Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(2-Hydroxybenzylideneamino)-benzonitrile

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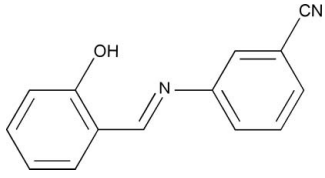
Received 21 January 2008; accepted 25 February 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.056; wR factor = 0.122; data-to-parameter ratio = 8.4.

In the title molecule, $C_{14}H_{10}N_2O$, an intramolecular O—H···N hydrogen bond contributes to the essential coplanarity of the two benzene rings, which form a dihedral angle of 6.04 (18)°.

Related literature

For related crystal structures, see: Kosar *et al.* (2005); Cheng *et al.* (2005, 2006).



Experimental

Crystal data

$C_{14}H_{10}N_2O$
M_r = 222.24
Orthorhombic, $Pca2_1$
a = 26.397 (5) Å
b = 3.9211 (8) Å
c = 10.773 (2) Å
V = 1115.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.22 × 0.05 × 0.05 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.812, T_{max} = 1.000
(expected range = 0.809–0.996)
9995 measured reflections
1339 independent reflections
901 reflections with $I > 2\sigma(I)$
R_{int} = 0.116

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.121
S = 1.05
1339 reflections
160 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1B···N1	0.82 (2)	1.89 (4)	2.623 (4)	149 (7)

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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

HJX acknowledges a Start-up Grant from Southeast University, People's Republic of China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2384).

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supplementary materials

Acta Cryst. (2008). E**64**, o638 [**doi:10.1107/S1600536808005242**]

3-(2-Hydroxybenzylideneamino)benzonitrile

H.-J. Xu, X.-X. Gong and H. Wang

Comment

Schiff base compounds have attracted great attention for many years. These compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism, photochromism and thermochromism. Here, we report the crystal structure of the title compound.

In the title compound (Fig. 1), all bond lengths are within normal ranges. The C7=N1 bond length of 1.277 (4)Å is a typical double bond, similar to the corresponding bond lengths in 4-methoxy-2-[(4-nitrophenyl)iminomethyl]phenol (Kosar *et al.*, 2005). The molecule is almost planar and displays a *trans* configuration with respect to the C7=N1 double bond. The dihedral angle between the benzene rings is 6.04 (18)°. Strong intramolecular O—H···N hydrogen-bond interaction (Talbe I), similar to the reported earlier (Cheng *et al.*, 2005, 2006), is observed in the molecule.

Experimental

3-Aminobenzonitrile and salicylaldehyde were available commercially and were used without further purification. 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 crystals were obtained by recrystallization from ethyl alcohol (yield: 82%). For the X-ray diffraction analysis, suitable single crystals were obtained after one week by slow evaporation from an ethyl alcohol solution.

Refinement

C-bound H atoms were geometrically positioned (C—H 0.93 Å) and refined as riding with U_{iso}(H)= 1.2Ueq(C). Atom H1B was located on a difference map and refined isotropically with bon restraint O1—H1B = 0.82 (2) Å. In the absence of significant anomalous scatterers, 1124 Friedel pairs were merged.

Figures

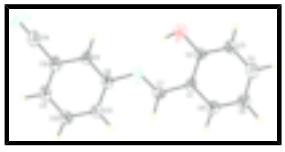

Fig. 1. The molecular structure of the title compound with atomic numbering and displacement ellipsoids drawn at the 30% probability level.

