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X-Ray Crystallographic data for (+)-77

Structure Description:

The crystal and molecular structures and absolute configuration of the (D)-*threo*- 2-amino-1-(4-nitrophenyl)propane-1,3-diol salt of (+)-**77** have been determined from three-dimensional X-ray diffraction data collected at reduced temperature. Figure 1 displays an ORTEPII drawing of the (D)-threo-2-amino-1-(4-nitrophenyl)-1,3-propanediol salt of (+)-**77** showing the absolute stereochemistry. The view shown is of that orientation of the dichlorophenyl ring in which the chlorine atom has an occupancy of 60%. The configuration was found to be 3(S), 5(R).

There is an extensive array of hydrogen bonds in the structure with all possible donors participating. An intramolecular hydrogen bond from the hydroxyl at C3 to the ionized carboxylate oxygen O4 is observed. All other interactions are intermolecular in nature, including a bifurcated contact for one of the amino hydrogens. Metrical details are:

Donor ----H---Acceptor	D...A (Å)	H...A (Å)	D - H...A(°)
O3---H3---O4	2.660(4)	1.95	144
O23---H23---O2	3.074(5)	2.24	180
O24---H24---O4	2.813(4)	2.00	165
N1---H22A---O4	2.859(4)	1.99	163
N1---H22A---O5	3.094(5)	2.38	136
N1---H22B---O5	2.770(5)	1.88	169
N1---H22C---O5	3.062(4)	2.29	143

Experimental

The sample was recrystallized by slow evaporation from a mixture of ethanol and isopropanol to obtain crystals suitable for study. Lattice parameters were determined from the setting angles of 25 reflections well distributed in reciprocal space measured on an Enraf Nonius CAD-4 diffractometer. Intensity data were collected on the diffractometer using graphite monochromated copper radiation and an ω–2θ variable speed scan technique. Three orientation controls were monitored to assess any crystal movement during the experiment. The intensities of three standard reflections measured at the beginning, end and every three hours of exposure time showed a maximum variation of 10% over the course of the experiment. Data were corrected for this variation and for Lorentz and polarization effects. A semiempirical correction was made for absorption. Equivalent reflections, but not Friedel opposites, were averaged, R_{int} = 0.03. Crystal data and refinement details are presented in Table 1.

The structure was solved by direct methods using the SHELXS program series and refined using the SHELXL-93 refinement program. Atomic positions were initially refined with isotropic temperature factors and subsequently with anisotropic displacement parameters. The dichlorophenyl ring was found to be disordered in a static way. A two-fold rotation about a vector defined by atoms C12, C15 and chlorine 2 results in two positions for chlorine atom 1, which were modeled with site occupancy factors of 65 and 35 percent. The function minimized in least-squares refinement was $\Sigma w(F_o^2 - F_c^2)^2$. Weights, w, were eventually assigned to the data as $w = 1/[\sigma^2(F_o^2) + (0.1177P)^2]$ where $P = [MAX(F_o^2,0) + 2F_c^2]/3$. Positional parameters for hydrogen atoms attached to heteroatoms were refined under constraints. Hydrogen atoms attached to carbon were included in the final model in calculated positions based on geometrical considerations with isotropic displacement factors assigned as $1.2(U_{eq})$ of the attached atom ($1.4(U_{eq})$ for amino, hydroxyl and methyl hydrogens). The full-matrix least-squares refinement (on F^2) converged (max $\Delta/\sigma = 0.005$) to values of the conventional crystallographic residuals R = 0.062 for observed data and R = 0.074 (wR2 = 0.170) for all data. A final difference

Fourier map was featureless with residual density between ±0.26 eÅ^{-3}. Values of the neutral atom scattering factors were taken from the International Tables for X-ray Crystallography.

