Inorganic Chemistry
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Table S1. Crystal data and structure refinement for 1.

Empirical formula	C57H39F6Mn3N3O13.2(CH3CN)
Formula weight	1334.84
Temperature	223(2) K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	C2/c
Unit cell dimensions	a = 15.774(2) A alpha = 90 deg. b = 17.269(2) A beta = 91.11(1) deg. c = 21.411(2) A gamma = 90 deg.
Volume	5831.3(11) A^3
Z	4
Density (calculated)	1.520 Mg/m^3
Absorption coefficient	0.708 mm^-1
F(000)	2704
Crystal size	0.57 x 0.19 x 0.19 mm
Theta range for data collection	2.54 to 25.00 deg.
Index ranges	-18<=h<=18, 0<=k<=20, 0<=l<=25
Reflections collected	5111
Independent reflections	5111 [R(int) = 0.0000]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5111 / 0 / 418
Goodness-of-fit on F^2	0.971
Final R indices [I>2sigma(I)]	R1 = 0.0800, wR2 = 0.2103
R indices (all data)	R1 = 0.1479, wR2 = 0.2469
Largest diff. peak and hole	1.061 and -1.018 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mn(1)	872(1)	8473(1)	2918(1)	29(1)
Mn(2)	0	10161(1)	2500	30(1)
O(12)	0	9009(4)	2500	21(1)
O(1)	1811(3)	9022(3)	2467(2)	35(1)
O(2)	1359(3)	10243(3)	2361(3)	42(1)
O(3)	1018(3)	9247(3)	3680(2)	36(1)
O(4)	-201(3)	10253(3)	1558(2)	37(1)
O(5)	86(3)	7826(3)	3436(2)	34(1)
O(6)	998(3)	7593(3)	2219(2)	35(1)
N(1)	0	11455(6)	2500	44(2)
N(2)	1845(4)	7838(3)	3382(3)	36(2)
C(1)	505(6)	11842(6)	2893(4)	59(3)
C(2)	500(7)	12643(6)	2912(6)	80(4)
C(3)	0	13027(9)	2500	66(4)
C(4)	2503(5)	7613(5)	3089(5)	50(2)
C(5)	3119(7)	7149(7)	3380(5)	72(3)
C(6)	3025(7)	6900(6)	3960(6)	72(3)
C(7)	2290(7)	7142(6)	4272(5)	73(3)
C(8)	1729(6)	7615(6)	3967(4)	56(3)
F(1)	2766(5)	11085(4)	2689(4)	45(2)
F(1B)*	2910(7)	8799(6)	1511(5)	64(3)
C(9)	1886(4)	9743(4)	2326(3)	27(2)
C(10)	3122(5)	10647(4)	2261(4)	38(2)
C(11)	2761(4)	9944(4)	2088(3)	29(2)
C(12)	3921(5)	10854(5)	2062(5)	54(3)
C(13)	4333(5)	10369(5)	1661(5)	55(3)
C(14)	3970(6)	9672(5)	1486(4)	50(2)
C(15)	3210(5)	9463(5)	1694(4)	39(2)
C(16)	675(4)	9880(4)	3803(3)	27(2)
F(2)	1724(5)	9194(4)	4794(3)	32(2)
F(2B)*	-3(9)	11300(8)	4278(6)	87(4)
C(17)	843(4)	10214(4)	4438(3)	28(2)
C(18)	1377(5)	9853(5)	4881(4)	44(2)
C(19)	1504(6)	10165(6)	5478(4)	51(2)
C(20)	1121(6)	10855(5)	5633(4)	48(2)
C(21)	635(6)	11222(5)	5211(4)	48(2)
C(22)	493(5)	10906(5)	4613(4)	39(2)
C(23)	-638(5)	7547(4)	3295(3)	27(2)
F(3)	-2428(4)	7404(4)	3483(3)	84(2)
C(24)	-1048(5)	7092(4)	3811(4)	34(2)
C(25)	-1901(5)	7044(5)	3879(4)	47(2)
C(26)	-2271(7)	6677(7)	4376(5)	73(3)
C(27)	-1750(7)	6320(7)	4812(5)	73(3)
C(28) S	-891(7)	6329(6)	4748(5)	69(3)
C(29)	-537(6)	6731(5)	4266(4)	45(2)
N(9)	3971(11)	8839(13)	4577(9)	208(10)
C(90)	3669(8)	9145(10)	4189(8)	108(5)

C(91)	3220(8)	9547(8)	3714(5)	86(4)

* occupancy 0.5

Table S3. Bond lengths [A] and angles [deg] for 1.

Mn(1)-O(12)	1.871(3)
Mn(1)-O(5)	2.017(5)
Mn(1)-O(1)	2.021(5)
Mn(1)-N(2)	2.118(7)
Mn(1)-O(3)	2.118(5)
Mn(1)-O(6)	2.145(5)
Mn(2)-O(12)	1.990(6)
Mn(2)-O(4)	2.041(5)
Mn(2)-O(4)#1	2.042(5)
Mn(2)-O(2)	2.174(5)
Mn(2)-O(2)#1	2.174(5)
Mn(2)-N(1)	2.234(10)
O(12)-Mn(1)#1	1.871(3)
O(1)-C(9)	1.287(9)
O(2)-C(9)	1.203(8)
O(3)-C(16)	1.251(8)
O(4)-C(16)#1	1.245(8)
O(5)-C(23)	1.270(9)
O(6)-C(23)#1	1.231(9)
N(1)-C(1)#1	1.329(10)
N(1)-C(1)	1.329(10)
N(2)-C(4)	1.283(10)
N(2)-C(8)	1.327(10)
C(1)-C(2)	1.38(2)
C(2)-C(3)	1.346(13)
C(3)-C(2)#1	1.346(13)
C(4)-C(5)	1.397(13)
C(5)-C(6)	1.325(14)
C(6)-C(7)	1.413(14)
C(7)-C(8)	1.361(13)
F(1)-C(10)	1.322(11)
F(1B)-C(15)	1.299(13)
C(9)-C(11)	1.521(10)
C(10)-C(12)	1.386(11)
C(10)-C(11)	1.387(10)
C(11)-C(15)	1.389(10)
C(12)-C(13)	1.371(12)
C(13)-C(14)	1.382(12)
C(14)-C(15)	1.336(11)
C(16)-O(4)#1	1.245(8)
C(16)-C(17)	1.495(10)
F(2)-C(18)	1.277(11)
F(2B)-C(22)	1.252(14)
C(17)-C(22)	1.373(10)
C(17)-C(18)	1.402(11)
C(18)-C(19)	1.398(11)
C(19)-C(20)	1.380(13)
C(20)-C(21)	1.334(12)
C(21)-C(22)	1.405(11)
C(23)-O(6)#1	1.231(9)
C(23)-C(24)	1.510(10)
F(3)-C(25)	1.330(10)
C(24)-C(25)	1.359(11)
C(24)-C(29)	1.399(11)
C(25)-C(26)	1.379(12)
C(26)-C(27)	1.377(14)

C(27)-C(28)	1.364(14)
C(28)-C(29)	1.371(11)
N(9)-C(90)	1.09(2)
C(90)-C(91)	1.41(2)
O(12)-Mn(1)-O(5)	94.8(2)
O(12)-Mn(1)-O(1)	94.5(2)
O(5)-Mn(1)-O(1)	170.7(2)
O(12)-Mn(1)-N(2)	178.4(2)
O(5)-Mn(1)-N(2)	84.4(2)
O(1)-Mn(1)-N(2)	86.3(2)
O(12)-Mn(1)-O(3)	97.2(2)
O(5)-Mn(1)-O(3)	89.2(2)
O(1)-Mn(1)-O(3)	90.1(2)
N(2)-Mn(1)-O(3)	84.2(2)
O(12)-Mn(1)-O(6)	95.4(2)
O(5)-Mn(1)-O(6)	93.3(2)
O(1)-Mn(1)-O(6)	85.4(2)
N(2)-Mn(1)-O(6)	83.4(2)
O(3)-Mn(1)-O(6)	167.0(2)
O(12)-Mn(2)-O(4)	94.46(14)
O(12)-Mn(2)-O(4)#1	94.46(14)
O(4)-Mn(2)-O(4)#1	171.1(3)
O(12)-Mn(2)-O(2)	93.74(14)
O(4)-Mn(2)-O(2)	89.6(2)
O(4)#1-Mn(2)-O(2)	89.8(2)
O(12)-Mn(2)-O(2)#1	93.74(14)
O(4)-Mn(2)-O(2)#1	89.8(2)
O(4)#1-Mn(2)-O(2)#1	89.6(2)
O(2)-Mn(2)-O(2)#1	172.5(3)
O(12)-Mn(2)-N(1)	180.000(3)
O(4)-Mn(2)-N(1)	85.54(14)
O(4)#1-Mn(2)-N(1)	85.54(14)
O(2)-Mn(2)-N(1)	86.26(14)
O(2)#1-Mn(2)-N(1)	86.26(14)
Mn(1)#1-O(12)-Mn(1)	120.7(3)
Mn(1)#1-O(12)-Mn(2)	119.6(2)
Mn(1)-O(12)-Mn(2)	119.6(2)
C(9)-O(1)-Mn(1)	129.6(4)
C(9)-O(2)-Mn(2)	130.3(5)
C(16)-O(3)-Mn(1)	132.3(5)
C(16)#1-O(4)-Mn(2)	130.8(5)
C(23)-O(5)-Mn(1)	129.8(5)
C(23)#1-O(6)-Mn(1)	128.5(5)
C(1)#1-N(1)-C(1)	119.5(12)
C(1)#1-N(1)-Mn(2)	120.2(6)
C(1)-N(1)-Mn(2)	120.2(6)
C(4)-N(2)-C(8)	120.1(8)
C(4)-N(2)-Mn(1)	120.9(6)
C(8)-N(2)-Mn(1)	118.8(6)
N(1)-C(1)-C(2)	121.2(10)
C(3)-C(2)-C(1)	118.5(11)
C(2)-C(3)-C(2)#1	121(2)
N(2)-C(4)-C(5)	121.2(9)
C(6)-C(5)-C(4)	121.0(10)
C(5)-C(6)-C(7)	117.0(10)
C(8)-C(7)-C(6)	118.9(10)
N(2)-C(8)-C(7)	121.8(9)
O(2)-C(9)-O(1)	127.8(7)
O(2)-C(9)-C(11)	119.4(7)

