contribute substantially to this crowding (see also Fig. 3).

Most bond lengths and angles (except those involving the disordered atoms) fall within normal ranges. The C(1)—C(2)—C(3) angle at 99·6 (3)° is somewhat compressed relative to the other four C—C—C angles in the cyclopentane ring, which average 105·5 (6)°.

Nucleophilic displacement of a methylsulfonate group requires that the incoming nucleophile approach from the back side of the CH_2 group, *i.e.* at 180° from the breaking C—O bond. In each case save one (assuming that the crystal structure represents a locus of solution conformations), this requires that the trajectory of the nucleophile take it directly past an adjacent $CH_2OSO_2CH_3$ group. The steric crowding introduced in this manner greatly decreases the rate of nucleophilic attack, and abstraction of a ring proton competes successfully.

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Structure of 2-Amino-2,6-dideoxy-α-D-glucopyranose-6-sulfonic Acid

BY R. VEGA, A. LÓPEZ-CASTRO AND R. MÁRQUEZ

Dpto de Optica y Sección de Física del Dpto de Investigaciones Físicas Químicas del CSIC, Universidad de Sevilla, Spain

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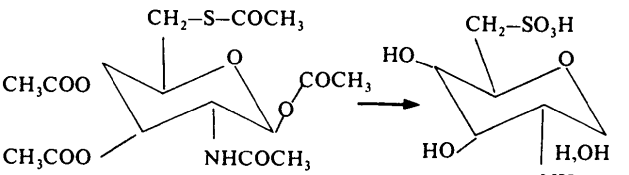
Abstract. $C_6H_{13}NO_7S$, $M_r = 243{\cdot}2$, monoclinic, $P2_1$, $a = 10{\cdot}818\ (2)$, $b = 5{\cdot}015\ (3)$, $c = 8{\cdot}838\ (2)$ Å, $\beta = 106{\cdot}77\ (2)°$, $V = 459{\cdot}1\ (3)$ Å^3, $Z = 2$, $D_x = 1{\cdot}76$, $D_m = 1{\cdot}74$ Mg m^{-3}, graphite-monochromated Mo $K\alpha$, $\lambda = 0{\cdot}7107$ Å, $\mu = 0{\cdot}35$ mm^{-1}, $F(000) = 256$, final $R = 0{\cdot}045$ for 1338 independent observed reflections (measured at 293 K). The conformation of the glucopyranose ring is a distorted chair. The N(1), O(21), O(31) and C(11) substituents are equatorial while the C(5)—O(51) bond is axial. The packing of the molecules is governed by van der Waals contacts and one H bond. The sulfonic ion is H-bonded to the amino group [N···O = 2·881 (6) Å].

Introduction. The crystal structure of 2-amino-2,6-dideoxy-α-D-glucopyranose-6-sulfonic acid has been determined as part of an investigation on conformational properties of sulfoaminosugars, which are of great interest because of their biological activity. Studies by chemical techniques have been very limited to date.

Aminosugar-sulfonic acids have been identified in hydrolysates of sulfite-treated glycoproteins and as a constituent of the cell-wall hydrolysates of *Halococcus* bacterium (Weber & Winzler, 1970; Reistad, 1977), although their structures have not been completely established. No other studies on these sulfoaminosugar derivatives have been published so far.

The compound (II) has been obtained by oxidation of 1,3,4-tri-*O*-acetyl-6-*S*-acetyl-*N*-acetyl-6-thio-β-D-glucosamine (I) with hydrogen peroxide (30%) in acetic acid and posterior deacetylation with Amberlite IR-120 (H^+) resin.



(I) (II)

A previous ^{1}H NMR study showed that in solution the α and β anomers appear to be in equilibrium, although the α anomer is dominant. The α anomer, which was synthesized in the Chemistry Department of

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Seville University (Fdez-Bolaños, Maya & Fdez-Bolaños-Guzman, 1986), is the first sulfoaminosugar derivative for which a crystal structure has been reported.

Experimental. D_m by flotation. Single crystal in the form of a colourless prism with approximate dimensions 0·17 × 0·30 × 0·21 mm used for intensity-data collection; preliminary Weissenberg photographs indicated crystals monoclinic with space group $P2_1$.

