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1,4-Dibromonaphthalene-2,3-diol

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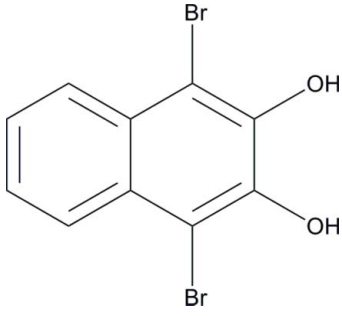
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.029; wR factor = 0.068; data-to-parameter ratio = 17.8.

In the title compound (r.m.s. deviation for the non-H atoms = 0.020 Å), $C_{10}H_6Br_2O_2$, an intramolecular O—H···O hydrogen bond generates an S(6) ring. In the crystal, the same H atom also forms an intermolecular O—H···O hydrogen bond, generating a C(2) chain propagating in [100]. The other O—H hydrogen forms a weak O—H···π interaction, and short Br···Br contacts [3.5972 (9) Å] also occur.

Related literature

For the synthesis, see: Lai *et al.* (1993). For a related structure, see: Ahn *et al.* (2009).



Experimental

Crystal data

$C_{10}H_6Br_2O_2$
M_r = 317.96
Orthorhombic, $P2_12_12_1$
a = 5.0928 (9) Å
b = 11.932 (2) Å
c = 15.779 (3) Å
V = 958.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 8.42 mm^{-1}
T = 298 K
0.16 × 0.12 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.356, T_{max} = 0.486
6339 measured reflections
2363 independent reflections
2156 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.068
S = 1.00
2363 reflections
133 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Absolute structure: Flack (1983), 899 Friedel pairs
Flack parameter: 0.034 (15)

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

*Cg*1 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···$Cg1^{i}$	0.82 (1)	2.94 (5)	3.441 (3)	122 (4)
O2—H2A···O2^{ii}	0.81 (1)	2.26 (2)	3.038 (3)	161 (4)
O2—H2A···O1	0.81 (1)	2.24 (4)	2.653 (4)	112 (4)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5940).

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supporting information

Acta Cryst. (2011). E**67**, o2009 [doi:10.1107/S1600536811026997]

1,4-Dibromonaphthalene-2,3-diol

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S1. Experimental

The title compound was synthesized according to the literature method (Lai *et al.*, 1993). Crystals of (I) were grown by slow evaporation of a chloroform-methanol (5:1) solution at room temperature.

S2. Refinement

All H atoms were positioned in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) =1.5U_{eq}(C).

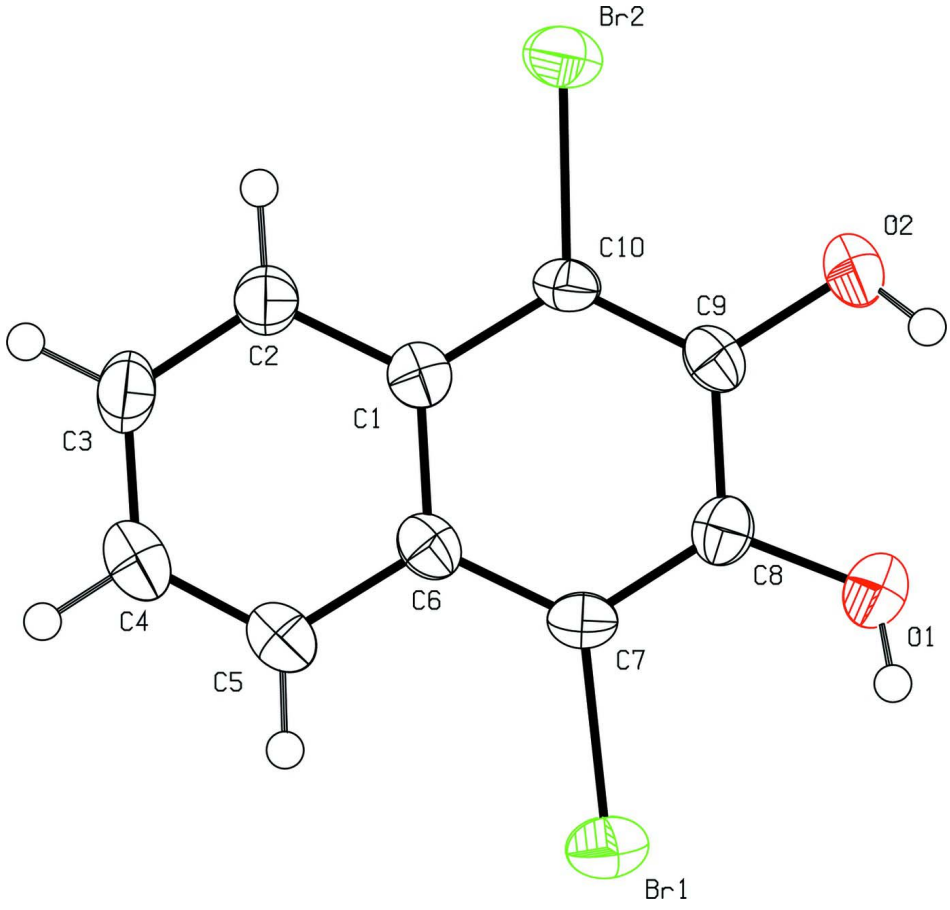

Figure 1

A view of (I), with displacement ellipsoids drawn at the 30% probability level.