The absolute stereochemistry of (+)-**77** was assigned based on Flack's absolute structure parameter which refined to a value of 0.05(5) for the correct antipode and of 0.93(5) for the inverted model. A purely statistical measure of the probability for correct absolute configuration assignment using a ratio of crystallographic residuals also was applied. The weighted R-factor ratio was 1.056 which allows for assignment of the configuration at the 99.5% confidence level. The configuration of the cation also is consistent with its known (R), (R) stereochemistry.

Table 1. Crystal and structure refinement data

Empirical formula	$[C_{18}H_{21}Cl_2O_5]^-$ $[C_9H_{13}NO_4]^+$
Formula weight	601.46
Temperature	223(2) K
Wavelength	1.54178 Å
Crystal size	0.01 x 0.2 x 0.5 mm
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 9.920(2) Å
	b = 5.321(1) Å β = 96.43(3)°
	c = 28.038(8) Å
Volume	1470.7(6) $Å^3$
Z	2
Density (calculated)	1.358 Mg/m^3
Absorption coefficient	2.449 mm^{-1}
Transmission coefficients	1.000 max, 0.832 min
F(000)	632
θ range for data collection	3.17 to 59.92°
Index ranges	$-11 \le h \le 10$, $-5 \le k \le 5$, $0 \le l \le 31$
Reflections collected	3671
Independent reflections	3638 (R_{int} = 0.0296)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3638 / 1 / 374
Goodness-of-fit on F^2	1.068
Final R indices [$I>2\sigma(I)$]	R1 = 0.0617, wR2 = 0.1577
R indices (all data)	R1 = 0.0743, wR2 = 0.1700
Absolute structure parameter	0.05(5)
Largest diff. peak and hole	0.261 and -0.237 $Å^{-3}$

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

	x/a	y/b	z/c	U(eq)
Cl(1)	14168(5)	11763(12)	5794(1)	154(2)
Cl(11)	10858(8)	5513(16)	5141(2)	137(3)
Cl(2)	13279(3)	11089(10)	3904(1)	171(2)
O(1)	8818(3)	8814(6)	8204(1)	45(1)
O(2)	9298(3)	8178(6)	8985(1)	40(1)
O(3)	6250(3)	8780(7)	8676(1)	48(1)
O(4)	6854(3)	8813(6)	9625(1)	44(1)
O(5)	8553(3)	11332(6)	9898(1)	47(1)
C(2)	8588(4)	9145(8)	8657(1)	36(1)
C(3)	7286(4)	10647(8)	8686(1)	36(1)
C(4)	7148(5)	11978(11)	8204(2)	51(1)
C(5)	7752(5)	10096(11)	7878(2)	51(1)
C(6)	8389(5)	11168(12)	7460(2)	58(1)
C(7)	9165(6)	9200(12)	7199(2)	66(2)
C(8)	9701(6)	10225(14)	6755(2)	72(2)
C(9)	10694(7)	8465(15)	6543(2)	81(2)
C(10)	11137(8)	9438(17)	6074(2)	92(2)
C(11)	12266(11)	7856(24)	5900(3)	135(4)
C(12)	12523(10)	8643(23)	5392(3)	112(3)
C(13)	13382(9)	10567(24)	5307(3)	114(3)
C(14)	13614(9)	11287(23)	4855(3)	114(3)
C(15)	12948(10)	10110(26)	4470(3)	121(4)
C(16)	12104(13)	8262(29)	4544(3)	150(5)
C(17)	11914(13)	7563(29)	4994(4)	159(5)
C(18)	7329(4)	12275(8)	9134(1)	37(1)
C(19)	7602(4)	10710(8)	9587(1)	36(1)
O(21)	5133(6)	5973(17)	7192(2)	135(3)
O(22)	3722(7)	3302(18)	6866(2)	147(3)
O(23)	334(3)	3568(6)	8873(1)	45(1)
O(24)	4013(3)	-1278(7)	9604(1)	54(1)
N(21)	4179(6)	4569(14)	7202(2)	87(2)
N(22)	1490(3)	997(7)	9665(1)	38(1)
C(20)	1983(5)	2283(11)	8106(2)	55(1)
C(21)	2573(6)	2523(13)	7686(2)	69(2)
C(22)	3552(5)	4318(11)	7651(2)	54(1)
C(23)	3980(5)	5843(11)	8025(2)	52(1)
C(24)	3405(4)	5590(9)	8447(2)	45(1)
C(25)	2406(4)	3830(9)	8495(1)	39(1)
C(26)	1771(4)	3578(9)	8958(1)	37(1)
C(27)	2182(4)	1142(8)	9222(1)	35(1)
C(28)	3711(4)	973(9)	9348(1)	39(1)

