organic compounds

2-(2-Hydroxybenzylideneamino)-benzonitrile

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The molecule of the title compound, $C_{14}H_{10}N_2O$, displays a *trans* configuration with respect to the C=N double bond. The molecule is roughly planar; the two aromatic rings make a dihedral angle of 9.3 (3)°. Such a planar conformation is induced by the strong intramolecular O—H···N hydrogen bond between the imine and hydroxyl groups.

Related literature

For the structures of similar Schiff base compounds, see: Cheng *et al.* (2005, 2006). For related literature, see: Chen *et al.* (2008); Elmah *et al.* (1999); May *et al.* (2004); Weber *et al.* (2007); Xu *et al.* (2008). For bond-length data, see: Allen *et al.* (1987).
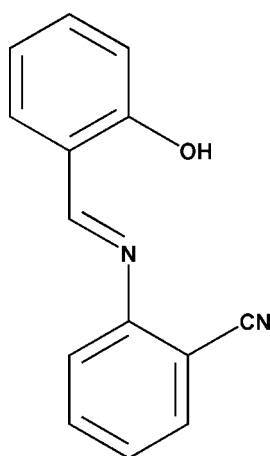
Experimental

Crystal data

$C_{14}H_{10}N_2O$ $M_r = 222.24$

Monoclinic, $P2_1$
$a = 4.7667$ (10) Å
$b = 16.190$ (3) Å
$c = 7.6714$ (15) Å
$\beta = 93.30$ (3)°
$V = 591.0$ (2) Å^3

$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 293$ (2) K
$0.20 \times 0.05 \times 0.05$ mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan
 (*CrystalClear*; Rigaku, 2005)
 $T_{min} = 0.981$, $T_{max} = 1.00$
 (expected range = 0.977–0.996)

5470 measured reflections
1201 independent reflections
633 reflections with $I > 2\sigma(I)$
$R_{int} = 0.105$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.136$
$S = 1.03$
1201 reflections
155 parameters

1 restraint
H-atom parameters constrained
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ 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	1.92	2.651 (6)	147

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2331).

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supporting information

2-(2-Hydroxybenzylideneamino)benzonitrile

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S1. Comment

The Schiff base compounds have received considerable attention for several decades, primarily due to their importance in the development of coordination chemistry related to magnetism (Weber, *et al.*, 2007), catalysis (Chen, *et al.*, 2008) and biological process (May, *et al.*,2004). Recently, we have reported a Schiff base compound (Xu, *et al.*, 2008). As an extention of our work on the structural characterization of Schiff base compounds, the title compound, (I), has been synthesized and its crystal structure is reported here.

As expected, the molecule displays a *trans* configuration about the central C7=N1 bond. The dihedral angle between the planes of the two aromatic rings is 9.34(0.29)°, showing that the conjugated part of the molecule is not entirely coplanar. A strong O – H ··· N intramolecular hydrogen-bond interaction is observed in the molecular structure (Fig. 1, Table 1) similar to the pervious reports (Xu *et al.,* 2008; Cheng *et al.*,2006, 2005).

All the bond lengths and bond angles in the compound are within normal ranges (Allen, *et al.*, 1987). The C7=N1 bond length of 1.292 (5) Å indicates a high degree of double-bond character comparable with the corresponding bond lengths in other Schiff bases (1.280 (2) Å; Elmah *et al.*, 1999).

S2. Experimental

All chemicals were obtained from commercial sources and used without further purification except for salicylaldehyde which is distiled under reduced pressure before use. 3-aminobenzonitrile (1.18 g, 10 mmol) and salicylaldehyde (1.22 g, 10 mmol) were dissolved in ethanol (20 ml). The mixture was heated to reflux for 4 h, then cooled to room temperature overnight and large amounts of a yellow precipitate were formed. Yellow crystal was obtained by recrystallization from ethyl alcohol(yield: 85%). ^{1}H-NMR(CDCl$_3$, 300 MHz): δ6.98 (t, 1 H), 7.08 (d, 1 H), 7.37(t, 2 H), 7.45 (t, 2 H), 7.69 (m, 2H), 8.72 (s, 1 H). Esi-MS: calcd for C$_{14}$H$_9$N$_2$O – H *m*/*z* 221.24, found 221.34. For the X-ray diffraction analysis, suitable single crystals of compound (I) were obtained after one week by slow evaporation from an ethyl alcohol solution.

S3. Refinement

All H atoms attached to C atoms and O atom were fixed geometrically and treated as riding with C—H = 0.93 Å and O—H = 0.82Å with U$_{iso}$(H) = 1.2U$_{eq}$(C) or U$_{iso}$(H) = 1.5U$_{eq}$(O).