1,4-Dibromonaphthalene-2,3-diol

Crystal data

$C_{10}H_6Br_2O_2$
$M_r = 317.96$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 5.0928$ (9) Å
$b = 11.932$ (2) Å
$c = 15.779$ (3) Å
$V = 958.9$ (3) Å^3
$Z = 4$
$F(000) = 608$
$D_x = 2.203$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3125 reflections
$\theta = 2.6$–$27.3°$
$\mu = 8.42$ mm^{-1}
$T = 298$ K
Block, colorless
0.16 × 0.12 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.356$, $T_{max} = 0.486$
6339 measured reflections
2363 independent reflections
2156 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.1°$
$h = -6 \rightarrow 5$
$k = -15 \rightarrow 15$
$l = -18 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.068$
$S = 1.00$
2363 reflections
133 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}
Absolute structure: Flack (1983), 899 Friedel pairs
Absolute structure parameter: 0.034 (15)

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	−0.18029 (8)	0.17357 (3)	0.16514 (2)	0.04109 (12)
Br2	0.61683 (7)	0.45789 (3)	0.40915 (2)	0.04028 (12)
C1	0.4056 (7)	0.3970 (3)	0.24593 (19)	0.0273 (7)

C2	0.5849 (7)	0.4724 (3)	0.2089 (2)	0.0331 (7)
H2	0.7024	0.5113	0.2431	0.040*
C3	0.5879 (8)	0.4891 (3)	0.1222 (2)	0.0409 (9)
H3	0.7077	0.5386	0.0982	0.049*
C4	0.4101 (8)	0.4313 (3)	0.0709 (2)	0.0423 (9)
H4	0.4103	0.4444	0.0128	0.051*
C5	0.2376 (8)	0.3569 (3)	0.1037 (2)	0.0360 (8)
H5	0.1239	0.3183	0.0679	0.043*
C6	0.2291 (7)	0.3372 (3)	0.19325 (18)	0.0285 (7)
C7	0.0531 (7)	0.2609 (3)	0.23054 (18)	0.0289 (7)
C8	0.0467 (7)	0.2438 (3)	0.31682 (19)	0.0291 (7)
C9	0.2215 (7)	0.3043 (3)	0.37007 (19)	0.0285 (7)
C10	0.3945 (7)	0.3778 (3)	0.33519 (19)	0.0267 (6)
O1	−0.1160 (6)	0.1729 (2)	0.35854 (16)	0.0424 (6)
H1A	−0.251 (5)	0.151 (4)	0.336 (3)	0.064*
O2	0.2141 (6)	0.2872 (2)	0.45569 (15)	0.0389 (6)
H2A	0.072 (5)	0.261 (4)	0.468 (3)	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0417 (2)	0.0386 (2)	0.04299 (19)	−0.00633 (18)	−0.00583 (16)	−0.00902 (16)
Br2	0.0427 (2)	0.0432 (2)	0.03491 (16)	−0.00489 (18)	−0.00972 (15)	−0.00380 (15)
C1	0.0291 (18)	0.0237 (15)	0.0290 (14)	0.0050 (14)	0.0019 (14)	−0.0014 (12)
C2	0.0373 (19)	0.0308 (18)	0.0311 (14)	−0.0022 (16)	0.0035 (14)	−0.0004 (14)
C3	0.046 (2)	0.041 (2)	0.0359 (16)	−0.0081 (18)	0.0107 (16)	0.0062 (16)
C4	0.051 (2)	0.048 (2)	0.0274 (15)	0.002 (2)	0.0016 (15)	0.0048 (15)
C5	0.042 (2)	0.0394 (19)	0.0269 (15)	0.0025 (16)	−0.0019 (14)	−0.0007 (14)
C6	0.0333 (19)	0.0274 (16)	0.0248 (13)	0.0058 (15)	0.0004 (12)	−0.0010 (13)
C7	0.0299 (18)	0.0271 (17)	0.0296 (15)	−0.0002 (14)	−0.0038 (13)	−0.0058 (13)
C8	0.0304 (18)	0.0238 (16)	0.0332 (15)	0.0018 (14)	0.0028 (13)	0.0027 (13)
C9	0.0329 (19)	0.0290 (17)	0.0235 (13)	0.0054 (14)	−0.0009 (13)	0.0020 (12)
C10	0.0298 (16)	0.0245 (15)	0.0256 (13)	−0.0004 (14)	−0.0059 (14)	−0.0037 (12)
O1	0.0440 (16)	0.0422 (15)	0.0408 (13)	−0.0125 (14)	0.0013 (12)	0.0070 (11)
O2	0.0422 (16)	0.0486 (15)	0.0258 (10)	−0.0055 (13)	0.0010 (10)	0.0066 (11)

