Inorganic Chemistry
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OAc)(MeL)$_2$][BF$_4$]$_2$.2MeCN (**1b**).

EXPERIMENTAL DETAILS

A. CRYSTAL DATA

Empirical Formula	$Mn_2B_2F_8O_4N_8C_{34}H_{43}$
Formula Weight	910.6
Crystal Colour, Habit	dark green, irregular shaped
Crystal dimensions (mm)	0.5 x 0.2 x 0.15
Crystal System	Triclinic
Lattice Type	P
No. of reflections used for unit cell determination (2θ range)	25 reflections (16<2θ<24)
Lattice parameters (A^o, deg.)	a= 10.283(2), b= 13.874(5) c= 16.152(5), α= 65.74(3) β= 84.24(2), γ= 78.06(2)
Space Group	$P\bar{1}$ (No.2)
Z value	2
D_{calc} (mg/m^3)	1.34
F(000)	934
μ(MoK$_\alpha$)/mm	0.41
min/max transmission coeff.	0.9066/0.9068
Volume (A^{o3})	2055.094(1.169)

B. INTENSITY MEASUREMENTS

Diffractometer	Cad4Mach
Radiation	MoK (λ= 0.71073A^o)
Temperature (K)	293
Scan Type	θ - 2θ
Scan Rate	variable
Scan Width	1.0 + 0.35tan0
2θ range(deg)	2 - 50
No. of reflections measured (2<2θ<45)	7894
No. of unique reflections	7220
Corrections	L_p, decay, absorption(analytical)

C. STRUCTURE SOLUTION AND REFINEMENT

Structure Solution	Direct Method
Refinement	Full matrix, least squares
Function minimized	$\Sigma w(\|F_o\| - \|F_c\|)^2$
Anomalous dispersion	applied (for non H atoms)
No. of observations (I>3σ(I))	3738
No. of variables	413
Reflection/Parameter ratio	9.051
Residuals: R;R_w	11.2 ; 11.9
Goodness of fit indicator	3.364
Max shift/error in final cycle	0.3877×10^{-1}
Avg shift/error in final cycle	0.1356×10^{-2}
Maximum peak in final diff. map	1.61 ; near C(21)
Minimum peak in final diff. map	-0.92

Non-Hydrogen Positional, Isotropic Displacement and Site Occupation Parameter

	x/a	y/b	z/c		U	PP
Mn(1)	0.2765(2)	0.7924(2)	0.1531(1)	*	0.044(1)	
Mn(2)	0.2350(2)	0.9578(2)	0.1980(2)	*	0.050(1)	
O(1)	0.1367(8)	0.8694(7)	0.1857(6)	*	0.049(4)	
O(2)	0.3752(8)	0.8593(7)	0.1881(6)	*	0.053(5)	
O(3)	0.2718(9)	0.8935(8)	0.0275(6)	*	0.055(5)	
O(4)	0.240(1)	1.0430(8)	0.0505(7)	*	0.071(5)	
N(1)	0.298(1)	0.6710(9)	0.2744(9)	*	0.060(6)	
N(2)	0.452(1)	0.695(1)	0.1267(9)	*	0.063(6)	
N(3)	0.156(1)	0.7113(9)	0.1163(8)	*	0.052(6)	
N(4)	0.215(1)	0.889(1)	0.3490(9)	*	0.070(7)	
N(5)	0.063(1)	1.069(1)	0.204(1)	*	0.079(8)	
N(6)	0.356(1)	1.057(1)	0.2080(9)	*	0.078(7)	
N(7)	0.230(2)	0.427(2)	0.258(2)	*	0.154(7)	
N(8)	0.738(3)	0.916(2)	0.572(2)	*	0.173(9)	
C(1)	0.256(1)	0.995(1)	0.001(1)	*	0.056(7)	
C(2)	0.261(2)	1.057(2)	-0.099(1)	*	0.09(1)	
C(3)	0.204(2)	0.649(1)	0.342(1)	*	0.075(9)	
C(4)	0.233(2)	0.562(2)	0.424(1)	*	0.09(1)	
C(5)	0.355(3)	0.501(2)	0.439(1)	*	0.10(1)	
C(6)	0.451(2)	0.525(2)	0.369(2)	*	0.10(1)	
C(7)	0.422(2)	0.607(1)	0.292(1)	*	0.066(8)	
C(8)	0.519(1)	0.643(1)	0.216(1)	*	0.074(9)	
C(9)	0.539(2)	0.766(2)	0.059(1)	*	0.09(1)	
C(10)	0.430(2)	0.613(1)	0.099(1)	*	0.08(1)	
C(11)	0.334(2)	0.657(2)	0.025(1)	*	0.08(1)	
C(12)	0.193(1)	0.662(1)	0.060(1)	*	0.062(8)	
C(13)	0.108(2)	0.608(1)	0.040(1)	*	0.08(1)	
C(14)	-0.017(2)	0.608(2)	0.078(1)	*	0.10(1)	
C(15)	-0.054(1)	0.657(1)	0.135(1)	*	0.08(1)	
C(16)	0.031(1)	0.710(1)	0.153(1)	*	0.065(8)	
C(17)	0.304(2)	0.818(2)	0.412(2)	*	0.136(5)	
C(18)	0.263(2)	0.780(2)	0.505(2)	*	0.148(7)	
C(19)	0.134(2)	0.821(2)	0.517(2)	*	0.144(7)	
C(20)	0.039(3)	0.893(2)	0.459(2)	*	0.149(7)	
C(21)	0.085(2)	0.923(2)	0.372(2)	*	0.128(5)	
C(22)	-0.005(2)	0.999(2)	0.302(1)	*	0.119(4)	
C(23)	-0.029(2)	1.096(2)	0.132(2)	*	0.124(4)	
C(24)	0.087(3)	1.155(2)	0.217(2)	*	0.149(7)	
C(25)	0.202(3)	1.204(2)	0.154(2)	*	0.160(9)	
C(26)	0.329(3)	1.161(2)	0.190(2)	*	0.147(7)	
C(27)	0.420(2)	1.224(2)	0.195(2)	*	0.137(6)	
C(28)	0.532(2)	1.155(2)	0.228(2)	*	0.134(5)	
C(29)	0.576(2)	1.046(2)	0.266(2)	*	0.143(6)	
C(30)	0.478(2)	1.010(2)	0.240(1)	*	0.110(3)	
C(31)	0.140(3)	0.418(2)	0.305(2)	*	0.143(7)	
C(32)	0.026(2)	0.417(2)	0.362(2)	*	0.131(5)	
C(33)	0.664(3)	0.882(3)	0.552(2)	*	0.182(9)	
C(34)	0.571(3)	0.821(3)	0.551(2)	*	0.183(8)	
B(1)	0.24109	0.62411	-0.20810		0.1000	
B(2)	-0.22272	0.72864	0.35818		0.1000	
F(1)	0.260(2)	0.533(1)	-0.128(1)		0.172(6)	
F(2)	0.228(3)	0.731(2)	-0.240(2)		0.138(9)	0.5000
F(2a)	0.265(4)	0.601(3)	-0.284(3)		0.07(1)	0.2500
F(2b)	0.228(4)	0.559(4)	-0.254(3)		0.09(1)	0.2500
F(3)	0.348(5)	0.625(4)	-0.163(3)		0.25(2)	0.5000
F(3a)	0.384(4)	0.628(3)	-0.247(3)		0.09(1)	0.2500
F(3b)	0.335(5)	0.625(3)	-0.277(3)		0.08(1)	0.2500
F(4)	0.103(3)	0.628(2)	-0.197(2)		0.15(1)	0.5000

F(4a)	0.238(3)	0.703(2)	-0.174(2)	0.046(7)	0.2500
F(4b)	0.136(5)	0.667(4)	-0.266(4)	0.13(2)	0.2500
F(5)	-0.200(3)	0.714(3)	0.437(2)	0.33(2)	
F(6)	-0.237(4)	0.847(3)	0.325(3)	0.19(1)	0.5000
F(6a)	-0.134(4)	0.791(3)	0.313(3)	0.08(1)	0.2500
F(6b)	-0.180(5)	0.803(4)	0.283(3)	0.08(1)	0.2500
F(7)	-0.353(3)	0.740(2)	0.387(2)	0.113(9)	0.5000
F(7a)	-0.130(6)	0.631(5)	0.384(5)	0.13(2)	0.2500
F(7b)	-0.350(5)	0.727(4)	0.348(3)	0.10(2)	0.2500
F(8)	-0.218(4)	0.650(3)	0.330(3)	0.19(1)	0.5000
F(8a)	-0.229(4)	0.726(4)	0.277(3)	0.10(1)	0.2500
F(8b)	-0.125(5)	0.658(4)	0.420(3)	0.09(1)	0.2500

Bond Distances (Angstroms)

Mn1-O1	1.778(9)
Mn1-O2	1.77(1)
Mn1-O3	1.934(9)
Mn1-N1	1.99(1)
Mn1-N2	2.14(1)
Mn1-N3	2.11(1)
Mn2-O1	1.82(1)
Mn2-O2	1.813(9)
Mn2-O4	2.18(1)
Mn2-N4	2.23(1)
Mn2-N5	2.12(1)
Mn2-N6	2.10(2)
O3-C1	1.28(2)
O4-C1	1.21(2)
N1-C3	1.36(2)
N1-C7	1.38(2)
N2-C8	1.49(2)
N2-C9	1.50(2)
N2-C10	1.44(3)
N3-C12	1.32(2)
N3-C16	1.35(2)
N4-C17	1.36(2)
N4-C21	1.39(2)
N5-C22	1.65(2)
N5-C23	1.45(3)
N5-C24	1.36(4)
N6-C26	1.32(3)
N6-C30	1.34(2)
C1-C2	1.49(2)
C3-C4	1.38(2)
C4-C5	1.34(3)
C5-C6	1.41(3)
C6-C7	1.30(2)
C7-C8	1.49(2)
C10-C11	1.48(3)
C11-C12	1.51(2)
C12-C13	1.40(3)
C13-C14	1.37(3)
C14-C15	1.34(4)
C15-C16	1.37(3)
C17-C18	1.43(3)
C18-C19	1.36(3)
C19-C20	1.35(3)
C20-C21	1.36(3)
C21-C22	1.44(3)
C24-C25	1.54(4)
C25-C26	1.39(4)
C26-C27	1.43(4)
C27-C28	1.33(3)
C28-C29	1.37(3)
C29-C30	1.38(4)

B2-F5	1.25(4)
B2-F6	1.48(4)
B2-F6a	1.34(4)
B2-F6b	1.33(4)
B2-F7	1.38(3)
B2-F7a	1.41(6)
B2-F7b	1.34(5)
B2-F8	1.34(6)
B2-F8a	1.33(6)
B2-F8b	1.40(4)
F5-F8b	1.08(6)
F6-F6a	1.22(6)
F6-F6b	1.13(7)
F6a-F6b	.65(7)
F6b-F8a	1.30(9)
F7-F7b	.72(7)
F7a-F8	1.23(9)
F7a-F8b	.8(1)
F7b-F8	1.63(7)
F7b-F8a	1.61(7)
F8-F8a	1.05(6)
N8-C33	1.11(6)
C33-C34	1.41(6)
B1-F1	1.38(1)
B1-F2	1.34(3)
B1-F2a	1.38(5)
B1-F2b	1.41(6)
B1-F3	1.38(6)
B1-F3a	1.54(4)
B1-F3b	1.40(5)
B1-F4	1.40(3)
B1-F4a	1.41(4)
B1-F4b	1.37(5)
F1-F3	1.59(6)
F2-F4a	.98(4)
F2-F4b	1.61(8)
F2a-F2b	.74(6)
F2a-F3a	1.59(8)
F2a-F3b	.89(8)
F2a-F4b	1.53(7)
F2b-F3b	1.50(8)
F2b-F4b	1.55(7)
F3-F3a	1.36(8)
F3-F4a	1.36(5)
F3a-F3b	.75(8)
F4-F4b	1.08(6)
N7-C31	1.13(4)
C31-C32	1.41(4)

$[Mn_2(L)(MeCO_2)_2](BF_4)_2 \cdot 2MeCN$ (**1b**).