Lattice parameters refined using 25 reflections in range $4 < \theta \leq 16°$. Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ radiation, ω–2θ mode, $2\theta_{max} = 60°$ ($-15 < h < 15, k \leq 7, l \leq 12$).

Two standard reflections $3\bar{1}0$ and $\bar{3}02$ monitored every 100 reflections showed only statistical fluctuations. 1477 independent reflections measured, $R_{int} = 0{\cdot}022$ from merging 68 equivalent reflections, 1338 observed with $I > 2\sigma(I)$. Lorentz–polarization but no absorption or extinction corrections.

Structure solved by direct methods (*MULTAN*80, Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980); 210 E values ($E > 1{\cdot}40$) used as input to *MULTAN* and the correct set with the highest figure of merit of 2·12 and residual value of 11·3 gave the approximate positions of the 15 nonhydrogen atoms. Scattering factors from *International Tables for X-ray Crystallography* (1974); full-matrix least-squares refinement based on F of the nonhydrogen atoms with isotropic temperature factors and unit weights gave $R = 0{\cdot}075$; with anisotropic temperature factors and weighting scheme $w = 1/\sigma^2(F)$, R was reduced to 0·054. A difference Fourier synthesis (calculated to a max. $\sin\theta/\lambda = 0{\cdot}4$ Å^{-1}) revealed positions of all H atoms.

Further refinement, with nonhydrogen atoms treated anisotropically and H atoms isotropically, produced convergence with $R = 0{\cdot}045$, $wR = 0{\cdot}050$ and $S = 2{\cdot}14$. In final cycle H atoms assigned isotropic thermal parameters equal to those of the bonded C atoms. A final difference Fourier synthesis showed $\Delta\rho = \pm 0{\cdot}3$ e Å^{-3}. $(\Delta/\sigma)_{max} = 0{\cdot}0004$.

The origin was defined by keeping the y coordinate of C(1) fixed. The absolute configuration was established from its chemical assignment. The *XRAY* system (Stewart, Kundell & Baldwin, 1970) computer program was used.

Discussion. Fractional atomic coordinates and equivalent isotropic temperature factors for nonhydrogen atoms are given in Table 1.* The molecule including bond distances and angles is shown in Fig. 1. The average C—H and O—H bond lengths are 0·99 (5) and 0·98 (4) Å, respectively.

Table 1. *Atomic coordinates* ($\times 10^4$) *and thermal parameters* (Å^2 $\times 10^4$) *for 2-amino-2,6-dideoxy-*D*-glucopyranose-6-sulfonic acid*

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*a_ia_j\cos(\mathbf{a}_i.\mathbf{a}_j)$.

	x	y	z	U_{eq}
S	2095 (1)	720	7365 (1)	202 (4)
O(51)	815 (3)	52 (8)	12135 (4)	265 (11)
O(1)	1508 (3)	−2319 (8)	10207 (3)	227 (10)
O(11)	1734 (4)	3146 (8)	7994 (5)	338 (13)
O(12)	2872 (3)	1189 (10)	6276 (4)	350 (14)
O(13)	980 (3)	−1003 (9)	6614 (4)	306 (11)
O(21)	4898 (3)	−799 (10)	12095 (4)	355 (13)
O(31)	4223 (3)	−4065 (10)	14484 (3)	305 (11)
N(1)	1572 (3)	−4358 (12)	14269 (4)	256 (11)
C(1)	2724 (4)	−996 (11)	10482 (5)	193 (11)
C(2)	3765 (4)	−2360 (11)	11808 (5)	215 (12)
C(3)	3315 (4)	−2609 (10)	13287 (5)	200 (12)
C(4)	2037 (4)	−4025 (11)	12842 (4)	183 (11)
C(5)	1041 (4)	−2556 (11)	11547 (5)	204 (12)
C(11)	3122 (4)	−1077 (11)	8965 (5)	208 (12)

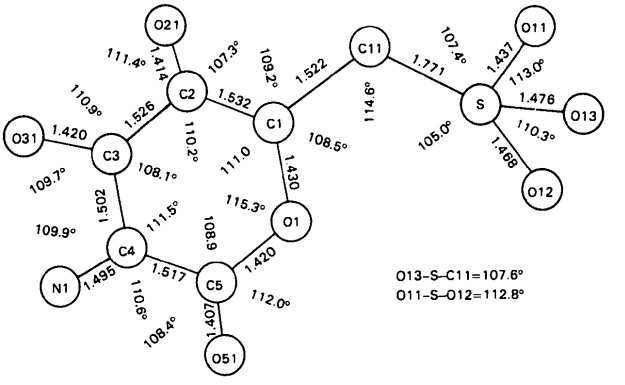

Fig. 1. Bond distances (Å) and angles (°). Maximum e.s.d.'s are 0·007 Å and 0·4°.

