

Table 1. Crystal data and structure refinement for **18g**.

Identification code	18g
Empirical formula	C ₁₆ H ₂₃ N O ₂
Formula weight	261.35
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 10.2983(8) Å α = 90°. b = 10.9460(9) Å β = 90°. c = 13.7850(12) Å γ = 90°.
Volume	1553.9(2) Å ³
Z	4
Density (calculated)	1.117 Mg/m ³
Absorption coefficient	0.073 mm ⁻¹
F(000)	568
Crystal size	0.39 x 0.59 x 0.70 mm ³
Theta range for data collection	2.38 to 26.02°.
Index ranges	-11 ≤ h ≤ 12, -13 ≤ k ≤ 9, -17 ≤ l ≤ 16
Reflections collected	8782
Independent reflections	3068 [R(int) = 0.0249]
Completeness to theta = 26.02°_100.0 %	
Absorption correction	SADABS
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3068 / 0 / 173
Goodness-of-fit on F ²	1.450
Final R indices [I > 2σ(I)]	R1 = 0.0645, wR2 = 0.1901
R indices (all data)	R1 = 0.0778, wR2 = 0.2024
Absolute structure parameter	0(2)
Extinction coefficient	0.046(8)
Largest diff. peak and hole	0.634 and -0.261 e.Å ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for **18g**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	10840(3)	-17929(2)	-12980(2)	108(1)
O(2)	9138(2)	-19094(2)	-13158(1)	69(1)
N	10639(2)	-20626(2)	-14357(2)	67(1)
C(1)	7276(3)	-20336(3)	-13801(2)	66(1)
C(2)	8677(2)	-20296(3)	-13406(2)	56(1)
C(3)	10438(3)	-18906(3)	-13215(2)	70(1)
C(4)	11289(3)	-19936(3)	-13589(2)	67(1)
C(5)	9443(2)	-20796(2)	-14235(2)	55(1)
C(6)	8470(3)	-21320(3)	-14930(2)	75(1)
C(7)	7764(4)	-22359(3)	-14390(3)	94(1)
C(8)	6890(3)	-21668(3)	-13661(2)	82(1)
C(9)	7466(3)	-20276(3)	-14918(2)	74(1)
C(10)	8005(4)	-19076(4)	-15297(3)	98(1)
C(11)	6243(5)	-20589(5)	-15506(3)	116(2)
C(12)	6367(3)	-19426(4)	-13332(3)	104(1)
C(13)	12511(3)	-19367(4)	-14021(3)	89(1)
C(14)	11648(4)	-20888(4)	-12791(3)	101(1)
C(15)	12378(5)	-20432(4)	-11971(4)	117(2)

C(16)	13572(5)	-20772(6)	-11777(4)	149(2)
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Table 3. Bond lengths [Å] and angles [°] for **18g**.

O(1)-C(3)	1.192(4)
O(2)-C(3)	1.357(3)
O(2)-C(2)	1.440(3)
N-C(5)	1.257(3)
N-C(4)	1.462(4)
C(1)-C(12)	1.512(5)
C(1)-C(8)	1.523(4)
C(1)-C(2)	1.543(4)
C(1)-C(9)	1.554(4)
C(2)-C(5)	1.493(4)
C(3)-C(4)	1.519(4)
C(4)-C(13)	1.524(4)
C(4)-C(14)	1.559(5)
C(5)-C(6)	1.500(4)
C(6)-C(7)	1.541(5)
C(6)-C(9)	1.541(5)
C(7)-C(8)	1.546(6)
C(9)-C(10)	1.519(5)
C(9)-C(11)	1.536(5)
C(14)-C(15)	1.446(6)
C(15)-C(16)	1.312(7)
C(3)-O(2)-C(2)	116.7(2)
C(5)-N-C(4)	115.3(2)
C(12)-C(1)-C(8)	114.5(3)
C(12)-C(1)-C(2)	114.1(3)
C(8)-C(1)-C(2)	103.1(2)
C(12)-C(1)-C(9)	118.3(3)
C(8)-C(1)-C(9)	101.4(3)
C(2)-C(1)-C(9)	103.4(2)
O(2)-C(2)-C(5)	110.0(2)
O(2)-C(2)-C(1)	114.7(2)
C(5)-C(2)-C(1)	102.3(2)
O(1)-C(3)-O(2)	117.6(3)
O(1)-C(3)-C(4)	123.9(3)
O(2)-C(3)-C(4)	118.5(2)
N-C(4)-C(3)	111.4(2)
N-C(4)-C(13)	107.8(3)
C(3)-C(4)-C(13)	107.8(3)
N-C(4)-C(14)	105.9(2)
C(3)-C(4)-C(14)	113.2(3)
C(13)-C(4)-C(14)	110.7(3)
N-C(5)-C(2)	124.5(2)
N-C(5)-C(6)	128.7(3)
C(2)-C(5)-C(6)	106.0(2)
C(5)-C(6)-C(7)	106.7(2)
C(5)-C(6)-C(9)	99.1(2)
C(7)-C(6)-C(9)	103.1(3)
C(6)-C(7)-C(8)	103.1(3)
C(1)-C(8)-C(7)	103.6(3)
C(10)-C(9)-C(11)	108.1(3)