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

Cl(1)-C(13)	1.625(10)	Cl(11)-C(17)	1.598(13)
Cl(2)-C(15)	1.737(8)	O(1)-C(2)	1.328(5)
O(1)-C(5)	1.484(5)	O(2)-C(2)	1.209(5)
O(3)-C(3)	1.427(5)	O(4)-C(19)	1.264(5)
O(5)-C(19)	1.256(5)	C(2)-C(3)	1.528(6)
C(3)-C(4)	1.519(6)	C(3)-C(18)	1.522(6)
C(4)-C(5)	1.524(7)	C(5)-C(6)	1.504(7)
C(6)-C(7)	1.533(8)	C(7)-C(8)	1.509(7)
C(8)-C(9)	1.528(9)	C(9)-C(10)	1.523(8)
C(10)-C(11)	1.524(11)	C(11)-C(12)	1.532(10)
C(12)-C(17)	1.34(2)	C(12)-C(13)	1.37(2)
C(13)-C(14)	1.367(11)	C(14)-C(15)	1.354(14)
C(15)-C(16)	1.32(2)	C(16)-C(17)	1.348(13)
C(18)-C(19)	1.516(6)	O(21)-N(21)	1.209(8)
O(22)-N(21)	1.204(8)	O(23)-C(26)	1.419(5)
O(24)-C(28)	1.411(6)	N(21)-C(22)	1.470(6)
N(22)-C(27)	1.486(5)	C(20)-C(21)	1.378(7)
C(20)-C(25)	1.394(7)	C(21)-C(22)	1.373(8)
C(22)-C(23)	1.358(7)	C(23)-C(24)	1.375(6)
C(24)-C(25)	1.382(6)	C(25)-C(26)	1.510(5)
C(26)-C(27)	1.526(6)	C(27)-C(28)	1.521(5)

Table 3.(cont.)