Bond Angles	(degrees)
Mn2-Mn1-O1	43.9(3)
Mn2-Mn1-O2	43.6(3)
Mn2-Mn1-O3	87.6(4)
Mn2-Mn1-N1	101.2(5)
Mn2-Mn1-N2	133.4(4)
Mn2-Mn1-N3	135.4(3)
O1-Mn1-N2	174.5(5)
O2-Mn1-N2	90.2(5)
O3-Mn1-N2	90.9(4)
N1-Mn1-N2	80.5(5)
N2-Mn1-N3	91.0(5)
Mn1-Mn2-O1	42.6(3)
Mn1-Mn2-O2	42.5(4)
Mn1-Mn2-O4	80.9(3)
Mn1-Mn2-N4	105.2(4)
Mn1-Mn2-N5	133.4(5)
Mn1-Mn2-N6	134.6(4)
O1-Mn2-O2	83.9(4)
O1-Mn2-O4	89.2(4)
O1-Mn2-N4	93.4(5)
O1-Mn2-N5	92.2(5)
O1-Mn2-N6	177.0(5)
O2-Mn2-O4	88.6(4)
O2-Mn2-N4	97.9(4)
O2-Mn2-N5	175.7(6)
O2-Mn2-N6	93.5(5)
O4-Mn2-N4	173.2(5)
O4-Mn2-N5	89.5(5)
O4-Mn2-N6	89.2(5)
N4-Mn2-N5	84.1(5)
N4-Mn2-N6	88.5(5)
N5-Mn2-N6	90.3(6)
O1-Mn1-O2	86.4(5)
O1-Mn1-O3	93.7(4)
O1-Mn1-N1	95.1(4)
O1-Mn1-N3	92.3(5)
O2-Mn1-O3	94.4(4)
O2-Mn1-N1	89.6(5)
O2-Mn1-N3	177.9(4)
O3-Mn1-N1	170.5(5)
O3-Mn1-N3	87.3(5)
N1-Mn1-N3	88.9(5)
O1-Mn2-O2	83.9(4)
O1-Mn2-N6	177.0(5)
O2-Mn2-N6	93.5(5)
Mn1-O1-Mn2	93.5(4)
Mn1-O2-Mn2	93.9(4)
Mn1-O3-C1	125(1)
Mn1-N1-C3	126.1(9)
Mn1-N1-C7	116.1(9)
C3-N1-C7	118(1)
C8-N2-C9	108(1)
C8-N2-C10	110(1)
C9-N2-C10	111(2)
Mn1-N3-C12	125(1)
Mn1-N3-C16	117(1)
C12-N3-C16	119(2)
C17-N4-C21	122(2)
C22-N5-C23	108(1)
C22-N5-C24	104(2)
C23-N5-C24	115(2)
Mn2-N6-C26	130(2)
Mn2-N6-C30	117(1)
C26-N6-C30	113(2)
O3-C1-O4	125(1)
O3-C1-C2	115(2)
O4-C1-C2	119(2)
N1-C3-C4	120(2)
C3-C4-C5	120(2)
C4-C5-C6	119(2)
C5-C6-C7	120(2)
N1-C7-C6	123(2)
N1-C7-C8	113(1)
C6-C7-C8	124(2)
N2-C8-C7	111(1)
N2-C10-C11	112(1)
C10-C11-C12	111(1)
N3-C12-C11	118(2)
N3-C12-C13	122(1)
C11-C12-C13	120(2)
C12-C13-C14	118(2)
C13-C14-C15	119(2)
C14-C15-C16	121(2)
N3-C16-C15	121(2)
N4-C17-C18	118(2)
C17-C18-C19	112(2)
C18-C19-C20	134(2)
C19-C20-C21	110(2)
N4-C21-C20	123(2)
N4-C21-C22	120(2)
C20-C21-C22	117(2)
N5-C22-C21	116(1)
N5-C24-C25	112(2)
C24-C25-C26	116(2)
N6-C26-C25	109(3)
N6-C26-C27	126(2)
C25-C26-C27	124(2)
C26-C27-C28	106(2)
C27-C28-C29	139(3)
C28-C29-C30	101(2)
N6-C30-C29	133(2)

F6-F6b-F6a	82(7)
F6-F6b-F8a	118(5)
F6a-F6b-F8a	121(7)
B2-F7-F7b	72(4)
B2-F7a-F8	60(3)
B2-F7a-F8b	72(5)
F8-F7a-F8b	130(7)
B2-F7b-F7	77(5)
B2-F7b-F8	52(3)
B2-F7b-F8a	53(3)
F7-F7b-F8	119(5)
F7-F7b-F8a	129(7)
F8-F7b-F8a	38(2)
B2-F8-F7a	67(4)
B2-F8-F7b	53(3)
B2-F8-F8a	67(4)
F7a-F8-F7b	111(5)
F7a-F8-F8a	114(6)
F7b-F8-F8a	70(4)
B2-F8a-F6b	61(4)
B2-F8a-F7b	53(3)
B2-F8a-F8	67(4)
F6b-F8a-F7b	96(5)
F6b-F8a-F8	121(6)
F7b-F8a-F8	72(4)
B2-F8b-F5	59(3)
B2-F8b-F7a	74(5)
F5-F8b-F7a	128(7)
N8-C33-C34	166(3)
F1-B1-F2	142(2)
F1-B1-F2a	112(2)
F1-B1-F2b	89(2)
F1-B1-F3	70(2)
F1-B1-F3a	102(2)
F1-B1-F3b	115(2)
F1-B1-F4	89(1)
F1-B1-F4a	100(1)
F1-B1-F4b	130(2)
F2-B1-F2a	105(2)
F2-B1-F2b	130(2)
F2-B1-F3	84(2)
F2-B1-F3a	85(2)
F2-B1-F3b	89(2)
F2-B1-F4	93(2)
F2-B1-F4a	42(2)
F2-B1-F4b	73(3)
F2a-B1-F2b	31(3)
F2a-B1-F3	119(3)
F2a-B1-F3a	66(3)
F2a-B1-F3b	37(3)
F2a-B1-F4	101(3)
F2a-B1-F4a	145(2)
F2a-B1-F4b	68(3)
F2b-B1-F3	130(3)
F2b-B1-F3a	89(3)
F2b-B1-F3b	64(3)
F2b-B1-F4	82(2)
F2b-B1-F4a	170(2)
F2b-B1-F4b	68(3)
F3-B1-F3a	55(3)
F3-B1-F3b	84(3)
F3-B1-F4	139(3)
F3-B1-F4a	58(2)
F3-B1-F4b	157(3)
F3a-B1-F3b	29(3)
F3a-B1-F4	165(2)
F3a-B1-F4a	95(2)
F3a-B1-F4b	120(3)
F3b-B1-F4	136(3)
F3b-B1-F4a	116(3)
F3b-B1-F4b	94(3)
F4-B1-F4a	93(2)
F4-B1-F4b	46(3)
F4a-B1-F4b	103(3)
B1-F1-F3	55(2)
B1-F2-F4a	73(2)
B1-F2-F4b	54(2)
F4a-F2-F4b	111(3)
B1-F2a-F2b	77(6)
B1-F2a-F3a	62(3)
B1-F2a-F3b	72(5)
B1-F2a-F4b	56(3)
F2b-F2a-F3a	121(6)
F2b-F2a-F3b	134(7)
F2b-F2a-F4b	77(5)
F3a-F2a-F3b	13(3)
F3a-F2a-F4b	108(5)
F3b-F2a-F4b	111(6)
B1-F2b-F2a	72(6)
B1-F2b-F3b	57(3)
B1-F2b-F4b	55(3)
F2a-F2b-F3b	26(5)
F2a-F2b-F4b	75(5)
F3b-F2b-F4b	83(4)
B1-F3-F1	55(2)
B1-F3-F3a	69(3)
B1-F3-F4a	62(3)
F1-F3-F3a	101(4)
F1-F3-F4a	92(3)
F3a-F3-F4a	106(4)
B1-F3a-F2a	52(2)
B1-F3a-F3	56(3)
B1-F3a-F3b	64(5)
F2a-F3a-F3	107(4)
F2a-F3a-F3b	16(4)
F3-F3a-F3b	121(6)
B1-F3b-F2a	70(4)
B1-F3b-F2b	58(3)
B1-F3b-F3a	87(6)
F2a-F3b-F2b	21(3)
F2a-F3b-F3a	151(7)
F2b-F3b-F3a	131(6)
B1-F4-F4b	65(3)
B1-F4a-F2	65(3)
B1-F4a-F3	60(3)
F2-F4a-F3	100(4)
B1-F4b-F2	53(3)
B1-F4b-F2a	57(3)
B1-F4b-F2b	58(3)
B1-F4b-F4	69(3)
F2-F4b-F2a	87(4)
F2-F4b-F2b	104(4)
F2-F4b-F4	93(5)
F2a-F4b-F2b	28(2)
F2a-F4b-F4	110(4)
F2b-F4b-F4	87(4)
N7-C31-C32	175(3)

