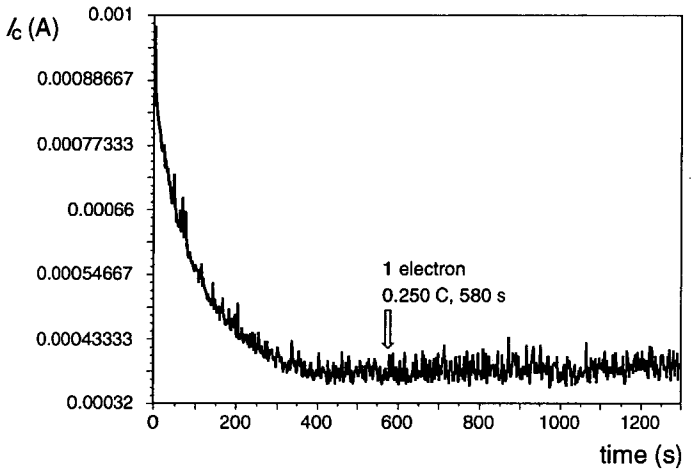
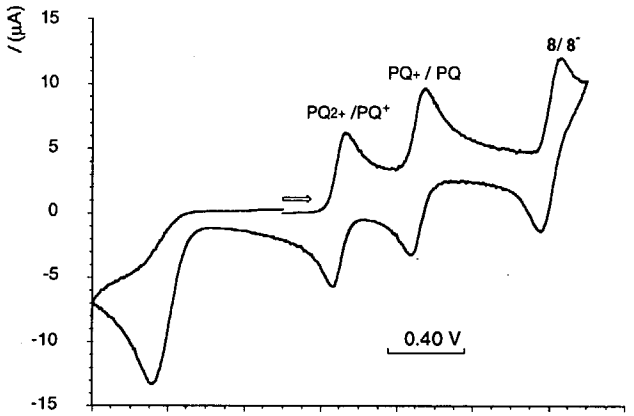
•Controlled-potential coulometry of a sample solution of complex **8** in CH_3CN (0.1 M $(n\text{-Bu})_4NPF_6$ as support electrolyte, separated cells, Pt-wire cathode, Pt-wire anode). Decay of the cathodic current (in A) upon electrolysis at a potential of -1.6V vs SCE (standard saturated calomel electrode) plotted vs. time (in s).



•Cyclic voltammetry of a mixture of complex **8** and 1,1'-dimethyl,4,4'-bipyridinium dihexafluorophosphate ($PQ^{2+}, 2PF_6$) in CH_3CN (scan rate = 200mV.s^{-1}, Pt-bead working electrode, Pt-wire counter electrode, Ag-wire pseudo-reference electrode).



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X-ray Diffraction Acquisition and Refinement Data

Compound **1b**

A.de Cian, J.-P. Collin, J.-P. Djukic, J. Fischer, C. Michon, M. Pfeffer, E. Ratkovic, D. Heiser, K. H. Dötz, N. Nieger

Table 1 : X-ray experimental data for **1b**

Formula	: $C_{30}H_{18}CrMnNO_6$
Molecular weight	: 595.42
Crystal system	: monoclinic
Space group	: P $2_1/c$
a(Å)	: 8.9761(2)
b(Å)	: 14.3301(5)
c(Å)	: 19.8900(7)
β(deg)	: 100.134(6)
V($Å^3$)	: 2518.5(3)
Z	: 4
Color	: red
Crystal dim(mm)	: 0.20*0.09*0.05
Dcalc($g.cm^{-3}$)	: 1.57
F000	: 1208
μ(mm^{-1})	: 0.980
Temperature(K)	: 173
Wavelength(Å)	: 0.71073
Radiation	: MoKα graphite monochromated
Diffractometer	: KappaCCD
Scan mode	: 'phi scans'
hkl limits	: -11,11/-17,18/-25,25
Theta limits(deg)	: 2.5/27.46
Number of data meas.	: 10143
Number of data with I > 3 σ(I)	: 4184
Weighting scheme	: $4Fo^2/(\sigma^2(Fo^2) + 0.0016\ Fo^4)$
Number of variables	: 352
R	: 0.028
Rw	: 0.040
GOF	: 1.011
Largest peak in final difference ($eÅ^{-3}$)	: 0.562

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Table of Positional Parameters and Their E.S.D.

Atom	x	y	z	Ueqv
MN	0.31024(3)	0.21773(2)	0.38856(1)	0.0153(1)
CR	0.26230(3)	0.19684(2)	0.53572(2)	0.0168(1)
C1	0.3079(2)	0.1402(1)	0.6209(1)	0.0234(9)
O1	0.3410(2)	0.1041(1)	0.67309(7)	0.0323(8)
C2	0.2224(2)	0.0745(1)	0.5032(1)	0.0211(9)
O2	0.1921(1)	-0.00048(9)	0.48561(7)	0.0315(8)
C3	0.4721(2)	0.1856(1)	0.5412(1)	0.0198(9)
O3	0.6022(1)	0.17595(9)	0.54986(7)	0.0280(7)
C4	0.0189(2)	0.2315(1)	0.5261(1)	0.0207(9)
C5	0.0996(2)	0.2777(1)	0.5836(1)	0.0232(9)
C6	0.2214(2)	0.3376(1)	0.5762(1)	0.0208(9)
C7	0.2616(2)	0.3505(1)	0.5124(1)	0.0181(9)
C8	0.1699(2)	0.3149(1)	0.44986(9)	0.0158(8)
C9	0.0600(2)	0.2435(1)	0.46145(9)	0.0163(8)
C10	-0.0045(2)	0.1834(1)	0.4033(1)	0.0169(8)
C11	-0.1531(2)	0.1528(1)	0.3894(1)	0.0231(9)
C12	-0.2013(2)	0.0979(1)	0.3328(1)	0.028(1)
C13	-0.0985(2)	0.0732(1)	0.2913(1)	0.029(1)
C14	0.0491(2)	0.1038(1)	0.3085(1)	0.024(1)
N	0.0969(1)	0.1587(1)	0.36290(8)	0.0170(7)
C15	0.4880(2)	0.2784(1)	0.41487(9)	0.0190(9)
O4	0.6027(1)	0.3156(1)	0.43098(7)	0.0278(7)
C16	0.3441(2)	0.2180(1)	0.3029(1)	0.0204(9)
O5	0.3713(1)	0.2122(1)	0.24807(7)	0.0351(8)
C17	0.4071(2)	0.1053(1)	0.4021(1)	0.0224(9)
O6	0.4754(1)	0.0368(1)	0.40626(8)	0.0352(7)
C18	0.1819(2)	0.3477(1)	0.38196(9)	0.0147(8)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C19	0.0336(2)	0.3540(1)	0.3302(1)	0.0163(8)
C20	-0.0994(2)	0.3841(1)	0.3511(1)	0.028(1)
C21	-0.2317(2)	0.3975(2)	0.3046(1)	0.035(1)
C22	-0.2354(2)	0.3818(2)	0.2358(1)	0.033(1)
C23	-0.1060(2)	0.3541(2)	0.2142(1)	0.034(1)
C24	0.0280(2)	0.3396(1)	0.2608(1)	0.024(1)
C25	0.2634(2)	0.4402(1)	0.37755(9)	0.0158(8)
C26	0.2203(2)	0.5196(1)	0.4115(1)	0.0235(9)
C27	0.2789(2)	0.6073(1)	0.4026(1)	0.026(1)
C28	0.3822(2)	0.6193(1)	0.3586(1)	0.024(1)
C29	0.4274(2)	0.5423(1)	0.3251(1)	0.0209(9)
C30	0.3685(2)	0.4538(1)	0.33413(9)	0.0171(9)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as one third of the trace of the orthogonalized Uij tensor.

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Table of Positional Parameters

Atom	x	y	z	Ueqv	
H1	-0.0636	0.1920	0.5309	0.0265	*
H2	0.0725	0.2688	0.6272	0.0301	*
H3	0.2758	0.3690	0.6149	0.0275	*
H4	0.3519	0.3837	0.5095	0.0238	*
H5	-0.2216	0.1696	0.4188	0.0306	*
H6	-0.3034	0.0773	0.3224	0.0383	*
H7	-0.1292	0.0359	0.2518	0.0393	*
H8	0.1199	0.0853	0.2808	0.0319	*
H9	-0.0989	0.3956	0.3982	0.0364	*
H10	-0.3207	0.4176	0.3201	0.0492	*
H11	-0.3266	0.3901	0.2039	0.0481	*
H12	-0.1070	0.3445	0.1668	0.0470	*
H13	0.1165	0.3197	0.2447	0.0329	*
H14	0.1491	0.5127	0.4412	0.0298	*
H15	0.2486	0.6593	0.4265	0.0344	*
H16	0.4211	0.6795	0.3516	0.0334	*
H17	0.4992	0.5497	0.2956	0.0279	*
H18	0.4004	0.4020	0.3104	0.0226	*

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
MN	.0148(1)	.0151(1)	.0162(1)	.0019(1)	.0037(1)	-.0000(1)
CR	.0186(1)	.0168(1)	.0151(1)	.0004(1)	.0034(1)	.0011(1)
C1	.0288(9)	.021(1)	.021(1)	-.0001(8)	.0061(8)	-.0027(9)
O1	.0561(8)	.0297(8)	.0201(7)	.0045(7)	.0047(6)	.0059(7)
C2	.0213(8)	.025(1)	.018(1)	.0027(7)	.0031(7)	.0054(9)
O2	.0415(7)	.0209(7)	.0362(9)	-.0026(6)	.0059(6)	-.0011(7)
C3	.0284(8)	.0144(9)	.019(1)	-.0000(8)	.0029(8)	.0019(9)
O3	.0218(6)	.0280(7)	.0358(8)	.0019(6)	.0010(6)	.0031(7)
C4	.0174(8)	.0223(9)	.023(1)	.0002(7)	.0074(7)	.0025(9)
C5	.0271(8)	.027(1)	.017(1)	.0051(8)	.0094(7)	.0020(9)
C6	.0234(8)	.0200(9)	.019(1)	.0022(8)	.0017(8)	-.0056(9)
C7	.0167(8)	.0164(9)	.022(1)	.0011(7)	.0032(7)	-.0001(9)
C8	.0140(7)	.0149(8)	.0189(9)	.0036(7)	.0037(7)	-.0014(8)
C9	.0141(7)	.0169(9)	.0182(9)	.0027(7)	.0026(7)	.0004(8)
C10	.0204(8)	.0122(8)	.0193(9)	.0011(7)	.0039(7)	.0044(8)
C11	.0188(8)	.0220(9)	.030(1)	.0004(7)	.0044(8)	.0034(9)
C12	.0197(8)	.028(1)	.038(1)	-.0067(8)	-.0020(9)	-.004(1)
C13	.030(1)	.026(1)	.031(1)	-.0045(8)	-.0045(9)	-.009(1)
C14	.0293(9)	.0197(9)	.024(1)	-.0005(8)	.0039(8)	-.0053(9)
N	.0194(6)	.0142(7)	.0179(8)	.0001(6)	.0021(6)	-.0004(7)
C15	.0210(8)	.0194(9)	.0169(9)	.0077(7)	.0050(7)	.0035(8)
O4	.0191(6)	.0335(8)	.0335(8)	-.0036(6)	.0026(6)	.0042(7)
C16	.0211(8)	.0157(9)	.026(1)	.0034(7)	.0041(8)	.0004(9)
O5	.0491(7)	.0367(8)	.0240(7)	.0110(6)	.0167(6)	.0009(7)
C17	.0222(8)	.024(1)	.021(1)	-.0009(8)	.0055(7)	.0002(9)
O6	.0394(7)	.0241(7)	.0459(9)	.0143(6)	.0125(6)	.0047(7)
C18	.0145(7)	.0150(8)	.0145(9)	.0016(7)	.0034(7)	-.0006(8)

Table of General Displacement Parameter Expressions (Continued)

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Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C19	.0163(7)	.0121(8)	.022(1)	-.0011(7)	.0021(7)	.0029(8)
C20	.0238(8)	.034(1)	.028(1)	.0101(8)	.0081(8)	.012(1)
C21	.0182(8)	.047(1)	.050(1)	.0083(9)	.0110(9)	.018(1)
C22	.0222(9)	.037(1)	.045(1)	.0009(9)	-.012(1)	.012(1)
C23	.036(1)	.038(1)	.029(1)	.008(1)	-.009(1)	-.006(1)
C24	.0222(8)	.032(1)	.021(1)	.0059(8)	-.0001(8)	-.005(1)
C25	.0149(7)	.0169(9)	.0157(9)	.0025(7)	-.0003(7)	.0018(8)
C26	.0238(8)	.0208(9)	.026(1)	.0013(7)	.0103(7)	-.0009(9)
C27	.0308(9)	.0188(9)	.029(1)	.0014(8)	.0028(8)	-.006(1)
C28	.0229(8)	.0187(9)	.034(1)	-.0061(8)	.0006(8)	.002(1)
C29	.0162(7)	.024(1)	.024(1)	-.0023(7)	.0018(7)	.0055(9)
C30	.0158(7)	.0189(9)	.0167(9)	.0029(7)	.0009(7)	.0009(8)

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
MN	C8	2.356(2)	C9	C10	1.476(3)
MN	N	2.074(1)	C10	C11	1.385(3)
MN	C15	1.812(2)	C10	N	1.363(2)
MN	C16	1.782(2)	C11	C12	1.379(3)
MN	C17	1.827(2)	C12	C13	1.387(3)
MN	C18	2.182(2)	C13	C14	1.380(3)
CR	C1	1.857(2)	C14	N	1.345(2)
CR	C2	1.880(2)	C15	O4	1.154(2)
CR	C3	1.874(2)	C16	O5	1.163(2)
CR	C4	2.216(2)	C17	O6	1.153(2)
CR	C5	2.207(2)	C18	C19	1.535(3)
CR	C6	2.226(2)	C18	C25	1.523(2)
CR	C7	2.250(2)	C19	C20	1.400(3)
CR	C9	2.233(2)	C19	C24	1.388(3)
C1	O1	1.152(2)	C20	C21	1.385(3)
C2	O2	1.148(2)	C21	C22	1.381(3)
C3	O3	1.158(2)	C22	C23	1.367(3)
C4	C5	1.407(3)	C23	C24	1.399(3)
C4	C9	1.409(3)	C25	C26	1.411(3)
C5	C6	1.418(3)	C25	C30	1.401(2)
C6	C7	1.391(3)	C26	C27	1.386(3)
C7	C8	1.458(3)	C27	C28	1.393(3)
C8	C9	1.467(2)	C28	C29	1.386(3)
C8	C18	1.452(3)	C29	C30	1.398(3)