O(1)-C(9)-C(11)	112.8(6)
F(1)-C(10)-C(12)	117.9(8)
F(1)-C(10)-C(11)	120.5(7)
C(12)-C(10)-C(11)	120.9(7)
C(10)-C(11)-C(15)	118.3(7)
C(10)-C(11)-C(9)	118.7(6)
C(15)-C(11)-C(9)	122.9(7)
C(13)-C(12)-C(10)	118.7(8)
C(12)-C(13)-C(14)	120.2(7)
C(15)-C(14)-C(13)	120.9(8)
F(1B)-C(15)-C(14)	117.5(8)
F(1B)-C(15)-C(11)	121.7(8)
C(14)-C(15)-C(11)	120.9(8)
O(4)#1-C(16)-O(3)	125.3(7)
O(4)#1-C(16)-C(17)	117.4(6)
O(3)-C(16)-C(17)	117.3(7)
C(22)-C(17)-C(18)	116.3(7)
C(22)-C(17)-C(16)	121.2(7)
C(18)-C(17)-C(16)	122.5(7)
F(2)-C(18)-C(19)	115.0(9)
F(2)-C(18)-C(17)	123.4(8)
C(19)-C(18)-C(17)	121.4(8)
C(20)-C(19)-C(18)	119.8(9)
C(21)-C(20)-C(19)	119.8(8)
C(20)-C(21)-C(22)	120.8(8)
F(2B)-C(22)-C(17)	124.6(9)
F(2B)-C(22)-C(21)	113.4(9)
C(17)-C(22)-C(21)	122.0(8)
O(6)#1-C(23)-O(5)	125.7(6)
O(6)#1-C(23)-C(24)	119.4(7)
O(5)-C(23)-C(24)	114.8(7)
C(25)-C(24)-C(29)	117.2(7)
C(25)-C(24)-C(23)	123.3(7)
C(29)-C(24)-C(23)	119.5(7)
F(3)-C(25)-C(24)	120.7(7)
F(3)-C(25)-C(26)	116.0(8)
C(24)-C(25)-C(26)	123.1(9)
C(27)-C(26)-C(25)	118.2(9)
C(28)-C(27)-C(26)	120.5(9)
C(27)-C(28)-C(29)	120.1(10)
C(28)-C(29)-C(24)	120.8(9)
N(9)-C(90)-C(91)	175(2)

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

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for 1. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mn(1)	32(1)	24(1)	33(1)	1(1)	10(1)	-2(1)
Mn(2)	29(1)	32(1)	31(1)	0	5(1)	0
O(12)	12(3)	25(4)	26(4)	0	-1(3)	0
O(1)	38(3)	23(3)	44(3)	10(2)	6(2)	4(2)
O(2)	30(3)	28(3)	68(4)	3(3)	11(3)	0(2)
O(3)	44(3)	34(3)	30(3)	-4(2)	-7(2)	7(3)
O(4)	50(3)	27(3)	34(3)	-4(2)	2(3)	-8(3)
O(5)	34(3)	36(3)	30(3)	9(2)	9(2)	-3(2)
O(6)	42(3)	28(3)	35(3)	-5(2)	8(3)	9(2)
N(1)	28(5)	59(7)	44(6)	0	3(4)	0
N(2)	47(4)	27(3)	35(4)	-1(3)	14(3)	1(3)
C(1)	42(5)	71(7)	64(6)	22(5)	-16(5)	-25(5)
C(2)	74(8)	61(7)	106(10)	10(7)	-27(7)	-32(6)
C(3)	54(9)	54(9)	91(12)	0	-4(8)	0
C(4)	37(5)	49(5)	64(6)	-5(5)	17(5)	9(4)
C(5)	56(7)	77(8)	83(8)	20(6)	15(6)	26(6)
C(6)	57(7)	71(7)	88(8)	26(6)	-7(6)	17(6)
C(7)	68(7)	83(8)	69(7)	33(6)	6(6)	10(6)
C(8)	58(6)	59(6)	50(6)	2(5)	4(5)	-14(5)
F(1)	41(5)	19(4)	77(7)	-25(4)	13(5)	-21(4)
F(1B)	80(8)	48(6)	65(7)	-12(5)	23(6)	-1(6)
C(9)	20(4)	36(4)	24(4)	-5(3)	1(3)	-2(3)
C(10)	30(4)	31(4)	52(5)	0(4)	1(4)	-1(3)
C(11)	29(4)	29(4)	29(4)	0(3)	4(3)	7(3)
C(12)	39(5)	29(4)	94(8)	-3(5)	15(5)	-19(4)
C(13)	41(5)	47(5)	77(7)	13(5)	33(5)	-8(4)
C(14)	51(5)	42(5)	58(6)	2(4)	30(5)	6(4)
C(15)	45(5)	32(5)	39(5)	3(4)	9(4)	11(4)
C(16)	22(4)	24(4)	35(4)	2(3)	8(3)	-4(3)
F(2)	54(5)	26(4)	16(4)	-6(3)	-11(4)	17(4)
F(2B)	100(10)	74(9)	89(9)	-26(7)	-1(8)	12(8)
C(17)	25(4)	30(4)	29(4)	-2(3)	6(3)	-5(3)
C(18)	43(5)	48(5)	41(5)	-3(4)	8(4)	-19(4)
C(19)	55(6)	67(6)	32(5)	-4(5)	4(4)	-17(5)
C(20)	51(6)	58(6)	36(5)	-18(5)	14(4)	-17(5)
C(21)	49(5)	39(5)	56(6)	-23(4)	20(5)	-6(4)
C(22)	33(5)	40(5)	46(5)	-4(4)	6(4)	0(4)
C(23)	28(4)	23(4)	31(4)	-5(3)	21(3)	8(3)
F(3)	44(3)	121(5)	88(5)	35(4)	21(3)	-6(3)
C(24)	36(4)	25(4)	41(5)	4(3)	6(4)	-4(3)
C(25)	37(5)	57(6)	47(5)	8(4)	12(4)	3(4)
C(26)	53(6)	99(9)	69(7)	5(6)	22(6)	-33(6)
C(27)	64(7)	107(9)	49(6)	25(6)	9(5)	-40(6)
C(28)	80(8)	69(7)	59(7)	26(5)	5(6)	-25(6)
C(29)	54(5)	35(5)	46(5)	8(4)	15(4)	-11(4)
N(9)	125(13)	291(25)	206(19)	129(18)	-54(13)	-24(15)
C(90)	61(8)	132(13)	129(13)	38(10)	-31(9)	-26(8)
C(91)	85(9)	100(10)	72(8)	18(7)	-19(7)	-24(7)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(1)	873(6)	11567(6)	3164(4)	71
H(2)	837(7)	12913(6)	3206(6)	97
H(3)	0	13571(9)	2500	80
H(4)	2572(5)	7764(5)	2671(5)	60
H(5)	3608(7)	7012(7)	3161(5)	87
H(6)	3430(7)	6577(6)	4155(6)	86
H(7)	2189(7)	6980(6)	4683(5)	87
H(8)	1246(6)	7788(6)	4177(4)	67
H(12)	4176(5)	11317(5)	2199(5)	65
H(13)	4864(5)	10512(5)	1505(5)	65
H(14)	4262(6)	9339(5)	1216(4)	60
H(19)	1851(6)	9905(6)	5773(4)	62
H(20)	1201(6)	11065(5)	6035(4)	58
H(21)	384(6)	11698(5)	5315(4)	58
H(26)	-2864(7)	6669(7)	4416(5)	88
H(27)	-1988(7)	6068(7)	5156(5)	88
H(28)	-542(7)	6060(6)	5035(5)	83
H(29)	56(6)	6765(5)	4242(4)	54
H(91A)	2624(11)	9411(38)	3727(25)	129
H(91B)	3443(36)	9407(37)	3310(6)	129
H(91C)	3284(45)	10100(8)	3778(23)	129

Table S6. Crystal data and structure refinement for Mn-3clbz(5)

Empirical formula	C52H36Cl6Mn3N2O14.1/2H2O
Formula weight	1299.36
Temperature	213(2) K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	P21/n
Unit cell dimensions	a = 15.172(2) A alpha = 90 deg. b = 17.603(2) A beta = 106.300(10) de c = 21.996(3) A gamma = 90 deg.
Volume	5638.4(12) A^3
Z	4
Density (calculated)	1.531 Mg/m^3
Absorption coefficient	0.987 mm^-1
F(000)	2636
Crystal size	0.61 x 0.46 x 0.23 mm
Theta range for data collection	1.51 to 22.50 deg.
Index ranges	-16<=h<=15, 0<=k<=18, 0<=l<=23
Reflections collected	7363
Independent reflections	7363 [R(int) = 0.0000]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7363 / 0 / 685
Goodness-of-fit on F^2	1.032
Final R indices [I>2sigma(I)]	R1 = 0.1175, wR2 = 0.3362
R indices (all data)	R1 = 0.2018, wR2 = 0.4002
Largest diff. peak and hole	1.358 and -2.185 e.A^-3