F5-B2-F6	93(2)
F5-B2-F6a	100(3)
F5-B2-F6b	125(3)
F5-B2-F7	83(2)
F5-B2-F7a	80(4)
F5-B2-F7b	112(3)
F5-B2-F8	124(2)
F5-B2-F8a	169(3)
F5-B2-F8b	48(3)
F6-B2-F6a	51(2)
F6-B2-F6b	47(3)
F6-B2-F7	88(2)
F6-B2-F7a	144(3)
F6-B2-F7b	97(3)
F6-B2-F8	142(2)
F6-B2-F8a	96(3)
F6-B2-F8b	122(3)
F6a-B2-F6b	28(3)
F6a-B2-F7	139(2)
F6a-B2-F7a	95(3)
F6a-B2-F7b	136(3)
F6a-B2-F8	111(3)
F6a-B2-F8a	81(3)
F6a-B2-F8b	90(3)
F6b-B2-F7	122(2)
F6b-B2-F7a	110(3)
F6b-B2-F7b	109(3)
F6b-B2-F8	100(3)
F6b-B2-F8a	59(4)
F6b-B2-F8b	116(3)
F7-B2-F7a	126(3)
F7-B2-F7b	31(3)
F7-B2-F8	100(2)
F7-B2-F8a	104(2)
F7-B2-F8b	119(2)
F7a-B2-F7b	119(4)
F7a-B2-F8	53(4)
F7a-B2-F8a	89(4)
F7a-B2-F8b	34(4)
F7b-B2-F8	75(3)
F7b-B2-F8a	74(3)
F7b-B2-F8b	133(3)
F8-B2-F8a	46(3)
F8-B2-F8b	86(3)
F8a-B2-F8b	121(3)
B2-F5-F8b	73(4)
B2-F6-F6a	59(3)
B2-F6-F6b	60(3)
F6a-F6-F6b	32(4)
B2-F6a-F6	70(3)
B2-F6a-F6b	75(6)
F6-F6a-F6b	67(6)
B2-F6b-F6	73(3)
B2-F6b-F6a	76(5)
B2-F6b-F8a	61(3)

Dihedral Angles (degrees)

O2-Mn1-O1-Mn2	11.5(4)
O3-Mn1-O1-Mn2	-82.7(5)
N1-Mn1-O1-Mn2	100.8(5)
N3-Mn1-O1-Mn2	-170.2(4)
O1-Mn1-O2-Mn2	-11.6(4)
O3-Mn1-O2-Mn2	81.9(4)
N1-Mn1-O2-Mn2	-106.8(5)
N3-Mn1-O2-Mn2	-64(*)
O1-Mn1-O3-C1	45(1)
O2-Mn1-O3-C1	-42(1)
N1-Mn1-O3-C1	-157(3)
N3-Mn1-O3-C1	137(1)
O1-Mn1-N1-C3	19(2)
O1-Mn1-N1-C7	-158(1)
O2-Mn1-N1-C3	105(2)
O2-Mn1-N1-C7	-72(1)
O3-Mn1-N1-C3	-140(3)
O3-Mn1-N1-C7	43(4)
N3-Mn1-N1-C3	-73(2)
N3-Mn1-N1-C7	110(1)
O1-Mn1-N3-C12	159(1)
O1-Mn1-N3-C16	-21.3(9)
O2-Mn1-N3-C12	-149(*)
O2-Mn1-N3-C16	31(*)
O3-Mn1-N3-C12	65(1)
O3-Mn1-N3-C16	-114.9(9)
N1-Mn1-N3-C12	-106(1)
N1-Mn1-N3-C16	73.8(9)
O2-Mn2-O1-Mn1	-11.3(4)
N6-Mn2-O1-Mn1	20(8)
O1-Mn2-O2-Mn1	11.4(4)
N6-Mn2-O2-Mn1	-167.1(4)
O1-Mn2-N6-C26	126(8)
O1-Mn2-N6-C30	-56(8)
O2-Mn2-N6-C26	157(2)
O2-Mn2-N6-C30	-26(1)
Mn1-O3-C1-O4	0(2)
Mn1-O3-C1-C2	177(1)
Mn1-N1-C3-C4	-179(2)
C7-N1-C3-C4	-1(3)
Mn1-N1-C7-C6	180(2)
Mn1-N1-C7-C8	2(2)
C3-N1-C7-C6	2(3)
C3-N1-C7-C8	-176(2)
C9-N2-C8-C7	158(2)
C10-N2-C8-C7	-80(2)
C8-N2-C10-C11	165(1)
C9-N2-C10-C11	-75(2)
Mn1-N3-C12-C11	4(2)
Mn1-N3-C12-C13	179(1)
C16-N3-C12-C11	-176(1)
C16-N3-C12-C13	0(2)
Mn1-N3-C16-C15	-179(1)
C12-N3-C16-C15	1(2)
C21-N4-C17-C18	0(4)
C17-N4-C21-C20	3(4)
C17-N4-C21-C22	180(2)
C23-N5-C22-C21	151(2)
C24-N5-C22-C21	-86(3)
C22-N5-C24-C25	155(2)

Mn2-N6-C26-C25	-4(3)
Mn2-N6-C26-C27	-177(2)
C30-N6-C26-C25	178(2)
C30-N6-C26-C27	5(4)
Mn2-N6-C30-C29	-171(2)
C26-N6-C30-C29	7(3)
N1-C3-C4-C5	1(4)
C3-C4-C5-C6	-2(4)
C4-C5-C6-C7	2(4)
C5-C6-C7-N1	-3(4)
C5-C6-C7-C8	175(2)
N1-C7-C8-N2	-32(2)
C6-C7-C8-N2	150(2)
N2-C10-C11-C12	-84(2)
C10-C11-C12-N3	53(2)
C10-C11-C12-C13	-122(2)
N3-C12-C13-C14	0(2)
C11-C12-C13-C14	176(1)
C12-C13-C14-C15	-1(2)
C13-C14-C15-C16	2(2)
C14-C15-C16-N3	-2(2)
N4-C17-C18-C19	1(4)
C17-C18-C19-C20	-4(6)
C18-C19-C20-C21	5(6)
C19-C20-C21-N4	-4(4)
C19-C20-C21-C22	179(3)
N4-C21-C22-N5	-20(4)
C20-C21-C22-N5	157(3)
N5-C24-C25-C26	-89(3)
C24-C25-C26-N6	60(4)
C24-C25-C26-C27	-126(3)
N6-C26-C27-C28	-4(4)
C25-C26-C27-C28	-177(3)
C26-C27-C28-C29	-10(5)
C27-C28-C29-C30	18(5)
C28-C29-C30-N6	-16(3)
F6-B2-F5-F8b	-132(4)
F6a-B2-F5-F8b	-81(4)
F6b-B2-F5-F8b	-95(4)
F7-B2-F5-F8b	141(4)
F7a-B2-F5-F8b	12(4)
F7b-B2-F5-F8b	130(4)
F8-B2-F5-F8b	43(4)
F8a-B2-F5-F8b	9(*)
F8b-B2-F5-F8b	0(4)
F5-B2-F6-F6a	100(4)
F5-B2-F6-F6b	137(4)
F6a-B2-F6-F6a	0(4)
F6a-B2-F6-F6b	37(4)
F6b-B2-F6-F6a	-37(4)
F6b-B2-F6-F6b	0(4)
F7-B2-F6-F6a	-177(4)
F7-B2-F6-F6b	-140(4)
F7a-B2-F6-F6a	23(7)
F7a-B2-F6-F6b	61(7)
F7b-B2-F6-F6a	-148(4)
F7b-B2-F6-F6b	-110(4)
F8-B2-F6-F6a	-74(5)
F8-B2-F6-F6b	-36(5)
F8a-B2-F6-F6a	-73(4)
F8a-B2-F6-F6b	-35(4)
F8b-B2-F6-F6a	60(4)
F8b-B2-F6-F6b	97(4)

F5-B2-F6a-F6b	-156(6)
F6-B2-F6a-F6	0(3)
F6-B2-F6a-F6b	-70(6)
F6b-B2-F6a-F6	70(6)
F6b-B2-F6a-F6b	0(7)
F7-B2-F6a-F6	5(5)
F7-B2-F6a-F6b	-65(8)
F7a-B2-F6a-F6	-167(4)
F7a-B2-F6a-F6b	124(7)
F7b-B2-F6a-F6	51(6)
F7b-B2-F6a-F6b	-19(9)
F8-B2-F6a-F6	141(3)
F8-B2-F6a-F6b	71(7)
F8a-B2-F6a-F6	106(4)
F8a-B2-F6a-F6b	36(6)
F8b-B2-F6a-F6	-133(4)
F8b-B2-F6a-F6b	157(7)
F5-B2-F6b-F6	-56(4)
F5-B2-F6b-F6a	30(7)
F5-B2-F6b-F8a	167(3)
F6-B2-F6b-F6	0(3)
F6-B2-F6b-F6a	85(7)
F6-B2-F6b-F8a	-137(4)
F6a-B2-F6b-F6	-85(7)
F6a-B2-F6b-F6a	0(6)
F6a-B2-F6b-F8a	137(7)
F7-B2-F6b-F6	50(5)
F7-B2-F6b-F6a	135(6)
F7-B2-F6b-F8a	-88(4)
F7a-B2-F6b-F6	-147(4)
F7a-B2-F6b-F6a	-62(8)
F7a-B2-F6b-F8a	75(4)
F7b-B2-F6b-F6	81(4)
F7b-B2-F6b-F6a	166(6)
F7b-B2-F6b-F8a	-57(4)
F8-B2-F6b-F6	158(3)
F8-B2-F6b-F6a	-116(6)
F8-B2-F6b-F8a	21(3)
F8a-B2-F6b-F6	137(4)
F8a-B2-F6b-F6a	-137(7)
F8a-B2-F6b-F8a	0(3)
F8b-B2-F6b-F6	-111(4)
F8b-B2-F6b-F6a	-26(8)
F8b-B2-F6b-F8a	112(4)
F5-B2-F7-F7b	-159(4)
F6-B2-F7-F7b	107(4)
F6a-B2-F7-F7b	104(6)
F6b-B2-F7-F7b	73(5)
F7a-B2-F7-F7b	-87(6)
F7b-B2-F7-F7b	0(5)
F8-B2-F7-F7b	-36(4)
F8a-B2-F7-F7b	12(5)
F8b-B2-F7-F7b	-127(5)
F5-B2-F7a-F8	148(4)
F5-B2-F7a-F8b	-17(5)
F6-B2-F7a-F8	-131(5)
F6-B2-F7a-F8b	64(8)
F6a-B2-F7a-F8	-113(4)
F6a-B2-F7a-F8b	82(6)
F6b-B2-F7a-F8	-88(4)
F6b-B2-F7a-F8b	107(6)
F7-B2-F7a-F8	74(4)
F7-B2-F7a-F8b	-90(6)