Bond lengths and angles about the six-membered ring are similar to those found in analogous compounds and the typical asymmetry of the endocyclic bonds O(1)–C(1) and O(1)–C(5) caused by the anomeric effects is observed.

The C–S bond length and the bond lengths and angles about the sulfonate group are comparable to those reported for other sulfonate structures (Solans, Plana & Font-Altaba, 1982; Barnes & Hawkinson, 1982; Brown, Ehrenberg & Yadav, 1984).

The conformation of the pyranose ring is a distorted chair; Cremer & Pople's (1975) puckering parameters for the sequence O(1)–C(1)–C(2)–C(3)–C(4)–C(5) are $Q = 0{\cdot}565$ (5) Å, $\varphi = 35$ (6)° and $\theta = 176$ (1)°. The asymmetry parameters of Nardelli (1983) are ΔC_s[C(1)] = 0·007 (3)° and ΔC_2[C(1)–O(1)] = 0·006 (2)°.

* Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42856 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The N(1), O(21), O(31) and C(11) substituents are equatorial, while the C(5)—O(51) bond is axial. Packing of the molecules in the unit cell is governed by van der Waals contacts and one H bond [N(1)···O(13)(x, y, $z+1$) = 2·881 (6) Å].

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Structure of 1-Acetonyl-2-[(2,4-dichlorophenyl)imino]imidazolidine Hydrochloride: a New Analgesic Compound

BY ALAIN CARPY AND ABDESLAM H'NAÏFI

Laboratoire de Chimie Analytique, ERA 890 *CNRS, Faculté de Pharmacie, Université de Bordeaux* II, *Place de la Victoire,* 33076 *Bordeaux CEDEX, France*

FRANZ ESSER

Boehringer Ingelheim KG, Abteilung Pharmachemie, Postfach 200, *D*-6507 *Ingelheim, Federal Republic of Germany*

AND HELMUT STÄHLE

Boehringer Ingelheim KG, Abteilung Medizin, Postfach 200, *D*-6507 *Ingelheim, Federal Republic of Germany*

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Abstract. $C_{12}H_{14}Cl_2N_3O^+.Cl^-$, $M_r = 322·5$, monoclinic, $P2_1/n$, $a = 17·930$ (1), $b = 9·427$ (3), $c = 18·008$ (3) Å, $\beta = 90·38$ (4)°, $V = 3043·2$ (3) Å^3, $Z = 8$ (two independent molecules), $D_x = 1·41$ g cm^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, $\mu = 54·1$ cm^{-1}, $F(000) = 1328$, room temperature, $R = 0·051$ for 3088 independent observed reflections. The title compound is structurally related to clonidine; however, its prevailing activity is one of producing analgesia (Boehringer Ingelheim, 1983). It is synthesized from 2-[(2,4-dichlorophenyl)imino]imidazolidine in two steps. The guanidine function is involved in the protonation process. The delocalization of the positive charge was evidenced by CNDO/2 calculations. The overall conformation in the crystal and in vacuum (PCILO calculations) is biplanar [with an angle of ~70 (1)° between the planes]. The two non-substituted N atoms of the guanidine group are involved in hydrogen bonds responsible for the crystalline cohesion.

Introduction. The title compound, named ESR 1276-CL, is structurally an analogue of clonidine (Catapressan®). The dominant property of clonidine is its hypotensive activity; however, the production of analgesia could also be established clinically (Tamsen & Gordh, 1984). Xylazine, another α-agonist, is in use as an analgesic compound in veterinary medicine (Kroneberg & Schlossman, 1971). The objective of the X-ray study at hand was to investigate whether the difference in activity profile between ESR 1276-CL and clonidine is paralleled by a difference in structure.

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