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 5. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

displacement parameters (A^2 x 10^3) for 5. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mn(1)	471(1)	8422(1)	2221(1)	32(1)
Mn(2)	-872(2)	9820(1)	2234(1)	41(1)
Mn(3)	-612(3)	9252(2)	835(2)	116(2)
O(13)	-314(6)	9165(5)	1808(4)	37(2)
OW1	-924(7)	9369(5)	-163(4)	42(2)
N(1)	-1596(8)	10559(6)	2623(6)	66(4)
C(1)	-2411(8)	10374(6)	2704(6)	90(7)
C(2)	-2969(7)	10865(9)	2910(7)	105(8)
C(3)	-2672(11)	11610(8)	3065(8)	104(8)
C(4)	-1843(12)	11793(5)	2992(8)	120(10)
C(5)	-1317(9)	11289(7)	2775(7)	100(8)
N(2)	1403(8)	7610(7)	2710(5)	38(3)
C(6)	1582(12)	7495(9)	3336(7)	54(4)
C(7)	2225(14)	6999(10)	3679(8)	71(6)
C(8)	2728(14)	6559(9)	3365(9)	63(5)
C(9)	2540(13)	6666(10)	2733(9)	62(5)
C(10)	1900(11)	7178(8)	2411(7)	44(4)
Cl(1)	471(4)	5453(3)	2756(3)	91(2)
O(1)	743(6)	9075(5)	860(4)	38(2)
O(2)	1469(6)	8773(5)	1863(4)	39(2)
C(11)	1449(10)	9042(8)	1312(7)	38(4)
C(12)	2682(8)	4339(7)	3775(6)	25(3)
C(13)	2535(10)	4333(8)	4347(7)	40(4)
C(14)	1740(13)	4675(12)	4447(9)	70(5)
C(15)	1103(11)	4990(10)	3984(9)	55(4)
C(16)	1276(11)	5017(9)	3379(9)	60(5)
C(17)	2065(10)	4658(8)	3278(8)	48(4)
Cl(2)	-952(6)	4611(3)	1166(5)	127(4)
Cl(2B)	-3178(31)	6059(19)	-442(17)	151(18)
O(3)	2(7)	7543(5)	1547(5)	42(2)
O(4)	-937(7)	8138(5)	706(5)	48(3)
C(18)	-629(11)	7545(9)	1045(8)	46(4)
C(19)	-1105(11)	6796(8)	792(8)	44(4)
C(20)	-830(13)	6155(9)	1066(10)	72(6)
C(21)	-1279(16)	5473(12)	807(13)	91(7)
C(22)	-1975(18)	5456(13)	308(14)	105(8)
C(23)	-2297(15)	6150(13)	-7(12)	98(8)
C(24)	-1830(12)	6818(9)	274(9)	66(5)
Cl(3)	2446(4)	2301(3)	4241(3)	101(2)
O(5)	288(7)	10219(5)	2803(5)	47(3)
O(6)	1100(7)	9137(6)	3028(5)	49(3)
C(25)	1019(12)	9834(9)	3060(7)	44(4)
C(26)	1851(11)	10260(9)	3441(7)	45(4)
C(27)	2698(13)	9958(9)	3573(9)	64(5)
C(28)	3438(15)	10360(12)	3865(12)	96(7)
C(29)	3366(15)	11064(13)	4078(11)	100(8)
C(30)	2548(15)	11407(10)	3978(8)	65(5)
C(31)	1800(12)	10997(10)	3679(8)	58(5)
Cl(4)	970(7)	13403(4)	2239(3)	154(4)
O(7)	-345(7)	10416(6)	840(5)	48(3)
O(8)	-823(7)	10779(5)	1662(5)	43(3)
C(32)	-492(9)	10890(8)	1224(9)	43(4)

C(33)	-220(10)	11716(8)	1123(7)	43(4)
C(34)	85(13)	12164(9)	1628(9)	64(5)
C(35)	434(14)	12883(11)	1577(10)	75(6)
C(36)	439(15)	13134(10)	990(11)	86(7)
C(37)	69(12)	12695(8)	476(10)	61(5)
C(38)	-242(11)	11990(8)	515(8)	50(4)
Cl(5)	-1232(3)	5759(2)	3976(2)	66(1)
O(9)	-1007(8)	9056(6)	2939(5)	57(3)
O(10)	-374(7)	8009(5)	2676(5)	47(3)
C(39)	-867(12)	8351(10)	2966(8)	52(4)
C(40)	-1364(7)	7879(5)	3331(5)	44(4)
C(41)	-2054(8)	8196(5)	3553(7)	79(6)
C(42)	-2489(8)	7760(7)	3910(7)	103(9)
C(43)	-2234(8)	7006(6)	4045(6)	73(6)
C(44)	-1544(8)	6690(4)	3823(6)	57(5)
C(45)	-1109(6)	7126(5)	3466(5)	50(4)
Cl(6)	-5238(7)	8056(7)	1541(6)	141(4)
Cl(6B)	-4492(12)	7434(15)	-307(7)	116(9)
O(11)	-2129(7)	9443(6)	1730(7)	56(3)
O(12)	-1958(7)	9433(6)	771(6)	56(3)
C(46)	-2354(11)	9271(9)	1157(11)	51(4)
C(47)	-3277(7)	8852(7)	941(8)	83(7)
C(48)	-3839(10)	8755(8)	1337(7)	91(8)
C(49)	-4636(9)	8325(9)	1136(10)	104(10)
C(50)	-4873(8)	7993(9)	539(11)	137(13)
C(51)	-4311(12)	8090(10)	142(9)	203(21)
C(52)	-3513(10)	8520(10)	343(8)	132(12)
OW2	-691(26)	9501(20)	5089(22)	175(22)

Pyridine ring N1-C5 has been fitted to
pyridine ring N2-C10 as a rigid group.

occupancy Cl2 0.8, Cl2B 0.2, Cl6 0.7, Cl6b 0.3, OW2 0.5

Table S8. Bond lengths [A] and angles [deg] for 5.

Mn(1)-O(13)	1.831(9)
Mn(1)-O(10)	1.973(10)
Mn(1)-O(2)	1.992(10)
Mn(1)-N(2)	2.084(12)
Mn(1)-O(3)	2.123(10)
Mn(1)-O(6)	2.166(10)
Mn(1)-Mn(2)	3.201(3)
Mn(1)-Mn(3)	3.364(5)
Mn(2)-O(13)	1.835(9)
Mn(2)-O(5)	1.979(11)
Mn(2)-O(11)	2.031(12)
Mn(2)-N(1)	2.038(9)
Mn(2)-O(9)	2.105(11)
Mn(2)-O(8)	2.119(10)
Mn(2)-Mn(3)	3.362(5)
Mn(3)-O(4)	2.023(10)
Mn(3)-O(12)	2.031(12)
Mn(3)-O(1)	2.065(10)
Mn(3)-O(13)	2.064(10)
Mn(3)-O(7)	2.088(11)
Mn(3)-OW1	2.123(10)

N(1)-C(1)	1.34
N(1)-C(5)	1.36
C(1)-C(2)	1.37
C(2)-C(3)	1.40
C(3)-C(4)	1.35
C(4)-C(5)	1.37
N(2)-C(6)	1.34(2)
N(2)-C(10)	1.36(2)
C(6)-C(7)	1.37(2)
C(7)-C(8)	1.40(3)
C(8)-C(9)	1.35(2)
C(9)-C(10)	1.37(2)
Cl(1)-C(16)	1.74(2)
O(1)-C(11)	1.24(2)
O(2)-C(11)	1.29(2)
C(11)-C(12)#1	1.48(2)
C(12)-C(13)	1.34(2)
C(12)-C(17)	1.35(2)
C(12)-C(11)#2	1.48(2)
C(13)-C(14)	1.42(2)
C(14)-C(15)	1.31(2)
C(15)-C(16)	1.43(2)
C(16)-C(17)	1.42(2)
Cl(2)-C(21)	1.72(2)
Cl(2B)-C(23)	1.42(4)
O(3)-C(18)	1.24(2)
O(4)-C(18)	1.29(2)
C(18)-C(19)	1.53(2)
C(19)-C(20)	1.29(2)
C(19)-C(24)	1.34(2)
C(20)-C(21)	1.42(3)
C(21)-C(22)	1.29(3)
C(22)-C(23)	1.42(3)
C(23)-C(24)	1.42(3)
Cl(3)-C(30)#3	1.70(2)
O(5)-C(25)	1.29(2)
O(6)-C(25)	1.24(2)
C(25)-C(26)	1.50(2)
C(26)-C(27)	1.34(2)
C(26)-C(31)	1.41(2)
C(27)-C(28)	1.33(3)
C(28)-C(29)	1.34(3)
C(29)-C(30)	1.34(3)
C(30)-C(31)	1.35(2)
C(30)-Cl(3)#4	1.70(2)
Cl(4)-C(35)	1.72(2)
O(7)-C(32)	1.25(2)
O(8)-C(32)	1.22(2)
C(32)-C(33)	1.54(2)
C(33)-C(34)	1.34(2)
C(33)-C(38)	1.41(2)
C(34)-C(35)	1.39(2)
C(35)-C(36)	1.37(3)
C(36)-C(37)	1.35(3)
C(37)-C(38)	1.34(2)
Cl(5)-C(44)	1.712(8)
O(9)-C(39)	1.26(2)
O(10)-C(39)	1.26(2)
C(39)-C(40)	1.50(2)
C(40)-C(41)	1.39

C(40)-C(45)	1.39
C(41)-C(42)	1.39
C(42)-C(43)	1.39
C(43)-C(44)	1.39
C(44)-C(45)	1.39
Cl(6)-C(49)	1.52(2)
Cl(6B)-C(51)	1.49(2)
O(11)-C(46)	1.25(2)
O(12)-C(46)	1.20(2)
C(46)-C(47)	1.54(2)
C(47)-C(48)	1.39
C(47)-C(52)	1.39
C(48)-C(49)	1.39
C(49)-C(50)	1.39
C(50)-C(51)	1.39
C(51)-C(52)	1.39