F7b-B2-F7a-F8	39(5)
F7b-B2-F7a-F8b	-126(5)
F8-B2-F7a-F8	0(3)
F8-B2-F7a-F8b	-165(7)
F8a-B2-F7a-F8	-32(4)
F8a-B2-F7a-F8b	163(6)
F8b-B2-F7a-F8	165(7)
F8b-B2-F7a-F8b	0(5)
F5-B2-F7b-F7	22(5)
F5-B2-F7b-F8	-122(3)
F5-B2-F7b-F8a	-170(3)
F6-B2-F7b-F7	-74(4)
F6-B2-F7b-F8	143(2)
F6-B2-F7b-F8a	94(3)
F6a-B2-F7b-F7	-111(5)
F6a-B2-F7b-F8	105(5)
F6a-B2-F7b-F8a	57(5)
F6b-B2-F7b-F7	-121(4)
F6b-B2-F7b-F8	96(3)
F6b-B2-F7b-F8a	48(4)
F7-B2-F7b-F7	0(3)
F7-B2-F7b-F8	-144(4)
F7-B2-F7b-F8a	168(5)
F7a-B2-F7b-F7	112(5)
F7a-B2-F7b-F8	-31(4)
F7a-B2-F7b-F8a	-79(4)
F8-B2-F7b-F7	144(4)
F8-B2-F7b-F8	0(2)
F8-B2-F7b-F8a	-48(3)
F8a-B2-F7b-F7	-168(5)
F8a-B2-F7b-F8	48(3)
F8a-B2-F7b-F8a	0(3)
F8b-B2-F7b-F7	74(6)
F8b-B2-F7b-F8	-70(5)
F8b-B2-F7b-F8a	-118(5)
F5-B2-F8-F7a	-39(4)
F5-B2-F8-F7b	106(3)
F5-B2-F8-F8a	-171(3)
F6-B2-F8-F7a	133(4)
F6-B2-F8-F7b	-81(4)
F6-B2-F8-F8a	1(5)
F6a-B2-F8-F7a	80(4)
F6a-B2-F8-F7b	-135(3)
F6a-B2-F8-F8a	-52(4)
F6b-B2-F8-F7a	107(4)
F6b-B2-F8-F7b	-107(3)
F6b-B2-F8-F8a	-25(4)
F7-B2-F8-F7a	-128(3)
F7-B2-F8-F7b	18(2)
F7-B2-F8-F8a	100(3)
F7a-B2-F8-F7a	0(4)
F7a-B2-F8-F7b	145(4)
F7a-B2-F8-F8a	-132(5)
F7b-B2-F8-F7a	-145(4)
F7b-B2-F8-F7b	0(3)
F7b-B2-F8-F8a	82(4)
F8a-B2-F8-F7a	132(5)
F8a-B2-F8-F7b	-82(4)
F8a-B2-F8-F8a	0(4)
F8b-B2-F8-F7a	-8(4)
F8b-B2-F8-F7b	137(3)
F8b-B2-F8-F8a	-141(4)
F5-B2-F8a-F6b	-111(*)
F5-B2-F8a-F7b	123(*)

F5-B2-F8a-F8	39(*)
F6-B2-F8a-F6b	30(3)
F6-B2-F8a-F7b	-95(3)
F6-B2-F8a-F8	-179(3)
F6a-B2-F8a-F6b	-19(3)
F6a-B2-F8a-F7b	-144(3)
F6a-B2-F8a-F8	132(4)
F6b-B2-F8a-F6b	0(3)
F6b-B2-F8a-F7b	-125(3)
F6b-B2-F8a-F8	151(4)
F7-B2-F8a-F6b	119(3)
F7-B2-F8a-F7b	-6(3)
F7-B2-F8a-F8	-90(3)
F7a-B2-F8a-F6b	-114(4)
F7a-B2-F8a-F7b	120(3)
F7a-B2-F8a-F8	36(4)
F7b-B2-F8a-F6b	125(3)
F7b-B2-F8a-F7b	0(3)
F7b-B2-F8a-F8	-84(4)
F8-B2-F8a-F6b	-151(4)
F8-B2-F8a-F7b	84(4)
F8-B2-F8a-F8	0(4)
F8b-B2-F8a-F6b	-103(4)
F8b-B2-F8a-F7b	132(3)
F8b-B2-F8a-F8	48(5)
F5-B2-F8b-F5	0(3)
F5-B2-F8b-F7a	158(7)
F6-B2-F8b-F5	61(4)
F6-B2-F8b-F7a	-141(5)
F6a-B2-F8b-F5	103(4)
F6a-B2-F8b-F7a	-99(6)
F6b-B2-F8b-F5	115(4)
F6b-B2-F8b-F7a	-87(6)
F7-B2-F8b-F5	-46(4)
F7-B2-F8b-F7a	112(5)
F7a-B2-F8b-F5	-158(7)
F7a-B2-F8b-F7a	0(6)
F7b-B2-F8b-F5	-80(6)
F7b-B2-F8b-F7a	77(7)
F8-B2-F8b-F5	-145(4)
F8-B2-F8b-F7a	12(5)
F8a-B2-F8b-F5	-178(4)
F8a-B2-F8b-F7a	-20(7)
B2-F5-F8b-B2	-.0001(1)
B2-F5-F8b-F7a	-28(8)
B2-F6-F6a-B2	-.0001(1)
B2-F6-F6a-F6b	82(6)
F6b-F6-F6a-B2	-82(6)
F6b-F6-F6a-F6b	0(6)
B2-F6-F6b-B2	-.0001(2)
B2-F6-F6b-F6a	-78(5)
B2-F6-F6b-F8a	42(3)
F6a-F6-F6b-B2	78(5)
F6a-F6-F6b-F6a	0(5)
F6a-F6-F6b-F8a	120(7)
B2-F6a-F6b-B2	-.0001(0)
B2-F6a-F6b-F6	75(3)
B2-F6a-F6b-F8a	-43(6)
F6-F6a-F6b-B2	-75(3)
F6-F6a-F6b-F6	0(3)
F6-F6a-F6b-F8a	-118(7)
B2-F6b-F8a-B2	-.0001(0)
B2-F6b-F8a-F7b	41(2)
B2-F6b-F8a-F8	-31(5)

F6-F6b-F8a-B2	-47(4)
F6-F6b-F8a-F7b	-6(5)
F6-F6b-F8a-F8	-79(7)
F6a-F6b-F8a-B2	50(8)
F6a-F6b-F8a-F7b	91(8)
F6a-F6b-F8a-F8	18(*)
B2-F7-F7b-B2	-.0001(0)
B2-F7-F7b-F8	33(4)
B2-F7-F7b-F8a	-12(5)
B2-F7a-F8-B2	-.0001(0)
B2-F7a-F8-F7b	-29(3)
B2-F7a-F8-F8a	48(5)
F8b-F7a-F8-B2	19(8)
F8b-F7a-F8-F7b	-10(*)
F8b-F7a-F8-F8a	67(*)
B2-F7a-F8b-B2	-.0001(2)
B2-F7a-F8b-F5	24(7)
F8-F7a-F8b-B2	-17(7)
F8-F7a-F8b-F5	7(*)
B2-F7b-F8-B2	-.0001(0)
B2-F7b-F8-F7a	34(4)
B2-F7b-F8-F8a	-75(5)
F7-F7b-F8-B2	-42(6)
F7-F7b-F8-F7a	-8(8)
F7-F7b-F8-F8a	-117(8)
F8a-F7b-F8-B2	75(5)
F8a-F7b-F8-F7a	109(6)
F8a-F7b-F8-F8a	0(5)
B2-F7b-F8a-B2	-.0001(1)
B2-F7b-F8a-F6b	-46(3)
B2-F7b-F8a-F8	74(4)
F7-F7b-F8a-B2	15(6)
F7-F7b-F8a-F6b	-31(7)
F7-F7b-F8a-F8	89(8)
F8-F7b-F8a-B2	-74(4)
F8-F7b-F8a-F6b	-120(6)
F8-F7b-F8a-F8	0(4)
B2-F8-F8a-B2	-.0001(0)
B2-F8-F8a-F6b	30(5)
B2-F8-F8a-F7b	-57(3)
F7a-F8-F8a-B2	-48(5)
F7a-F8-F8a-F6b	-19(8)
F7a-F8-F8a-F7b	-105(6)
F7b-F8-F8a-B2	57(3)
F7b-F8-F8a-F6b	86(6)
F7b-F8-F8a-F7b	0(3)
F2-B1-F1-F3	51(3)
F2a-B1-F1-F3	-114(3)
F2b-B1-F1-F3	-134(3)
F3-B1-F1-F3	0(3)
F3a-B1-F1-F3	-46(3)
F3b-B1-F1-F3	-73(4)
F4-B1-F1-F3	144(3)
F4a-B1-F1-F3	51(3)
F4b-B1-F1-F3	167(4)
F1-B1-F2-F4a	0(3)
F1-B1-F2-F4b	134(3)
F2a-B1-F2-F4a	166(3)
F2a-B1-F2-F4b	-60(3)
F2b-B1-F2-F4a	-173(3)
F2b-B1-F2-F4b	-40(4)
F3-B1-F2-F4a	48(3)
F3-B1-F2-F4b	-179(3)
F3a-B1-F2-F4a	103(3)