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Table of Bond Angles in Degrees

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C8	MN	N	79.26(6)	C2	CR	C9	88.19(8)
C8	MN	C15	95.25(7)	C3	CR	C4	171.79(8)
C8	MN	C16	133.63(8)	C3	CR	C5	138.99(8)
C8	MN	C17	136.70(8)	C3	CR	C6	106.53(8)
C8	MN	C18	37.08(7)	C3	CR	C7	93.55(7)
N	MN	C15	174.45(7)	C3	CR	C9	139.13(8)
N	MN	C16	94.09(8)	C4	CR	C5	37.09(7)
N	MN	C17	94.09(7)	C4	CR	C6	66.77(7)
N	MN	C18	83.04(6)	C4	CR	C7	78.24(7)
C15	MN	C16	89.15(9)	C4	CR	C9	36.94(7)
C15	MN	C17	90.46(8)	C5	CR	C6	37.31(7)
C15	MN	C18	92.11(7)	C5	CR	C7	66.25(7)
C16	MN	C17	89.23(9)	C5	CR	C9	66.74(7)
C16	MN	C18	96.76(8)	C6	CR	C7	36.21(7)
C17	MN	C18	173.52(8)	C6	CR	C9	78.53(7)
C1	CR	C2	84.52(9)	C7	CR	C9	66.30(7)
C1	CR	C3	81.46(9)	C5	C4	C9	120.3(2)
C1	CR	C4	103.45(8)	C4	C5	C6	119.8(2)
C1	CR	C5	83.84(8)	C5	C6	C7	120.2(2)
C1	CR	C6	95.17(8)	C6	C7	C8	122.2(2)
C1	CR	C7	127.42(8)	C7	C8	C9	113.9(2)
C1	CR	C9	139.24(7)	C7	C8	C18	123.8(2)
C2	CR	C3	93.93(8)	C9	C8	C18	122.3(2)
C2	CR	C4	93.09(8)	C4	C9	C8	121.3(2)
C2	CR	C5	122.49(8)	C4	C9	C10	120.9(2)
C2	CR	C6	159.29(7)	C8	C9	C10	117.8(2)
C2	CR	C7	147.97(8)	C9	C10	C11	124.9(2)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C9	C10	N	113.8(2)	C19	C20	C21	121.4(2)
C11	C10	N	121.3(2)	C20	C21	C22	120.5(2)
C10	C11	C12	119.8(2)	C21	C22	C23	119.0(2)
C11	C12	C13	119.0(2)	C22	C23	C24	120.9(2)
C12	C13	C14	118.8(2)	C19	C24	C23	120.9(2)
C13	C14	N	122.8(2)	C18	C25	C26	120.0(2)
C10	N	C14	118.3(2)	C18	C25	C30	122.6(2)
C8	C18	C19	116.4(1)	C26	C25	C30	117.0(2)
C8	C18	C25	116.8(2)	C25	C26	C27	121.9(2)
C19	C18	C25	106.2(1)	C26	C27	C28	120.1(2)
C18	C19	C20	120.2(2)	C27	C28	C29	119.2(2)
C18	C19	C24	122.2(2)	C28	C29	C30	120.7(2)
C20	C19	C24	117.2(2)	C25	C30	C29	121.1(2)

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Compound **1c**

Table 1 : X-ray experimental data for **1c**

Formula	: $C_{30}H_{16}CrMnNO_6$
Molecular weight	: 593.40
Crystal system	: monoclinic
Space group	: P $2_1/c$
a(Å)	: 9.6538(3)
b(Å)	: 15.0319(5)
c(Å)	: 17.5379(5)
β(deg)	: 100.773(5)
V(Å^3)	: 2500.2(1)
Z	: 4
Color	: orange
Crystal dim(mm)	: 0.18*0.12*0.08
Dcalc(g.cm^{-3})	: 1.58
F000	: 1200
μ(mm^{-1})	: 0.987
Temperature(K)	: 173
Wavelength(Å)	: 0.71073
Radiation	: MoKα graphite monochromated
Diffractometer	: KappaCCD
Scan mode	: 'phi scans'
hkl limits	: -12,12/-17,19/-22,22
Theta limits(deg)	: 2.5/27.46
Number of data meas.	: 10230
Number of data with I > 3 σ(I)	: 3727
Number of variables	: 352
R	: 0.033
Rw	: 0.060
GOF	: 1.073
Largest peak in final difference (eÅ^{-3})	: 0.357

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Table of Positional Parameters and Their E.S.D.

Atom	x	y	z	Ueqv
CR	0.25405(5)	0.35119(3)	0.01823(3)	0.0214(2)
C1	0.1669(3)	0.3561(2)	0.1029(2)	0.029(2)
O1	0.1093(2)	0.3629(2)	0.1541(1)	0.048(1)
C2	0.0895(4)	0.3986(2)	-0.0368(2)	0.040(2)
O2	-0.0150(3)	0.4261(2)	-0.0717(2)	0.064(2)
C3	0.3157(3)	0.4644(2)	0.0446(2)	0.032(2)
O3	0.3528(3)	0.5357(2)	0.0625(1)	0.052(1)
MN	0.74706(4)	0.25883(3)	0.17021(2)	0.0191(2)
C4	0.7507(3)	0.3753(2)	0.1501(2)	0.027(2)
O4	0.7518(3)	0.4504(1)	0.1375(1)	0.042(1)
C5	0.8317(3)	0.2343(2)	0.0898(2)	0.030(2)
O5	0.8846(2)	0.2178(2)	0.0381(1)	0.052(1)
C6	0.9104(3)	0.2663(2)	0.2378(2)	0.029(2)
O6	1.0104(3)	0.2732(2)	0.2848(1)	0.044(1)
C7	0.2220(3)	0.2201(2)	-0.0388(2)	0.023(1)
C8	0.2678(3)	0.2797(2)	-0.0900(2)	0.028(2)
C9	0.3919(3)	0.3277(2)	-0.0675(2)	0.026(1)
C10	0.4717(3)	0.3142(2)	0.0081(2)	0.023(1)
C11	0.4300(3)	0.2537(2)	0.0602(1)	0.020(1)
C12	0.2985(3)	0.2065(2)	0.0368(1)	0.021(1)
C13	0.2433(3)	0.1406(2)	0.0874(2)	0.022(1)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C14	0.2491(3)	0.1508(2)	0.1654(2)	0.028(2)
C15	0.1949(4)	0.0839(2)	0.2072(2)	0.036(2)
C16	0.1371(4)	0.0102(2)	0.1676(2)	0.038(2)
C17	0.1341(4)	0.0052(2)	0.0888(2)	0.036(2)
N	0.1849(3)	0.0685(2)	0.0481(1)	0.030(1)
C18	0.5278(3)	0.2301(2)	0.1341(2)	0.019(1)
C19	0.5470(3)	0.2698(2)	0.2102(2)	0.022(1)
C20	0.4974(3)	0.3507(2)	0.2386(2)	0.029(2)
C21	0.5404(3)	0.3722(2)	0.3137(2)	0.036(2)
C22	0.6318(3)	0.3172(2)	0.3665(2)	0.035(2)
C23	0.6824(3)	0.2395(2)	0.3425(2)	0.029(2)
C24	0.6409(3)	0.2141(2)	0.2638(1)	0.022(1)
C25	0.6757(3)	0.1374(2)	0.2211(2)	0.022(1)
C26	0.6007(3)	0.1464(2)	0.1424(2)	0.019(1)
C27	0.6154(3)	0.0783(2)	0.0873(2)	0.025(1)
C28	0.6977(3)	0.0072(2)	0.1110(2)	0.032(2)
C29	0.7693(3)	-0.0022(2)	0.1895(2)	0.032(2)
C30	0.7602(3)	0.0607(2)	0.2436(2)	0.028(1)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as one third of the trace of the orthogonalized Uij tensor.

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Table of Positional Parameters

Atom	x	y	z	Ueqv	
H1	0.1371	0.1879	-0.0555	0.0311	*
H2	0.2137	0.2874	-0.1406	0.0379	*
H3	0.4225	0.3687	-0.1022	0.0349	*
H4	0.5561	0.3473	0.0240	0.0306	*
H5	0.2897	0.2028	0.1911	0.0365	*
H6	0.1981	0.0896	0.2615	0.0464	*
H7	0.0997	-0.0367	0.1940	0.0492	*
H8	0.0935	-0.0461	0.0619	0.0499	*
H9	0.4350	0.3887	0.2050	0.0397	*
H10	0.5084	0.4264	0.3322	0.0473	*
H11	0.6581	0.3349	0.4192	0.0469	*
H12	0.7442	0.2031	0.3779	0.0392	*
H13	0.5680	0.0831	0.0349	0.0319	*
H14	0.7082	-0.0379	0.0745	0.0414	*
H15	0.8247	-0.0538	0.2042	0.0430	*
H16	0.8091	0.0538	0.2955	0.0376	*

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
CR	.0178(2)	.0220(2)	.0251(2)	-.0018(2)	-.0009(2)	.0031(2)
C1	.025(2)	.026(2)	.037(2)	-.006(1)	.007(1)	.002(1)
O1	.042(1)	.047(1)	.055(1)	-.007(1)	.022(1)	-.006(1)
C2	.039(2)	.041(2)	.039(2)	.010(2)	-.007(2)	-.006(2)
O2	.054(2)	.077(2)	.064(2)	.033(1)	-.026(1)	-.012(2)
C3	.028(2)	.031(2)	.039(2)	-.005(1)	.009(1)	.004(1)
O3	.061(2)	.032(1)	.072(1)	-.017(1)	.022(1)	-.010(1)
MN	.0160(2)	.0231(2)	.0189(2)	-.0016(2)	.0005(2)	.0015(2)
C4	.026(2)	.032(2)	.025(1)	-.003(1)	-.004(1)	-.001(1)
O4	.065(2)	.026(1)	.045(1)	-.006(1)	.001(1)	.005(1)
C5	.026(2)	.037(2)	.030(1)	-.011(1)	.003(1)	-.003(1)
O5	.045(1)	.073(2)	.042(1)	-.015(1)	.0232(9)	-.017(1)
C6	.024(2)	.037(2)	.028(1)	-.002(1)	.003(1)	.007(1)
O6	.026(1)	.075(2)	.044(1)	-.008(1)	-.014(1)	.014(1)
C7	.019(1)	.025(1)	.025(1)	-.005(1)	-.003(1)	-.004(1)
C8	.026(2)	.038(2)	.021(1)	-.001(1)	-.002(1)	.002(1)
C9	.025(2)	.033(2)	.021(1)	-.004(1)	.001(1)	.005(1)
C10	.016(1)	.030(1)	.024(1)	-.003(1)	.003(1)	.001(1)
C11	.015(1)	.023(1)	.023(1)	.001(1)	.001(1)	-.000(1)
C12	.019(1)	.020(1)	.022(1)	-.000(1)	.003(1)	-.000(1)
C13	.016(1)	.021(1)	.031(1)	.001(1)	.000(1)	.000(1)
C14	.029(2)	.026(1)	.029(1)	-.005(1)	.003(1)	-.003(1)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C15	.041(2)	.033(2)	.033(1)	-.005(2)	.008(1)	.004(1)
C16	.039(2)	.031(2)	.043(2)	-.010(2)	.008(1)	.011(1)
C17	.043(2)	.026(2)	.043(2)	-.013(2)	.001(2)	.000(1)
N	.032(1)	.025(1)	.032(1)	-.006(1)	.001(1)	-.001(1)

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C18	.013(1)	.024(1)	.022(1)	-.002(1)	.000(1)	.001(1)
C19	.017(1)	.025(1)	.024(1)	.000(1)	.002(1)	.001(1)
C20	.021(1)	.036(2)	.033(2)	.006(1)	.001(1)	-.007(1)
C21	.030(2)	.042(2)	.037(2)	.004(2)	.006(1)	-.015(1)
C22	.030(2)	.053(2)	.026(1)	-.005(2)	.007(1)	-.009(1)
C23	.025(2)	.041(2)	.023(1)	-.001(1)	.004(1)	.004(1)
C24	.018(1)	.032(1)	.019(1)	-.002(1)	.002(1)	.001(1)
C25	.018(1)	.024(1)	.024(1)	-.003(1)	.004(1)	.004(1)
C26	.013(1)	.024(1)	.021(1)	-.004(1)	.002(1)	.002(1)
C27	.025(1)	.026(1)	.023(1)	-.006(1)	.006(1)	.001(1)
C28	.032(2)	.024(1)	.042(2)	-.000(1)	.014(1)	-.002(1)
C29	.025(2)	.027(2)	.048(2)	.005(1)	.008(1)	.005(1)
C30	.022(2)	.031(2)	.032(1)	.001(1)	.002(1)	.012(1)

