

Table 1. Crystal data and structure refinement for struct5a.

Identification code	struct5a
Empirical formula	C12 H6 Mn N2 O4
Formula weight	297.13
Temperature	343(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 12.1736(10) Å α = 90°. b = 14.6323(12) Å β = 131.210(1)°. c = 9.0078(8) Å γ = 90°.
Volume	1207.09(18) Å ³
Z	4
Calculated density	1.635 Mg/m ³
Absorption coefficient	1.104 mm ⁻¹
F(000)	596
Crystal size	0.28 x 0.08 x 0.07 mm ³
Theta range for data collection	2.62 to 24.94°.
Limiting indices	-14 ≤ h ≤ 14, -17 ≤ k ≤ 17, -10 ≤ l ≤ 10
Reflections collected	4647
Independent reflections	1061 [R(int) = 0.0260]
Completeness to theta = 24.94°	99.8%
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.855
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1061 / 0 / 87
Goodness-of-fit on F ²	1.146
Final R indices [I > 2σ(I)]	R1 = 0.0381, wR2 = 0.0852
R indices (all data)	R1 = 0.0438, wR2 = 0.0876
Largest diff. peak and hole	0.545 and -0.231 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct5a. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Mn(1)	0	321(1)	2500	22(1)
N(1)	982(2)	1632(2)	2232(3)	24(1)
C(1)	606(3)	2441(2)	2495(4)	22(1)
C(2)	1333(3)	3242(2)	2782(4)	25(1)
C(3)	2411(3)	3236(2)	2667(4)	24(1)
C(4)	2730(3)	2416(2)	2263(5)	32(1)
C(5)	2024(3)	1634(2)	2103(5)	32(1)
C(6)	3236(3)	4109(2)	3069(4)	26(1)
O(1)	3628(2)	4242(1)	2117(3)	40(1)
O(2)	3439(2)	4634(1)	4328(3)	30(1)

Table 3. Bond lengths [Å] and angles [°] for struct5a.

Mn(1)-O(2)#1	2.1505(19)
Mn(1)-O(2)#2	2.1505(19)
Mn(1)-O(1)#3	2.155(2)
Mn(1)-O(1)#4	2.155(2)
Mn(1)-N(1)	2.355(2)
Mn(1)-N(1)#5	2.355(2)
N(1)-C(1)	1.346(3)
N(1)-C(5)	1.348(3)
C(1)-C(2)	1.386(4)
C(1)-C(1)#5	1.482(5)
C(2)-C(3)	1.383(4)
C(3)-C(4)	1.382(4)
C(3)-C(6)	1.514(4)
C(4)-C(5)	1.380(4)
C(6)-O(1)	1.241(3)
C(6)-O(2)	1.253(3)
O(1)-Mn(1)#6	2.155(2)
O(2)-Mn(1)#1	2.1505(19)
O(2)#1-Mn(1)-O(2)#2	176.53(10)
O(2)#1-Mn(1)-O(1)#3	98.52(8)
O(2)#2-Mn(1)-O(1)#3	84.05(8)
O(2)#1-Mn(1)-O(1)#4	84.05(8)
O(2)#2-Mn(1)-O(1)#4	98.52(8)
O(1)#3-Mn(1)-O(1)#4	85.77(12)
O(2)#1-Mn(1)-N(1)	92.73(8)
O(2)#2-Mn(1)-N(1)	84.44(8)
O(1)#3-Mn(1)-N(1)	166.57(9)
O(1)#4-Mn(1)-N(1)	102.76(8)
O(2)#1-Mn(1)-N(1)#5	84.44(8)
O(2)#2-Mn(1)-N(1)#5	92.73(8)
O(1)#3-Mn(1)-N(1)#5	102.76(8)
O(1)#4-Mn(1)-N(1)#5	166.57(9)
N(1)-Mn(1)-N(1)#5	70.93(11)
C(1)-N(1)-C(5)	117.4(2)

C(1)-N(1)-Mn(1)	116.42(17)
C(5)-N(1)-Mn(1)	125.52(17)
N(1)-C(1)-C(2)	121.9(2)
N(1)-C(1)-C(1)#5	117.13(15)
C(2)-C(1)-C(1)#5	120.98(16)
C(3)-C(2)-C(1)	120.1(2)
C(4)-C(3)-C(2)	118.0(2)
C(4)-C(3)-C(6)	122.6(2)
C(2)-C(3)-C(6)	119.3(2)
C(5)-C(4)-C(3)	119.0(3)
N(1)-C(5)-C(4)	123.3(3)
O(1)-C(6)-O(2)	126.4(2)
O(1)-C(6)-C(3)	117.6(2)
O(2)-C(6)-C(3)	116.0(2)
C(6)-O(1)-Mn(1)#6	127.93(19)
C(6)-O(2)-Mn(1)#1	134.11(17)

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1/2, -y+1/2, -z+1$ #2 $x-1/2, -y+1/2, z-1/2$
 #3 $x-1/2, y-1/2, z$ #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 struct5a.

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)	26 (1)	15 (1)	36 (1)	0	25 (1)	0
N (1)	27 (1)	18 (1)	36 (1)	-3 (1)	24 (1)	-1 (1)
C (1)	23 (1)	20 (1)	28 (1)	2 (1)	18 (1)	2 (1)
C (2)	27 (1)	17 (1)	37 (2)	-1 (1)	24 (1)	1 (1)
C (3)	26 (1)	23 (1)	28 (2)	0 (1)	20 (1)	-2 (1)
C (4)	38 (2)	27 (2)	51 (2)	-7 (1)	38 (2)	-6 (1)
C (5)	37 (2)	23 (1)	53 (2)	-7 (1)	37 (2)	-3 (1)
C (6)	21 (1)	20 (1)	34 (2)	3 (1)	17 (1)	-1 (1)
O (1)	54 (1)	35 (1)	56 (1)	-9 (1)	47 (1)	-18 (1)
O (2)	33 (1)	21 (1)	36 (1)	-3 (1)	22 (1)	-1 (1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct5a.

	x	y	z	U(eq)
H(2)	1095	3784	3051	30
H(4)	3409	2391	2102	39
H(5)	2280	1081	1895	39

