

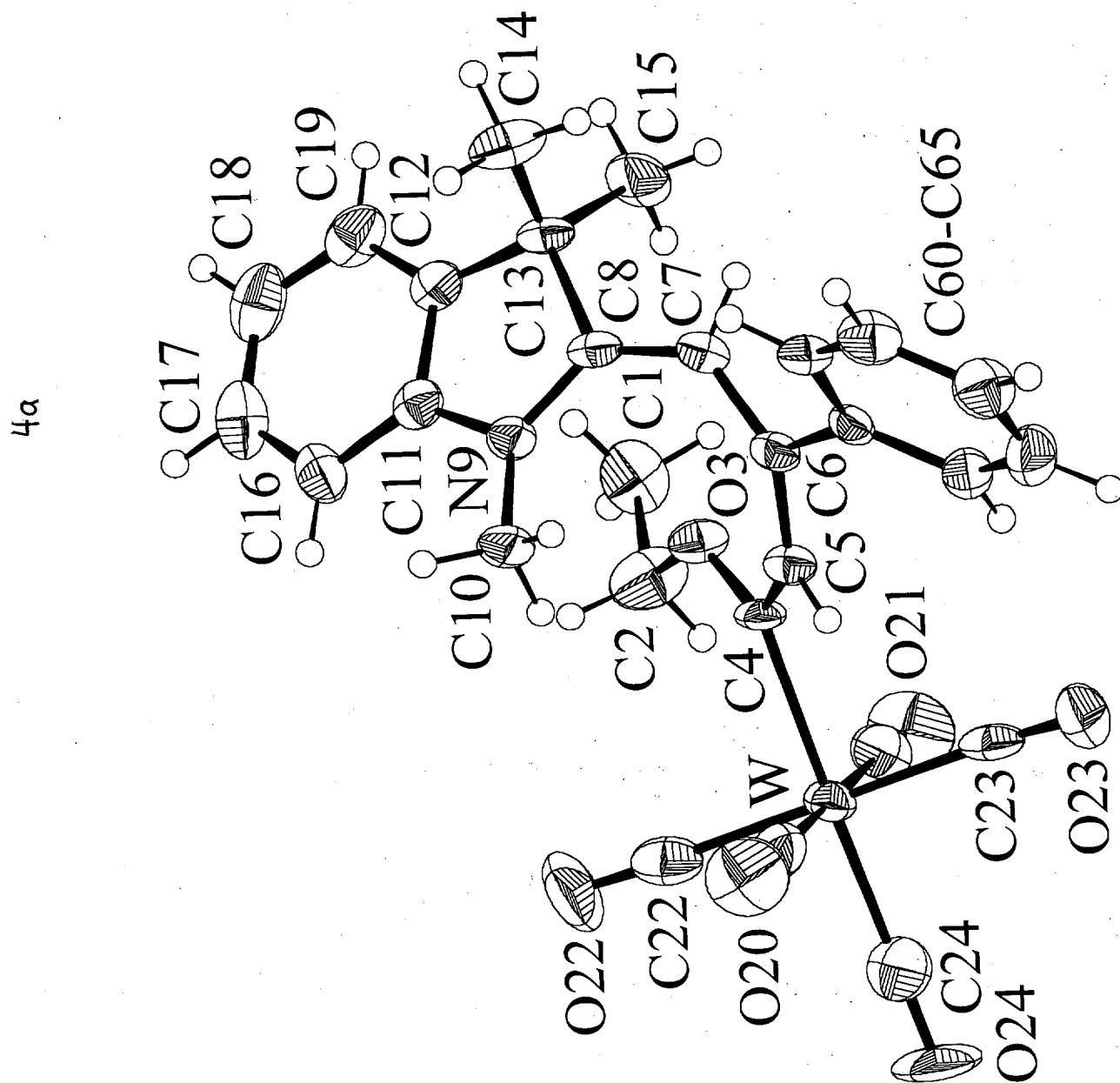


Table 1. Crystal data and structure refinement for **4a**

Identification code	AUM_940
Empirical formula	C ₂₈ H ₂₅ N O ₆ W
Formula weight	655.34
Temperature	223(2) K
Wavelength	0.71073 Å
Crystal system, space group	triclinic, P-1
Unit cell dimensions	a = 10.104(1) Å α = 99.66(1)°. b = 11.408(1) Å β = 93.66(1)°. c = 12.796(1) Å γ = 114.62(1)°.
Volume	1307.0(3) Å ³
Z, Calculated density	2, 1.665 Mg/m ³
Absorption coefficient	4.461 mm ⁻¹
F(000)	644
Crystal size	0.40 x 0.20 x 0.10 mm
Theta range for data collection	2.57 to 26.27°.
Limiting indices	-11<=h<=12, -14<=k<=0, -15<=l<=15
Reflections collected / unique	5550 / 5275 [R(int) = 0.0522]
Completeness to theta = 26.27	99.9 %
Max. and min. transmission	0.6640 and 0.2685
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5275 / 0 / 329
Goodness-of-fit on F ²	1.063
Final R indices [I>2σ(I)]	R1 = 0.0592, wR ² = 0.1458
R indices (all data)	R1 = 0.0693, wR ² = 0.1532
Largest diff. peak and hole	3.265 and -4.651 eÅ ⁻³

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

	x	y	z	U(eq)
C(1)	3116(12)	6492(11)	4389(6)	56(2)
C(2)	3156(13)	5358(9)	3706(6)	60(3)
O(3)	2903(6)	5379(5)	2582(4)	35(1)
C(4)	2347(7)	4287(6)	1824(5)	28(1)
C(5)	2329(7)	4523(6)	777(5)	29(1)
C(6)	2674(7)	5667(6)	384(5)	27(1)
C(65)	740(9)	4399(8)	-1255(6)	36(2)
C(60)	2084(7)	5453(6)	-771(5)	26(1)
C(61)	2921(8)	6280(7)	-1408(6)	34(1)
C(62)	2459(10)	6031(8)	-2495(6)	43(2)
C(64)	285(9)	4166(9)	-2338(7)	48(2)
C(63)	1134(10)	4973(9)	-2966(6)	48(2)
C(7)	3442(8)	7027(7)	930(5)	30(1)
C(8)	4565(8)	7640(6)	1766(5)	29(1)
N(9)	5510(6)	7201(5)	2148(5)	31(1)
C(10)	5757(9)	6100(7)	1601(7)	41(2)
C(11)	6402(8)	8057(7)	3096(5)	32(1)
C(12)	6106(8)	9154(7)	3312(5)	33(1)
C(13)	5003(8)	9047(6)	2405(5)	31(1)
C(14)	5748(12)	10032(8)	1720(7)	51(2)
C(15)	3662(10)	9205(9)	2790(7)	48(2)
C(16)	7414(8)	7894(9)	3774(6)	43(2)
C(17)	8130(9)	8879(10)	4676(7)	52(2)
C(18)	7860(10)	9972(11)	4900(7)	55(2)
C(19)	6849(9)	10106(8)	4220(6)	45(2)
C(20)	2433(10)	1776(9)	826(8)	48(2)
O(20)	3074(10)	1598(9)	146(7)	77(2)
C(21)	277(10)	2538(9)	3196(8)	49(2)
O(21)	-359(10)	2694(9)	3897(7)	74(2)
C(22)	3111(11)	2434(9)	3054(7)	47(2)
O(22)	4149(8)	2628(10)	3602(7)	75(2)
C(23)	-363(10)	1878(7)	903(7)	38(2)
O(23)	-1319(7)	1652(8)	259(6)	58(2)
C(24)	417(11)	208(10)	2047(8)	54(2)
O(24)	-82(10)	-882(6)	2055(7)	77(2)
W	1354(1)	2161(1)	2007(1)	32(1)

Table 3. Bond lengths [Å] and angles [°] for **4a**

C(1)-C(2)	1.451(13)
C(2)-O(3)	1.450(9)
O(3)-C(4)	1.323(8)
C(4)-C(5)	1.411(9)
C(4)-W	2.267(6)
C(5)-C(6)	1.393(9)
C(6)-C(7)	1.436(9)
C(6)-C(60)	1.498(9)
C(65)-C(64)	1.377(11)
C(65)-C(60)	1.399(10)
C(60)-C(61)	1.397(9)
C(61)-C(62)	1.381(10)
C(62)-C(63)	1.386(12)
C(64)-C(63)	1.381(12)
C(7)-C(8)	1.361(10)
C(8)-N(9)	1.350(9)
C(8)-C(13)	1.537(8)
N(9)-C(11)	1.402(9)
N(9)-C(10)	1.456(8)
C(11)-C(16)	1.390(11)
C(11)-C(12)	1.393(10)
C(12)-C(19)	1.371(10)
C(12)-C(13)	1.509(10)
C(13)-C(14)	1.518(10)
C(13)-C(15)	1.540(10)
C(16)-C(17)	1.378(12)
C(17)-C(18)	1.372(15)
C(18)-C(19)	1.373(14)
C(20)-O(20)	1.157(12)
C(20)-W	2.013(9)
C(21)-O(21)	1.167(12)
C(21)-W	2.017(10)
C(22)-O(22)	1.140(12)
C(22)-W	2.035(10)
C(23)-O(23)	1.139(11)
C(23)-W	2.044(9)
C(24)-O(24)	1.132(12)
C(24)-W	2.037(10)
O(3)-C(2)-C(1)	111.2(8)
C(4)-O(3)-C(2)	122.1(6)
O(3)-C(4)-C(5)	113.4(6)
O(3)-C(4)-W	128.6(5)
C(5)-C(4)-W	117.9(5)
C(6)-C(5)-C(4)	132.8(6)
C(5)-C(6)-C(7)	129.9(6)
C(5)-C(6)-C(60)	115.4(6)
C(7)-C(6)-C(60)	114.6(6)
C(64)-C(65)-C(60)	120.5(7)
C(61)-C(60)-C(65)	118.2(6)
C(61)-C(60)-C(6)	119.8(6)
C(65)-C(60)-C(6)	121.9(6)
C(62)-C(61)-C(60)	120.8(7)
C(61)-C(62)-C(63)	120.3(7)
C(65)-C(64)-C(63)	120.9(7)
C(64)-C(63)-C(62)	119.3(7)
C(8)-C(7)-C(6)	131.3(6)
N(9)-C(8)-C(7)	128.6(6)
N(9)-C(8)-C(13)	108.4(6)
C(7)-C(8)-C(13)	122.9(6)
C(8)-N(9)-C(11)	111.2(5)
C(8)-N(9)-C(10)	126.0(6)
C(11)-N(9)-C(10)	122.2(6)
C(16)-C(11)-C(12)	122.2(7)
C(16)-C(11)-N(9)	128.5(7)
C(12)-C(11)-N(9)	109.3(6)
C(19)-C(12)-C(11)	118.6(7)
C(19)-C(12)-C(13)	132.7(7)
C(11)-C(12)-C(13)	108.7(6)
C(12)-C(13)-C(14)	110.3(7)