C(2)-O(1)-C(5)	110.0(3)	O(2)-C(2)-O(1)	121.6(4)
O(2)-C(2)-C(3)	127.3(3)	O(1)-C(2)-C(3)	110.9(3)
O(3)-C(3)-C(4)	108.3(3)	O(3)-C(3)-C(18)	111.4(3)
C(4)-C(3)-C(18)	117.4(4)	O(3)-C(3)-C(2)	104.2(3)
C(4)-C(3)-C(2)	100.9(3)	C(18)-C(3)-C(2)	113.3(3)
C(3)-C(4)-C(5)	103.1(4)	O(1)-C(5)-C(6)	108.8(4)
O(1)-C(5)-C(4)	103.4(3)	C(6)-C(5)-C(4)	116.5(5)
C(5)-C(6)-C(7)	112.9(5)	C(8)-C(7)-C(6)	112.9(5)
C(7)-C(8)-C(9)	113.7(6)	C(10)-C(9)-C(8)	112.9(6)
C(9)-C(10)-C(11)	112.5(7)	C(10)-C(11)-C(12)	110.6(8)
C(17)-C(12)-C(13)	114.0(8)	C(17)-C(12)-C(11)	123.5(11)
C(13)-C(12)-C(11)	122.5(10)	C(14)-C(13)-C(12)	122.9(10)
C(14)-C(13)-Cl(1)	123.7(10)	C(12)-C(13)-Cl(1)	113.3(7)
C(15)-C(14)-C(13)	119.4(10)	C(16)-C(15)-C(14)	118.7(8)
C(16)-C(15)-Cl(2)	123.6(9)	C(14)-C(15)-Cl(2)	117.7(9)
C(15)-C(16)-C(17)	120.6(11)	C(12)-C(17)-C(16)	124.4(12)
C(12)-C(17)-Cl(11)	109.0(8)	C(16)-C(17)-Cl(11)	126.4(10)
C(19)-C(18)-C(3)	111.3(3)	O(5)-C(19)-O(4)	123.6(4)
O(5)-C(19)-C(18)	119.1(4)	O(4)-C(19)-C(18)	117.3(3)
O(22)-N(21)-O(21)	123.7(6)	O(22)-N(21)-C(22)	117.3(6)
O(21)-N(21)-C(22)	119.0(5)	C(21)-C(20)-C(25)	119.7(5)
C(22)-C(21)-C(20)	119.8(5)	C(23)-C(22)-C(21)	121.5(4)
C(23)-C(22)-N(21)	118.8(5)	C(21)-C(22)-N(21)	119.7(5)
C(22)-C(23)-C(24)	118.9(5)	C(23)-C(24)-C(25)	121.4(4)
C(24)-C(25)-C(20)	118.7(4)	C(24)-C(25)-C(26)	121.1(4)
C(20)-C(25)-C(26)	120.2(4)	O(23)-C(26)-C(25)	111.4(3)
O(23)-C(26)-C(27)	106.6(3)	C(25)-C(26)-C(27)	112.3(3)
N(22)-C(27)-C(28)	110.2(3)	N(22)-C(27)-C(26)	109.1(3)
C(28)-C(27)-C(26)	111.6(3)	O(24)-C(28)-C(27)	108.5(3)

Table 4. Torsion angles [°].

