4-(2-Hydroxyphenyliminomethylene)phenol

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The asymmetric unit of the title compound, $C_{13}H_{11}NO_2$, consists of two crystallographically independent molecules which are essentially planar and are approximately orthogonal to each other. These two molecules are linked by an O—H···O hydrogen bond and display two intramolecular O—H···N hydrogen bonds.

Comment

Schiff bases have been extensively used as ligands in the field of coordination chemistry (Calligaris *et al.*, 1972; Garnovski *et al.*, 1993). Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Cohen *et al.*, 1964; Moustakali *et al.*, 1978; Hadjoudis *et al.*, 1987). Based on studies of some thermochromic and photochromic Schiff base compounds, it has been proposed that molecules exhibiting monochromism are planar, while those exhibiting photochromism are non-planar (Moustakali *et al.*, 1978). Our structural investigations of Schiff bases (Kazak *et al.*, 2000; Ersanlı *et al.*, 2003; Odabaşoğlu *et al.*, 2003) have led us to examine the title compound, (I).

(I)
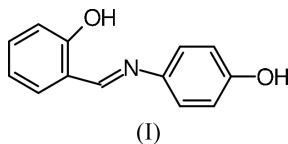
The asymmetric unit of (I) consists of two crystallographically independent, but nearly identical, molecules (*A* and *B*) linked by an O—H···O hydrogen bond (Fig. 1 and
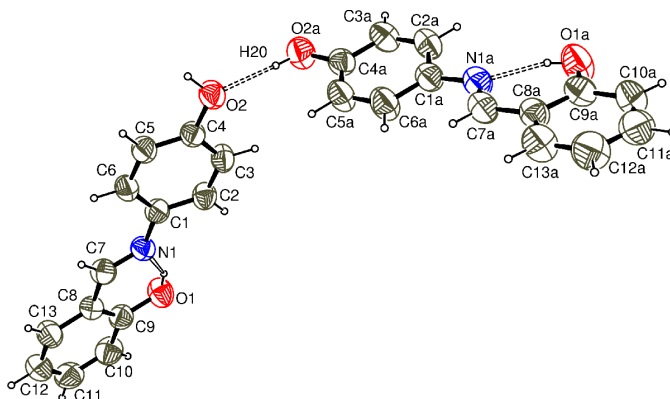

Figure 1
ORTEP view (Burnett & Johnson, 1996; Farrugia, 1997) of the asymmetric unit of (I), showing the atom-labelling scheme. Ellipsoids are drawn at the 50% probability level. H atoms are represented as spheres of arbitrary radius. The open dashed lines indicate hydrogen bonds.
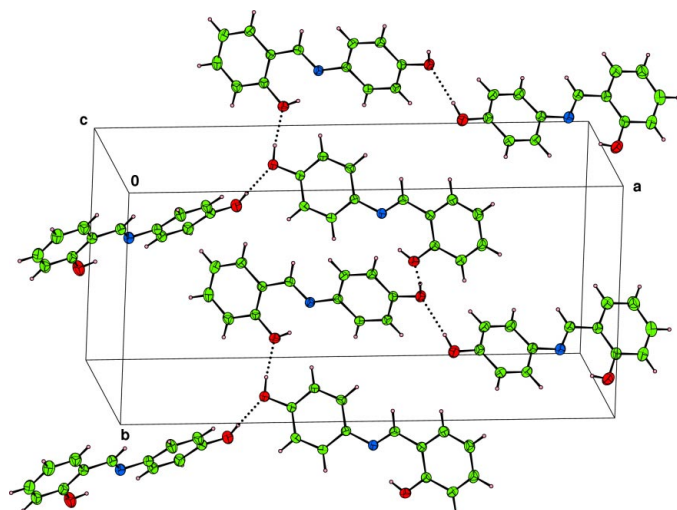
Figure 2
CAMERON (Watkin et al., 1996) packing diagram for (I), showing the O—H···O hydrogen-bonding intercations as dashed lines. Ellipsoids are drawn at the 20% probability level. The H atoms are represented as spheres of arbitrary radius.

