

Table 1. Crystal data and structure refinement for structure16.

Identification code	structure16	
Empirical formula	C12 H8 N2 O4	
Formula weight	244.20	
Temperature	173 (2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	$a = 3.6250(10)$ Å $b = 14.644(5)$ Å $c = 18.649(7)$ Å	$\alpha = 90^\circ$. $\beta = 91.199(5)^\circ$. $\gamma = 90^\circ$.
Volume	989.8 (6) Å ³	
Z	4	
Calculated density	1.639 Mg/m ³	
Absorption coefficient	0.126 mm ⁻¹	
F(000)	504	
Crystal size	0.4 x 0.15 x 0.1 mm ³	
Theta range for data collection	2.18 to 23.29°.	
Limiting indices	-4 ≤ h ≤ 4, -16 ≤ k ≤ 16, -20 ≤ l ≤ 20	
Reflections collected	4020	
Independent reflections	1396 [R(int) = 0.0380]	
Completeness to theta = 23.29°	99.9%	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.833	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	1396 / 4 / 169	
Goodness-of-fit on F ²	1.025	
Final R indices [I > 2σ(I)]	R1 = 0.0329, wR2 = 0.0718	
R indices (all data)	R1 = 0.0370, wR2 = 0.0745	
Absolute structure parameter	0.7(14)	
Largest diff. peak and hole	0.167 and -0.152 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct16. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	493(8)	3796(2)	-2229(2)	22(1)
C(2)	1500(8)	4682(2)	-2385(2)	23(1)
C(3)	1990(8)	5293(2)	-1826(2)	18(1)
C(4)	1482(8)	4992(2)	-1130(1)	19(1)
C(5)	534(7)	4088(2)	-1015(1)	18(1)
C(6)	118(7)	3696(2)	-279(1)	18(1)
C(7)	985(7)	2788(2)	-146(1)	18(1)
C(8)	425(8)	2426(2)	529(2)	18(1)
C(9)	-904(8)	2994(2)	1060(1)	20(1)
C(10)	-1580(8)	3896(2)	896(2)	22(1)
C(11)	1153(8)	1436(2)	679(2)	20(1)
C(12)	3050(9)	6259(2)	-1985(2)	23(1)
N(1)	0(6)	3497(2)	-1565(1)	20(1)
N(2)	-1100(6)	4246(2)	239(1)	20(1)
O(1)	530(6)	1085(1)	1249(1)	35(1)
O(2)	2488(6)	1013(1)	123(1)	30(1)
O(3)	4510(6)	6485(1)	-2528(1)	32(1)
O(4)	2241(6)	6814(1)	-1450(1)	27(1)

Table 3. Bond lengths [Å] and angles [°] for struct16.

C(1)-N(1)	1.329(3)
C(1)-C(2)	1.380(4)
C(2)-C(3)	1.382(4)
C(3)-C(4)	1.386(4)
C(3)-C(12)	1.498(4)
C(4)-C(5)	1.385(4)
C(5)-N(1)	1.353(3)
C(5)-C(6)	1.500(3)
C(6)-N(2)	1.339(3)
C(6)-C(7)	1.387(4)
C(7)-C(8)	1.384(3)
C(8)-C(9)	1.387(4)
C(8)-C(11)	1.499(4)
C(9)-C(10)	1.377(4)
C(10)-N(2)	1.344(4)
C(11)-O(1)	1.205(3)
C(11)-O(2)	1.309(3)
C(12)-O(3)	1.198(3)
C(12)-O(4)	1.326(4)
N(1)-C(1)-C(2)	123.2(3)
C(1)-C(2)-C(3)	118.7(3)
C(2)-C(3)-C(4)	118.8(3)
C(2)-C(3)-C(12)	119.5(2)
C(4)-C(3)-C(12)	121.7(3)
C(5)-C(4)-C(3)	119.2(3)
N(1)-C(5)-C(4)	121.8(2)
N(1)-C(5)-C(6)	115.7(2)
C(4)-C(5)-C(6)	122.6(2)
N(2)-C(6)-C(7)	121.7(2)
N(2)-C(6)-C(5)	118.0(2)
C(7)-C(6)-C(5)	120.3(2)
C(8)-C(7)-C(6)	119.5(2)
C(7)-C(8)-C(9)	118.6(2)
C(7)-C(8)-C(11)	120.8(2)
C(9)-C(8)-C(11)	120.5(3)
C(10)-C(9)-C(8)	118.7(3)
N(2)-C(10)-C(9)	122.8(3)
O(1)-C(11)-O(2)	125.1(3)
O(1)-C(11)-C(8)	122.8(3)
O(2)-C(11)-C(8)	112.1(2)
O(3)-C(12)-O(4)	125.2(3)
O(3)-C(12)-C(3)	123.2(3)
O(4)-C(12)-C(3)	111.6(3)
C(1)-N(1)-C(5)	118.4(2)
C(6)-N(2)-C(10)	118.6(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct16.
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}
C (1)	30 (2)	19 (2)	16 (2)	-2 (1)	1 (1)	-2 (1)
C (2)	28 (2)	23 (2)	18 (2)	1 (1)	2 (1)	-1 (1)
C (3)	19 (2)	15 (2)	22 (2)	2 (1)	3 (1)	1 (1)
C (4)	19 (2)	19 (2)	20 (2)	-4 (1)	2 (1)	4 (1)
C (5)	17 (2)	15 (2)	21 (2)	2 (1)	2 (1)	-1 (1)
C (6)	18 (2)	14 (2)	23 (2)	0 (1)	1 (1)	-2 (1)
C (7)	17 (2)	19 (2)	19 (2)	-4 (1)	-1 (1)	-1 (1)
C (8)	18 (2)	15 (2)	21 (2)	-1 (1)	1 (1)	0 (1)
C (9)	22 (2)	20 (2)	18 (2)	3 (1)	-3 (1)	1 (1)
C (10)	22 (2)	20 (2)	24 (2)	-4 (1)	1 (1)	0 (1)
C (11)	24 (2)	19 (2)	17 (2)	1 (2)	0 (1)	0 (2)
C (12)	25 (2)	20 (2)	25 (2)	-2 (2)	-3 (1)	2 (1)
N (1)	23 (1)	16 (1)	20 (1)	-3 (1)	-4 (1)	-2 (1)
N (2)	25 (1)	17 (1)	19 (1)	0 (1)	2 (1)	2 (1)
O (1)	62 (2)	20 (1)	24 (1)	6 (1)	11 (1)	8 (1)
O (2)	51 (2)	13 (1)	27 (1)	3 (1)	11 (1)	7 (1)
O (3)	47 (2)	26 (1)	22 (1)	4 (1)	13 (1)	-7 (1)
O (4)	42 (1)	13 (1)	27 (1)	-3 (1)	5 (1)	-8 (1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct16.

	x	y	z	U(eq)
H(1)	135	3380	-2615	26
H(2)	1850	4868	-2866	28
H(4)	1781	5400	-738	23
H(7)	1955	2418	-515	22
H(9)	-1339	2764	1527	24
H(10)	-2422	4288	1264	26
H(2A)	2800 (90)	436 (14)	231 (16)	41
H(4A)	3250 (80)	7346 (15)	-1487 (18)	41