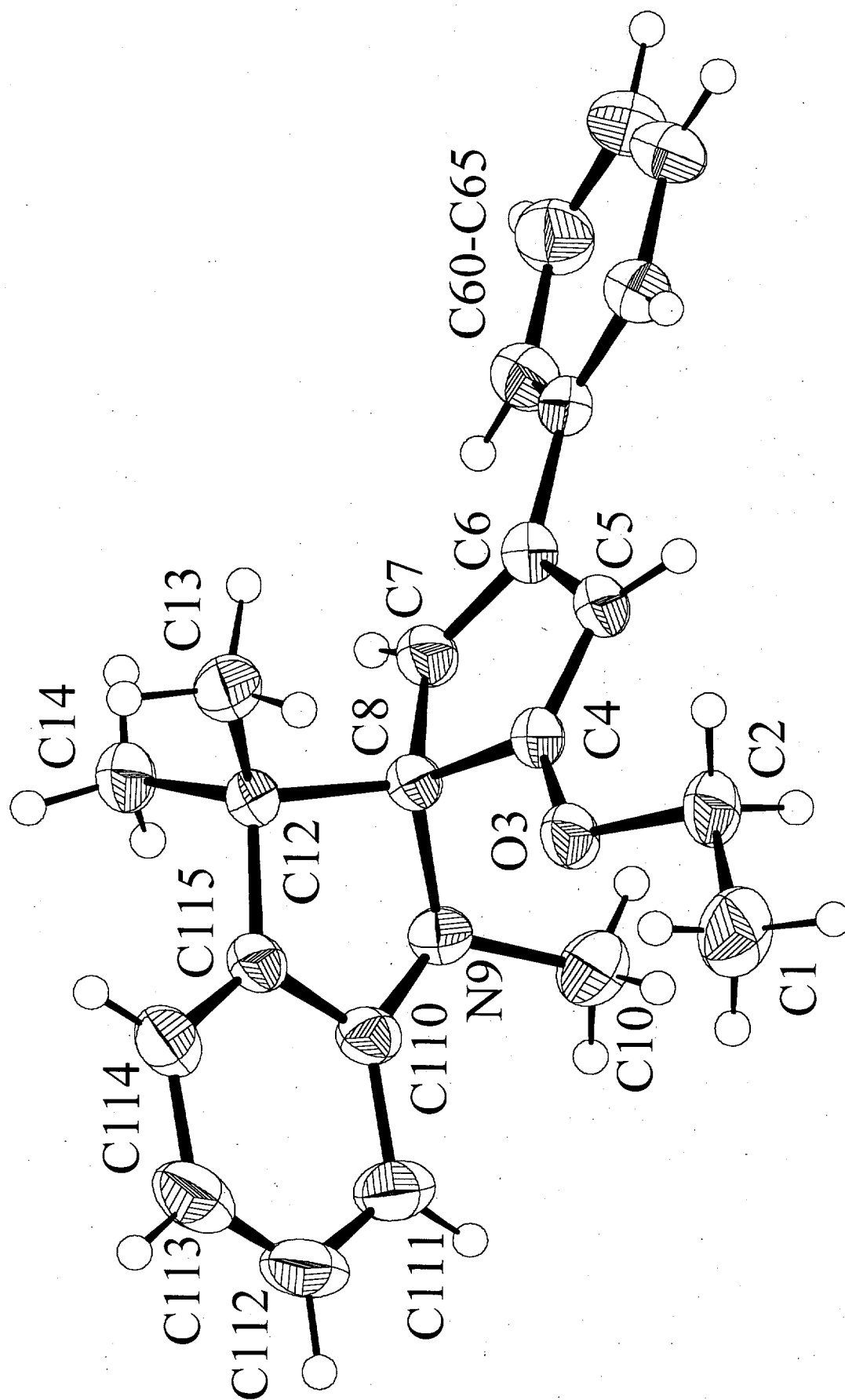
C(12)-C(13)-C(8)	101.2(5)
C(14)-C(13)-C(8)	109.5(6)
C(12)-C(13)-C(15)	113.1(6)
C(14)-C(13)-C(15)	111.0(7)
C(8)-C(13)-C(15)	111.4(6)
C(17)-C(16)-C(11)	116.9(8)
C(18)-C(17)-C(16)	121.8(8)
C(17)-C(18)-C(19)	120.2(8)
C(12)-C(19)-C(18)	120.4(8)
O(20)-C(20)-W	177.8(9)
O(21)-C(21)-W	176.5(9)
O(22)-C(22)-W	175.9(8)
O(23)-C(23)-W	175.9(7)
O(24)-C(24)-W	178.5(9)
C(20)-W-C(21)	179.6(3)
C(20)-W-C(22)	87.0(4)
C(21)-W-C(22)	92.7(4)
C(20)-W-C(24)	89.3(4)
C(21)-W-C(24)	90.4(4)
C(22)-W-C(24)	89.5(4)
C(20)-W-C(23)	90.6(3)
C(21)-W-C(23)	89.7(3)
C(22)-W-C(23)	177.6(3)
C(24)-W-C(23)	90.7(4)
C(20)-W-C(4)	87.8(3)
C(21)-W-C(4)	92.5(3)
C(22)-W-C(4)	93.6(3)
C(24)-W-C(4)	175.6(3)
C(23)-W-C(4)	86.0(3)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4a**
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	66(6)	73(6)	32(4)	1(4)	5(4)	37(5)
C(2)	90(7)	47(5)	33(4)	13(3)	0(4)	20(5)
O(3)	49(3)	27(2)	30(2)	10(2)	9(2)	17(2)
C(4)	31(3)	19(3)	41(3)	17(3)	13(3)	13(3)
C(5)	35(3)	26(3)	31(3)	8(2)	11(3)	17(3)
C(6)	30(3)	27(3)	33(3)	9(2)	10(2)	19(3)
C(65)	33(4)	36(4)	41(4)	15(3)	5(3)	13(3)
C(60)	26(3)	28(3)	33(3)	9(2)	7(2)	18(3)
C(61)	40(4)	25(3)	41(4)	13(3)	6(3)	16(3)
C(62)	56(5)	45(4)	34(4)	19(3)	8(3)	24(4)
C(64)	38(4)	46(5)	49(4)	10(4)	-7(3)	12(4)
C(63)	57(5)	50(5)	36(4)	11(3)	-1(3)	24(4)
C(7)	38(4)	30(3)	31(3)	8(3)	6(3)	22(3)
C(8)	36(3)	19(3)	35(3)	8(2)	13(3)	15(3)
N(9)	30(3)	25(3)	38(3)	3(2)	7(2)	15(2)
C(10)	40(4)	28(4)	58(4)	3(3)	10(3)	22(3)
C(11)	29(3)	30(3)	36(3)	8(3)	12(3)	11(3)
C(12)	30(3)	30(3)	37(3)	3(3)	14(3)	12(3)
C(13)	43(4)	18(3)	35(3)	4(2)	11(3)	17(3)
C(14)	77(6)	29(4)	46(4)	12(3)	17(4)	18(4)
C(15)	56(5)	45(5)	53(5)	-5(4)	7(4)	35(4)
C(16)	34(4)	52(5)	47(4)	15(3)	5(3)	22(4)
C(17)	35(4)	73(6)	43(4)	12(4)	5(3)	18(4)
C(18)	41(5)	62(6)	42(4)	-6(4)	4(3)	9(4)
C(19)	42(4)	37(4)	48(4)	-2(3)	15(3)	13(3)
C(20)	38(4)	35(4)	66(5)	-1(4)	7(4)	14(3)
O(20)	78(5)	78(6)	85(5)	8(4)	42(5)	44(5)
C(21)	48(5)	47(5)	59(5)	16(4)	9(4)	25(4)
O(21)	85(6)	91(6)	72(5)	34(4)	48(4)	51(5)
C(22)	64(6)	37(4)	50(4)	23(3)	21(4)	25(4)
O(22)	54(4)	101(7)	85(5)	39(5)	-7(4)	43(4)
C(23)	51(5)	22(3)	49(4)	19(3)	21(4)	18(3)
O(23)	42(3)	60(4)	72(4)	22(3)	-5(3)	22(3)
C(24)	49(5)	56(6)	61(5)	21(4)	20(4)	22(4)
O(24)	93(6)	27(3)	126(7)	44(4)	41(5)	27(4)
W	33(1)	29(1)	44(1)	18(1)	11(1)	17(1)

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

	x	y	z	U(eq)
H(1A)	3941	7291	4316	84
H(1B)	3179	6404	5130	84
H(1C)	2202	6537	4180	84
H(2A)	4117	5361	3873	72
H(2B)	2400	4546	3849	72
H(5)	2023	3756	237	34
H(65)	143	3845	-839	44
H(61)	3808	7015	-1093	41
H(62)	3047	6582	-2917	51
H(64)	-617	3449	-2654	57
H(63)	817	4805	-3706	57
H(7)	3111	7593	665	36
H(10A)	5200	5319	1872	61
H(10B)	6798	6316	1730	61
H(10C)	5440	5931	837	61
H(14A)	6056	10921	2132	77
H(14B)	5062	9875	1089	77
H(14C)	6602	9928	1502	77
H(15A)	3180	8543	3199	73
H(15B)	2975	9094	2174	73
H(15C)	3984	10078	3238	73
H(16)	7602	7147	3624	51
H(17)	8822	8800	5152	62
H(18)	8369	10630	5520	66
H(19)	6666	10855	4379	54



6a

Table 1. Crystal data and structure refinement for **6a**.

Identification code	AUM_747
Empirical formula	C ₂₃ H ₂₅ N O
Formula weight	331.44
Temperature	223(2) K
Wavelength	1.54178 Å
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a = 8.443(1) Å α = 101.79(1)° b = 9.047(1) Å β = 106.43(1)° c = 13.215(2) Å γ = 94.18(1)°
Volume	938.5(2) Å ³
Z	2
Density (calculated)	1.173 Mg/m ³
Absorption coefficient	0.546 mm ⁻¹
F(000)	356
Crystal size	1.00 x 0.50 x 0.30 mm
Theta range for data collection	3.59 to 74.24°
Index ranges	-10 ≤ h ≤ 10, -11 ≤ k ≤ 11, 0 ≤ l ≤ 16
Reflections collected	3993
Independent reflections	3823 [R(int) = 0.0182]
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3823 / 0 / 231
Goodness-of-fit on F ²	1.106
Final R indices [I > 2σ(I)]	R ₁ = 0.0491, wR ² = 0.1405
R indices (all data)	R ₁ = 0.0503, wR ² = 0.1418
Extinction coefficient	0.017(2)
Largest diff. peak and hole	0.298 and -0.229 eÅ ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **6a**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	2885(3)	5138(2)	8549(2)	57(1)
C(2)	2739(2)	5231(2)	7410(1)	40(1)
O(3)	2864(1)	6817(1)	7379(1)	35(1)
C(4)	2657(2)	7081(1)	6385(1)	30(1)
C(5)	2608(2)	6150(1)	5445(1)	34(1)
C(6)	2197(2)	7011(1)	4590(1)	32(1)
C(60)	2119(2)	6379(2)	3456(1)	33(1)
C(61)	1331(2)	7060(2)	2629(1)	41(1)
C(62)	1311(2)	6492(2)	1572(1)	49(1)
C(63)	2062(2)	5208(2)	1312(1)	51(1)
C(64)	2824(2)	4520(2)	2118(1)	49(1)
C(65)	2868(2)	5094(2)	3183(1)	40(1)
C(7)	1958(2)	8430(2)	5025(1)	34(1)
C(8)	2314(2)	8670(1)	6233(1)	29(1)
N(9)	934(1)	9150(1)	6649(1)	34(1)
C(10)	-560(2)	8045(2)	6326(1)	48(1)
C(110)	1648(2)	9876(2)	7745(1)	33(1)
C(111)	889(2)	10140(2)	8557(1)	46(1)
C(112)	1860(2)	10936(2)	9589(1)	53(1)
C(113)	3526(2)	11438(2)	9813(1)	51(1)
C(114)	4286(2)	11170(2)	8992(1)	42(1)
C(115)	3339(2)	10382(1)	7967(1)	32(1)
C(12)	3802(2)	9963(1)	6927(1)	31(1)
C(13)	5503(2)	9427(2)	7063(1)	43(1)
C(14)	3740(2)	11361(2)	6426(1)	43(1)

Table 3. Bond lengths [Å] and angles [°] for **6a**.

