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3-Hydroxy-*N*′-(2-hydroxybenzylidene)-benzohydrazide

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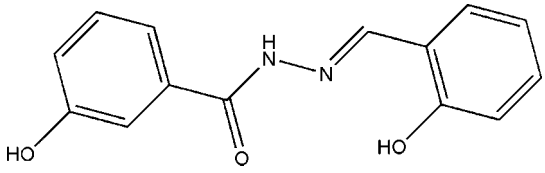
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.119; data-to-parameter ratio = 15.4.

The title compound, $C_{14}H_{12}N_2O_3$, was synthesized by the condensation of salicylaldehyde with 3-hydroxybenzohydrazide. The dihedral angle between the two benzene rings is 12.4 (2)°. The 2-hydroxy group forms an intramolecular O—H···N hydrogen bond with the imide N atom. Molecules are linked through intermolecular O—H···O and N—H···O hydrogen bonds into a two-dimensional polymeric structure parallel to the *ab* plane.

Related literature

For related literature, see: Ali *et al.* (2005); Eltayeb *et al.* (2008); Habibi *et al.* (2007); Jing *et al.* (2006); Ling *et al.* (2008); Peng & You (2007); Peng & Zhou (2007); Peng, Ping & Song (2007); Peng, Yang & Zhou (2006); Peng, Zhou & Yang (2006); Yehye *et al.* (2008*a*,*b*).



Experimental

Crystal data

$C_{14}H_{12}N_2O_3$
M_r = 256.26
Orthorhombic, *Pbca*
a = 14.405 (2) Å
b = 9.661 (1) Å
c = 17.905 (2) Å
V = 2491.8 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.23 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.978, T_{max} = 0.981
13415 measured reflections
2720 independent reflections
1869 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.118
S = 1.03
2720 reflections
177 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.13 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	1.88	2.6010 (19)	146
O3—H3···O2^{i}	0.82	1.81	2.5946 (16)	159
N2—H2···O3^{ii}	0.895 (9)	2.119 (10)	3.0062 (18)	171.0 (18)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2164).

References

Ali, H. M., Kamalul Aripin, N. F. & Ng, S. W. (2005). *Acta Cryst.* E**61**, m433–m434.
Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Eltayeb, N. E., Teoh, S. G., Chantrapromma, S., Fun, H.-K. & Adnan, R. (2008). *Acta Cryst.* E**64**, m912–m913.
Habibi, M. H., Montazerozohori, M., Lalegani, A., Mokhtari, R., Harrington, R. W. & Clegg, W. (2007). *Acta Cryst.* E**63**, m2933–m2934.
Jing, Z.-L., Zhao, Y.-L., Chen, X. & Yu, M. (2006). *Acta Cryst.* E**62**, o4087–o4088.
Ling, C.-H., Chen, Y.-B., Huang, J.-A., Ji, C. & Liu, P. (2008). *Acta Cryst.* E**64**, o948.
Peng, S.-J., Ping, W.-J. & Song, L.-B. (2007). *Z. Kristallogr. New Cryst. S*truct. **222**, 425–426.
Peng, S.-J., Yang, T. & Zhou, C.-S. (2006). *Acta Cryst.* E**62**, m235–m236.
Peng, S.-J. & You, Z.-L. (2007). *J. Chem. Crystallogr.* **37**, 415–419.
Peng, S.-J. & Zhou, C.-S. (2007). *Acta Cryst.* E**63**, m3185.
Peng, S.-J., Zhou, C.-S. & Yang, T. (2006). *Acta Cryst.* E**62**, m1147–m1149.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yehye, W. A., Ariffin, A. & Ng, S. W. (2008*a*). *Acta Cryst.* E**64**, o960.
Yehye, W. A., Ariffin, A. & Ng, S. W. (2008*b*). *Acta Cryst.* E**64**, o1452.

supporting information

Acta Cryst. (2008). E**64**, o1864 [doi:10.1107/S1600536808027426]

3-Hydroxy-*N*′-(2-hydroxybenzylidene)benzohydrazide

San-Jun Peng and Hai-Yun Hou

S1. Comment

Schiff bases derived from the condensation of aldehydes with primary amines play an important role in coordination chemistry (Ali *et al.*, 2005; Eltayeb *et al.*, 2008; Habibi *et al.*, 2007). Recently, we have reported synthesis and crystal structure of some Schiff base complexes (Peng, Yang & Zhou, 2006; Peng, Zhou & Yang, 2006; Peng *et al.*, 2007; Peng & You, 2007; Peng & Zhou, 2007). We report herein the crystal structure of the title compound, Fig. 1.

