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## N'-(4-Hydroxybenzylidene)-3-methoxybenzohydrazide

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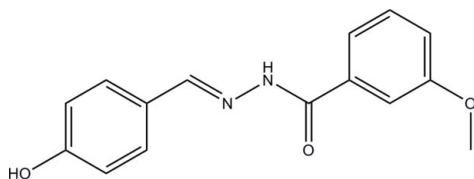
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.061;  $wR$  factor = 0.117; data-to-parameter ratio = 13.5.

In the title compound,  $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_3$ , the dihedral angle between the two benzene rings is  $47.9(3)^\circ$ . In the crystal, molecules are linked through  $\text{N}-\text{H}\cdots\text{O}$ ,  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds, forming layers parallel to the  $ab$  plane.

## Related literature

For general background to hydrazones, see: Rasras *et al.* (2010); Pyta *et al.* (2010); Angelusiu *et al.* (2010). For related structures, see: Fun *et al.* (2008); Singh & Singh (2010); Ahmad *et al.* (2010); Tang (2010, 2011). For reference bond-length data, see: Allen *et al.* (1987).



## Experimental

## Crystal data

 $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_3$  $M_r = 270.28$ Orthorhombic,  $Pbca$  $a = 13.221(2)$  Å $b = 9.5336(18)$  Å $c = 21.620(2)$  Å $V = 2725.1(7)$  Å<sup>3</sup> $Z = 8$ Mo  $K\alpha$  radiation $\mu = 0.09$  mm<sup>-1</sup> $T = 298$  K $0.23 \times 0.21 \times 0.20$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) $T_{\min} = 0.979$ ,  $T_{\max} = 0.982$ 18234 measured reflections  
2531 independent reflections  
1805 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.069$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.061$  $wR(F^2) = 0.117$  $S = 1.11$ 

2531 reflections

188 parameters

2 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\max} = 0.18$  e Å<sup>-3</sup> $\Delta\rho_{\min} = -0.20$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H2}\cdots\text{O2}^{\text{i}}$	0.90 (1)	2.13 (1)	3.000 (2)	162 (3)
$\text{O1}-\text{H1}\cdots\text{N1}^{\text{ii}}$	0.85 (1)	2.11 (1)	2.959 (2)	176 (3)
$\text{O1}-\text{H1}\cdots\text{O2}^{\text{ii}}$	0.85 (1)	2.53 (3)	2.969 (2)	113 (3)

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5225).

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## supporting information

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***N'*-(4-Hydroxybenzylidene)-3-methoxybenzohydrazide****Chun-Bao Tang****S1. Comment**

Hydrazone compounds have received much attention in biological and structural chemistry in the last years (Rasras *et al.*, 2010; Pyta *et al.*, 2010; Angelusiu *et al.*, 2010; Fun *et al.*, 2008; Singh & Singh, 2010; Ahmad *et al.*, 2010). As a continuation of our work on the structural study on such compounds (Tang, 2010, 2011), the author reports herein the crystal structure of the title new hydrazone compound (Fig. 1).

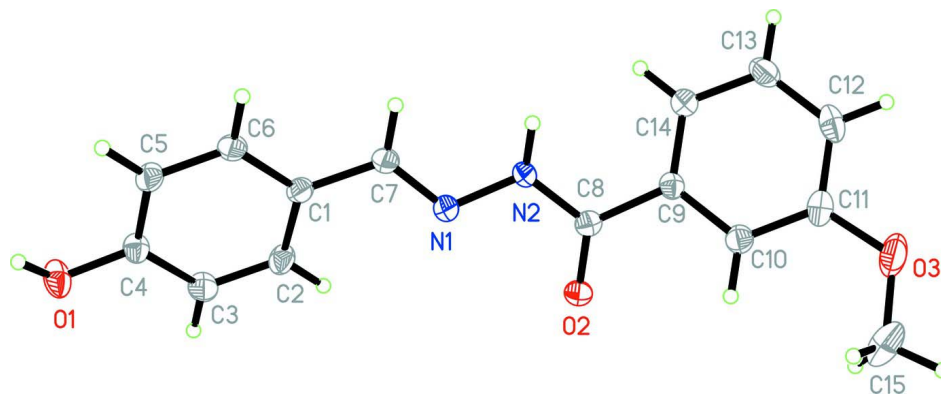
In the molecule of the title compound, the dihedral angle between the two benzene rings is 47.9 (3)°. Bond lengths in the compound are normal (Allen *et al.*, 1987) and comparable to those in the similar compounds the author reported previously. In the crystal structure, molecules are linked through intermolecular N—H···O, O—H···O, and O—H···N hydrogen bonds (Table 1), forming layers parallel to the *ab* plane.