C(1)-C(2)	1.495(2)
C(2)-O(3)	1.440(2)
O(3)-C(4)	1.349(2)
C(4)-C(5)	1.339(2)
C(4)-C(8)	1.528(2)
C(5)-C(6)	1.477(2)
C(6)-C(7)	1.349(2)
C(6)-C(60)	1.472(2)
C(60)-C(61)	1.393(2)
C(60)-C(65)	1.394(2)
C(61)-C(62)	1.382(2)
C(62)-C(63)	1.392(3)
C(63)-C(64)	1.370(3)
C(64)-C(65)	1.386(2)
C(7)-C(8)	1.505(2)
C(8)-N(9)	1.479(2)
C(8)-C(12)	1.576(2)
N(9)-C(110)	1.398(2)
N(9)-C(10)	1.452(2)
C(110)-C(111)	1.388(2)
C(110)-C(115)	1.395(2)
C(111)-C(112)	1.389(2)
C(112)-C(113)	1.374(3)
C(113)-C(114)	1.398(2)
C(114)-C(115)	1.376(2)
C(115)-C(12)	1.516(2)
C(12)-C(13)	1.524(2)
C(12)-C(14)	1.540(2)
O(3)-C(2)-C(1)	108.02(12)
C(4)-O(3)-C(2)	114.91(10)
C(5)-C(4)-O(3)	131.06(12)
C(5)-C(4)-C(8)	111.10(11)
O(3)-C(4)-C(8)	117.73(10)
C(4)-C(5)-C(6)	107.98(11)
C(7)-C(6)-C(60)	127.08(12)
C(7)-C(6)-C(5)	109.43(11)
C(60)-C(6)-C(5)	123.47(12)
C(61)-C(60)-C(65)	118.11(13)
C(61)-C(60)-C(6)	121.23(12)
C(65)-C(60)-C(6)	120.65(13)
C(62)-C(61)-C(60)	120.97(14)
C(61)-C(62)-C(63)	120.2(2)
C(64)-C(63)-C(62)	119.18(14)
C(63)-C(64)-C(65)	120.9(2)
C(64)-C(65)-C(60)	120.59(14)
C(6)-C(7)-C(8)	110.39(11)
N(9)-C(8)-C(7)	115.12(11)
N(9)-C(8)-C(4)	111.22(10)
C(7)-C(8)-C(4)	100.90(10)
N(9)-C(8)-C(12)	102.33(9)
C(7)-C(8)-C(12)	114.49(10)
C(4)-C(8)-C(12)	113.25(10)
C(110)-N(9)-C(10)	119.14(12)
C(110)-N(9)-C(8)	106.81(10)
C(10)-N(9)-C(8)	116.61(11)
C(111)-C(110)-C(115)	120.75(14)
C(111)-C(110)-N(9)	128.59(14)
C(115)-C(110)-N(9)	110.65(11)
C(110)-C(111)-C(112)	117.9(2)
C(113)-C(112)-C(111)	121.6(2)
C(112)-C(113)-C(114)	120.3(2)
C(115)-C(114)-C(113)	118.7(2)
C(114)-C(115)-C(110)	120.73(13)
C(114)-C(115)-C(12)	130.40(13)
C(110)-C(115)-C(12)	108.83(11)
C(115)-C(12)-C(13)	114.80(12)
C(115)-C(12)-C(14)	108.22(10)
C(13)-C(12)-C(14)	109.44(12)
C(115)-C(12)-C(8)	100.24(10)

C(13)-C(12)-C(8)	112.92(10)
C(14)-C(12)-C(8)	110.88(11)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **6a**.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	76(1)	48(1)	53(1)	26(1)	21(1)	1(1)
C(2)	51(1)	26(1)	47(1)	14(1)	17(1)	2(1)
O(3)	50(1)	24(1)	35(1)	9(1)	17(1)	4(1)
C(4)	36(1)	23(1)	34(1)	7(1)	14(1)	2(1)
C(5)	43(1)	23(1)	38(1)	5(1)	17(1)	3(1)
C(6)	35(1)	28(1)	34(1)	4(1)	14(1)	0(1)
C(60)	35(1)	29(1)	34(1)	2(1)	15(1)	-4(1)
C(61)	45(1)	39(1)	37(1)	5(1)	13(1)	5(1)
C(62)	58(1)	52(1)	35(1)	8(1)	12(1)	4(1)
C(63)	64(1)	53(1)	37(1)	0(1)	23(1)	1(1)
C(64)	63(1)	41(1)	46(1)	1(1)	29(1)	8(1)
C(65)	49(1)	35(1)	41(1)	5(1)	20(1)	5(1)
C(7)	42(1)	28(1)	34(1)	8(1)	15(1)	5(1)
C(8)	34(1)	23(1)	34(1)	6(1)	15(1)	5(1)
N(9)	32(1)	34(1)	38(1)	7(1)	15(1)	6(1)
C(10)	35(1)	53(1)	56(1)	9(1)	15(1)	0(1)
C(110)	40(1)	29(1)	37(1)	10(1)	18(1)	11(1)
C(111)	51(1)	50(1)	49(1)	14(1)	30(1)	16(1)
C(112)	78(1)	51(1)	43(1)	11(1)	36(1)	21(1)
C(113)	76(1)	41(1)	34(1)	2(1)	18(1)	12(1)
C(114)	52(1)	32(1)	40(1)	4(1)	13(1)	5(1)
C(115)	40(1)	23(1)	36(1)	7(1)	16(1)	7(1)
C(12)	35(1)	23(1)	37(1)	4(1)	16(1)	2(1)
C(13)	35(1)	39(1)	56(1)	5(1)	21(1)	4(1)
C(14)	59(1)	27(1)	48(1)	9(1)	25(1)	1(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **6a**.

	x	y	z	U(eq)
H(1A)	2737(19)	4077(2)	8580(3)	85
H(1B)	2033(12)	5651(15)	8781(5)	85
H(1C)	3978(7)	5626(16)	9024(2)	85
H(2A)	3632(2)	4766(2)	7181(1)	48
H(2B)	1665(2)	4684(2)	6916(1)	48
H(5)	2801(2)	5128(1)	5347(1)	41
H(61)	805(2)	7919(2)	2793(1)	49
H(62)	788(2)	6975(2)	1025(1)	59
H(63)	2047(2)	4817(2)	593(1)	62
H(64)	3324(2)	3646(2)	1947(1)	59
H(65)	3406(2)	4614(2)	3727(1)	49
H(7)	1617(2)	9164(2)	4628(1)	41
H(10A)	-826(10)	7552(11)	5563(3)	73
H(10B)	-1481(4)	8561(3)	6447(10)	73
H(10C)	-371(6)	7285(9)	6753(8)	73
H(111)	-247(2)	9792(2)	8413(1)	55
H(112)	1366(2)	11135(2)	10148(1)	64
H(113)	4157(2)	11963(2)	10520(1)	61
H(114)	5421(2)	11523(2)	9138(1)	50
H(13A)	5624(6)	9025(13)	6354(1)	65
H(13B)	5597(6)	8635(10)	7464(9)	65
H(13C)	6372(2)	10279(3)	7456(9)	65
H(14A)	4041(15)	11117(5)	5761(5)	64
H(14B)	4520(11)	12210(4)	6935(4)	64
H(14C)	2622(4)	11635(9)	6267(9)	64

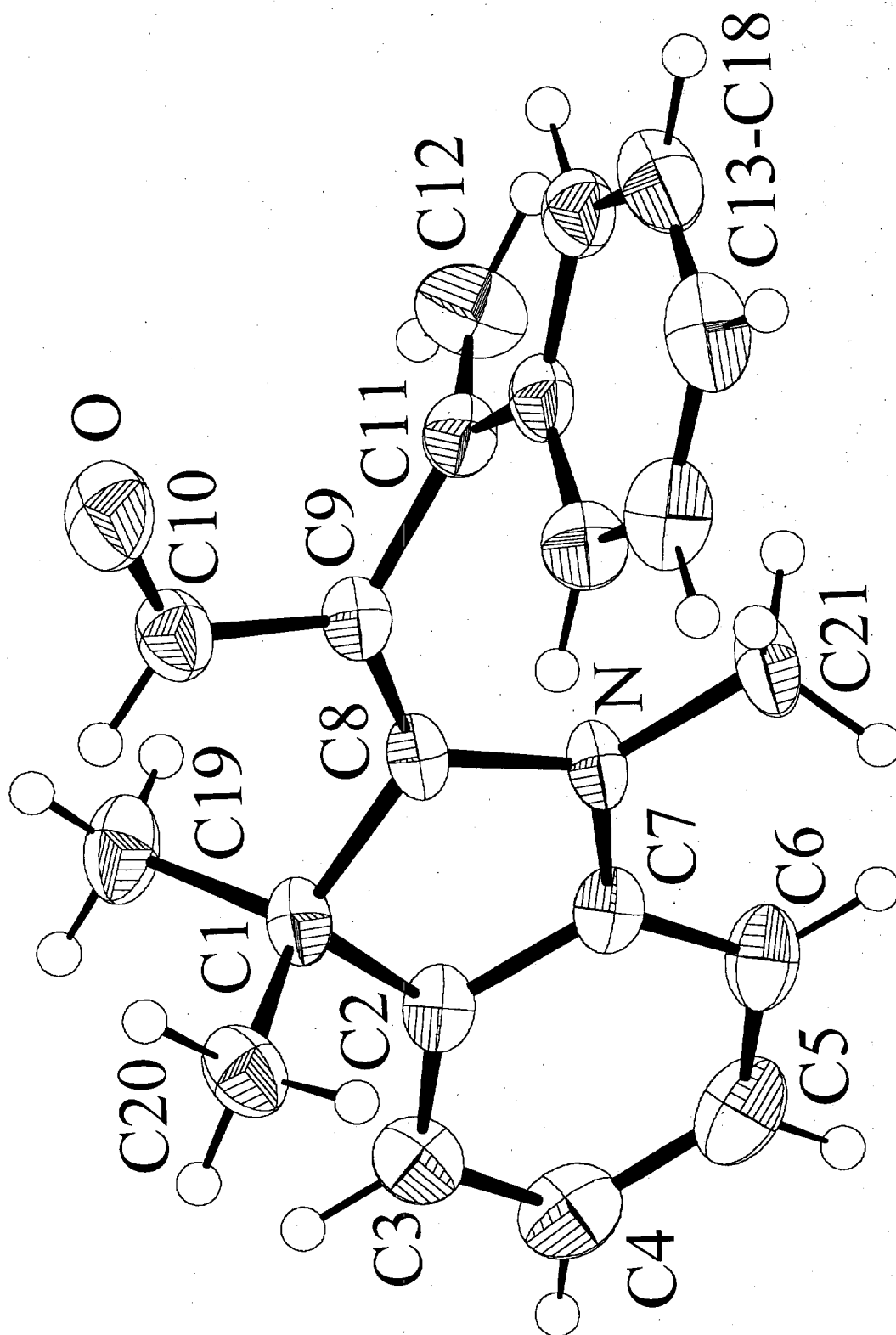


Table 1. Crystal data and structure refinement for **7a**.