All the bond lengths are comparable to those observed in other similar compounds (Yehye *et al.*, 2008*a,b*; Jing *et al.*, 2006; Ling *et al.*, 2008). The molecule is not planar and the dihedral angle between the two benzene rings is 12.4 (2)°. There is an intramolecular O–H···N hydrogen bond (Table 1) in each molecule of the compound. The molecules are linked through intermolecular O–H···O and N–H···O hydrogen bonds (Table 1), forming layers parallel to the *ab* plane (Fig. 2).

S2. Experimental

3-Hydroxybenzohydrazide (0.1 mmol, 15.2 mg) and salicylaldehyde (0.1 mmol, 12.2 mg) were stirred at 318 K in methanol (10 ml) for 30 min. The filtrate was kept open to slowly evaporate for a few days, depositing colorless block-like crystals of the title compound.

S3. Refinement

The atom H2 attached to N2 was located in a difference Fourier map and refined with N–H distance restrained to 0.90 (1) Å, and with U_{iso} set to 0.08 Å^2. All H atoms bound to carbon and oxygen were refined using riding models with d(C–H) = 0.93 Å, d(O–H) = 0.82 Å, U_{iso} = 1.2U_{eq}(C) and 1.5U_{eq}(O).

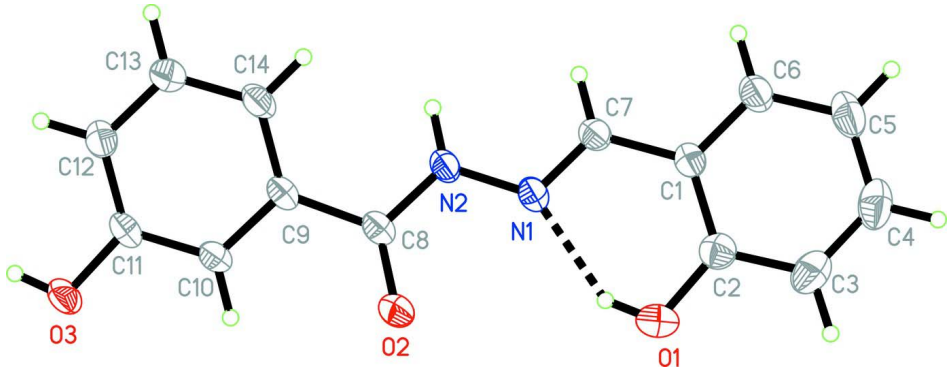

Figure 1

The molecular structure of the title compound, showing the atom-numbering scheme and 30% probability displacement ellipsoids. H atoms are shown as spheres of arbitrary radii.

