Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,4-Dibromo-6-(4-iodophenylimino-methyl)phenol

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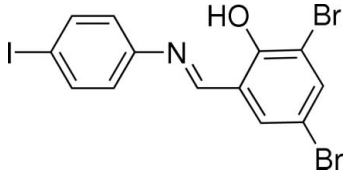
Received 2 November 2007; accepted 3 November 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.014 Å; R factor = 0.067; wR factor = 0.197; data-to-parameter ratio = 15.0.

The molecular skeleton of the title Schiff base compound, $C_{13}H_8Br_2INO$, is essentially planar due to an intramolecular N—H···O hydrogen bond; the two aromatic rings make a dihedral angle of 4.4 (5)°. The crystal packing exhibits short intermolecular I···Br contacts of 3.7226 (16) Å.

Related literature

For related crystal structures, see: Zheng *et al.* (2005); Özek *et al.* (2007); Guo (2007). For general background, see: Yeap *et al.* (2003).



Experimental

Crystal data

$C_{13}H_8Br_2INO$
M_r = 480.92
Triclinic, $P\overline{1}$
a = 8.0213 (17) Å
b = 8.5936 (18) Å
c = 11.290 (2) Å
α = 87.066 (3)°
β = 76.541 (4)°
γ = 66.203 (3)°
V = 691.7 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 8.08 mm^{-1}
T = 294 (2) K
0.14 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.334, T_{max} = 0.447
3478 measured reflections
2455 independent reflections
1802 reflections with $I > 2\sigma$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.197
S = 1.00
2455 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.19 e Å^{-3}
$\Delta\rho_{min}$ = −2.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	2.02	2.588 (10)	126

Data collection: *SMART* (Bruker 1997); cell refinement: *SAINT* (Bruker 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We thank Tianjin Polytechnic University for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2344).

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supplementary materials

Acta Cryst. (2007). E**63**, o4640 [**doi:10.1107/S1600536807055675**]

2,4-Dibromo-6-(4-iodophenyliminomethyl)phenol

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Comment

Schiff bases are important in diverse fields of chemistry and biochemistry owing to their biological activities, photochromism and so on (Yeap *et al.*, 2003). Thus, the chemists are prompted to generate the derivatives by introducing different substituents into the existing skeleton of the molecule (Zheng *et al.*, 2005; Özek *et al.*, 2007; Guo, 2007). Here, we report the structure of the title compound, (I) (Fig. 1), a new Schiff base, which was prepared by reaction of 3,5-dibromo-2-hydroxybenzaldehyde with 4-iodobenzenamine.

In (I), two aromatic substituents lie *trans* to each other across the C=N bond. The molecule is almost planar, with a dihedral angle of 4.4 (5)° between the aromatic rings. Intramolecular O1—H1···N1 hydrogen bonding generates an S(6) ring motif. The crystal packing exhibits short intermolecular I1···Br2^{i} (*d*[I1···Br2]=3.7226 (16) Å, symmetry code: (i) −1 + *x*,1 + *y*,-1 + *z*) contacts.

Experimental

The title compound, (I), was prepared by reaction of 3,5-dibromo-2-hydroxybenzaldehyde (1.4 g, 5 mmol) with 4-iodobenzenamine (1.2 g 5.5 mol) in 30 ml of 95% ethanol. The mixture was stirred and heated in air at reflux temperature for 30 min, after which 40 ml distilled water was added, the resulting product was separated by filtration (2.2 g, yield 91.7%). The pure product (0.5 g) was heated and dissolved in 20 ml of 1,2-dichloroethane. Single crystals were obtained from this solution by slow evaporation over a period of 2 days at room temperature.

Refinement

Atom H1 was found in difference Fourier map, but placed in idealized position with O—H = 0.82 Å and refined as riding, with U_{iso}(H) = 1.5 U_{eq} (O). C-bound H atoms were geometrically positioned (C—H 0.93 Å) and refined as riding, with U_{iso}(H) = 1.2 U_{eq}(C).

Figures

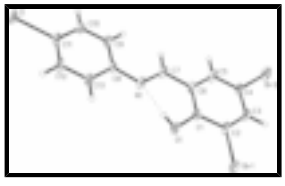

Fig. 1. The molecular structure of (I) with the atomic numbering and displacement ellipsoids drawn at the 30% probability level. Dashed line indicates hydrogen bond.

