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N′-(4-Hydroxybenzylidene)-2-methylbenzohydrazide

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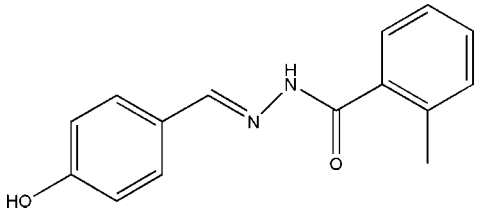
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.101; data-to-parameter ratio = 9.2.

The title hydrazone compound, $C_{15}H_{14}N_2O_2$, was prepared by the condensation of 4-hydroxybenzaldehyde with 2-methylbenzohydrazide in methanol. The dihedral angle between the two benzene rings is 42.3 (2)°. In the crystal structure, molecules are linked by intermolecular O—H···O, O—H···N and N—H···O hydrogen bonds, forming a three-dimensional framework.

Related literature

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



Experimental

Crystal data

$C_{15}H_{14}N_2O_2$
M_r = 254.28
Orthorhombic, $P2_12_12_1$
a = 7.6900 (15) Å
b = 11.701 (2) Å
c = 14.471 (3) Å
V = 1302.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.983, T_{max} = 0.984
10755 measured reflections
1634 independent reflections
1502 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.101
S = 1.12
1634 reflections
177 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.96	2.7657 (18)	166
O1—H1···N1^{i}	0.82	2.52	2.995 (2)	118
N2—H2···O1^{ii}	0.91 (1)	2.14 (1)	2.995 (2)	158 (2)

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

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: *SHELXTL*.

Financial support from the Jiaying University research fund is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5176).

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supporting information

Acta Cryst. (2010). E**66**, o2482 [doi:10.1107/S1600536810035063]

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S1. Comment

Hydrazone compounds have been received much attention in biological chemistry and structural chemistry in the last few years (Rasras *et al.*, 2010; Pyta *et al.*, 2010; Angelusiu *et al.*, 2010; Fun *et al.*, 2008; Singh & Singh, 2010; Ahmad *et al.*, 2010). In the present paper, the author reports the crystal structure of the title new hydrazone compound (Fig. 1).

In the title molecule, the dihedral angle between the two benzene rings is 42.3 (2)°. The torsion angles C1—C7—N1—N2, C7—N1—N2—C8 and N1—N2—C8—C9 are 2.9 (2), 0.9 (2), and 0.2 (2)°, respectively. All the bond lengths are within normal values (Allen *et al.*, 1987).

In the crystal structure of the compound, molecules are linked through O–H···O, O–H···N, and N–H···O intermolecular hydrogen bonds (Table 1), forming a three-dimensional network (Fig. 2).

S2. Experimental

4-Hydroxybenzaldehyde (0.1 mmol, 12.2 mg) and 3-methylbenzohydrazide (0.1 mmol, 15.0 mg) were dissolved in methanol (20 ml). The mixture was stirred at reflux for 10 min to give a clear colourless solution. Colourless block-shaped crystals of the compound were formed by slow evaporation of the solvent over several days.

S3. Refinement

Atom H2 was located in a difference Fourier map and refined isotropically, with the N–H distance restrained to 0.90 (1) Å [U_{iso}(H) = 0.08 Å^2]. Other H atoms were constrained to ideal geometries, with C–H = 0.93–0.96 Å, O–H = 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(C15 and O1). In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