Geometric parameters (Å, º)

Br1—C7	1.888 (3)	C5—C6	1.434 (4)
Br2—C10	1.886 (3)	C5—H5	0.9300
C1—C2	1.409 (5)	C6—C7	1.407 (5)
C1—C6	1.417 (5)	C7—C8	1.377 (4)
C1—C10	1.428 (4)	C8—O1	1.355 (4)
C2—C3	1.383 (4)	C8—C9	1.421 (5)
C2—H2	0.9300	C9—C10	1.359 (5)
C3—C4	1.397 (5)	C9—O2	1.367 (4)
C3—H3	0.9300	O1—H1A	0.819 (10)
C4—C5	1.352 (5)	O2—H2A	0.810 (10)

C4—H4	0.9300		
C2—C1—C6	119.3 (3)	C7—C6—C5	122.5 (3)
C2—C1—C10	122.5 (3)	C1—C6—C5	118.5 (3)
C6—C1—C10	118.2 (3)	C8—C7—C6	121.6 (3)
C3—C2—C1	120.6 (3)	C8—C7—Br1	116.4 (3)
C3—C2—H2	119.7	C6—C7—Br1	122.0 (2)
C1—C2—H2	119.7	O1—C8—C7	126.0 (3)
C2—C3—C4	119.7 (3)	O1—C8—C9	114.4 (3)
C2—C3—H3	120.1	C7—C8—C9	119.6 (3)
C4—C3—H3	120.1	C10—C9—O2	121.0 (3)
C5—C4—C3	121.6 (3)	C10—C9—C8	119.6 (3)
C5—C4—H4	119.2	O2—C9—C8	119.4 (3)
C3—C4—H4	119.2	C9—C10—C1	121.9 (3)
C4—C5—C6	120.3 (3)	C9—C10—Br2	117.7 (2)
C4—C5—H5	119.9	C1—C10—Br2	120.4 (2)
C6—C5—H5	119.9	C8—O1—H1A	120 (3)
C7—C6—C1	119.0 (3)	C9—O2—H2A	108 (3)
C6—C1—C2—C3	0.7 (5)	Br1—C7—C8—O1	−2.0 (5)
C10—C1—C2—C3	−179.5 (3)	C6—C7—C8—C9	0.0 (5)
C1—C2—C3—C4	0.5 (6)	Br1—C7—C8—C9	178.4 (2)
C2—C3—C4—C5	−1.6 (6)	O1—C8—C9—C10	179.8 (3)
C3—C4—C5—C6	1.4 (6)	C7—C8—C9—C10	−0.5 (5)
C2—C1—C6—C7	179.1 (3)	O1—C8—C9—O2	0.3 (5)
C10—C1—C6—C7	−0.7 (5)	C7—C8—C9—O2	179.9 (3)
C2—C1—C6—C5	−0.8 (5)	O2—C9—C10—C1	180.0 (3)
C10—C1—C6—C5	179.4 (3)	C8—C9—C10—C1	0.4 (5)
C4—C5—C6—C7	179.8 (3)	O2—C9—C10—Br2	−1.7 (4)
C4—C5—C6—C1	−0.2 (5)	C8—C9—C10—Br2	178.8 (2)
C1—C6—C7—C8	0.6 (5)	C2—C1—C10—C9	−179.6 (3)
C5—C6—C7—C8	−179.5 (3)	C6—C1—C10—C9	0.2 (5)
C1—C6—C7—Br1	−177.7 (2)	C2—C1—C10—Br2	2.0 (4)
C5—C6—C7—Br1	2.2 (5)	C6—C1—C10—Br2	−178.1 (2)
C6—C7—C8—O1	179.6 (3)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···*Cg*1^{i}	0.82 (1)	2.94 (5)	3.441 (3)	122 (4)
O2—H2*A*···O2^{ii}	0.81 (1)	2.26 (2)	3.038 (3)	161 (4)
O2—H2*A*···O1	0.81 (1)	2.24 (4)	2.653 (4)	112 (4)

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