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X-Ray Crystallography

Supplementary Material

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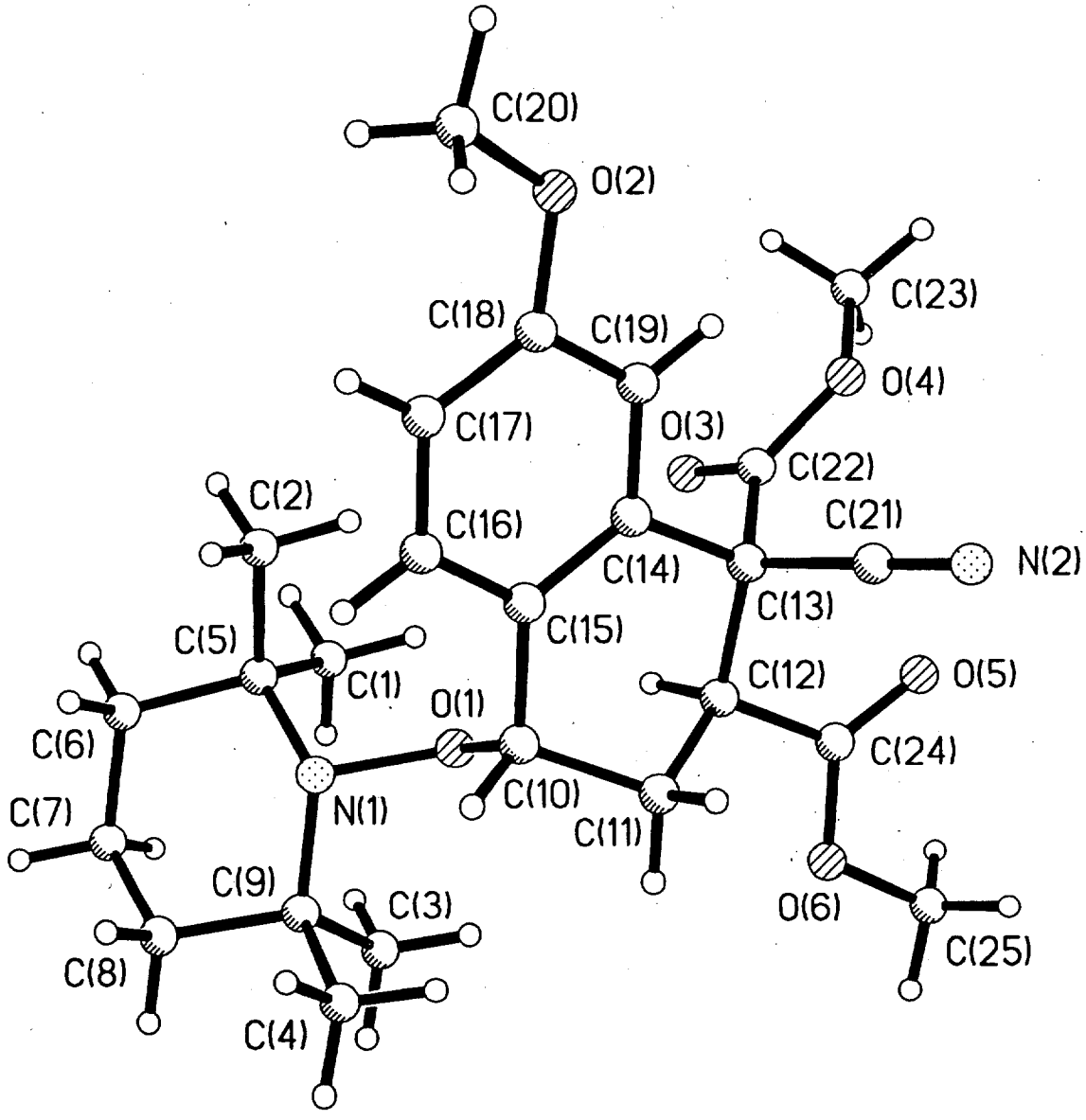

Table 1. Crystal data and structure refinement for 1.

