

Table 1. Crystal data and structure refinement for structure4.

Identification code	structure4
Empirical formula	C19.33 H15.33 Mn1.33 N3.33 O6
Formula weight	463.60
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 15.6193(9) Å α = 90°. b = 10.3503(6) Å β = 102.400(1)°. c = 16.8723(10) Å γ = 90°.
Volume	2664.0(3) Å ³
Z	6
Calculated density	1.734 Mg/m ³
Absorption coefficient	1.018 mm ⁻¹
F(000)	1416
Crystal size	0.18 x 0.17 x 0.03 mm ³
Theta range for data collection	2.38 to 25.00°.
Limiting indices	-18<= <i>h</i> <=17, -12<= <i>k</i> <=12, -20<= <i>l</i> <=19
Reflections collected	8622
Independent reflections	2345 [R(int) = 0.0275]
Completeness to theta = 25.00°	99.9%
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.821
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2345 / 2 / 237
Goodness-of-fit on F ²	1.312
Final R indices [I>2sigma(I)]	R1 = 0.0444, wR2 = 0.0947
R indices (all data)	R1 = 0.0467, wR2 = 0.0956
Largest diff. peak and hole	0.398 and -0.261 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mn(1)	1433(1)	989(1)	238(1)	11(1)
C(1)	1045(2)	-38(3)	1939(2)	17(1)
C(2)	1227(2)	-603(3)	2696(2)	18(1)
C(3)	1904(2)	-1488(3)	2878(2)	15(1)
C(4)	2376(2)	-1769(3)	2286(2)	16(1)
C(5)	2165(2)	-1141(3)	1543(2)	14(1)
C(6)	2728(2)	-1263(3)	940(2)	13(1)
C(7)	3289(2)	-2302(3)	928(2)	14(1)
C(8)	3886(2)	-2253(3)	430(2)	14(1)
C(9)	3901(2)	-1160(3)	-41(2)	20(1)
C(10)	3289(2)	-202(3)	-36(2)	21(1)
C(11)	2170(2)	-2092(3)	3718(2)	13(1)
C(12)	4528(2)	-3342(3)	414(2)	14(1)
C(13)	-290(5)	3340(8)	2798(5)	31(2)
C(14)	229(8)	4722(11)	1844(5)	73(4)
C(15)	-741(10)	5573(18)	2750(13)	81(7)
C(16)	1042(9)	5460(20)	2121(11)	59(4)
C(17)	-189(7)	6592(9)	3232(6)	50(2)
O(1)	2895(1)	-2659(2)	3865(1)	17(1)
O(2)	1659(2)	-1936(2)	4190(1)	17(1)
O(3)	4272(1)	-4464(2)	530(1)	15(1)
O(4)	5260(1)	-3012(2)	303(1)	18(1)
O(5)	-80(70)	2379(5)	2440(80)	43(11)
N(1)	1499(2)	-283(2)	1365(2)	15(1)
N(2)	2695(2)	-245(2)	429(2)	15(1)
N(3)	-257(5)	4513(6)	2486(7)	47(3)

Table 3. Bond lengths [Å] and angles [°] for struct4.

Mn(1)-O(2)#1	2.117(2)
Mn(1)-O(4)#2	2.126(2)
Mn(1)-O(1)#3	2.161(2)
Mn(1)-O(3)#4	2.184(2)
Mn(1)-N(1)	2.298(3)
Mn(1)-N(2)	2.313(3)
C(1)-N(1)	1.340(4)
C(1)-C(2)	1.378(5)
C(2)-C(3)	1.383(5)
C(3)-C(4)	1.393(4)
C(3)-C(11)	1.524(4)
C(4)-C(5)	1.388(4)
C(5)-N(1)	1.352(4)
C(5)-C(6)	1.487(4)
C(6)-N(2)	1.355(4)
C(6)-C(7)	1.391(4)
C(7)-C(8)	1.384(4)
C(8)-C(9)	1.385(4)
C(8)-C(12)	1.513(4)
C(9)-C(10)	1.378(5)
C(10)-N(2)	1.338(4)
C(11)-O(2)	1.252(4)
C(11)-O(1)	1.252(4)
C(12)-O(4)	1.245(4)
C(12)-O(3)	1.258(4)
C(13)-O(5)	1.25(9)
C(13)-N(3)	1.330(11)
C(14)-N(3)	1.466(13)
C(14)-C(16)	1.467(18)
C(15)-N(3)	1.456(16)
C(15)-C(17)	1.489(18)
O(1)-Mn(1)#5	2.161(2)

