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2,4-Dibromonaphthalen-1-ol

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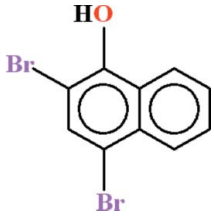
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.009 Å; R factor = 0.042; wR factor = 0.089; data-to-parameter ratio = 18.8.

In the essentially planar (r.m.s. deviation = 0.023 Å) title compound, $C_{10}H_6Br_2O$, an intramolecular O—H···Br hydrogen bond generates an $S(5)$ ring. In the crystal, molecules are linked by an ···O—H···O—H···O— $C(2)$ chain extending along [100], which involves the same H atom that participates in the intramolecular hydrogen bond. Aromatic π–π interactions [centroid–centroid separation = 3.737 (4) Å] help to consolidate the packing.

Related literature

For a related structure, see: Chanh *et al.* (1973): For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{10}H_6Br_2O$
M_r = 301.97
Orthorhombic, $P2_12_12_1$
a = 4.1225 (3) Å
b = 14.4441 (11) Å
c = 16.0490 (14) Å
V = 955.65 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 8.44 mm^{-1}
T = 296 K
0.32 × 0.14 × 0.12 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.254, T_{max} = 0.365
5060 measured reflections
2239 independent reflections
1410 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.089
S = 0.96
2239 reflections
119 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Absolute structure: Flack (1983), 863 Friedel pairs
Flack parameter: −0.01 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···Br1	0.82	2.60	3.107 (5)	122
O1—H1···O1^{i}	0.82	2.21	2.893 (6)	141

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6335).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chanh, N. B., Haget, Y., Leroy, F. & Hannoteaux, F. (1973). *Acta Cryst.* B**29**, 1469–1473.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2011). E**67**, o2199 [doi:10.1107/S160053681103011X]

2,4-Dibromonaphthalen-1-ol

Abdul Rauf Raza, Aeysha Sultan and M. Nawaz Tahir

S1. Comment

The crystal structure of 2-bromonaphthalene (Chanh, *et al.*, 1973) has been published which is related to the title compound (Fig. 1).

The molecule of the title compound is planar with r.m.s. deviation of 0.0234 Å. The Br2 atom has maximum deviation from the mean plane and its value is 0.0574 (27) Å. There exists an intra-molecular hydrogen bond of O—H···Br type (Table 1, Fig. 1) and complete S(5) ring motif (Bernstein *et al.*, 1995). The molecules are stabilized in the form of polymeric chains due to intermolecular H-bonding of O—H···O type (Table 1, Fig. 2). Due to these hydrogen bonds a chain of ···O—H···O—H···O— exists. The π–π interactions between the benzene rings (C1—C6) and (C1/C6—C10) of the naphthalen group at a distance of 3.737 (4) Å help to consolidate the packing.

S2. Experimental

Bromine (2.9 ml, 9.2 g, 30 mmol, 2 eq) was added as drops to an ice-chilled solution of α,β-unsaturated-1-tetralone (2.2 g, 15 mmol, 1 eq) in $CHCl_3$ (50 ml) and was stirred for 1 h. Et_3N (3 ml, 2.2 g, 22 mmol, 1.5 eq) was added to the reaction mixture followed by 2 h stirring at room temperature. After the commencement of reaction, the reaction mixture was neutralized with aq HCl (15 ml). The organic layer was washed with H_2O (3 × 25 ml), dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to afford the colorless needles of (I).

Yield: 2.4 g, 52%, m.p. 499 K.

S3. Refinement

The H-atoms were positioned geometrically with (O–H = 0.82, C–H = 0.93 Å) and refined as riding with U_{iso}(H) = xU_{eq}(C, O), where x = 1.5 for hydroxy and x = 1.2 for aryl H-atoms.

