

Table 1. Crystal data and structure refinement for structure5.

Identification code	structure5
Empirical formula	C12 H10 Mn N2 O6
Formula weight	333.16
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 11.9505(9) Å $\alpha = 90^\circ$. b = 14.5679(11) Å $\beta = 127.791(1)^\circ$. c = 9.2494(7) Å $\gamma = 90^\circ$.
Volume	1272.51(17) Å ³
Z	4
Calculated density	1.739 Mg/m ³
Absorption coefficient	1.068 mm ⁻¹
F(000)	676
Crystal size	0.38 x 0.09 x 0.08 mm ³
Theta range for data collection	2.57 to 28.29°.
Limiting indices	-15<=h<=15, -19<=k<=19, -11<=l<=12
Reflections collected	6153
Independent reflections	1500 [R(int) = 0.0259]
Completeness to theta = 28.29°	94.6%
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.855
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1500 / 0 / 105
Goodness-of-fit on F ²	1.219
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.0954
R indices (all data)	R1 = 0.0415, wR2 = 0.0966
Largest diff. peak and hole	0.497 and -0.244 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct5. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Mn(1)	0	348(1)	2500	11(1)
N(1)	1061(2)	1617(1)	2322(3)	14(1)
C(1)	651(2)	2423(1)	2568(3)	13(1)
C(2)	1406(2)	3226(1)	2957(3)	14(1)
C(3)	2566(2)	3225(2)	2952(3)	14(1)
C(4)	2945(2)	2408(2)	2584(3)	18(1)
C(5)	2191(2)	1616(2)	2324(3)	18(1)
C(6)	3334(2)	4116(1)	3305(3)	14(1)
O(1)	3643(2)	4298(1)	2256(2)	19(1)
O(2)	3544(2)	4625(1)	4541(2)	17(1)
O(3)	626(5)	4862(3)	-448(6)	36(1)
O(3')	637(5)	4453(5)	-1067(7)	54(2)

Table 3. Bond lengths [Å] and angles [°] for struct5.

Mn(1)-O(1)#1	2.1383(15)
Mn(1)-O(1)#2	2.1383(15)
Mn(1)-O(2)#3	2.1643(16)
Mn(1)-O(2)#4	2.1643(16)
Mn(1)-N(1)#5	2.3038(18)
Mn(1)-N(1)	2.3038(18)
N(1)-C(1)	1.344(3)
N(1)-C(5)	1.349(3)
C(1)-C(2)	1.384(3)
C(1)-C(1)#5	1.482(4)
C(2)-C(3)	1.388(3)
C(3)-C(4)	1.387(3)
C(3)-C(6)	1.506(3)
C(4)-C(5)	1.391(3)
C(6)-O(2)	1.253(3)
C(6)-O(1)	1.259(3)
O(1)-Mn(1)#6	2.1383(15)
O(2)-Mn(1)#3	2.1643(16)
O(3)-O(3')	0.832(6)
O(1)#1-Mn(1)-O(1)#2	88.69(9)
O(1)#1-Mn(1)-O(2)#3	96.69(6)
O(1)#2-Mn(1)-O(2)#3	84.80(6)
O(1)#1-Mn(1)-O(2)#4	84.80(6)
O(1)#2-Mn(1)-O(2)#4	96.69(6)
O(2)#3-Mn(1)-O(2)#4	177.92(8)
O(1)#1-Mn(1)-N(1)#5	99.57(6)
O(1)#2-Mn(1)-N(1)#5	168.93(7)
O(2)#3-Mn(1)-N(1)#5	86.91(6)
O(2)#4-Mn(1)-N(1)#5	91.42(6)
O(1)#1-Mn(1)-N(1)	168.93(6)
O(1)#2-Mn(1)-N(1)	99.57(6)
O(2)#3-Mn(1)-N(1)	91.42(6)
O(2)#4-Mn(1)-N(1)	86.91(6)
N(1)#5-Mn(1)-N(1)	73.28(9)

C(1)-N(1)-C(5)	117.94(18)
C(1)-N(1)-Mn(1)	114.52(13)
C(5)-N(1)-Mn(1)	126.41(15)
N(1)-C(1)-C(2)	122.36(18)
N(1)-C(1)-C(1)#5	117.27(12)
C(2)-C(1)-C(1)#5	120.37(12)
C(1)-C(2)-C(3)	119.40(19)
C(4)-C(3)-C(2)	118.6(2)
C(4)-C(3)-C(6)	122.98(19)
C(2)-C(3)-C(6)	118.38(19)
C(3)-C(4)-C(5)	118.62(19)
N(1)-C(5)-C(4)	122.8(2)
O(2)-C(6)-O(1)	126.04(19)
O(2)-C(6)-C(3)	117.56(19)
O(1)-C(6)-C(3)	116.30(19)
C(6)-O(1)-Mn(1)#6	129.13(14)
C(6)-O(2)-Mn(1)#3	136.13(14)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct5.

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)	13 (1)	7 (1)	17 (1)	0	11 (1)	0
N (1)	15 (1)	11 (1)	20 (1)	0 (1)	12 (1)	-1 (1)
C (1)	14 (1)	12 (1)	14 (1)	1 (1)	9 (1)	1 (1)
C (2)	15 (1)	10 (1)	19 (1)	0 (1)	11 (1)	0 (1)
C (3)	15 (1)	13 (1)	15 (1)	1 (1)	9 (1)	-2 (1)
C (4)	19 (1)	14 (1)	28 (1)	-3 (1)	18 (1)	-1 (1)
C (5)	20 (1)	13 (1)	29 (1)	-3 (1)	19 (1)	0 (1)
C (6)	11 (1)	11 (1)	17 (1)	3 (1)	7 (1)	1 (1)
O (1)	23 (1)	17 (1)	23 (1)	-2 (1)	17 (1)	-6 (1)
O (2)	18 (1)	12 (1)	19 (1)	-1 (1)	10 (1)	-1 (1)
O (3)	32 (2)	42 (3)	25 (2)	5 (2)	13 (2)	3 (2)
O (3')	31 (2)	94 (5)	29 (3)	6 (3)	14 (2)	-3 (3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct5.

	x	y	z	U(eq)
H(2)	1134	3774	3224	17
H(4)	3703	2391	2511	22
H(5)	2484	1051	2141	22