O(2)-Mn(1) #6	2.117(2)
O(3)-Mn(1) #4	2.184(2)
O(4)-Mn(1) #7	2.126(2)

O(2) #1-Mn(1) -O(4) #2	96.80(9)
O(2) #1-Mn(1) -O(1) #3	98.18(8)
O(4) #2-Mn(1) -O(1) #3	86.80(8)
O(2) #1-Mn(1) -O(3) #4	89.55(8)
O(4) #2-Mn(1) -O(3) #4	92.98(8)
O(1) #3-Mn(1) -O(3) #4	172.24(8)
O(2) #1-Mn(1) -N(1)	166.17(9)
O(4) #2-Mn(1) -N(1)	97.02(9)
O(1) #3-Mn(1) -N(1)	82.07(9)
O(3) #4-Mn(1) -N(1)	90.26(9)
O(2) #1-Mn(1) -N(2)	94.68(9)
O(4) #2-Mn(1) -N(2)	168.30(9)
O(1) #3-Mn(1) -N(2)	89.32(9)
O(3) #4-Mn(1) -N(2)	89.37(9)
N(1) -Mn(1) -N(2)	71.49(9)
N(1) -C(1) -C(2)	123.6(3)
C(1) -C(2) -C(3)	118.8(3)
C(2) -C(3) -C(4)	118.4(3)
C(2) -C(3) -C(11)	121.3(3)
C(4) -C(3) -C(11)	120.1(3)
C(5) -C(4) -C(3)	119.4(3)
N(1) -C(5) -C(4)	122.0(3)
N(1) -C(5) -C(6)	116.4(3)
C(4) -C(5) -C(6)	121.2(3)
N(2) -C(6) -C(7)	122.1(3)
N(2) -C(6) -C(5)	115.0(3)
C(7) -C(6) -C(5)	122.8(3)
C(8) -C(7) -C(6)	119.2(3)
C(7) -C(8) -C(9)	118.4(3)
C(7) -C(8) -C(12)	121.2(3)
C(9) -C(8) -C(12)	120.4(3)

C(10)-C(9)-C(8)	119.1(3)
N(2)-C(10)-C(9)	123.3(3)
O(2)-C(11)-O(1)	127.4(3)
O(2)-C(11)-C(3)	117.1(3)
O(1)-C(11)-C(3)	115.5(3)
O(4)-C(12)-O(3)	127.6(3)
O(4)-C(12)-C(8)	115.6(3)
O(3)-C(12)-C(8)	116.8(3)
O(5)-C(13)-N(3)	120(5)
N(3)-C(14)-C(16)	113.0(10)
N(3)-C(15)-C(17)	115.0(12)
C(11)-O(1)-Mn(1) #5	136.5(2)
C(11)-O(2)-Mn(1) #6	146.5(2)
C(12)-O(3)-Mn(1) #4	135.34(19)
C(12)-O(4)-Mn(1) #7	134.7(2)
C(1)-N(1)-C(5)	117.8(3)
C(1)-N(1)-Mn(1)	123.5(2)
C(5)-N(1)-Mn(1)	117.11(19)
C(10)-N(2)-C(6)	117.5(3)
C(10)-N(2)-Mn(1)	125.3(2)
C(6)-N(2)-Mn(1)	115.66(19)
C(13)-N(3)-C(15)	120.0(12)
C(13)-N(3)-C(14)	119.9(8)
C(15)-N(3)-C(14)	120.1(12)