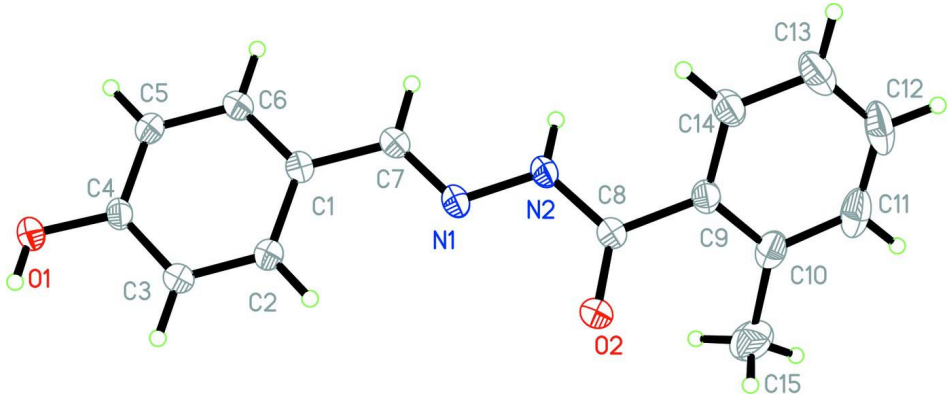

Figure 1

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

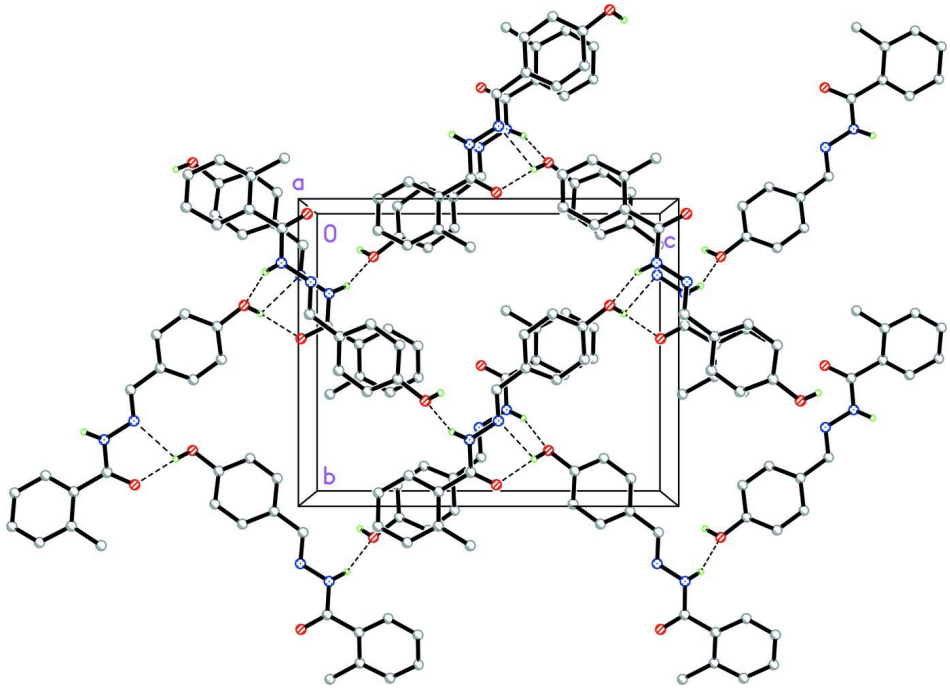

Figure 2

Molecular packing of the title compound, with hydrogen bonds shown as dashed lines.

