

Table 1. Crystal data and structure refinement for Structure19.

Identification code	Structure19
Empirical formula	C10 H15 N2 O2
Formula weight	195.24
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)
Unit cell dimensions	a = 8.9038(7) Å $\alpha = 90^\circ$. b = 11.1419(9) Å $\beta = 94.797(2)^\circ$. c = 10.8140(8) Å $\gamma = 90^\circ$.
Volume	1069.05(14) Å ³
Z	4
Calculated density	1.213 Mg/m ³
Absorption coefficient	0.086 mm ⁻¹
F(000)	420
Crystal size	0.28 x 0.25 x 0.13 mm ³
Theta range for data collection	1.89 to 29.97°.
Limiting indices	-10<=h<=12, -15<=k<=15, -15<=l<=8
Reflections collected	8278
Independent reflections	5731 [R(int) = 0.0220]
Completeness to theta = 29.97°	96.6 %
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.325
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5731 / 1 / 253
Goodness-of-fit on F ²	0.992
Final R indices [I>2sigma(I)]	R1 = 0.0649, wR2 = 0.1516
R indices (all data)	R1 = 0.0809, wR2 = 0.1622
Absolute structure parameter	0.3(13)
Largest diff. peak and hole	0.509 and -0.342 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for STRUCT19. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(3)	2997(2)	8989(2)	9166(2)	29(1)
N(1)	301(2)	8114(2)	12885(2)	24(1)
O(4)	2954(2)	10846(2)	8391(2)	31(1)
N(2)	-373(2)	11181(2)	11890(2)	26(1)
C(8)	1484(2)	10448(2)	10068(2)	19(1)
C(5)	-246(2)	9234(2)	12888(2)	18(1)
O(1)	-3057(2)	10304(2)	15620(2)	35(1)
C(3)	-1656(2)	8823(2)	14640(2)	20(1)
O(2)	-3366(2)	8381(2)	16126(2)	38(1)
N(4)	4270(2)	6334(2)	2432(2)	21(1)
N(3)	3959(2)	8050(2)	7067(2)	19(1)
C(11)	-2789(3)	9200(2)	15541(2)	24(1)
C(6)	197(2)	10055(2)	11890(2)	18(1)
C(4)	-1199(2)	9629(2)	13764(2)	19(1)
C(7)	1131(2)	9666(2)	11000(2)	17(1)
C(12)	2565(2)	10059(2)	9121(2)	21(1)
C(10)	-39(3)	11913(2)	10976(2)	29(1)
C(9)	885(3)	11600(2)	10047(2)	24(1)
C(1)	-124(3)	7350(2)	13745(2)	27(1)
C(2)	-1114(3)	7661(2)	14621(2)	25(1)
C(17)	3097(3)	6265(2)	1373(2)	27(1)
C(14)	2704(3)	8198(2)	6072(2)	28(1)
C(13)	4165(3)	6783(2)	7488(2)	26(1)
C(18)	4529(3)	7557(2)	2971(2)	30(1)
C(16)	2714(3)	9451(2)	5546(3)	38(1)
C(19)	2944(3)	4987(3)	899(3)	36(1)
C(15)	5498(3)	6694(2)	8440(2)	33(1)
C(20)	5306(3)	8380(3)	2111(3)	40(1)

Table 3. Bond lengths [Å] and angles [°] for STRUCT19.

O(3)-C(12)	1.252 (3)
N(1)-C(1)	1.338 (3)
N(1)-C(5)	1.339 (3)
O(4)-C(12)	1.248 (3)
N(2)-C(10)	1.334 (3)
N(2)-C(6)	1.354 (3)
C(8)-C(7)	1.388 (3)
C(8)-C(9)	1.389 (3)
C(8)-C(12)	1.525 (3)
C(5)-C(4)	1.395 (3)
C(5)-C(6)	1.492 (3)
O(1)-C(11)	1.257 (3)
C(3)-C(2)	1.383 (3)
C(3)-C(4)	1.390 (3)
C(3)-C(11)	1.519 (3)
O(2)-C(11)	1.246 (3)
N(4)-C(17)	1.485 (3)
N(4)-C(18)	1.493 (3)
N(3)-C(13)	1.490 (3)
N(3)-C(14)	1.494 (3)
C(6)-C(7)	1.393 (3)
C(10)-C(9)	1.395 (3)
C(1)-C(2)	1.391 (3)
C(17)-C(19)	1.516 (4)
C(14)-C(16)	1.507 (4)
C(13)-C(15)	1.508 (3)
C(18)-C(20)	1.515 (4)
C(1)-N(1)-C(5)	117.85 (19)
C(10)-N(2)-C(6)	117.39 (19)
C(7)-C(8)-C(9)	118.83 (19)
C(7)-C(8)-C(12)	120.2 (2)
C(9)-C(8)-C(12)	120.9 (2)
N(1)-C(5)-C(4)	122.5 (2)
N(1)-C(5)-C(6)	116.82 (17)
C(4)-C(5)-C(6)	120.69 (19)
C(2)-C(3)-C(4)	118.2 (2)
C(2)-C(3)-C(11)	121.3 (2)
C(4)-C(3)-C(11)	120.4 (2)
C(17)-N(4)-C(18)	115.07 (19)
C(13)-N(3)-C(14)	112.99 (18)
O(2)-C(11)-O(1)	126.4 (2)
O(2)-C(11)-C(3)	116.6 (2)
O(1)-C(11)-C(3)	117.0 (2)
N(2)-C(6)-C(7)	122.2 (2)
N(2)-C(6)-C(5)	116.53 (17)
C(7)-C(6)-C(5)	121.22 (19)
C(3)-C(4)-C(5)	119.2 (2)
C(8)-C(7)-C(6)	119.4 (2)
O(4)-C(12)-O(3)	126.3 (2)
O(4)-C(12)-C(8)	116.7 (2)
O(3)-C(12)-C(8)	117.0 (2)
N(2)-C(10)-C(9)	124.2 (2)
C(8)-C(9)-C(10)	117.9 (2)
N(1)-C(1)-C(2)	123.2 (2)
C(3)-C(2)-C(1)	119.0 (2)
N(4)-C(17)-C(19)	110.3 (2)

