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The crystal structure of 6-bromohexanoic acid, $C_6H_{11}BrO_2$

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Abstract

$C_6H_{11}BrO_2$, monoclinic, $P2_1/n$ (no. 14), $a = 10.6730(14)$ Å, $b = 5.2781(6)$ Å, $c = 14.7781(18)$ Å, $\beta = 109.610(4)^\circ$, $V = 784.21(17)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0225$, $wR_{ref}(F^2) = 0.0564$, $T = 200(2)$ 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 material

The compound was obtained commercially (Sigma Aldrich). Crystals suitable for the diffraction study were taken directly from the provided product.

Experimental details

Carbon-bound H atoms were placed in calculated positions (C–H 0.99 Å) and were included in the refinement in the riding model approximation, with $U(H)$ set to $1.2 U_{eq}(C)$.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.57 × 0.54 × 0.27 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	5.17 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	28.4°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	7266, 1944, 0.025
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1622
$N(param)_{refined}$:	84
Programs:	Bruker [1, 2], SHELX [3], WinGX/ORTEP [4], Mercury [5], PLATON [6]

The H atom of the hydroxyl group was 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 suite [3]), with $U(H)$ set to $1.5 U_{eq}(O)$.

Comment

The synthesis of alkylarsonic acids can be achieved easily by means of the Meyer reaction, which involves a nucleophilic substitution reaction employing arsenite as the nucleophile [7]. In an attempt to synthesize a polyfunctional member of this compound class the title compound was chosen as the starting material. To prevent accidentally characterizing the title compound instead of the intended arsonic acid and in continuation of our own studies into the structural aspects of carboxylic acids [8–13], the structure of the substrate was determined. Structural information about the homologous series of ω -bromo alkanic acids for a maximum of 10 carbon atoms is otherwise limited exclusively to bromoacetic acid [14].

The structure solution shows the presence of a derivative of hexanoic acid bearing a bromo substituent in ω position. The C–Br bond length of 1.9549(19) Å as well as the C–O bond lengths of 1.215(2) and 1.315(2) Å are in good agreement with comparable bonding patterns in compounds whose metrical parameters have been deposited with the Cambridge Structural Database [15]. The hydrocarbon chain adopts an ideal zig-zag conformation.

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

Atom	x	y	z	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Br1	0.71652 (2)	0.94843 (4)	0.65878 (2)	0.03851 (9)
O1	0.50025 (17)	0.2173 (3)	0.07297 (10)	0.0508 (4)
H1	0.486055	0.269487	0.016716	0.076*
O2	0.55600 (18)	0.6200 (3)	0.10813 (10)	0.0552 (4)
C1	0.54244 (18)	0.4060 (4)	0.13367 (14)	0.0359 (4)
C2	0.57476 (19)	0.3316 (4)	0.23689 (13)	0.0365 (4)
H2A	0.657561	0.230102	0.256967	0.044*
H2B	0.502382	0.223005	0.242981	0.044*
C3	0.5926 (2)	0.5566 (4)	0.30397 (14)	0.0372 (4)
H3A	0.505618	0.641811	0.290785	0.045*
H3B	0.653982	0.679231	0.290148	0.045*
C4	0.6469 (2)	0.4853 (4)	0.40977 (14)	0.0368 (4)
H4A	0.735673	0.406706	0.424119	0.044*
H4B	0.587308	0.358960	0.423743	0.044*
C5	0.65831 (18)	0.7164 (4)	0.47411 (12)	0.0357 (4)
H5A	0.715882	0.844305	0.458635	0.043*
H5B	0.569062	0.792352	0.460515	0.043*
C6	0.7149 (2)	0.6520 (4)	0.57911 (13)	0.0384 (4)
H6A	0.806787	0.587673	0.594028	0.046*
H6B	0.660936	0.516239	0.594111	0.046*

In the crystal, the formation of centrosymmetric dimers based on hydrogen bonding between the carboxyl groups of two neighboring molecules of the title compound is observed. In terms of graph-set analysis [16, 17], the descriptor for these contacts at the unary level is R_2^2 (8).

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