O(13)-Mn(1)-O(10)	95.2(4)
O(13)-Mn(1)-O(2)	92.5(4)
O(10)-Mn(1)-O(2)	171.7(4)
O(13)-Mn(1)-N(2)	177.6(4)
O(10)-Mn(1)-N(2)	86.0(4)
O(2)-Mn(1)-N(2)	86.3(4)
O(13)-Mn(1)-O(3)	97.5(4)
O(10)-Mn(1)-O(3)	87.0(4)
O(2)-Mn(1)-O(3)	95.4(4)
N(2)-Mn(1)-O(3)	84.7(4)
O(13)-Mn(1)-O(6)	93.8(4)
O(10)-Mn(1)-O(6)	89.9(4)
O(2)-Mn(1)-O(6)	86.2(4)
N(2)-Mn(1)-O(6)	84.1(4)
O(3)-Mn(1)-O(6)	168.5(4)
O(13)-Mn(1)-Mn(2)	29.2(3)
O(10)-Mn(1)-Mn(2)	76.9(3)
O(2)-Mn(1)-Mn(2)	108.7(3)
N(2)-Mn(1)-Mn(2)	149.8(3)
O(3)-Mn(1)-Mn(2)	118.5(3)
O(6)-Mn(1)-Mn(2)	71.4(3)
O(13)-Mn(1)-Mn(3)	32.3(3)
O(10)-Mn(1)-Mn(3)	113.4(3)
O(2)-Mn(1)-Mn(3)	74.9(3)
N(2)-Mn(1)-Mn(3)	148.6(3)
O(3)-Mn(1)-Mn(3)	72.6(3)
O(6)-Mn(1)-Mn(3)	118.7(3)
Mn(2)-Mn(1)-Mn(3)	61.54(10)
O(13)-Mn(2)-O(5)	95.1(4)
O(13)-Mn(2)-O(11)	90.7(4)
O(5)-Mn(2)-O(11)	173.5(5)
O(13)-Mn(2)-N(1)	174.1(5)
O(5)-Mn(2)-N(1)	89.9(5)
O(11)-Mn(2)-N(1)	84.5(5)
O(13)-Mn(2)-O(9)	97.4(4)
O(5)-Mn(2)-O(9)	90.8(4)
O(11)-Mn(2)-O(9)	85.6(5)
N(1)-Mn(2)-O(9)	85.6(4)
O(13)-Mn(2)-O(8)	95.7(4)
O(5)-Mn(2)-O(8)	85.4(4)
O(11)-Mn(2)-O(8)	96.9(4)
N(1)-Mn(2)-O(8)	81.6(4)
O(9)-Mn(2)-O(8)	166.7(4)

O(13)-Mn(2)-Mn(1)	29.1(3)
O(5)-Mn(2)-Mn(1)	79.8(3)
O(11)-Mn(2)-Mn(1)	104.3(3)
N(1)-Mn(2)-Mn(1)	156.0(4)
O(9)-Mn(2)-Mn(1)	73.1(3)
O(8)-Mn(2)-Mn(1)	118.6(3)
O(13)-Mn(2)-Mn(3)	32.5(3)
O(5)-Mn(2)-Mn(3)	111.8(3)
O(11)-Mn(2)-Mn(3)	74.7(4)
N(1)-Mn(2)-Mn(3)	142.1(4)
O(9)-Mn(2)-Mn(3)	123.0(3)
O(8)-Mn(2)-Mn(3)	70.2(3)
Mn(1)-Mn(2)-Mn(3)	61.62(9)
O(4)-Mn(3)-O(12)	86.7(5)
O(4)-Mn(3)-O(1)	93.4(4)
O(12)-Mn(3)-O(1)	177.6(5)
O(4)-Mn(3)-O(13)	92.8(4)
O(12)-Mn(3)-O(13)	90.4(5)
O(1)-Mn(3)-O(13)	92.0(4)
O(4)-Mn(3)-O(7)	172.5(5)
O(12)-Mn(3)-O(7)	92.1(5)
O(1)-Mn(3)-O(7)	87.6(4)
O(13)-Mn(3)-O(7)	94.7(4)
O(4)-Mn(3)-OW1	88.5(4)
O(12)-Mn(3)-OW1	89.2(5)
O(1)-Mn(3)-OW1	88.5(4)
O(13)-Mn(3)-OW1	178.6(4)
O(7)-Mn(3)-OW1	84.0(4)
O(4)-Mn(3)-Mn(2)	109.3(3)
O(12)-Mn(3)-Mn(2)	69.1(4)
O(1)-Mn(3)-Mn(2)	113.1(3)
O(13)-Mn(3)-Mn(2)	28.5(2)
O(7)-Mn(3)-Mn(2)	77.0(3)
OW1-Mn(3)-Mn(2)	150.3(3)
O(4)-Mn(3)-Mn(1)	75.2(3)
O(12)-Mn(3)-Mn(1)	110.9(4)
O(1)-Mn(3)-Mn(1)	71.4(3)
O(13)-Mn(3)-Mn(1)	28.3(2)
O(7)-Mn(3)-Mn(1)	112.1(3)
OW1-Mn(3)-Mn(1)	152.9(3)
Mn(2)-Mn(3)-Mn(1)	56.84(9)
Mn(1)-O(13)-Mn(2)	121.6(5)
Mn(1)-O(13)-Mn(3)	119.3(5)
Mn(2)-O(13)-Mn(3)	119.0(5)
C(1)-N(1)-C(5)	115.4
C(1)-N(1)-Mn(2)	121.9(7)
C(5)-N(1)-Mn(2)	122.5(7)
N(1)-C(1)-C(2)	124.7
C(1)-C(2)-C(3)	119.0
C(4)-C(3)-C(2)	116.3
C(3)-C(4)-C(5)	122.7
N(1)-C(5)-C(4)	121.8
C(6)-N(2)-C(10)	115.5(13)
C(6)-N(2)-Mn(1)	123.1(11)
C(10)-N(2)-Mn(1)	121.4(9)
N(2)-C(6)-C(7)	125(2)
C(6)-C(7)-C(8)	119(2)
C(9)-C(8)-C(7)	116(2)
C(8)-C(9)-C(10)	123(2)
N(2)-C(10)-C(9)	122(2)

C(11)-O(1)-Mn(3)	131.1(9)
C(11)-O(2)-Mn(1)	131.6(9)
O(1)-C(11)-O(2)	123.7(13)
O(1)-C(11)-C(12)#1	118.7(13)
O(2)-C(11)-C(12)#1	117.6(13)
C(13)-C(12)-C(17)	120.3(13)
C(13)-C(12)-C(11)#2	120.7(12)
C(17)-C(12)-C(11)#2	118.9(13)
C(12)-C(13)-C(14)	121(2)
C(15)-C(14)-C(13)	122(2)
C(14)-C(15)-C(16)	117(2)
C(17)-C(16)-C(15)	121(2)
C(17)-C(16)-Cl(1)	121(2)
C(15)-C(16)-Cl(1)	118.5(13)
C(12)-C(17)-C(16)	119(2)
C(18)-O(3)-Mn(1)	129.9(10)
C(18)-O(4)-Mn(3)	131.8(9)
O(3)-C(18)-O(4)	125.5(13)
O(3)-C(18)-C(19)	119(2)
O(4)-C(18)-C(19)	115.3(14)
C(20)-C(19)-C(24)	120(2)
C(20)-C(19)-C(18)	122(2)
C(24)-C(19)-C(18)	118(2)
C(19)-C(20)-C(21)	120(2)
C(22)-C(21)-C(20)	123(2)
C(22)-C(21)-Cl(2)	116(2)
C(20)-C(21)-Cl(2)	121(2)
C(21)-C(22)-C(23)	119(2)
C(24)-C(23)-C(22)	116(2)
C(24)-C(23)-Cl(2B)	130(2)
C(22)-C(23)-Cl(2B)	111(2)
C(19)-C(24)-C(23)	122(2)
C(25)-O(5)-Mn(2)	126.6(9)
C(25)-O(6)-Mn(1)	126.6(10)
O(6)-C(25)-O(5)	125.7(14)
O(6)-C(25)-C(26)	116(2)
O(5)-C(25)-C(26)	117.9(13)
C(27)-C(26)-C(31)	116(2)
C(27)-C(26)-C(25)	121.7(14)
C(31)-C(26)-C(25)	123(2)
C(28)-C(27)-C(26)	121(2)
C(27)-C(28)-C(29)	121(2)
C(30)-C(29)-C(28)	121(2)
C(29)-C(30)-C(31)	117(2)
C(29)-C(30)-Cl(3)#4	122(2)
C(31)-C(30)-Cl(3)#4	121(2)
C(30)-C(31)-C(26)	123(2)
C(32)-O(7)-Mn(3)	126.0(10)
C(32)-O(8)-Mn(2)	133.4(9)
O(8)-C(32)-O(7)	128.0(13)
O(8)-C(32)-C(33)	117(2)
O(7)-C(32)-C(33)	115(2)
C(34)-C(33)-C(38)	120(2)
C(34)-C(33)-C(32)	119(2)
C(38)-C(33)-C(32)	121.5(14)
C(33)-C(34)-C(35)	122(2)
C(36)-C(35)-C(34)	118(2)
C(36)-C(35)-Cl(4)	120(2)
C(34)-C(35)-Cl(4)	121(2)
C(37)-C(36)-C(35)	120(2)

C(38)-C(37)-C(36)	123(2)
C(37)-C(38)-C(33)	118(2)
C(39)-O(9)-Mn(2)	128.0(10)
C(39)-O(10)-Mn(1)	130.0(10)
O(9)-C(39)-O(10)	124.1(14)
O(9)-C(39)-C(40)	118.0(14)
O(10)-C(39)-C(40)	117.8(14)
C(41)-C(40)-C(45)	120.0
C(41)-C(40)-C(39)	120.5(10)
C(45)-C(40)-C(39)	119.4(9)
C(42)-C(41)-C(40)	120.0
C(41)-C(42)-C(43)	120.0
C(44)-C(43)-C(42)	120.0
C(45)-C(44)-C(43)	120.0
C(45)-C(44)-Cl(5)	119.4(6)
C(43)-C(44)-Cl(5)	120.6(6)
C(44)-C(45)-C(40)	120.0
C(46)-O(11)-Mn(2)	125.4(11)
C(46)-O(12)-Mn(3)	127.2(11)
O(12)-C(46)-O(11)	127(2)
O(12)-C(46)-C(47)	119(2)
O(11)-C(46)-C(47)	113(2)
C(48)-C(47)-C(52)	120.0
C(48)-C(47)-C(46)	122.1(13)
C(52)-C(47)-C(46)	117.7(13)
C(49)-C(48)-C(47)	120.0
C(48)-C(49)-C(50)	120.0
C(48)-C(49)-Cl(6)	126.6(14)
C(50)-C(49)-Cl(6)	113(2)
C(49)-C(50)-C(51)	120.0
C(52)-C(51)-C(50)	120.0
C(52)-C(51)-Cl(6B)	128(2)
C(50)-C(51)-Cl(6B)	107(2)
C(51)-C(52)-C(47)	120.0