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
CR	C1	1.840(3)	C5	O5	1.148(4)
CR	C2	1.842(4)	C6	O6	1.151(4)
CR	C3	1.833(4)	C7	C8	1.397(5)
CR	C7	2.206(3)	C7	C12	1.406(4)
CR	C8	2.207(3)	C8	C9	1.391(5)
CR	C9	2.215(3)	C9	C10	1.419(4)
CR	C10	2.212(3)	C10	C11	1.400(4)
CR	C11	2.260(3)	C11	C12	1.445(4)
CR	C12	2.229(3)	C11	C18	1.496(4)
C1	O1	1.146(4)	C12	C13	1.494(4)
C2	O2	1.154(4)	C13	C14	1.368(4)
C3	O3	1.155(4)	C13	N	1.349(4)
MN	C4	1.788(3)	C14	C15	1.402(4)
MN	C5	1.796(3)	C15	C16	1.370(5)
MN	C6	1.790(4)	C16	C17	1.378(5)
MN	C18	2.137(3)	C17	N	1.336(4)
MN	C19	2.180(3)	C18	C19	1.443(4)
MN	C24	2.197(3)	C18	C26	1.436(4)
MN	C25	2.198(3)	C19	C20	1.431(4)
MN	C26	2.199(3)	C19	C24	1.445(4)
C4	O4	1.150(4)	C20	C21	1.343(5)

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Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C21	C22	1.419(5)	C25	C30	1.425(4)
C22	C23	1.363(5)	C26	C27	1.433(4)
C23	C24	1.415(4)	C27	C28	1.351(5)
C24	C25	1.449(4)	C28	C29	1.428(5)
C25	C26	1.439(4)	C29	C30	1.352(5)

Table of Bond Angles in Degrees

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C1	CR	C2	85.9(2)	C7	CR	C8	36.9(1)
C1	CR	C3	86.3(1)	C7	CR	C9	66.5(1)
C1	CR	C7	110.8(1)	C7	CR	C10	78.1(1)
C1	CR	C8	145.5(1)	C7	CR	C11	66.5(1)
C1	CR	C9	167.9(1)	C7	CR	C12	37.0(1)
C1	CR	C10	131.2(1)	C8	CR	C9	36.7(1)
C1	CR	C11	101.1(1)	C8	CR	C10	66.3(1)
C1	CR	C12	91.5(1)	C8	CR	C11	78.6(1)
C2	CR	C3	88.9(2)	C8	CR	C12	67.0(1)
C2	CR	C7	94.3(1)	C9	CR	C10	37.4(1)
C2	CR	C8	85.6(1)	C9	CR	C11	66.9(1)
C2	CR	C9	105.9(1)	C9	CR	C12	79.6(1)
C2	CR	C10	142.6(1)	C10	CR	C11	36.5(1)
C2	CR	C11	160.8(1)	C10	CR	C12	66.8(1)
C2	CR	C12	125.3(1)	C11	CR	C12	37.6(1)
C3	CR	C7	162.8(1)	C4	MN	C5	91.0(2)
C3	CR	C8	126.9(1)	C4	MN	C6	91.3(2)
C3	CR	C9	96.4(1)	C4	MN	C18	101.2(1)
C3	CR	C10	89.1(1)	C4	MN	C19	92.3(1)
C3	CR	C11	109.3(1)	C4	MN	C24	118.5(1)
C3	CR	C12	145.5(1)	C4	MN	C25	155.9(1)

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Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C4	MN	C26	138.1(1)	C25	MN	C26	38.2(1)
C5	MN	C6	93.4(2)	MN	C4	O4	179.2(3)
C5	MN	C18	107.2(1)	MN	C5	O5	179.2(3)
C5	MN	C19	146.0(1)	MN	C6	O6	175.5(3)
C5	MN	C24	150.3(1)	C8	C7	C12	121.7(3)
C5	MN	C25	111.8(1)	C7	C8	C9	120.7(3)
C5	MN	C26	92.1(1)	C8	C9	C10	118.6(3)
C6	MN	C18	155.5(1)	C9	C10	C11	122.1(3)
C6	MN	C19	120.4(1)	C10	C11	C12	118.5(3)
C6	MN	C24	90.0(1)	C10	C11	C18	120.5(3)
C6	MN	C25	95.0(1)	C12	C11	C18	120.6(3)
C6	MN	C26	130.1(1)	C7	C12	C11	118.4(3)
C18	MN	C19	39.0(1)	C7	C12	C13	118.2(3)
C18	MN	C24	65.5(1)	C11	C12	C13	123.3(3)
C18	MN	C25	65.4(1)	C12	C13	C14	124.6(3)
C18	MN	C26	38.7(1)	C12	C13	N	113.0(3)
C19	MN	C24	38.5(1)	C14	C13	N	122.4(3)
C19	MN	C25	64.5(1)	C13	C14	C15	119.6(3)
C19	MN	C26	63.8(1)	C14	C15	C16	118.1(3)
C24	MN	C25	38.5(1)	C15	C16	C17	118.9(3)
C24	MN	C26	63.9(1)	C16	C17	N	123.8(3)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C13	N	C17	117.3(3)	C19	C24	C23	120.5(3)
MN	C18	C11	129.7(2)	C19	C24	C25	107.6(3)
MN	C18	C19	72.1(2)	C23	C24	C25	131.9(3)
MN	C18	C26	73.0(2)	MN	C25	C24	70.7(2)
C11	C18	C19	130.9(3)	MN	C25	C26	70.9(2)
C11	C18	C26	121.0(3)	MN	C25	C30	125.3(2)
C19	C18	C26	107.0(3)	C24	C25	C26	107.3(3)
MN	C19	C18	68.9(2)	C24	C25	C30	132.6(3)
MN	C19	C20	123.4(2)	C26	C25	C30	120.1(3)
MN	C19	C24	71.4(2)	MN	C26	C18	68.4(2)
C18	C19	C20	132.9(3)	MN	C26	C25	70.9(2)
C18	C19	C24	108.6(3)	MN	C26	C27	123.9(2)
C20	C19	C24	118.4(3)	C18	C26	C25	109.2(3)
C19	C20	C21	118.9(3)	C18	C26	C27	131.7(3)
C20	C21	C22	122.7(3)	C25	C26	C27	119.0(3)
C21	C22	C23	120.9(3)	C26	C27	C28	118.9(3)
C22	C23	C24	118.6(3)	C27	C28	C29	121.7(3)
MN	C24	C19	70.1(2)	C28	C29	C30	121.6(3)
MN	C24	C23	124.0(2)	C25	C30	C29	118.6(3)
MN	C24	C25	70.8(2)				

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Compound **2b**

Table 1. X-ray experimental data for **2b**

Formula	$C_{28}H_{20}MnNO_3$
Molecular weight	473.41
Crystal system	orthorhombic
Space group	P b c a
a(Å)	11.8883(2)
b(Å)	17.0308(2)
c(Å)	21.9813(4)
$V(Å^3)$	4450.5(1)
Z	8
Color	red
Crystal dim(mm)	0.20*0.20*0.16
$Dcalc(gcm^{-3})$	1.41
F000	1952
$\mu(mm^{-1})$	0.624
Trans. min and max	0.9078/1.1867
Temperature(K)	173
Wavelength(Å)	0.71073
Radiation	MoKα graphite monochromated
Diffractometer	KappaCCD
Scan mode	'phi scans'
hkl limits	-16,16/-22,22/-30,30
Theta limits(deg)	2.5/30.03
Number of data meas.	12128
Number of data with I > 3 σ(I)	3412
Number of variables	298
R	0.036
Rw	0.050
GOF	1.057
Largest peak in final difference ($eÅ^{-3}$)	0.404

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Table of Positional Parameters and Their E.S.D.

Atom	x	y	z	Ueqv
MN	0.73080(3)	0.33369(2)	0.54196(2)	0.0221(2)
C1	0.8038(2)	0.4201(1)	0.5149(1)	0.031(1)
O1	0.8467(2)	0.47480(9)	0.49486(9)	0.048(1)
C2	0.6741(2)	0.3236(1)	0.4653(1)	0.028(1)
O2	0.6452(2)	0.3177(1)	0.41572(8)	0.043(1)
C3	0.8486(2)	0.2711(1)	0.5300(1)	0.026(1)
O3	0.9220(1)	0.22741(9)	0.52434(8)	0.040(1)
N	0.6294(1)	0.2461(1)	0.57067(8)	0.0223(9)
C4	0.5441(2)	0.2855(1)	0.5970(1)	0.021(1)
C5	0.4497(2)	0.2485(1)	0.6210(1)	0.024(1)
C6	0.4483(2)	0.1672(1)	0.6170(1)	0.031(1)
C7	0.5357(2)	0.1264(1)	0.5907(1)	0.032(1)
C8	0.6261(2)	0.1674(1)	0.5678(1)	0.029(1)
C9	0.3566(2)	0.2928(1)	0.6517(1)	0.038(1)
C10	0.5675(2)	0.3715(1)	0.5956(1)	0.021(1)
C11	0.4820(2)	0.4227(1)	0.5734(1)	0.028(1)
C12	0.4942(2)	0.5019(1)	0.5751(1)	0.032(1)
C13	0.5938(2)	0.5343(1)	0.5986(1)	0.029(1)
C14	0.6776(2)	0.4876(1)	0.6197(1)	0.027(1)
C15	0.6698(2)	0.4031(1)	0.6208(1)	0.021(1)
C16	0.7656(2)	0.3534(1)	0.6378(1)	0.022(1)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C17	0.8720(2)	0.3948(1)	0.6583(1)	0.025(1)
C18	0.9716(2)	0.3969(1)	0.6253(1)	0.033(1)
C19	1.0675(2)	0.4332(1)	0.6490(1)	0.038(1)
C20	1.0657(2)	0.4685(1)	0.7049(1)	0.038(1)
C21	0.9679(2)	0.4672(1)	0.7390(1)	0.038(1)
C22	0.8730(2)	0.4305(1)	0.7158(1)	0.033(1)
C23	0.7458(2)	0.2830(1)	0.6787(1)	0.022(1)
C24	0.6528(2)	0.2770(1)	0.7172(1)	0.026(1)
C25	0.6380(2)	0.2110(1)	0.7538(1)	0.034(1)
C26	0.7163(2)	0.1515(1)	0.7540(1)	0.035(1)
C27	0.8110(2)	0.1583(1)	0.7181(1)	0.033(1)
C28	0.8253(2)	0.2230(1)	0.6805(1)	0.028(1)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as one third of the trace of the orthogonalized Uij tensor.

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Table of Positional Parameters

Atom	x	y	z	Ueqv	
H1	0.3858	0.1391	0.6328	0.0400	*
H2	0.5336	0.0707	0.5884	0.0430	*
H3	0.6869	0.1397	0.5497	0.0378	*
H4	0.3003	0.2569	0.6649	0.0497	*
H5	0.3858	0.3202	0.6859	0.0497	*
H6	0.3246	0.3292	0.6239	0.0497	*
H7	0.4150	0.4009	0.5571	0.0365	*
H8	0.4359	0.5351	0.5606	0.0422	*
H9	0.6026	0.5897	0.5997	0.0398	*
H10	0.7445	0.5116	0.6343	0.0349	*
H11	0.9746	0.3733	0.5862	0.0435	*
H12	1.1351	0.4334	0.6259	0.0521	*
H13	1.1312	0.4937	0.7202	0.0541	*
H14	0.9659	0.4912	0.7780	0.0503	*
H15	0.8063	0.4296	0.7397	0.0430	*
H16	0.5990	0.3182	0.7185	0.0339	*
H17	0.5732	0.2071	0.7790	0.0452	*
H18	0.7053	0.1062	0.7785	0.0462	*
H19	0.8668	0.1184	0.7191	0.0441	*
H20	0.8904	0.2264	0.6556	0.0369	*

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
MN	.0226(2)	.0222(2)	.0217(2)	.0014(2)	.0030(2)	-.0005(1)
C1	.032(1)	.034(1)	.027(1)	-.000(1)	.006(1)	-.002(1)
O1	.062(1)	.0356(9)	.049(1)	-.012(1)	.017(1)	.0080(9)
C2	.026(1)	.031(1)	.029(1)	.005(1)	.003(1)	-.000(1)
O2	.047(1)	.061(1)	.0273(9)	.010(1)	-.0036(9)	-.0046(9)
C3	.028(1)	.028(1)	.023(1)	-.003(1)	.004(1)	.001(1)
O3	.037(1)	.0427(9)	.039(1)	.0148(9)	.0081(9)	-.0007(8)
N	.0213(9)	.0228(8)	.0228(9)	.0003(9)	-.0022(8)	.0000(8)
C4	.021(1)	.025(1)	.017(1)	.001(1)	-.006(1)	-.0011(9)
C5	.021(1)	.031(1)	.021(1)	-.001(1)	-.003(1)	-.002(1)
C6	.027(1)	.032(1)	.034(1)	-.008(1)	-.004(1)	.006(1)
C7	.037(1)	.022(1)	.041(1)	-.004(1)	-.006(1)	.001(1)
C8	.027(1)	.024(1)	.037(1)	.004(1)	-.004(1)	-.003(1)
C9	.031(1)	.040(1)	.044(2)	-.005(1)	.010(1)	-.002(1)
C10	.020(1)	.025(1)	.019(1)	.001(1)	.0019(9)	-.0012(9)
C11	.028(1)	.032(1)	.025(1)	.004(1)	-.002(1)	.000(1)
C12	.039(1)	.029(1)	.029(1)	.012(1)	-.003(1)	.003(1)
C13	.042(1)	.020(1)	.030(1)	.004(1)	.002(1)	.000(1)
C14	.030(1)	.022(1)	.028(1)	-.002(1)	.004(1)	-.003(1)
C15	.023(1)	.023(1)	.018(1)	.001(1)	.004(1)	-.0007(9)
C16	.021(1)	.022(1)	.023(1)	.001(1)	.001(1)	-.0025(9)
C17	.024(1)	.0210(9)	.030(1)	.001(1)	-.005(1)	.002(1)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C18	.027(1)	.034(1)	.039(1)	-.001(1)	-.000(1)	-.000(1)
C19	.027(1)	.037(1)	.056(2)	-.005(1)	.000(1)	.004(1)
C20	.033(1)	.025(1)	.067(2)	-.003(1)	-.019(1)	.001(1)
C21	.040(1)	.029(1)	.047(2)	.001(1)	-.017(1)	-.007(1)