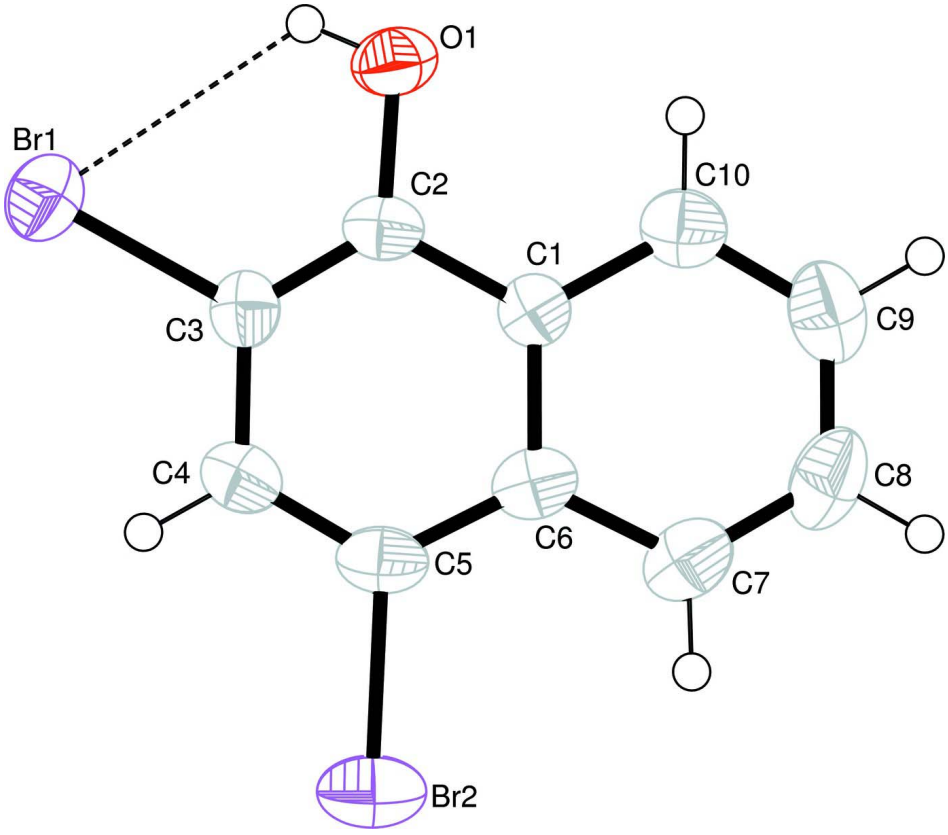

Figure 1

View of the title compound with displacement ellipsoids drawn at the 50% probability level. The dotted line indicates the intramolecular H-bond.

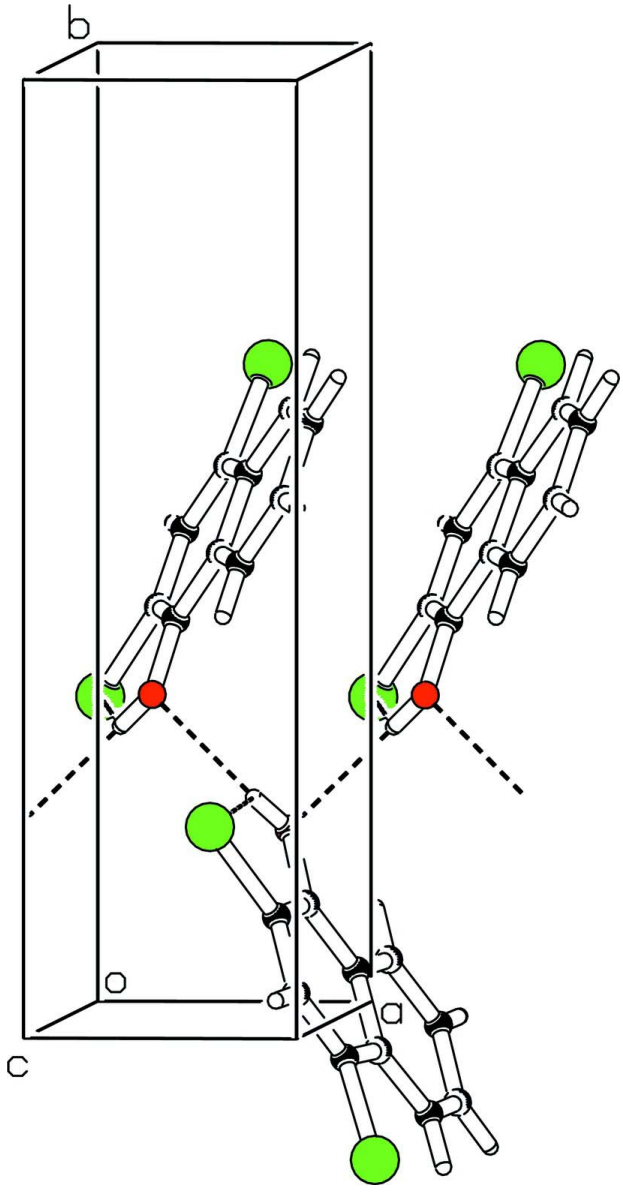

Figure 2

The partial packing of (I), which shows that molecules form polymeric chains.

