Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N′-(2-Hydroxy-1,2-diphenylethylidene)-benzohydrazide

Ming-zhi Song

College of Chemistry and Chemical Technology, Binzhou University, Binzhou 256600, Shandong, People's Republic of China
Correspondence e-mail: fanchuangang2009@163.com

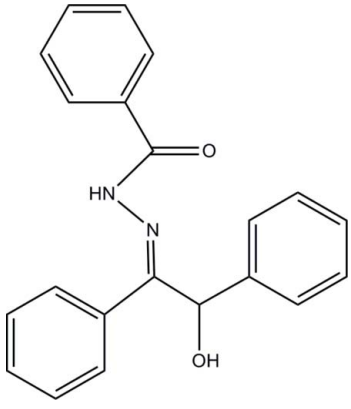
Received 6 September 2010; accepted 25 September 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.040; wR factor = 0.097; data-to-parameter ratio = 7.7.

In the title compound, $C_{21}H_{18}N_2O_2$, the amino group is involved in an intramolecular N—H···O hydrogen bond. The rings make dihedral angles of 37.9 (2), 64.4 (2) and 83.6 (2)°. In the crystal, intermolecular O—H···N and O—H···O hydrogen bonds link the molecules into chains running along [100].

Related literature

For related structures, see: Fun *et al.*(2008); Nie (2008); Seijas *et al.* (2007). For general background to the biological activity of Schiff bases and their metal complexes, see: Chakraborty *et al.* (1996); Jeewoth *et al.* (1999).



Experimental

Crystal data

$C_{21}H_{18}N_2O_2$
M_r = 330.37
Orthorhombic, $P2_12_12_1$
a = 7.7318 (8) Å
b = 11.0653 (12) Å
c = 19.725 (2) Å
V = 1687.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.41 × 0.16 × 0.13 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.966, T_{max} = 0.989
7865 measured reflections
1729 independent reflections
1051 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.097
S = 1.07
1729 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 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
O2—H2···O1^{i}	0.82	2.45	2.998 (4)	125
O2—H2···N2^{i}	0.82	2.20	2.992 (4)	164
N1—H1···O2	0.86	2.12	2.715 (4)	126

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, -z$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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*.

The author acknowledges financial support by the Foundation of Binzhou University (grant No. BZXYQNLG2005013).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2764).

References

Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chakraborty, J. & Patel, R. N. (1996). *J. Indian Chem. Soc.* **73**, 191–195.
Fun, H.-K., Patil, P. S., Jebas, S. R., Sujith, K. V. & Kalluraya, B. (2008). *Acta Cryst.* E**64**, o1594–o1595.
Jeewoth, T., Bhowon, M. G. & Wah, H. L. K. (1999). *Transition Met. Chem.* **24**, 445–448.
Nie, Y. (2008). *Acta Cryst.* E**64**, o471.
Seijas, L. E., Delgado, G. E., Mora, A. J., Bahsas, A. & Briceño, A. (2007). *Acta Cryst.* C**63**, o303–o305.
Sheldrick, G. M. (2007). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2010). E**66**, o2692 [doi:10.1107/S1600536810038365]

N′-(2-Hydroxy-1,2-diphenylethylidene)benzohydrazide

Ming-zhi Song

S1. Comment

Schiff bases and their metal complexes were reported to exhibit fungicidal, bactericidal, antiviral, and antitubercular activity (Chakraborty *et al.*, 1996; Jeewoth *et al.*, 1999). Herewith we present the title compound (I), which is a new Shiff base compound.

In (I) (Fig. 1), the bond lengths and angles are normal and comparable to those observed in similar compounds (Nie *et al.*, 2008; Fun *et al.*, 2008) The C=N (C8=N2) bond length in the molecule is 1.287 (3) Å. Two benzene rings - C2—C7 and C16—C21, respectively - form a dihedral angle of 37.94 (7) °. The amino group is involved in formation of intramolecular N—H···O hydrogen bond (Table 1), while intermolecular O—H···N and O—H···O hydrogen bonds (Table 1) link the molecules into chains running in direction [100].

S2. Experimental

Benzoin (5 mmol), benzohydrazide (5 mmol) and methanol (10 ml) were mixed in 50 ml flask. After stirring for 2 h at 373 K, the resulting mixture was recrystalized from methanol, affording the title compound as a colorless crystalline solid. Elemental analysis: calculated for $C_{21}H_{18}N_2O_2$: C 76.34, H 5.49, N 8.48%; found: C 76.21, H 5.56, N 8.54%.

S3. Refinement

All H atoms were placed in geometrically idealized positions (N—H 0.86, O—H= 0.82 and C—H = 0.93–0.98 Å) and treated as riding on their parent atoms, with U_{iso}(H) = 1.2U-1.5U_{eq} of the parent atom. Due to the absence of any significant anomalous scatterers in the molecule, the 1239 Friedel pairs were merged before the final refinement.

