Supporting Information:

Preparation and Structural characterization of Transition Metal Complexes Featuring the Cymantrenyl(bromo)boryl Ligand

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Experimental Section

1. General considerations

All manipulations were conducted either under an atmosphere of dry argon or *in vacuo* using standard Schlenk line or glove-box techniques. Solvents (toluene, benzene and hexane) were purified by distillation from appropriate drying agents (sodium and sodium wire) under dry argon, immediately prior to use. Deuterated solvent (C_6D_6) were degassed by three freeze-pump-thaw cycles and stored over molecular sieves in the glove-box. NMR: Bruker DRX 300 at 300.13 MHz (^{1}H, internal standard TMS), 75.47MHz (^{13}C{^{1}H}, APT, internal standard TMS), Bruker Avance 500 at 500.13 MHz (^{1}H, internal standard TMS), 160.46 MHz (^{11}B, $BF_3{\cdot}OEt_2$ in C_6D_6 as external standard) and 125.76MHz (^{13}C{^{1}H}, APT, internal standard TMS). IR spectra for compounds **3** and **4** were recorded as toluene solutions between KBr plates on a Bruker Vector 22 FT-IR-spectrometer. Microanalyses for C, H and N were performed by Mr C. P. Kneis (University of Wuerzburg) on a Leco CHNS-932 instrument.

2. Synthetic procedures

[(η^5-C_5H_5)$(OC)_2$Fe{B(Br)Cym}] (3). K[(η^5-C_5H_5)Fe$(CO)_2$] (0.53 g, 2.45 mmol) was suspended in toluene (10 mL) and a solution of cymantrenyl(dibromo)borane (**1**) (0.92 g, 2.45 mmol) in toluene (10 mL) was added. After stirring for 30 min, all volatiles were removed *in vacuo* and the residue was treated with hexane (20 mL). The remaining solid was removed by centrifugation. The dark red solution was concentrated *in vacuo* to 10 mL and stored at –30 °C for 2 days, yielding **3** as a dark red solid (0.39 g, 34 %). ^{1}H NMR (C_6D_6): δ 5.13 (m, 2H, C_5H_4B), 4.23 (m, 2H, C_5H_4B), 4.18 (s, 5H, C_5H_5); ^{13}C{^{1}H} NMR (C_6D_6): δ 224.8 (CO), 214.6 (CO), 95.0 (C_5H_4B), 86.44 (C_5H_4B), 85.9 (C_5H_5); ^{11}B{^{1}H} NMR (C_6D_6): δ 102.2 (br, s). IR ν(C=O) 2045 (w), 2025 (bm), 1999 (ws), 1940 (b) cm^{-1}. Anal. Calcd for $C_{15}H_9BBrFeMnO_5$: C, 38.27; H, 1.93. Found: C, 38.65; H, 2.28.

[(η^5-C_5Me_5)$(OC)_2$Fe{B(Br)Cym}] (4). Na[(η^5-C_5Me_5)Fe$(CO)_2$] (0.63 g, 2.33 mmol) were suspended in toluene (10 mL) and a solution of cymantrenyl(dibromo)borane (**1**) (0.87 g, 2.33 mmol) in toluene (10 mL) was added. After stirring for 30 min, all volatiles were removed *in vacuo* and the residue was treated with hexane (20 mL). The remaining solid was removed by centrifugation. The dark red solution was concentrated *in vacuo* to 10 mL and stored at –30 °C for 2 days, yielding **4** as a red crystalline solid (0.58 g, 46 %). ^{1}H NMR (C_6D_6): δ 5.21 (m, 2H, C_5H_4B), 4.22 (m, 2H, C_5H_4B), 1.42 (s, 15H, C_5Me_5); $^{13}C\{^1H\}$ NMR (C_6D_6): δ 224.8 (CO), 216.4 (CO), 96.5 (C_5Me_5), 94.1 (C_5H_4B), 86.2 (C_5H_4B), 9.9 (C_5Me_5) ; $^{11}B\{^1H\}$ NMR (C_6D_6): δ 106.1 (br, s). IR ν(C=O) 2022 (bm), 1976 (bw), 1922 (bs) cm^{-1}. Anal. Calcd for $C_{20}H_{19}BBrFeMnO_5$: C, 44.41; H, 3.54. Found: C, 44.09; H, 3.77.