Identification code	AUM_802
Empirical formula	C ₂₁ H ₂₁ N O
Formula weight	303.39
Temperature	223(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, P2 ₁ /n (No. 14)
Unit cell dimensions	a = 11.641(1) Å b = 8.886(1) Å β = 103.09(1)° c = 16.540(1) Å
Volume	1666.5(3) Å ³
Z, Calculated density	4, 1.209 Mg/m ³
Absorption coefficient	0.074 mm ⁻¹
F(000)	648
Crystal size	0.60 x 0.60 x 0.40 mm
Theta range for data collection	2.42 to 26.28°.
Index ranges	-14 ≤ h ≤ 0, -11 ≤ k ≤ 0, -20 ≤ l ≤ 20
Reflections collected / unique	3536 / 3369 [R(int) = 0.0346]
Completeness to 2theta = 26.28	93.6%
Max. and min. transmission	0.9711 and 0.9572
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3369 / 0 / 211
Goodness-of-fit on F ²	1.039
Final R indices [I > 2σ(I)]	R1 = 0.0659, wR ² = 0.1961
R indices (all data)	R1 = 0.0883, wR ² = 0.2161
Largest diff. peak and hole	0.384 and -0.428 eÅ ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7a**.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O	8984(2)	8775(2)	-889(1)	54(1)
N	6283(1)	7812(2)	852(1)	31(1)
C(1)	7639(2)	9798(2)	1254(1)	30(1)
C(2)	6805(2)	9639(2)	1829(1)	30(1)
C(3)	6741(2)	10439(2)	2531(1)	38(1)
C(4)	5874(2)	10070(3)	2951(1)	45(1)
C(5)	5091(2)	8904(3)	2672(1)	45(1)
C(6)	5147(2)	8095(2)	1967(1)	39(1)
C(7)	6023(2)	8479(2)	1560(1)	30(1)
C(8)	7188(2)	8553(2)	606(1)	28(1)
C(9)	7564(2)	8256(2)	-110(1)	31(1)
C(10)	8617(2)	8957(2)	-258(1)	39(1)
C(11)	6891(2)	7325(2)	-816(1)	33(1)
C(12)	5869(2)	7834(3)	-1252(2)	51(1)
C(13)	7415(2)	5881(2)	-1015(1)	31(1)
C(14)	8243(2)	5137(2)	-419(1)	39(1)
C(15)	8707(2)	3755(2)	-583(2)	46(1)
C(16)	8352(2)	3112(3)	-1352(2)	49(1)
C(17)	7549(2)	3853(3)	-1966(2)	47(1)
C(18)	7079(2)	5225(2)	-1801(1)	37(1)
C(19)	7496(2)	11364(2)	850(2)	46(1)
C(20)	8910(2)	9532(2)	1755(1)	40(1)
C(21)	5737(2)	6401(2)	538(2)	42(1)

Table 3. Bond lengths [Å] and angles [°] for **7a**.

O-C(10)	1.223(2)
N-C(8)	1.380(2)
N-C(7)	1.404(2)
N-C(21)	1.448(2)
C(1)-C(2)	1.512(3)
C(1)-C(19)	1.536(2)
C(1)-C(20)	1.541(3)
C(1)-C(8)	1.547(2)
C(2)-C(3)	1.378(3)
C(2)-C(7)	1.381(3)
C(3)-C(4)	1.388(3)
C(4)-C(5)	1.388(3)
C(5)-C(6)	1.383(3)
C(6)-C(7)	1.387(3)
C(8)-C(9)	1.378(3)
C(9)-C(10)	1.445(3)
C(9)-C(11)	1.498(3)
C(11)-C(12)	1.323(3)
C(11)-C(13)	1.490(3)
C(13)-C(14)	1.381(3)
C(13)-C(18)	1.398(3)
C(14)-C(15)	1.393(3)
C(15)-C(16)	1.370(3)
C(16)-C(17)	1.382(4)
C(17)-C(18)	1.387(3)
C(8)-N-C(7)	111.59(15)
C(8)-N-C(21)	127.58(16)
C(7)-N-C(21)	120.27(15)
C(2)-C(1)-C(19)	109.64(15)
C(2)-C(1)-C(20)	108.74(16)
C(19)-C(1)-C(20)	111.71(17)
C(2)-C(1)-C(8)	101.72(14)
C(19)-C(1)-C(8)	111.12(16)
C(20)-C(1)-C(8)	113.38(15)
C(3)-C(2)-C(7)	119.97(18)
C(3)-C(2)-C(1)	130.32(18)
C(7)-C(2)-C(1)	109.71(16)
C(2)-C(3)-C(4)	119.0(2)
C(3)-C(4)-C(5)	120.5(2)
C(6)-C(5)-C(4)	121.02(19)
C(5)-C(6)-C(7)	117.5(2)
C(2)-C(7)-C(6)	122.04(18)
C(2)-C(7)-N	109.44(15)
C(6)-C(7)-N	128.52(18)
C(9)-C(8)-N	125.05(17)
C(9)-C(8)-C(1)	127.48(16)
N-C(8)-C(1)	107.40(15)
C(8)-C(9)-C(10)	120.67(17)
C(8)-C(9)-C(11)	124.34(17)
C(10)-C(9)-C(11)	114.79(16)
O-C(10)-C(9)	124.13(19)
C(12)-C(11)-C(9)	122.45(19)
C(12)-C(11)-C(13)	118.84(19)
C(13)-C(11)-C(9)	118.69(17)
C(14)-C(13)-C(18)	117.85(18)
C(14)-C(13)-C(11)	120.62(17)
C(18)-C(13)-C(11)	121.52(18)
C(13)-C(14)-C(15)	121.5(2)
C(16)-C(15)-C(14)	120.0(2)
C(15)-C(16)-C(17)	119.6(2)
C(16)-C(17)-C(18)	120.4(2)
C(17)-C(18)-C(13)	120.6(2)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7a**.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O	54(1)	62(1)	56(1)	-10(1)	35(1)	-17(1)
N	29(1)	24(1)	44(1)	-4(1)	15(1)	-7(1)
C(1)	31(1)	23(1)	41(1)	-3(1)	15(1)	-3(1)
C(2)	28(1)	25(1)	40(1)	2(1)	13(1)	3(1)
C(3)	37(1)	37(1)	42(1)	-6(1)	11(1)	4(1)
C(4)	49(1)	48(1)	43(1)	-2(1)	21(1)	13(1)
C(5)	43(1)	47(1)	53(1)	11(1)	29(1)	11(1)
C(6)	32(1)	33(1)	58(1)	6(1)	22(1)	2(1)
C(7)	28(1)	25(1)	39(1)	3(1)	12(1)	3(1)
C(8)	23(1)	21(1)	42(1)	1(1)	10(1)	-2(1)
C(9)	30(1)	27(1)	37(1)	-1(1)	12(1)	-2(1)
C(10)	37(1)	41(1)	44(1)	-7(1)	18(1)	-10(1)
C(11)	35(1)	31(1)	36(1)	1(1)	13(1)	-2(1)
C(12)	47(1)	48(1)	52(1)	-8(1)	1(1)	11(1)
C(13)	29(1)	29(1)	38(1)	-1(1)	15(1)	-6(1)
C(14)	40(1)	37(1)	41(1)	-3(1)	13(1)	0(1)
C(15)	39(1)	38(1)	64(1)	5(1)	20(1)	6(1)
C(16)	46(1)	37(1)	72(2)	-10(1)	32(1)	-2(1)
C(17)	48(1)	47(1)	53(1)	-20(1)	29(1)	-15(1)
C(18)	39(1)	39(1)	39(1)	-2(1)	17(1)	-9(1)
C(19)	59(1)	24(1)	59(1)	3(1)	24(1)	-2(1)
C(20)	30(1)	43(1)	47(1)	-9(1)	11(1)	-6(1)
C(21)	44(1)	29(1)	58(1)	-9(1)	22(1)	-15(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7a**.

	x	y	z	U(eq)
H(3)	7276	11222	2722	46
H(4)	5816	10613	3427	54
H(5)	4513	8661	2966	54
H(6)	4611	7313	1772	47
H(10)	9048	9592	156	47
H(12A)	5446	7278	-1706	61
H(12B)	5567	8751	-1107	61
H(14)	8499	5573	109	47
H(15)	9264	3264	-166	55
H(16)	8654	2171	-1461	58
H(17)	7319	3426	-2498	56
H(18)	6531	5718	-2223	45
H(19A)	6688	11492	540	68
H(19B)	8026	11460	477	68
H(19C)	7682	12129	1278	68
H(20A)	9075	10199	2232	59
H(20B)	9459	9734	1407	59
H(20C)	8994	8495	1943	59
H(21A)	5022	6601	121	63
H(21B)	5545	5832	990	63
H(21C)	6279	5824	292	63

9a

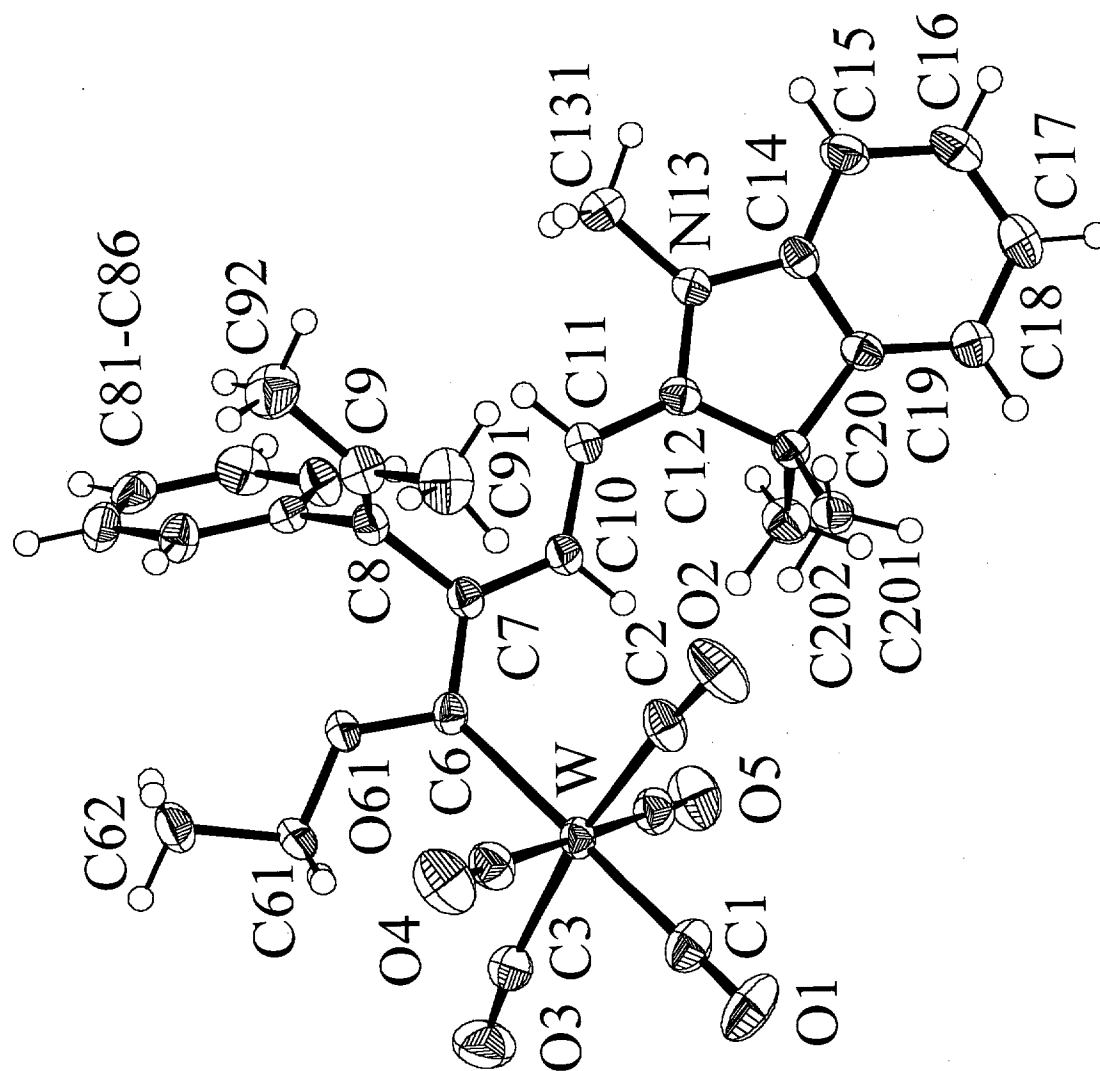


Table 1. Crystal data and structure refinement for **9a**.