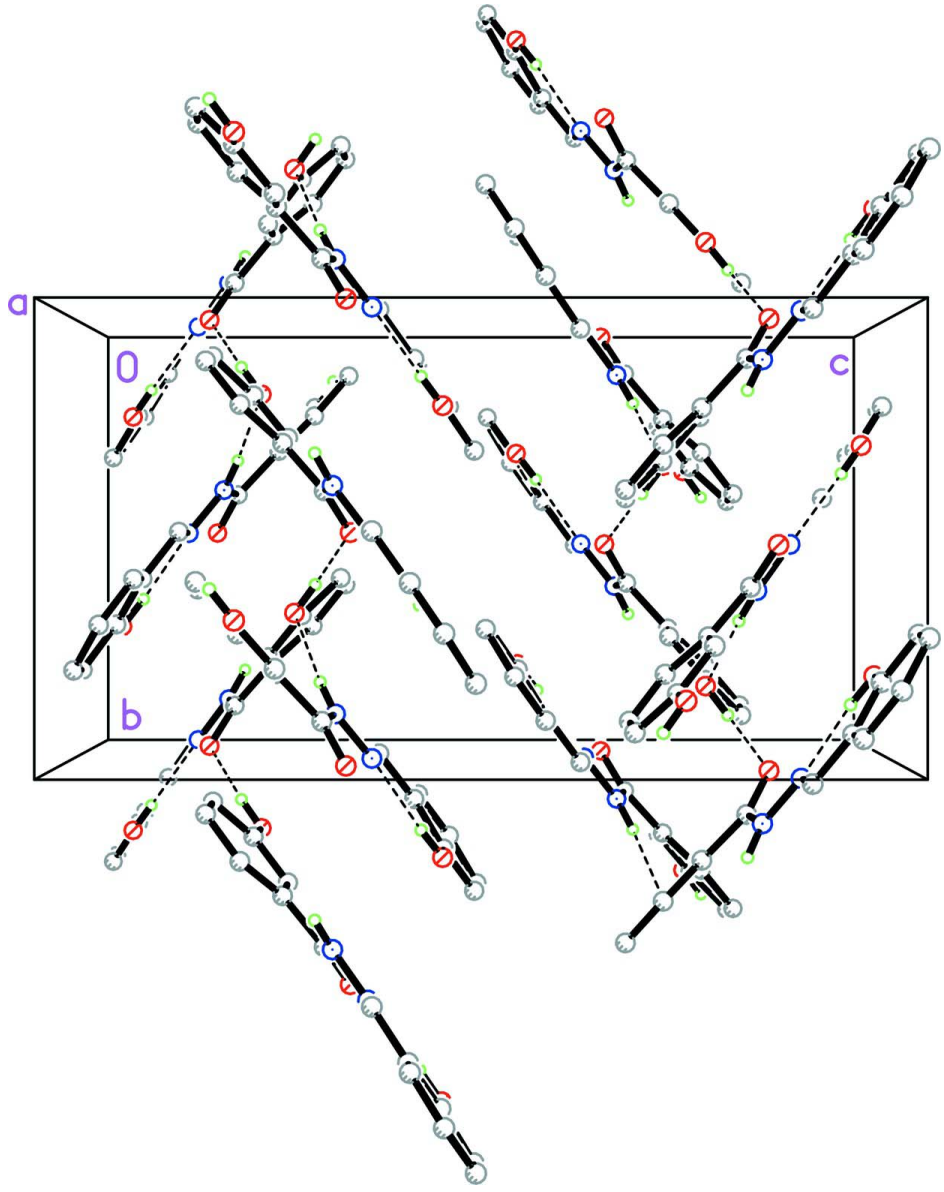

Figure 2

Packing diagram, viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

3-Hydroxy-*N*′-(2-hydroxybenzylidene)benzohydrazide

Crystal data

$C_{14}H_{12}N_2O_3$
$M_r = 256.26$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 14.405$ (2) Å
$b = 9.661$ (1) Å
$c = 17.905$ (2) Å
$V = 2491.8$ (5) Å^3
$Z = 8$
$F(000) = 1072$
$D_x = 1.366$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3092 reflections
$\theta = 2.7$–$26.0°$
$\mu = 0.10$ mm^{-1}
$T = 298$ K
Block, colorless
0.23 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.978, T_{max} = 0.981
13415 measured reflections
2720 independent reflections
1869 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 27.0°, θ_{min} = 2.3°
h = −15→18
k = −11→12
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.119
S = 1.03
2720 reflections
177 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 0.3997P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
O1	0.16163 (8)	1.20579 (14)	0.04590 (8)	0.0677 (4)
H1	0.1829	1.1427	0.0713	0.102*
O2	0.33625 (7)	0.98665 (12)	0.15618 (6)	0.0524 (3)
O3	0.56381 (7)	0.66767 (12)	0.27314 (7)	0.0548 (3)
H3	0.5826	0.6036	0.2991	0.082*
N1	0.15527 (8)	0.98711 (13)	0.13048 (7)	0.0419 (3)
N2	0.19669 (8)	0.88568 (13)	0.17276 (8)	0.0436 (3)
C1	0.01929 (10)	1.09152 (16)	0.08195 (8)	0.0409 (4)
C2	0.06764 (12)	1.19810 (18)	0.04586 (9)	0.0493 (4)
C3	0.01833 (15)	1.3000 (2)	0.00834 (11)	0.0668 (5)
H3A	0.0501	1.3716	−0.0152	0.080*
C4	−0.07686 (16)	1.2964 (2)	0.00557 (11)	0.0709 (6)
H4	−0.1089	1.3653	−0.0200	0.085*
C5	−0.12534 (13)	1.1922 (2)	0.04022 (11)	0.0663 (6)
H5	−0.1898	1.1900	0.0380	0.080*