F3a-B1-F2-F4b	-123(3)
F3b-B1-F2-F4a	132(3)
F3b-B1-F2-F4b	-95(3)
F4-B1-F2-F4a	-92(3)
F4-B1-F2-F4b	42(3)
F4a-B1-F2-F4a	0(2)
F4a-B1-F2-F4b	133(3)
F4b-B1-F2-F4a	-133(3)
F4b-B1-F2-F4b	0(4)
F1-B1-F2a-F2b	-42(5)
F1-B1-F2a-F3a	94(2)
F1-B1-F2a-F3b	103(3)
F1-B1-F2a-F4b	-126(3)
F2-B1-F2a-F2b	148(4)
F2-B1-F2a-F3a	-77(2)
F2-B1-F2a-F3b	-68(4)
F2-B1-F2a-F4b	64(3)
F2b-B1-F2a-F2b	0(5)
F2b-B1-F2a-F3a	136(5)
F2b-B1-F2a-F3b	145(6)
F2b-B1-F2a-F4b	-83(5)
F3-B1-F2a-F2b	-121(5)
F3-B1-F2a-F3a	14(3)
F3-B1-F2a-F3b	23(4)
F3-B1-F2a-F4b	155(3)
F3a-B1-F2a-F2b	-136(5)
F3a-B1-F2a-F3a	0(2)
F3a-B1-F2a-F3b	9(3)
F3a-B1-F2a-F4b	141(3)
F3b-B1-F2a-F2b	-145(6)
F3b-B1-F2a-F3a	-9(3)
F3b-B1-F2a-F3b	0(4)
F3b-B1-F2a-F4b	132(4)
F4-B1-F2a-F2b	52(5)
F4-B1-F2a-F3a	-173(2)
F4-B1-F2a-F3b	-164(3)
F4-B1-F2a-F4b	-32(3)
F4a-B1-F2a-F2b	163(4)
F4a-B1-F2a-F3a	-61(4)
F4a-B1-F2a-F3b	-52(5)
F4a-B1-F2a-F4b	80(4)
F4b-B1-F2a-F2b	83(5)
F4b-B1-F2a-F3a	-141(3)
F4b-B1-F2a-F3b	-132(4)
F4b-B1-F2a-F4b	0(4)
F1-B1-F2b-F2a	142(4)
F1-B1-F2b-F3b	119(2)
F1-B1-F2b-F4b	-135(3)
F2-B1-F2b-F2a	-42(5)
F2-B1-F2b-F3b	-65(3)
F2-B1-F2b-F4b	41(3)
F2a-B1-F2b-F2a	0(5)
F2a-B1-F2b-F3b	-23(4)
F2a-B1-F2b-F4b	84(5)
F3-B1-F2b-F2a	79(5)
F3-B1-F2b-F3b	56(4)
F3-B1-F2b-F4b	163(3)
F3a-B1-F2b-F2a	39(5)
F3a-B1-F2b-F3b	17(2)
F3a-B1-F2b-F4b	123(3)
F3b-B1-F2b-F2a	23(4)
F3b-B1-F2b-F3b	0(3)
F3b-B1-F2b-F4b	106(3)
F4-B1-F2b-F2a	-129(5)

F4-B1-F2b-F3b	-152(2)
F4-B1-F2b-F4b	-45(3)
F4a-B1-F2b-F2a	-70(*)
F4a-B1-F2b-F3b	-93(*)
F4a-B1-F2b-F4b	14(*)
F4b-B1-F2b-F2a	-84(5)
F4b-B1-F2b-F3b	-106(3)
F4b-B1-F2b-F4b	0(3)
F1-B1-F3-F1	0(1)
F1-B1-F3-F3a	-121(3)
F1-B1-F3-F4a	116(2)
F2-B1-F3-F1	-151(2)
F2-B1-F3-F3a	88(3)
F2-B1-F3-F4a	-35(2)
F2a-B1-F3-F1	105(2)
F2a-B1-F3-F3a	-16(4)
F2a-B1-F3-F4a	-139(2)
F2b-B1-F3-F1	71(3)
F2b-B1-F3-F3a	-51(4)
F2b-B1-F3-F4a	-174(3)
F3a-B1-F3-F1	121(3)
F3a-B1-F3-F3a	0(3)
F3a-B1-F3-F4a	-123(3)
F3b-B1-F3-F1	119(2)
F3b-B1-F3-F3a	-2(3)
F3b-B1-F3-F4a	-125(2)
F4-B1-F3-F1	-64(3)
F4-B1-F3-F3a	175(3)
F4-B1-F3-F4a	51(4)
F4a-B1-F3-F1	-116(2)
F4a-B1-F3-F3a	123(3)
F4a-B1-F3-F4a	0(2)
F4b-B1-F3-F1	-154(8)
F4b-B1-F3-F3a	85(9)
F4b-B1-F3-F4a	-39(9)
F1-B1-F3a-F2a	-109(2)
F1-B1-F3a-F3	55(3)
F1-B1-F3a-F3b	-121(4)
F2-B1-F3a-F2a	109(2)
F2-B1-F3a-F3	-86(3)
F2-B1-F3a-F3b	98(5)
F2a-B1-F3a-F2a	0(2)
F2a-B1-F3a-F3	165(3)
F2a-B1-F3a-F3b	-11(4)
F2b-B1-F3a-F2a	-21(2)
F2b-B1-F3a-F3	144(3)
F2b-B1-F3a-F3b	-32(5)
F3-B1-F3a-F2a	-165(3)
F3-B1-F3a-F3	0(3)
F3-B1-F3a-F3b	-176(6)
F3b-B1-F3a-F2a	11(4)
F3b-B1-F3a-F3	176(6)
F3b-B1-F3a-F3b	0(5)
F4-B1-F3a-F2a	29(9)
F4-B1-F3a-F3	-166(8)
F4-B1-F3a-F3b	18(*)
F4a-B1-F3a-F2a	150(2)
F4a-B1-F3a-F3	-46(3)
F4a-B1-F3a-F3b	138(5)
F4b-B1-F3a-F2a	42(4)
F4b-B1-F3a-F3	-153(4)
F4b-B1-F3a-F3b	31(6)
F1-B1-F3b-F2a	-94(4)
F1-B1-F3b-F2b	-75(3)

F1-B1-F3b-F3a	68(5)
F2-B1-F3b-F2a	117(4)
F2-B1-F3b-F2b	136(2)
F2-B1-F3b-F3a	-80(5)
F2a-B1-F3b-F2a	0(4)
F2a-B1-F3b-F2b	19(3)
F2a-B1-F3b-F3a	163(6)
F2b-B1-F3b-F2a	-19(3)
F2b-B1-F3b-F2b	0(2)
F2b-B1-F3b-F3a	144(5)
F3-B1-F3b-F2a	-160(4)
F3-B1-F3b-F2b	-141(3)
F3-B1-F3b-F3a	3(5)
F3a-B1-F3b-F2a	-163(6)
F3a-B1-F3b-F2b	-144(5)
F3a-B1-F3b-F3a	0(4)
F4-B1-F3b-F2a	24(5)
F4-B1-F3b-F2b	43(3)
F4-B1-F3b-F3a	-173(4)
F4a-B1-F3b-F2a	150(3)
F4a-B1-F3b-F2b	169(2)
F4a-B1-F3b-F3a	-47(5)
F4b-B1-F3b-F2a	44(4)
F4b-B1-F3b-F2b	63(3)
F4b-B1-F3b-F3a	-153(5)
F1-B1-F4-F4b	155(4)
F2-B1-F4-F4b	-63(5)
F2a-B1-F4-F4b	43(5)
F2b-B1-F4-F4b	67(5)
F3-B1-F4-F4b	-146(5)
F3a-B1-F4-F4b	16(*)
F3b-B1-F4-F4b	28(5)
F4a-B1-F4-F4b	-105(4)
F4b-B1-F4-F4b	0(6)
F1-B1-F4a-F2	-179(2)
F1-B1-F4a-F3	-60(2)
F2-B1-F4a-F2	0(3)
F2-B1-F4a-F3	120(3)
F2a-B1-F4a-F2	-23(5)
F2a-B1-F4a-F3	96(4)
F2b-B1-F4a-F2	32(*)
F2b-B1-F4a-F3	152(*)
F3-B1-F4a-F2	-120(3)
F3-B1-F4a-F3	0(3)
F3a-B1-F4a-F2	-76(3)
F3a-B1-F4a-F3	44(3)
F3b-B1-F4a-F2	-55(3)
F3b-B1-F4a-F3	64(3)
F4-B1-F4a-F2	91(2)
F4-B1-F4a-F3	-149(3)
F4b-B1-F4a-F2	46(3)
F4b-B1-F4a-F3	165(3)
F1-B1-F4b-F2	-144(2)
F1-B1-F4b-F2a	101(3)
F1-B1-F4b-F2b	68(4)
F1-B1-F4b-F4	-33(6)
F2-B1-F4b-F2	0(2)
F2-B1-F4b-F2a	-115(3)
F2-B1-F4b-F2b	-148(3)
F2-B1-F4b-F4	112(4)
F2a-B1-F4b-F2	115(3)
F2a-B1-F4b-F2a	0(3)
F2a-B1-F4b-F2b	-33(3)
F2a-B1-F4b-F4	-134(5)

F2b-B1-F4b-F2	148(3)
F2b-B1-F4b-F2a	33(3)
F2b-B1-F4b-F2b	0(3)
F2b-B1-F4b-F4	-101(4)
F3-B1-F4b-F2	3(9)
F3-B1-F4b-F2a	-111(8)
F3-B1-F4b-F2b	-145(8)
F3-B1-F4b-F4	115(7)
F3a-B1-F4b-F2	73(3)
F3a-B1-F4b-F2a	-41(4)
F3a-B1-F4b-F2b	-75(4)
F3a-B1-F4b-F4	-175(3)
F3b-B1-F4b-F2	88(3)
F3b-B1-F4b-F2a	-27(3)
F3b-B1-F4b-F2b	-60(3)
F3b-B1-F4b-F4	-161(4)
F4-B1-F4b-F2	-112(4)
F4-B1-F4b-F2a	134(5)
F4-B1-F4b-F2b	101(4)
F4-B1-F4b-F4	0(3)
F4a-B1-F4b-F2	-30(2)
F4a-B1-F4b-F2a	-144(2)
F4a-B1-F4b-F2b	-178(2)
F4a-B1-F4b-F4	82(4)
B1-F1-F3-B1	-.0001(3)
B1-F1-F3-F3a	54(3)
B1-F1-F3-F4a	-53(2)
B1-F2-F4a-B1	-.0001
B1-F2-F4a-F3	-50(3)
F4b-F2-F4a-B1	-39(3)
F4b-F2-F4a-F3	-89(4)
B1-F2-F4b-B1	-.0001(3)
B1-F2-F4b-F2a	49(2)
B1-F2-F4b-F2b	28(2)
B1-F2-F4b-F4	-60(3)
F4a-F2-F4b-B1	48(3)
F4a-F2-F4b-F2a	98(4)
F4a-F2-F4b-F2b	76(4)
F4a-F2-F4b-F4	-12(5)
B1-F2a-F2b-B1	-.0001
B1-F2a-F2b-F3b	49(9)
B1-F2a-F2b-F4b	-57(3)
F3a-F2a-F2b-B1	-46(5)
F3a-F2a-F2b-F3b	3(6)
F3a-F2a-F2b-F4b	-103(6)
F3b-F2a-F2b-B1	-49(9)
F3b-F2a-F2b-F3b	0(6)
F3b-F2a-F2b-F4b	-107(*)
F4b-F2a-F2b-B1	57(3)
F4b-F2a-F2b-F3b	107(*)
F4b-F2a-F2b-F4b	0(4)
B1-F2a-F3a-B1	-.0001(0)
B1-F2a-F3a-F3	-13(3)
B1-F2a-F3a-F3b	138(*)
F2b-F2a-F3a-B1	52(7)
F2b-F2a-F3a-F3	39(8)
F2b-F2a-F3a-F3b	-169(*)
F3b-F2a-F3a-B1	-138(*)
F3b-F2a-F3a-F3	-152(*)
F3b-F2a-F3a-F3b	0(*)
F4b-F2a-F3a-B1	-33(3)
F4b-F2a-F3a-F3	-47(4)
F4b-F2a-F3a-F3b	105(*)
B1-F2a-F3b-B1	-.0001(2)

