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2-(Hydrazonomethyl)phenol

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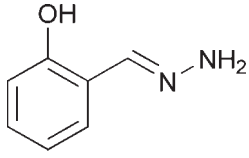
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.110; data-to-parameter ratio = 12.9.

The conformation of the title compound, $C_7H_8N_2O$, is stabilized by an intramolecular O—H···N hydrogen bond. The crystal structure shows intermolecular N—H···O hydrogen bonds.

Related literature

For Schiff bases as mixed-donor ligands in coordination chemistry, see: Lee *et al.* (2005). For the pharmaceutical and medicinal activity of Schiff bases, see: Sriram *et al.* (2006); Hao (2009); Bedia *et al.* (2006).



Experimental

Crystal data

$C_7H_8N_2O$
M_r = 136.15
Monoclinic, $P2_1/c$
a = 14.1010 (11) Å
b = 6.0062 (5) Å
c = 8.1979 (6) Å
β = 102.5250 (10)°
V = 677.78 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.46 × 0.45 × 0.35 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.959, T_{max} = 0.968
3351 measured reflections
1203 independent reflections
1081 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.110
S = 1.06
1203 reflections
93 parameters
.
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.86	2.56	3.3076 (17)	145
N2—H2B···O1^{ii}	0.86	2.23	3.0530 (16)	160
O1—H1···N1	0.82	1.89	2.6109 (15)	147

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* (Sheldrick, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5112).

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supporting information

Acta Cryst. (2009). E**65**, o3023 [doi:10.1107/S1600536809045504]

2-(Hydrazonomethyl)phenol

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S1. Comment

Schiff bases are one of the most prevalent and important mixed-donor ligand in coordination chemistry (Lee *et al.*, 2005). Recently, the synthesis, structure and properties of Schiff base complexes have stimulated much more interest for their noteworthy contributions in pharmaceutical and medicinal activity (Sriram *et al.*, 2006; Hao 2009; Bedia *et al.*, 2006).

The X-ray structural analysis confirmed the assignment of the structure of the title compound(I). The molecular structure is depicted in Fig. 1, and the crystal packing of the title compound(I) is depicted in Fig. 2. In the crystal structure,intermolecular N—H···O, N—H···N and intramolecular O—H···N hydrogen bonds contribute to form the title compound(I).

S2. Experimental

35% of hydrazine hydrate (0.50 mL, 10 mmol) and salicylidence (0.52 mL, 5 mmol) were mixed in 50.0 mL ethanol and refluxed for 3 h. When the solution was cooled to room temperature, a light yellow solid was obtained, and light yellow block shaped crystals were formed from the filtrate by slow evaporation of the solution in air after a few days. The yield of the isolated yellow solid was 0.62 g.(90%).

S3. Refinement

H atoms attached to C were placed in geometrically idealized positions with Csp^2—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). H atoms bonded to N and O were located in a difference map. They were refined using a riding model with O—H = 0.82 Å and N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N) or 1.5U_{eq}(O).

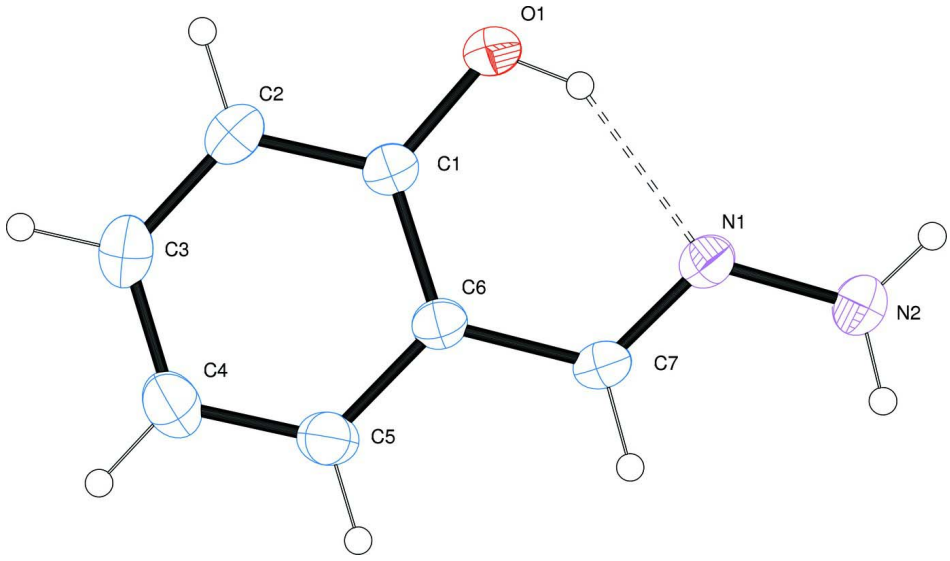

Figure 1

A view of the title compound with displacement ellipsoids drawn at the 30% probability level. Dashed line indicates hydrogen bonding interactions.