C(5)-O(1)-C(2)-O(2)	176.9(4)	C(5)-O(1)-C(2)-C(3)	1.9(5)
O(2)-C(2)-C(3)-O(3)	-84.6(5)	O(1)-C(2)-C(3)-O(3)	90.1(4)
O(2)-C(2)-C(3)-C(4)	163.2(4)	O(1)-C(2)-C(3)-C(4)	-22.2(5)
O(2)-C(2)-C(3)-C(18)	36.8(6)	O(1)-C(2)-C(3)-C(18)	-148.6(3)
O(3)-C(3)-C(4)-C(5)	-76.9(4)	C(18)-C(3)-C(4)-C(5)	155.8(4)
C(2)-C(3)-C(4)-C(5)	32.2(5)	C(2)-O(1)-C(5)-C(6)	143.7(4)
C(2)-O(1)-C(5)-C(4)	19.3(5)	C(3)-C(4)-C(5)-O(1)	-32.1(5)
C(3)-C(4)-C(5)-C(6)	-151.4(4)	O(1)-C(5)-C(6)-C(7)	54.5(5)
C(4)-C(5)-C(6)-C(7)	170.8(4)	C(5)-C(6)-C(7)-C(8)	175.0(4)
C(6)-C(7)-C(8)-C(9)	169.2(5)	C(7)-C(8)-C(9)-C(10)	175.5(6)
C(8)-C(9)-C(10)-C(11)	172.4(8)	C(9)-C(10)-C(11)-C(12)	171.1(8)
C(10)-C(11)-C(12)-C(17)	-92(2)	C(10)-C(11)-C(12)-C(13)	86.2(12)
C(17)-C(12)-C(13)-C(14)	-1(2)	C(11)-C(12)-C(13)-C(14)	-179.8(9)
C(17)-C(12)-C(13)-Cl(1)	-177.1(10)	C(11)-C(12)-C(13)-Cl(1)	4.2(12)
C(12)-C(13)-C(14)-C(15)	2(2)	Cl(1)-C(13)-C(14)-C(15)	177.4(9)
C(13)-C(14)-C(15)-C(16)	-1(2)	C(13)-C(14)-C(15)-Cl(2)	-179.9(8)
C(14)-C(15)-C(16)-C(17)	0(2)	Cl(2)-C(15)-C(16)-C(17)	178.6(11)
C(13)-C(12)-C(17)-C(16)	0(2)	C(11)-C(12)-C(17)-C(16)	178.5(13)
C(13)-C(12)-C(17)-Cl(11)	-175.5(8)	C(11)-C(12)-C(17)-Cl(11)	3(2)
C(15)-C(16)-C(17)-C(12)	1(2)	C(15)-C(16)-C(17)-Cl(11)	175.3(12)
O(3)-C(3)-C(18)-C(19)	59.6(4)	C(4)-C(3)-C(18)-C(19)	-174.6(4)
C(2)-C(3)-C(18)-C(19)	-57.6(5)	C(3)-C(18)-C(19)-O(5)	127.6(4)
C(3)-C(18)-C(19)-O(4)	-51.7(5)	C(25)-C(20)-C(21)-C(22)	-1.4(9)
C(20)-C(21)-C(22)-C(23)	1.5(9)	C(20)-C(21)-C(22)-N(21)	-180.0(6)
O(22)-N(21)-C(22)-C(23)	-175.5(7)	O(21)-N(21)-C(22)-C(23)	6.2(9)
O(22)-N(21)-C(22)-C(21)	5.9(10)	O(21)-N(21)-C(22)-C(21)	-172.5(8)
C(21)-C(22)-C(23)-C(24)	-0.7(8)	N(21)-C(22)-C(23)-C(24)	-179.3(5)
C(22)-C(23)-C(24)-C(25)	-0.2(7)	C(23)-C(24)-C(25)-C(20)	0.2(7)
C(23)-C(24)-C(25)-C(26)	-179.5(4)	C(21)-C(20)-C(25)-C(24)	0.6(8)
C(21)-C(20)-C(25)-C(26)	-179.7(5)	C(24)-C(25)-C(26)-O(23)	130.4(4)
C(20)-C(25)-C(26)-O(23)	-49.3(6)	C(24)-C(25)-C(26)-C(27)	-110.1(5)
C(20)-C(25)-C(26)-C(27)	70.2(5)	O(23)-C(26)-C(27)-N(22)	-56.2(4)
C(25)-C(26)-C(27)-N(22)	-178.4(3)	O(23)-C(26)-C(27)-C(28)	-178.2(3)
C(25)-C(26)-C(27)-C(28)	59.5(4)	N(22)-C(27)-C(28)-O(24)	56.8(4)
C(26)-C(27)-C(28)-O(24)	178.2(3)		

