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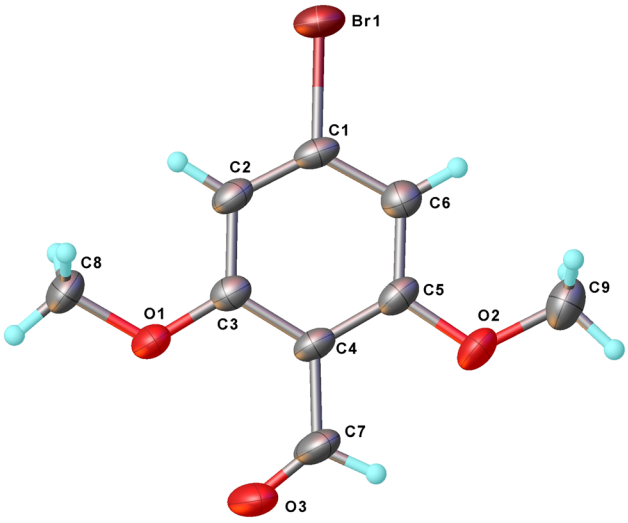
The crystal structure of 4-bromo-2,6-dimethoxybenzaldehyde, $C_9H_9BrO_3$



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Abstract

$C_9H_9BrO_3$, monoclinic, $C2/c$ (no. 15), a = 19.8576(5) Å, b = 4.1080(2) Å, c = 23.1284(8) Å, β = 94.983(3)°, V = 1879.57(12) Å^3, Z = 8, $R_{gt}(F)$ = 0.0416, $wR_{ref}(F^2)$ = 0.1155, T = 297 K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data. The list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

1 Source of materials

The title compound was bought from Shanghai Bide Pharmatech Co., Ltd. About 20 mg powder was placed into a 10 ml penicillin bottle, followed by addition of 3 ml ethanol. After all the powder was disolved in ethanol, the penicillin bottle was left open and placed in a fume hood. After 5 days, needle-shaped crystals were harvested.

Table 1: Data collection and handling.

Crystal:	Needle, colourless
Size:	0.20 × 0.05 × 0.05 mm
Wavelength:	Cu $K\alpha$ radiation (1.54178 Å)
μ:	5.76 mm^{-1}
Diffractometer, scan mode:	XtaLAB Synergy R, ω-scans
θ_{max}, completeness:	76.6°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7846, 1842, 0.087
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 1,535
$N(param)_{refined}$:	120
Programs:	Rigaku[1], OLEX2[2], SHELX[3,4]

2 Experimental details

The positions of hydrogen atoms were calculated geometrically and refined using the riding model. Their coordinates and displacement parameters were constrained to ride on the carrier atom.

3 Comment

The title compound is a key intermediate in the synthesis of many bioactive molecules.[5–7]

The titled compound was crystallized in $C2/c$ space group with one molecule in its asymmetric unit. The bond lengths and angles within these moieties are in the expected ranges.[8] All non-hydrogen atoms are essentially coplanar. Only a weak hydrogen bond between C8–H8C and O3$^{1-x,1-y,1-z}$ is observed with D···A length of 3.325(5) Å. Some π–π interaction exists between adjacent aromatic rings with centroid-to-centroid distance of 4.108(2) Å and interplanar distance of 3.5429(15) Å.

Author contribution: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Conflict of interest: The authors declare no conflicts of interest regarding this article.

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