Identification code	3lea	
Empirical formula	C25 H34 N2 O6	
Formula weight	458.54	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 8.3693(17) Å	α= 90°.
	b = 24.434(5) Å	β= 106.237(3)°.
	c = 12.512(3) Å	γ = 90°.
Volume	2456.7(9) $Å^3$	
Z	4	
Density (calculated)	1.240 Mg/m^3	
Absorption coefficient	0.088 mm^{-1}	
F(000)	984	
Crystal size	0.61 x 0.45 x 0.36 mm^3	
Theta range for data collection	2.38 to 26.40°.	
Index ranges	-10<=h<=8, -22<=k<=30, -10<=l<=15	
Reflections collected	17648	
Independent reflections	5025 [R(int) = 0.0428]	
Completeness to theta = 26.40°	99.6 %	
Max. and min. transmission	0.9689 and 0.9481	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5025 / 0 / 300	
Goodness-of-fit on F^2	1.009	
Final R indices [I>2sigma(I)]	R1 = 0.0442, wR2 = 0.1024	
R indices (all data)	R1 = 0.0777, wR2 = 0.1139	
Largest diff. peak and hole	0.246 and -0.215 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4664(1)	3948(1)	8493(1)	28(1)
O(2)	1114(2)	2019(1)	10456(1)	42(1)
O(3)	5133(2)	3886(1)	11838(1)	34(1)
O(4)	5780(1)	3109(1)	12813(1)	30(1)
O(5)	9064(2)	3579(1)	12112(1)	45(1)
O(6)	9604(2)	3910(1)	10593(1)	50(1)
N(1)	3451(2)	4138(1)	7482(1)	28(1)
N(2)	7851(2)	2242(1)	11627(1)	40(1)
C(1)	2942(2)	4872(1)	8813(2)	40(1)
C(2)	1128(2)	4053(1)	8292(2)	44(1)
C(3)	5757(2)	4829(1)	7456(2)	42(1)
C(4)	5303(3)	3989(1)	6304(2)	48(1)
C(5)	2197(2)	4463(1)	7874(2)	33(1)
C(6)	1058(2)	4756(1)	6862(2)	46(1)
C(7)	1993(3)	5098(1)	6228(2)	51(1)
C(8)	3169(3)	4722(1)	5847(2)	49(1)
C(9)	4428(2)	4428(1)	6810(2)	35(1)
C(10)	5047(2)	3368(1)	8497(1)	26(1)
C(11)	6857(2)	3334(1)	9189(1)	28(1)
C(12)	6949(2)	3525(1)	10369(1)	25(1)
C(13)	6049(2)	3124(1)	10956(1)	23(1)
C(14)	4400(2)	2913(1)	10155(1)	24(1)
C(15)	3960(2)	3023(1)	9010(1)	24(1)
C(16)	2493(2)	2790(1)	8349(1)	28(1)
C(17)	1498(2)	2452(1)	8784(1)	30(1)
C(18)	1966(2)	2348(1)	9918(1)	29(1)
C(19)	3407(2)	2580(1)	10598(1)	28(1)
C(20)	-265(2)	1722(1)	9797(2)	42(1)
C(21)	7095(2)	2633(1)	11358(1)	27(1)
C(22)	5627(2)	3422(1)	11923(1)	24(1)
C(23)	5323(2)	3372(1)	13728(1)	37(1)
C(24)	8649(2)	3661(1)	11127(2)	30(1)
C(25)	11243(3)	4070(1)	11277(2)	73(1)

Table 3. Bond lengths [Å] and angles [°] for 1.

