Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,4-Dibromo-6-(2-hydroxyethyliminiomethyl)-phenolate

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.024
wR factor = 0.055
Data-to-parameter ratio = 16.2

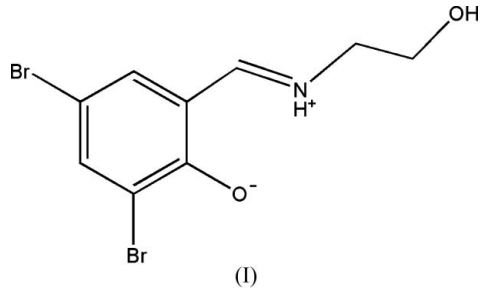
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 4 September 2006
Accepted 7 September 2006

The title Schiff base compound, $C_9H_9Br_2NO_2$, synthesized by the reaction of 3,5-dibromo-2-hydroxybenzaldehyde and 2-aminoethanol in ethanol solution, crystallizes in a zwitterionic form. The molecule adopts a *trans* configuration about the central C=N bond. In the crystal structure, O—H···O intermolecular hydrogen bonds link the molecules into ribbons along the *c* axis.

Comment

Shiff bases play an important role in coordination chemistry and have demonstrated significant biological activity; new examples are being tested for their antitumor, antimicrobial and antiviral activity (Maheswari *et al.*, 2006; Tarafder *et al.*, 2002; Cukurovali *et al.*, 2002; Ali *et al.*, 2002). As an extension of our work (Sun *et al.*, 2004) on the structural characterization of Schiff base compounds, the title compound, (I), is reported here.



(I)

The title molecule exists in a zwitterionic form with a strong intramolecular N—H···O hydrogen bond (Table 1) between the NH^+ group and the phenolate O^- group, as shown in Fig. 1. All the bond lengths are within normal ranges (Allen *et al.*, 1987). The N1=C7 [1.277 (5) Å] and N1—C8 [1.451 (4) Å] bond distances are comparable to the corresponding values [1.261 (2) and 1.457 (2) Å] observed in another Schiff base compound (Sun *et al.*, 2004). As expected, the molecule adopts a *trans* configuration about the central C=N bond. Atoms C7, N1, Br1, Br2 and O1 are nearly coplanar with the C1–C6 benzene ring, the r.m.s. deviation of the fitted atoms being 0.054 (3) Å. The C8—N1—C7—C6, C7—N1—C8—C9 and N1—C8—C9—O2 torsion angles are 175.0 (3), 119.2 (4) and −71.0 (4)°, respectively.

In the crystal structure, O2—H2···O2^{i} (symmetry code as given in Table 1) intermolecular hydrogen bonds link the molecules into ribbons along the *c* axis (Fig. 2). In addition, Br1···Br1^{ii} [3.5538 (6) Å] and Br1···Br1^{iii} [3.5538 (6) Å] short contacts are observed [symmetry codes: (ii) $-\frac{1}{2}-x, y, \frac{1}{2}+z$; (iii) $-\frac{1}{2}-x, y, -\frac{1}{2}+z$].

Experimental

All the chemicals were obtained from commercial sources and used without purification. 3,5-Dibromo-2-hydroxybenzaldehyde (0.56 g, 2 mmol) and an equimolar quantity of 2-aminoethanol (0.12 g, 2 mmol) were dissolved in ethanol (15 ml). The mixture was stirred for 30 min at room temperature, giving a clear yellow solution which was allowed to stand in air for 12 d, after which time yellow prism-shaped crystals of (I) formed at the bottom of the vessel on slow evaporation of the ethanol. (yield 79.2%; m.p. 418–420 K). Analysis found: C 33.39, H 2.78, N 4.30%; calculated for $C_9H_9Br_2NO_2$: C 33.47, H 2.81, N 4.34%.