Identification code	AUM1388
Empirical formula	C ₃₂ H ₃₁ N O ₆ W
Formula weight	709.43
Temperature	198(2) K
Wavelength	0.71073 Å
Crystal system, space group	triclinic, P1bar (No. 2)
Unit cell dimensions	a = 10.712(1) Å α = 79.48(1)°. b = 10.861(1) Å β = 88.40(1)°. c = 14.835(1) Å γ = 62.35(1)°.
Volume	1499.9(2) Å ³
Z, Calculated density	2, 1.571 Mg/m ³
Absorption coefficient	3.894 mm ⁻¹
F(000)	704
Crystal size	0.25 x 0.20 x 0.10 mm
Theta range for data collection	2.15 to 27.52°
Limiting indices	-13<=h<=13, -14<=k<=13, -17<=l<=19
Reflections collected / unique	9934 / 6811 [R(int) = 0.0294]
Completeness to theta = 27.52	98.7 %
Max. and min. transmission	0.6968 and 0.4427
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6811 / 0 / 367
Goodness-of-fit on F ²	1.009
Final R indices [I>2σ(I)]	R1 = 0.0234, wR ² = 0.0583
R indices (all data)	R1 = 0.0259, wR ² = 0.0598
Largest diff. peak and hole	1.077 and -1.212 eÅ ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **9a**.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	1559(4)	2241(3)	1340(2)	40(1)
O(1)	1052(3)	3437(2)	1121(2)	62(1)
C(2)	4246(3)	98(3)	1216(2)	34(1)
O(2)	5186(3)	204(3)	930(2)	54(1)
C(3)	487(3)	489(3)	2145(2)	37(1)
O(3)	-613(3)	837(3)	2393(2)	59(1)
C(4)	1909(3)	69(3)	400(2)	35(1)
O(4)	1614(3)	56(3)	-328(2)	57(1)
C(5)	2911(3)	81(3)	3023(2)	33(1)
O(5)	3130(3)	54(3)	3777(2)	50(1)
W	2431(1)	120(1)	1701(1)	26(1)
C(6)	3472(3)	-2264(3)	1947(2)	24(1)
O(61)	2853(2)	-3019(2)	1761(2)	30(1)
C(61)	1335(3)	-2427(3)	1637(2)	37(1)
C(62)	1036(3)	-3577(3)	1444(2)	39(1)
C(7)	4957(3)	-3238(3)	2155(2)	25(1)
C(8)	5544(3)	-4679(3)	1901(2)	25(1)
C(81)	5267(3)	-5754(3)	2528(2)	25(1)
C(82)	5675(3)	-6100(3)	3459(2)	33(1)
C(83)	5455(3)	-7137(3)	4038(2)	37(1)
C(84)	4803(3)	-7810(3)	3704(2)	33(1)
C(85)	4358(3)	-7443(3)	2785(2)	36(1)
C(86)	4591(3)	-6422(3)	2201(2)	32(1)
C(9)	6281(3)	-4953(3)	1153(2)	32(1)
C(91)	6542(4)	-3846(4)	531(2)	48(1)
C(92)	6953(4)	-6378(4)	871(2)	45(1)
C(10)	5832(3)	-2883(3)	2584(2)	24(1)
C(11)	7272(3)	-3793(3)	2841(2)	27(1)
C(12)	8185(3)	-3480(3)	3257(2)	24(1)
N(13)	9574(2)	-4439(2)	3483(2)	27(1)
C(131)	10203(3)	-5906(3)	3377(2)	39(1)
C(14)	10311(3)	-3840(3)	3837(2)	26(1)
C(15)	11748(3)	-4424(3)	4073(2)	34(1)
C(16)	12208(3)	-3575(4)	4395(2)	43(1)
C(17)	11290(3)	-2200(4)	4486(2)	44(1)
C(18)	9851(3)	-1627(3)	4231(2)	37(1)
C(19)	9376(3)	-2452(3)	3907(2)	26(1)
C(20)	7918(3)	-2097(3)	3546(2)	24(1)
C(201)	6904(3)	-1793(3)	4324(2)	34(1)
C(202)	7388(3)	-845(3)	2739(2)	31(1)

Table 3. Bond lengths [Å] and angles [°] for **9a**.

C(1)-O(1)	1.135(4)
C(1)-W	2.012(3)
C(2)-O(2)	1.128(4)
C(2)-W	2.046(3)
C(3)-O(3)	1.132(4)
C(3)-W	2.044(3)
C(4)-O(4)	1.138(4)
C(4)-W	2.042(3)
C(5)-O(5)	1.142(4)
C(5)-W	2.029(3)
W-C(6)	2.254(2)
C(6)-O(61)	1.335(3)
C(6)-C(7)	1.446(4)
O(61)-C(61)	1.448(3)
C(61)-C(62)	1.500(4)
C(7)-C(10)	1.376(4)
C(7)-C(8)	1.508(4)
C(8)-C(9)	1.341(4)
C(8)-C(81)	1.491(4)
C(81)-C(86)	1.387(4)
C(81)-C(82)	1.390(4)
C(82)-C(83)	1.394(4)
C(83)-C(84)	1.375(5)
C(84)-C(85)	1.381(5)
C(85)-C(86)	1.391(4)
C(9)-C(91)	1.505(4)
C(9)-C(92)	1.508(4)
C(10)-C(11)	1.408(4)
C(11)-C(12)	1.368(4)
C(12)-N(13)	1.369(3)
C(12)-C(20)	1.534(3)
N(13)-C(14)	1.395(4)
N(13)-C(131)	1.450(3)
C(14)-C(15)	1.391(4)
C(14)-C(19)	1.392(4)
C(15)-C(16)	1.385(5)
C(16)-C(17)	1.385(5)
C(17)-C(18)	1.401(4)
C(18)-C(19)	1.374(4)
C(19)-C(20)	1.512(4)
C(20)-C(202)	1.526(4)
C(20)-C(201)	1.536(3)
O(1)-C(1)-W	178.6(4)
O(2)-C(2)-W	174.3(3)
O(3)-C(3)-W	172.5(3)
O(4)-C(4)-W	179.3(3)
O(5)-C(5)-W	177.1(3)
C(1)-W-C(5)	94.10(13)
C(1)-W-C(4)	88.47(13)
C(5)-W-C(4)	176.53(11)
C(1)-W-C(3)	84.86(13)
C(5)-W-C(3)	84.82(13)
C(4)-W-C(3)	93.09(13)
C(1)-W-C(2)	85.91(13)
C(5)-W-C(2)	95.02(12)
C(4)-W-C(2)	87.49(12)
C(3)-W-C(2)	170.74(12)
C(1)-W-C(6)	173.79(11)
C(5)-W-C(6)	91.32(11)
C(4)-W-C(6)	86.25(11)
C(3)-W-C(6)	98.67(11)
C(2)-W-C(6)	90.59(11)
O(61)-C(6)-C(7)	107.0(2)
O(61)-C(6)-W	124.74(18)
C(7)-C(6)-W	127.31(18)
C(6)-O(61)-C(61)	122.3(2)
O(61)-C(61)-C(62)	107.2(2)
C(10)-C(7)-C(6)	121.5(2)
C(10)-C(7)-C(8)	119.7(2)

C(6)-C(7)-C(8)	118.8(2)
C(9)-C(8)-C(81)	123.0(2)
C(9)-C(8)-C(7)	120.6(2)
C(81)-C(8)-C(7)	116.4(2)
C(86)-C(81)-C(82)	118.4(3)
C(86)-C(81)-C(8)	121.1(2)
C(82)-C(81)-C(8)	120.4(2)
C(81)-C(82)-C(83)	120.3(3)
C(84)-C(83)-C(82)	120.8(3)
C(83)-C(84)-C(85)	119.2(3)
C(84)-C(85)-C(86)	120.3(3)
C(81)-C(86)-C(85)	120.9(3)
C(8)-C(9)-C(91)	121.9(3)
C(8)-C(9)-C(92)	124.1(3)
C(91)-C(9)-C(92)	114.0(3)
C(7)-C(10)-C(11)	124.7(2)
C(12)-C(11)-C(10)	126.7(2)
C(11)-C(12)-N(13)	122.6(2)
C(11)-C(12)-C(20)	129.5(2)
N(13)-C(12)-C(20)	107.9(2)
C(12)-N(13)-C(14)	111.8(2)
C(12)-N(13)-C(131)	124.2(2)
C(14)-N(13)-C(131)	124.0(2)
C(15)-C(14)-C(19)	121.5(3)
C(15)-C(14)-N(13)	129.3(3)
C(19)-C(14)-N(13)	109.2(2)
C(16)-C(15)-C(14)	117.3(3)
C(15)-C(16)-C(17)	122.1(3)
C(16)-C(17)-C(18)	119.6(3)
C(19)-C(18)-C(17)	119.1(3)
C(18)-C(19)-C(14)	120.4(3)
C(18)-C(19)-C(20)	130.4(2)
C(14)-C(19)-C(20)	109.1(2)
C(19)-C(20)-C(202)	110.5(2)
C(19)-C(20)-C(12)	101.8(2)
C(202)-C(20)-C(12)	112.5(2)
C(19)-C(20)-C(201)	109.8(2)
C(202)-C(20)-C(201)	111.4(2)
C(12)-C(20)-C(201)	110.4(2)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **9a**.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	49(2)	31(2)	42(2)	-4(1)	6(1)	-21(1)
O(1)	87(2)	26(1)	68(2)	-4(1)	10(2)	-25(1)
C(2)	39(2)	45(2)	26(1)	-1(1)	-3(1)	-28(1)
O(2)	49(1)	92(2)	35(1)	0(1)	1(1)	-49(2)
C(3)	33(2)	29(1)	49(2)	-3(1)	0(1)	-16(1)
O(3)	34(1)	50(1)	86(2)	-3(1)	13(1)	-18(1)
C(4)	34(1)	38(2)	34(2)	0(1)	-3(1)	-19(1)
O(4)	60(2)	81(2)	36(1)	-5(1)	-10(1)	-39(2)
C(5)	34(1)	34(1)	36(2)	-8(1)	6(1)	-20(1)
O(5)	61(2)	67(2)	35(1)	-16(1)	4(1)	-38(1)
W	28(1)	23(1)	29(1)	-2(1)	0(1)	-15(1)
C(6)	28(1)	23(1)	23(1)	-2(1)	0(1)	-15(1)
O(61)	25(1)	26(1)	43(1)	-4(1)	-4(1)	-15(1)
C(61)	25(1)	33(1)	55(2)	-6(1)	-4(1)	-17(1)
C(62)	36(2)	44(2)	48(2)	-12(1)	4(1)	-29(1)
C(7)	26(1)	26(1)	25(1)	-3(1)	1(1)	-16(1)
C(8)	27(1)	27(1)	25(1)	-5(1)	-1(1)	-15(1)
C(81)	23(1)	23(1)	28(1)	-6(1)	2(1)	-10(1)
C(82)	34(1)	38(2)	32(2)	-5(1)	2(1)	-23(1)
C(83)	35(2)	40(2)	30(2)	2(1)	3(1)	-18(1)
C(84)	32(1)	24(1)	43(2)	-7(1)	13(1)	-13(1)
C(85)	39(2)	29(1)	48(2)	-14(1)	8(1)	-21(1)
C(86)	39(2)	32(1)	31(2)	-9(1)	0(1)	-19(1)
C(9)	35(1)	36(1)	27(1)	-5(1)	2(1)	-19(1)
C(91)	65(2)	59(2)	30(2)	-6(2)	13(2)	-39(2)
C(92)	48(2)	47(2)	42(2)	-19(2)	13(2)	-21(2)
C(10)	24(1)	26(1)	25(1)	-3(1)	1(1)	-14(1)
C(11)	26(1)	27(1)	30(1)	-6(1)	1(1)	-14(1)
C(12)	22(1)	26(1)	23(1)	-3(1)	3(1)	-11(1)
N(13)	23(1)	24(1)	32(1)	-5(1)	-2(1)	-10(1)
C(131)	33(2)	27(1)	54(2)	-10(1)	-2(1)	-10(1)
C(14)	27(1)	30(1)	23(1)	-3(1)	0(1)	-15(1)
C(15)	23(1)	36(2)	37(2)	-7(1)	-5(1)	-9(1)
C(16)	27(1)	50(2)	49(2)	-8(2)	-9(1)	-16(1)
C(17)	39(2)	52(2)	51(2)	-14(2)	-8(1)	-27(2)
C(18)	36(2)	36(2)	42(2)	-11(1)	-3(1)	-18(1)
C(19)	24(1)	31(1)	24(1)	-5(1)	0(1)	-12(1)
C(20)	22(1)	26(1)	26(1)	-6(1)	1(1)	-12(1)
C(201)	31(1)	43(2)	31(2)	-14(1)	8(1)	-18(1)
C(202)	31(1)	30(1)	33(2)	-2(1)	-3(1)	-15(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **9a**.