Table 2). The two molecules make a dihedral angle of 73.07 (4)°. They are both roughly planar, the largest deviation being 0.225 (2) Å at C2 for molecule A and 0.160 (2) Å at atom C6A for molecule B. However, the benzene ring C1–C6 (C1A–C6A) is slightly twisted with respect to the C1—N1=C7—C8 (C1A—N1A=C7A—C8A) moiety, as indicated by the value of the dihedral angle between these planes 12.3 (1)° [9.7 (3)°]. The two other benzene rings, C8–C13 and C8A–C13A, are less twisted with respect to the imino groups, the dihedral angles being 3.5 (1) and 1.1 (3)°, respectively.

The C—O (hydroxyl) bonds [1.350 (2) and 1.355 (3) Å in molecules A and B, respectively] indicate single-bond character, whereas the N—C bonds [1.286 (2) and 1.278 (3) Å in molecules A and B, respectively] show double-bond character. These bond lengths are consistent with typical values reported in related compounds (Kevran et al., 1996; Elerman & Elmalı, 1998). The enol–imine tautomeric form is favoured over the keto–amine form.

There are strong intramolecular hydrogen bonds O1—H1···N1 and O1A—H1A···N1A (Table 2). The sum of the van der Walls radii of O and N (3.07 Å; Bondi, 1964) is significantly longer than the O···N hydrogen-bond length; similar results were observed in N-(3,5-dichlorophenyl)-naphthaldimine [2.570 (3) Å; Elmali et al., 1998] and in 5-chloro-2-[(2-hydroxybenzylidene)aminomethyl]phenol [2.599 (3) Å; Kevran et al., 1996]. The packing of the molecules within the crystals is governed by O—H···O hydrogen-bonding interactions (Table 2 and Fig. 2)

Experimental

The title compound, (I), was prepared as described by Ersanlı et al. (2003), using salicylaldehyde and 4-hydroxyaniline as starting materials. The product was recrystallized from ethanol and well shaped crystals of (I) were obtained by slow evaporation of an ethanol solution (yield 85%; m.p. 405–407 K).

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.423 (2)	C7—N1	1.285 (2)
C1A—N1A	1.418 (2)	C7A—N1A	1.278 (2)
C4—O2	1.3741 (19)	C9—O1	1.350 (2)
C4A—O2A	1.375 (2)	C9A—O1A	1.355 (2)
C2—C1—N1	116.91 (15)	N1—C7—C8	121.68 (16)
C6—C1—N1	124.66 (15)	N1A—C7A—C8A	122.08 (18)
C2A—C1A—N1A	116.90 (17)	O1—C9—C10	119.97 (16)
C6A—C1A—N1A	125.13 (19)	O1—C9—C8	120.53 (15)
C3—C4—O2	118.30 (15)	O1A—C9A—C10A	118.5 (2)
O2—C4—C5	122.13 (15)	O1A—C9A—C8A	121.35 (19)
C5A—C4A—O2A	122.93 (17)	C7—N1—C1	124.07 (14)
C3A—C4A—O2A	117.69 (18)	C7A—N1A—C1A	122.12 (17)
C1—N1—C7—C8	179.91 (15)	N1A—C7A—C8A—C9A	−0.8 (3)
N1—C7—C8—C9	−3.4 (3)	C7—N1—C1—C6	−12.5 (3)
N1—C7—C8—C13	176.67 (17)	C7—N1—C1—C2	167.90 (17)
C1A—N1A—C7A—C8A	179.57 (17)	C7A—N1A—C1A—C6A	−9.9 (3)
N1A—C7A—C8A—C13A	179.57 (18)	C7A—N1A—C1A—C2A	170.83 (17)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.81	2.5465 (19)	149
O1A—H1A···N1A	0.82	1.86	2.591 (2)	147
O2—H21···O1^i	0.878 (14)	1.889 (14)	2.757 (2)	169.9 (18)
O2A—H20···O2	0.847 (15)	2.006 (15)	2.852 (2)	177 (2)

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

All H atoms, except for those of the two terminal hydroxy groups (O2 and O2A), were placed in calculated positions (O—H = 0.82 Å and C—H = 0.93 Å), with U_{iso} values constrained to be 1.5U_{eq} of the carrier atom for the hydroxyl-group H atom and 1.2U_{eq} for the remaining H atoms. The coordinates of the H atoms of the two

terminal hydroxy groups were refined with the O—H distances restrained to 0.82 (2) Å and isotropic displacement parameters constrained to be $1.2U_{eq}(O)$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996), *ORTEP*-3 *for Window*s (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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