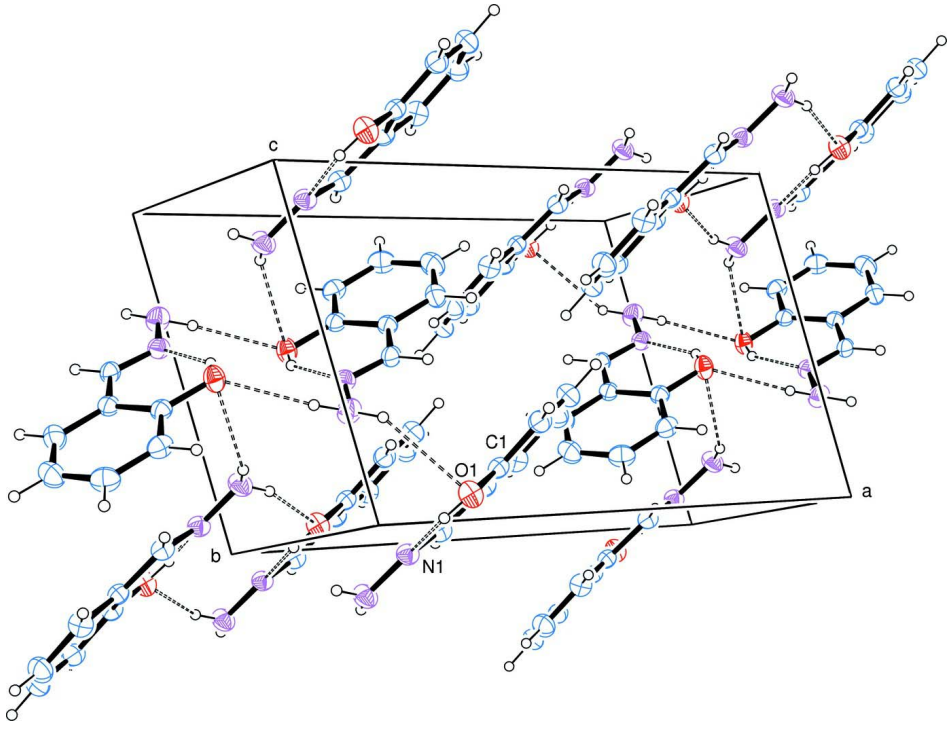

Figure 2

Crystal packing of the title compound.

2-(Hydrazonomethyl)phenol

Crystal data

$C_7H_8N_2O$
$M_r = 136.15$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.1010\ (11)$ Å
$b = 6.0062\ (5)$ Å
$c = 8.1979\ (6)$ Å
$\beta = 102.525\ (1)°$
$V = 677.78\ (9)$ Å^3
$Z = 4$
$F(000) = 288$
$D_x = 1.334$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2298 reflections
$\theta = 3.0–28.4°$
$\mu = 0.09$ mm^{-1}
$T = 296$ K
Block, yellow
0.46 × 0.45 × 0.35 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.959$, $T_{max} = 0.968$
3351 measured reflections
1203 independent reflections
1081 reflections with $I > 2\sigma(I)$
$R_{int} = 0.013$
$\theta_{max} = 25.1°$, $\theta_{min} = 3.0°$
$h = -15\rightarrow16$
$k = -6\rightarrow7$
$l = -9\rightarrow8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.110$
$S = 1.06$
1203 reflections
93 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.1774P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.129 (12)

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 $F^2 > \sigma(F^2)$ 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}
C1	0.22022 (10)	−0.1162 (2)	0.13139 (16)	0.0374 (4)
C2	0.27892 (11)	−0.2576 (3)	0.24310 (18)	0.0462 (4)
H2	0.2554	−0.3958	0.2670	0.055*

