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3,5-Dibromo-2-hydroxybenzoic acid

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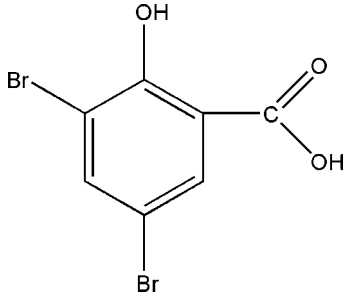
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.031; wR factor = 0.061; data-to-parameter ratio = 14.4.

The title compound, $C_7H_4Br_2O_3$, has an intramolecular O—H···O=C hydrogen bond and aggregates to form hydrogen-bonded dimers *via* O—H···O interactions. The formation of zigzag one-dimensional molecular tapes *via* C—H···Br interactions and π–π stacking interactions (interplanar separation = 3.42 Å) completes the crystal structure.

Related literature

For related literature, see: Chiari *et al.* (1981); Jin & Xiao (2005).



Experimental

Crystal data

$C_7H_4Br_2O_3$
M_r = 295.92
Monoclinic, $C2/c$
a = 10.770 (3) Å
b = 11.082 (3) Å
c = 14.879 (4) Å
β = 105.606 (3)°
V = 1710.4 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 9.44 mm^{-1}
T = 293 (2) K
0.50 × 0.31 × 0.21 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.088, T_{max} = 0.243
(expected range = 0.050–0.138)
6362 measured reflections
1599 independent reflections
1286 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.061
S = 1.79
1599 reflections
111 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.87	2.684 (3)	175
O3—H3···O2	0.82	1.93	2.648 (3)	145
C3—H3A···Br1^{ii}	0.93	2.89	3.810 (3)	172

Symmetry codes: (i) $-x+\frac{5}{2}, -y-\frac{1}{2}, -z+1$; (ii) $-x+\frac{5}{2}, -y+\frac{1}{2}, -z+1$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2052).

References

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Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supporting information

Acta Cryst. (2008). E**64**, o3 [https://doi.org/10.1107/S1600536807062320]

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S1. Comment

The compound 2-hydroxybenzoic acid (salicylic acid) and its derivatives have been widely studied as medicines or important active pharmaceutical intermediates (Chiari *et al.*, 1981; Jin & Xiao, 2005). Herein, we report the crystal structure of the title compound, (I).

In (I) (Fig. 1), the atoms O1, O2, O3, Br1, Br2, C1 and aromatic ring {C2,···,C7} are essentially coplanar with a mean deviation of 0.014 Å. The crystal packing is stabilized by intramolecular and intermolecular O—H···O and C—H···Br hydrogen bonds (Table 1).

S2. Experimental

Crystals appropriate for data collection were obtained by recrystallization from ethanol (m.p. 500–501 K).

S3. Refinement

The hydroxyl H atom and the carboxylate H atom were located from difference Fourier map but were refined using the riding model with O—H distance restrained to 0.82Å and U_{iso}(H) = 1.5Ueq(O); while all other H atoms were placed at geometrical idealized positions with C—H = 0.93Å and U_{iso}(H) = 1.2Ueq(C).