C(10)-C(9)-C(6)	113.1(3)
C(11)-C(9)-C(6)	112.3(3)
C(10)-C(9)-C(1)	115.0(3)
C(11)-C(9)-C(1)	114.2(3)
C(6)-C(9)-C(1)	93.7(2)
C(15)-C(14)-C(4)	116.3(4)
C(16)-C(15)-C(14)	123.3(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **18g**. 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(1)	89(2)	82(2)	152(2)	-51(2)	-7(2)	-21(1)
O(2)	58(1)	69(1)	79(1)	-23(1)	3(1)	-2(1)
N	57(1)	48(1)	95(2)	-8(1)	9(1)	3(1)
C(1)	51(1)	77(2)	70(2)	5(1)	-7(1)	-1(1)
C(2)	50(1)	63(2)	56(1)	2(1)	-5(1)	-4(1)
C(3)	59(2)	67(2)	84(2)	-17(2)	-13(1)	-6(1)
C(4)	46(1)	67(2)	89(2)	1(2)	-3(1)	-3(1)
C(5)	57(1)	39(1)	69(1)	-5(1)	1(1)	0(1)
C(6)	86(2)	70(2)	68(2)	-12(1)	-4(2)	-15(2)
C(7)	103(3)	66(2)	113(2)	0(2)	-29(2)	-34(2)
C(8)	68(2)	93(2)	85(2)	13(2)	-8(2)	-26(2)
C(9)	69(2)	86(2)	68(2)	15(2)	-17(1)	-10(2)
C(10)	102(3)	91(2)	100(2)	41(2)	-12(2)	-4(2)
C(11)	99(3)	163(4)	85(2)	24(3)	-42(2)	-26(3)
C(12)	54(2)	135(4)	124(3)	-8(3)	9(2)	13(2)
C(13)	60(2)	93(2)	114(2)	5(2)	6(2)	-16(2)
C(14)	65(2)	105(3)	132(3)	30(3)	-28(2)	-8(2)
C(15)	115(4)	108(3)	130(3)	-26(3)	-12(3)	-4(3)
C(16)	98(3)	209(6)	139(4)	66(4)	-60(3)	-40(4)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **18g**.

	x	y	z	U(eq)
H(2A)	8755	-20839	-12843	68
H(6A)	8811	-21535	-15571	89
H(7A)	8377	-22885	-14056	113
H(7B)	7249	-22848	-14833	113
H(8A)	5979	-21791	-13809	98
H(8B)	7057	-21933	-13002	98
H(10A)	8104	-19123	-15989	146
H(10B)	8834	-18920	-15004	146
H(10C)	7418	-18425	-15138	146
H(11A)	6434	-20536	-16186	173
H(11B)	5564	-20022	-15347	173
H(11C)	5966	-21403	-15351	173
H(12A)	6333	-19575	-12646	157
H(12B)	5514	-19514	-13603	157
H(12C)	6678	-18612	-13448	157

H(13A)	12271	-18776	-14503	134
H(13B)	13031	-19994	-14314	134
H(13C)	12999	-18973	-13517	134
H(14A)	10850	-21248	-12550	121
H(14B)	12147	-21537	-13093	121
H(15A)	11981	-19870	-11562	141
H(16A)	13990	-21333	-12176	179
H(16B)	14000	-20452	-11240	179