	x	y	z	U(eq)
H(61A)	956	-1610	1118	44
H(61B)	886	-2101	2200	44
H(62A)	1436	-3850	866	58
H(62B)	12	-3231	1392	58
H(62C)	1463	-4400	1946	58
H(82)	6105	-5627	3703	39
H(83)	5760	-7382	4670	44
H(84)	4660	-8519	4102	40
H(85)	3891	-7889	2551	43
H(86)	4282	-6180	1570	39
H(91A)	5975	-2924	706	71
H(91B)	6274	-3794	-106	71
H(91C)	7545	-4100	589	71
H(92A)	6822	-7065	1337	67
H(92B)	7965	-6694	812	67
H(92C)	6510	-6300	280	67
H(10)	5436	-1956	2716	29
H(11)	7649	-4721	2712	32
H(13A)	9760	-6394	3776	59
H(13B)	11218	-6369	3549	59
H(13C)	10057	-5945	2736	59
H(15)	12387	-5367	4015	41
H(16)	13184	-3947	4559	51
H(17)	11633	-1649	4720	53
H(18)	9212	-680	4281	44
H(20A)	7261	-2623	4824	51
H(20B)	5967	-1587	4090	51
H(20C)	6837	-976	4554	51
H(20D)	7438	-46	2924	47
H(20E)	6407	-565	2555	47
H(20F)	7978	-1118	2221	47

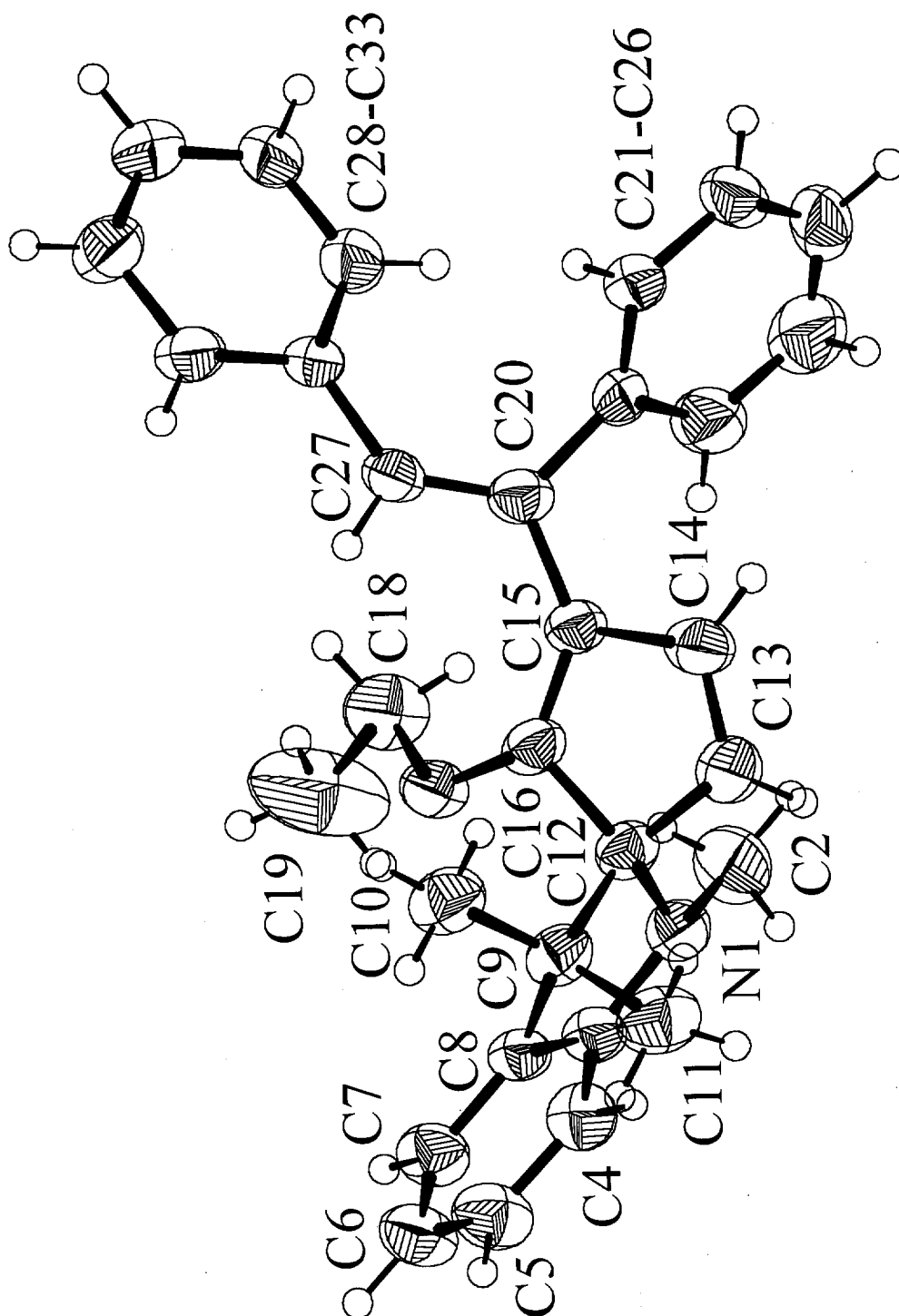


Table 1. Crystal data and structure refinement for 10c.

Identification code	AUM1490
Empirical formula	C ₃₃ H ₃₄ N ₂ O
Formula weight	474.62
Temperature	223(2) K
Wavelength	1.54178 Å
Crystal system, space group	monoclinic, P2 ₁ /c (No. 14)
Unit cell dimensions	a = 8.694(3) Å b = 16.319(4) Å β = 94.15(2)° c = 19.886(4) Å
Volume	2814.0(13) Å ³
Z, Calculated density	4, 1.120 Mg/m ³
Absorption coefficient	0.517 mm ⁻¹
F(000)	1016
Crystal size	0.25 x 0.15 x 0.05 mm
Theta range for data collection	3.51 to 57.50°.
Limiting indices	-9<=h<=9, -17<=k<=0, 0<=l<=21
Reflections collected / unique	3988 / 3859 [R(int) = 0.0688]
Completeness to theta = 57.50	99.9 %
Max. and min. transmission	0.9746 and 0.8816
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3859 / 0 / 330
Goodness-of-fit on F ²	1.004
Final R indices [I>2σ(I)]	R1 = 0.0663, wR ² = 0.1465
R indices (all data)	R1 = 0.2286, wR ² = 0.2135
Largest diff. peak and hole	0.237 and -0.212 eÅ ⁻³

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

	x	y	z	U(eq)
N(1)	2883(5)	1351(3)	4124(2)	46(1)
C(2)	4464(6)	1044(4)	4105(3)	68(2)
C(3)	2306(6)	1889(4)	3624(3)	43(2)
C(4)	2800(7)	2004(4)	2975(3)	50(2)
C(5)	1999(7)	2571(4)	2563(3)	60(2)
C(6)	781(7)	3005(4)	2774(3)	59(2)
C(7)	282(6)	2875(4)	3420(3)	51(2)
C(8)	1063(6)	2325(4)	3838(3)	39(1)
C(9)	749(6)	2041(4)	4545(3)	44(2)
C(10)	289(7)	2721(4)	5016(3)	59(2)
C(11)	-552(6)	1389(4)	4483(3)	64(2)
C(12)	2340(6)	1636(4)	4775(3)	42(2)
C(13)	2281(7)	969(4)	5290(3)	56(2)
C(14)	3244(7)	1154(4)	5815(3)	56(2)
C(15)	4007(6)	1952(4)	5740(3)	40(2)
C(16)	3496(6)	2233(4)	5119(3)	43(2)
O(17)	3876(4)	2884(2)	4760(2)	49(1)
C(18)	5384(7)	3212(4)	4842(3)	68(2)
C(19)	5703(9)	3667(7)	4254(4)	146(5)
C(20)	5110(6)	2298(4)	6264(3)	44(2)
C(21)	6165(6)	1679(3)	6599(3)	39(2)
C(22)	6229(6)	1560(3)	7295(3)	44(2)
C(23)	7126(7)	939(4)	7584(3)	55(2)
C(24)	7951(7)	427(4)	7198(4)	68(2)
C(25)	7907(8)	542(4)	6512(4)	77(2)
C(26)	7007(7)	1155(4)	6219(3)	64(2)
C(27)	5067(6)	3094(4)	6415(3)	42(2)
C(28)	6118(6)	3601(3)	6854(3)	36(1)
C(29)	7604(6)	3380(4)	7076(3)	51(2)
C(30)	8519(7)	3893(4)	7491(3)	53(2)
C(31)	7966(7)	4638(4)	7688(3)	58(2)
C(32)	6497(7)	4868(4)	7468(3)	56(2)
C(33)	5576(6)	4358(4)	7053(3)	47(2)
N(34)	8629(11)	-216(7)	9060(5)	136(4)
C(35)	9895(15)	-98(6)	9080(5)	101(4)
C(36)	11534(10)	73(6)	9131(4)	113(3)

Table 3. Bond lengths [Å] and angles [°] for **10c**.