2,4-Dibromonaphthalen-1-ol

Crystal data

$C_{10}H_6Br_2O$
$M_r = 301.97$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 4.1225\ (3)$ Å
$b = 14.4441\ (11)$ Å
$c = 16.0490\ (14)$ Å
$V = 955.65\ (13)$ Å^3
$Z = 4$
$F(000) = 576$
$D_x = 2.099$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1410 reflections
$\theta = 2.8–27.9°$
$\mu = 8.44$ mm^{-1}
$T = 296$ K
Needle, colorless
0.32 × 0.14 × 0.12 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.60 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.254, T_{max} = 0.365
5060 measured reflections
2239 independent reflections
1410 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 27.9°, θ_{min} = 2.8°
h = −5→5
k = −15→19
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.089
S = 0.96
2239 reflections
119 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
$w = 1/[\sigma^2(F_o^2) + (0.0309P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Absolute structure: Flack (1983), 863 Friedel pairs
Absolute structure parameter: −0.01 (3)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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	0.45967 (15)	0.18900 (4)	0.18041 (4)	0.0493 (2)
Br2	1.06884 (18)	−0.15734 (4)	0.19773 (5)	0.0624 (3)
O1	0.6998 (11)	0.1798 (3)	−0.0029 (3)	0.0463 (16)
C1	0.9478 (14)	0.0326 (3)	0.0024 (3)	0.0333 (17)
C2	0.7730 (14)	0.1034 (4)	0.0449 (4)	0.0343 (19)
C3	0.6882 (14)	0.0934 (4)	0.1244 (4)	0.036 (2)
C4	0.7718 (13)	0.0149 (4)	0.1698 (4)	0.039 (2)
C5	0.9399 (15)	−0.0536 (4)	0.1318 (4)	0.0417 (19)
C6	1.0379 (14)	−0.0490 (4)	0.0474 (3)	0.0377 (19)
C7	1.2132 (16)	−0.1172 (4)	0.0024 (5)	0.048 (3)
C8	1.2958 (16)	−0.1080 (5)	−0.0777 (4)	0.058 (3)
C9	1.2149 (16)	−0.0287 (5)	−0.1202 (5)	0.059 (3)
C10	1.0428 (15)	0.0408 (4)	−0.0816 (3)	0.045 (2)
H1	0.57717	0.21391	0.02304	0.0692*
H4	0.71293	0.00947	0.22552	0.0471*

H7	1.27375	−0.17112	0.03010	0.0583*
H8	1.40791	−0.15515	−0.10460	0.0694*
H9	1.27695	−0.02190	−0.17559	0.0702*
H10	0.98850	0.09384	−0.11132	0.0537*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0513 (4)	0.0432 (3)	0.0535 (4)	−0.0002 (3)	0.0022 (4)	−0.0087 (3)
Br2	0.0679 (5)	0.0465 (4)	0.0727 (5)	0.0007 (3)	−0.0084 (4)	0.0200 (4)
O1	0.049 (3)	0.034 (2)	0.056 (3)	0.002 (2)	0.002 (2)	0.007 (2)
C1	0.030 (3)	0.036 (3)	0.034 (3)	−0.005 (3)	−0.008 (3)	−0.005 (3)
C2	0.034 (3)	0.030 (3)	0.039 (4)	−0.008 (3)	−0.009 (3)	0.003 (3)
C3	0.033 (3)	0.036 (4)	0.038 (4)	−0.008 (3)	0.000 (3)	−0.006 (3)
C4	0.041 (4)	0.039 (3)	0.038 (4)	−0.008 (3)	−0.006 (3)	0.005 (3)
C5	0.039 (3)	0.037 (3)	0.049 (4)	−0.006 (3)	−0.014 (3)	0.008 (3)
C6	0.033 (3)	0.031 (3)	0.049 (4)	−0.007 (3)	−0.012 (3)	−0.002 (3)
C7	0.047 (4)	0.042 (4)	0.056 (5)	0.004 (3)	−0.017 (4)	−0.012 (4)
C8	0.052 (4)	0.063 (5)	0.059 (6)	0.011 (4)	−0.004 (4)	−0.026 (5)
C9	0.052 (5)	0.081 (6)	0.043 (5)	−0.001 (4)	0.003 (4)	−0.006 (4)
C10	0.042 (4)	0.049 (3)	0.044 (4)	−0.002 (3)	−0.012 (3)	0.001 (3)