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

Table S9. Anisotropic displacement parameters (A^2 x 10^3) for 5. The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mn(1)	39(1)	22(1)	37(1)	2(1)	15(1)	-1(1)
Mn(2)	45(1)	28(1)	60(2)	0(1)	29(1)	-1(1)
Mn(3)	113(3)	100(3)	130(4)	5(3)	28(3)	-3(2)
O(13)	38(6)	21(5)	52(6)	-1(4)	16(5)	-2(4)
OW1	49(6)	32(6)	40(6)	1(5)	4(5)	4(5)
N(1)	67(10)	44(9)	117(13)	3(8)	77(10)	-11(7)
C(1)	110(18)	87(16)	83(15)	-9(13)	41(14)	26(14)
C(2)	94(17)	131(22)	81(16)	-32(15)	11(13)	41(16)
C(3)	152(24)	44(13)	127(21)	-25(13)	61(19)	-1(14)
C(4)	181(29)	69(16)	138(23)	13(15)	90(22)	47(18)
C(5)	145(22)	78(16)	105(18)	-4(14)	83(17)	24(16)

N(2)	40(7)	47(8)	26(7)	1(6)	4(6)	-13(6)
C(6)	72(12)	47(10)	43(11)	1(8)	13(9)	-10(9)
C(7)	113(17)	59(12)	29(10)	12(9)	1(11)	-4(12)
C(8)	95(14)	32(9)	56(12)	7(9)	12(11)	3(9)
C(9)	76(13)	51(11)	63(13)	-1(9)	23(10)	8(10)
C(10)	57(10)	37(9)	38(9)	11(7)	13(8)	9(8)
Cl(1)	60(3)	103(4)	93(4)	5(3)	-7(3)	35(3)
O(1)	28(5)	51(6)	29(6)	0(5)	-2(5)	-6(5)
O(2)	41(6)	33(5)	39(6)	5(5)	4(5)	-7(5)
C(11)	45(10)	27(8)	40(10)	-5(7)	10(8)	-11(7)
C(12)	23(7)	16(7)	32(8)	1(6)	4(6)	9(6)
C(13)	34(9)	48(10)	40(10)	-2(7)	13(7)	-2(7)
C(14)	63(13)	94(15)	56(12)	1(11)	20(11)	-12(11)
C(15)	41(10)	69(12)	59(12)	-12(10)	19(9)	0(9)
C(16)	31(9)	35(9)	96(15)	-13(9)	-11(9)	0(7)
C(17)	41(10)	39(9)	60(11)	-16(8)	11(8)	-11(8)
Cl(2)	120(6)	25(3)	193(9)	15(4)	-25(6)	-12(4)
Cl(2B)	201(41)	86(23)	102(25)	13(19)	-62(27)	-22(25)
O(3)	44(6)	29(5)	51(7)	-4(5)	8(6)	-4(5)
O(4)	63(7)	26(6)	47(6)	6(5)	5(5)	-6(5)
C(18)	32(9)	44(10)	65(12)	-28(9)	20(9)	-11(8)
C(19)	49(10)	21(9)	59(11)	-7(7)	8(9)	-6(7)
C(20)	65(12)	28(10)	116(17)	-5(10)	12(11)	-21(9)
C(21)	72(15)	63(14)	131(21)	36(14)	19(15)	3(12)
C(22)	86(18)	64(16)	164(26)	-7(16)	31(18)	-7(13)
C(23)	78(15)	74(16)	120(20)	8(14)	-11(14)	-23(13)
C(24)	68(12)	37(10)	79(13)	-2(9)	-6(11)	-18(9)
Cl(3)	104(4)	62(3)	137(5)	-47(3)	34(4)	-27(3)
O(5)	52(7)	32(6)	61(7)	-12(5)	24(6)	-7(5)
O(6)	73(8)	33(7)	40(6)	-6(5)	13(6)	-4(5)
C(25)	60(11)	37(10)	40(9)	-15(8)	23(8)	-13(9)
C(26)	55(11)	42(10)	41(9)	-7(8)	18(8)	-1(8)
C(27)	71(13)	31(9)	84(14)	-11(9)	12(11)	2(9)
C(28)	67(15)	65(15)	132(20)	-9(14)	-10(14)	-6(12)
C(29)	66(15)	70(16)	125(20)	-13(14)	-40(14)	-25(13)
C(30)	80(14)	51(12)	56(12)	-11(9)	3(11)	-17(11)
C(31)	64(12)	56(11)	64(12)	-7(9)	31(10)	-1(10)
Cl(4)	246(10)	91(5)	106(5)	-44(4)	20(6)	-85(6)
O(7)	71(8)	23(6)	50(7)	-6(5)	18(6)	-4(5)
O(8)	46(6)	32(6)	58(7)	6(5)	29(6)	-3(5)
C(32)	19(8)	26(9)	72(12)	18(9)	-7(8)	-9(6)
C(33)	56(10)	21(8)	45(10)	-15(7)	3(8)	0(7)
C(34)	80(13)	47(11)	59(12)	-4(9)	11(10)	-7(10)
C(35)	95(16)	61(13)	67(13)	-14(11)	18(11)	-39(11)
C(36)	109(18)	28(10)	112(19)	0(12)	16(14)	-27(11)
C(37)	78(13)	21(9)	91(14)	15(9)	37(11)	-4(8)
C(38)	71(11)	36(10)	47(10)	8(8)	25(9)	16(8)
Cl(5)	65(3)	46(3)	96(4)	20(2)	37(3)	-5(2)
O(9)	76(8)	30(7)	81(8)	1(6)	49(7)	-6(6)
O(10)	55(7)	31(6)	67(7)	-3(5)	38(6)	-1(5)
C(39)	59(11)	48(12)	55(11)	6(9)	25(9)	-16(9)
C(40)	40(9)	35(9)	68(11)	9(8)	34(8)	9(7)
C(41)	86(15)	54(12)	107(17)	13(11)	45(13)	9(11)
C(42)	128(20)	65(14)	155(23)	48(14)	103(18)	36(14)
C(43)	71(13)	68(13)	95(15)	19(11)	46(12)	16(11)
C(44)	46(10)	40(10)	88(13)	17(9)	24(10)	0(8)
C(45)	50(10)	38(10)	68(11)	1(8)	30(9)	-15(8)
Cl(6)	94(7)	151(10)	189(11)	12(8)	58(7)	-20(7)
Cl(6B)	77(12)	235(26)	24(8)	-27(11)	-4(7)	-102(15)
O(11)	37(6)	35(6)	104(10)	8(7)	31(7)	-2(5)

O(12)	41(6)	60(8)	71(8)	19(6)	21(6)	10(6)
C(46)	38(10)	28(9)	80(14)	8(9)	4(10)	-3(7)
C(47)	25(10)	31(10)	182(24)	21(12)	11(13)	8(8)
C(48)	35(11)	73(14)	160(22)	63(14)	21(12)	5(10)
C(49)	61(15)	81(16)	185(28)	79(18)	57(17)	2(12)
C(50)	72(19)	97(21)	246(42)	20(24)	50(24)	7(16)
C(51)	69(20)	119(26)	362(60)	-63(33)	-35(29)	4(19)
C(52)	60(15)	107(20)	216(31)	-101(21)	20(17)	-44(14)
OW2	175(34)	134(29)	294(51)	172(34)	192(38)	118(27)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 51.

	x	y	z	U(eq)
H(6)	1242(12)	7776(9)	3555(7)	65
H(7)	2327(14)	6954(10)	4119(8)	85
H(8)	3172(14)	6208(9)	3581(9)	75
H(9)	2863(13)	6378(10)	2506(9)	75
H(10)	1800(11)	7232(8)	1972(7)	53
H(13)	2964(10)	4098(8)	4688(7)	48
H(14)	1667(13)	4676(12)	4857(9)	84
H(15)	560(11)	5187(10)	4048(9)	67
H(17)	2152(10)	4645(8)	2872(8)	57
H(20)	-334(13)	6141(9)	1435(10)	87
H(22)	-2262(18)	4994(13)	156(14)	126
H(24)	-2035(12)	7291(9)	91(9)	80
H(27)	2769(13)	9453(9)	3456(9)	77
H(28)	4024(15)	10146(12)	3923(12)	115
H(29)	3900(15)	11323(13)	4303(11)	120
H(31)	1217(12)	11213(10)	3627(8)	70
H(34)	62(13)	11989(9)	2027(9)	76
H(36)	697(15)	13609(10)	943(11)	104
H(37)	29(12)	12894(8)	73(10)	73
H(38)	-466(11)	11689(8)	152(8)	60

Table S11. Crystal data and structure refinement for 6.