In the absence of significant anomalous scattering, the absolute structure could not be reliably determined and then the Friedel pairs were merged and any references to the Flack parameter were removed.
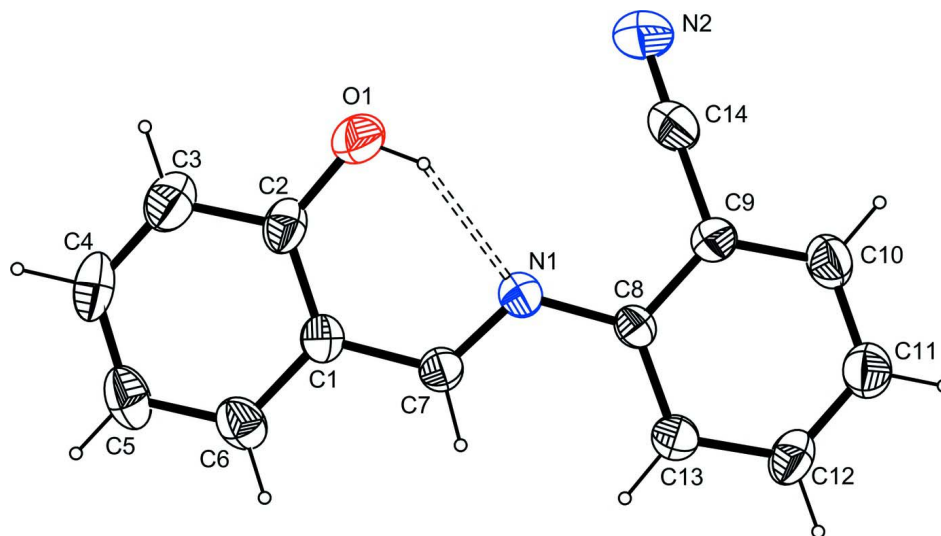
Figure 1

A view of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as smal spheres of arbitrary radii. Intramolecular H bond is shown as dashed line.

2-(2-Hydroxybenzylideneamino)benzonitrile

Crystal data

$C_{14}H_{10}N_2O$	$F(000) = 232$
$M_r = 222.24$	$D_x = 1.249$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2yb	Cell parameters from 4123 reflections
$a = 4.7667$ (10) Å	$\theta = 3.7–28.7°$
$b = 16.190$ (3) Å	$\mu = 0.08$ mm^{-1}
$c = 7.6714$ (15) Å	$T = 293$ K
$\beta = 93.30$ (3)°	Block, colorless
$V = 591.0$ (2) Å^3	$0.20 \times 0.05 \times 0.05$ mm
$Z = 2$	

Data collection

Rigaku Mercury2 diffractometer	5470 measured reflections
Radiation source: fine-focus sealed tube	1201 independent reflections
Graphite monochromator	633 reflections with $I > 2\sigma(I)$
Detector resolution: 13.6612 pixels mm^{-1}	$R_{int} = 0.105$
ω scans	$\theta_{max} = 26.0°$, $\theta_{min} = 3.7°$
Absorption correction: multi-scan	$h = -5\rightarrow5$
(*CrystalClear*; Rigaku, 2005)	$k = -19\rightarrow19$
$T_{min} = 0.981$, $T_{max} = 1.00$	$l = -9\rightarrow9$

Refinement

Refinement on F^2	1 restraint
Least-squares matrix: full	Primary atom site location: structure-invariant direct methods
$R[F^2 > 2\sigma(F^2)] = 0.061$	
$wR(F^2) = 0.136$	Secondary atom site location: difference Fourier map
$S = 1.03$	
1201 reflections	Hydrogen site location: inferred from neighbouring sites
155 parameters	

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.048P)^2]$

 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.15$ e Å^{-3}

$\Delta\rho_{min} = -0.18$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.0060 (10)	0.5064 (3)	0.8304 (7)	0.0474 (15)
C2	−0.0982 (11)	0.5462 (4)	0.6745 (9)	0.0580 (16)
C3	−0.2999 (13)	0.6076 (4)	0.6777 (10)	0.076 (2)
H3	−0.3594	0.6343	0.5747	0.091*
C4	−0.4118 (14)	0.6293 (4)	0.8306 (12)	0.0747 (19)
H4	−0.5453	0.6712	0.8303	0.090*
C5	−0.3320 (12)	0.5906 (4)	0.9860 (10)	0.073 (2)
H5	−0.4150	0.6047	1.0887	0.087*
C6	−0.1256 (11)	0.5303 (4)	0.9858 (8)	0.0639 (16)
H6	−0.0652	0.5052	1.0904	0.077*
C7	0.2044 (10)	0.4416 (3)	0.8361 (7)	0.0480 (14)
H7	0.2592	0.4179	0.9431	0.058*
C8	0.5180 (10)	0.3518 (3)	0.7054 (6)	0.0431 (14)
C9	0.6040 (10)	0.3216 (3)	0.5473 (7)	0.0526 (15)
C10	0.7977 (11)	0.2575 (4)	0.5400 (8)	0.0657 (17)
H10	0.8484	0.2375	0.4326	0.079*
C11	0.9127 (13)	0.2241 (4)	0.6912 (9)	0.0685 (18)
H11	1.0417	0.1812	0.6877	0.082*
C12	0.8365 (11)	0.2546 (4)	0.8477 (9)	0.0623 (17)
H12	0.9182	0.2324	0.9503	0.075*
C13	0.6393 (11)	0.3180 (3)	0.8582 (7)	0.0565 (15)
H13	0.5899	0.3373	0.9664	0.068*
C14	0.4758 (15)	0.3547 (5)	0.3888 (9)	0.093 (2)
N1	0.3182 (9)	0.4157 (2)	0.6972 (5)	0.0459 (11)
N2	0.3736 (15)	0.3796 (5)	0.2608 (8)	0.147 (3)
O1	0.0028 (9)	0.5256 (3)	0.5203 (5)	0.0815 (14)
H1	0.1174	0.4881	0.5348	0.122*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.040 (3)	0.047 (4)	0.055 (4)	−0.003 (3)	0.005 (3)	−0.002 (3)

