

Table 1. Crystal data and structure refinement for struct22.

Identification code	struct22
Empirical formula	C18 H20 N2 O4
Formula weight	328.36
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 5.8683(7) Å α = 74.578(2) °. b = 6.8410(8) Å β = 81.482(2) °. c = 10.7485(13) Å γ = 81.131(2) °.
Volume	408.38(8) Å ³
Z	1
Calculated density	1.335 Mg/m ³
Absorption coefficient	0.095 mm ⁻¹
F(000)	174
Crystal size	0.40 x 0.09 x 0.05 mm ³
Theta range for data collection	1.98 to 25.00 °.
Limiting indices	-6 ≤ h ≤ 6, -8 ≤ k ≤ 8, -12 ≤ l ≤ 12
Reflections collected	3620
Independent reflections	1430 [R(int) = 0.0200]
Completeness to theta = 25.00°	99.8 %
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.900
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1430 / 0 / 111
Goodness-of-fit on F ²	1.046
Final R indices [I > 2sigma(I)]	R1 = 0.0382, wR2 = 0.0956
R indices (all data)	R1 = 0.0448, wR2 = 0.0997
Largest diff. peak and hole	0.198 and -0.176 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct22. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(2)	1135(2)	8793(1)	7026(1)	26(1)
O(1)	3061(2)	11463(2)	6897(1)	33(1)
N(1)	-4043(2)	12359(2)	10031(1)	27(1)
C(3)	-484(2)	11096(2)	8291(1)	23(1)
C(5)	-4027(2)	10609(2)	9693(1)	22(1)
C(4)	-2289(2)	9934(2)	8814(1)	23(1)
C(6)	1449(2)	10488(2)	7341(1)	25(1)
C(2)	-478(2)	12895(2)	8651(1)	26(1)
C(1)	-2291(3)	13463(2)	9508(1)	28(1)
C(7)	2856(2)	8143(2)	6028(1)	27(1)
C(8)	1631(3)	6983(2)	5377(2)	33(1)
C(9)	4921(3)	6906(3)	6648(2)	41(1)

Table 3. Bond lengths [Å] and angles [°] for struct22.

O(2)-C(6)	1.3369(17)
O(2)-C(7)	1.4700(16)
O(1)-C(6)	1.2080(17)
N(1)-C(1)	1.3362(19)
N(1)-C(5)	1.3384(18)
C(3)-C(4)	1.384(2)
C(3)-C(2)	1.385(2)
C(3)-C(6)	1.4964(19)
C(5)-C(4)	1.3953(19)
C(5)-C(5)#1	1.487(3)
C(2)-C(1)	1.380(2)
C(7)-C(9)	1.501(2)
C(7)-C(8)	1.502(2)
C(6)-O(2)-C(7)	116.42(11)
C(1)-N(1)-C(5)	117.63(12)
C(4)-C(3)-C(2)	118.80(13)
C(4)-C(3)-C(6)	122.35(13)
C(2)-C(3)-C(6)	118.85(13)
N(1)-C(5)-C(4)	122.57(13)
N(1)-C(5)-C(5)#1	116.55(15)
C(4)-C(5)-C(5)#1	120.88(15)
C(3)-C(4)-C(5)	118.80(13)
O(1)-C(6)-O(2)	124.77(13)
O(1)-C(6)-C(3)	123.14(13)
O(2)-C(6)-C(3)	112.07(12)
C(1)-C(2)-C(3)	118.44(13)
N(1)-C(1)-C(2)	123.75(13)
O(2)-C(7)-C(9)	109.61(12)
O(2)-C(7)-C(8)	106.34(11)
C(9)-C(7)-C(8)	113.55(13)

Symmetry transformations used to generate equivalent atoms:

#1 -x-1, -y+2, -z+2

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct22.
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}
O(2)	25(1)	29(1)	27(1)	-13(1)	6(1)	-5(1)
O(1)	28(1)	36(1)	37(1)	-14(1)	8(1)	-10(1)
N(1)	27(1)	24(1)	28(1)	-9(1)	1(1)	0(1)
C(3)	23(1)	25(1)	20(1)	-6(1)	-2(1)	1(1)
C(5)	21(1)	24(1)	21(1)	-7(1)	-3(1)	4(1)
C(4)	23(1)	24(1)	22(1)	-9(1)	-3(1)	0(1)
C(6)	23(1)	27(1)	23(1)	-7(1)	-1(1)	-2(1)
C(2)	25(1)	26(1)	27(1)	-6(1)	0(1)	-3(1)
C(1)	31(1)	23(1)	33(1)	-10(1)	-1(1)	-2(1)
C(7)	25(1)	32(1)	25(1)	-13(1)	9(1)	-4(1)
C(8)	36(1)	35(1)	27(1)	-12(1)	1(1)	-3(1)
C(9)	28(1)	53(1)	48(1)	-27(1)	-2(1)	4(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct22.

	x	y	z	U(eq)
H(4)	-2343	8698	8580	27
H(2)	746	13717	8316	32
H(1)	-2294	14710	9739	34
H(7)	3367	9380	5374	33
H(8A)	187	7804	5101	49
H(8B)	1274	5695	5988	49
H(8C)	2634	6694	4617	49
H(9A)	5592	7725	7091	62
H(9B)	6085	6508	5978	62
H(9C)	4436	5679	7280	62