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C22	.034(1)	.031(1)	.034(1)	-.001(1)	-.003(1)	-.004(1)
C23	.025(1)	.021(1)	.020(1)	-.0006(9)	-.004(1)	-.0026(9)
C24	.024(1)	.031(1)	.023(1)	.002(1)	-.005(1)	-.001(1)
C25	.027(1)	.048(1)	.029(1)	-.009(1)	-.001(1)	.007(1)
C26	.044(2)	.029(1)	.034(1)	-.009(1)	-.010(1)	.007(1)
C27	.042(1)	.025(1)	.035(1)	.006(1)	-.008(1)	-.000(1)
C28	.031(1)	.028(1)	.026(1)	.003(1)	.001(1)	-.000(1)

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
MN	C1	1.808(3)	C11	C12	1.357(3)
MN	C2	1.822(3)	C12	C13	1.405(4)
MN	C3	1.779(3)	C13	C14	1.357(3)
MN	N	2.019(2)	C14	C15	1.441(3)
MN	C15	2.221(2)	C15	C16	1.468(3)
MN	C16	2.173(2)	C16	C17	1.517(3)
C1	O1	1.150(3)	C16	C23	1.516(3)
C2	O2	1.148(3)	C17	C18	1.388(4)
C3	O3	1.154(3)	C17	C22	1.404(4)
N	C4	1.347(3)	C18	C19	1.397(4)
N	C8	1.342(3)	C19	C20	1.368(4)
C4	C5	1.392(3)	C20	C21	1.384(4)
C4	C10	1.492(3)	C21	C22	1.387(3)
C5	C6	1.388(3)	C23	C24	1.396(3)
C5	C9	1.499(3)	C23	C28	1.393(3)
C6	C7	1.377(4)	C24	C25	1.393(3)
C7	C8	1.378(4)	C25	C26	1.376(4)
C10	C11	1.425(3)	C26	C27	1.380(4)
C10	C15	1.441(3)	C27	C28	1.387(3)

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Table of Bond Angles in Degrees

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C1	MN	C2	87.2(1)	N	C4	C5	123.1(2)
C1	MN	C3	93.5(1)	N	C4	C10	109.9(2)
C1	MN	N	172.0(1)	C5	C4	C10	127.1(2)
C1	MN	C15	88.8(1)	C4	C5	C6	115.9(2)
C1	MN	C16	95.8(1)	C4	C5	C9	122.6(2)
C2	MN	C3	95.6(1)	C6	C5	C9	121.5(2)
C2	MN	N	89.9(1)	C5	C6	C7	121.5(2)
C2	MN	C15	130.6(1)	C6	C7	C8	119.1(2)
C2	MN	C16	168.8(1)	N	C8	C7	120.8(2)
C3	MN	N	94.20(9)	C4	C10	C11	118.4(2)
C3	MN	C15	133.7(1)	C4	C10	C15	121.1(2)
C3	MN	C16	94.9(1)	C11	C10	C15	120.3(2)
N	MN	C15	87.37(8)	C10	C11	C12	121.5(2)
N	MN	C16	85.67(8)	C11	C12	C13	119.4(2)
C15	MN	C16	39.01(8)	C12	C13	C14	120.9(2)
MN	C1	O1	176.2(3)	C13	C14	C15	123.0(2)
MN	C2	O2	175.7(2)	MN	C15	C10	77.1(1)
MN	C3	O3	176.2(2)	MN	C15	C14	119.7(2)
MN	N	C4	102.5(1)	MN	C15	C16	68.7(1)
MN	N	C8	137.7(2)	C10	C15	C14	114.9(2)
C4	N	C8	119.7(2)	C10	C15	C16	122.5(2)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C14	C15	C16	122.0(2)	C19	C20	C21	119.5(3)
MN	C16	C15	72.2(1)	C20	C21	C22	119.5(3)
MN	C16	C17	121.2(2)	C17	C22	C21	122.2(3)
MN	C16	C23	115.0(2)	C16	C23	C24	122.7(2)
C15	C16	C17	117.0(2)	C16	C23	C28	119.4(2)
C15	C16	C23	119.1(2)	C24	C23	C28	117.8(2)
C17	C16	C23	108.7(2)	C23	C24	C25	120.7(2)
C16	C17	C18	124.7(2)	C24	C25	C26	120.6(2)
C16	C17	C22	118.4(2)	C25	C26	C27	119.3(2)
C18	C17	C22	116.8(2)	C26	C27	C28	120.5(2)
C17	C18	C19	120.9(3)	C23	C28	C27	121.1(2)
C18	C19	C20	121.0(3)				

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Compound **3c**

Table 1 : X-ray experimental data for **3c**

Formula	: $C_{52}H_{32}Mn_2N_2O_6$
Molecular weight	: 890.72
Crystal system	: monoclinic
Space group	: P $2_1/n$
a(Å)	: 15.6887(7)
b(Å)	: 16.7698(9)
c(Å)	: 15.9857(7)
β(deg)	: 93.588(5)
V(Å^3)	: 4197.5(3)
Z	: 4
Color	: dark blue
Crystal dim(mm)	: 0.20*0.14*0.10
Dcalc(gcm-3)	: 1.41
F000	: 1824
_(mm-1)	: 0.657
Temperature(K)	: 294
Wavelength(Å)	: 0.71073
Radiation	: MoK_ graphite monochromated
Diffractometer	: KappaCCD
Scan mode	: 'phi scans'
hkl limits	: -20,20/-21,20/-20,20
Theta limits(deg)	: 2.5/27.51
Number of data meas.	: 16708
Number of data with I > 3 _(I)	: 3947
Number of variables	: 559
R	: 0.035
Rw	: 0.040
GOF	: 1.040
Largest peak in final difference (eÅ-3)	: 0.289

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Table of Positional Parameters and Their E.S.D.

Atom	x	y	z	Ueqv
MN1	0.28683(3)	0.18729(3)	0.32886(3)	0.0374(3)
MN2	0.65448(3)	0.09686(3)	0.16454(3)	0.0341(3)
C1	0.1903(1)	0.1668(2)	0.3794(1)	0.049(2)
O1	0.1292(1)	0.1580(2)	0.4147(1)	0.079(2)
C2	0.3379(2)	0.1985(3)	0.4334(2)	0.065(3)
O2	0.3647(1)	0.2033(3)	0.5009(1)	0.107(3)
C3	0.2466(2)	0.2863(2)	0.3194(2)	0.053(2)
O3	0.2163(1)	0.3491(1)	0.3172(1)	0.080(2)
C4	0.2419(2)	0.1370(2)	0.2097(2)	0.032(2)
C5	0.1476(2)	0.1345(2)	0.1805(2)	0.037(2)
C6	0.0912(2)	0.1963(2)	0.1926(2)	0.049(2)
C7	0.0068(2)	0.1927(3)	0.1606(2)	0.061(3)
C8	-0.0229(2)	0.1280(3)	0.1170(2)	0.062(3)
C9	0.0312(2)	0.0656(2)	0.1044(2)	0.065(3)
C10	0.1163(2)	0.0694(2)	0.1343(2)	0.055(2)
C11	0.2912(1)	0.1610(2)	0.1347(1)	0.031(2)
C12	0.3345(1)	0.1059(2)	0.0891(1)	0.043(2)
C13	0.3776(2)	0.1286(2)	0.0198(2)	0.053(2)
C14	0.3761(2)	0.2064(2)	-0.0054(2)	0.058(2)
C15	0.3315(1)	0.2614(2)	0.0371(1)	0.054(2)
C16	0.2892(1)	0.2391(2)	0.1062(1)	0.045(2)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C17	0.2736(2)	0.0719(2)	0.2634(2)	0.031(2)
C18	0.2176(2)	0.0143(2)	0.2980(2)	0.038(2)
C19	0.2450(2)	-0.0428(2)	0.3527(2)	0.046(2)
C20	0.3306(2)	-0.0482(2)	0.3800(2)	0.047(2)
C21	0.3870(2)	0.0056(2)	0.3527(2)	0.040(2)
C22	0.3607(2)	0.0669(2)	0.2963(2)	0.031(2)
C23	0.4257(1)	0.1231(2)	0.2662(1)	0.028(2)
N1	0.4017(1)	0.1983(1)	0.2745(1)	0.030(1)
C24	0.4530(1)	0.2579(2)	0.2472(1)	0.034(2)
C25	0.5267(1)	0.2383(2)	0.2055(1)	0.033(2)
C26	0.5746(2)	0.2996(2)	0.1715(2)	0.052(2)
C27	0.5545(2)	0.3766(2)	0.1860(2)	0.062(2)
C28	0.4860(1)	0.3960(2)	0.2332(1)	0.058(2)
C29	0.4348(1)	0.3383(2)	0.2621(2)	0.046(2)
C30	0.7370(2)	0.0308(2)	0.1338(2)	0.047(2)
O4	0.7907(1)	-0.0089(2)	0.1104(1)	0.076(2)
C31	0.6099(2)	0.0932(2)	0.0569(2)	0.051(2)
O5	0.5879(1)	0.0910(2)	-0.0129(1)	0.081(2)
C32	0.7260(2)	0.1760(2)	0.1471(2)	0.044(2)
O6	0.7747(1)	0.2255(2)	0.1350(1)	0.067(2)
C33	0.6853(2)	0.0837(2)	0.2971(2)	0.032(2)

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Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv	
C34	0.6501(1)	0.1492(2)	0.3509(1)	0.034(2)	
C35	0.5910(1)	0.1334(2)	0.4098(1)	0.043(2)	
C36	0.5642(2)	0.1934(3)	0.4618(2)	0.059(2)	
C37	0.5964(2)	0.2688(2)	0.4560(2)	0.072(3)	
C38	0.6553(1)	0.2857(2)	0.3993(1)	0.067(3)	
C39	0.6828(1)	0.2259(2)	0.3479(1)	0.051(2)	
C40	0.7750(2)	0.0672(2)	0.3344(2)	0.034(2)	
C41	0.7857(2)	0.0304(2)	0.4129(2)	0.045(2)	
C42	0.8644(2)	0.0262(2)	0.4565(2)	0.048(2)	
C43	0.9342(2)	0.0602(2)	0.4238(2)	0.049(2)	
C44	0.9265(2)	0.0952(2)	0.3469(2)	0.050(2)	
C45	0.8481(2)	0.0982(2)	0.3024(2)	0.044(2)	
C46	0.6321(1)	0.0156(2)	0.2706(1)	0.033(2)	
C47	0.6643(2)	-0.0642(2)	0.2701(2)	0.041(2)	
C48	0.6181(2)	-0.1265(2)	0.2380(2)	0.047(2)	
C49	0.5356(1)	-0.1160(2)	0.2025(1)	0.045(2)	
C50	0.5009(1)	-0.0421(2)	0.1999(1)	0.038(2)	
C51	0.5469(1)	0.0249(2)	0.2322(1)	0.031(2)	
C52	0.5048(1)	0.1041(2)	0.2339(1)	0.026(2)	
N2	0.5522(1)	0.1602(1)	0.2016(1)	0.031(1)	

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as one third of the trace of the orthogonalized Uij tensor.

Table of Positional Parameters

Atom	x	y	z	Ueqv	
H1	0.1105	0.2420	0.2234	0.0663	*
H2	-0.0305	0.2361	0.1693	0.0878	*
H3	-0.0807	0.1259	0.0955	0.0925	*
H4	0.0106	0.0195	0.0751	0.0866	*

H5	0.1537	0.0267	0.1229	0.0725	*
H6	0.3348	0.0515	0.1055	0.0556	*
H7	0.4080	0.0901	-0.0101	0.0705	*
H8	0.4062	0.2222	-0.0525	0.0771	*
H9	0.3295	0.3153	0.0188	0.0718	*
H10	0.2581	0.2779	0.1350	0.0585	*
H11	0.1584	0.0166	0.2815	0.0504	*
H12	0.2052	-0.0797	0.3729	0.0603	*
H13	0.3495	-0.0894	0.4175	0.0616	*
H14	0.4454	0.0021	0.3720	0.0529	*
H15	0.6210	0.2870	0.1383	0.0716	*
H16	0.5877	0.4179	0.1637	0.0942	*
H17	0.4749	0.4504	0.2454	0.0900	*
H18	0.3868	0.3524	0.2924	0.0671	*
H19	0.5687	0.0811	0.4146	0.0587	*
H20	0.5234	0.1821	0.5017	0.0842	*
H21	0.5776	0.3097	0.4916	0.0949	*

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Table of Positional Parameters (cont.)