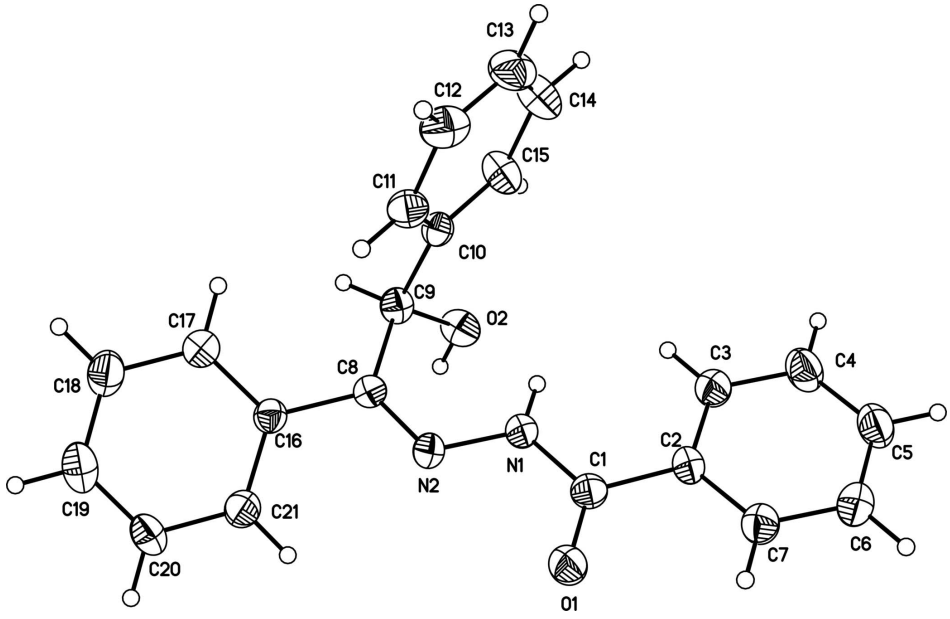


Figure 1

lThe molecular structure of (I) showing the atomic numbering scheme and 30% probability displacement ellipsoids.

N′-(2-Hydroxy-1,2-diphenylethylidene)benzohydrazide

Crystal data

$C_{21}H_{18}N_2O_2$
M_r = 330.37
Orthorhombic, $P2_12_12_1$
a = 7.7318 (8) Å
b = 11.0653 (12) Å
c = 19.725 (2) Å
V = 1687.5 (3) Å^3
Z = 4
F(000) = 696
D_x = 1.300 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1315 reflections
θ = 2.8–19.7°
μ = 0.09 mm^{-1}
T = 298 K
Needle, colourless
0.41 × 0.16 × 0.13 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.966, T_{max} = 0.989
7865 measured reflections
1729 independent reflections
1051 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 25.0°, θ_{min} = 2.1°
h = −9→8
k = −13→13
l = −10→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.097
S = 1.07
1729 reflections
226 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

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0315P)^2 + 0.2666P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.6095 (4)	0.7285 (3)	0.07224 (14)	0.0466 (9)
H1	0.5711	0.6582	0.0833	0.056*
N2	0.6267 (4)	0.7612 (3)	0.00542 (16)	0.0445 (9)
O1	0.7060 (4)	0.9121 (2)	0.10546 (13)	0.0550 (8)
O2	0.3956 (3)	0.5524 (2)	0.02563 (13)	0.0547 (8)
H2	0.3161	0.5939	0.0110	0.082*
C1	0.6551 (5)	0.8107 (4)	0.1207 (2)	0.0441 (10)
C2	0.6408 (5)	0.7712 (3)	0.19238 (19)	0.0424 (10)
C3	0.5837 (6)	0.6586 (4)	0.2127 (2)	0.0538 (12)
H3	0.5485	0.6025	0.1805	0.065*
C4	0.5787 (6)	0.6288 (4)	0.2806 (2)	0.0634 (13)
H4	0.5385	0.5531	0.2939	0.076*
C5	0.6324 (6)	0.7097 (4)	0.3285 (2)	0.0638 (13)
H5	0.6309	0.6890	0.3742	0.077*
C6	0.6885 (7)	0.8213 (4)	0.3087 (2)	0.0666 (14)
H6	0.7230	0.8774	0.3410	0.080*
C7	0.6939 (5)	0.8510 (4)	0.2408 (2)	0.0543 (11)
H7	0.7344	0.9267	0.2279	0.065*
C8	0.5919 (5)	0.6798 (3)	−0.03926 (18)	0.0416 (10)
C9	0.5351 (5)	0.5513 (3)	−0.0227 (2)	0.0443 (10)
H9	0.4936	0.5132	−0.0645	0.053*
C10	0.6779 (5)	0.4743 (3)	0.00625 (18)	0.0404 (10)
C11	0.8474 (5)	0.4869 (3)	−0.0146 (2)	0.0513 (11)
H11	0.8759	0.5474	−0.0453	0.062*
C12	0.9764 (6)	0.4104 (4)	0.0096 (2)	0.0650 (13)
H12	1.0900	0.4197	−0.0050	0.078*
C13	0.9345 (7)	0.3213 (4)	0.0551 (2)	0.0692 (14)
H13	1.0199	0.2697	0.0714	0.083*
C14	0.7678 (7)	0.3084 (4)	0.0766 (3)	0.0781 (15)
H14	0.7401	0.2484	0.1077	0.094*
C15	0.6399 (6)	0.3839 (4)	0.0523 (2)	0.0622 (12)
H15	0.5267	0.3739	0.0672	0.075*