N(1)-C(3)	1.391(7)
N(1)-C(2)	1.466(6)
N(1)-C(12)	1.485(6)
C(3)-C(8)	1.386(7)
C(3)-C(4)	1.403(7)
C(4)-C(5)	1.390(8)
C(5)-C(6)	1.364(8)
C(6)-C(7)	1.401(8)
C(7)-C(8)	1.371(7)
C(8)-C(9)	1.523(7)
C(9)-C(10)	1.523(7)
C(9)-C(11)	1.551(7)
C(9)-C(12)	1.571(7)
C(12)-C(13)	1.497(7)
C(12)-C(16)	1.526(7)
C(13)-C(14)	1.325(7)
C(14)-C(15)	1.473(8)
C(15)-C(16)	1.361(7)
C(15)-C(20)	1.477(7)
C(16)-O(17)	1.335(6)
O(17)-C(18)	1.414(6)
C(18)-C(19)	1.431(8)
C(20)-C(27)	1.334(7)
C(20)-C(21)	1.489(7)
C(21)-C(26)	1.384(7)
C(21)-C(22)	1.395(7)
C(22)-C(23)	1.378(7)
C(23)-C(24)	1.371(8)
C(24)-C(25)	1.374(9)
C(25)-C(26)	1.373(8)
C(27)-C(28)	1.471(7)
C(28)-C(29)	1.383(7)
C(28)-C(33)	1.390(7)
C(29)-C(30)	1.385(7)
C(30)-C(31)	1.375(8)
C(31)-C(32)	1.372(7)
C(32)-C(33)	1.385(7)
N(34)-C(35)	1.115(11)
C(35)-C(36)	1.448(12)
C(3)-N(1)-C(2)	119.3(5)
C(3)-N(1)-C(12)	107.7(4)
C(2)-N(1)-C(12)	119.1(5)
C(8)-C(3)-N(1)	110.7(5)
C(8)-C(3)-C(4)	120.8(5)
N(1)-C(3)-C(4)	128.5(5)
C(5)-C(4)-C(3)	117.2(6)
C(6)-C(5)-C(4)	122.1(6)
C(5)-C(6)-C(7)	120.1(6)
C(8)-C(7)-C(6)	118.9(6)
C(7)-C(8)-C(3)	120.8(5)
C(7)-C(8)-C(9)	130.2(5)
C(3)-C(8)-C(9)	108.9(5)
C(8)-C(9)-C(10)	114.8(5)
C(8)-C(9)-C(11)	108.3(4)
C(10)-C(9)-C(11)	109.0(5)
C(8)-C(9)-C(12)	100.6(4)
C(10)-C(9)-C(12)	113.1(4)
C(11)-C(9)-C(12)	110.8(5)
N(1)-C(12)-C(13)	113.5(5)
N(1)-C(12)-C(16)	110.5(4)
C(13)-C(12)-C(16)	102.2(5)
N(1)-C(12)-C(9)	101.9(4)
C(13)-C(12)-C(9)	115.6(5)
C(16)-C(12)-C(9)	113.5(5)
C(14)-C(13)-C(12)	108.8(5)
C(13)-C(14)-C(15)	112.6(5)
C(16)-C(15)-C(14)	105.7(5)
C(16)-C(15)-C(20)	131.6(5)
C(14)-C(15)-C(20)	122.7(5)

O(17)-C(16)-C(15)	132.6(5)
O(17)-C(16)-C(12)	116.7(5)
C(15)-C(16)-C(12)	110.6(5)
C(16)-O(17)-C(18)	120.1(4)
O(17)-C(18)-C(19)	109.6(6)
C(27)-C(20)-C(15)	120.2(5)
C(27)-C(20)-C(21)	125.9(5)
C(15)-C(20)-C(21)	113.8(5)
C(26)-C(21)-C(22)	118.1(6)
C(26)-C(21)-C(20)	120.5(5)
C(22)-C(21)-C(20)	121.1(5)
C(23)-C(22)-C(21)	119.7(6)
C(24)-C(23)-C(22)	121.2(6)
C(23)-C(24)-C(25)	119.6(6)
C(26)-C(25)-C(24)	119.6(7)
C(25)-C(26)-C(21)	121.7(7)
C(20)-C(27)-C(28)	130.9(5)
C(29)-C(28)-C(33)	118.0(5)
C(29)-C(28)-C(27)	124.6(5)
C(33)-C(28)-C(27)	117.4(5)
C(28)-C(29)-C(30)	121.0(6)
C(31)-C(30)-C(29)	120.5(6)
C(32)-C(31)-C(30)	119.1(6)
C(31)-C(32)-C(33)	120.7(6)
C(32)-C(33)-C(28)	120.7(5)
N(34)-C(35)-C(36)	177.8(12)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **10c**.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
N(1)	40(3)	48(3)	49(3)	-6(3)	0(2)	5(2)
C(2)	48(4)	69(5)	85(5)	-2(4)	-2(4)	16(4)
C(3)	40(3)	47(4)	42(4)	-1(3)	-6(3)	-4(3)
C(4)	48(4)	55(4)	48(4)	-4(3)	9(3)	4(3)
C(5)	54(4)	72(5)	52(4)	14(4)	2(3)	-10(4)
C(6)	50(4)	68(5)	57(4)	14(4)	-8(3)	-3(4)
C(7)	38(3)	60(5)	55(4)	-1(4)	-2(3)	6(3)
C(8)	34(3)	46(4)	37(3)	-3(3)	-4(3)	1(3)
C(9)	36(3)	51(4)	45(4)	-9(3)	4(3)	-2(3)
C(10)	56(4)	68(5)	52(4)	-13(4)	1(3)	3(3)
C(11)	54(4)	79(5)	59(4)	-1(4)	-3(3)	-14(4)
C(12)	41(3)	44(4)	41(4)	-1(3)	1(3)	-9(3)
C(13)	57(4)	47(4)	61(4)	6(4)	-6(3)	-16(3)
C(14)	64(4)	55(5)	46(4)	10(3)	-13(3)	-10(4)
C(15)	41(3)	42(4)	36(3)	2(3)	-3(3)	-8(3)
C(16)	40(3)	45(4)	43(4)	-4(3)	-5(3)	-8(3)
O(17)	43(2)	51(3)	52(3)	15(2)	-9(2)	-17(2)
C(18)	54(4)	80(5)	69(5)	18(4)	3(3)	-28(4)
C(19)	104(7)	212(12)	117(8)	89(8)	-22(6)	-76(7)
C(20)	40(3)	49(4)	41(4)	2(3)	-4(3)	-5(3)
C(21)	37(3)	34(4)	45(4)	-2(3)	-6(3)	-4(3)
C(22)	44(3)	43(4)	44(4)	0(3)	-5(3)	-4(3)
C(23)	46(4)	51(4)	64(4)	17(4)	-15(3)	-8(3)
C(24)	48(4)	43(5)	107(7)	-1(5)	-24(4)	8(3)
C(25)	71(5)	71(6)	88(6)	-25(5)	-8(4)	21(4)
C(26)	60(4)	66(5)	63(5)	-11(4)	-11(4)	18(4)
C(27)	41(3)	44(4)	39(3)	10(3)	-6(3)	-4(3)
C(28)	34(3)	42(4)	31(3)	1(3)	-2(3)	3(3)
C(29)	47(4)	45(4)	59(4)	4(3)	-7(3)	-1(3)
C(30)	51(4)	45(4)	60(4)	6(4)	-16(3)	4(3)
C(31)	56(4)	59(5)	56(4)	-6(4)	-13(3)	-3(4)
C(32)	54(4)	57(4)	57(4)	-16(4)	-2(3)	1(3)
C(33)	43(3)	56(4)	41(4)	-7(3)	-5(3)	5(3)
N(34)	131(7)	167(8)	112(7)	31(6)	26(6)	64(8)
C(35)	139(9)	104(8)	64(6)	19(5)	27(7)	71(9)
C(36)	119(8)	145(9)	77(6)	4(6)	23(6)	58(7)

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

	x	y	z	U(eq)
H(2A)	4574	765	3681	102
H(2B)	4684	664	4475	102
H(2C)	5181	1500	4149	102
H(4)	3639	1709	2825	60
H(5)	2306	2659	2126	71
H(6)	276	3391	2485	71
H(7)	-574	3160	3563	61
H(10A)	1062	3150	5033	88
H(10B)	211	2499	5465	88
H(10C)	-700	2946	4851	88
H(11A)	-1468	1626	4253	96
H(11B)	-786	1211	4930	96
H(11C)	-216	924	4229	96
H(13)	1662	497	5248	67
H(14)	3421	814	6194	67
H(18A)	6134	2766	4914	81
H(18B)	5473	3571	5238	81
H(19A)	5497	3328	3857	219
H(19B)	6778	3832	4286	219
H(19C)	5053	4151	4219	219
H(22)	5663	1902	7567	53
H(23)	7173	865	8053	66
H(24)	8543	0	7401	81
H(25)	8490	203	6245	93
H(26)	6961	1220	5749	76
H(27)	4223	3379	6206	50
H(29)	8000	2873	6944	61
H(30)	9524	3731	7638	64
H(31)	8586	4986	7970	69
H(32)	6112	5377	7599	67
H(33)	4574	4526	6905	56
H(36A)	11910	89	9602	170
H(36B)	11720	598	8923	170
H(36C)	12071	-354	8902	170