Atom	x	y	z	Ueqv	
H22	0.6774	0.3382	0.3952	0.0897	*
H23	0.7251	0.2376	0.3096	0.0665	*
H24	0.7375	0.0076	0.4369	0.0593	*
H25	0.8701	-0.0003	0.5091	0.0633	*
H26	0.9879	0.0595	0.4547	0.0669	*
H27	0.9753	0.1176	0.3236	0.0684	*
H28	0.8443	0.1222	0.2485	0.0589	*
H29	0.7206	-0.0739	0.2933	0.0547	*
H30	0.6424	-0.1784	0.2397	0.0646	*
H31	0.5038	-0.1603	0.1804	0.0593	*
H32	0.4445	-0.0350	0.1759	0.0496	*

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
MN1	.0307(3)	.0401(3)	.0427(3)	-.0011(3)	.0073(2)	-.0049(3)
MN2	.0298(3)	.0378(3)	.0352(3)	.0020(2)	.0048(2)	.0003(3)
C1	.048(2)	.052(2)	.047(2)	-.003(2)	.007(2)	-.005(2)
O1	.054(1)	.106(2)	.085(2)	-.016(2)	.037(1)	-.001(2)
C2	.042(2)	.125(3)	.051(2)	-.002(3)	.009(2)	-.037(2)
O2	.066(2)	.329(5)	.057(2)	.007(3)	-.005(2)	-.078(3)
C3	.041(2)	.048(2)	.074(2)	-.002(2)	.018(2)	-.008(2)
O3	.076(2)	.050(2)	.136(2)	.019(1)	.039(2)	.002(2)
C4	.028(2)	.033(2)	.037(2)	-.002(2)	.004(1)	.005(2)
C5	.029(2)	.046(2)	.039(2)	-.002(2)	-.001(2)	.007(2)
C6	.034(2)	.068(2)	.050(2)	.004(2)	.002(2)	.002(2)
C7	.035(2)	.105(3)	.063(3)	.018(2)	.006(2)	.007(3)
C8	.035(2)	.122(4)	.056(2)	-.014(2)	-.002(2)	.018(3)
C9	.054(2)	.085(3)	.058(2)	-.030(2)	-.012(2)	.006(2)
C10	.048(2)	.057(2)	.061(2)	-.005(2)	-.005(2)	.006(2)
C11	.025(2)	.035(2)	.035(2)	.001(2)	-.005(2)	.001(2)
C12	.045(2)	.040(2)	.043(2)	.006(2)	-.001(2)	.002(2)
C13	.056(2)	.069(2)	.039(2)	.010(2)	.010(2)	-.004(2)
C14	.066(2)	.073(3)	.041(2)	-.006(2)	.017(2)	.009(2)
C15	.071(2)	.045(2)	.051(2)	-.008(2)	.009(2)	.013(2)
C16	.048(2)	.039(2)	.048(2)	.002(2)	.007(2)	.004(2)
C17	.029(2)	.031(2)	.033(2)	-.003(2)	.003(1)	-.004(2)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C18	.030(2)	.040(2)	.046(2)	-.008(2)	.001(2)	-.000(2)
C19	.054(2)	.041(2)	.046(2)	-.007(2)	.012(2)	.009(2)
C20	.054(2)	.048(2)	.040(2)	.003(2)	-.002(2)	.014(2)
C21	.039(2)	.043(2)	.040(2)	-.001(2)	-.004(2)	.010(2)

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C22	.029(2)	.032(2)	.032(2)	-.001(1)	.003(1)	-.001(2)
C23	.028(2)	.030(2)	.026(2)	.001(2)	-.005(1)	.000(2)
N1	.023(1)	.034(1)	.035(1)	-.001(1)	-.002(1)	-.004(1)
C24	.026(2)	.032(2)	.049(2)	-.002(2)	-.004(2)	.001(2)
C25	.026(2)	.032(2)	.044(2)	.002(2)	-.001(2)	.005(2)
C26	.039(2)	.040(2)	.088(3)	.003(2)	.020(2)	.021(2)
C27	.048(2)	.038(2)	.134(3)	.006(2)	.023(2)	.032(2)
C28	.046(2)	.032(2)	.130(4)	.008(2)	.015(2)	-.002(2)
C29	.034(2)	.032(2)	.090(3)	-.000(2)	.016(2)	-.002(2)
C30	.043(2)	.051(2)	.048(2)	-.002(2)	.007(2)	-.005(2)
O4	.061(2)	.072(2)	.100(2)	.021(1)	.027(1)	-.018(2)
C31	.045(2)	.069(2)	.043(2)	.004(2)	.006(2)	-.003(2)
O5	.089(2)	.142(3)	.042(2)	.017(2)	-.005(1)	-.009(2)
C32	.033(2)	.054(2)	.047(2)	.006(2)	.012(1)	.007(2)
O6	.046(1)	.066(2)	.096(2)	-.011(1)	.017(1)	.018(2)
C33	.029(2)	.035(2)	.033(2)	.004(2)	.002(1)	.003(2)
C34	.029(2)	.039(2)	.035(2)	.005(2)	-.007(2)	.000(2)
C35	.034(2)	.062(2)	.038(2)	.005(2)	-.005(2)	-.003(2)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C36	.048(2)	.104(3)	.042(2)	.019(2)	-.001(2)	-.025(2)
C37	.074(3)	.079(3)	.063(3)	.029(2)	-.017(2)	-.036(2)
C38	.087(3)	.051(2)	.067(3)	.003(2)	-.014(2)	-.018(2)
C39	.056(2)	.045(2)	.051(2)	-.002(2)	-.004(2)	-.006(2)
C40	.031(2)	.032(2)	.039(2)	.003(2)	.000(2)	-.001(2)
C41	.032(2)	.056(2)	.049(2)	.008(2)	.005(2)	.004(2)
C42	.041(2)	.062(2)	.043(2)	.015(2)	-.001(2)	.006(2)
C43	.033(2)	.058(2)	.061(2)	.007(2)	-.014(2)	.001(2)
C44	.031(2)	.060(2)	.067(2)	-.002(2)	-.002(2)	.010(2)
C45	.030(2)	.054(2)	.051(2)	-.001(2)	-.003(2)	.009(2)
C46	.030(2)	.035(2)	.035(2)	.003(2)	.003(1)	.002(2)

C47	.034(2)	.039(2)	.053(2)	.009(2)	.000(2)	.005(2)
C48	.052(2)	.030(2)	.067(2)	.004(2)	.006(2)	.002(2)
C49	.046(2)	.035(2)	.056(2)	-.002(2)	.002(2)	-.005(2)
C50	.031(2)	.039(2)	.044(2)	-.001(2)	-.000(2)	-.001(2)
C51	.029(2)	.029(2)	.035(2)	.001(1)	.003(1)	.001(2)
C52	.024(2)	.031(2)	.025(2)	.001(2)	-.003(1)	.001(2)
N2	.028(1)	.034(1)	.031(1)	.002(1)	-.001(1)	.005(1)

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Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
MN1	C1	1.795(4)	C7	C8	1.356(7)
MN1	C2	1.818(5)	C8	C9	1.370(7)
MN1	C3	1.780(4)	C9	C10	1.390(6)
MN1	C4	2.161(4)	C11	C12	1.382(5)
MN1	C17	2.203(3)	C11	C16	1.387(5)
MN1	N1	2.057(3)	C12	C13	1.385(5)
MN2	C30	1.797(4)	C13	C14	1.365(6)
MN2	C31	1.819(5)	C14	C15	1.365(5)
MN2	C32	1.772(4)	C15	C16	1.376(5)
MN2	C33	2.154(4)	C17	C18	1.439(4)
MN2	C46	2.220(3)	C17	C22	1.437(5)
MN2	N2	2.043(3)	C18	C19	1.348(5)
C1	O1	1.151(4)	C19	C20	1.389(6)
C2	O2	1.135(5)	C20	C21	1.356(5)
C3	O3	1.154(4)	C21	C22	1.412(5)
C4	C5	1.523(5)	C22	C23	1.491(4)
C4	C11	1.521(5)	C23	N1	1.325(4)
C4	C17	1.457(5)	C23	C52	1.410(4)
C5	C6	1.385(5)	N1	C24	1.371(4)
C5	C10	1.391(5)	C24	C25	1.408(4)
C6	C7	1.390(6)	C24	C29	1.403(5)

Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C25	C26	1.404(5)	C38	C39	1.382(5)
C25	N2	1.372(4)	C40	C41	1.398(5)
C26	C27	1.352(5)	C40	C45	1.388(5)
C27	C28	1.390(6)	C41	C42	1.382(5)
C28	C29	1.357(5)	C42	C43	1.367(5)
C30	O4	1.153(4)	C43	C44	1.360(6)
C31	O5	1.146(5)	C44	C45	1.381(5)
C32	O6	1.152(4)	C46	C47	1.431(5)
C33	C34	1.520(5)	C46	C51	1.444(5)
C33	C40	1.520(5)	C47	C48	1.356(5)
C33	C46	1.462(5)	C48	C49	1.391(5)
C34	C35	1.387(5)	C49	C50	1.353(5)
C34	C39	1.388(5)	C50	C51	1.413(5)
C35	C36	1.388(5)	C51	C52	1.485(4)
C36	C37	1.366(7)	C52	N2	1.325(4)
C37	C38	1.365(7)			

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Table of Bond Angles in Degrees

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C1	MN1	C2	86.7(2)	C31	MN2	C33	167.6(2)
C1	MN1	C3	85.0(2)	C31	MN2	C46	129.2(2)
C1	MN1	C4	94.8(2)	C31	MN2	N2	91.7(2)
C1	MN1	C17	89.3(1)	C32	MN2	C33	97.3(2)
C1	MN1	N1	173.7(2)	C32	MN2	C46	135.4(2)
C2	MN1	C3	96.6(2)	C32	MN2	N2	99.9(1)
C2	MN1	C4	162.2(2)	C33	MN2	C46	39.0(1)
C2	MN1	C17	123.4(2)	C33	MN2	N2	84.2(1)
C2	MN1	N1	91.8(2)	C46	MN2	N2	86.2(1)
C3	MN1	C4	101.3(2)	MN1	C1	O1	175.6(4)
C3	MN1	C17	139.2(2)	MN1	C2	O2	175.1(4)
C3	MN1	N1	101.3(1)	MN1	C3	O3	175.2(4)
C4	MN1	C17	39.0(1)	MN1	C4	C5	122.5(2)
C4	MN1	N1	84.8(1)	MN1	C4	C11	115.9(2)
C17	MN1	N1	86.4(1)	MN1	C4	C17	72.1(2)
C30	MN2	C31	87.8(2)	C5	C4	C11	107.4(3)
C30	MN2	C32	86.8(2)	C5	C4	C17	116.7(3)
C30	MN2	C33	94.9(2)	C11	C4	C17	119.3(3)
C30	MN2	C46	88.9(1)	C4	C5	C6	123.6(4)
C30	MN2	N2	173.2(1)	C4	C5	C10	119.3(3)
C31	MN2	C32	94.9(2)	C6	C5	C10	117.0(4)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C5	C6	C7	121.2(4)	C19	C20	C21	119.6(4)
C6	C7	C8	120.9(4)	C20	C21	C22	121.3(4)
C7	C8	C9	119.3(4)	C17	C22	C21	120.7(3)
C8	C9	C10	120.4(4)	C17	C22	C23	119.9(3)
C5	C10	C9	121.2(4)	C21	C22	C23	119.2(3)
C4	C11	C12	122.1(3)	C22	C23	N1	111.4(3)
C4	C11	C16	120.4(3)	C22	C23	C52	127.6(3)
C12	C11	C16	117.3(3)	N1	C23	C52	121.0(3)
C11	C12	C13	121.3(3)	MN1	N1	C23	102.7(2)
C12	C13	C14	119.9(4)	MN1	N1	C24	138.3(2)
C13	C14	C15	120.0(4)	C23	N1	C24	119.0(3)
C14	C15	C16	120.2(4)	N1	C24	C25	119.8(3)
C11	C16	C15	121.3(3)	N1	C24	C29	121.1(3)
MN1	C17	C4	68.9(2)	C25	C24	C29	119.1(3)
MN1	C17	C18	116.6(2)	C24	C25	C26	119.3(3)
MN1	C17	C22	79.5(2)	C24	C25	N2	119.6(3)
C4	C17	C18	122.4(3)	C26	C25	N2	121.0(3)
C4	C17	C22	122.8(3)	C25	C26	C27	119.7(3)
C18	C17	C22	114.1(3)	C26	C27	C28	121.0(4)
C17	C18	C19	123.3(3)	C27	C28	C29	120.7(4)
C18	C19	C20	120.9(3)	C24	C29	C28	119.8(3)

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Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
MN2	C30	O4	176.2(4)	C41	C42	C43	119.8(4)
MN2	C31	O5	174.8(4)	C42	C43	C44	119.8(4)
MN2	C32	O6	177.5(3)	C43	C44	C45	120.5(4)
MN2	C33	C34	114.6(2)	C40	C45	C44	121.7(4)
MN2	C33	C40	123.4(2)	MN2	C46	C33	68.1(2)
MN2	C33	C46	72.9(2)	MN2	C46	C47	119.8(2)
C34	C33	C40	105.6(3)	MN2	C46	C51	78.2(2)
C34	C33	C46	120.5(3)	C33	C46	C47	122.4(3)
C40	C33	C46	118.0(3)	C33	C46	C51	122.4(3)
C33	C34	C35	121.9(3)	C47	C46	C51	114.6(3)
C33	C34	C39	120.1(3)	C46	C47	C48	122.8(4)
C35	C34	C39	117.7(3)	C47	C48	C49	121.3(3)
C34	C35	C36	120.6(4)	C48	C49	C50	119.4(4)
C35	C36	C37	120.2(4)	C49	C50	C51	121.4(4)
C36	C37	C38	120.4(4)	C46	C51	C50	120.5(3)
C37	C38	C39	119.6(4)	C46	C51	C52	119.3(3)
C34	C39	C38	121.5(4)	C50	C51	C52	120.0(3)
C33	C40	C41	119.4(3)	C23	C52	C51	127.8(3)
C33	C40	C45	123.6(3)	C23	C52	N2	120.7(3)
C41	C40	C45	116.1(4)	C51	C52	N2	111.6(3)
C40	C41	C42	122.0(3)	MN2	N2	C25	138.3(2)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
MN2	N2	C52	102.3(2)	C25	N2	C52	119.2(3)

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Compound 3d

Table 1 : X-ray experimental data for 3d

Formula	: C53H30Cl2Mn2N2O6 : C52H28Mn2N2O6•CH2Cl2
Molecular weight	: 971.62
Crystal system	: orthorhombic
Space group	: P b c a
a(Å)	: 14.8379(2)
b(Å)	: 35.4532(3)
c(Å)	: 16.3323(5)
V(Å3)	: 8591.6(3)
Z	: 8
Color	: yellow
Crystal dim(mm)	: 0.16*0.13*0.10
Dcalc(gcm-3)	: 1.50
F000	: 3952
$\mu(mm^{-1})$	: 0.769
Trans. min and max	: 0.8063/1.0000
Temperature(K)	: 173
Wavelength(Å)	: 0.71073
Radiation	: MoKα graphite monochromated
Diffractometer	: KappaCCD
Scan mode	: 'phi scans'
hkl limits	: -19,19/-21,21/-45,45
Theta limits(deg)	: 2.5/27.48
Number of data meas.	: 19157
Number of data with I > 3 σ(I)	: 3614
Number of variables	: 586
R	: 0.051
Rw	: 0.082
GOF	: 1.415
Largest peak in final difference ($eÅ^{-3}$)	: 0.589

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Table of Positional Parameters and Their E.S.D.