2,4-Dibromo-6-(4-iodophenyliminomethyl)phenol

Crystal data

$C_{13}H_8Br_2INO$	$Z = 2$
$M_r = 480.92$	$F_{000} = 448$
Triclinic, $P\overline{1}$	$D_x = 2.309$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.0213$ (17) Å	Cell parameters from 1701 reflections
$b = 8.5936$ (18) Å	$\theta = 2.6$–26.4°
$c = 11.290$ (2) Å	$\mu = 8.08$ mm^{-1}
$\alpha = 87.066$ (3)°	$T = 294$ (2) K
$\beta = 76.541$ (4)°	Prism, red
$\gamma = 66.203$ (3)°	0.14 × 0.12 × 0.10 mm
$V = 691.7$ (2) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	2455 independent reflections
Radiation source: fine-focus sealed tube	1802 reflections with $I > 2\sigma$
Monochromator: graphite	$R_{int} = 0.043$
$T = 294$(2) K	$\theta_{max} = 25.1^\circ$
φ and ω scans	$\theta_{min} = 1.9^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -6 \rightarrow 9$
$T_{min} = 0.334$, $T_{max} = 0.447$	$k = -9 \rightarrow 10$
3478 measured reflections	$l = -10 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.067$	H-atom parameters constrained
$wR(F^2) = 0.197$	$w = 1/[\sigma^2(F_o^2) + (0.1364P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = <0.001$
2455 reflections	$\Delta\rho_{max} = 2.19$ e Å^{-3}
164 parameters	$\Delta\rho_{min} = -2.26$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
I1	0.29339 (10)	0.87433 (9)	0.00531 (6)	0.0523 (3)
N1	0.6493 (10)	0.6165 (10)	0.4578 (7)	0.0363 (18)
O1	0.7096 (10)	0.7011 (8)	0.6555 (6)	0.0471 (17)
H1	0.7162	0.7249	0.5837	0.071*
Br1	0.87718 (17)	0.65091 (14)	0.87405 (10)	0.0578 (4)
Br2	1.19331 (18)	−0.03821 (13)	0.69717 (11)	0.0579 (4)
C1	0.8181 (11)	0.5375 (11)	0.6621 (8)	0.0313 (19)
C2	0.9089 (13)	0.4830 (12)	0.7589 (8)	0.038 (2)
C3	1.0183 (13)	0.3134 (12)	0.7704 (8)	0.037 (2)
H3	1.0751	0.2788	0.8357	0.044*
C4	1.0406 (13)	0.1962 (12)	0.6813 (8)	0.039 (2)
C5	0.9571 (14)	0.2448 (13)	0.5844 (9)	0.043 (2)
H5	0.9754	0.1635	0.5260	0.052*
C6	0.8464 (12)	0.4136 (12)	0.5735 (8)	0.033 (2)
C7	0.7600 (13)	0.4619 (13)	0.4687 (8)	0.038 (2)
H7	0.7859	0.3793	0.4091	0.046*
C8	0.5710 (11)	0.6631 (11)	0.3539 (8)	0.0306 (19)
C9	0.5922 (14)	0.5538 (13)	0.2609 (9)	0.043 (2)
H9	0.6612	0.4377	0.2648	0.052*
C10	0.5139 (14)	0.6122 (13)	0.1631 (9)	0.044 (2)
H10	0.5266	0.5363	0.1024	0.053*
C11	0.4142 (13)	0.7881 (12)	0.1555 (8)	0.038 (2)
C12	0.3925 (14)	0.8980 (12)	0.2458 (9)	0.043 (2)
H12	0.3259	1.0143	0.2409	0.052*
C13	0.4693 (13)	0.8370 (13)	0.3450 (9)	0.041 (2)
H13	0.4531	0.9130	0.4067	0.050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0699 (5)	0.0484 (5)	0.0438 (5)	−0.0146 (4)	−0.0420 (4)	0.0128 (3)
N1	0.044 (4)	0.038 (5)	0.036 (4)	−0.018 (4)	−0.026 (3)	0.012 (3)

O1	0.064 (4)	0.029 (4)	0.046 (4)	−0.004 (3)	−0.035 (3)	0.003 (3)
Br1	0.0766 (8)	0.0456 (7)	0.0464 (7)	−0.0061 (6)	−0.0382 (6)	−0.0035 (5)
Br2	0.0851 (8)	0.0310 (6)	0.0618 (7)	−0.0127 (6)	−0.0468 (6)	0.0138 (5)
C1	0.033 (4)	0.028 (5)	0.034 (4)	−0.010 (4)	−0.016 (4)	0.006 (4)
C2	0.045 (5)	0.044 (6)	0.035 (5)	−0.018 (4)	−0.028 (4)	0.014 (4)
C3	0.048 (5)	0.039 (6)	0.031 (4)	−0.019 (4)	−0.023 (4)	0.008 (4)
C4	0.043 (5)	0.037 (5)	0.038 (5)	−0.010 (4)	−0.027 (4)	0.015 (4)
C5	0.059 (6)	0.039 (6)	0.048 (5)	−0.026 (5)	−0.037 (5)	0.015 (4)
C6	0.036 (4)	0.036 (5)	0.036 (5)	−0.015 (4)	−0.024 (4)	0.016 (4)
C7	0.050 (5)	0.041 (6)	0.039 (5)	−0.025 (5)	−0.029 (4)	0.012 (4)
C8	0.032 (4)	0.031 (5)	0.034 (5)	−0.012 (4)	−0.021 (4)	0.009 (4)
C9	0.055 (6)	0.034 (5)	0.041 (5)	−0.010 (5)	−0.026 (5)	0.007 (4)
C10	0.053 (6)	0.037 (6)	0.038 (5)	−0.008 (5)	−0.025 (4)	0.001 (4)
C11	0.043 (5)	0.043 (6)	0.034 (5)	−0.015 (4)	−0.025 (4)	0.011 (4)
C12	0.059 (6)	0.028 (5)	0.051 (6)	−0.014 (4)	−0.039 (5)	0.014 (4)
C13	0.053 (5)	0.036 (5)	0.039 (5)	−0.012 (4)	−0.030 (4)	0.002 (4)