**S2. Experimental**

4-Hydroxybenzaldehyde (0.1 mmol, 12.2 mg) and 3-methoxybenzohydrazide (0.1 mmol, 16.6 mg) were dissolved in methanol (20 ml). The mixture was stirred at reflux for 10 min to give a clear colourless solution. Colourless needle-shaped crystals of the compound were formed by slow evaporation of the solvent over several days.

**S3. Refinement**

The amino and hydroxyl H atoms were located in a difference Fourier map and refined isotropically, with the O—H and N—H distances restrained to 0.85 (1) and 0.90 (1) Å, respectively. Other H atoms were constrained to ideal geometries and refined as riding, with  $C_{sp^2}-H = 0.93$  Å, and  $C(\text{methyl})-H = 0.96$  Å;  $U_{iso}(H) = 1.2U_{eq}(C)$  and  $1.5U_{eq}(C_{\text{methyl}})$ .

**Figure 1**

The molecular structure of the compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

***N'*-(4-Hydroxybenzylidene)-3-methoxybenzohydrazide***Crystal data*C<sub>15</sub>H<sub>14</sub>N<sub>2</sub>O<sub>3</sub> $M_r = 270.28$ Orthorhombic, *Pbca* $a = 13.221 (2) \text{ \AA}$  $b = 9.5336 (18) \text{ \AA}$  $c = 21.620 (2) \text{ \AA}$  $V = 2725.1 (7) \text{ \AA}^3$  $Z = 8$  $F(000) = 1136$  $D_x = 1.318 \text{ Mg m}^{-3}$ Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$ 

Cell parameters from 2706 reflections

 $\theta = 2.4\text{--}24.6^\circ$  $\mu = 0.09 \text{ mm}^{-1}$  $T = 298 \text{ K}$ 

Cut from needle, colorless

 $0.23 \times 0.21 \times 0.20 \text{ mm}$ *Data collection*Bruker SMART CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\omega$  scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.979$ ,  $T_{\max} = 0.982$ 

18234 measured reflections

2531 independent reflections

1805 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.069$  $\theta_{\text{max}} = 25.5^\circ$ ,  $\theta_{\text{min}} = 2.4^\circ$  $h = -16 \rightarrow 16$  $k = -11 \rightarrow 11$  $l = -22 \rightarrow 26$ *Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.061$  $wR(F^2) = 0.117$  $S = 1.11$ 

2531 reflections

188 parameters

2 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sitesH atoms treated by a mixture of independent  
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.712P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} < 0.001$  $\Delta\rho_{\text{max}} = 0.18 \text{ e \AA}^{-3}$  $\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$ *Special details*

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.84363 (13)	0.96516 (19)	0.63698 (8)	0.0335 (5)
N2	0.76637 (13)	0.89157 (18)	0.60808 (9)	0.0331 (5)
O1	1.24869 (13)	1.15604 (17)	0.77207 (8)	0.0491 (5)
O2	0.67126 (11)	1.08925 (16)	0.60246 (8)	0.0416 (4)