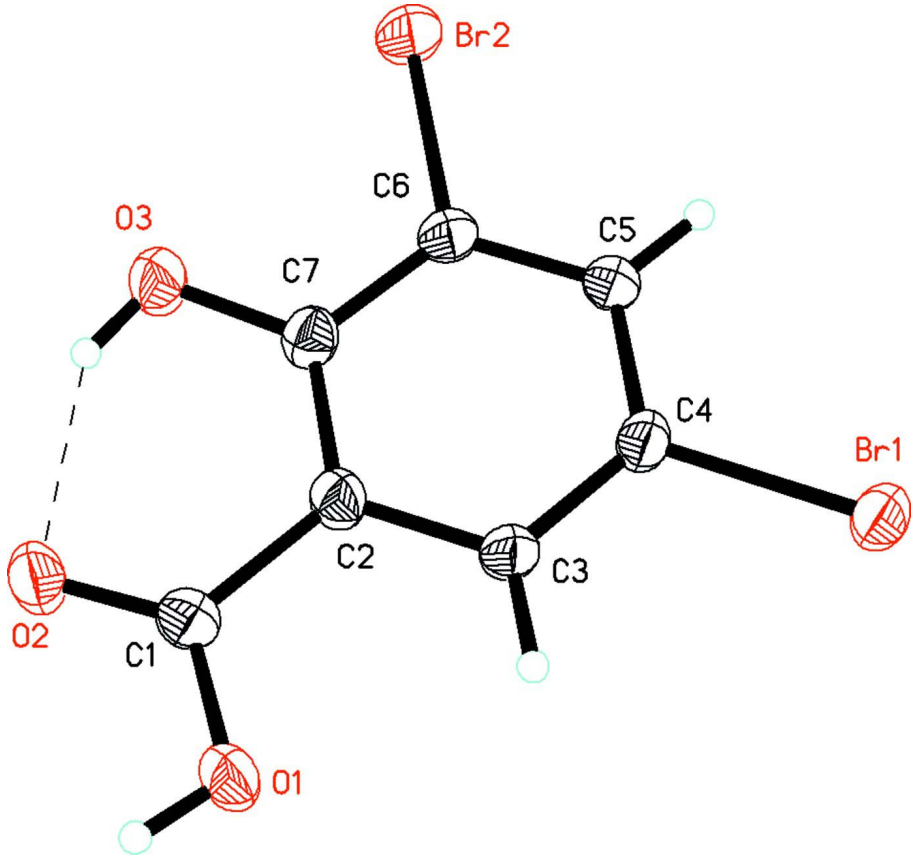

Figure 1

The molecular structure of the title compound depicted with 30% probability displacement ellipsoids.

3,5-Dibromo-2-hydroxybenzoic acid

Crystal data

$C_7H_4Br_2O_3$
$M_r = 295.92$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 10.770\ (3)$ Å
$b = 11.082\ (3)$ Å
$c = 14.879\ (4)$ Å
$\beta = 105.606\ (3)°$
$V = 1710.4\ (8)$ Å^3
$Z = 8$

$F(000) = 1120$
$D_x = 2.298$ Mg m^{-3}
Melting point: 500 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2346 reflections
$\theta = 2.7–26.3°$
$\mu = 9.44$ mm^{-1}
$T = 293$ K
Block, light-yellow
0.50 × 0.31 × 0.21 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.088$, $T_{max} = 0.243$

6362 measured reflections
1599 independent reflections
1286 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.7°$
$h = -13\rightarrow13$
$k = -13\rightarrow13$
$l = -17\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.061$
$S = 1.79$
1599 reflections
111 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2)]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.82$ e Å^{-3}
$\Delta\rho_{min} = -0.81$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.
Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	1.06441 (4)	0.35585 (3)	0.42603 (3)	0.07017 (19)
Br2	0.68570 (4)	0.02983 (4)	0.22295 (3)	0.05891 (17)
O1	1.2480 (2)	−0.0861 (2)	0.49804 (18)	0.0543 (7)
H1	1.2875	−0.1464	0.5219	0.081*
O2	1.1105 (2)	−0.2248 (2)	0.41973 (16)	0.0545 (7)
O3	0.8866 (2)	−0.1506 (2)	0.31093 (18)	0.0560 (7)
H3	0.9422	−0.2005	0.3341	0.084*
C1	1.1390 (3)	−0.1185 (3)	0.4393 (2)	0.0422 (9)
C2	1.0523 (3)	−0.0171 (3)	0.3998 (2)	0.0376 (8)
C3	1.0907 (3)	0.1018 (3)	0.4246 (2)	0.0403 (9)
H3A	1.1712	0.1172	0.4654	0.048*
C4	1.0092 (3)	0.1959 (3)	0.3885 (2)	0.0412 (9)
C5	0.8890 (3)	0.1766 (3)	0.3280 (2)	0.0414 (9)
H5	0.8349	0.2410	0.3040	0.050*
C6	0.8509 (3)	0.0593 (3)	0.3040 (2)	0.0395 (9)
C7	0.9306 (3)	−0.0390 (3)	0.3386 (2)	0.0387 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0482 (3)	0.0329 (2)	0.1040 (4)	−0.00311 (18)	−0.0233 (2)	0.0025 (2)
Br2	0.0371 (2)	0.0526 (3)	0.0726 (3)	−0.00593 (18)	−0.0101 (2)	−0.0044 (2)
O1	0.0511 (16)	0.0353 (14)	0.0606 (17)	0.0064 (12)	−0.0126 (13)	0.0036 (12)
O2	0.0583 (17)	0.0327 (15)	0.0596 (17)	0.0041 (12)	−0.0064 (13)	−0.0017 (12)
O3	0.0514 (16)	0.0348 (15)	0.0690 (18)	−0.0019 (12)	−0.0056 (13)	−0.0074 (13)