N(3)-C(14)-C(16)	110.3(2)
N(3)-C(13)-C(15)	109.92(19)
N(4)-C(18)-C(20)	112.1(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for STRUCT19.
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(3)	35(1)	29(1)	25(1)	-3(1)	17(1)	3(1)
N(1)	25(1)	25(1)	23(1)	0(1)	11(1)	3(1)
O(4)	30(1)	35(1)	29(1)	3(1)	17(1)	1(1)
N(2)	30(1)	24(1)	25(1)	3(1)	12(1)	8(1)
C(8)	17(1)	24(1)	17(1)	-1(1)	5(1)	-2(1)
C(5)	17(1)	23(1)	15(1)	-2(1)	4(1)	1(1)
O(1)	43(1)	30(1)	35(1)	-1(1)	25(1)	5(1)
C(3)	19(1)	24(1)	18(1)	-1(1)	5(1)	-1(1)
O(2)	37(1)	36(1)	45(1)	8(1)	28(1)	2(1)
N(4)	23(1)	19(1)	24(1)	1(1)	11(1)	-1(1)
N(3)	20(1)	20(1)	18(1)	-3(1)	3(1)	-2(1)
C(11)	23(1)	30(1)	20(1)	-1(1)	10(1)	3(1)
C(6)	17(1)	22(1)	16(1)	1(1)	4(1)	0(1)
C(4)	18(1)	22(1)	17(1)	0(1)	5(1)	1(1)
C(7)	18(1)	18(1)	17(1)	-3(1)	5(1)	3(1)
C(12)	19(1)	26(1)	18(1)	-2(1)	6(1)	-1(1)
C(10)	33(1)	23(1)	32(1)	7(1)	13(1)	10(1)
C(9)	27(1)	26(1)	22(1)	8(1)	9(1)	2(1)
C(1)	36(1)	19(1)	30(1)	2(1)	14(1)	3(1)
C(2)	29(1)	22(1)	25(1)	1(1)	11(1)	-3(1)
C(17)	28(1)	25(1)	27(1)	3(1)	8(1)	5(1)
C(14)	25(1)	34(1)	23(1)	-5(1)	-1(1)	3(1)
C(13)	25(1)	22(1)	30(1)	2(1)	5(1)	-3(1)
C(18)	36(1)	24(1)	32(1)	-4(1)	5(1)	2(1)
C(16)	49(2)	34(2)	28(1)	1(1)	-14(1)	9(1)
C(19)	38(1)	35(2)	35(1)	-6(1)	-3(1)	1(1)
C(15)	34(1)	29(1)	36(1)	10(1)	-1(1)	-1(1)
C(20)	48(2)	22(1)	47(2)	5(1)	-1(1)	-8(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for STRUCT19.

	x	y	z	U(eq)
H(4A)	5164	6055	2172	26
H(4B)	3999	5828	3048	26
H(3A)	4841	8318	6775	23
H(3B)	3767	8520	7735	23
H(4)	-1533	10439	13763	22
H(7)	1524	8872	11030	21
H(10)	-457	12697	10956	34
H(9)	1098	12157	9419	29
H(1)	269	6557	13757	33
H(2)	-1414	7083	15198	30
H(17A)	3376	6799	697	32
H(17B)	2120	6542	1643	32
H(14A)	1728	8045	6419	33
H(14B)	2820	7608	5403	33
H(13A)	4331	6264	6770	31
H(13B)	3245	6503	7854	31
H(18A)	5154	7489	3769	37
H(18B)	3549	7912	3143	37
H(16A)	1887	9536	4894	57
H(16B)	3676	9597	5194	57
H(16C)	2584	10034	6207	57
H(19A)	2172	4955	198	54
H(19B)	2649	4463	1565	54
H(19C)	3911	4717	627	54
H(15A)	5626	5859	8714	50
H(15B)	5326	7203	9154	50
H(15C)	6410	6962	8072	50
H(20A)	5452	9172	2498	59
H(20B)	4682	8461	1324	59
H(20C)	6288	8041	1953	59

