F(8)-C(15)-F(9)	105.2(2)
F(7)-C(15)-C(11)	113.0(2)
F(8)-C(15)-C(11)	113.2(2)
F(9)-C(15)-C(11)	113.0(2)
F(10)-C(16)-F(11)	106.2(3)
F(10)-C(16)-F(12)	106.3(3)
F(11)-C(16)-F(12)	104.1(3)
F(10)-C(16)-C(13)	114.1(3)
F(11)-C(16)-C(13)	113.4(3)
F(12)-C(16)-C(13)	112.0(2)
C(1)#2-B(1)-C(1)	111.8(3)
C(1)#2-B(1)-C(9)	108.27(12)
C(1)-B(1)-C(9)	108.20(11)
C(1)#2-B(1)-C(9)#2	108.20(11)
C(1)-B(1)-C(9)#2	108.27(12)
C(9)-B(1)-C(9)#2	112.2(3)

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

Table 7.4 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **10**

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}
N(1)	29(2)	70(3)	49(2)	0	25(2)	0
C(17)	62(2)	42(2)	64(2)	-5(2)	40(2)	2(2)
C(19)	67(3)	76(3)	60(3)	11(2)	40(2)	10(2)
C(18)	77(3)	92(4)	75(3)	-1(3)	38(3)	-39(3)
C(1)	23(1)	30(1)	22(1)	-1(1)	17(1)	2(1)
C(2)	23(1)	28(1)	24(1)	0(1)	17(1)	1(1)
C(3)	22(1)	36(2)	22(1)	0(1)	14(1)	4(1)
C(4)	29(1)	36(2)	25(1)	7(1)	17(1)	9(1)
C(5)	31(1)	31(1)	30(1)	1(1)	22(1)	1(1)
C(6)	23(1)	31(1)	26(1)	0(1)	17(1)	1(1)
C(7)	24(1)	38(2)	27(1)	1(1)	15(1)	5(1)
C(8)	43(2)	40(2)	44(2)	9(1)	27(2)	1(1)
C(9)	20(1)	29(1)	19(1)	-2(1)	13(1)	-2(1)
C(10)	24(1)	26(1)	24(1)	-1(1)	17(1)	-1(1)
C(11)	24(1)	37(2)	23(1)	-4(1)	17(1)	-2(1)
C(12)	29(1)	40(2)	32(1)	-1(1)	23(1)	4(1)
C(13)	28(1)	33(1)	29(1)	2(1)	19(1)	3(1)
C(14)	26(1)	34(1)	23(1)	1(1)	17(1)	0(1)
C(15)	32(1)	39(2)	29(1)	-4(1)	23(1)	-2(1)
C(16)	42(2)	39(2)	43(2)	6(1)	31(2)	8(1)
B(1)	22(2)	27(2)	21(2)	0	14(2)	0
F(1)	30(1)	87(2)	57(1)	-44(1)	23(1)	-10(1)
F(2)	39(1)	90(2)	46(1)	-17(1)	31(1)	-22(1)
F(3)	25(1)	72(2)	61(1)	27(1)	5(1)	4(1)
F(4)	62(1)	60(1)	67(2)	19(1)	20(1)	-25(1)
F(5)	153(3)	81(2)	115(2)	-1(2)	117(2)	-26(2)
F(6)	70(2)	44(1)	111(2)	33(1)	54(2)	14(1)
F(7)	80(2)	99(2)	50(1)	-32(1)	51(1)	-57(1)
F(8)	110(2)	57(1)	88(2)	17(1)	91(2)	25(1)
F(9)	48(1)	83(2)	45(1)	25(1)	35(1)	12(1)
F(10)	95(2)	53(1)	91(2)	28(1)	79(2)	38(1)
F(11)	87(2)	54(1)	50(1)	21(1)	48(1)	28(1)
F(12)	58(1)	41(1)	102(2)	19(1)	38(1)	-2(1)

Table 7.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **10**

	x	y	z	U(eq)
H(1A)	10266	3209	2377	62
H(1B)	9734	3209	2623	62
H(17)	10374	4439	3702	70
H(19A)	10642	3111	4609	107
H(19B)	11426	3714	5411	107
H(19C)	11376	2980	4659	107
H(18A)	11491	3930	3484	140
H(18B)	11652	4683	4305	140
H(18C)	10930	4749	2887	140
H(2)	8323	1025	5498	29
H(4)	7773	3021	3448	37
H(6)	10069	2741	6703	32
H(10)	10466	1475	6244	30
H(12)	11679	-638	6770	39
H(14)	10716	-392	8224	32