Table 5. Anisotropic displacement parameters [$Å^2$ x 10^3].
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U_{11}	U_{33}	U_{33}	U_{13}	U_{23}	U_{12}
Cl(1)	133(3)	248(6)	84(2)	-30(3)	27(2)	-49(4)
Cl(11)	171(7)	162(7)	80(3)	-23(4)	18(3)	-88(6)
Cl(2)	152(2)	289(5)	80(1)	51(2)	45(1)	17(3)
O(1)	41(2)	54(2)	41(2)	0(1)	9(1)	5(2)
O(2)	30(2)	41(2)	48(2)	3(1)	1(1)	8(1)
O(3)	29(2)	63(2)	53(2)	-6(2)	4(1)	-11(2)
O(4)	31(2)	51(2)	51(2)	11(1)	10(1)	1(1)
O(5)	33(2)	59(2)	48(2)	-7(1)	1(1)	7(2)
C(2)	30(2)	37(2)	42(2)	-4(2)	6(2)	-3(2)
C(3)	21(2)	43(2)	45(2)	4(2)	3(2)	-1(2)
C(4)	37(3)	64(3)	52(2)	8(2)	3(2)	14(2)
C(5)	39(3)	67(3)	45(2)	6(2)	-2(2)	4(2)
C(6)	54(3)	74(3)	45(2)	5(2)	3(2)	1(3)
C(7)	78(4)	77(4)	44(2)	-2(2)	12(2)	-12(3)
C(8)	74(4)	93(4)	50(3)	3(3)	16(2)	5(3)
C(9)	96(5)	92(5)	59(3)	0(3)	22(3)	-2(4)
C(10)	95(5)	124(6)	63(3)	12(3)	36(3)	18(4)
C(11)	147(8)	172(10)	100(6)	35(6)	68(6)	49(8)
C(12)	124(7)	140(8)	84(5)	14(5)	61(5)	23(6)
C(13)	103(6)	170(10)	73(4)	-1(5)	34(4)	24(7)
C(14)	99(6)	156(9)	96(5)	18(6)	46(4)	-9(6)
C(15)	113(7)	190(11)	65(4)	12(5)	24(4)	20(7)
C(16)	157(10)	207(13)	95(6)	-17(7)	55(6)	-65(10)
C(17)	177(11)	216(14)	95(6)	-17(7)	68(7)	-59(10)
C(18)	24(2)	38(2)	50(2)	2(2)	8(2)	3(2)
C(19)	26(2)	41(2)	43(2)	0(2)	8(2)	5(2)
O(21)	117(4)	223(8)	72(3)	-1(4)	39(3)	-78(5)
O(22)	166(6)	221(8)	61(3)	-30(4)	37(3)	-68(6)
O(23)	27(1)	47(2)	61(2)	2(1)	5(1)	3(1)
O(24)	28(2)	71(2)	62(2)	17(2)	4(1)	5(2)
N(21)	76(3)	144(6)	44(2)	-4(3)	8(2)	-21(4)
N(22)	26(2)	45(2)	45(2)	-4(2)	6(1)	-5(2)
C(20)	46(3)	72(3)	47(2)	-8(2)	3(2)	-18(2)
C(21)	60(3)	101(5)	46(3)	-15(3)	-1(2)	-19(3)
C(22)	41(3)	78(4)	45(2)	3(2)	6(2)	-7(3)
C(23)	39(2)	65(3)	54(3)	8(2)	5(2)	-5(2)
C(24)	38(2)	50(3)	49(2)	-3(2)	8(2)	-7(2)
C(25)	26(2)	45(2)	45(2)	3(2)	3(1)	1(2)
C(26)	24(2)	41(2)	47(2)	-2(2)	6(1)	-2(2)
C(27)	22(2)	41(2)	42(2)	-1(2)	5(1)	-3(2)
C(28)	25(2)	51(3)	42(2)	1(2)	4(1)	-1(2)

Table 6. Hydrogen atom coordinates (x 10^4) and isotropic temperature factors ($Å^2$ x 10^3).