Geometric parameters (Å, º)

Br1—C3	1.898 (6)	C5—C6	1.415 (8)
Br2—C5	1.910 (6)	C6—C7	1.419 (9)
O1—C2	1.377 (7)	C7—C8	1.337 (10)
O1—H1	0.8200	C8—C9	1.374 (10)
C1—C2	1.425 (8)	C9—C10	1.377 (9)
C1—C10	1.409 (7)	C4—H4	0.9300
C1—C6	1.431 (7)	C7—H7	0.9300
C2—C3	1.331 (9)	C8—H8	0.9300
C3—C4	1.391 (8)	C9—H9	0.9300
C4—C5	1.353 (8)	C10—H10	0.9300
C2—O1—H1	110.00	C1—C6—C5	116.6 (5)
C2—C1—C6	118.7 (5)	C6—C7—C8	123.4 (6)
C2—C1—C10	122.6 (5)	C7—C8—C9	119.9 (7)
C6—C1—C10	118.7 (5)	C8—C9—C10	120.6 (7)
O1—C2—C1	114.8 (5)	C1—C10—C9	120.8 (5)
O1—C2—C3	124.3 (5)	C3—C4—H4	121.00
C1—C2—C3	120.9 (5)	C5—C4—H4	120.00
Br1—C3—C4	117.9 (5)	C6—C7—H7	118.00
C2—C3—C4	121.7 (6)	C8—C7—H7	118.00
Br1—C3—C2	120.4 (5)	C7—C8—H8	120.00
C3—C4—C5	119.1 (6)	C9—C8—H8	120.00
Br2—C5—C6	119.2 (4)	C8—C9—H9	120.00
C4—C5—C6	122.9 (6)	C10—C9—H9	120.00

Br2—C5—C4	117.8 (5)	C1—C10—H10	120.00
C1—C6—C7	116.6 (5)	C9—C10—H10	120.00
C5—C6—C7	126.9 (6)		
C6—C1—C2—O1	179.3 (5)	Br1—C3—C4—C5	−178.8 (4)
C6—C1—C2—C3	−1.5 (8)	C2—C3—C4—C5	−0.9 (9)
C10—C1—C2—O1	1.0 (8)	C3—C4—C5—Br2	176.9 (4)
C10—C1—C2—C3	−179.8 (6)	C3—C4—C5—C6	0.5 (9)
C2—C1—C6—C5	1.0 (8)	Br2—C5—C6—C1	−176.9 (4)
C2—C1—C6—C7	−179.7 (5)	Br2—C5—C6—C7	3.8 (9)
C10—C1—C6—C5	179.4 (5)	C4—C5—C6—C1	−0.5 (9)
C10—C1—C6—C7	−1.3 (8)	C4—C5—C6—C7	−179.8 (6)
C2—C1—C10—C9	179.2 (6)	C1—C6—C7—C8	0.4 (9)
C6—C1—C10—C9	0.9 (9)	C5—C6—C7—C8	179.6 (6)
O1—C2—C3—Br1	−1.5 (8)	C6—C7—C8—C9	1.0 (10)
O1—C2—C3—C4	−179.4 (5)	C7—C8—C9—C10	−1.5 (10)
C1—C2—C3—Br1	179.3 (4)	C8—C9—C10—C1	0.5 (10)
C1—C2—C3—C4	1.4 (9)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···Br1	0.82	2.60	3.107 (5)	122
O1—H1···O1^{i}	0.82	2.21	2.893 (6)	141

Symmetry code: (i) $x-1/2, -y+1/2, -z$.