Crystal data

$C_9H_9Br_2NO_2$
M_r = 322.99
Orthorhombic, *Aba*2
a = 18.7541 (9) Å
b = 21.9752 (11) Å
c = 5.0082 (3) Å
V = 2064.01 (19) Å^3
Z = 8
D_x = 2.079 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 7.83 mm^{-1}
T = 295 (2) K
Prism, yellow
0.50 × 0.14 × 0.14 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.111, T_{max} = 0.407
(expected range = 0.091–0.334)
10642 measured reflections
2139 independent reflections
2009 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 26.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.055
S = 1.00
2139 reflections
132 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0326P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.92 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0081 (3)
Absolute structure: Flack (1983), 936 Friedel pairs
Flack parameter: 0.027 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.897 (10)	1.83 (2)	2.563 (4)	138 (3)
O2—H2···O2^{i}	0.82	2.10	2.867 (2)	157

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

The H atom on the imino N atom was located in a difference map and refined with an N—H distance restraint of 0.90 (1) Å. Other H atoms were positioned geometrically (O—H = 0.82 Å and C—H = 0.93 or 0.97 Å) and constrained to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(O) for the hydroxyl H atom or 1.2U_{eq}(C) for other atoms

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT-Plus* (Bruker, 2002); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

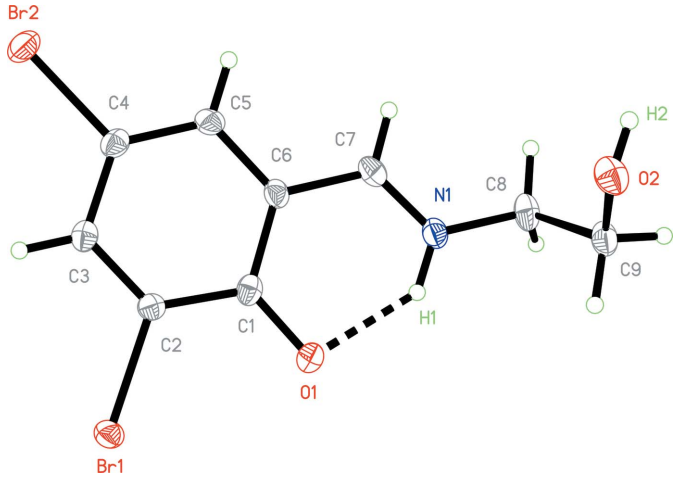


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. The N—H···O hydrogen bond is shown as a dashed line.

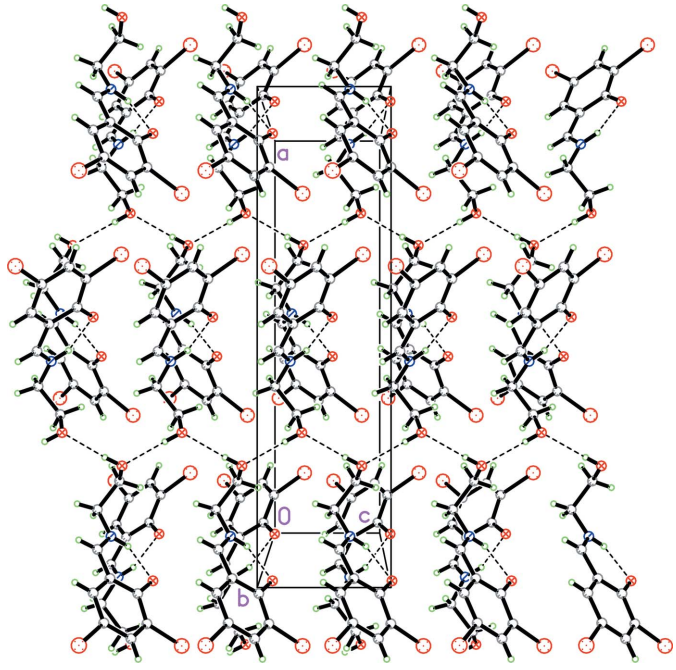


Figure 2
The packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

The work was supported by the National Natural Science Foundation of China (grant Nos. 30270245 and 30470247) and Qufu Normal University for Science and Technology.

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