Atom	x	y	z	Ueqv
MN1	1.13242(8)	0.10226(3)	0.49421(7)	0.0201(5)
MN2	0.55251(8)	0.08461(3)	0.51944(7)	0.0196(5)
C1	1.2370(5)	0.1006(2)	0.4352(4)	0.024(4)
O1	1.3022(4)	0.0986(1)	0.3987(3)	0.037(3)
C2	1.1858(6)	0.1238(2)	0.5789(5)	0.039(5)
O2	1.2194(5)	0.1378(2)	0.6358(3)	0.071(4)
C3	1.1507(5)	0.0571(2)	0.5371(5)	0.026(4)
O3	1.1626(4)	0.0277(1)	0.5676(4)	0.044(4)
C4	0.5151(5)	0.1112(2)	0.4302(5)	0.023(4)
O4	0.4960(4)	0.1284(1)	0.3741(3)	0.037(3)
C5	0.5484(5)	0.0436(2)	0.4580(4)	0.026(4)
O5	0.5476(4)	0.0163(1)	0.4184(3)	0.037(3)
C6	0.4409(5)	0.0758(2)	0.5549(5)	0.027(4)
O6	0.3686(4)	0.0697(1)	0.5773(3)	0.039(3)
C7	1.0329(5)	0.1478(2)	0.4913(4)	0.018(4)
C8	1.0448(5)	0.1829(2)	0.5346(4)	0.024(4)
C9	1.0870(6)	0.2112(2)	0.4955(5)	0.031(4)
C10	1.1204(6)	0.2072(2)	0.4142(5)	0.033(5)
C11	1.1139(5)	0.1750(2)	0.3731(5)	0.031(4)
C12	1.0697(5)	0.1447(2)	0.4108(4)	0.017(4)
C13	1.0515(5)	0.1070(2)	0.3813(4)	0.021(4)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C14	0.9991(5)	0.0885(2)	0.4432(4)	0.019(4)
C15	0.9912(5)	0.1118(2)	0.5138(4)	0.018(4)
C16	1.0682(5)	0.0895(2)	0.3055(4)	0.024(4)
C17	1.0359(6)	0.0543(2)	0.2927(5)	0.031(4)
C18	0.9840(6)	0.0355(2)	0.3530(5)	0.031(5)
C19	0.9657(5)	0.0507(2)	0.4266(4)	0.023(4)
C20	0.9341(5)	0.1039(2)	0.5860(4)	0.020(4)
C21	0.9433(5)	0.0687(2)	0.6265(4)	0.024(4)
C22	0.8922(5)	0.0590(2)	0.6941(4)	0.026(4)
C23	0.8305(5)	0.0847(2)	0.7260(4)	0.024(4)
C24	0.8199(5)	0.1191(2)	0.6884(4)	0.021(4)
C25	0.8680(5)	0.1291(2)	0.6168(4)	0.021(4)
C26	0.8484(5)	0.1671(2)	0.5805(5)	0.019(4)
N1	0.8608(4)	0.1950(1)	0.6342(3)	0.025(3)
C27	0.8533(5)	0.2310(2)	0.6048(5)	0.026(4)
C28	0.8326(5)	0.2375(2)	0.5220(5)	0.023(4)
N2	0.8148(4)	0.2078(1)	0.4698(4)	0.023(3)
C29	0.8214(5)	0.1735(2)	0.4979(4)	0.017(4)
C30	0.8695(6)	0.2620(2)	0.6580(5)	0.034(5)
C31	0.8691(6)	0.2974(2)	0.6296(5)	0.044(5)
C32	0.8503(6)	0.3037(2)	0.5474(6)	0.032(5)

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Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C33	0.8321(6)	0.2744(2)	0.4930(5)	0.034(5)
C34	0.8039(5)	0.1437(2)	0.4353(4)	0.018(4)
C35	0.8498(5)	0.1478(2)	0.3608(4)	0.021(4)
C36	0.8422(5)	0.1228(2)	0.2993(4)	0.024(4)
C37	0.7876(6)	0.0923(2)	0.3078(4)	0.025(4)
C38	0.7390(5)	0.0879(2)	0.3788(4)	0.025(4)
C39	0.7449(5)	0.1123(2)	0.4447(4)	0.015(4)
C40	0.6272(5)	0.0740(2)	0.6325(4)	0.024(4)
C41	0.6145(6)	0.0438(2)	0.6883(5)	0.031(5)
C42	0.6589(6)	0.0103(2)	0.6746(5)	0.032(5)
C43	0.7170(6)	0.0065(2)	0.6072(5)	0.030(5)
C44	0.7311(5)	0.0355(2)	0.5519(5)	0.026(4)
C45	0.6868(5)	0.0704(2)	0.5645(4)	0.018(4)
C46	0.6881(5)	0.1058(2)	0.5183(4)	0.014(4)
C47	0.6345(5)	0.1326(2)	0.5642(4)	0.019(4)
C48	0.5943(5)	0.1128(2)	0.6332(4)	0.019(4)
C49	0.6099(5)	0.1708(2)	0.5501(5)	0.026(4)
C50	0.5540(6)	0.1887(2)	0.6038(5)	0.031(5)
C51	0.5173(6)	0.1698(2)	0.6719(5)	0.035(5)
C52	0.5357(5)	0.1336(2)	0.6872(4)	0.028(5)
C53	0.6998(6)	0.2283(2)	0.3042(5)	0.046(5)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
CL1	0.6855(2)	0.27600(6)	0.2841(2)	0.083(2)
CL2	0.6010(2)	0.20618(8)	0.3354(2)	0.075(2)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as one third of the trace of the orthogonalized Uij tensor.

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Table of Positional Parameters

Atom	x	y	z	Ueqv	
H1	1.0234	0.1859	0.5891	0.0317	*
H2	1.0949	0.2346	0.5229	0.0428	*
H3	1.1482	0.2282	0.3885	0.0451	*
H4	1.1385	0.1725	0.3196	0.0419	*
H5	1.1015	0.1022	0.2641	0.0330	*
H6	1.0483	0.0420	0.2423	0.0412	*
H7	0.9611	0.0111	0.3409	0.0403	*
H8	0.9320	0.0372	0.4665	0.0301	*
H9	0.9863	0.0512	0.6064	0.0316	*
H10	0.8992	0.0349	0.7186	0.0334	*
H11	0.7961	0.0785	0.7732	0.0338	*
H12	0.7789	0.1368	0.7113	0.0275	*
H13	0.8807	0.2575	0.7144	0.0448	*
H14	0.8815	0.3179	0.6651	0.0575	*
H15	0.8498	0.3289	0.5276	0.0614	*
H16	0.8196	0.2796	0.4371	0.0465	*
H17	0.8878	0.1691	0.3536	0.0285	*
H18	0.8750	0.1265	0.2500	0.0325	*
H19	0.7831	0.0742	0.2651	0.0341	*
H20	0.6993	0.0670	0.3829	0.0331	*
H21	0.5759	0.0467	0.7343	0.0408	*

Table of Positional Parameters (cont.)

Atom	x	y	z	Ueqv	
H22	0.6503	-0.0104	0.7109	0.0425	*
H23	0.7477	-0.0167	0.5992	0.0427	*
H24	0.7698	0.0320	0.5062	0.0364	*
H25	0.6324	0.1838	0.5035	0.0339	*
H26	0.5394	0.2145	0.5951	0.0448	*
H27	0.4785	0.1832	0.7080	0.0463	*
H28	0.5101	0.1215	0.7337	0.0401	*
H29	0.7435	0.2256	0.3464	0.0603	*
H30	0.7209	0.2163	0.2559	0.0603	*

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Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
MN1	.0197(6)	.0200(5)	.0207(6)	.0022(5)	.0008(6)	.0009(5)
MN2	.0177(6)	.0222(5)	.0192(5)	-.0020(5)	-.0004(6)	-.0004(5)
C1	.032(5)	.015(3)	.027(4)	-.000(4)	-.005(4)	.006(3)
O1	.024(3)	.056(3)	.036(3)	-.001(3)	.012(3)	-.001(3)
C2	.033(5)	.044(4)	.040(5)	.021(4)	-.017(5)	-.003(4)
O2	.095(5)	.069(4)	.054(4)	.038(4)	-.048(4)	-.027(3)
C3	.021(5)	.023(4)	.038(5)	-.001(4)	.002(4)	-.004(3)
O3	.031(4)	.044(3)	.063(4)	.003(3)	.005(4)	.016(3)
C4	.015(4)	.021(3)	.037(4)	-.008(3)	.004(4)	-.012(3)
O4	.043(4)	.047(3)	.025(3)	.003(3)	-.012(3)	.014(3)
C5	.026(5)	.024(4)	.027(4)	-.007(4)	.002(4)	.005(3)
O5	.048(4)	.028(3)	.038(3)	-.008(3)	-.000(3)	-.009(2)
C6	.018(5)	.043(4)	.026(4)	-.007(4)	-.008(4)	-.002(4)
O6	.024(3)	.079(4)	.032(3)	-.009(3)	.000(3)	-.008(3)
C7	.018(4)	.011(3)	.029(4)	.006(3)	-.002(4)	.007(3)
C8	.019(4)	.033(4)	.021(4)	.006(4)	-.000(4)	-.003(3)
C9	.030(5)	.019(3)	.050(5)	-.004(4)	-.005(5)	.004(4)
C10	.032(5)	.022(4)	.050(5)	-.005(4)	.007(5)	.015(4)
C11	.021(5)	.042(4)	.033(5)	-.005(4)	.010(4)	.013(4)
C12	.019(4)	.012(3)	.024(4)	.000(3)	.004(4)	.003(3)
C13	.018(4)	.025(4)	.020(4)	.012(3)	.002(4)	.007(3)
C14	.020(4)	.021(3)	.016(4)	.004(4)	-.001(4)	.002(3)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C15	.020(4)	.022(3)	.014(4)	-.001(3)	.001(4)	.002(3)
C16	.029(5)	.031(4)	.016(4)	.007(4)	-.001(4)	-.002(3)
C17	.042(6)	.030(4)	.023(4)	.012(4)	.007(4)	-.003(3)
C18	.030(5)	.031(4)	.031(5)	.005(4)	-.011(5)	-.011(4)

C19	.021(5)	.025(4)	.024(4)	.001(4)	-.001(4)	.001(3)
C20	.018(4)	.020(3)	.022(4)	.001(3)	-.003(4)	.001(3)
C21	.022(5)	.033(4)	.019(4)	-.001(4)	-.002(4)	-.002(3)
C22	.029(5)	.023(4)	.025(4)	-.001(4)	-.004(4)	.006(3)
C23	.017(4)	.043(4)	.018(4)	-.006(4)	-.003(4)	-.000(4)
C24	.018(4)	.029(4)	.017(4)	.003(4)	-.003(4)	-.009(3)
C25	.020(4)	.025(3)	.020(4)	-.005(4)	-.003(4)	-.005(3)
C26	.009(4)	.029(4)	.026(4)	.000(3)	.005(4)	.002(3)
N1	.028(4)	.027(3)	.021(3)	-.003(3)	-.001(4)	-.006(3)
C27	.019(5)	.023(4)	.039(5)	.001(4)	.010(4)	.001(3)
C28	.019(4)	.016(3)	.040(5)	-.002(3)	.004(4)	-.003(3)
N2	.022(4)	.019(3)	.031(4)	.000(3)	-.002(3)	.006(3)
C29	.008(4)	.024(3)	.024(4)	.003(3)	.003(4)	-.001(3)
C30	.035(5)	.027(4)	.041(5)	-.007(4)	.009(5)	-.018(4)
C31	.045(6)	.036(4)	.051(5)	.001(5)	.001(6)	-.014(4)
C32	.031(5)	.011(4)	.100(7)	-.002(4)	.015(6)	-.005(4)
C33	.032(5)	.024(4)	.051(5)	.002(4)	.003(5)	.004(4)
C34	.019(4)	.014(3)	.023(4)	.000(3)	-.007(4)	.003(3)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C35	.030(5)	.021(3)	.015(4)	-.001(4)	.003(4)	.010(3)
C36	.027(5)	.033(4)	.015(4)	-.004(4)	.002(4)	.008(3)
C37	.036(5)	.028(4)	.015(4)	.008(4)	.000(4)	-.003(3)
C38	.027(5)	.020(4)	.030(4)	-.003(4)	-.002(4)	-.007(3)
C39	.013(4)	.020(3)	.013(3)	.004(3)	.002(4)	.000(3)
C40	.021(4)	.029(4)	.023(4)	-.002(4)	-.001(4)	.002(3)
C41	.028(5)	.040(4)	.026(4)	-.004(4)	.007(4)	.008(4)
C42	.035(5)	.026(4)	.037(5)	-.002(4)	.001(5)	.004(4)
C43	.039(5)	.017(4)	.042(5)	.010(4)	.007(5)	-.001(4)
C44	.016(4)	.039(4)	.029(4)	.003(4)	-.001(4)	-.009(4)
C45	.010(4)	.026(4)	.024(4)	-.002(3)	-.000(4)	-.006(3)

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C46	.015(4)	.009(3)	.020(4)	-.005(3)	-.004(4)	-.002(3)
C47	.011(4)	.031(4)	.020(4)	.001(4)	-.002(4)	-.003(3)
C48	.022(4)	.015(3)	.019(4)	-.001(3)	.003(4)	-.000(3)
C49	.021(5)	.030(4)	.027(4)	-.000(4)	-.001(4)	.003(4)
C50	.034(5)	.017(4)	.052(5)	-.000(4)	.012(5)	.005(4)
C51	.026(5)	.034(4)	.047(5)	.005(4)	.005(5)	-.009(4)
C52	.016(5)	.050(5)	.026(4)	-.007(4)	.011(4)	-.001(4)
C53	.046(6)	.057(5)	.035(5)	-.017(5)	-.001(5)	.005(4)
CL1	.130(3)	.062(1)	.071(2)	.030(2)	.028(2)	.018(1)
CL2	.074(2)	.128(2)	.044(2)	-.048(2)	.015(2)	-.011(2)