3-(2-Hydroxybenzylideneamino)benzonitrile

Crystal data

$C_{14}H_{10}N_2O$ F_{000} = 464

M_r = 222.24	D_x = 1.324 Mg m^{-3}
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2c -2ac	Cell parameters from 8294 reflections
a = 26.397 (5) Å	θ = 3.0–27.6º
b = 3.9211 (8) Å	μ = 0.09 mm^{-1}
c = 10.773 (2) Å	T = 293 (2) K
V = 1115.1 (4) Å^3	Stick, yellow
Z = 4	0.22 × 0.05 × 0.05 mm

Data collection

Rigaku Mercury2 diffractometer	1339 independent reflections
Radiation source: fine-focus sealed tube	901 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.116
Detector resolution: 13.6612 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 3.1º
ω scans	h = −34→34
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	k = −5→5
T_{min} = 0.812, T_{max} = 1.00	l = −13→13
9995 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.056	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.121	$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
1339 reflections	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
160 parameters	$\Delta\rho_{min}$ = −0.16 e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
N1	0.45687 (11)	0.2218 (7)	0.2697 (3)	0.0473 (8)
C1	0.54425 (12)	0.2407 (8)	0.3273 (3)	0.0427 (8)
C9	0.37076 (12)	0.2616 (9)	0.2071 (3)	0.0457 (9)
H9A	0.3823	0.3718	0.1360	0.055*
C6	0.57995 (14)	0.1614 (9)	0.4188 (3)	0.0559 (10)
H6A	0.5694	0.0602	0.4924	0.067*
C8	0.40534 (12)	0.1480 (8)	0.2952 (3)	0.0451 (8)
C7	0.49124 (12)	0.1608 (8)	0.3501 (3)	0.0460 (9)
H7A	0.4821	0.0624	0.4254	0.055*
C3	0.61133 (14)	0.4649 (10)	0.2017 (3)	0.0570 (11)
H3A	0.6223	0.5715	0.1294	0.068*
C2	0.56072 (13)	0.3894 (9)	0.2167 (3)	0.0468 (9)
C12	0.33597 (14)	−0.0682 (10)	0.4162 (4)	0.0601 (10)
H12A	0.3245	−0.1800	0.4869	0.072*
C10	0.31905 (13)	0.2118 (9)	0.2243 (3)	0.0510 (10)
C11	0.30193 (13)	0.0476 (9)	0.3297 (3)	0.0572 (11)
H11A	0.2674	0.0157	0.3421	0.069*
C14	0.28378 (13)	0.3427 (10)	0.1343 (4)	0.0585 (10)
O1	0.52789 (11)	0.4688 (8)	0.1250 (3)	0.0683 (8)
C5	0.63050 (14)	0.2312 (10)	0.4013 (4)	0.0629 (11)
H5A	0.6540	0.1756	0.4622	0.076*
C4	0.64585 (14)	0.3839 (10)	0.2928 (4)	0.0632 (11)
H4A	0.6800	0.4331	0.2808	0.076*
C13	0.38733 (13)	−0.0193 (10)	0.3986 (3)	0.0542 (10)
H13A	0.4101	−0.1006	0.4575	0.065*
N2	0.25591 (14)	0.4542 (10)	0.0648 (4)	0.0896 (13)
H1B	0.4999 (10)	0.396 (12)	0.145 (7)	0.13 (2)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0426 (18)	0.0517 (18)	0.0474 (16)	0.0006 (13)	−0.0038 (14)	−0.0007 (13)
C1	0.038 (2)	0.0449 (17)	0.045 (2)	0.0021 (14)	0.0015 (17)	−0.0035 (16)
C9	0.042 (2)	0.048 (2)	0.046 (2)	0.0029 (16)	0.0022 (17)	−0.0027 (17)
C6	0.053 (2)	0.058 (2)	0.057 (2)	0.0006 (18)	−0.005 (2)	0.0031 (19)
C8	0.0392 (19)	0.0456 (19)	0.051 (2)	−0.0018 (15)	0.0032 (17)	−0.0088 (17)
C7	0.052 (2)	0.0445 (19)	0.042 (2)	0.0000 (16)	0.0045 (17)	0.0015 (17)
C3	0.054 (3)	0.061 (3)	0.056 (2)	−0.0065 (18)	0.0091 (19)	−0.0002 (19)
C2	0.047 (2)	0.051 (2)	0.042 (2)	−0.0009 (16)	0.0012 (16)	−0.0012 (18)