Empirical formula	C52H36Br6Mn3N2O14.1/4H2O
Formula weight	1561.61
Temperature	213(2) K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	P21/n
Unit cell dimensions	a = 15.553(3) A alpha = 90 deg. b = 17.884(2) A beta = 106.95(1) deg. c = 21.997(4) A gamma = 90 deg.
Volume	5853(2) A^3
Z	4
Density (calculated)	1.772 Mg/m^3
Absorption coefficient	4.773 mm^-1
F(000)	3060
Crystal size	0.53 x 0.34 x 0.34 mm
Theta range for data collection	1.78 to 25.00 deg.
Index ranges	-18<=h<=17, 0<=k<=21, 0<=l<=26
Reflections collected	10299
Independent reflections	10299 [R(int) = 0.0000]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10291 / 0 / 683
Goodness-of-fit on F^2	0.901
Final R indices [I>2sigma(I)]	R1 = 0.1148, wR2 = 0.2769
R indices (all data)	R1 = 0.2876, wR2 = 0.3504
Extinction coefficient	0.0000(2)
Largest diff. peak and hole	1.497 and -1.756 e.A^-3
Empirical Absoprtion correction	DIFABS (PLATON, A.L. Spek, Acta Cryst. A46 (1990) C34)
Transmission factors (Min./max.)	0.187/1.000

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 6. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mn(1)	496(2)	8415(1)	2208(1)	37(1)
Mn(2)	-818(2)	9787(1)	2228(1)	46(1)
Mn(3)	-588(4)	9251(3)	829(3)	160(2)
O(13)	-265(7)	9155(5)	1806(5)	34(3)
OW1	-912(7)	9376(6)	-180(5)	40(3)
N(1)	-1543(9)	10512(6)	2643(6)	64(5)
C(1)	-2369(10)	10285(7)	2703(7)	91(8)
C(2)	-2880(9)	10776(11)	2946(9)	115(10)
C(3)	-2565(13)	11493(9)	3128(8)	113(10)
C(4)	-1739(14)	11720(6)	3068(9)	123(11)
C(5)	-1228(10)	11230(7)	2825(8)	107(9)
N(2)	1415(9)	7617(7)	2682(7)	42(3)
C(6)	1610(12)	7530(9)	3313(8)	48(5)
C(7)	2222(16)	7027(11)	3645(10)	75(7)
C(8)	2657(13)	6581(10)	3308(11)	59(6)
C(9)	2486(15)	6680(11)	2688(10)	70(6)
C(10)	1846(13)	7182(10)	2383(9)	56(5)
Br(1)	484(2)	5493(1)	2725(1)	86(1)
O(1)	735(7)	9093(6)	852(5)	40(3)
O(2)	1467(7)	8757(6)	1842(6)	50(3)
C(11)	1444(11)	9047(9)	1306(9)	42(4)
C(12)	2719(11)	4331(8)	3770(8)	37(4)
C(13)	2577(11)	4288(11)	4355(10)	55(5)
C(14)	1850(17)	4595(13)	4474(10)	78(7)
C(15)	1200(15)	4965(12)	4017(10)	69(6)
C(16)	1344(13)	4986(10)	3399(11)	69(7)
C(17)	2078(12)	4680(8)	3273(9)	46(5)
Br(2)	-947(2)	4585(1)	1093(2)	128(2)
Br(2B)	-3479(15)	6123(12)	-339(11)	75(7)
O(3)	-6(8)	7545(6)	1500(6)	49(3)
O(4)	-923(8)	8153(5)	711(5)	50(3)
C(18)	-649(12)	7567(10)	1006(9)	49(5)
C(19)	-1103(12)	6847(8)	770(8)	43(4)
C(20)	-833(14)	6172(10)	1025(9)	68(6)
C(21)	-1319(15)	5530(11)	747(12)	74(6)
C(22)	-2054(15)	5561(12)	250(12)	93(8)
C(23)	-2349(17)	6246(12)	-12(14)	112(10)
C(24)	-1867(14)	6890(11)	241(11)	75(6)
Br(3)	2456(2)	2292(1)	4292(2)	108(1)
O(5)	337(8)	10184(6)	2817(6)	51(3)
O(6)	1124(8)	9117(6)	3007(5)	48(3)
C(25)	1018(13)	9807(10)	3065(8)	43(4)
C(26)	1878(12)	10234(9)	3459(9)	46(4)
C(27)	2670(15)	9915(11)	3548(9)	66(6)
C(28)	3440(18)	10278(13)	3843(13)	99(9)
C(29)	3358(16)	11013(14)	4109(11)	90(8)
C(30)	2543(15)	11318(10)	4009(9)	61(6)
C(31)	1777(12)	10918(11)	3678(9)	58(5)
Br(4)	1082(2)	13388(1)	2280(1)	116(1)
O(7)	-339(8)	10383(5)	845(5)	48(3)

O(8)	-750(8)	10749(5)	1676(5)	46(3)
C(32)	-458(10)	10881(8)	1217(8)	35(4)
C(33)	-226(11)	11664(9)	1117(8)	38(4)
C(34)	132(11)	12109(10)	1629(8)	47(5)
C(35)	478(13)	12820(10)	1553(10)	59(5)
C(36)	416(14)	13100(10)	963(12)	73(7)
C(37)	4(13)	12653(9)	430(9)	55(5)
C(38)	-251(12)	11933(9)	519(9)	58(6)
Br(5)	-1210(2)	5676(1)	3931(1)	73(1)
O(9)	-958(9)	9003(6)	2925(6)	64(4)
O(10)	-324(9)	7987(6)	2678(6)	58(3)
C(39)	-849(13)	8329(10)	2929(9)	56(5)
C(40)	-1340(10)	7829(6)	3261(7)	62(6)
C(41)	-2065(11)	8128(5)	3426(9)	133(13)
C(42)	-2531(10)	7691(8)	3748(9)	120(11)
C(43)	-2270(10)	6955(7)	3903(8)	94(8)
C(44)	-1545(9)	6657(5)	3737(7)	64(6)
C(45)	-1079(8)	7094(6)	3416(6)	54(5)
Br(6)	-5173(3)	8079(2)	1540(3)	125(2)
Br(6B)	-4584(7)	7510(8)	-319(5)	139(5)
O(11)	-2026(9)	9411(6)	1725(8)	64(4)
O(12)	-1872(9)	9438(9)	766(7)	69(4)
C(46)	-2245(14)	9284(10)	1114(14)	67(7)
C(47)	-3193(8)	8845(6)	945(10)	104(10)
C(48)	-3730(13)	8719(6)	1341(8)	113(11)
C(49)	-4537(12)	8334(6)	1114(11)	133(15)
C(50)	-4807(7)	8076(7)	491(11)	194(26)
C(51)	-4270(11)	8202(7)	95(8)	204(24)
C(52)	-3463(10)	8587(6)	322(9)	150(16)
OW2	-3959(26)	4258(7)	144(18)	59(16)

Table S13. Bond lengths [A] and angles [deg] for 6.

Mn(1)-O(13)	1.824(10)
Mn(1)-O(2)	2.003(12)
Mn(1)-O(10)	2.012(12)
Mn(1)-N(2)	2.072(13)
Mn(1)-O(6)	2.149(11)
Mn(1)-O(3)	2.179(11)
Mn(1)-Mn(2)	3.202(3)
Mn(1)-Mn(3)	3.362(7)
Mn(2)-O(13)	1.830(10)
Mn(2)-O(11)	2.00(2)
Mn(2)-O(5)	2.015(12)
Mn(2)-N(1)	2.095(10)
Mn(2)-O(8)	2.127(11)
Mn(2)-O(9)	2.134(11)
Mn(2)-Mn(3)	3.340(7)
Mn(3)-O(12)	1.99(2)
Mn(3)-O(4)	2.028(11)
Mn(3)-O(7)	2.060(11)
Mn(3)-O(1)	2.064(12)
Mn(3)-O(13)	2.066(12)
Mn(3)-OW1	2.140(12)
Mn(3)-C(46)	2.83(3)
N(1)-C(1)	1.39
N(1)-C(5)	1.39
C(1)-C(2)	1.39
C(2)-C(3)	1.39
C(3)-C(4)	1.39
C(4)-C(5)	1.39
N(2)-C(10)	1.32(2)
N(2)-C(6)	1.34(2)
C(6)-C(7)	1.36(2)
C(7)-C(8)	1.39(3)
C(8)-C(9)	1.32(3)
C(9)-C(10)	1.36(3)
Br(1)-C(16)	1.91(2)
O(1)-C(11)	1.26(2)
O(2)-C(11)	1.28(2)
C(11)-C(12)#1	1.45(2)
C(12)-C(13)	1.37(2)
C(12)-C(17)	1.39(2)
C(12)-C(11)#2	1.45(2)
C(13)-C(14)	1.35(3)
C(14)-C(15)	1.37(3)
C(15)-C(16)	1.44(3)
C(16)-C(17)	1.37(3)
Br(2)-C(21)	1.88(2)
Br(2B)-C(23)	1.71(3)
O(3)-C(18)	1.24(2)
O(4)-C(18)	1.24(2)
C(18)-C(19)	1.49(2)
C(19)-C(20)	1.35(2)
C(19)-C(24)	1.40(3)
C(20)-C(21)	1.41(3)
C(21)-C(22)	1.33(3)
C(22)-C(23)	1.38(3)
C(23)-C(24)	1.40(3)

Br(3)-C(30)#3	1.87(2)
O(5)-C(25)	1.24(2)
O(6)-C(25)	1.26(2)
C(25)-C(26)	1.56(2)
C(26)-C(27)	1.32(2)
C(26)-C(31)	1.34(2)
C(27)-C(28)	1.35(3)
C(28)-C(29)	1.46(3)
C(29)-C(30)	1.34(3)
C(30)-C(31)	1.40(2)
C(30)-Br(3)#4	1.87(2)
Br(4)-C(35)	1.90(2)
O(7)-C(32)	1.26(2)
O(8)-C(32)	1.24(2)
C(32)-C(33)	1.48(2)
C(33)-C(34)	1.36(2)
C(33)-C(38)	1.39(2)
C(34)-C(35)	1.41(2)
C(35)-C(36)	1.37(3)
C(36)-C(37)	1.41(3)
C(37)-C(38)	1.38(2)
Br(5)-C(44)	1.843(9)
O(9)-C(39)	1.22(2)
O(10)-C(39)	1.27(2)
C(39)-C(40)	1.49(2)
C(40)-C(41)	1.39
C(40)-C(45)	1.39
C(41)-C(42)	1.39
C(42)-C(43)	1.39
C(43)-C(44)	1.39
C(44)-C(45)	1.39
Br(6)-C(49)	1.61(2)
Br(6B)-C(51)	1.53(2)
Br(6B)-C(50)	2.16(2)
O(11)-C(46)	1.31(3)
O(12)-C(46)	1.12(3)
C(46)-C(47)	1.61(2)
C(47)-C(48)	1.39
C(47)-C(52)	1.39
C(48)-C(49)	1.39
C(49)-C(50)	1.39
C(50)-C(51)	1.39
C(51)-C(52)	1.39