C6	−0.07735 (11)	1.0909 (2)	0.07839 (9)	0.0533 (4)
H6	−0.1102	1.0207	0.1022	0.064*
C7	0.06694 (10)	0.98419 (16)	0.12381 (9)	0.0423 (4)
H7	0.0331	0.9131	0.1458	0.051*
C8	0.28882 (10)	0.89504 (16)	0.18561 (8)	0.0411 (4)
C9	0.32990 (9)	0.78911 (16)	0.23665 (9)	0.0396 (4)
C10	0.42602 (10)	0.77388 (16)	0.23447 (9)	0.0402 (4)
H10	0.4612	0.8302	0.2033	0.048*
C11	0.46926 (9)	0.67575 (16)	0.27832 (9)	0.0407 (4)
C12	0.41777 (11)	0.59119 (18)	0.32492 (9)	0.0474 (4)
H12	0.4468	0.5240	0.3538	0.057*
C13	0.32267 (11)	0.6079 (2)	0.32798 (10)	0.0561 (5)
H13	0.2878	0.5519	0.3596	0.067*
C14	0.27860 (11)	0.70631 (19)	0.28484 (9)	0.0517 (4)
H14	0.2146	0.7172	0.2880	0.062*
H2	0.1622 (12)	0.8175 (16)	0.1921 (11)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0516 (7)	0.0702 (10)	0.0815 (10)	−0.0133 (6)	0.0067 (6)	0.0162 (7)
O2	0.0375 (6)	0.0518 (7)	0.0680 (8)	−0.0079 (5)	−0.0066 (5)	0.0050 (6)
O3	0.0286 (5)	0.0524 (7)	0.0835 (9)	0.0054 (5)	−0.0026 (5)	0.0072 (6)
N1	0.0331 (6)	0.0436 (8)	0.0488 (7)	0.0030 (5)	−0.0044 (5)	−0.0028 (6)
N2	0.0297 (6)	0.0423 (8)	0.0586 (8)	0.0007 (5)	−0.0060 (6)	0.0025 (6)
C1	0.0378 (8)	0.0462 (9)	0.0387 (8)	0.0039 (7)	−0.0007 (6)	−0.0018 (7)
C2	0.0507 (10)	0.0523 (10)	0.0448 (9)	−0.0009 (8)	0.0011 (7)	−0.0004 (8)
C3	0.0846 (15)	0.0592 (12)	0.0566 (11)	0.0036 (10)	0.0013 (10)	0.0144 (9)
C4	0.0794 (14)	0.0749 (14)	0.0583 (12)	0.0259 (11)	−0.0111 (11)	0.0105 (10)
C5	0.0491 (10)	0.0885 (15)	0.0614 (12)	0.0206 (10)	−0.0073 (9)	0.0031 (11)
C6	0.0401 (9)	0.0672 (12)	0.0525 (10)	0.0064 (8)	−0.0014 (7)	0.0054 (9)
C7	0.0359 (8)	0.0434 (9)	0.0476 (9)	−0.0005 (6)	0.0000 (7)	0.0001 (7)
C8	0.0312 (7)	0.0424 (9)	0.0497 (9)	−0.0003 (7)	−0.0027 (6)	−0.0081 (7)
C9	0.0286 (7)	0.0440 (9)	0.0461 (8)	−0.0005 (6)	−0.0040 (6)	−0.0075 (7)
C10	0.0296 (7)	0.0395 (8)	0.0516 (9)	−0.0022 (6)	0.0002 (6)	−0.0050 (7)
C11	0.0275 (7)	0.0417 (8)	0.0529 (9)	0.0026 (6)	−0.0050 (7)	−0.0113 (7)
C12	0.0414 (8)	0.0540 (10)	0.0467 (9)	0.0054 (7)	−0.0046 (7)	0.0004 (8)
C13	0.0394 (9)	0.0740 (13)	0.0548 (10)	−0.0012 (8)	0.0048 (7)	0.0130 (9)
C14	0.0282 (7)	0.0729 (12)	0.0541 (10)	0.0016 (7)	0.0006 (7)	0.0026 (9)