Geometric parameters (Å, °)

I1—C11	2.102 (9)	C5—H5	0.9300
N1—C7	1.285 (12)	C6—C7	1.467 (11)
N1—C8	1.423 (10)	C7—H7	0.9300
O1—C1	1.331 (10)	C8—C9	1.378 (13)
O1—H1	0.8200	C8—C13	1.396 (13)
Br1—C2	1.892 (10)	C9—C10	1.370 (13)
Br2—C4	1.914 (9)	C9—H9	0.9300
C1—C2	1.409 (12)	C10—C11	1.406 (13)
C1—C6	1.411 (13)	C10—H10	0.9300
C2—C3	1.383 (13)	C11—C12	1.359 (14)
C3—C4	1.390 (14)	C12—C13	1.381 (12)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.374 (12)	C13—H13	0.9300
C5—C6	1.379 (13)		
C7—N1—C8	120.7 (8)	N1—C7—H7	119.4
C1—O1—H1	109.5	C6—C7—H7	119.4
O1—C1—C2	120.4 (8)	C9—C8—C13	118.1 (8)
O1—C1—C6	121.7 (8)	C9—C8—N1	126.1 (8)
C2—C1—C6	117.9 (8)	C13—C8—N1	115.8 (8)
C3—C2—C1	121.9 (9)	C10—C9—C8	121.6 (9)
C3—C2—Br1	120.5 (6)	C10—C9—H9	119.2
C1—C2—Br1	117.6 (7)	C8—C9—H9	119.2
C2—C3—C4	118.0 (8)	C9—C10—C11	119.3 (9)
C2—C3—H3	121.0	C9—C10—H10	120.4
C4—C3—H3	121.0	C11—C10—H10	120.4
C5—C4—C3	121.9 (9)	C12—C11—C10	120.0 (8)
C5—C4—Br2	120.4 (8)	C12—C11—I1	121.4 (7)
C3—C4—Br2	117.8 (6)	C10—C11—I1	118.6 (7)
C4—C5—C6	120.2 (10)	C11—C12—C13	120.0 (9)
C4—C5—H5	119.9	C11—C12—H12	120.0

C6—C5—H5	119.9	C13—C12—H12	120.0
C5—C6—C1	120.1 (8)	C12—C13—C8	121.0 (9)
C5—C6—C7	119.0 (9)	C12—C13—H13	119.5
C1—C6—C7	120.8 (8)	C8—C13—H13	119.5
N1—C7—C6	121.1 (9)		
O1—C1—C2—C3	178.1 (8)	C8—N1—C7—C6	178.0 (8)
C6—C1—C2—C3	−1.9 (13)	C5—C6—C7—N1	176.9 (9)
O1—C1—C2—Br1	−2.1 (12)	C1—C6—C7—N1	−3.5 (14)
C6—C1—C2—Br1	177.9 (6)	C7—N1—C8—C9	4.3 (14)
C1—C2—C3—C4	1.4 (14)	C7—N1—C8—C13	−173.3 (9)
Br1—C2—C3—C4	−178.3 (7)	C13—C8—C9—C10	−1.0 (15)
C2—C3—C4—C5	−0.2 (14)	N1—C8—C9—C10	−178.6 (9)
C2—C3—C4—Br2	179.7 (7)	C8—C9—C10—C11	1.8 (16)
C3—C4—C5—C6	−0.4 (15)	C9—C10—C11—C12	−1.5 (16)
Br2—C4—C5—C6	179.7 (7)	C9—C10—C11—I1	−179.4 (8)
C4—C5—C6—C1	−0.1 (14)	C10—C11—C12—C13	0.4 (15)
C4—C5—C6—C7	179.6 (9)	I1—C11—C12—C13	178.2 (8)
O1—C1—C6—C5	−178.9 (9)	C11—C12—C13—C8	0.5 (16)
C2—C1—C6—C5	1.2 (13)	C9—C8—C13—C12	−0.2 (15)
O1—C1—C6—C7	1.5 (13)	N1—C8—C13—C12	177.7 (9)
C2—C1—C6—C7	−178.5 (8)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	2.02	2.588 (10)	126

Fig. 1