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2-Hydroxy-*N*′-[(1*E*)-1-(2-hydroxy-5-methylphenyl)-2-phenylethylidene]benzohydrazide

Guo-Fang He,[a] Jian-Min Dou[b] and Jian-Guo Chang[a]*

[a]Department of Materials Science and Chemical Engineering, Taishan University, 271021 Taian, Shandong, People's Republic of China, and [b]School of Chemistry and Chemical Engineering, Liaocheng University, 252059 Liaocheng, Shandong, People's Republic of China

Correspondence e-mail: tsucjg@163.com

Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.114
Data-to-parameter ratio = 13.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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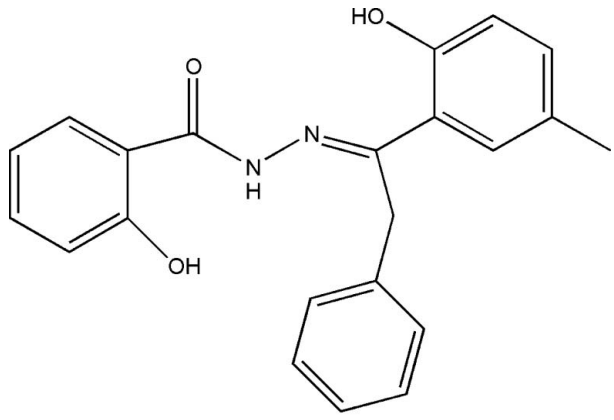
The title compound, $C_{22}H_{20}N_2O_3$, displays a *trans* configuration with respect to the C=N double bond. The crystal structure is stabilized by intramolecular O—H···N and N—H···O and intermolecular O—H···O hydrogen bonds.

Comment

The chemistry of arylhydrazones continues to attract much attention due to their ability to coordinate to metal ions (Singh *et al.*, 1982; Salem, 1998) and their biological activity (Singh *et al.*, 1982; Carcelli *et al.*, 1995). As an extension of our work on the structural characterization of arylhydrazone derivatives, the title compound, (I), was synthesized.



(I)

The title molecule displays a *trans* configuration with respect to the C7=N1 double bond (Fig. 1). The three benzene rings, C1–C6 (*A*), C17–C22 (*B*) and C9–C14 (*C*) make dihedral angles of 19.02 (9) (*A*/*B*), 79.17 (5) (*A*/*C*) and 88.39 (5)° (*B*/*C*). Intramolecular N—H···O and O—H···N hydrogen bonds stabilize the conformation of the molecule, while O—H···O intermolecular hydrogen bonds lead to the formation of an infinite chain, graph set *C*(6) (Etter *et al.*, 1990), extending along the *a* axis (Table 1 and Fig. 2).

Experimental

2-Hydroxybenzoylhydrazine (0.02 mol, 3.04 g) was dissolved in anhydrous ethanol (50 ml), and 1-(2-hydroxy-5-methylphenyl)-2-phenylethanone (0.02 mol, 4.52 g) was added. The reaction mixture was refluxed for 6 h with stirring. The resulting precipitate was collected by filtration, washed several times with ethanol and dried *in vacuo* (yield 81%). The compound (2.0 mmol, 0.72 g) was dissolved in dimethylformamide (30 ml) and allowed to stand at room temperature for 30 d, yielding yellow single crystals suitable for X-ray diffraction.

Crystal data

$C_{22}H_{20}N_2O_3$
M_r = 360.40
Triclinic, $P\overline{1}$
a = 6.7401 (11) Å
b = 10.4033 (17) Å
c = 14.065 (2) Å
α = 79.475 (6)°
β = 80.193 (6)°
γ = 78.639 (6)°
V = 941.4 (3) Å^3
Z = 2
D_x = 1.271 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 273 (2) K
Block, yellow
0.35 × 0.24 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
10775 measured reflections
3292 independent reflections
2663 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.114
S = 1.03
3292 reflections
247 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2 + 0.1919P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.26 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
O3—H3···N2	0.82	1.83	2.5468 (15)	145
N1—H1···O1	0.86	1.96	2.6338 (15)	134
O1—H1A···O2^{i}	0.82	1.88	2.6850 (15)	169

Symmetry code: (i) $x+1, y, z$.

All H atoms were positioned geometrically and treated as riding on their parent atoms, with methyl C—H = 0.96 Å, aromatic C—H = 0.93 Å, O—H = 0.82 Å and N—H = 0.86 Å, and with U_{iso}(H) = 1.5U_{eq}(methyl C,O) and 1.2U_{eq}(aromatic C,N).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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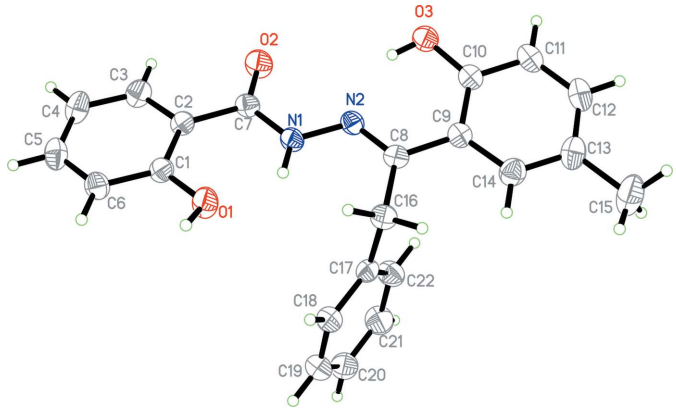

Figure 1
The molecular structure of compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

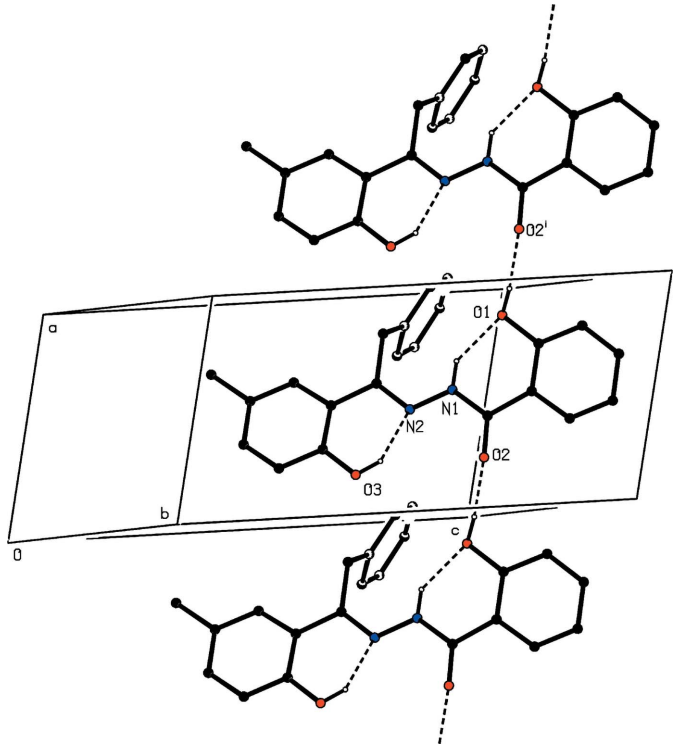

Figure 2
Partial packing view showing O—H···N, N—H···O and O—H···O hydrogen bonds and the formation of an infinite chain. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry code: (i) 1 + x, y, z.]

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