C1	0.039 (2)	0.043 (2)	0.041 (2)	0.0019 (17)	0.0051 (17)	0.0040 (17)
C2	0.040 (2)	0.033 (2)	0.037 (2)	0.0013 (16)	0.0032 (17)	0.0044 (15)
C3	0.0332 (19)	0.037 (2)	0.043 (2)	−0.0024 (16)	−0.0032 (16)	0.0013 (16)
C4	0.041 (2)	0.0296 (19)	0.047 (2)	−0.0045 (15)	0.0024 (18)	0.0026 (16)
C5	0.0325 (19)	0.036 (2)	0.050 (2)	0.0017 (16)	0.0011 (17)	0.0028 (17)
C6	0.0326 (19)	0.041 (2)	0.041 (2)	−0.0032 (16)	0.0026 (16)	−0.0023 (16)
C7	0.042 (2)	0.035 (2)	0.037 (2)	−0.0032 (17)	0.0082 (17)	−0.0017 (16)

Geometric parameters (Å, º)

Br1—C4	1.905 (3)	C2—C3	1.401 (4)
Br2—C6	1.890 (3)	C2—C7	1.402 (5)
O1—C1	1.311 (4)	C3—C4	1.375 (5)
O1—H1	0.8200	C3—H3A	0.9300
O2—C1	1.233 (4)	C4—C5	1.381 (5)
O3—C7	1.348 (4)	C5—C6	1.380 (4)
O3—H3	0.8200	C5—H5	0.9300
C1—C2	1.478 (5)	C6—C7	1.397 (5)
C1—O1—H1	109.5	C3—C4—Br1	118.3 (3)
C7—O3—H3	109.5	C5—C4—Br1	119.9 (3)
O2—C1—O1	122.7 (3)	C6—C5—C4	118.4 (3)
O2—C1—C2	122.9 (3)	C6—C5—H5	120.8
O1—C1—C2	114.4 (3)	C4—C5—H5	120.8
C3—C2—C7	119.5 (3)	C5—C6—C7	122.0 (3)
C3—C2—C1	120.0 (3)	C5—C6—Br2	119.4 (3)
C7—C2—C1	120.4 (3)	C7—C6—Br2	118.6 (3)
C4—C3—C2	119.9 (3)	O3—C7—C6	118.2 (3)
C4—C3—H3A	120.1	O3—C7—C2	123.2 (3)
C2—C3—H3A	120.1	C6—C7—C2	118.5 (3)
C3—C4—C5	121.7 (3)		
O2—C1—C2—C3	−179.7 (3)	C4—C5—C6—C7	−0.5 (5)
O1—C1—C2—C3	1.3 (5)	C4—C5—C6—Br2	179.0 (3)
O2—C1—C2—C7	1.2 (6)	C5—C6—C7—O3	−179.3 (3)
O1—C1—C2—C7	−177.8 (3)	Br2—C6—C7—O3	1.2 (4)
C7—C2—C3—C4	−0.3 (5)	C5—C6—C7—C2	0.5 (5)
C1—C2—C3—C4	−179.3 (3)	Br2—C6—C7—C2	−179.0 (2)
C2—C3—C4—C5	0.2 (5)	C3—C2—C7—O3	179.7 (3)
C2—C3—C4—Br1	178.9 (2)	C1—C2—C7—O3	−1.2 (5)
C3—C4—C5—C6	0.2 (5)	C3—C2—C7—C6	−0.1 (5)
Br1—C4—C5—C6	−178.5 (2)	C1—C2—C7—C6	179.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.87	2.684 (3)	175

O3—H3···O2	0.82	1.93	2.648 (3)	145
C3—H3*A*···Br1^{ii}	0.93	2.89	3.810 (3)	172

Symmetry codes: (i) −*x*+5/2, −*y*−1/2, −*z*+1; (ii) −*x*+5/2, −*y*+1/2, −*z*+1.