General Procedure for X-ray Crystallography.

X-ray structure determination of compounds **2** and **4**:

A crystal of appropriate size was mounted on a glass fiber with silicone grease. The crystal was transferred to a Bruker SMART APEX diffractometer with CCD area detector, centered in the beam, and cooled by a nitrogen flow low-temperature apparatus to an appropriate temperature. Preliminary orientation matrix and cell constants were determined by collection of 100 frames, followed by spot integration and least-squares refinement. A hemisphere of data was collected [1]. The raw data were integrated with SAINT [2]. Cell dimensions were calculated from all reflections. Data analysis was performed with XPREP [3]. The data were corrected for Lorentz and polarization effects and an empirical absorption correction based on comparison of redundant and equivalent reflections was applied with SADABS [4]. The structures were solved via direct methods and refined with the SHELX software package and expanded using Fourier techniques [5]. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were assigned idealized positions and were included in structure factor calculations.

Crystallographic data for the structural analyses have been deposited with the Cambridge Crystallographic Data Centre, CCDC, with codes CCDC 605601 and CCDC 605602. Copies of this information may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge, CB2 1EZ [fax +44-1223-336033 or e-mail deposit@ccdc.cam.ac.uk or http://www.ccdc.cam.ac.uk]. This material is available free of charge via the Internet at http://pubs.acs.org.

[1] *SMART NT ver.5.63,* Area-Detector Software Package; Bruker Advanced *X*-ray Solutions, Inc.: Madison, WI, 1997-2001.

[2] *Saint+ NT ver. 6.45,* Area-Detector Integration Program; Bruker Advanced *X*-ray Solutions, Inc.: Madison, WI, 1997-2003.

[3] *XPREP ver. 6.10,* Part of the SHELXTL Crystal Structure Determination Package; Bruker Advanced *X*-ray Solutions, Inc.: Madison, WI, 1997-2001.

[4] Sheldrick, G. *SADABS ver. 2.10,* Area Detector Absorption Correction Program; 2002.

[5] Sheldrick, G. *SHELXS-97*: structure solution and *SHELXL*-97: structure refinement programs; 1997.

Table 1. Crystal data and structure refinement for [{(η^5-C_5H_3Me)$Mn(CO)_3$}BBr_2] (**2**).

Identification code	fs035	
Empirical formula	C9 H6 B Br2 Mn O3	
Formula weight	387.71	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 10.0066(7) Å	α = 90°
	b = 10.5736(8) Å	β = 90°
	c = 22.9813(17) Å	γ = 90°
Volume	2431.6(3) $Å^3$	
Z	8	
Density (calculated)	2.118 Mg/m^3	
Absorption coefficient	7.643 mm^{-1}	
F(000)	1472	

Crystal size	0.32 x 0.14 x 0.12 mm
θ range for data collection	2.70 to 26.12°
Index ranges	-12<=h<=12, -13<=k<=13, -28<=l<=28
Reflections collected	27308
Independent reflections	2413 [R_{int} = 0.0403]
Completeness to θ = 26.12°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.40 and 0.19476
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2413 / 0 / 145
Goodness-of-fit on F^2	S = 1.062
R indices [for 2039 reflections with I>2σ(I)]	R_1 = 0.0290, wR_2 = 0.0626
R indices (for all 2413 data)	R_1 = 0.0389, wR_2 = 0.0659
Largest diff. peak and hole	0.869 and -0.348 eÅ^{-3}

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

	x	y	z	U(eq)
Br(1)	1598(1)	3296(1)	2867(1)	44(1)
Mn(1)	4793(1)	2838(1)	3966(1)	24(1)
Br(2)	644(1)	2498(1)	4176(1)	45(1)
O(3)	4765(3)	4985(2)	3147(1)	43(1)
O(2)	3503(2)	4262(2)	4915(1)	41(1)
O(1)	7502(2)	3431(2)	4380(1)	45(1)
C(11)	3239(3)	1667(3)	3665(1)	29(1)
C(12)	4367(3)	1558(3)	3276(1)	31(1)
C(14)	5059(3)	857(3)	4167(2)	35(1)
C(15)	3713(3)	1202(3)	4217(1)	32(1)
C(1)	6442(3)	3220(3)	4222(1)	31(1)
C(3)	4777(3)	4160(3)	3469(1)	29(1)
B(1)	1975(4)	2412(3)	3578(2)	30(1)
C(2)	4020(3)	3726(3)	4546(1)	29(1)
C(13)	5465(3)	1066(3)	3577(1)	33(1)
C(16)	6814(4)	722(4)	3333(2)	48(1)

Table 3. Bond lengths [Å] and angles [°] for **2**.