Symmetry transformations used to generate equivalent atoms:

#1 $x, -y, z-1/2$ #2 $x-1/2, y+1/2, z$ #3 $-x+1/2, y+1/2, -z+1/2$
#4 $-x+1/2, -y-1/2, -z$ #5 $-x+1/2, y-1/2, -z+1/2$
#6 $x, -y, z+1/2$ #7 $x+1/2, y-1/2, z$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct4.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2[h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn (1)	11 (1)	12 (1)	10 (1)	0 (1)	3 (1)	2 (1)
C (1)	14 (2)	19 (2)	20 (2)	1 (1)	4 (1)	5 (1)
C (2)	20 (2)	23 (2)	14 (2)	0 (1)	9 (1)	3 (1)
C (3)	16 (2)	15 (2)	12 (2)	0 (1)	2 (1)	0 (1)
C (4)	17 (2)	13 (2)	17 (2)	1 (1)	4 (1)	4 (1)
C (5)	14 (2)	12 (2)	15 (2)	-1 (1)	4 (1)	0 (1)
C (6)	11 (2)	14 (2)	11 (2)	-2 (1)	-1 (1)	-1 (1)
C (7)	15 (2)	15 (2)	9 (1)	3 (1)	-1 (1)	1 (1)
C (8)	11 (2)	16 (2)	13 (2)	-4 (1)	0 (1)	-3 (1)
C (9)	19 (2)	21 (2)	24 (2)	6 (1)	13 (1)	5 (1)
C (10)	20 (2)	24 (2)	21 (2)	9 (1)	7 (1)	3 (1)
C (11)	18 (2)	9 (1)	13 (2)	-3 (1)	3 (1)	-2 (1)
C (12)	15 (2)	16 (2)	9 (2)	-2 (1)	2 (1)	2 (1)
C (13)	31 (4)	33 (4)	25 (4)	2 (3)	-4 (3)	-2 (3)
C (14)	128 (11)	67 (7)	17 (5)	11 (4)	0 (6)	-58 (7)
C (15)	82 (13)	33 (7)	114 (16)	-6 (8)	-14 (11)	10 (9)
C (16)	43 (8)	79 (10)	46 (7)	-4 (6)	-8 (6)	14 (7)
C (17)	56 (6)	48 (6)	46 (6)	-8 (4)	13 (5)	-11 (5)
O (1)	16 (1)	21 (1)	15 (1)	4 (1)	3 (1)	5 (1)
O (2)	22 (1)	21 (1)	10 (1)	0 (1)	6 (1)	2 (1)
O (3)	18 (1)	14 (1)	15 (1)	-2 (1)	4 (1)	0 (1)
O (4)	12 (1)	17 (1)	26 (1)	-1 (1)	8 (1)	3 (1)
O (5)	40 (30)	32 (2)	60 (30)	1 (6)	10 (20)	-3 (6)
N (1)	16 (1)	16 (1)	12 (1)	1 (1)	3 (1)	2 (1)
N (2)	16 (1)	17 (1)	13 (1)	3 (1)	4 (1)	3 (1)
N (3)	69 (8)	29 (3)	36 (4)	5 (4)	-6 (7)	-2 (3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct4.

	x	y	z	U(eq)
H(1)	573	558	1816	21
H(2)	893	-389	3086	22
H(4)	2837	-2385	2390	19
H(7)	3263	-3038	1259	16
H(9)	4327	-1072	-363	24
H(10)	3289	525	-380	25
H(13)	-474	3232	3296	38
H(14A)	-150	5192	1390	88
H(14B)	373	3873	1636	88
H(15A)	-1136	5213	3082	98
H(15B)	-1112	5980	2265	98
H(16A)	1416	5362	1726	88
H(16B)	1352	5125	2649	88
H(16C)	902	6371	2172	88
H(17A)	-552	7128	3508	75
H(17B)	71	7133	2869	75
H(17C)	279	6186	3636	75