N′-(4-Hydroxybenzylidene)-2-methylbenzohydrazide

Crystal data

$C_{15}H_{14}N_2O_2$
$M_r = 254.28$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 7.6900\ (15)$ Å
$b = 11.701\ (2)$ Å
$c = 14.471\ (3)$ Å
$V = 1302.1\ (4)$ Å^3
$Z = 4$
$F(000) = 536$
$D_x = 1.297$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4917 reflections
$\theta = 2.2$–$27.1°$
$\mu = 0.09$ mm^{-1}
$T = 298$ K
Block, colourless
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.983$, $T_{max} = 0.984$
10755 measured reflections
1634 independent reflections
1502 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.2°$
$h = -9\rightarrow9$
$k = -14\rightarrow14$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.101$
$S = 1.12$
1634 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
$w = 1/[\sigma^2(F_o^2) + (0.0604P)^2 + 0.1042P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-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 $F^2 > 2\text{sigma}(F^2)$ 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}
N1	0.1045 (2)	0.76789 (13)	0.47260 (10)	0.0442 (4)
N2	0.1260 (2)	0.70443 (13)	0.55210 (10)	0.0433 (4)
O1	0.1276 (2)	1.15917 (11)	0.16838 (8)	0.0439 (3)
H1	0.0660	1.1323	0.1275	0.066*
O2	0.0277 (2)	0.54745 (11)	0.47842 (8)	0.0480 (4)
C1	0.1310 (2)	0.94736 (15)	0.39752 (11)	0.0369 (4)
C2	0.0694 (2)	0.90743 (16)	0.31255 (12)	0.0397 (4)
H2A	0.0288	0.8328	0.3080	0.048*
C3	0.0675 (2)	0.97611 (15)	0.23590 (12)	0.0391 (4)
H3	0.0264	0.9482	0.1799	0.047*
C4	0.1276 (2)	1.08777 (15)	0.24249 (11)	0.0345 (4)
C5	0.1884 (3)	1.12934 (16)	0.32573 (13)	0.0416 (4)
H5	0.2283	1.2042	0.3300	0.050*
C6	0.1899 (3)	1.05962 (16)	0.40250 (12)	0.0427 (4)
H6	0.2309	1.0880	0.4584	0.051*
C7	0.1410 (3)	0.87360 (15)	0.47796 (12)	0.0402 (4)
H7	0.1747	0.9043	0.5345	0.048*
C8	0.0859 (2)	0.59215 (15)	0.54852 (11)	0.0375 (4)
C9	0.1113 (2)	0.52835 (15)	0.63685 (12)	0.0389 (4)
C10	0.1715 (3)	0.41533 (17)	0.63644 (15)	0.0483 (5)
C11	0.1871 (3)	0.3609 (2)	0.7213 (2)	0.0631 (7)
H11	0.2286	0.2863	0.7229	0.076*
C12	0.1439 (3)	0.4126 (3)	0.80218 (18)	0.0703 (8)
H12	0.1559	0.3732	0.8576	0.084*
C13	0.0828 (3)	0.5227 (2)	0.80235 (14)	0.0649 (7)
H13	0.0519	0.5579	0.8576	0.078*
C14	0.0678 (3)	0.5808 (2)	0.71959 (13)	0.0498 (5)
H14	0.0280	0.6559	0.7194	0.060*
C15	0.2224 (4)	0.3530 (2)	0.5498 (2)	0.0763 (8)