Br(1)-B(1)	1.920(4)
Mn(1)-C(1)	1.797(3)
Mn(1)-C(2)	1.804(3)
Mn(1)-C(3)	1.806(3)
Mn(1)-C(11)	2.104(3)
Mn(1)-C(15)	2.119(3)
Mn(1)-C(12)	2.129(3)
Mn(1)-C(14)	2.161(3)
Mn(1)-C(13)	2.182(3)
Br(2)-B(1)	1.915(4)
O(3)-C(3)	1.144(4)
O(2)-C(2)	1.143(4)
O(1)-C(1)	1.143(4)
C(11)-C(15)	1.440(4)
C(11)-C(12)	1.445(4)
C(11)-B(1)	1.504(5)
C(12)-C(13)	1.399(4)
C(14)-C(15)	1.400(5)
C(14)-C(13)	1.431(4)
C(13)-C(16)	1.507(4)
C(1)-Mn(1)-C(2)	92.02(13)
C(1)-Mn(1)-C(3)	92.37(14)
C(2)-Mn(1)-C(3)	93.50(13)
C(1)-Mn(1)-C(11)	156.61(13)
C(2)-Mn(1)-C(11)	103.42(13)
C(3)-Mn(1)-C(11)	103.93(13)
C(1)-Mn(1)-C(15)	124.24(14)
C(2)-Mn(1)-C(15)	90.29(13)
C(3)-Mn(1)-C(15)	143.05(13)
C(11)-Mn(1)-C(15)	39.86(12)
C(1)-Mn(1)-C(12)	124.78(13)
C(2)-Mn(1)-C(12)	142.70(13)
C(3)-Mn(1)-C(12)	91.05(13)
C(11)-Mn(1)-C(12)	39.92(11)
C(15)-Mn(1)-C(12)	65.27(12)

C(1)-Mn(1)-C(14)	92.02(14)
C(2)-Mn(1)-C(14)	113.56(13)
C(3)-Mn(1)-C(14)	152.40(13)
C(11)-Mn(1)-C(14)	65.83(13)
C(15)-Mn(1)-C(14)	38.18(12)
C(12)-Mn(1)-C(14)	64.35(13)
C(1)-Mn(1)-C(13)	92.53(13)
C(2)-Mn(1)-C(13)	151.81(13)
C(3)-Mn(1)-C(13)	114.08(13)
C(11)-Mn(1)-C(13)	65.65(12)
C(15)-Mn(1)-C(13)	64.40(12)
C(12)-Mn(1)-C(13)	37.85(12)
C(14)-Mn(1)-C(13)	38.47(12)
C(15)-C(11)-C(12)	105.1(3)
C(15)-C(11)-B(1)	125.0(3)
C(12)-C(11)-B(1)	128.0(3)
C(15)-C(11)-Mn(1)	70.62(17)
C(12)-C(11)-Mn(1)	70.94(17)
B(1)-C(11)-Mn(1)	110.9(2)
C(13)-C(12)-C(11)	109.6(3)
C(13)-C(12)-Mn(1)	73.13(18)
C(11)-C(12)-Mn(1)	69.14(17)
C(15)-C(14)-C(13)	108.1(3)
C(15)-C(14)-Mn(1)	69.29(17)
C(13)-C(14)-Mn(1)	71.54(17)
C(14)-C(15)-C(11)	109.4(3)
C(14)-C(15)-Mn(1)	72.54(18)
C(11)-C(15)-Mn(1)	69.52(16)
O(1)-C(1)-Mn(1)	178.1(3)
O(3)-C(3)-Mn(1)	179.0(3)
C(11)-B(1)-Br(2)	120.9(3)
C(11)-B(1)-Br(1)	122.3(2)
Br(2)-B(1)-Br(1)	116.80(19)
O(2)-C(2)-Mn(1)	178.1(3)
C(12)-C(13)-C(14)	107.7(3)
C(12)-C(13)-C(16)	127.5(3)
C(14)-C(13)-C(16)	124.7(3)
C(12)-C(13)-Mn(1)	69.02(17)

C(14)-C(13)-Mn(1)	69.98(17)
C(16)-C(13)-Mn(1)	129.5(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2**.