B1-F2a-F3b-F2b	-51(*)
B1-F2a-F3b-F3a	-38(*)
F2b-F2a-F3b-B1	51(*)
F2b-F2a-F3b-F2b	0(8)
F2b-F2a-F3b-F3a	13(*)
F3a-F2a-F3b-B1	38(*)
F3a-F2a-F3b-F2b	-13(*)
F3a-F2a-F3b-F3a	0(*)
F4b-F2a-F3b-B1	-41(3)
F4b-F2a-F3b-F2b	-92(*)
F4b-F2a-F3b-F3a	-79(*)
B1-F2a-F4b-B1	-.0001(1)
B1-F2a-F4b-F2	-46(2)
B1-F2a-F4b-F2b	83(6)
B1-F2a-F4b-F4	46(5)
F2b-F2a-F4b-B1	-83(6)
F2b-F2a-F4b-F2	-129(6)
F2b-F2a-F4b-F2b	0(6)
F2b-F2a-F4b-F4	-37(8)
F3a-F2a-F4b-B1	36(3)
F3a-F2a-F4b-F2	-10(3)
F3a-F2a-F4b-F2b	119(6)
F3a-F2a-F4b-F4	82(6)
F3b-F2a-F4b-B1	49(4)
F3b-F2a-F4b-F2	3(5)
F3b-F2a-F4b-F2b	132(8)
F3b-F2a-F4b-F4	95(7)
B1-F2b-F3b-B1	-.0001
B1-F2b-F3b-F2a	121(*)
B1-F2b-F3b-F3a	-51(8)
F2a-F2b-F3b-B1	-121(*)
F2a-F2b-F3b-F2a	0(*)
F2a-F2b-F3b-F3a	-172(*)
F4b-F2b-F3b-B1	-52(3)
F4b-F2b-F3b-F2a	69(*)
F4b-F2b-F3b-F3a	-103(9)
B1-F2b-F4b-B1	-.0001(3)
B1-F2b-F4b-F2	-26(2)
B1-F2b-F4b-F2a	-79(6)
B1-F2b-F4b-F4	67(4)
F2a-F2b-F4b-B1	79(6)
F2a-F2b-F4b-F2	53(6)
F2a-F2b-F4b-F2a	0(6)
F2a-F2b-F4b-F4	146(7)
F3b-F2b-F4b-B1	54(3)
F3b-F2b-F4b-F2	28(4)
F3b-F2b-F4b-F2a	-25(5)
F3b-F2b-F4b-F4	121(5)
B1-F3-F3a-B1	-.0001(2)
B1-F3-F3a-F2a	13(3)
B1-F3-F3a-F3b	4(6)
F1-F3-F3a-B1	-45(2)
F1-F3-F3a-F2a	-33(4)
F1-F3-F3a-F3b	-41(7)
F4a-F3-F3a-B1	50(3)
F4a-F3-F3a-F2a	63(5)
F4a-F3-F3a-F3b	54(8)
B1-F3-F4a-B1	-.0001(3)
B1-F3-F4a-F2	53(3)
F1-F3-F4a-B1	47(2)
F1-F3-F4a-F2	101(4)
F3a-F3-F4a-B1	-54(4)
F3a-F3-F4a-F2	-1(5)
B1-F3a-F3b-B1	-.0001(3)

B1-F3a-F3b-F2a	36(*)
B1-F3a-F3b-F2b	42(6)
F2a-F3a-F3b-B1	-36(*)
F2a-F3a-F3b-F2a	0(9)
F2a-F3a-F3b-F2b	6(*)
F3-F3a-F3b-B1	-4(5)
F3-F3a-F3b-F2a	32(*)
F3-F3a-F3b-F2b	38(*)
B1-F4-F4b-B1	-.0001
B1-F4-F4b-F2	48(2)
B1-F4-F4b-F2a	-40(4)
B1-F4-F4b-F2b	-56(3)

Atomic Anisotropic Displacement Parameters

	U11	U22	U33	U12	U13	U23
Mn(1)	.032(1)	.049(1)	.062(1)	-.0134(9)	.006(1)	-.030(1)
Mn(2)	.042(1)	.051(1)	.071(2)	-.019(1)	.013(1)	-.036(1)
O(1)	.032(5)	.051(5)	.080(7)	-.014(4)	.008(4)	-.039(5)
O(2)	.035(5)	.060(6)	.083(7)	-.018(4)	.008(5)	-.044(6)
O(3)	.052(6)	.058(6)	.065(7)	-.021(5)	.006(5)	-.030(5)
O(4)	.082(8)	.062(7)	.079(8)	-.023(6)	.016(6)	-.037(6)
N(1)	.033(6)	.066(8)	.10(1)	-.012(6)	-.001(6)	-.051(8)
N(2)	.042(7)	.081(9)	.078(9)	-.013(6)	.019(7)	-.045(8)
N(3)	.038(6)	.063(8)	.066(8)	-.022(6)	.005(6)	-.032(7)
N(4)	.063(8)	.063(8)	.10(1)	-.022(7)	.003(7)	-.047(8)
N(5)	.055(8)	.068(9)	.14(1)	-.009(7)	-.005(8)	-.066(9)
N(6)	.10(1)	.08(1)	.076(9)	-.053(9)	.044(8)	-.056(8)
C(1)	.045(8)	.07(1)	.06(1)	-.027(7)	.008(7)	-.028(9)
C(2)	.10(1)	.09(1)	.09(1)	-.04(1)	-.00(1)	-.03(1)
C(3)	.09(1)	.08(1)	.08(1)	-.04(1)	.01(1)	-.05(1)
C(4)	.11(2)	.09(1)	.09(2)	-.05(1)	.01(1)	-.03(1)
C(5)	.13(2)	.08(1)	.07(1)	-.04(1)	-.03(1)	-.01(1)
C(6)	.11(2)	.09(1)	.10(2)	-.02(1)	-.03(1)	-.03(1)
C(7)	.08(1)	.06(1)	.07(1)	-.018(9)	-.018(9)	-.023(9)
C(8)	.042(9)	.08(1)	.09(1)	.005(8)	-.005(9)	-.04(1)
C(9)	.05(1)	.12(2)	.12(2)	-.04(1)	.04(1)	-.07(1)
C(10)	.06(1)	.09(1)	.12(2)	-.016(9)	.01(1)	-.07(1)
C(11)	.07(1)	.11(1)	.09(1)	-.02(1)	.01(1)	-.06(1)
C(12)	.07(1)	.06(1)	.07(1)	-.023(8)	.008(8)	-.036(9)
C(13)	.11(1)	.08(1)	.09(1)	-.04(1)	.00(1)	-.06(1)
C(14)	.09(1)	.11(2)	.12(2)	-.06(1)	-.00(1)	-.06(1)
C(15)	.046(9)	.10(1)	.11(2)	-.042(9)	.001(9)	-.05(1)
C(16)	.043(8)	.07(1)	.08(1)	-.022(8)	-.001(8)	-.029(9)

Table S7. Hydrogen atom coordinates of $[Mn^{III,IV}_2(\mu\text{-}O)_2(\mu\text{-}OAc)(MeL)_2]\,[BF_4]_2.2MeCN$ (**1b**).

Hydrogen Positional and Isotropic Displacement Parameters

	x/a	y/b	z/c	U
H(3)	0.1119	0.6909	0.3315	0.100
H(4)	0.1619	0.5486	0.4720	0.100
H(5)	0.3727	0.4402	0.4974	0.100
H(6)	0.5418	0.4777	0.3834	0.100
H(16)	0.0004	0.7410	0.2009	0.150
H(13)	0.1403	0.5708	-0.0009	0.150
H(14)	-0.0732	0.5673	0.0672	0.150
H(15)	-0.1416	0.6595	0.1596	0.150
H(17)	0.3934	0.7933	0.3921	0.150
H(18)	0.3246	0.7333	0.5496	0.150
H(19)	0.1152	0.7939	0.5864	0.150
H(20)	-0.0400	0.9046	0.4800	0.150
H(30)	0.4938	0.9287	0.2606	0.150
H(27)	0.3942	1.2993	0.1772	0.150
H(28)	0.5967	1.2014	0.2339	0.150
H(29)	0.6474	1.0184	0.2810	0.150
H(81)	0.5626	0.6965	0.2249	0.150
H(82)	0.5889	0.5854	0.2165	0.150
H(101)	0.3892	0.5600	0.1514	0.150
H(102)	0.5100	0.5784	0.0828	0.150
H(111)	0.3449	0.7304	-0.0183	0.150
H(112)	0.3467	0.6143	-0.0120	0.150
H(221)	-0.0629	0.9673	0.2818	0.150
H(222)	-0.0548	1.0550	0.3177	0.150
H(241)	0.1191	1.1314	0.2854	0.150
H(242)	0.0049	1.2091	0.2196	0.150
H(251)	0.1842	1.1902	0.1008	0.150
H(252)	0.1731	1.2834	0.1337	0.150
H(91)	0.5545	0.8216	0.0747	0.150
H(92)	0.6227	0.7240	0.0508	0.150
H(93)	0.4952	0.8004	-0.0006	0.150
H(231)	-0.0481	1.0317	0.1293	0.150
H(232)	-0.1119	1.1390	0.1399	0.150
H(233)	0.0115	1.1364	0.0743	0.150
H(21)	0.3473	1.0353	-0.1221	0.150
H(22)	0.1938	1.0425	-0.1268	0.150
H(23)	0.2485	1.1361	-0.1221	0.150
H(321)	0.0510	0.4733	0.3810	0.200
H(322)	-0.0318	0.4551	0.3140	0.200
H(323)	-0.0488	0.4141	0.4066	0.200
H(341)	0.4668	1.2016	0.3863	0.200
H(342)	0.3495	1.2617	0.4269	0.200
H(343)	0.4823	1.2384	0.4531	0.200

Table S8. Summary of plane calculations of $[Mn^{III,IV}_2(\mu\text{-}O)_2(\mu\text{-}OAc)(MeL)_2][BF_4]_2.2MeCN$ (**1b**).