C2	0.052 (3)	0.044 (4)	0.079 (5)	0.005 (3)	0.013 (3)	0.011 (3)
C3	0.067 (5)	0.068 (5)	0.094 (6)	0.010 (4)	0.014 (4)	0.020 (4)
C4	0.063 (4)	0.043 (4)	0.119 (6)	0.012 (4)	0.013 (4)	−0.001 (4)
C5	0.051 (4)	0.079 (5)	0.089 (5)	0.002 (3)	0.014 (4)	−0.029 (4)
C6	0.054 (4)	0.075 (5)	0.062 (4)	−0.004 (4)	−0.002 (3)	−0.020 (3)
C7	0.043 (3)	0.053 (4)	0.047 (4)	0.002 (3)	−0.003 (2)	−0.005 (3)
C8	0.046 (3)	0.042 (4)	0.042 (3)	−0.002 (3)	0.004 (2)	−0.006 (2)
C9	0.050 (3)	0.060 (4)	0.048 (4)	0.004 (3)	0.001 (3)	0.003 (3)
C10	0.065 (4)	0.068 (5)	0.065 (4)	0.009 (3)	0.005 (3)	−0.017 (3)
C11	0.060 (4)	0.072 (5)	0.073 (5)	0.007 (4)	0.004 (3)	−0.005 (4)
C12	0.056 (4)	0.052 (4)	0.080 (5)	0.010 (3)	0.006 (3)	0.017 (3)
C13	0.059 (4)	0.061 (4)	0.050 (4)	0.006 (3)	0.010 (3)	0.007 (3)
C14	0.093 (5)	0.135 (7)	0.052 (4)	0.042 (5)	0.005 (4)	−0.012 (4)
N1	0.049 (3)	0.041 (3)	0.048 (3)	−0.003 (2)	0.0079 (19)	0.000 (2)
N2	0.162 (7)	0.225 (9)	0.053 (4)	0.106 (6)	−0.002 (4)	0.010 (5)
O1	0.085 (3)	0.092 (4)	0.069 (3)	0.028 (2)	0.020 (2)	0.030 (2)

Geometric parameters (Å, º)

C1—C6	1.405 (7)	C8—C13	1.389 (7)
C1—C2	1.406 (7)	C8—C9	1.391 (6)
C1—C7	1.450 (6)	C8—N1	1.406 (6)
C2—O1	1.345 (7)	C9—C10	1.393 (7)
C2—C3	1.385 (8)	C9—C14	1.433 (9)
C3—C4	1.363 (9)	C10—C11	1.365 (8)
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.381 (9)	C11—C12	1.366 (8)
C4—H4	0.9300	C11—H11	0.9300
C5—C6	1.387 (8)	C12—C13	1.397 (7)
C5—H5	0.9300	C12—H12	0.9300
C6—H6	0.9300	C13—H13	0.9300
C7—N1	1.293 (5)	C14—N2	1.144 (7)
C7—H7	0.9300	O1—H1	0.8200
C6—C1—C2	118.3 (5)	C13—C8—C9	117.9 (5)
C6—C1—C7	119.1 (5)	C13—C8—N1	125.2 (5)
C2—C1—C7	122.6 (5)	C9—C8—N1	116.9 (4)
O1—C2—C3	118.5 (6)	C8—C9—C10	121.8 (5)
O1—C2—C1	121.7 (5)	C8—C9—C14	118.4 (5)
C3—C2—C1	119.8 (6)	C10—C9—C14	119.7 (5)
C4—C3—C2	120.5 (6)	C11—C10—C9	119.7 (6)
C4—C3—H3	119.8	C11—C10—H10	120.2
C2—C3—H3	119.8	C9—C10—H10	120.2
C3—C4—C5	121.6 (6)	C10—C11—C12	119.3 (6)
C3—C4—H4	119.2	C10—C11—H11	120.3
C5—C4—H4	119.2	C12—C11—H11	120.3
C4—C5—C6	118.6 (6)	C11—C12—C13	122.0 (6)
C4—C5—H5	120.7	C11—C12—H12	119.0

C6—C5—H5	120.7	C13—C12—H12	119.0
C5—C6—C1	121.2 (6)	C8—C13—C12	119.3 (5)
C5—C6—H6	119.4	C8—C13—H13	120.3
C1—C6—H6	119.4	C12—C13—H13	120.3
N1—C7—C1	122.1 (4)	N2—C14—C9	178.6 (8)
N1—C7—H7	118.9	C7—N1—C8	121.1 (4)
C1—C7—H7	118.9	C2—O1—H1	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.92	2.651 (6)	147