O3	0.31857 (12)	0.8832 (2)	0.55817 (10)	0.0676 (6)
C1	1.00898 (16)	0.9639 (2)	0.68058 (11)	0.0327 (5)
C2	1.02194 (17)	1.1091 (2)	0.67981 (12)	0.0390 (6)
H2A	0.9757	1.1648	0.6586	0.047*
C3	1.10217 (17)	1.1714 (2)	0.70994 (11)	0.0414 (6)
H3	1.1102	1.2682	0.7084	0.050*
C4	1.17085 (16)	1.0898 (2)	0.74251 (11)	0.0340 (6)
C5	1.16016 (17)	0.9463 (2)	0.74303 (11)	0.0378 (6)
H5	1.2064	0.8911	0.7645	0.045*
C6	1.08096 (16)	0.8842 (2)	0.71180 (12)	0.0384 (6)
H6	1.0755	0.7869	0.7116	0.046*
C7	0.92309 (16)	0.8958 (2)	0.65072 (11)	0.0338 (6)
H7	0.9263	0.8005	0.6416	0.041*
C8	0.68050 (16)	0.9628 (2)	0.59326 (10)	0.0311 (5)
C9	0.59785 (15)	0.8768 (2)	0.56562 (10)	0.0300 (5)
C10	0.49867 (16)	0.9232 (2)	0.57510 (11)	0.0365 (6)
H10	0.4868	1.0042	0.5980	0.044*
C11	0.41857 (17)	0.8491 (3)	0.55060 (12)	0.0429 (6)
C12	0.43747 (19)	0.7307 (3)	0.51536 (13)	0.0495 (7)
H12	0.3837	0.6808	0.4985	0.059*
C13	0.53502 (19)	0.6863 (3)	0.50505 (12)	0.0463 (7)
H13	0.5467	0.6076	0.4807	0.056*
C14	0.61629 (17)	0.7580 (2)	0.53071 (10)	0.0375 (6)
H14	0.6821	0.7266	0.5245	0.045*
C15	0.2946 (2)	1.0000 (4)	0.59606 (15)	0.0752 (10)
H15A	0.3231	0.9867	0.6365	0.113*
H15B	0.2224	1.0087	0.5994	0.113*
H15C	0.3219	1.0838	0.5779	0.113*
H2	0.770 (2)	0.7974 (11)	0.6051 (14)	0.090*
H1	1.276 (2)	1.104 (3)	0.7996 (13)	0.113*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0297 (10)	0.0310 (10)	0.0398 (12)	-0.0013 (9)	-0.0022 (9)	-0.0029 (9)
N2	0.0288 (10)	0.0267 (10)	0.0439 (12)	-0.0026 (9)	-0.0047 (9)	-0.0049 (9)
O1	0.0510 (10)	0.0357 (10)	0.0607 (13)	-0.0157 (8)	-0.0214 (10)	0.0127 (9)
O2	0.0395 (9)	0.0267 (9)	0.0587 (12)	0.0026 (7)	-0.0059 (8)	-0.0060 (8)
O3	0.0298 (10)	0.0944 (16)	0.0784 (15)	-0.0011 (10)	-0.0039 (10)	-0.0058 (13)
C1	0.0298 (12)	0.0289 (12)	0.0393 (14)	0.0024 (10)	0.0001 (11)	0.0002 (11)
C2	0.0347 (13)	0.0336 (13)	0.0486 (16)	0.0032 (11)	-0.0085 (11)	0.0082 (12)
C3	0.0468 (15)	0.0241 (12)	0.0532 (17)	-0.0039 (11)	-0.0067 (13)	0.0065 (12)
C4	0.0332 (12)	0.0319 (12)	0.0370 (14)	-0.0054 (10)	-0.0027 (11)	0.0053 (11)
C5	0.0375 (13)	0.0275 (12)	0.0483 (16)	0.0020 (10)	-0.0085 (12)	0.0070 (11)
C6	0.0391 (13)	0.0218 (12)	0.0544 (17)	-0.0015 (10)	-0.0041 (12)	0.0001 (11)
C7	0.0346 (13)	0.0261 (12)	0.0406 (15)	-0.0007 (10)	-0.0007 (11)	-0.0012 (11)
C8	0.0320 (12)	0.0305 (13)	0.0307 (14)	0.0004 (10)	0.0033 (10)	0.0018 (11)
C9	0.0305 (12)	0.0274 (12)	0.0322 (14)	-0.0029 (9)	-0.0020 (10)	0.0049 (11)