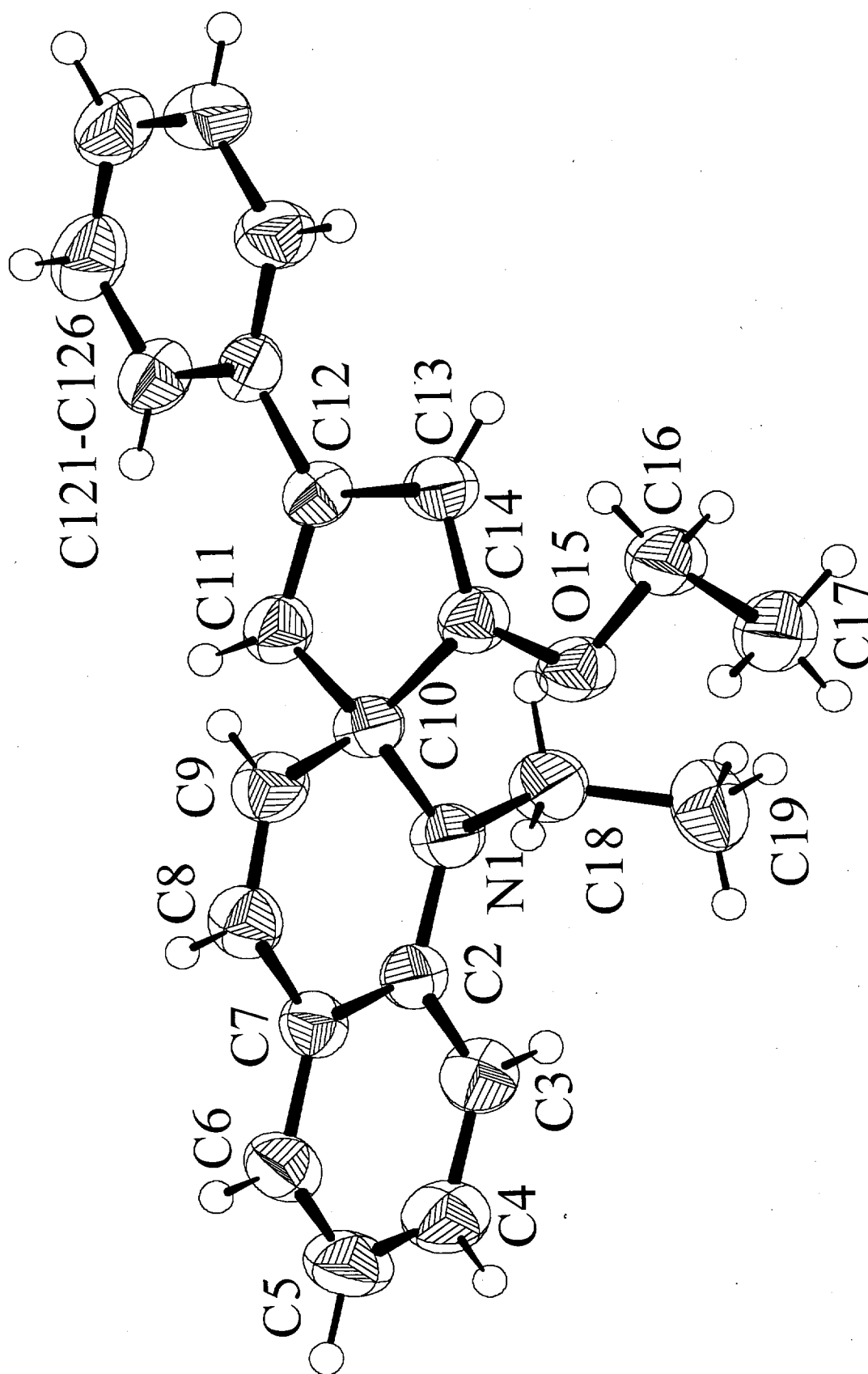


Table 1. Crystal data and structure refinement for **16b**.

Identification code	AUM1035
Empirical formula	C ₂₆ H ₂₆ N O
Formula weight	368.48
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, P2 ₁ /n (No.14)
Unit cell dimensions	a = 11.100(1) Å b = 16.841(1) Å β = 95.05(1)° c = 11.111(1) Å
Volume	2069.0(3) Å ³
Z, Calculated density	4, 1.183 Mg/m ³
Absorption coefficient	0.071 mm ⁻¹
F(000)	788
Crystal size	0.45 x 0.30 x 0.20 mm
Theta range for data collection	2.97 to 30.46°.
Index ranges	-11<=h<=13, -24<=k<=18, -15<=l<=10
Reflections collected / unique	12070 / 5834 [R(int) = 0.0345]
Completeness to 2theta = 30.46	89.9%
Max. and min. transmission	0.9859 and 0.9687
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5834 / 0 / 255.
Goodness-of-fit on F ²	0.999
Final R indices [I>2σ(I)]	R1 = 0.0566, wR ² = 0.1364
R indices (all data)	R1 = 0.0883, wR ² = 0.1595
Largest diff. peak and hole	0.222 and -0.234 eÅ ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **16b**.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(1)	5545(1)	2338(1)	7666(1)	46(1)
C(2)	5706(1)	2926(1)	8528(1)	39(1)
C(3)	4723(1)	3277(1)	9037(1)	50(1)
C(4)	4907(2)	3858(1)	9912(2)	60(1)
C(5)	6051(2)	4109(1)	10315(2)	62(1)
C(6)	7027(2)	3768(1)	9821(1)	52(1)
C(7)	6878(1)	3184(1)	8939(1)	42(1)
C(8)	7896(1)	2826(1)	8414(1)	49(1)
C(9)	7744(1)	2299(1)	7535(1)	50(1)
C(10)	6520(1)	2029(1)	6995(1)	43(1)
C(11)	6402(1)	2233(1)	5659(1)	45(1)
C(12)	6417(1)	1573(1)	4984(1)	42(1)
C(13)	6483(1)	873(1)	5784(1)	47(1)
C(14)	6512(1)	1121(1)	6929(1)	44(1)
O(15)	6575(1)	714(1)	7972(1)	50(1)
C(16)	6620(2)	-136(1)	7835(1)	54(1)
C(17)	6672(2)	-507(1)	9063(2)	64(1)
C(18)	4324(1)	2087(1)	7215(1)	53(1)
C(19)	3759(2)	1511(1)	8047(2)	69(1)
C(121)	6404(1)	1516(1)	3658(1)	41(1)
C(122)	6090(1)	2160(1)	2915(1)	51(1)
C(123)	6115(2)	2104(1)	1678(2)	60(1)
C(124)	6458(2)	1413(1)	1154(1)	62(1)
C(125)	6773(2)	771(1)	1870(2)	63(1)
C(126)	6737(2)	817(1)	3110(1)	53(1)
C(21)	9762(3)	392(3)	-1055(4)	128(1)
C(22)	9612(3)	753(2)	-18(6)	127(1)
C(23)	9848(3)	373(4)	1044(4)	132(1)

Table 3. Bond lengths [Å] and angles [°] for 16b.

N(1)-C(2)	1.3788(17)
N(1)-C(10)	1.4634(18)
N(1)-C(18)	1.4647(19)
C(2)-C(3)	1.4022(19)
C(2)-C(7)	1.408(2)
C(3)-C(4)	1.382(2)
C(4)-C(5)	1.375(3)
C(5)-C(6)	1.383(2)
C(6)-C(7)	1.388(2)
C(7)-C(8)	1.447(2)
C(8)-C(9)	1.320(2)
C(9)-C(10)	1.506(2)
C(10)-C(11)	1.5185(19)
C(10)-C(14)	1.530(2)
C(11)-C(12)	1.342(2)
C(12)-C(13)	1.4750(19)
C(12)-C(121)	1.4752(18)
C(13)-C(14)	1.3366(19)
C(14)-O(15)	1.3427(16)
O(15)-C(16)	1.4416(18)
C(16)-C(17)	1.497(2)
C(18)-C(19)	1.513(2)
C(121)-C(126)	1.389(2)
C(121)-C(122)	1.389(2)
C(122)-C(123)	1.380(2)
C(123)-C(124)	1.369(3)
C(124)-C(125)	1.370(3)
C(125)-C(126)	1.384(2)
C(21)-C(22)	1.327(5)
C(21)-C(23)#1	1.358(5)
C(22)-C(23)	1.348(5)
C(23)-C(21)#1	1.358(5)
C(2)-N(1)-C(10)	123.57(11)
C(2)-N(1)-C(18)	120.30(12)
C(10)-N(1)-C(18)	115.26(12)
N(1)-C(2)-C(3)	121.66(13)
N(1)-C(2)-C(7)	120.40(12)
C(3)-C(2)-C(7)	117.93(13)
C(4)-C(3)-C(2)	120.66(15)
C(5)-C(4)-C(3)	121.45(15)
C(4)-C(5)-C(6)	118.45(15)
C(5)-C(6)-C(7)	121.73(15)
C(6)-C(7)-C(2)	119.78(13)
C(6)-C(7)-C(8)	122.01(14)
C(2)-C(7)-C(8)	118.21(13)
C(9)-C(8)-C(7)	121.66(14)
C(8)-C(9)-C(10)	123.34(13)
N(1)-C(10)-C(9)	111.81(11)
N(1)-C(10)-C(11)	114.41(12)
C(9)-C(10)-C(11)	108.59(12)
N(1)-C(10)-C(14)	112.22(11)
C(9)-C(10)-C(14)	108.78(12)
C(11)-C(10)-C(14)	100.36(11)
C(12)-C(11)-C(10)	110.76(12)
C(11)-C(12)-C(13)	109.12(12)
C(11)-C(12)-C(121)	127.78(13)
C(13)-C(12)-C(121)	123.09(12)
C(14)-C(13)-C(12)	108.63(13)
C(13)-C(14)-O(15)	131.03(14)
C(13)-C(14)-C(10)	110.98(12)
O(15)-C(14)-C(10)	117.95(12)
C(14)-O(15)-C(16)	114.55(11)
O(15)-C(16)-C(17)	108.50(13)
N(1)-C(18)-C(19)	113.39(14)
C(126)-C(121)-C(122)	117.62(13)
C(126)-C(121)-C(12)	120.88(13)
C(122)-C(121)-C(12)	121.48(13)
C(123)-C(122)-C(121)	120.78(15)
C(124)-C(123)-C(122)	120.81(16)

C(123)-C(124)-C(125)	119.38(15)
C(124)-C(125)-C(126)	120.31(16)
C(125)-C(126)-C(121)	121.08(15)
C(22)-C(21)-C(23)#1	119.4(4)
C(21)-C(22)-C(23)	120.8(3)
C(22)-C(23)-C(21)#1	119.8(3)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **16b**.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
N(1)	38(1)	54(1)	45(1)	-10(1)	4(1)	-2(1)
C(2)	45(1)	35(1)	37(1)	4(1)	3(1)	5(1)
C(3)	47(1)	48(1)	56(1)	2(1)	6(1)	9(1)
C(4)	69(1)	47(1)	64(1)	-3(1)	15(1)	16(1)
C(5)	84(1)	42(1)	61(1)	-11(1)	8(1)	5(1)
C(6)	64(1)	40(1)	52(1)	-1(1)	0(1)	-4(1)
C(7)	48(1)	37(1)	41(1)	4(1)	2(1)	0(1)
C(8)	41(1)	52(1)	53(1)	-1(1)	1(1)	-2(1)
C(9)	42(1)	55(1)	54(1)	-4(1)	9(1)	4(1)
C(10)	46(1)	43(1)	39(1)	-3(1)	7(1)	1(1)
C(11)	51(1)	43(1)	43(1)	4(1)	8(1)	1(1)
C(12)	45(1)	45(1)	37(1)	2(1)	6(1)	1(1)
C(13)	60(1)	41(1)	40(1)	0(1)	6(1)	3(1)
C(14)	50(1)	44(1)	38(1)	2(1)	4(1)	2(1)
O(15)	68(1)	46(1)	35(1)	2(1)	5(1)	6(1)
C(16)	73(1)	45(1)	43(1)	1(1)	4(1)	2(1)
C(17)	89(1)	55(1)	49(1)	11(1)	8(1)	2(1)
C(18)	43(1)	66(1)	50(1)	-7(1)	1(1)	-6(1)
C(19)	55(1)	63(1)	89(1)	3(1)	8(1)	-10(1)
C(121)	38(1)	48(1)	37(1)	2(1)	5(1)	-3(1)
C(122)	54(1)	53(1)	46(1)	7(1)	11(1)	3(1)
C(123)	67(1)	69(1)	45(1)	16(1)	7(1)	-4(1)
C(124)	73(1)	78(1)	37(1)	1(1)	8(1)	-14(1)
C(125)	81(1)	64(1)	45(1)	-11(1)	11(1)	-5(1)
C(126)	67(1)	51(1)	42(1)	-1(1)	5(1)	1(1)
C(21)	85(2)	160(4)	138(3)	26(3)	6(2)	-11(2)
C(22)	76(2)	81(2)	223(4)	-17(3)	11(2)	0(1)
C(23)	81(2)	173(4)	143(3)	-72(3)	22(2)	-16(2)