C12	0.056 (2)	0.065 (3)	0.060 (2)	−0.0083 (19)	0.006 (2)	0.006 (2)
C10	0.042 (2)	0.054 (2)	0.057 (2)	0.0035 (17)	0.0024 (19)	−0.0148 (19)
C11	0.0399 (19)	0.061 (2)	0.071 (3)	−0.0074 (17)	0.0068 (19)	−0.013 (2)
C14	0.044 (2)	0.065 (3)	0.067 (2)	0.0038 (18)	−0.006 (2)	−0.011 (2)
O1	0.0590 (17)	0.092 (2)	0.0540 (15)	−0.0015 (16)	−0.0059 (17)	0.0190 (16)
C5	0.049 (2)	0.070 (3)	0.070 (3)	0.007 (2)	−0.011 (2)	0.002 (2)
C4	0.047 (2)	0.064 (2)	0.079 (3)	−0.0066 (19)	0.004 (2)	−0.008 (2)
C13	0.047 (2)	0.060 (2)	0.056 (2)	−0.0005 (17)	0.0015 (18)	0.007 (2)
N2	0.066 (2)	0.097 (3)	0.105 (3)	0.012 (2)	−0.032 (2)	−0.004 (2)

Geometric parameters (Å, °)

N1—C7	1.277 (4)	C3—H3A	0.9300
N1—C8	1.418 (4)	C2—O1	1.351 (4)
C1—C2	1.396 (4)	C12—C11	1.372 (5)
C1—C6	1.398 (5)	C12—C13	1.382 (5)
C1—C7	1.455 (4)	C12—H12A	0.9300
C9—C8	1.390 (4)	C10—C11	1.381 (5)
C9—C10	1.391 (4)	C10—C14	1.439 (5)
C9—H9A	0.9300	C11—H11A	0.9300
C6—C5	1.375 (5)	C14—N2	1.137 (5)
C6—H6A	0.9300	O1—H1B	0.82 (2)
C8—C13	1.377 (5)	C5—C4	1.374 (5)
C7—H7A	0.9300	C5—H5A	0.9300
C3—C4	1.376 (5)	C4—H4A	0.9300
C3—C2	1.378 (4)	C13—H13A	0.9300
C7—N1—C8	120.8 (3)	C3—C2—C1	119.5 (3)
C2—C1—C6	119.0 (3)	C11—C12—C13	120.2 (3)
C2—C1—C7	122.2 (3)	C11—C12—H12A	119.9
C6—C1—C7	118.8 (3)	C13—C12—H12A	119.9
C8—C9—C10	120.5 (3)	C11—C10—C9	119.8 (3)
C8—C9—H9A	119.7	C11—C10—C14	120.6 (3)
C10—C9—H9A	119.7	C9—C10—C14	119.6 (4)
C5—C6—C1	120.9 (4)	C12—C11—C10	119.9 (3)
C5—C6—H6A	119.6	C12—C11—H11A	120.1
C1—C6—H6A	119.6	C10—C11—H11A	120.1
C13—C8—C9	118.6 (3)	N2—C14—C10	178.2 (5)
C13—C8—N1	125.8 (3)	C2—O1—H1B	108 (5)
C9—C8—N1	115.6 (3)	C4—C5—C6	119.3 (4)
N1—C7—C1	121.9 (3)	C4—C5—H5A	120.4
N1—C7—H7A	119.0	C6—C5—H5A	120.4
C1—C7—H7A	119.0	C3—C4—C5	120.8 (3)
C4—C3—C2	120.5 (4)	C3—C4—H4A	119.6
C4—C3—H3A	119.7	C5—C4—H4A	119.6
C2—C3—H3A	119.7	C12—C13—C8	121.0 (3)
O1—C2—C3	119.1 (3)	C12—C13—H13A	119.5
O1—C2—C1	121.4 (3)	C8—C13—H13A	119.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1B···N1	0.82 (2)	1.89 (4)	2.623 (4)	149 (7)

Fig. 1