C10	0.0357 (13)	0.0350 (13)	0.0389 (15)	0.0000 (10)	-0.0014 (11)	0.0012 (11)
C11	0.0317 (13)	0.0542 (16)	0.0427 (16)	-0.0045 (12)	-0.0032 (12)	0.0085 (13)
C12	0.0420 (15)	0.0547 (17)	0.0518 (18)	-0.0145 (13)	-0.0148 (13)	0.0015 (14)
C13	0.0521 (16)	0.0382 (14)	0.0486 (17)	-0.0050 (12)	-0.0090 (14)	-0.0092 (12)
C14	0.0356 (13)	0.0344 (13)	0.0426 (15)	-0.0008 (11)	-0.0021 (11)	-0.0028 (12)
C15	0.0442 (17)	0.107 (3)	0.074 (2)	0.0198 (17)	0.0123 (16)	0.008 (2)

*Geometric parameters (Å, °)*

N1—C7	1.277 (3)	C5—H5	0.9300
N1—N2	1.388 (2)	C6—H6	0.9300
N2—C8	1.361 (3)	C7—H7	0.9300
N2—H2	0.901 (10)	C8—C9	1.491 (3)
O1—C4	1.366 (3)	C9—C14	1.382 (3)
O1—H1	0.853 (10)	C9—C10	1.399 (3)
O2—C8	1.228 (2)	C10—C11	1.379 (3)
O3—C11	1.371 (3)	C10—H10	0.9300
O3—C15	1.419 (3)	C11—C12	1.384 (4)
C1—C6	1.392 (3)	C12—C13	1.376 (3)
C1—C2	1.395 (3)	C12—H12	0.9300
C1—C7	1.459 (3)	C13—C14	1.389 (3)
C2—C3	1.379 (3)	C13—H13	0.9300
C2—H2A	0.9300	C14—H14	0.9300
C3—C4	1.387 (3)	C15—H15A	0.9600
C3—H3	0.9300	C15—H15B	0.9600
C4—C5	1.376 (3)	C15—H15C	0.9600
C5—C6	1.379 (3)		
C7—N1—N2	116.64 (18)	O2—C8—N2	122.3 (2)
C8—N2—N1	117.87 (17)	O2—C8—C9	122.15 (19)
C8—N2—H2	121.7 (19)	N2—C8—C9	115.51 (19)
N1—N2—H2	119.8 (19)	C14—C9—C10	120.3 (2)
C4—O1—H1	112 (2)	C14—C9—C8	122.69 (19)
C11—O3—C15	118.1 (2)	C10—C9—C8	117.0 (2)
C6—C1—C2	117.6 (2)	C11—C10—C9	120.1 (2)
C6—C1—C7	120.3 (2)	C11—C10—H10	120.0
C2—C1—C7	122.1 (2)	C9—C10—H10	120.0
C3—C2—C1	121.1 (2)	O3—C11—C10	125.0 (2)
C3—C2—H2A	119.5	O3—C11—C12	115.7 (2)
C1—C2—H2A	119.5	C10—C11—C12	119.4 (2)
C2—C3—C4	120.1 (2)	C13—C12—C11	120.6 (2)
C2—C3—H3	119.9	C13—C12—H12	119.7
C4—C3—H3	119.9	C11—C12—H12	119.7
O1—C4—C5	122.2 (2)	C12—C13—C14	120.6 (2)
O1—C4—C3	118.13 (19)	C12—C13—H13	119.7
C5—C4—C3	119.6 (2)	C14—C13—H13	119.7
C4—C5—C6	120.1 (2)	C9—C14—C13	119.0 (2)
C4—C5—H5	120.0	C9—C14—H14	120.5

C6—C5—H5	120.0	C13—C14—H14	120.5
C5—C6—C1	121.5 (2)	O3—C15—H15A	109.5
C5—C6—H6	119.3	O3—C15—H15B	109.5
C1—C6—H6	119.3	H15A—C15—H15B	109.5
N1—C7—C1	120.9 (2)	O3—C15—H15C	109.5
N1—C7—H7	119.6	H15A—C15—H15C	109.5
C1—C7—H7	119.6	H15B—C15—H15C	109.5

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H2...O2 <sup>i</sup>	0.90 (1)	2.13 (1)	3.000 (2)	162 (3)
O1—H1...N1 <sup>ii</sup>	0.85 (1)	2.11 (1)	2.959 (2)	176 (3)
O1—H1...O2 <sup>ii</sup>	0.85 (1)	2.53 (3)	2.969 (2)	113 (3)

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