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2-Hydroxy-*N*′-[(1*E*,2*E*)-3-phenylprop-2-enylidene]benzohydrazide

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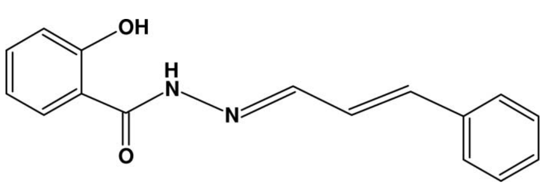
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.124; data-to-parameter ratio = 13.1.

In molecule of the title compound, $C_{16}H_{14}N_2O_2$, the two aromatic rings form a dihedral angle of 6.93 (3)° and an intramolecular N—H···O hydrogen bond occurs. In the crystal structure, intermolecular O—H···O hydrogen bonds link the molecules into zigzag chains running in the [10$\overline{1}$] direction.

Related literature

For the coordination chemistry of Schiff bases, see: Garnovskii *et al.* (1993); Musie *et al.* (2001); Paul *et al.* (2002); Shi *et al.* (2007). For Schiff bases and biological systems, see: Anderson *et al.* (1997). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{16}H_{14}N_2O_2$
M_r = 266.29
Monoclinic, $P2_1/n$
a = 4.8892 (6) Å
b = 26.563 (3) Å
c = 10.7367 (13) Å
β = 102.305 (2)°
V = 1362.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 K
0.15 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.987, T_{max} = 0.991
7141 measured reflections
2395 independent reflections
1354 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.123
S = 1.05
2395 reflections
183 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1	0.86	1.97	2.6348 (19)	133
O1—H1···O2^i	0.82	2.10	2.804 (3)	144

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2440).

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supplementary materials

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2-Hydroxy-*N*'-[(1*E*,2*E*)-3-phenylprop-2-enylidene]benzohydrazide

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Comment

In recent years, a number of Schiff-bases have been investigated in terms of their coordination chemistry (Garnovskii *et al.*, 1993; Musie *et al.*, 2001; Paul *et al.*, 2002; Shi *et al.*, 2007;) and biological systems (Anderson *et al.*, 1997). In order to search for new Schiff-bases with higher bioactivity, the title compound, (I), was synthesized and its crystal structure determined.

In (I) (Fig. 1), the bond lengths and angles are in good agreement with the expected values (Allen *et al.*, 1987). The intramolecular N—H···O hydrogen bond (Table 1) influences the molecular conformation. In the crystal, the molecules are linked into infinite chains along direction [10-1] by O—H···O hydrogen bonds (Table 1).

Experimental

The title compound was synthesized by the reaction of 2-Hydroxy-benzoic acid hydrazide(1 mmol, 152.2 mg) with 3-Phenyl-propenal (1 mmol, 132.2 mg) in ethanol(20 ml) under reflux conditions (348 K) for 6 h. The solvent was removed and the solid product recrystallized from tetrahydrofuran. After six days colorless crystals suitable for X-ray diffraction study were obtained. Yield, 226.3 mg, 85%. m.p. 239–241 K. Analysis calculated for $C_{16}H_{14}N_2O_2$: C 72.16, H 5.30, N 10.52%; found: C 71.73, H 5.34, N 10.48%.

Refinement

All H atoms were placed in idealized positions (C—H = 0.93— 0.97 Å, N—H = 0.86 Å) and refined as riding, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C, N).

Figures

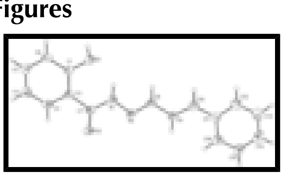

Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

2-Hydroxy-*N*'-[(1*E*,2*E*)-3-phenylprop-2- enylidene]benzohydrazide

Crystal data

$C_{16}H_{14}N_2O_2$	F_{000} = 560
M_r = 266.29	D_x = 1.298 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 932 reflections

$a = 4.8892$ (6) Å	$\theta = 3.6–21.4$°
$b = 26.563$ (3) Å	$\mu = 0.09$ mm^{-1}
$c = 10.7367$ (13) Å	$T = 295$ K
$\beta = 102.305$ (2)°	Block, colourless
$V = 1362.4$ (3) Å^3	0.15 × 0.12 × 0.10 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	2395 independent reflections
Radiation source: fine-focus sealed tube	1354 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.038$
$T = 295$ K	$\theta_{max} = 25.1$°
φ and ω scans	$\theta_{min} = 2.5$°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -5\rightarrow5$
$T_{min} = 0.987$, $T_{max} = 0.991$	$k = -21\rightarrow31$
7141 measured reflections	$l = -12\rightarrow12$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.047$	$w = 1/[\sigma^2(F_o^2) + (0.0505P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.124$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.05$	$\Delta\rho_{max} = 0.14$ e Å^{-3}
2395 reflections	$\Delta\rho_{min} = -0.13$ e Å^{-3}
183 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997a), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.008 (2)
Secondary atom site location: difference Fourier map	