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}
Br(1)	48(1)	46(1)	40(1)	0(1)	-13(1)	3(1)
Mn(1)	22(1)	23(1)	26(1)	0(1)	2(1)	2(1)
Br(2)	30(1)	47(1)	57(1)	-3(1)	13(1)	3(1)
O(3)	54(2)	33(1)	41(1)	8(1)	4(1)	0(1)
O(2)	43(1)	44(1)	37(1)	-11(1)	3(1)	11(1)
O(1)	25(1)	57(2)	52(1)	-7(1)	-3(1)	2(1)
C(11)	29(2)	23(1)	35(2)	-5(1)	4(1)	-6(1)
C(12)	36(2)	24(2)	31(2)	-6(1)	4(1)	-1(1)
C(14)	38(2)	24(2)	42(2)	5(1)	3(1)	6(1)
C(15)	37(2)	24(2)	36(2)	3(1)	8(1)	-1(1)
C(1)	29(2)	33(2)	31(2)	-3(1)	4(1)	5(1)
C(3)	28(2)	29(2)	31(2)	-3(1)	1(1)	0(1)
B(1)	31(2)	27(2)	34(2)	-5(1)	2(1)	-7(2)
C(2)	27(2)	27(2)	33(2)	1(1)	-3(1)	1(1)
C(13)	36(2)	22(2)	41(2)	-1(1)	7(1)	5(1)
C(16)	45(2)	47(2)	53(2)	4(2)	15(2)	20(2)

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

	x	y	z	U(eq)
H(12A)	4358	1781	2853	37
H(14A)	5630	505	4485	42
H(15A)	3161	1121	4578	39
H(16A)	6794	-151	3191	72
H(16B)	7493	802	3639	72
H(16C)	7033	1293	3011	72

Table 1. Crystal data and structure refinement for [(η^5-C_5Me_5)$(OC)_2$Fe{B(Cym)Br}] (**4**).

Identification code	fs026	
Empirical formula	C20 H19 B Br Fe Mn O5	
Formula weight	540.86	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 8.5509(10) Å	α = 90°
	b = 15.5135(19) Å	β = 90°
	c = 32.237(4) Å	γ = 90°
Volume	4276.4(9) $Å^3$	
Z	8	
Density (calculated)	1.680 Mg/m^3	
Absorption coefficient	3.165 mm^{-1}	
F(000)	2160	
Crystal size	0.26 x 0.20 x 0.18 mm	
θ range for data collection	1.26 to 26.08°	
Index ranges	-10<=h<=10, -19<=k<=19, -39<=l<=39	
Reflections collected	51603	
Independent reflections	4226 [R_{int} = 0.0445]	
Completeness to θ = 26.08°	99.6 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.57 and 0.4494
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4226 / 0 / 262
Goodness-of-fit on F^2	S = 1.082
R indices [for 3633 reflections with $I>2\sigma(I)$]	$R_1 = 0.0430$, $wR_2 = 0.1175$
R indices (for all 4226 data)	$R_1 = 0.0511$, $wR_2 = 0.1227$
Largest diff. peak and hole	0.765 and -0.677 $eÅ^{-3}$

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

	x	y	z	U(eq)
Fe(1)	721(1)	5948(1)	1525(1)	28(1)
Br(1)	3309(1)	4315(1)	1703(1)	55(1)
Mn(1)	2448(1)	4003(1)	452(1)	33(1)
O(1)	671(3)	6594(2)	681(1)	44(1)
C(4)	4413(5)	3758(3)	617(1)	40(1)
C(1)	707(4)	6323(2)	1010(1)	31(1)
C(21)	18(5)	5730(3)	2140(1)	40(1)
O(2)	3771(4)	6632(2)	1727(1)	54(1)
C(22)	-769(4)	5135(2)	1876(1)	38(1)
C(24)	-1452(4)	6521(2)	1681(1)	35(1)
O(3)	3424(5)	5749(2)	211(1)	74(1)
B(1)	1651(5)	4832(3)	1353(1)	33(1)
C(15)	174(4)	4398(2)	648(1)	37(1)
C(23)	-1652(4)	5623(3)	1586(1)	36(1)
O(4)	5640(4)	3599(2)	725(1)	59(1)
C(3)	3025(5)	5069(3)	308(1)	48(1)
C(2)	2589(5)	6350(3)	1640(1)	38(1)
C(5)	2829(5)	3598(3)	-57(1)	52(1)
C(12)	1534(5)	3310(2)	963(1)	40(1)
C(11)	1135(4)	4212(2)	1006(1)	34(1)
C(25)	-431(5)	6588(2)	2019(1)	38(1)
C(14)	27(5)	3653(3)	407(1)	46(1)
C(30)	24(6)	7393(3)	2245(1)	57(1)
O(5)	3050(5)	3325(3)	-384(1)	81(1)
C(13)	863(5)	2976(3)	607(1)	49(1)
C(29)	-2271(5)	7257(3)	1466(1)	54(1)
C(26)	1027(6)	5509(4)	2507(1)	61(1)
C(27)	-840(6)	4180(3)	1941(2)	62(1)
C(28)	-2764(5)	5261(3)	1274(2)	57(1)