PLANE NUMBER 1
==========

EQUATION OF PLANE AS AX+BY+CZ=D, XYZ IN FRACTIONAL AND ORTHOGONAL UNITS

A	B	C	D	ESDA	ESDB	ESDC	ESDD
-.3375	-5.2920	11.0732	-2.5912	.0612	.0757	.0694	.0770
.0312	-.7273	.6856	-2.5912	.0062	.0063	.0043	.0770

ATOM		DIST(A)	ESDD	X	Y	Z
Mn1	DEFINING	.0000	.0025	.2765	.7924	.1531
O1	DEFINING	.0000	.0141	.1367	.8694	.1857
O2	DEFINING	.0000	.0145	.3752	.8593	.1881

PLANE NUMBER 2
==========

EQUATION OF PLANE AS AX+BY+CZ=D, XYZ IN FRACTIONAL AND ORTHOGONAL UNITS

A	B	C	D	ESDA	ESDB	ESDC	ESDD
-.2133	-1.6953	13.8032	1.0597	.0611	.0776	.0473	.0867
-.0124	-.5192	.8546	1.0597	.0062	.0063	.0029	.0867

ANGLE BETWEEN PLANES/LINES 1 2 15.614 ESD .461

ATOM		DIST(A)	ESDD	X	Y	Z
Mn2	DEFINING	-.0000	.0026	.2350	.9578	.1980
O1	DEFINING	-.0000	.0141	.1367	.8694	.1857
O2	DEFINING	-.0000	.0145	.3752	.8593	.1881

PLANE NUMBER 3
==========

EQUATION OF PLANE AS AX+BY+CZ=D, XYZ IN FRACTIONAL AND ORTHOGONAL UNITS

A	B	C	D	ESDA	ESDB	ESDC	ESDD
10.2682	2.1626	1.4905	4.7801	.0011	.0211	.0452	.0177
.9873	.1294	.0923	4.7801	.0003	.0021	.0028	.0177

<CHI**2>	<GOODNESS OF FIT>	<N-3>
3.5092	1.3246	2

ANGLE BETWEEN PLANES/LINES 1 3 90.002 ESD .394

ANGLE BETWEEN PLANES/LINES 2 3 90.034 ESD .394

ATOM		DIST(A)	ESDD	X	Y	Z
Mn1	DEFINING	.0007	.0029	.2765	.7924	.1531
O3	DEFINING	-.0163	.0124	.2718	.8935	.0275
C1	DEFINING	.0003	.0198	.2558	.9953	.0012
O4	DEFINING	.0180	.0139	.2403	1.0430	.0505
Mn2	DEFINING	-.0007	.0031	.2350	.9578	.1980

PLANE NUMBER 4
==========

EQUATION OF PLANE AS AX+BY+CZ=D, XYZ IN FRACTIONAL AND ORTHOGONAL UNITS

A	B	C	D	ESDA	ESDB	ESDC	ESDD
4.9069	12.3340	11.0725	12.7823	.0829	.0568	.1030	.0063
.2937	.6662	.6855	12.7823	.0083	.0053	.0064	.0063

<CHI**2>	<GOODNESS OF FIT>	<N-3>
.5792	.4394	3

ANGLE BETWEEN PLANES/LINES 1 4 90.309 ESD .606

ANGLE BETWEEN PLANES/LINES 2 4 76.330 ESD .595

ANGLE BETWEEN PLANES/LINES 3 4 63.931 ESD .530

ATOM		DIST(A)	ESDD	X	Y	Z
N1	DEFINING	-.0049	.0169	.2982	.6710	.2744
C3	DEFINING	.0045	.0230	.2041	.6486	.3419
C4	DEFINING	-.0022	.0281	.2331	.5625	.4244
C5	DEFINING	.0055	.0310	.3546	.5015	.4391
C6	DEFINING	-.0135	.0294	.4510	.5247	.3689
C7	DEFINING	.0097	.0213	.4222	.6068	.2923

PLANE NUMBER 5
==========

EQUATION OF PLANE AS AX+BY+CZ=D, XYZ IN FRACTIONAL AND ORTHOGONAL UNITS

A	B	C	D	ESDA	ESDB	ESDC	ESDD
2.5519	-7.1690	8.0797	-3.7648	.0764	.0698	.1090	.0730
.3495	-.7922	.5002	-3.7648	.0077	.0077	.0067	.0730

<CHI**2>	<GOODNESS OF FIT>	<N-3>
.2615	.2952	3

ANGLE BETWEEN PLANES/LINES 1 5 21.556 ESD .560

ANGLE BETWEEN PLANES/LINES 2 5 33.444 ESD .561

ANGLE BETWEEN PLANES/LINES 3 5 73.218 ESD .478

ANGLE BETWEEN PLANES/LINES 4 5 94.713 ESD .664

ATOM		DIST(A)	ESDD	X	Y	Z
N3	DEFINING	.0025	.0146	.1555	.7113	.1163
C12	DEFINING	-.0021	.0190	.1928	.6621	.0604
C13	DEFINING	.0016	.0236	.1084	.6081	.0396
C14	DEFINING	-.0046	.0268	-.0170	.6079	.0782
C15	DEFINING	.0074	.0245	-.0536	.6572	.1350
C16	DEFINING	-.0061	.0199	.0314	.7100	.1534

PLANE NUMBER 6
==========

EQUATION OF PLANE AS AX+BY+CZ=D, XYZ IN FRACTIONAL AND ORTHOGONAL UNITS

A	B	C	D	ESDA	ESDB	ESDC	ESDD
5.0080	13.2012	7.5928	15.4538	.1002	.0486	.1438	.0541
.2951	.8318	.4701	15.4538	.0100	.0056	.0089	.0541

<CHI**2>	<GOODNESS OF FIT>	<N-3>
.8902	.5447	3

ANGLE BETWEEN PLANES/LINES 1 6 105.875 ESD .686

ANGLE BETWEEN PLANES/LINES 2 6 91.937 ESD .670

ANGLE BETWEEN PLANES/LINES 3 6 63.744 ESD .644

ANGLE BETWEEN PLANES/LINES 4 6 15.619 ESD .756

ANGLE BETWEEN PLANES/LINES 5 6 108.704 ESD .758

ATOM		DIST(A)	ESDD	X	Y	Z
N4	DEFINING	.0014	.0177	.2148	.8885	.3490
C17	DEFINING	.0017	.0298	.3045	.8182	.4121
C18	DEFINING	.0042	.0347	.2630	.7805	.5054
C19	DEFINING	-.0169	.0338	.1339	.8215	.5165
C20	DEFINING	.0220	.0345	.0391	.8934	.4591
C21	DEFINING	-.0138	.0300	.0855	.9232	.3721

PLANE NUMBER 7
==========

EQUATION OF PLANE AS AX+BY+CZ=D, XYZ IN FRACTIONAL AND ORTHOGONAL UNITS

A	B	C	D	ESDA	ESDB	ESDC	ESDD
-3.2691	2.3444	14.5352	4.3411	.0983	.1436	.0676	.1768
-.3764	-.2202	.8999	4.3411	.0100	.0115	.0042	.1768

<CHI**2>	<GOODNESS OF FIT>	<N-3>
17.9362	2.4451	3

ANGLE BETWEEN PLANES/LINES 1 7 40.061 ESD .731

ANGLE BETWEEN PLANES/LINES 2 7 27.371 ESD .731

ANGLE BETWEEN PLANES/LINES 3 7 108.486 ESD .609

ANGLE BETWEEN PLANES/LINES 4 7 68.923 ESD .751

ANGLE BETWEEN PLANES/LINES 5 7 60.459 ESD .800

ANGLE BETWEEN PLANES/LINES 6 7 82.602 ESD .805

ATOM		DIST(A)	ESDD	X	Y	Z
N6	DEFINING	-.0028	.0181	.3560	1.0571	.2080
C26	DEFINING	.0618	.0328	.3291	1.1608	.1897
C27	DEFINING	-.0110	.0332	.4197	1.2238	.1949
C28	DEFINING	-.0597	.0315	.5315	1.1552	.2278
C29	DEFINING	.0906	.0330	.5762	1.0464	.2657
C30	DEFINING	-.0478	.0270	.4784	1.0102	.2400

PLANE NUMBER 8

EQUATION OF PLANE AS AX+BY+CZ=D, XYZ IN FRACTIONAL AND ORTHOGONAL UNITS

A	B	C	D	ESDA	ESDB	ESDC	ESDD
-.2245	-3.4740	12.5932	-.8768	.0608	.0216	.0156	.0334
.0140	-.6260	.7797	-.8768	.0060	.0018	.0010	.0334

<CHI**2>	<GOODNESS OF FIT>	<N-3>
393.293	19.8316	1

ANGLE BETWEEN PLANES/LINES 1 8 7.989 ESD .338

ANGLE BETWEEN PLANES/LINES 2 8 7.634 ESD .324

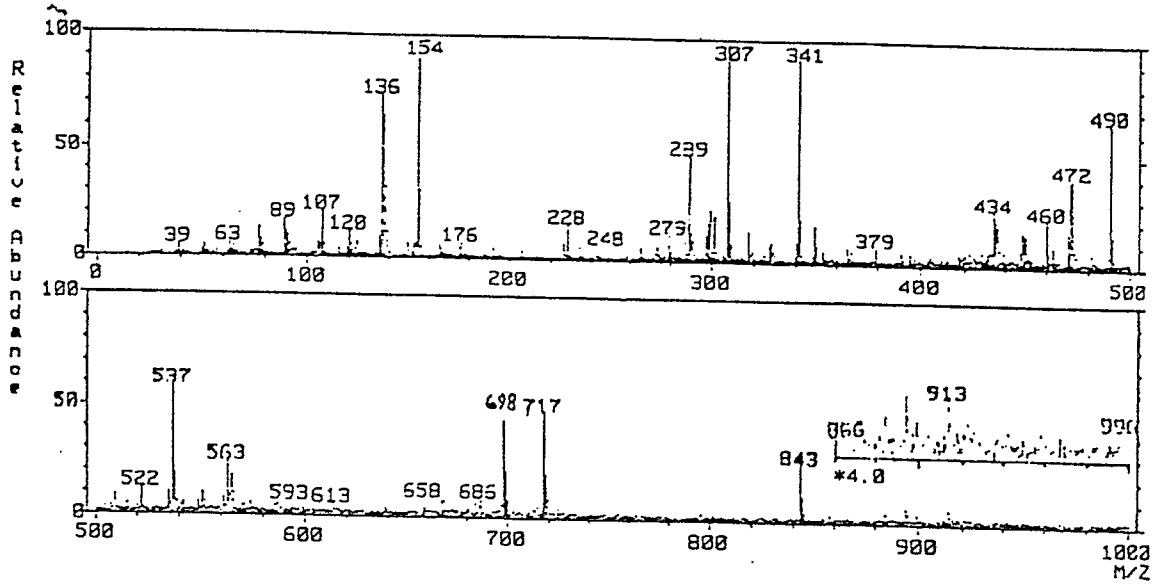
ANGLE BETWEEN PLANES/LINES 3 8 89.723 ESD .393

ATOM		DIST(A)	ESDD	X	Y	Z
Mn1	DEFINING	-.0098	.0030	.2765	.7924	.1531
O1	DEFINING	.1638	.0123	.1367	.8694	.1857
Mn2	DEFINING	-.0094	.0030	.2350	.9578	.1980
O2	DEFINING	.1761	.0126	.3752	.8593	.1881

Table S9. Magnetic data of $[Mn^{IV}_2(\mu\text{-}O)_2(\mu\text{-}OAc)(MeL)_2][ClO_4]_2.H_2O$ (**3**).