C3	0.37226 (12)	−0.1944 (3)	0.3192 (2)	0.0546 (5)
H3	0.4111	−0.2898	0.3948	0.065*
C4	0.40836 (11)	0.0097 (3)	0.2837 (2)	0.0568 (5)
H4	0.4715	0.0513	0.3339	0.068*
C5	0.34970 (11)	0.1512 (3)	0.17277 (19)	0.0487 (4)
H5	0.3743	0.2881	0.1487	0.058*
C6	0.25465 (9)	0.0945 (2)	0.09582 (16)	0.0372 (4)
C7	0.19290 (10)	0.2536 (2)	−0.01248 (16)	0.0392 (4)
H7	0.2190	0.3883	−0.0376	0.047*
N1	0.10354 (8)	0.21085 (19)	−0.07344 (14)	0.0407 (3)
N2	0.04759 (9)	0.3659 (2)	−0.17427 (15)	0.0507 (4)
H2A	0.0693	0.4889	−0.2059	0.061*
H2B	−0.0089	0.3460	−0.1530	0.061*
O1	0.12928 (7)	−0.18636 (16)	0.05811 (13)	0.0476 (3)
H1	0.0993	−0.0840	0.0039	0.071*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0428 (8)	0.0355 (7)	0.0358 (7)	−0.0005 (6)	0.0127 (6)	−0.0036 (5)
C2	0.0587 (9)	0.0381 (8)	0.0439 (8)	0.0040 (6)	0.0157 (7)	0.0026 (6)
C3	0.0576 (10)	0.0566 (10)	0.0467 (9)	0.0148 (8)	0.0050 (7)	0.0038 (7)
C4	0.0439 (8)	0.0645 (11)	0.0574 (10)	0.0009 (8)	0.0007 (7)	−0.0041 (8)
C5	0.0468 (8)	0.0447 (8)	0.0543 (9)	−0.0070 (6)	0.0106 (7)	−0.0034 (7)
C6	0.0418 (7)	0.0351 (7)	0.0363 (7)	−0.0016 (6)	0.0118 (5)	−0.0038 (5)
C7	0.0471 (8)	0.0323 (7)	0.0399 (7)	−0.0060 (6)	0.0130 (6)	0.0003 (6)
N1	0.0468 (7)	0.0364 (6)	0.0385 (6)	−0.0013 (5)	0.0083 (5)	0.0020 (5)
N2	0.0523 (8)	0.0466 (8)	0.0522 (8)	0.0037 (6)	0.0092 (6)	0.0140 (6)
O1	0.0451 (6)	0.0353 (6)	0.0607 (7)	−0.0054 (4)	0.0078 (5)	0.0039 (5)

Geometric parameters (Å, º)

C1—O1	1.3597 (16)	C5—C6	1.3941 (19)
C1—C2	1.384 (2)	C5—H5	0.9300
C1—C6	1.409 (2)	C6—C7	1.4574 (19)
C2—C3	1.382 (2)	C7—N1	1.2768 (18)
C2—H2	0.9300	C7—H7	0.9300
C3—C4	1.382 (2)	N1—N2	1.3749 (16)
C3—H3	0.9300	N2—H2A	0.8604
C4—C5	1.381 (2)	N2—H2B	0.8604
C4—H4	0.9300	O1—H1	0.8200
O1—C1—C2	118.26 (12)	C4—C5—H5	119.1
O1—C1—C6	121.42 (12)	C6—C5—H5	119.1
C2—C1—C6	120.32 (13)	C5—C6—C1	117.79 (13)
C3—C2—C1	120.28 (14)	C5—C6—C7	120.29 (13)
C3—C2—H2	119.9	C1—C6—C7	121.88 (12)
C1—C2—H2	119.9	N1—C7—C6	121.00 (12)

C2—C3—C4	120.46 (15)	N1—C7—H7	119.5
C2—C3—H3	119.8	C6—C7—H7	119.5
C4—C3—H3	119.8	C7—N1—N2	119.21 (12)
C5—C4—C3	119.27 (15)	N1—N2—H2A	124.6
C5—C4—H4	120.4	N1—N2—H2B	102.7
C3—C4—H4	120.4	H2A—N2—H2B	125.9
C4—C5—C6	121.86 (14)	C1—O1—H1	109.5
O1—C1—C2—C3	179.29 (13)	O1—C1—C6—C5	−178.27 (12)
C6—C1—C2—C3	−0.8 (2)	C2—C1—C6—C5	1.82 (19)
C1—C2—C3—C4	−0.5 (2)	O1—C1—C6—C7	4.02 (19)
C2—C3—C4—C5	0.8 (2)	C2—C1—C6—C7	−175.89 (12)
C3—C4—C5—C6	0.3 (2)	C5—C6—C7—N1	−174.54 (13)
C4—C5—C6—C1	−1.6 (2)	C1—C6—C7—N1	3.1 (2)
C4—C5—C6—C7	176.17 (13)	C6—C7—N1—N2	179.61 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1^{i}	0.86	2.56	3.3076 (17)	145
N2—H2*B*···O1^{ii}	0.86	2.23	3.0530 (16)	160
O1—H1···N1	0.82	1.89	2.6109 (15)	147

Symmetry codes: (i) x, $-y+1/2$, $z-1/2$; (ii) $-x$, $-y$, $-z$.