Table 3. Bond lengths [Å] and angles [°] for **4**.

Fe(1)-C(2)	1.755(4)
Fe(1)-C(1)	1.759(4)
Fe(1)-B(1)	1.983(4)
Fe(1)-C(21)	2.098(4)
Fe(1)-C(23)	2.100(4)
Fe(1)-C(25)	2.120(4)
Fe(1)-C(24)	2.120(4)
Fe(1)-C(22)	2.120(4)
Br(1)-B(1)	1.981(4)
Mn(1)-C(3)	1.787(4)
Mn(1)-C(5)	1.788(5)
Mn(1)-C(4)	1.804(4)
Mn(1)-C(12)	2.119(4)
Mn(1)-C(15)	2.134(4)
Mn(1)-C(11)	2.136(4)
Mn(1)-C(14)	2.144(4)
Mn(1)-C(13)	2.150(4)
O(1)-C(1)	1.140(4)
C(4)-O(4)	1.133(5)
C(21)-C(22)	1.423(5)
C(21)-C(25)	1.439(6)
C(21)-C(26)	1.504(6)
O(2)-C(2)	1.137(5)
C(22)-C(23)	1.422(6)
C(22)-C(27)	1.497(5)
C(24)-C(25)	1.400(5)
C(24)-C(23)	1.436(5)
C(24)-C(29)	1.509(6)
O(3)-C(3)	1.151(5)
B(1)-C(11)	1.539(6)
C(15)-C(14)	1.398(5)
C(15)-C(11)	1.447(5)
C(23)-C(28)	1.493(6)
C(5)-O(5)	1.150(5)
C(12)-C(13)	1.386(6)
C(12)-C(11)	1.448(5)

C(25)-C(30)	1.497(5)
C(14)-C(13)	1.425(6)

C(2)-Fe(1)-C(1)	95.03(16)
C(2)-Fe(1)-B(1)	90.25(18)
C(1)-Fe(1)-B(1)	91.57(16)
C(2)-Fe(1)-C(21)	96.80(16)
C(1)-Fe(1)-C(21)	160.46(16)
B(1)-Fe(1)-C(21)	103.84(16)
C(2)-Fe(1)-C(23)	160.97(17)
C(1)-Fe(1)-C(23)	99.24(16)
B(1)-Fe(1)-C(23)	101.81(16)
C(21)-Fe(1)-C(23)	66.21(16)
C(2)-Fe(1)-C(25)	95.60(17)
C(1)-Fe(1)-C(25)	123.38(16)
B(1)-Fe(1)-C(25)	143.67(16)
C(21)-Fe(1)-C(25)	39.89(15)
C(23)-Fe(1)-C(25)	66.00(14)
C(2)-Fe(1)-C(24)	126.76(17)
C(1)-Fe(1)-C(24)	94.51(15)
B(1)-Fe(1)-C(24)	141.59(16)
C(21)-Fe(1)-C(24)	65.95(15)
C(23)-Fe(1)-C(24)	39.79(14)
C(25)-Fe(1)-C(24)	38.57(15)
C(2)-Fe(1)-C(22)	130.21(16)
C(1)-Fe(1)-C(22)	134.19(16)
B(1)-Fe(1)-C(22)	82.64(16)
C(21)-Fe(1)-C(22)	39.44(15)
C(23)-Fe(1)-C(22)	39.40(16)
C(25)-Fe(1)-C(22)	66.31(14)
C(24)-Fe(1)-C(22)	66.19(15)
C(3)-Mn(1)-C(5)	92.1(2)
C(3)-Mn(1)-C(4)	90.83(19)
C(5)-Mn(1)-C(4)	91.53(18)
C(3)-Mn(1)-C(12)	140.74(17)
C(5)-Mn(1)-C(12)	127.1(2)
C(4)-Mn(1)-C(12)	90.37(17)
C(3)-Mn(1)-C(15)	93.65(17)