T[a]	$10^3\chi_M$(exptl)[b]	$10^3\chi_M$calc)[b]	μ_{eff}[c]	T[a]	$10^3\chi_M$(exptl)[b]	$10^3\chi_M$calc)[b]	μ_{eff}[c]
300	4.391	4.888	2.30	120	6.319	6.047	1.74
280	4.504	4.951	2.25	100	6.972	6.450	1.67
260	4.709	5.023	2.21	81	7.792	7.140	1.59
240	4.875	5.104	2.16	63	9.159	8.430	1.52
220	5.044	5.199	2.11	53	10.310	9.669	1.48
200	5.256	5.309	2.05	43	12.009	11.585	1.44
180	5.429	5.439	1.98	34	13.987	14.337	1.38
160	5.765	5.595	1.92	25	18.811	19.098	1.37
140	6.022	5.788	1.84				

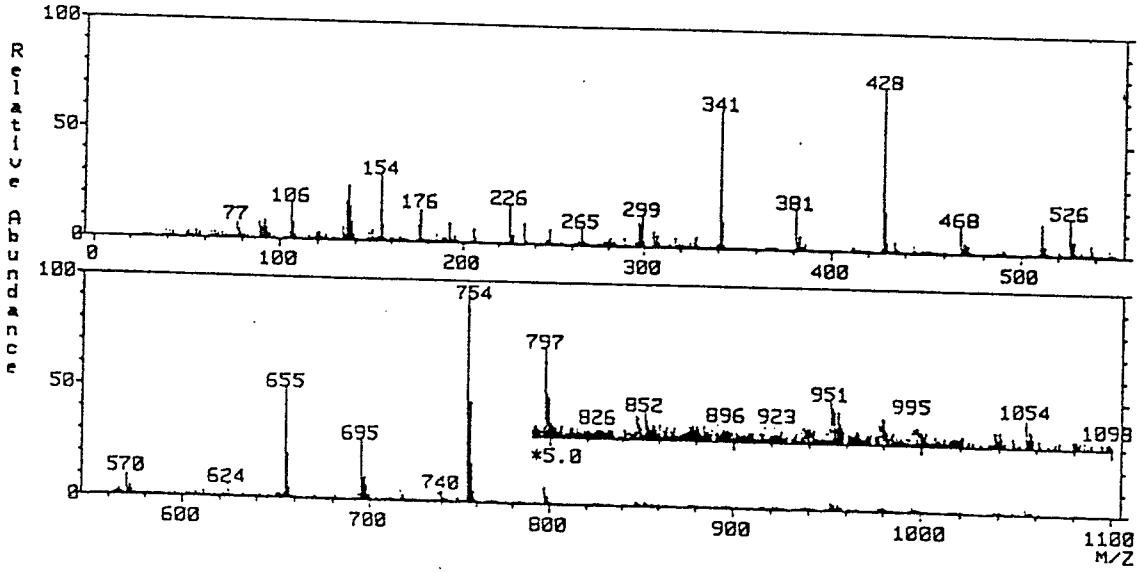
[a] ^oK. [b] χ_M values are in $cm^3\ mol^{-1}$. [c] μ_{eff} values (in μ_B) are calculated using the expression: $\mu_{eff} = 2.828\ (\chi_M\ T)^{1/2}$.



III, III

PF_6^-

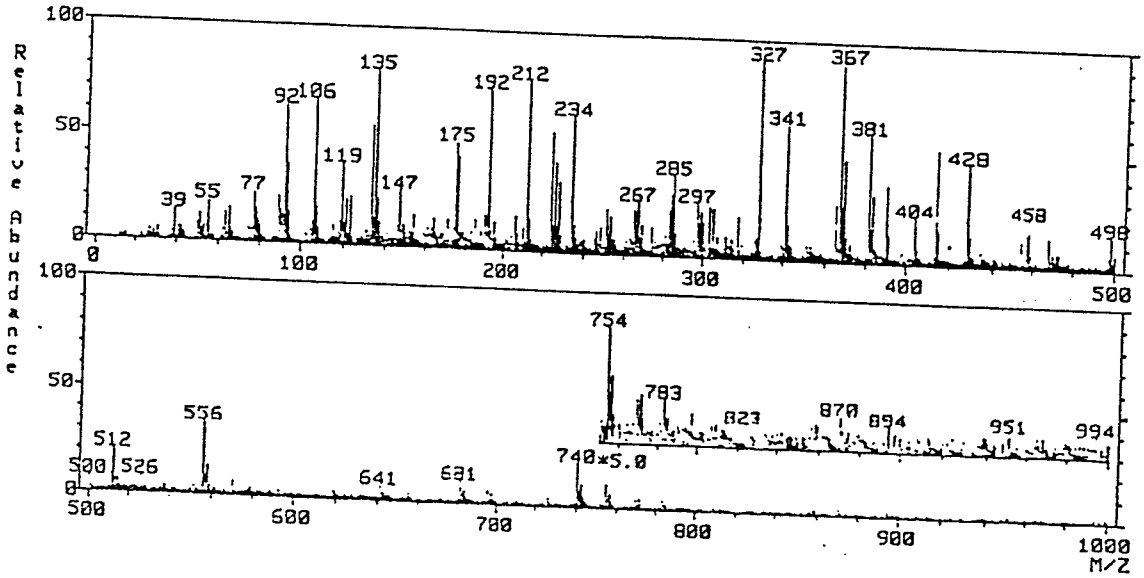
2a



III, IV

1a

ClO_4^-



IV, IV

3

$CH_3CO_2^-$

Figure S1

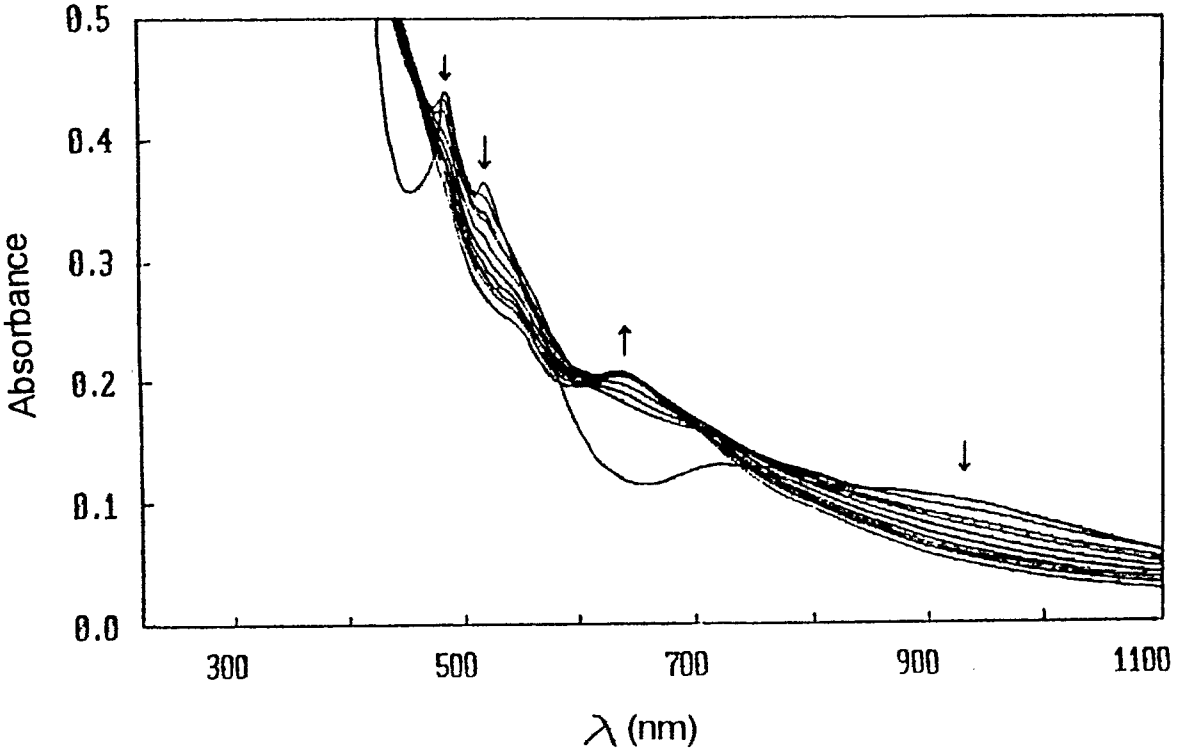


Figure S2

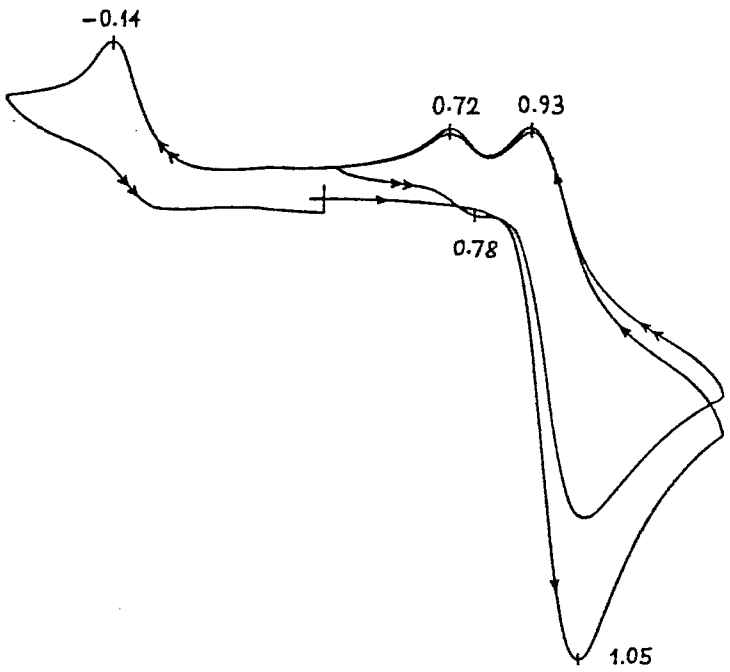


Figure S3