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
MN1	C1	1.83(1)	C8	C9	1.34(1)
MN1	C2	1.77(1)	C9	C10	1.42(1)
MN1	C3	1.768(9)	C10	C11	1.33(1)
MN1	C7	2.190(7)	C11	C12	1.40(1)
MN1	C15	2.147(8)	C12	C13	1.45(1)
MN2	C4	1.821(9)	C13	C14	1.43(1)
MN2	C5	1.768(8)	C13	C16	1.41(1)
MN2	C6	1.781(9)	C14	C15	1.42(1)
MN2	C40	2.185(8)	C14	C19	1.46(1)
MN2	C45	2.183(8)	C15	C20	1.48(1)
MN2	C46	2.148(8)	C16	C17	1.35(1)
MN2	C48	2.199(7)	C17	C18	1.42(1)
C1	O1	1.139(9)	C18	C19	1.35(1)
C2	O2	1.17(1)	C20	C21	1.42(1)
C3	O3	1.169(9)	C20	C25	1.42(1)
C4	O4	1.138(9)	C21	C22	1.38(1)
C5	O5	1.163(9)	C22	C23	1.39(1)
C6	O6	1.15(1)	C23	C24	1.38(1)
C7	C8	1.44(1)	C24	C25	1.41(1)
C7	C12	1.43(1)	C25	C26	1.50(1)
C7	C15	1.47(1)	C26	N1	1.334(9)

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Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C26	C29	1.42(1)	C40	C41	1.42(1)
N1	C27	1.370(9)	C40	C45	1.43(1)
C27	C28	1.41(1)	C40	C48	1.46(1)
C27	C30	1.42(1)	C41	C42	1.38(1)
C28	N2	1.38(1)	C42	C43	1.41(1)
C28	C33	1.39(1)	C43	C44	1.38(1)
N2	C29	1.307(9)	C44	C45	1.42(1)
C29	C34	1.49(1)	C45	C46	1.47(1)
C30	C31	1.34(1)	C46	C47	1.45(1)
C31	C32	1.39(1)	C47	C48	1.46(1)
C32	C33	1.39(1)	C47	C49	1.42(1)
C34	C35	1.40(1)	C48	C52	1.44(1)
C34	C39	1.42(1)	C49	C50	1.36(1)
C35	C36	1.34(1)	C50	C51	1.41(1)
C36	C37	1.36(1)	C51	C52	1.34(1)
C37	C38	1.37(1)	C53	CL1	1.736(9)
C38	C39	1.38(1)	C53	CL2	1.74(1)
C39	C46	1.49(1)			

Table of Bond Angles in Degrees

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C1	MN1	C2	92.7(4)	C6	MN2	C40	99.6(3)
C1	MN1	C3	92.9(4)	C6	MN2	C45	134.3(3)
C1	MN1	C7	125.8(3)	C6	MN2	C46	159.2(3)
C1	MN1	C15	155.8(3)	C6	MN2	C48	93.9(3)
C2	MN1	C3	90.7(4)	C40	MN2	C45	38.1(3)
C2	MN1	C7	90.0(3)	C40	MN2	C46	65.9(3)
C2	MN1	C15	104.6(4)	C40	MN2	C48	38.9(3)
C3	MN1	C7	141.3(3)	C45	MN2	C46	39.6(3)
C3	MN1	C15	103.5(3)	C45	MN2	C48	64.1(3)
C7	MN1	C15	39.5(3)	C46	MN2	C48	65.4(3)
C4	MN2	C5	87.7(3)	MN1	C1	O1	178.3(7)
C4	MN2	C6	93.9(4)	MN1	C2	O2	178(1)
C4	MN2	C40	156.8(3)	MN1	C3	O3	178.1(8)
C4	MN2	C45	131.9(3)	MN2	C4	O4	176.6(7)
C4	MN2	C46	95.6(3)	MN2	C5	O5	178.4(8)
C4	MN2	C48	121.8(3)	MN2	C6	O6	179.3(8)
C5	MN2	C6	90.4(4)	MN1	C7	C8	122.9(6)
C5	MN2	C40	110.8(3)	MN1	C7	C12	72.8(4)
C5	MN2	C45	91.9(3)	MN1	C7	C15	68.7(4)
C5	MN2	C46	108.4(3)	C8	C7	C12	118.2(7)
C5	MN2	C48	149.7(3)	C8	C7	C15	132.8(7)

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Bond Angles (cont.)

At 1	At 2	At 3	Angle
C12	C7	C15	108.9(6)
C7	C8	C9	117.8(7)
C8	C9	C10	122.0(8)
C9	C10	C11	122.2(7)
C10	C11	C12	118.0(8)
C7	C12	C11	121.6(7)
C7	C12	C13	107.9(6)
C11	C12	C13	130.5(8)
C12	C13	C14	106.8(7)
C12	C13	C16	131.9(7)
C14	C13	C16	121.0(7)
C13	C14	C15	110.5(6)
C13	C14	C19	118.3(7)
C15	C14	C19	131.1(7)
MN1	C15	C7	71.8(4)
MN1	C15	C14	73.0(5)
MN1	C15	C20	130.4(5)
C7	C15	C14	105.5(6)
C7	C15	C20	127.4(6)
C14	C15	C20	125.7(7)
C13	C16	C17	118.7(8)
C16	C17	C18	121.3(7)
C17	C18	C19	122.8(7)
C14	C19	C18	117.8(8)
C15	C20	C21	118.9(7)
C15	C20	C25	124.0(6)
C21	C20	C25	117.0(7)
C20	C21	C22	122.6(7)
C21	C22	C23	119.7(7)
C22	C23	C24	119.2(7)
C23	C24	C25	122.2(7)
C20	C25	C24	119.0(7)
C20	C25	C26	123.9(7)
C24	C25	C26	117.0(7)
C25	C26	N1	112.2(7)
C25	C26	C29	124.8(7)
N1	C26	C29	122.9(7)
C26	N1	C27	116.8(7)
N1	C27	C28	120.3(7)
N1	C27	C30	119.6(8)
C28	C27	C30	120.0(7)
C27	C28	N2	120.9(7)

Bond Angles (cont.)

At 1	At 2	At 3	Angle
C27	C28	C33	118.7(7)
N2	C28	C33	120.4(8)
C28	N2	C29	118.7(7)
C26	C29	N2	120.1(7)
C26	C29	C34	125.8(7)
N2	C29	C34	114.0(7)
C27	C30	C31	120.8(9)
C30	C31	C32	119.2(8)
C31	C32	C33	122.3(8)
C28	C33	C32	119.0(9)
C29	C34	C35	115.7(6)
C29	C34	C39	125.9(7)
C35	C34	C39	118.3(7)
C34	C35	C36	122.6(7)
C35	C36	C37	119.9(7)
C36	C37	C38	119.2(7)
C37	C38	C39	123.6(7)
C34	C39	C38	116.3(7)
C34	C39	C46	123.7(6)
C38	C39	C46	119.9(7)
MN2	C40	C41	127.2(6)
MN2	C40	C45	70.8(4)
MN2	C40	C48	71.1(4)
C41	C40	C45	121.0(7)
C41	C40	C48	131.4(8)
C45	C40	C48	107.5(6)
C40	C41	C42	119.0(8)
C41	C42	C43	120.1(7)
C42	C43	C44	122.3(7)
C43	C44	C45	119.0(8)
MN2	C45	C40	71.1(5)
MN2	C45	C44	125.2(6)
MN2	C45	C46	68.9(4)
C40	C45	C44	118.7(7)
C40	C45	C46	109.3(6)
C44	C45	C46	131.9(7)
MN2	C46	C39	126.3(5)
MN2	C46	C45	71.5(4)
MN2	C46	C47	73.2(4)
C39	C46	C45	123.7(6)
C39	C46	C47	129.0(6)
C45	C46	C47	106.8(6)

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Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C46	C47	C48	108.0(6)	C40	C48	C52	133.5(7)
C46	C47	C49	133.0(7)	C47	C48	C52	118.3(7)
C48	C47	C49	118.7(7)	C47	C49	C50	119.7(7)
MN2	C48	C40	70.1(4)	C49	C50	C51	121.5(7)
MN2	C48	C47	71.4(4)	C50	C51	C52	121.8(8)
MN2	C48	C52	125.4(6)	C48	C52	C51	120.0(7)
C40	C48	C47	108.1(7)	CL1	C53	CL2	113.1(6)

Compound **3e**

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Table 1 : X-ray experimental data for **3e**

Formula	: $C_{55}H_{39}AgBF_4Mn_2N_2O_9$:$C_{53}H_{31}AgMn_2N_2O_6 \cdot BF_4 \cdot 2CH_3OH$
Molecular weight	: 1176.48
Crystal system	: orthorhombic
Space group	: P 2_1 2_1 2_1
a(Å)	: 13.6186(5)
b(Å)	: 15.1375(7)
c(Å)	: 25.032(1)
V(A3)	: 5160.5(4)
Z	: 4
Color	: red
Crystal dim(mm)	: 0.12*0.10*0.08
Dcalc(gcm^{-3})	: 1.51
F000	: 2372
μ(mm^{-1})	: 0.930
Trans. min and max	: 0.8920/0.928
Temperature(K)	: 173
Wavelength(Å)	: 0.71073
Radiation	: MoKα graphite monochromated
Diffractometer	: KappaCCD
Scan mode	: 'phi scans'
hkl limits	: -17,17/-19,19/-32,32
Theta limits(deg)	: 2.5/27.48
Number of data meas.	: 11811
Number of data with I > 3 σ(I)	: 3656
Number of variables	: 634
R	: 0.058
Rw	: 0.080
GOF	: 1.513
Largest peak in final difference ($eÅ^{-3}$)	: 0.959

Table of Positional Parameters and Their E.S.D.

Atom	x	y	z	Ueqv
AG	0.84699(6)	0.29846(6)	0.45854(3)	0.0347(4)
MN1	0.7833(1)	-0.1075(1)	0.51419(6)	0.0357(8)
MN2	0.4117(1)	0.1737(1)	0.29627(6)	0.0353(8)
C1	0.8275(9)	-0.1896(8)	0.4711(5)	0.051(7)
O1	0.8518(7)	-0.2439(7)	0.4402(3)	0.087(6)
C2	0.8963(8)	-0.0483(7)	0.5111(4)	0.037(6)
O2	0.9692(6)	-0.0091(6)	0.5080(3)	0.058(5)
C3	0.827(1)	-0.1716(9)	0.5724(4)	0.057(7)
O3	0.8545(6)	-0.2095(6)	0.6076(3)	0.065(5)
C4	0.2957(9)	0.1952(8)	0.3277(4)	0.045(6)
O4	0.7228(6)	0.2913(6)	0.6500(3)	0.062(5)
C5	0.3819(8)	0.2382(9)	0.2410(4)	0.046(6)
O5	0.8634(8)	0.2141(6)	0.7967(3)	0.078(6)
C6	0.3592(8)	0.0799(8)	0.2662(4)	0.043(6)
O6	0.8237(7)	0.4836(6)	0.7527(3)	0.073(6)
C7	0.7275(7)	0.0492(7)	0.4310(4)	0.033(5)
C8	0.7840(7)	0.0126(8)	0.3881(4)	0.037(6)
C9	0.8126(9)	0.0588(9)	0.3445(4)	0.049(7)
C10	0.7894(8)	0.1476(8)	0.3410(4)	0.046(6)
C11	0.7360(7)	0.1871(7)	0.3815(4)	0.031(5)
C12	0.7024(7)	0.1410(7)	0.4265(3)	0.027(5)

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Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C13	0.6477(7)	0.1913(7)	0.4646(3)	0.034(5)
N1	0.6927(6)	0.2639(6)	0.4830(3)	0.031(4)
C14	0.6458(6)	0.3168(7)	0.5193(4)	0.025(5)
C15	0.6916(8)	0.3939(8)	0.5392(4)	0.046(6)
C16	0.6472(8)	0.4462(7)	0.5763(4)	0.036(6)
C17	0.5534(8)	0.4220(8)	0.5949(4)	0.042(6)
C18	0.5092(8)	0.3493(8)	0.5785(4)	0.039(6)
C19	0.5511(7)	0.2940(6)	0.5381(3)	0.027(5)
N2	1.0063(5)	0.2765(6)	0.4832(3)	0.029(4)
C20	0.5494(7)	0.1721(7)	0.4814(3)	0.026(5)
C21	0.4918(6)	0.0945(7)	0.4639(4)	0.027(5)
C22	0.4593(7)	0.0390(7)	0.5048(4)	0.028(5)
C23	0.4051(8)	-0.0384(7)	0.4930(4)	0.042(6)
C24	0.3828(8)	-0.0571(7)	0.4412(5)	0.040(6)
C25	0.4106(8)	-0.0003(7)	0.4008(4)	0.037(6)
C26	0.4660(7)	0.0767(7)	0.4117(4)	0.027(5)
O7	0.8428(9)	0.3850(7)	0.3819(3)	0.094(7)
C27	0.910(2)	0.374(1)	0.3332(7)	0.14(2)
C28	0.6961(7)	-0.0098(7)	0.4743(4)	0.030(5)
C29	0.6492(7)	-0.0944(7)	0.4667(3)	0.035(5)
C30	0.6232(8)	-0.1418(8)	0.4193(4)	0.042(6)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C31	0.5817(9)	-0.2212(9)	0.4236(4)	0.053(7)
C32	1.060(1)	0.7598(9)	0.5259(5)	0.062(8)
C33	0.5806(9)	-0.2155(8)	0.5193(4)	0.054(7)
C34	0.6249(7)	-0.1320(7)	0.5160(4)	0.038(6)
C35	0.6493(8)	-0.0653(8)	0.5576(4)	0.040(6)
C36	0.6334(9)	-0.0668(9)	0.6136(4)	0.051(7)
C37	0.659(1)	0.0045(9)	0.6407(4)	0.053(7)
C38	0.705(1)	0.0787(9)	0.6188(4)	0.052(7)
C39	0.7238(8)	0.0832(7)	0.5632(4)	0.041(6)
C40	0.6916(7)	0.0083(7)	0.5309(4)	0.030(5)
C41	0.4936(7)	0.1309(7)	0.3667(4)	0.029(5)
C42	0.4984(8)	0.2275(7)	0.3643(4)	0.037(6)
C43	0.4631(8)	0.2946(7)	0.3969(4)	0.038(6)
C44	0.478(1)	0.3802(8)	0.3856(4)	0.050(7)
C45	0.5291(9)	0.4072(9)	0.3391(5)	0.061(8)
C46	0.560(1)	0.3448(9)	0.3004(4)	0.056(7)
C47	0.5439(7)	0.2513(8)	0.3122(4)	0.038(6)
C48	0.5697(9)	0.1734(7)	0.2823(4)	0.043(6)
C49	0.6191(8)	0.1612(9)	0.2364(4)	0.050(7)
C50	0.641(1)	0.078(1)	0.2207(4)	0.062(8)
C51	0.617(1)	0.0026(9)	0.2521(4)	0.058(7)

