

Table 1. Crystal data and structure refinement for struct20.

Identification code	struct20
Empirical formula	C14 H12 N2 O4
Formula weight	272.26
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	$a = 3.8060(10) \text{ Å}$ $\alpha = 90^\circ$. $b = 5.864(2) \text{ Å}$ $\beta = 93.704(6)^\circ$. $c = 27.625(3) \text{ Å}$ $\gamma = 90^\circ$.
Volume	615.3(3) Å ³
Z	2
Calculated density	1.470 Mg/m ³
Absorption coefficient	0.110 mm ⁻¹
F(000)	284
Crystal size	0.25 x 0.18 x 0.02 mm ³
Theta range for data collection	2.96 to 25.03 °.
Limiting indices	-4<=h<=4, 0<=k<=6, 0<=l<=32
Reflections collected	3156
Independent reflections	1804 [R(int) = 0.0373]
Completeness to theta = 25.03°	99.1 %
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.678
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1804 / 0 / 93
Goodness-of-fit on F ²	1.125
Final R indices [I>2sigma(I)]	R1 = 0.0721, wR2 = 0.1807
R indices (all data)	R1 = 0.0939, wR2 = 0.1873
Largest diff. peak and hole	0.282 and -0.247 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct20. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	-1990 (7)	-2665 (4)	162 (1)	20 (1)
C(5)	-304 (8)	-661 (5)	224 (1)	18 (1)
C(4)	854 (8)	161 (5)	680 (1)	21 (1)
C(3)	325 (8)	-1182 (5)	1083 (1)	20 (1)
C(2)	-1348 (8)	-3272 (5)	1018 (1)	23 (1)
C(1)	-2474 (8)	-3932 (5)	555 (1)	22 (1)
C(6)	1502 (9)	-454 (5)	1588 (1)	23 (1)
C(7)	4158 (9)	2507 (6)	2065 (1)	31 (1)
O(1)	1296 (7)	-1605 (4)	1943 (1)	37 (1)
O(2)	2885 (6)	1655 (4)	1595 (1)	28 (1)

Table 3. Bond lengths [Å] and angles [°] for struct20.

N(1)-C(1)	1.338(4)
N(1)-C(5)	1.345(4)
C(5)-C(4)	1.395(4)
C(5)-C(5)#1	1.489(6)
C(4)-C(3)	1.388(4)
C(3)-C(2)	1.387(4)
C(3)-C(6)	1.499(4)
C(2)-C(1)	1.379(4)
C(6)-O(1)	1.198(4)
C(6)-O(2)	1.344(4)
C(7)-O(2)	1.446(4)
C(1)-N(1)-C(5)	118.2(3)
N(1)-C(5)-C(4)	122.5(3)
N(1)-C(5)-C(5)#1	116.6(3)
C(4)-C(5)-C(5)#1	120.9(3)
C(3)-C(4)-C(5)	118.3(3)
C(2)-C(3)-C(4)	119.1(3)
C(2)-C(3)-C(6)	118.6(3)
C(4)-C(3)-C(6)	122.2(3)
C(1)-C(2)-C(3)	118.7(3)
N(1)-C(1)-C(2)	123.1(3)
O(1)-C(6)-O(2)	123.5(3)
O(1)-C(6)-C(3)	124.8(3)
O(2)-C(6)-C(3)	111.7(3)
C(6)-O(2)-C(7)	116.1(2)

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

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct20.
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}
N(1)	20 (1)	16 (1)	25 (2)	-1 (1)	-1 (1)	0 (1)
C(5)	15 (2)	16 (2)	23 (2)	0 (1)	0 (1)	2 (1)
C(4)	25 (2)	15 (2)	24 (2)	-2 (1)	4 (1)	0 (1)
C(3)	18 (2)	20 (2)	22 (2)	-2 (1)	2 (1)	4 (1)
C(2)	23 (2)	22 (2)	25 (2)	4 (1)	2 (1)	1 (1)
C(1)	26 (2)	16 (2)	25 (2)	-1 (1)	5 (1)	0 (1)
C(6)	21 (2)	24 (2)	23 (2)	0 (1)	3 (1)	4 (1)
C(7)	41 (2)	31 (2)	21 (2)	-7 (1)	0 (2)	-5 (2)
O(1)	58 (2)	31 (1)	21 (1)	5 (1)	-1 (1)	-10 (1)
O(2)	40 (1)	23 (1)	21 (1)	-2 (1)	-3 (1)	-5 (1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct20.

	x	y	z	U(eq)
H(4)	1976	1604	715	26
H(2)	-1711	-4229	1288	28
H(1)	-3649	-5355	512	27
H(7A)	5032	4068	2032	47
H(7B)	6073	1530	2199	47
H(7C)	2233	2502	2284	47