C16	0.6030 (5)	0.7188 (3)	−0.11073 (19)	0.0414 (10)
C17	0.6508 (6)	0.6403 (4)	−0.16168 (19)	0.0547 (11)
H17	0.6767	0.5604	−0.1512	0.066*
C18	0.6607 (6)	0.6793 (4)	−0.2285 (2)	0.0632 (13)
H18	0.6950	0.6262	−0.2624	0.076*
C19	0.6194 (6)	0.7971 (4)	−0.2443 (2)	0.0664 (14)
H19	0.6252	0.8235	−0.2890	0.080*
C20	0.5702 (6)	0.8749 (4)	−0.1946 (2)	0.0565 (12)
H20	0.5415	0.9543	−0.2053	0.068*
C21	0.5628 (5)	0.8365 (3)	−0.1283 (2)	0.0511 (11)
H21	0.5301	0.8907	−0.0947	0.061*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.062 (3)	0.0403 (18)	0.038 (2)	−0.0013 (18)	−0.0013 (18)	0.0009 (16)
N2	0.053 (2)	0.0448 (18)	0.0352 (18)	0.0040 (18)	0.0059 (17)	0.0001 (15)
O1	0.066 (2)	0.0506 (16)	0.0487 (17)	−0.0063 (15)	−0.0034 (16)	0.0039 (15)
O2	0.0445 (17)	0.0555 (16)	0.0642 (18)	−0.0006 (14)	0.0037 (16)	0.0091 (14)
C1	0.040 (2)	0.045 (3)	0.047 (3)	0.007 (2)	0.001 (2)	0.001 (2)
C2	0.040 (3)	0.050 (2)	0.037 (2)	0.001 (2)	0.000 (2)	0.005 (2)
C3	0.064 (3)	0.050 (3)	0.048 (3)	−0.004 (2)	−0.004 (2)	0.000 (2)
C4	0.074 (4)	0.064 (3)	0.052 (3)	−0.009 (3)	−0.001 (3)	0.015 (3)
C5	0.073 (4)	0.072 (3)	0.047 (3)	0.005 (3)	−0.001 (3)	0.012 (3)
C6	0.090 (4)	0.064 (3)	0.045 (3)	0.000 (3)	−0.003 (3)	−0.005 (2)
C7	0.060 (3)	0.054 (3)	0.050 (3)	−0.002 (2)	−0.005 (2)	0.000 (2)
C8	0.046 (3)	0.039 (2)	0.040 (2)	0.003 (2)	−0.001 (2)	−0.002 (2)
C9	0.043 (2)	0.047 (2)	0.043 (2)	−0.005 (2)	−0.002 (2)	0.000 (2)
C10	0.043 (2)	0.041 (2)	0.037 (2)	−0.0017 (19)	−0.006 (2)	−0.004 (2)
C11	0.051 (3)	0.045 (2)	0.057 (3)	−0.003 (2)	0.000 (3)	−0.002 (2)
C12	0.056 (3)	0.059 (3)	0.080 (3)	0.002 (3)	−0.012 (3)	−0.012 (3)
C13	0.067 (4)	0.063 (3)	0.078 (3)	0.015 (3)	−0.029 (3)	−0.003 (3)
C14	0.080 (4)	0.079 (4)	0.075 (3)	0.006 (3)	−0.013 (3)	0.028 (3)
C15	0.059 (3)	0.070 (3)	0.057 (3)	0.001 (3)	−0.002 (3)	0.018 (3)
C16	0.042 (3)	0.043 (2)	0.040 (2)	−0.001 (2)	0.004 (2)	0.000 (2)
C17	0.064 (3)	0.051 (2)	0.049 (2)	0.004 (3)	0.002 (2)	−0.002 (2)
C18	0.075 (3)	0.067 (3)	0.047 (3)	−0.014 (3)	0.007 (3)	−0.005 (3)
C19	0.070 (3)	0.084 (4)	0.045 (3)	−0.015 (3)	0.000 (3)	0.008 (3)
C20	0.064 (3)	0.056 (3)	0.049 (3)	−0.006 (3)	0.002 (2)	0.015 (2)
C21	0.057 (3)	0.049 (3)	0.047 (3)	−0.003 (2)	0.004 (2)	−0.003 (2)

