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5-Bromosalicylic acid

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.048
wR factor = 0.111
Data-to-parameter ratio = 14.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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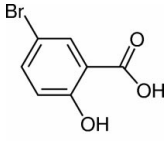
The title compound, $C_7H_5BrO_3$, crystallizes with two independent molecules in the asymmetric unit. All the O atoms in the two molecules contribute to the formation of a three-dimensional hydrogen-bonded network.

Comment

The asymmetric unit of the title complex, (I), consists of two independent molecules of 5-bromosalicylic acid (Fig. 1). In both independent molecules, the bond lengths and angles are in the normal ranges. The C—C bond lengths of the benzene rings are in the range 1.353 (7)–1.404 (7) Å, the C5—Br1 bond length is 1.904 (5) Å and the Br2—C12 bond length is 1.897 (5) Å. The C1—C6 and C8—C13 rings are planar, with a mean deviation of 0.0033 Å. The benzene rings of the two independent molecules in the asymmetric unit are almost perpendicular to one another, with a dihedral angle of 89.1 (3)°.



(I)

All the O atoms in the two independent molecules contribute to the formation of intermolecular hydrogen bonds, so forming a three-dimensional network (details are given in Table 1 and Fig. 2).

Experimental

Crystals of compound (I) were obtained by evaporation of an ethanol–water (1:2 *v*/*v*, 10 ml) solution of 5-bromosalicylic acid (1 mmol, 0.22 g). Colorless crystals of (I) were collected, washed with water and dried in a vacuum using $CaCl_2$ (yield 42.5%). Elemental analysis found: C 38.68, H 2.40, Br 36.77%; calculated for $C_7H_5BrO_3$: C 38.74, H 2.32, Br 36.82%.

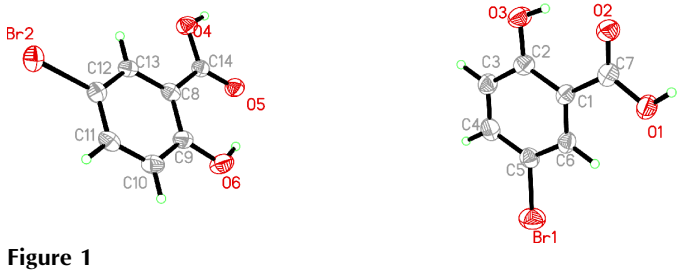


Figure 1
The structure of the asymmetric unit of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Crystal data

$C_7H_5BrO_3$
M_r = 217.02
Triclinic, $P\overline{1}$
a = 4.8050 (10) Å
b = 12.047 (2) Å
c = 14.666 (3) Å
α = 114.06 (3)°
β = 90.40 (3)°
γ = 101.19 (3)°
V = 756.9 (3) Å^3
Z = 4
D_x = 1.904 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2884 reflections
θ = 6–27.5°
μ = 5.38 mm^{-1}
T = 293 (2) K
Rod, colorless
0.14 × 0.06 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.514, T_{max} = 0.767
5095 measured reflections
2884 independent reflections
1786 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 26.0°
$h = -5 \rightarrow 5$
$k = -14 \rightarrow 14$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.111
S = 0.95
2884 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0474P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O2^{i}	0.85	1.83	2.681 (5)	179
O3—H3B···O2	0.85	1.87	2.614 (5)	145
O4—H4B···O5^{ii}	0.85	1.80	2.648 (5)	177
O6—H6C···O5	0.85	1.90	2.633 (5)	144

Symmetry codes: (i) $2-x, -y, 2-z$; (ii) $-x, 1-y, 1-z$.

All the H atoms were placed in geometrically idealized positions (C—H = 0.96 Å and O—H = 0.85 Å) and allowed to ride on their parent atoms with U_{iso}(H) = 0.08 Å^2.

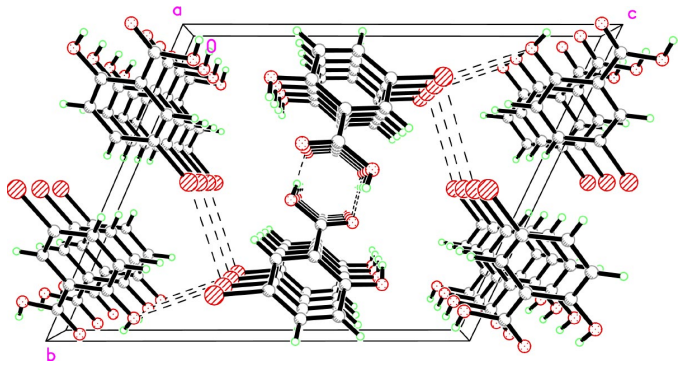


Figure 2
The crystal packing of (I), showing the O—H···O hydrogen-bonding interactions as dashed lines.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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References

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version. 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.