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Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv	
C52	0.5678(8)	0.0118(8)	0.2998(4)	0.042(6)	
C53	0.5437(7)	0.0993(8)	0.3168(4)	0.037(6)	
C54	0.931(2)	-0.380(2)	0.2690(9)	0.18(1)	*
O8	0.869(2)	-0.332(1)	0.3134(7)	0.211(8)	*
C55	0.297(2)	0.071(2)	0.1012(9)	0.17(1)	*
O9	0.191(1)	0.053(1)	0.1221(6)	0.154(5)	*
B1	0.324(2)	0.154(2)	0.8209(8)	0.111(7)	*
F1	0.338(3)	0.242(2)	0.820(1)	0.20(1)	*
F2	0.391(1)	0.0834(9)	0.8104(5)	0.153(4)	*
F3	0.217(2)	0.139(2)	0.8197(8)	0.131(7)	*
F4	0.328(2)	0.167(1)	0.8739(7)	0.111(6)	*
F1a	0.320(2)	0.201(1)	0.7796(7)	0.110(6)	*
F3A	0.265(2)	0.121(2)	0.8510(7)	0.123(7)	*
F4a	0.404(2)	0.221(2)	0.8490(9)	0.151(9)	*

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as one third of the trace of the orthogonalized Uij tensor. Starred atoms were refined isotropically.

Table of Positional Parameters

Atom	x	y	z	Ueqv	
H1	0.8025	-0.0478	0.3904	0.0507	*
H2	0.8482	0.0307	0.3167	0.0654	*
H3	0.8100	0.1812	0.3110	0.0606	*
H4	0.7214	0.2483	0.3787	0.0444	*
H5	0.7548	0.4097	0.5263	0.0603	*
H6	0.6787	0.4978	0.5892	0.0506	*
H7	0.5211	0.4589	0.6201	0.0560	*
H8	0.4480	0.3332	0.5938	0.0525	*
H9	0.4737	0.0533	0.5409	0.0425	*
H10	0.3846	-0.0768	0.5209	0.0555	*
H11	0.3480	-0.1097	0.4327	0.0603	*
H12	0.3921	-0.0131	0.3650	0.0484	*
H13	0.6354	-0.1169	0.3851	0.0555	*
H14	0.5661	-0.2529	0.3920	0.0728	*
H15	0.5309	-0.3168	0.4759	0.0805	*
H16	0.5655	-0.2405	0.5531	0.0711	*
H17	0.6056	-0.1168	0.6308	0.0687	*
H18	0.6457	0.0052	0.6780	0.0740	*
H19	0.7229	0.1265	0.6413	0.0780	*
H20	0.7561	0.1326	0.5477	0.0535	*
H21	0.4274	0.2795	0.4282	0.0501	*

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Table of Positional Parameters (cont.)

Atom	x	y	z	Ueqv	
H22	0.4538	0.4239	0.4094	0.0664	*
H23	0.5425	0.4681	0.3337	0.0870	*
H24	0.5908	0.3630	0.2681	0.0725	*
H25	0.6383	0.2103	0.2153	0.0679	*
H26	0.6737	0.0693	0.1876	0.0875	*
H27	0.6358	-0.0546	0.2400	0.0790	*
H28	0.5504	-0.0382	0.3207	0.0578	*

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
AG	.0195(3)	.0449(4)	.0478(4)	-.0001(4)	-.0006(4)	.0004(4)
MN1	.0287(8)	.0365(9)	.0432(8)	.0045(9)	-.0049(8)	-.0031(8)
MN2	.0302(8)	.0420(9)	.0347(7)	-.0001(9)	-.0050(7)	-.0017(8)
C1	.042(7)	.042(7)	.075(7)	.011(6)	-.007(6)	-.004(6)
O1	.090(6)	.094(6)	.078(5)	.050(6)	-.036(5)	-.044(5)
C2	.031(5)	.032(6)	.053(6)	.006(5)	-.007(5)	-.003(5)
O2	.046(5)	.059(5)	.071(5)	-.007(5)	.002(4)	-.001(5)
C3	.063(8)	.055(8)	.053(6)	.005(8)	.002(6)	-.003(6)
O3	.068(5)	.085(6)	.048(4)	.031(6)	-.009(4)	.025(4)
C4	.046(6)	.040(7)	.048(5)	.001(7)	-.017(5)	.006(6)
O4	.041(4)	.072(6)	.080(5)	.001(5)	-.015(4)	-.004(5)
C5	.032(6)	.068(8)	.044(6)	-.005(6)	.000(5)	-.014(6)
O5	.116(8)	.071(6)	.058(4)	-.001(7)	.017(5)	.041(4)
C6	.029(5)	.063(8)	.045(5)	.016(6)	-.006(5)	-.010(6)
O6	.055(5)	.076(6)	.093(6)	-.015(5)	.014(5)	-.043(5)
C7	.025(5)	.047(7)	.029(5)	-.005(6)	-.002(5)	-.000(5)
C8	.023(5)	.057(7)	.037(5)	.010(6)	.006(5)	-.000(6)
C9	.035(6)	.064(8)	.052(6)	-.008(7)	.003(5)	-.015(6)
C10	.037(6)	.060(8)	.043(6)	-.008(7)	.003(5)	-.000(6)
C11	.016(4)	.043(7)	.043(5)	-.007(5)	-.002(4)	-.003(6)
C12	.016(4)	.047(7)	.025(5)	.001(5)	-.005(4)	.002(5)
C13	.032(5)	.032(6)	.038(5)	-.003(6)	-.005(5)	.006(5)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
N1	.021(4)	.034(5)	.044(4)	.001(4)	.001(4)	.001(4)
C14	.009(4)	.040(6)	.045(5)	.004(5)	-.001(4)	-.001(5)
C15	.037(6)	.047(7)	.055(6)	-.006(6)	.002(6)	-.004(6)
C16	.027(5)	.029(6)	.061(6)	.006(6)	-.007(6)	-.005(5)

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C17	.032(6)	.056(7)	.041(5)	.013(6)	.007(5)	.000(6)
C18	.028(5)	.045(7)	.048(6)	.002(6)	-.007(5)	-.007(6)
C19	.019(4)	.025(5)	.039(5)	-.002(5)	-.004(4)	.000(5)
N2	.020(4)	.051(6)	.024(4)	-.007(4)	-.002(3)	-.004(4)
C20	.022(5)	.036(6)	.023(4)	.002(5)	-.002(4)	.003(5)
C21	.015(4)	.038(6)	.033(5)	.001(5)	.011(4)	.002(5)
C22	.012(4)	.037(6)	.049(6)	-.003(5)	-.001(5)	.006(5)
C23	.047(6)	.036(6)	.045(6)	-.004(6)	-.005(6)	.015(5)
C24	.031(6)	.024(6)	.084(7)	.005(5)	-.013(6)	-.005(6)
C25	.032(6)	.042(6)	.038(5)	-.004(6)	-.003(5)	.002(5)
C26	.016(4)	.033(6)	.039(5)	.008(5)	.005(4)	-.004(5)
O7	.113(8)	.111(7)	.066(5)	-.042(8)	-.018(6)	.039(5)
C27	.21(2)	.09(1)	.15(1)	-.01(2)	.09(1)	-.03(1)
C28	.016(4)	.041(6)	.042(5)	.009(5)	-.009(4)	-.004(5)
C29	.032(5)	.045(6)	.030(5)	.024(6)	.002(5)	-.002(5)
C30	.037(6)	.037(7)	.054(6)	-.005(6)	-.005(5)	-.001(6)
C31	.035(6)	.08(1)	.050(6)	-.003(8)	.002(6)	.001(7)
C32	.059(8)	.058(8)	.068(7)	.022(8)	.009(7)	-.000(7)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C33	.051(7)	.052(8)	.061(6)	-.003(7)	-.003(6)	.014(6)
C34	.026(5)	.037(6)	.058(6)	-.001(5)	-.003(5)	.017(6)
C35	.028(5)	.049(7)	.047(5)	.009(6)	-.007(5)	-.005(5)
C36	.055(7)	.068(8)	.036(5)	.008(7)	.003(6)	.006(6)
C37	.078(9)	.063(8)	.030(5)	.001(9)	.005(6)	.002(6)
C38	.080(9)	.077(9)	.023(5)	.017(9)	-.000(6)	-.006(6)
C39	.036(6)	.039(6)	.048(6)	.010(6)	-.009(5)	-.005(5)
C40	.023(5)	.034(6)	.035(5)	.010(5)	.005(4)	.006(5)
C41	.019(5)	.023(6)	.058(6)	-.001(5)	-.005(5)	-.005(5)
C42	.042(6)	.027(6)	.046(6)	-.004(6)	-.017(5)	.000(5)
C43	.041(6)	.038(6)	.037(5)	.009(6)	-.004(5)	-.005(6)

C44	.065(8)	.046(7)	.042(6)	.002(7)	-.007(6)	-.001(6)
C45	.051(7)	.040(8)	.110(9)	.003(7)	-.043(7)	-.007(8)
C46	.050(7)	.060(8)	.057(6)	.002(7)	.004(6)	.013(7)
C47	.021(5)	.054(7)	.046(6)	-.002(6)	-.005(5)	.007(6)
C48	.040(6)	.042(7)	.046(6)	-.004(6)	-.006(5)	.012(6)
C49	.042(6)	.073(9)	.041(6)	-.011(7)	.011(5)	-.002(6)
C50	.048(7)	.11(1)	.047(6)	-.004(9)	.009(6)	.000(8)
C51	.061(8)	.083(9)	.039(6)	.023(8)	.006(6)	-.025(7)
C52	.026(5)	.043(6)	.065(6)	.014(6)	-.009(6)	.006(6)
C53	.025(5)	.054(7)	.038(5)	.007(6)	-.003(5)	-.004(6)

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Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
AG	N1	2.251(9)	C3	O3	1.12(2)
AG	N2	2.281(9)	C4	O4	1.16(2)
AG	O7	2.32(1)	C5	O5	1.21(2)
MN1	C1	1.75(1)	C6	O6	1.18(2)
MN1	C2	1.78(1)	C7	C8	1.43(2)
MN1	C3	1.85(2)	C7	C12	1.44(2)
MN1	C28	2.14(1)	C7	C28	1.47(2)
MN1	C29	2.19(1)	C8	C9	1.35(2)
MN1	C34	2.19(1)	C9	C10	1.38(2)
MN1	C35	2.22(1)	C10	C11	1.38(2)
MN1	C40	2.19(1)	C11	C12	1.40(2)
MN2	C4	1.79(1)	C12	C13	1.43(2)
MN2	C5	1.74(2)	C13	N1	1.34(1)
MN2	C6	1.76(2)	C13	C20	1.43(2)
MN2	C41	2.19(1)	N1	C14	1.37(1)
MN2	C42	2.23(1)	C14	C15	1.41(2)
MN2	C47	2.19(1)	C14	C19	1.41(1)
MN2	C48	2.18(1)	C15	C16	1.36(2)
MN2	C53	2.18(1)	C16	C17	1.41(2)
C1	O1	1.18(2)	C17	C18	1.32(2)
C2	O2	1.16(1)	C18	C19	1.43(2)

Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C19	N2	1.34(1)	C35	C40	1.42(2)
N2	C20	1.32(1)	C36	C37	1.32(2)
C20	C21	1.48(2)	C37	C38	1.39(2)
C21	C22	1.40(2)	C38	C39	1.42(2)
C21	C26	1.38(2)	C39	C40	1.46(2)
C22	C23	1.42(2)	C41	C42	1.47(2)
C23	C24	1.36(2)	C41	C53	1.50(2)
C24	C25	1.38(2)	C42	C43	1.39(2)
C25	C26	1.42(2)	C42	C47	1.49(2)
C26	C41	1.44(2)	C43	C44	1.34(2)
O7	C27	1.54(3)	C44	C45	1.41(2)
C28	C29	1.44(2)	C45	C46	1.42(2)
C28	C40	1.45(2)	C46	C47	1.46(2)
C29	C30	1.43(2)	C47	C48	1.44(2)
C29	C34	1.40(2)	C48	C49	1.34(2)
C30	C31	1.33(2)	C48	C53	1.46(2)
C31	C32	1.43(2)	C49	C50	1.36(2)
C32	C33	1.34(2)	C50	C51	1.42(2)
C33	C34	1.40(2)	C51	C52	1.38(2)
C34	C35	1.49(2)	C52	C53	1.43(2)
C35	C36	1.42(2)	C54	O8	1.57(4)

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