Geometric parameters (Å, º)

O1—C2	1.356 (2)	C4—H4	0.9300
O1—H1	0.8200	C5—C6	1.380 (3)
O2—C8	1.2360 (18)	C5—H5	0.9300
O3—C11	1.3673 (17)	C6—H6	0.9300
O3—H3	0.8200	C7—H7	0.9300
N1—C7	1.2784 (18)	C8—C9	1.494 (2)

N1—N2	1.3745 (18)	C9—C14	1.389 (2)
N2—C8	1.3499 (18)	C9—C10	1.3928 (19)
N2—H2	0.895 (9)	C10—C11	1.379 (2)
C1—C6	1.394 (2)	C10—H10	0.9300
C1—C2	1.401 (2)	C11—C12	1.383 (2)
C1—C7	1.452 (2)	C12—C13	1.380 (2)
C2—C3	1.388 (2)	C12—H12	0.9300
C3—C4	1.373 (3)	C13—C14	1.380 (2)
C3—H3A	0.9300	C13—H13	0.9300
C4—C5	1.373 (3)	C14—H14	0.9300
C2—O1—H1	109.5	N1—C7—C1	120.20 (14)
C11—O3—H3	109.5	N1—C7—H7	119.9
C7—N1—N2	117.88 (13)	C1—C7—H7	119.9
C8—N2—N1	118.21 (13)	O2—C8—N2	121.25 (14)
C8—N2—H2	122.0 (13)	O2—C8—C9	122.15 (13)
N1—N2—H2	119.8 (13)	N2—C8—C9	116.60 (13)
C6—C1—C2	118.60 (15)	C14—C9—C10	119.03 (14)
C6—C1—C7	119.53 (15)	C14—C9—C8	124.29 (13)
C2—C1—C7	121.86 (14)	C10—C9—C8	116.68 (13)
O1—C2—C3	118.19 (16)	C11—C10—C9	120.37 (14)
O1—C2—C1	122.45 (15)	C11—C10—H10	119.8
C3—C2—C1	119.36 (17)	C9—C10—H10	119.8
C4—C3—C2	120.71 (19)	O3—C11—C10	116.77 (14)
C4—C3—H3A	119.6	O3—C11—C12	122.77 (14)
C2—C3—H3A	119.6	C10—C11—C12	120.46 (13)
C3—C4—C5	120.68 (18)	C13—C12—C11	119.15 (15)
C3—C4—H4	119.7	C13—C12—H12	120.4
C5—C4—H4	119.7	C11—C12—H12	120.4
C4—C5—C6	119.29 (18)	C14—C13—C12	120.98 (16)
C4—C5—H5	120.4	C14—C13—H13	119.5
C6—C5—H5	120.4	C12—C13—H13	119.5
C5—C6—C1	121.34 (18)	C13—C14—C9	119.98 (14)
C5—C6—H6	119.3	C13—C14—H14	120.0
C1—C6—H6	119.3	C9—C14—H14	120.0

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.88	2.6010 (19)	146
O3—H3···O2^{i}	0.82	1.81	2.5946 (16)	159
N2—H2···O3^{ii}	0.90 (1)	2.12 (1)	3.0062 (18)	171 (2)

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