O(13)-Mn(1)-O(2)	92.3(4)
O(13)-Mn(1)-O(10)	96.1(5)
O(2)-Mn(1)-O(10)	171.1(5)
O(13)-Mn(1)-N(2)	176.9(5)
O(2)-Mn(1)-N(2)	85.6(5)
O(10)-Mn(1)-N(2)	85.9(5)
O(13)-Mn(1)-O(6)	92.8(4)
O(2)-Mn(1)-O(6)	86.2(5)
O(10)-Mn(1)-O(6)	90.4(5)
N(2)-Mn(1)-O(6)	84.8(5)
O(13)-Mn(1)-O(3)	97.1(4)
O(2)-Mn(1)-O(3)	94.9(4)
O(10)-Mn(1)-O(3)	87.0(5)
N(2)-Mn(1)-O(3)	85.4(5)
O(6)-Mn(1)-O(3)	170.0(4)
O(13)-Mn(1)-Mn(2)	28.8(3)

O(2)-Mn(1)-Mn(2)	109.3(3)
O(10)-Mn(1)-Mn(2)	77.3(4)
N(2)-Mn(1)-Mn(2)	150.5(4)
O(6)-Mn(1)-Mn(2)	71.4(3)
O(3)-Mn(1)-Mn(2)	117.3(3)
O(13)-Mn(1)-Mn(3)	32.3(3)
O(2)-Mn(1)-Mn(3)	74.9(3)
O(10)-Mn(1)-Mn(3)	114.0(4)
N(2)-Mn(1)-Mn(3)	148.3(4)
O(6)-Mn(1)-Mn(3)	117.8(3)
O(3)-Mn(1)-Mn(3)	72.0(3)
Mn(2)-Mn(1)-Mn(3)	61.12(13)
O(13)-Mn(2)-O(11)	91.0(5)
O(13)-Mn(2)-O(5)	94.7(5)
O(11)-Mn(2)-O(5)	173.4(6)
O(13)-Mn(2)-N(1)	175.2(5)
O(11)-Mn(2)-N(1)	84.9(6)
O(5)-Mn(2)-N(1)	89.6(5)
O(13)-Mn(2)-O(8)	95.8(4)
O(11)-Mn(2)-O(8)	98.7(5)
O(5)-Mn(2)-O(8)	84.1(5)
N(1)-Mn(2)-O(8)	82.5(5)
O(13)-Mn(2)-O(9)	97.0(5)
O(11)-Mn(2)-O(9)	84.3(6)
O(5)-Mn(2)-O(9)	91.6(5)
N(1)-Mn(2)-O(9)	85.0(5)
O(8)-Mn(2)-O(9)	166.8(5)
O(13)-Mn(2)-Mn(1)	28.7(3)
O(11)-Mn(2)-Mn(1)	103.6(3)
O(5)-Mn(2)-Mn(1)	80.0(3)
N(1)-Mn(2)-Mn(1)	155.1(4)
O(8)-Mn(2)-Mn(1)	118.3(3)
O(9)-Mn(2)-Mn(1)	72.9(3)
O(13)-Mn(2)-Mn(3)	33.1(3)
O(11)-Mn(2)-Mn(3)	74.3(4)
O(5)-Mn(2)-Mn(3)	112.3(4)
N(1)-Mn(2)-Mn(3)	142.7(4)
O(8)-Mn(2)-Mn(3)	70.7(3)
O(9)-Mn(2)-Mn(3)	122.3(4)
Mn(1)-Mn(2)-Mn(3)	61.79(12)
O(12)-Mn(3)-O(4)	86.5(6)
O(12)-Mn(3)-O(7)	90.9(6)
O(4)-Mn(3)-O(7)	173.5(6)
O(12)-Mn(3)-O(1)	176.9(7)
O(4)-Mn(3)-O(1)	95.0(5)
O(7)-Mn(3)-O(1)	87.3(5)
O(12)-Mn(3)-O(13)	91.3(6)
O(4)-Mn(3)-O(13)	91.6(5)
O(7)-Mn(3)-O(13)	94.4(5)
O(1)-Mn(3)-O(13)	91.4(5)
O(12)-Mn(3)-OW1	89.0(6)
O(4)-Mn(3)-OW1	89.7(5)
O(7)-Mn(3)-OW1	84.3(5)
O(1)-Mn(3)-OW1	88.3(5)
O(13)-Mn(3)-OW1	178.7(5)
O(12)-Mn(3)-C(46)	18.2(6)
O(4)-Mn(3)-C(46)	80.3(6)
O(7)-Mn(3)-C(46)	98.9(6)
O(1)-Mn(3)-C(46)	164.9(7)
O(13)-Mn(3)-C(46)	74.5(7)

OW1-Mn(3)-C(46)	105.9(7)
O(12)-Mn(3)-Mn(2)	69.0(5)
O(4)-Mn(3)-Mn(2)	107.6(4)
O(7)-Mn(3)-Mn(2)	76.9(4)
O(1)-Mn(3)-Mn(2)	113.0(4)
O(13)-Mn(3)-Mn(2)	28.9(3)
OW1-Mn(3)-Mn(2)	150.4(4)
C(46)-Mn(3)-Mn(2)	55.9(5)
O(12)-Mn(3)-Mn(1)	111.5(5)
O(4)-Mn(3)-Mn(1)	74.2(4)
O(7)-Mn(3)-Mn(1)	112.3(4)
O(1)-Mn(3)-Mn(1)	71.5(3)
O(13)-Mn(3)-Mn(1)	28.2(3)
OW1-Mn(3)-Mn(1)	152.5(4)
C(46)-Mn(3)-Mn(1)	93.4(6)
Mn(2)-Mn(3)-Mn(1)	57.08(12)
Mn(1)-O(13)-Mn(2)	122.4(5)
Mn(1)-O(13)-Mn(3)	119.5(5)
Mn(2)-O(13)-Mn(3)	118.0(5)
C(1)-N(1)-C(5)	120.0
C(1)-N(1)-Mn(2)	119.4(8)
C(5)-N(1)-Mn(2)	120.5(8)
C(2)-C(1)-N(1)	120.0
C(1)-C(2)-C(3)	120.0
C(4)-C(3)-C(2)	120.0
C(3)-C(4)-C(5)	120.0
C(4)-C(5)-N(1)	120.0
C(10)-N(2)-C(6)	117(2)
C(10)-N(2)-Mn(1)	122.1(12)
C(6)-N(2)-Mn(1)	121.0(12)
N(2)-C(6)-C(7)	123(2)
C(6)-C(7)-C(8)	118(2)
C(9)-C(8)-C(7)	119(2)
C(8)-C(9)-C(10)	120(2)
N(2)-C(10)-C(9)	123(2)
C(11)-O(1)-Mn(3)	131.8(11)
C(11)-O(2)-Mn(1)	132.3(10)
O(1)-C(11)-O(2)	123(2)
O(1)-C(11)-C(12)#1	120(2)
O(2)-C(11)-C(12)#1	117.6(14)
C(13)-C(12)-C(17)	119(2)
C(13)-C(12)-C(11)#2	119(2)
C(17)-C(12)-C(11)#2	122(2)
C(14)-C(13)-C(12)	122(2)
C(13)-C(14)-C(15)	122(2)
C(14)-C(15)-C(16)	115(2)
C(17)-C(16)-C(15)	123(2)
C(17)-C(16)-Br(1)	118(2)
C(15)-C(16)-Br(1)	119(2)
C(16)-C(17)-C(12)	118(2)
C(18)-O(3)-Mn(1)	129.2(11)
C(18)-O(4)-Mn(3)	135.6(12)
O(4)-C(18)-O(3)	123(2)
O(4)-C(18)-C(19)	120(2)
O(3)-C(18)-C(19)	117(2)
C(20)-C(19)-C(24)	119(2)
C(20)-C(19)-C(18)	125(2)
C(24)-C(19)-C(18)	116(2)
C(19)-C(20)-C(21)	119(2)
C(22)-C(21)-C(20)	123(2)

C(22)-C(21)-Br(2)	117(2)
C(20)-C(21)-Br(2)	120(2)
C(21)-C(22)-C(23)	119(2)
C(22)-C(23)-C(24)	120(2)
C(22)-C(23)-Br(2B)	104(2)
C(24)-C(23)-Br(2B)	130(2)
C(23)-C(24)-C(19)	121(2)
C(25)-O(5)-Mn(2)	125.3(11)
C(25)-O(6)-Mn(1)	128.0(11)
O(5)-C(25)-O(6)	128(2)
O(5)-C(25)-C(26)	117.4(14)
O(6)-C(25)-C(26)	115(2)
C(27)-C(26)-C(31)	123(2)
C(27)-C(26)-C(25)	119(2)
C(31)-C(26)-C(25)	118(2)
C(26)-C(27)-C(28)	122(2)
C(27)-C(28)-C(29)	117(2)
C(30)-C(29)-C(28)	119(2)
C(29)-C(30)-C(31)	120(2)
C(29)-C(30)-Br(3)#4	119(2)
C(31)-C(30)-Br(3)#4	121(2)
C(26)-C(31)-C(30)	119(2)
C(32)-O(7)-Mn(3)	130.0(10)
C(32)-O(8)-Mn(2)	135.0(10)
O(8)-C(32)-O(7)	123.5(13)
O(8)-C(32)-C(33)	118(2)
O(7)-C(32)-C(33)	119(2)
C(34)-C(33)-C(38)	118(2)
C(34)-C(33)-C(32)	120(2)
C(38)-C(33)-C(32)	122(2)
C(33)-C(34)-C(35)	121(2)
C(36)-C(35)-C(34)	121(2)
C(36)-C(35)-Br(4)	119(2)
C(34)-C(35)-Br(4)	120(2)
C(35)-C(36)-C(37)	118(2)
C(38)-C(37)-C(36)	119(2)
C(37)-C(38)-C(33)	122(2)
C(39)-O(9)-Mn(2)	127.8(13)
C(39)-O(10)-Mn(1)	128.8(11)
O(9)-C(39)-O(10)	125(2)
O(9)-C(39)-C(40)	120(2)
O(10)-C(39)-C(40)	114(2)
C(41)-C(40)-C(45)	120.0
C(41)-C(40)-C(39)	117.9(11)
C(45)-C(40)-C(39)	122.1(11)
C(40)-C(41)-C(42)	120.0
C(41)-C(42)-C(43)	120.0
C(44)-C(43)-C(42)	120.0
C(45)-C(44)-C(43)	120.0
C(45)-C(44)-Br(5)	119.9(7)
C(43)-C(44)-Br(5)	120.1(7)
C(44)-C(45)-C(40)	120.0
C(51)-Br(6B)-C(50)	39.8(6)
C(46)-O(11)-Mn(2)	123.3(14)
C(46)-O(12)-Mn(3)	128(2)
O(12)-C(46)-O(11)	129(2)
O(12)-C(46)-C(47)	126(2)
O(11)-C(46)-C(47)	106(2)
O(12)-C(46)-Mn(3)	33.5(11)
O(11)-C(46)-Mn(3)	104.5(13)

