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Redetermination of the crystal structure of 2-amino-2-methyl-propane-1,3-diol, $C_4H_{11}NO_2$

Table 1: Data collection and handling.

Crystal:	Colourless blocks
Size:	0.59 × 0.53 × 0.35 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.10 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	28.3°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	6559, 1422, 0.016
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1299
$N(\text{param})_{\text{refined}}$:	75
Programs:	Bruker [1, 2], SHELX [3], WinGX/ORTEP [4], Mercury [5], PLATON [6]

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Abstract

$C_4H_{11}NO_2$, monoclinic, $P2_1/n$ (no. 14), $a = 6.0864(4)$ Å, $b = 10.9696(8)$ Å, $c = 8.5928(5)$ Å, $\beta = 93.360(3)^\circ$, $V = 572.72(7)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0307$, $wR_{\text{ref}}(F^2) = 0.0891$, $T = 200$ K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of materials

The compound was obtained commercially (Merck). Crystals were taken directly from the provided product.

Carbon-bound H atoms were placed in calculated positions (C–H 0.99 Å for methylene groups) and were

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.75720 (9)	0.32652 (6)	0.52692 (7)	0.02653 (17)
H1	0.861363	0.306999	0.590497	0.040*
O2	0.52222 (11)	0.55170 (6)	0.29563 (8)	0.03188 (18)
H2	0.436659	0.585810	0.355318	0.048*
N1	0.59156 (12)	0.22262 (6)	0.23927 (8)	0.02410 (18)
C1	0.66847 (12)	0.35027 (7)	0.25099 (9)	0.01995 (18)
C2	0.76768 (15)	0.38609 (9)	0.09854 (10)	0.0298 (2)
H2A	0.657587	0.374985	0.011835	0.045*
H2B	0.895809	0.334561	0.082129	0.045*
H2C	0.813381	0.471728	0.103728	0.045*
C3	0.84325 (13)	0.36530 (8)	0.38456 (9)	0.02338 (19)
H3A	0.974613	0.316158	0.363340	0.028*
H3B	0.888401	0.451857	0.393101	0.028*
C4	0.46442 (13)	0.42694 (7)	0.27876 (9)	0.02309 (19)
H4A	0.355016	0.417145	0.189757	0.028*
H4B	0.396708	0.398216	0.374115	0.028*
H1A	0.548 (2)	0.2002 (12)	0.3331 (16)	0.037 (3)*
H1B	0.704 (2)	0.1733 (13)	0.2192 (15)	0.039 (3)*

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included in the refinement in the riding model approximation, with $U(\text{H})$ set to $1.2U_{\text{eq}}(\text{C})$. The H atoms of the methyl group were allowed to rotate with a fixed angle around the C–C bond to best fit the experimental electron density (HFIX 137 in the SHELX program [2]), with $U(\text{H})$ set to $1.5U_{\text{eq}}(\text{C})$. The H atoms of the hydroxyl groups were

allowed to rotate with a fixed angle around the C–O bond to best fit the experimental electron density (HFIX 147 in the SHELX program [2]), with $U(\text{H})$ set to $1.5U_{\text{eq}}(\text{O})$. Both nitrogen-bound H atoms were refined freely.

Comment

Chelate ligands have found widespread use in coordination chemistry due to the increased stability of coordination compounds they can form in comparison to monodentate ligands [7]. Aminols are particularly interesting in this aspect as they offer different donor sites of markedly diverging acidity as potential bonding partners. Upon variation of the substitution pattern on the hydrocarbon backbone, the acidity of the donor sites can be varied over a wide range and they may serve as probes for establishing the rules in which pK_a range coordination to various central atoms of variable Lewis acidity can be observed. Furthermore, the spatial pretense of the substitution pattern can also be exploited to enable unusual coordination numbers. The title compound was chosen as it features one amino group next to two alcohol groups and can give rise to either five-membered heteroleptic chelate rings or six-membered homoleptic chelate rings. While the unit cell dimensions of the aminole are apparent in the literature no 3D coordinates have been deposited [8]. The crystal and molecular structures of similar aminols have been reported earlier [9–16].

The structure shows the expected connectivity. The C–O bond lengths of 1.4184(10) and 1.4237(10) Å as well as the C–N bond length of 1.4780(10) Å are in agreement with values reported for similar compounds deposited with the Cambridge Structural Database [17].

In the crystal, classical hydrogen bonds of the O–H...O, O–H...N and N–H...O type are apparent that employ all hydrogen atoms bonded to heteroatoms as donors as well as all heteroatoms as acceptors. One of the hydrogen atoms of the amino group establishes an intramolecular hydrogen bond to one of the hydroxyl groups. In terms of graph-set analysis [18], the descriptor for these hydrogen bonds is $S(5)C_1^1(5)C_1^1(5)R_2^2(12)$. In total, the molecules are connected to a three-dimensional network.

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