C(5)-Mn(1)-C(15)	122.64(17)
C(4)-Mn(1)-C(15)	145.27(16)
C(12)-Mn(1)-C(15)	65.11(15)
C(3)-Mn(1)-C(11)	102.87(16)
C(5)-Mn(1)-C(11)	156.60(19)
C(4)-Mn(1)-C(11)	105.94(16)
C(12)-Mn(1)-C(11)	39.78(13)
C(15)-Mn(1)-C(11)	39.61(14)
C(3)-Mn(1)-C(14)	118.91(19)
C(5)-Mn(1)-C(14)	91.41(19)
C(4)-Mn(1)-C(14)	149.98(18)
C(12)-Mn(1)-C(14)	64.43(17)
C(15)-Mn(1)-C(14)	38.15(14)
C(11)-Mn(1)-C(14)	65.67(15)
C(3)-Mn(1)-C(13)	156.95(18)
C(5)-Mn(1)-C(13)	93.8(2)
C(4)-Mn(1)-C(13)	111.23(17)
C(12)-Mn(1)-C(13)	37.87(16)
C(15)-Mn(1)-C(13)	64.52(15)
C(11)-Mn(1)-C(13)	65.60(15)
C(14)-Mn(1)-C(13)	38.75(16)
O(4)-C(4)-Mn(1)	179.1(4)
O(1)-C(1)-Fe(1)	177.4(3)
C(22)-C(21)-C(25)	108.2(3)
C(22)-C(21)-C(26)	126.3(4)
C(25)-C(21)-C(26)	125.3(4)
C(22)-C(21)-Fe(1)	71.1(2)
C(25)-C(21)-Fe(1)	70.9(2)
C(26)-C(21)-Fe(1)	128.0(3)
C(23)-C(22)-C(21)	107.4(3)
C(23)-C(22)-C(27)	126.7(4)
C(21)-C(22)-C(27)	125.3(4)
C(23)-C(22)-Fe(1)	69.5(2)
C(21)-C(22)-Fe(1)	69.4(2)
C(27)-C(22)-Fe(1)	133.4(3)
C(25)-C(24)-C(23)	108.2(3)
C(25)-C(24)-C(29)	126.2(4)
C(23)-C(24)-C(29)	125.5(4)

C(25)-C(24)-Fe(1)	70.7(2)
C(23)-C(24)-Fe(1)	69.3(2)
C(29)-C(24)-Fe(1)	128.0(3)
C(11)-B(1)-Br(1)	111.4(3)
C(11)-B(1)-Fe(1)	129.3(3)
Br(1)-B(1)-Fe(1)	118.7(2)
C(14)-C(15)-C(11)	109.3(3)
C(14)-C(15)-Mn(1)	71.3(2)
C(11)-C(15)-Mn(1)	70.2(2)
C(22)-C(23)-C(24)	108.2(3)
C(22)-C(23)-C(28)	125.5(4)
C(24)-C(23)-C(28)	125.8(4)
C(22)-C(23)-Fe(1)	71.1(2)
C(24)-C(23)-Fe(1)	70.9(2)
C(28)-C(23)-Fe(1)	130.0(3)
O(3)-C(3)-Mn(1)	178.6(4)
O(2)-C(2)-Fe(1)	177.1(4)
O(5)-C(5)-Mn(1)	178.6(5)
C(13)-C(12)-C(11)	110.0(4)
C(13)-C(12)-Mn(1)	72.3(2)
C(11)-C(12)-Mn(1)	70.7(2)
C(15)-C(11)-C(12)	104.5(3)
C(15)-C(11)-B(1)	128.2(3)
C(12)-C(11)-B(1)	127.3(3)
C(15)-C(11)-Mn(1)	70.1(2)
C(12)-C(11)-Mn(1)	69.5(2)
B(1)-C(11)-Mn(1)	123.5(3)
C(24)-C(25)-C(21)	107.9(3)
C(24)-C(25)-C(30)	127.0(4)
C(21)-C(25)-C(30)	124.8(4)
C(24)-C(25)-Fe(1)	70.7(2)
C(21)-C(25)-Fe(1)	69.2(2)
C(30)-C(25)-Fe(1)	129.5(3)
C(15)-C(14)-C(13)	108.2(4)
C(15)-C(14)-Mn(1)	70.5(2)
C(13)-C(14)-Mn(1)	70.9(2)
C(12)-C(13)-C(14)	107.9(3)
C(12)-C(13)-Mn(1)	69.8(2)