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}
O1	0.5440 (4)	0.26610 (6)	0.08347 (14)	0.0702 (5)
H1	0.6201	0.2633	0.0227	0.105*
O2	0.4213 (4)	0.27755 (6)	0.45173 (13)	0.0687 (5)
N1	0.2766 (4)	0.24015 (6)	0.26236 (15)	0.0508 (5)
H1A	0.2861	0.2378	0.1835	0.061*
N2	0.1041 (4)	0.20892 (7)	0.31262 (16)	0.0513 (5)
C1	0.6656 (4)	0.30391 (8)	0.15959 (19)	0.0483 (6)
C2	0.6118 (4)	0.30864 (8)	0.28157 (18)	0.0450 (5)
C3	0.7379 (5)	0.34777 (9)	0.3569 (2)	0.0634 (7)
H3	0.7048	0.3513	0.4386	0.076*
C4	0.9102 (6)	0.38164 (9)	0.3154 (2)	0.0736 (8)
H4	0.9898	0.4080	0.3676	0.088*
C5	0.9638 (5)	0.37611 (9)	0.1959 (2)	0.0662 (7)
H5	1.0826	0.3986	0.1674	0.079*
C6	0.8438 (5)	0.33774 (9)	0.1184 (2)	0.0606 (7)
H6	0.8818	0.3343	0.0375	0.073*
C7	0.4304 (5)	0.27445 (8)	0.33872 (19)	0.0476 (6)
C8	−0.0380 (5)	0.17709 (8)	0.2358 (2)	0.0529 (6)
H8	−0.0220	0.1766	0.1510	0.064*
C9	−0.2215 (5)	0.14220 (8)	0.2788 (2)	0.0530 (6)
H9	−0.2416	0.1442	0.3628	0.064*
C10	−0.3630 (5)	0.10743 (9)	0.2044 (2)	0.0576 (6)
H10	−0.3419	0.1072	0.1203	0.069*
C11	−0.5490 (5)	0.06929 (8)	0.2383 (2)	0.0529 (6)
C12	−0.6805 (5)	0.03509 (10)	0.1480 (2)	0.0739 (8)
H12	−0.6499	0.0369	0.0655	0.089*
C13	−0.8563 (6)	−0.00161 (11)	0.1777 (3)	0.0842 (9)
H13	−0.9404	−0.0244	0.1156	0.101*
C14	−0.9071 (6)	−0.00457 (10)	0.2973 (3)	0.0761 (8)
H14	−1.0287	−0.0288	0.3169	0.091*
C15	−0.7772 (6)	0.02847 (10)	0.3879 (3)	0.0807 (8)
H15	−0.8084	0.0264	0.4702	0.097*
C16	−0.6002 (5)	0.06496 (9)	0.3590 (2)	0.0670 (7)
H16	−0.5137	0.0871	0.4223	0.080*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0858 (13)	0.0893 (13)	0.0482 (9)	−0.0339 (10)	0.0428 (9)	−0.0229 (9)
O2	0.0900 (14)	0.0857 (12)	0.0392 (9)	−0.0137 (9)	0.0337 (8)	−0.0060 (8)
N1	0.0615 (13)	0.0615 (12)	0.0363 (9)	−0.0068 (10)	0.0257 (9)	0.0017 (9)
N2	0.0587 (13)	0.0596 (12)	0.0424 (10)	−0.0030 (10)	0.0263 (9)	0.0069 (9)
C1	0.0531 (15)	0.0568 (14)	0.0384 (12)	−0.0055 (11)	0.0174 (10)	−0.0034 (10)
C2	0.0509 (15)	0.0505 (13)	0.0366 (11)	0.0016 (11)	0.0158 (10)	0.0003 (10)