Geometric parameters (Å, º)

N1—C1	1.366 (4)	C10—C11	1.380 (5)
N1—N2	1.373 (4)	C10—C15	1.383 (5)
N1—H1	0.8600	C11—C12	1.392 (5)
N2—C8	1.288 (4)	C11—H11	0.9300
O1—C1	1.226 (4)	C12—C13	1.372 (6)

O2—C9	1.439 (4)	C12—H12	0.9300
O2—H2	0.8200	C13—C14	1.365 (7)
C1—C2	1.485 (5)	C13—H13	0.9300
C2—C7	1.365 (5)	C14—C15	1.379 (6)
C2—C3	1.381 (5)	C14—H14	0.9300
C3—C4	1.380 (5)	C15—H15	0.9300
C3—H3	0.9300	C16—C17	1.379 (5)
C4—C5	1.366 (5)	C16—C21	1.383 (5)
C4—H4	0.9300	C17—C18	1.389 (5)
C5—C6	1.366 (6)	C17—H17	0.9300
C5—H5	0.9300	C18—C19	1.378 (6)
C6—C7	1.378 (5)	C18—H18	0.9300
C6—H6	0.9300	C19—C20	1.359 (5)
C7—H7	0.9300	C19—H19	0.9300
C8—C16	1.477 (5)	C20—C21	1.375 (5)
C8—C9	1.524 (5)	C20—H20	0.9300
C9—C10	1.507 (5)	C21—H21	0.9300
C9—H9	0.9800		

C1—N1—N2	118.1 (3)	C11—C10—C9	121.7 (3)
C1—N1—H1	121.0	C15—C10—C9	120.1 (4)
N2—N1—H1	121.0	C10—C11—C12	121.1 (4)
C8—N2—N1	116.9 (3)	C10—C11—H11	119.4
C9—O2—H2	109.5	C12—C11—H11	119.4
O1—C1—N1	121.4 (4)	C13—C12—C11	119.4 (4)
O1—C1—C2	121.8 (4)	C13—C12—H12	120.3
N1—C1—C2	116.8 (4)	C11—C12—H12	120.3
C7—C2—C3	118.4 (4)	C14—C13—C12	120.1 (4)
C7—C2—C1	117.0 (3)	C14—C13—H13	120.0
C3—C2—C1	124.5 (4)	C12—C13—H13	120.0
C4—C3—C2	120.4 (4)	C13—C14—C15	120.4 (4)
C4—C3—H3	119.8	C13—C14—H14	119.8
C2—C3—H3	119.8	C15—C14—H14	119.8
C5—C4—C3	120.3 (4)	C14—C15—C10	120.9 (4)
C5—C4—H4	119.8	C14—C15—H15	119.6
C3—C4—H4	119.8	C10—C15—H15	119.6
C4—C5—C6	119.5 (4)	C17—C16—C21	118.1 (4)
C4—C5—H5	120.3	C17—C16—C8	121.8 (3)
C6—C5—H5	120.3	C21—C16—C8	120.1 (3)
C5—C6—C7	120.2 (4)	C16—C17—C18	120.7 (4)
C5—C6—H6	119.9	C16—C17—H17	119.7
C7—C6—H6	119.9	C18—C17—H17	119.7
C2—C7—C6	121.1 (4)	C19—C18—C17	119.7 (4)
C2—C7—H7	119.5	C19—C18—H18	120.1
C6—C7—H7	119.5	C17—C18—H18	120.1
N2—C8—C16	115.9 (3)	C20—C19—C18	120.1 (4)
N2—C8—C9	124.4 (3)	C20—C19—H19	120.0
C16—C8—C9	119.6 (3)	C18—C19—H19	120.0

O2—C9—C10	107.7 (3)	C19—C20—C21	120.1 (4)
O2—C9—C8	110.5 (3)	C19—C20—H20	120.0
C10—C9—C8	113.5 (3)	C21—C20—H20	120.0
O2—C9—H9	108.4	C20—C21—C16	121.3 (4)
C10—C9—H9	108.4	C20—C21—H21	119.3
C8—C9—H9	108.4	C16—C21—H21	119.3
C11—C10—C15	118.1 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.82	2.45	2.998 (4)	125
O2—H2···N2^{i}	0.82	2.20	2.992 (4)	164
N1—H1···O2	0.86	2.12	2.715 (4)	126

Symmetry code: (i) $x-1/2, -y+3/2, -z$.