O(1)-C(10)	1.4502(18)
O(1)-N(1)	1.4597(16)
O(2)-C(18)	1.3688(19)
O(2)-C(20)	1.417(2)
O(3)-C(22)	1.2029(18)
O(4)-C(22)	1.3265(19)
O(4)-C(23)	1.4544(19)
O(5)-C(24)	1.201(2)
O(6)-C(24)	1.324(2)
O(6)-C(25)	1.453(2)
N(1)-C(9)	1.504(2)
N(1)-C(5)	1.504(2)
N(2)-C(21)	1.143(2)
C(1)-C(5)	1.536(2)
C(2)-C(5)	1.530(2)
C(3)-C(9)	1.532(2)
C(4)-C(9)	1.532(3)
C(5)-C(6)	1.533(2)
C(6)-C(7)	1.512(3)
C(7)-C(8)	1.518(3)
C(8)-C(9)	1.539(3)
C(10)-C(15)	1.510(2)
C(10)-C(11)	1.523(2)
C(11)-C(12)	1.531(2)
C(12)-C(24)	1.510(2)
C(12)-C(13)	1.542(2)
C(13)-C(21)	1.486(2)
C(13)-C(22)	1.535(2)
C(13)-C(14)	1.550(2)
C(14)-C(19)	1.384(2)
C(14)-C(15)	1.401(2)
C(15)-C(16)	1.396(2)
C(16)-C(17)	1.387(2)
C(17)-C(18)	1.386(2)
C(18)-C(19)	1.388(2)

C(10)-O(1)-N(1)	114.41(11)
C(18)-O(2)-C(20)	117.79(13)
C(22)-O(4)-C(23)	114.97(13)
C(24)-O(6)-C(25)	115.47(15)
O(1)-N(1)-C(9)	106.22(12)
O(1)-N(1)-C(5)	105.38(11)
C(9)-N(1)-C(5)	118.13(12)
N(1)-C(5)-C(2)	107.07(13)
N(1)-C(5)-C(6)	107.86(15)
C(2)-C(5)-C(6)	107.48(15)
N(1)-C(5)-C(1)	114.97(14)
C(2)-C(5)-C(1)	108.46(15)
C(6)-C(5)-C(1)	110.71(15)
C(7)-C(6)-C(5)	113.43(16)
C(6)-C(7)-C(8)	107.81(16)
C(7)-C(8)-C(9)	113.51(16)
N(1)-C(9)-C(4)	107.35(13)
N(1)-C(9)-C(3)	115.78(14)
C(4)-C(9)-C(3)	107.80(16)
N(1)-C(9)-C(8)	107.26(15)
C(4)-C(9)-C(8)	107.73(16)
C(3)-C(9)-C(8)	110.62(15)
O(1)-C(10)-C(15)	112.84(12)
O(1)-C(10)-C(11)	103.87(12)
C(15)-C(10)-C(11)	110.42(13)
C(10)-C(11)-C(12)	107.75(13)
C(24)-C(12)-C(11)	117.20(13)
C(24)-C(12)-C(13)	109.95(13)
C(11)-C(12)-C(13)	111.43(13)
C(21)-C(13)-C(22)	111.04(13)
C(21)-C(13)-C(12)	110.77(13)
C(22)-C(13)-C(12)	108.85(12)
C(21)-C(13)-C(14)	106.58(12)
C(22)-C(13)-C(14)	107.92(12)
C(12)-C(13)-C(14)	111.63(13)
C(19)-C(14)-C(15)	120.45(14)
C(19)-C(14)-C(13)	117.50(14)
C(15)-C(14)-C(13)	121.94(13)
C(16)-C(15)-C(14)	117.57(14)