C3	0.083 (2)	0.0703 (17)	0.0416 (13)	−0.0132 (14)	0.0247 (12)	−0.0088 (12)
C4	0.097 (2)	0.0700 (18)	0.0568 (16)	−0.0233 (15)	0.0219 (15)	−0.0121 (13)
C5	0.0740 (19)	0.0696 (17)	0.0575 (15)	−0.0225 (14)	0.0192 (14)	0.0020 (13)
C6	0.0701 (18)	0.0765 (17)	0.0412 (12)	−0.0134 (13)	0.0252 (12)	0.0026 (12)
C7	0.0552 (15)	0.0547 (14)	0.0383 (12)	0.0047 (11)	0.0218 (11)	0.0002 (11)
C8	0.0614 (17)	0.0631 (15)	0.0377 (12)	−0.0015 (12)	0.0183 (11)	0.0042 (11)
C9	0.0580 (16)	0.0613 (15)	0.0440 (13)	−0.0030 (12)	0.0205 (11)	0.0068 (11)
C10	0.0613 (17)	0.0687 (16)	0.0444 (13)	−0.0007 (13)	0.0151 (12)	0.0044 (12)
C11	0.0528 (16)	0.0563 (15)	0.0501 (14)	0.0024 (12)	0.0118 (11)	0.0029 (12)
C12	0.079 (2)	0.086 (2)	0.0571 (16)	−0.0149 (16)	0.0147 (14)	−0.0071 (14)
C13	0.082 (2)	0.082 (2)	0.085 (2)	−0.0215 (16)	0.0086 (17)	−0.0090 (16)
C14	0.0696 (19)	0.0665 (19)	0.093 (2)	−0.0088 (14)	0.0189 (16)	0.0139 (16)
C15	0.092 (2)	0.082 (2)	0.0768 (18)	−0.0177 (16)	0.0376 (17)	0.0056 (16)
C16	0.076 (2)	0.0684 (17)	0.0609 (16)	−0.0142 (13)	0.0244 (14)	−0.0028 (12)

Geometric parameters (Å, °)

O1—C1	1.350 (2)	C8—C9	1.433 (3)
O1—H1	0.8200	C8—H8	0.9300
O2—C7	1.226 (2)	C9—C10	1.317 (3)
N1—C7	1.344 (2)	C9—H9	0.9300
N1—N2	1.373 (2)	C10—C11	1.458 (3)
N1—H1A	0.8600	C10—H10	0.9300
N2—C8	1.278 (2)	C11—C16	1.376 (3)
C1—C6	1.388 (3)	C11—C12	1.383 (3)
C1—C2	1.395 (3)	C12—C13	1.381 (3)
C2—C3	1.379 (3)	C12—H12	0.9300
C2—C7	1.490 (3)	C13—C14	1.361 (3)
C3—C4	1.370 (3)	C13—H13	0.9300
C3—H3	0.9300	C14—C15	1.362 (3)
C4—C5	1.371 (3)	C14—H14	0.9300
C4—H4	0.9300	C15—C16	1.378 (3)
C5—C6	1.366 (3)	C15—H15	0.9300
C5—H5	0.9300	C16—H16	0.9300
C6—H6	0.9300		
C1—O1—H1	109.5	N2—C8—H8	119.6
C7—N1—N2	118.73 (17)	C9—C8—H8	119.6
C7—N1—H1A	120.6	C10—C9—C8	122.9 (2)
N2—N1—H1A	120.6	C10—C9—H9	118.6
C8—N2—N1	116.17 (17)	C8—C9—H9	118.6
O1—C1—C6	120.93 (18)	C9—C10—C11	127.6 (2)
O1—C1—C2	119.23 (18)	C9—C10—H10	116.2
C6—C1—C2	119.8 (2)	C11—C10—H10	116.2
C3—C2—C1	117.9 (2)	C16—C11—C12	117.0 (2)
C3—C2—C7	116.66 (18)	C16—C11—C10	122.8 (2)
C1—C2—C7	125.41 (19)	C12—C11—C10	120.2 (2)
C4—C3—C2	122.2 (2)	C13—C12—C11	121.4 (2)
C4—C3—H3	118.9	C13—C12—H12	119.3
C2—C3—H3	118.9	C11—C12—H12	119.3

C3—C4—C5	119.2 (2)	C14—C13—C12	120.4 (3)
C3—C4—H4	120.4	C14—C13—H13	119.8
C5—C4—H4	120.4	C12—C13—H13	119.8
C6—C5—C4	120.5 (2)	C13—C14—C15	119.0 (3)
C6—C5—H5	119.8	C13—C14—H14	120.5
C4—C5—H5	119.8	C15—C14—H14	120.5
C5—C6—C1	120.4 (2)	C14—C15—C16	120.8 (3)
C5—C6—H6	119.8	C14—C15—H15	119.6
C1—C6—H6	119.8	C16—C15—H15	119.6
O2—C7—N1	121.0 (2)	C11—C16—C15	121.3 (2)
O2—C7—C2	121.1 (2)	C11—C16—H16	119.3
N1—C7—C2	117.84 (17)	C15—C16—H16	119.3
N2—C8—C9	120.8 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1	0.86	1.97	2.6348 (19)	133
O1—H1···O2^{i}	0.82	2.10	2.804 (3)	144
O1—H1···N2^{i}	0.82	2.36	3.057 (3)	144

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

Fig. 1