	x/a	y/b	z/c	U(eq)
H(3)	6205(41)	8248(81)	8952(3)	67
H(4A)	7656(5)	13561(11)	8222(2)	61
H(4B)	6195(5)	12324(11)	8092(2)	61
H(5A)	7048(5)	8860(11)	7758(2)	61
H(6A)	9014(5)	12519(12)	7575(2)	69
H(6B)	7677(5)	11905(12)	7232(2)	69
H(7A)	9927(6)	8571(12)	7420(2)	79
H(7B)	8562(6)	7779(12)	7109(2)	79
H(8A)	10155(6)	11830(14)	6835(2)	86
H(8B)	8934(6)	10556(14)	6512(2)	86
H(9A)	11498(7)	8243(15)	6776(2)	97
H(9B)	10267(7)	6816(15)	6486(2)	97
H(10A)	11453(8)	11176(17)	6119(2)	111
H(10B)	10355(8)	9441(17)	5827(2)	111
H(11A)	12011(11)	6077(24)	5900(3)	162
H(11B)	13100(11)	8069(24)	6119(3)	162
H(13A)	13810(9)	11484(24)	5568(3)	136
H(14A)	14230(9)	12587(23)	4812(3)	137
H(16A)	11632(13)	7429(29)	4281(3)	180
H(17A)	11281(13)	6283(29)	5032(4)	191
H(18A)	8043(4)	13545(8)	9128(1)	44
H(18B)	6461(4)	13151(8)	9136(1)	44
H(23)	54(3)	2113(93)	8904(12)	63
H(24)	4844(7)	-1526(59)	9631(19)	75
H(22A)	1871(22)	2105(43)	9883(4)	54
H(22B)	1575(28)	-566(18)	9787(6)	54
H(22C)	605(8)	1364(59)	9594(2)	54
H(20A)	1298(5)	1083(11)	8129(2)	66
H(21A)	2306(6)	1461(13)	7424(2)	83
H(23A)	4657(5)	7052(11)	7997(2)	63
H(24A)	3699(4)	6638(9)	8708(2)	55
H(26A)	2061(4)	5017(9)	9168(1)	45
H(27A)	1880(4)	-293(8)	9012(1)	42
H(28A)	4161(4)	985(9)	9054(1)	47
H(28B)	4037(4)	2419(9)	9545(1)	47

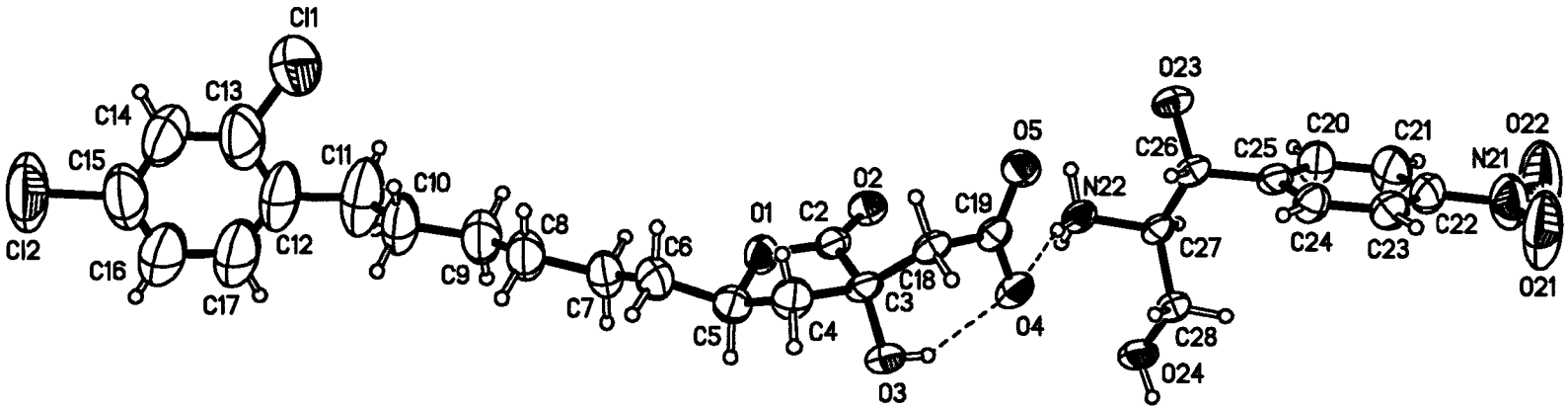

Figure 1. A view of (+)-**77** from its crystal structure showing the numbering scheme employed. Anisotropic displacement ellipsoids for non-hydrogen atoms are shown at the 50% probability level. Hydrogen atoms are displayed with an arbitrarily small radius. Several hydrogen bonds are shown as dashed lines. The view shown is of that orientation of the dichlorophenyl ring in which the chlorine atom has an occupancy of 60%.