C(47)-C(46)-Mn(3)	140(2)
C(48)-C(47)-C(52)	120.0
C(48)-C(47)-C(46)	128(2)
C(52)-C(47)-C(46)	113(2)
C(49)-C(48)-C(47)	120.0
C(48)-C(49)-C(50)	120.0
C(48)-C(49)-Br(6)	125.0(13)
C(50)-C(49)-Br(6)	114.7(12)
C(51)-C(50)-C(49)	120.0
C(51)-C(50)-Br(6B)	44.7(6)
C(49)-C(50)-Br(6B)	153.2(6)
C(50)-C(51)-C(52)	120.0
C(50)-C(51)-Br(6B)	95.5(10)
C(52)-C(51)-Br(6B)	135.5(11)
C(51)-C(52)-C(47)	120.0

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

Table S14. Anisotropic displacement parameters (A^2 x 10^3) for 6. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mn(1)	40(2)	43(1)	32(2)	3(1)	15(1)	-3(1)
Mn(2)	51(2)	45(1)	53(2)	-1(1)	32(2)	-3(1)
Mn(3)	166(6)	136(4)	166(6)	5(4)	27(4)	-1(4)
O(13)	47(7)	35(5)	25(6)	-6(4)	17(5)	-5(5)
OW1	36(7)	64(6)	19(6)	-6(5)	7(5)	8(5)
N(1)	92(14)	62(9)	64(12)	-10(8)	60(10)	-21(9)
C(1)	113(22)	115(19)	59(17)	-13(14)	45(15)	-9(17)
C(2)	153(28)	115(21)	97(22)	11(17)	71(20)	58(20)
C(3)	141(27)	65(15)	142(26)	-4(15)	54(22)	54(16)
C(4)	116(25)	118(21)	160(30)	-25(20)	80(23)	29(19)
C(5)	173(29)	76(15)	94(21)	6(14)	74(20)	18(17)
N(2)	44(9)	52(8)	30(9)	11(7)	12(7)	-1(7)
C(6)	63(13)	53(9)	25(11)	0(8)	9(9)	-6(9)
C(7)	93(18)	75(13)	44(14)	4(11)	-1(13)	-3(13)
C(8)	50(13)	45(10)	81(17)	21(11)	16(12)	-2(9)
C(9)	82(16)	74(13)	53(15)	-18(11)	19(12)	22(12)
C(10)	57(13)	63(11)	45(13)	3(10)	11(11)	-3(10)
Br(1)	55(2)	111(2)	82(2)	1(1)	7(1)	22(1)
O(1)	23(6)	71(7)	29(7)	-3(5)	13(6)	-3(5)
O(2)	43(8)	57(6)	40(8)	8(6)	-4(6)	-1(6)
C(11)	22(10)	53(9)	37(11)	-9(8)	-11(9)	5(7)
C(12)	36(10)	47(8)	38(11)	-7(8)	27(8)	12(8)
C(13)	19(10)	95(13)	66(15)	3(11)	33(10)	-9(9)
C(14)	92(19)	109(17)	34(13)	-2(12)	20(13)	-12(15)
C(15)	81(17)	96(15)	50(15)	-28(12)	50(14)	-16(13)
C(16)	39(13)	54(11)	94(19)	-11(11)	-12(12)	-5(9)
C(17)	47(12)	35(8)	53(12)	2(8)	10(10)	5(8)
Br(2)	121(3)	53(1)	172(4)	12(2)	-19(2)	-12(2)
Br(2B)	64(15)	84(13)	65(15)	-8(11)	-1(12)	-39(12)
O(3)	39(8)	62(7)	42(8)	-7(6)	6(6)	1(6)
O(4)	62(8)	36(6)	50(8)	5(5)	11(7)	-2(5)
C(18)	39(12)	67(11)	35(12)	-2(9)	2(9)	9(9)
C(19)	60(13)	33(8)	40(11)	-7(7)	21(10)	-18(8)
C(20)	84(16)	56(11)	52(14)	-5(10)	1(12)	-3(11)
C(21)	65(16)	64(12)	94(19)	4(12)	25(14)	-6(11)
C(22)	62(16)	73(14)	121(23)	-37(14)	-8(15)	-14(12)
C(23)	85(19)	57(13)	158(27)	-32(15)	-22(17)	-11(12)
C(24)	67(15)	63(12)	84(17)	-15(11)	6(13)	-7(11)
Br(3)	102(2)	85(2)	129(3)	-48(2)	18(2)	-19(2)
O(5)	54(9)	53(7)	52(8)	-7(6)	23(7)	3(6)
O(6)	51(8)	56(7)	38(8)	-12(5)	14(6)	-5(6)
C(25)	61(13)	56(10)	24(10)	-8(8)	31(9)	-4(10)
C(26)	33(11)	54(10)	54(13)	5(9)	15(9)	-3(8)
C(27)	64(15)	71(12)	56(14)	-13(10)	6(12)	-8(12)
C(28)	92(20)	74(15)	121(24)	5(15)	16(17)	-17(14)
C(29)	64(17)	114(19)	75(18)	39(15)	-9(14)	-37(15)
C(30)	62(15)	67(12)	46(13)	-8(9)	2(11)	-18(11)
C(31)	34(11)	81(13)	67(15)	-9(11)	26(10)	-14(10)
Br(4)	160(3)	82(2)	88(2)	-29(2)	9(2)	-43(2)
O(7)	81(9)	32(5)	36(7)	1(5)	26(7)	-7(6)

O(8)	55(8)	40(6)	41(8)	5(5)	11(6)	-12(5)
C(32)	24(9)	42(9)	35(11)	10(8)	3(8)	-5(7)
C(33)	44(11)	54(9)	23(10)	0(8)	19(8)	-4(8)
C(34)	39(11)	81(12)	17(10)	-3(9)	5(8)	-2(9)
C(35)	54(13)	50(10)	67(15)	-10(10)	9(11)	-9(9)
C(36)	66(15)	49(10)	115(22)	0(13)	44(15)	-6(10)
C(37)	79(15)	54(10)	41(12)	15(9)	31(11)	16(10)
C(38)	43(12)	56(10)	59(14)	-8(10)	-12(10)	12(9)
Br(5)	70(2)	67(1)	93(2)	18(1)	41(1)	-6(1)
O(9)	89(11)	50(7)	74(10)	22(6)	56(9)	6(7)
O(10)	71(10)	50(7)	66(10)	4(6)	41(8)	-12(6)
C(39)	47(12)	64(12)	63(14)	-5(10)	25(11)	13(10)
C(40)	67(14)	60(11)	83(16)	2(10)	61(13)	-25(10)
C(41)	219(37)	78(16)	158(29)	23(17)	144(28)	-17(19)
C(42)	146(27)	82(16)	163(29)	35(18)	94(23)	41(17)
C(43)	92(19)	57(12)	154(25)	41(14)	69(18)	15(12)
C(44)	57(14)	67(11)	91(17)	4(11)	58(13)	-8(10)
C(45)	65(13)	50(10)	50(13)	18(9)	23(10)	-15(9)
Br(6)	70(3)	133(3)	182(5)	36(3)	55(3)	-7(2)
Br(6B)	77(7)	258(14)	66(6)	-40(8)	-3(5)	-79(8)
O(11)	52(9)	49(7)	99(12)	7(8)	34(9)	-1(6)
O(12)	32(9)	111(12)	68(11)	3(9)	18(7)	10(8)
C(46)	40(14)	47(11)	94(21)	-15(12)	-14(14)	8(10)
C(47)	24(13)	60(12)	205(33)	-8(16)	-1(17)	11(10)
C(48)	59(17)	93(17)	207(34)	17(19)	69(21)	-1(14)
C(49)	55(19)	141(26)	208(40)	88(26)	45(22)	-8(17)
C(50)	56(22)	107(23)	387(75)	99(37)	12(34)	-3(18)
C(51)	10(14)	134(26)	402(67)	-45(33)	-45(24)	17(15)
C(52)	41(16)	110(20)	253(41)	-87(24)	-29(20)	21(14)
OW2	84(37)	94(33)	37(30)	-47(26)	75(29)	-61(30)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 6.

	x	y	z	U(eq)
H(6)	1310(12)	7832(9)	3536(8)	58
H(7)	2348(16)	6982(11)	4088(10)	90
H(8)	3068(13)	6212(10)	3518(11)	71
H(9)	2805(15)	6407(11)	2459(10)	84
H(10)	1704(13)	7220(10)	1939(9)	67
H(13)	3001(11)	4036(11)	4684(10)	66
H(14)	1787(17)	4553(13)	4885(10)	93
H(15)	699(15)	5189(12)	4101(10)	83
H(17)	2149(12)	4703(8)	2863(9)	55
H(20)	-328(14)	6128(10)	1383(9)	81
H(22)	-2365(15)	5121(12)	82(12)	111
H(24)	-2057(14)	7357(11)	54(11)	90
H(27)	2698(15)	9424(11)	3403(9)	80
H(28)	4005(18)	10067(13)	3875(13)	119
H(29)	3873(16)	11269(14)	4349(11)	109
H(31)	1202(12)	11126(11)	3609(9)	70
H(34)	148(11)	11942(10)	2037(8)	56
H(36)	641(14)	13577(10)	915(12)	87
H(37)	-96(13)	12845(9)	18(9)	66
H(38)	-447(12)	11614(9)	165(9)	70