C(14)-C(13)-Mn(1) 70.4(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **4**.

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}
Fe(1)	30(1)	27(1)	27(1)	1(1)	2(1)	-7(1)
Br(1)	56(1)	57(1)	51(1)	7(1)	-11(1)	8(1)
Mn(1)	35(1)	31(1)	34(1)	-4(1)	-2(1)	3(1)
O(1)	58(2)	40(1)	33(1)	4(1)	4(1)	3(1)
C(4)	41(2)	41(2)	38(2)	1(2)	-1(2)	-5(2)
C(1)	32(2)	25(2)	34(2)	-2(1)	1(1)	-1(1)
C(21)	40(2)	48(2)	32(2)	5(2)	7(2)	-11(2)
O(2)	46(2)	60(2)	57(2)	10(2)	-10(1)	-22(2)
C(22)	41(2)	34(2)	40(2)	2(2)	13(2)	-8(2)
C(24)	37(2)	35(2)	33(2)	-3(1)	12(2)	-1(2)
O(3)	79(3)	47(2)	96(3)	19(2)	40(2)	5(2)
B(1)	32(2)	37(2)	31(2)	9(2)	-1(2)	-1(2)
C(15)	30(2)	36(2)	44(2)	-6(2)	-2(2)	1(2)
C(23)	30(2)	41(2)	38(2)	-10(2)	10(2)	-11(2)
O(4)	41(2)	67(2)	70(2)	8(2)	-14(2)	-2(2)
C(3)	49(2)	44(2)	50(2)	2(2)	14(2)	8(2)
C(2)	40(2)	41(2)	33(2)	9(2)	0(2)	-9(2)
C(5)	40(2)	65(3)	51(3)	-12(2)	-7(2)	18(2)
C(12)	44(2)	27(2)	50(2)	4(2)	4(2)	-2(2)
C(11)	33(2)	31(2)	38(2)	2(1)	3(2)	-1(1)
C(25)	44(2)	39(2)	31(2)	-5(2)	12(2)	-15(2)
C(14)	37(2)	48(2)	53(2)	-14(2)	-7(2)	-3(2)
C(30)	74(3)	50(2)	47(2)	-18(2)	18(2)	-28(2)
O(5)	68(2)	124(3)	51(2)	-38(2)	-7(2)	35(2)
C(13)	48(2)	31(2)	67(3)	-10(2)	2(2)	-7(2)
C(29)	49(2)	54(3)	58(3)	4(2)	16(2)	18(2)
C(26)	63(3)	91(4)	29(2)	14(2)	1(2)	-3(3)
C(27)	64(3)	37(2)	84(4)	8(2)	28(3)	-11(2)

C(28)	36(2)	78(3)	58(3)	-24(2)	4(2)	-12(2)

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

	x	y	z	U(eq)
H(15A)	-321	4967	585	44
H(12A)	2174	2972	1166	48
H(14A)	-588	3600	144	55
H(30A)	-758	7521	2458	85
H(30B)	79	7874	2048	85
H(30C)	1048	7312	2375	85
H(13A)	938	2366	509	59
H(29A)	-3257	7382	1608	80
H(29B)	-2487	7099	1177	80
H(29C)	-1601	7770	1472	80
H(26A)	369	5446	2754	92
H(26B)	1791	5970	2552	92
H(26C)	1577	4966	2453	92
H(27A)	-1703	4042	2129	93
H(27B)	148	3981	2061	93
H(27C)	-1010	3894	1674	93
H(28A)	-3793	5184	1403	86
H(28B)	-2376	4702	1176	86
H(28C)	-2854	5658	1039	86