C(16)-C(15)-C(10)	120.73(14)
C(14)-C(15)-C(10)	121.68(14)
C(17)-C(16)-C(15)	122.42(15)
C(18)-C(17)-C(16)	118.80(15)
O(2)-C(18)-C(17)	125.04(15)
O(2)-C(18)-C(19)	114.90(14)
C(17)-C(18)-C(19)	120.06(15)
C(14)-C(19)-C(18)	120.70(15)
N(2)-C(21)-C(13)	176.72(18)
O(3)-C(22)-O(4)	124.59(15)
O(3)-C(22)-C(13)	121.83(14)
O(4)-C(22)-C(13)	113.49(13)
O(5)-C(24)-O(6)	123.57(16)
O(5)-C(24)-C(12)	123.98(15)
O(6)-C(24)-C(12)	112.35(14)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	37(1)	25(1)	20(1)	2(1)	2(1)	0(1)
O(2)	38(1)	58(1)	28(1)	-1(1)	6(1)	-24(1)
O(3)	41(1)	27(1)	36(1)	-1(1)	14(1)	4(1)
O(4)	40(1)	30(1)	22(1)	0(1)	11(1)	0(1)
O(5)	39(1)	60(1)	31(1)	8(1)	-1(1)	-15(1)
O(6)	31(1)	83(1)	37(1)	0(1)	10(1)	-21(1)
N(1)	34(1)	27(1)	20(1)	5(1)	3(1)	-1(1)
N(2)	42(1)	33(1)	43(1)	2(1)	8(1)	6(1)
C(1)	48(1)	34(1)	39(1)	-4(1)	13(1)	6(1)
C(2)	40(1)	39(1)	56(1)	5(1)	21(1)	2(1)
C(3)	45(1)	31(1)	54(1)	2(1)	21(1)	-7(1)
C(4)	82(2)	36(1)	40(1)	1(1)	39(1)	-4(1)
C(5)	35(1)	30(1)	34(1)	4(1)	7(1)	1(1)
C(6)	42(1)	39(1)	48(1)	7(1)	-3(1)	3(1)
C(7)	59(1)	39(1)	43(1)	16(1)	-4(1)	3(1)
C(8)	74(2)	43(1)	29(1)	11(1)	10(1)	-8(1)
C(9)	50(1)	28(1)	29(1)	4(1)	16(1)	-5(1)
C(10)	36(1)	23(1)	21(1)	0(1)	9(1)	0(1)
C(11)	30(1)	30(1)	27(1)	3(1)	11(1)	1(1)
C(12)	25(1)	26(1)	25(1)	2(1)	7(1)	0(1)
C(13)	24(1)	22(1)	22(1)	0(1)	5(1)	1(1)
C(14)	25(1)	23(1)	22(1)	0(1)	5(1)	2(1)
C(15)	28(1)	23(1)	22(1)	0(1)	5(1)	2(1)
C(16)	33(1)	29(1)	20(1)	0(1)	3(1)	1(1)
C(17)	27(1)	32(1)	27(1)	-4(1)	2(1)	-3(1)
C(18)	30(1)	31(1)	27(1)	0(1)	8(1)	-5(1)
C(19)	30(1)	32(1)	20(1)	1(1)	4(1)	-2(1)
C(20)	37(1)	50(1)	37(1)	-4(1)	7(1)	-19(1)
C(21)	28(1)	28(1)	24(1)	-3(1)	6(1)	-2(1)
C(22)	21(1)	26(1)	23(1)	0(1)	4(1)	-4(1)
C(23)	49(1)	40(1)	26(1)	-6(1)	17(1)	-3(1)
C(24)	27(1)	31(1)	31(1)	2(1)	9(1)	0(1)
C(25)	33(1)	131(2)	53(2)	-6(2)	10(1)	-37(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 1.

	x	y	z	U(eq)
H(1A)	3665	4677	9451	60
H(1B)	2043	5053	9039	60
H(1C)	3595	5147	8548	60
H(2A)	641	3788	7701	65
H(2B)	235	4248	8499	65
H(2C)	1821	3859	8943	65
H(3A)	6547	4635	8065	62
H(3B)	5224	5124	7763	62
H(3C)	6350	4985	6954	62
H(4A)	6115	3795	6901	72
H(4B)	5877	4163	5809	72
H(4C)	4477	3729	5878	72
H(6A)	385	4479	6351	55
H(6B)	281	4996	7115	55
H(7A)	2629	5390	6714	61
H(7B)	1203	5272	5577	61
H(8A)	3785	4939	5424	59
H(8B)	2506	4444	5336	59
H(10A)	4940	3242	7720	31
H(11A)	7560	3570	8862	34
H(11B)	7262	2952	9204	34
H(12A)	6297	3874	10279	30
H(16A)	2165	2865	7574	34
H(17A)	514	2295	8312	35
H(19A)	3716	2510	11375	33
H(20A)	-758	1505	10282	63
H(20B)	107	1478	9293	63
H(20C)	-1096	1978	9361	63
H(23A)	5556	3123	14367	56
H(23B)	4134	3461	13496	56
H(23C)	5971	3709	13937	56
H(25A)	11814	4280	10826	109
H(25B)	11893	3742	11569	109
H(25C)	11128	4296	11898	109