H15A	0.1196	0.3306	0.5167	0.114*
H15B	0.2886	0.2863	0.5656	0.114*
H15C	0.2915	0.4024	0.5116	0.114*
H2	0.190 (3)	0.733 (2)	0.5994 (13)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0618 (10)	0.0404 (8)	0.0303 (7)	−0.0046 (8)	−0.0064 (7)	0.0072 (6)
N2	0.0622 (10)	0.0384 (8)	0.0294 (7)	−0.0076 (8)	−0.0103 (7)	0.0068 (6)
O1	0.0610 (8)	0.0385 (6)	0.0322 (6)	−0.0012 (6)	−0.0033 (6)	0.0082 (5)
O2	0.0697 (9)	0.0413 (7)	0.0329 (6)	−0.0064 (7)	−0.0078 (6)	−0.0010 (6)
C1	0.0426 (9)	0.0353 (8)	0.0327 (8)	0.0014 (8)	−0.0021 (7)	0.0036 (7)
C2	0.0499 (10)	0.0322 (8)	0.0371 (9)	−0.0036 (8)	−0.0030 (8)	0.0023 (7)
C3	0.0485 (10)	0.0373 (9)	0.0316 (8)	0.0001 (8)	−0.0038 (7)	−0.0014 (7)
C4	0.0380 (8)	0.0335 (8)	0.0319 (8)	0.0054 (7)	0.0010 (7)	0.0054 (7)
C5	0.0537 (11)	0.0304 (8)	0.0407 (9)	−0.0019 (8)	−0.0045 (8)	0.0012 (7)
C6	0.0566 (11)	0.0393 (9)	0.0322 (8)	−0.0018 (9)	−0.0088 (8)	−0.0008 (8)
C7	0.0504 (10)	0.0396 (9)	0.0305 (8)	−0.0009 (8)	−0.0039 (8)	0.0016 (8)
C8	0.0437 (9)	0.0370 (8)	0.0317 (8)	−0.0007 (8)	−0.0010 (7)	0.0020 (7)
C9	0.0414 (9)	0.0390 (9)	0.0361 (8)	−0.0069 (8)	−0.0055 (8)	0.0068 (7)
C10	0.0468 (11)	0.0388 (9)	0.0592 (12)	−0.0054 (8)	−0.0076 (9)	0.0087 (9)
C11	0.0553 (13)	0.0510 (12)	0.0831 (17)	−0.0073 (10)	−0.0172 (13)	0.0303 (13)
C12	0.0643 (14)	0.0870 (18)	0.0594 (14)	−0.0195 (15)	−0.0179 (11)	0.0431 (14)
C13	0.0711 (15)	0.0877 (19)	0.0361 (10)	−0.0117 (14)	−0.0034 (10)	0.0141 (11)
C14	0.0590 (12)	0.0541 (11)	0.0364 (9)	−0.0040 (10)	−0.0023 (9)	0.0065 (9)
C15	0.092 (2)	0.0484 (12)	0.0880 (18)	0.0146 (14)	−0.0047 (17)	−0.0092 (14)

Geometric parameters (Å, º)

N1—C7	1.271 (2)	C6—H6	0.93
N1—N2	1.379 (2)	C7—H7	0.93
N2—C8	1.350 (2)	C8—C9	1.493 (2)
N2—H2	0.907 (10)	C9—C14	1.387 (3)
O1—C4	1.3594 (19)	C9—C10	1.401 (3)
O1—H1	0.82	C10—C11	1.389 (3)
O2—C8	1.226 (2)	C10—C15	1.503 (3)
C1—C6	1.391 (3)	C11—C12	1.358 (4)
C1—C2	1.398 (2)	C11—H11	0.93
C1—C7	1.451 (2)	C12—C13	1.371 (4)
C2—C3	1.370 (2)	C12—H12	0.93
C2—H2A	0.93	C13—C14	1.382 (3)
C3—C4	1.389 (3)	C13—H13	0.93
C3—H3	0.93	C14—H14	0.93
C4—C5	1.381 (2)	C15—H15A	0.96
C5—C6	1.378 (2)	C15—H15B	0.96
C5—H5	0.93	C15—H15C	0.96

C7—N1—N2	116.54 (15)	O2—C8—C9	122.87 (16)
C8—N2—N1	117.68 (14)	N2—C8—C9	115.07 (15)
C8—N2—H2	120.6 (17)	C14—C9—C10	120.08 (17)
N1—N2—H2	119.9 (17)	C14—C9—C8	119.10 (17)
C4—O1—H1	109.5	C10—C9—C8	120.77 (17)
C6—C1—C2	118.12 (15)	C11—C10—C9	117.2 (2)
C6—C1—C7	120.18 (16)	C11—C10—C15	119.6 (2)
C2—C1—C7	121.65 (16)	C9—C10—C15	123.19 (19)
C3—C2—C1	121.31 (16)	C12—C11—C10	122.5 (2)
C3—C2—H2A	119.3	C12—C11—H11	118.8
C1—C2—H2A	119.3	C10—C11—H11	118.8
C2—C3—C4	119.52 (16)	C11—C12—C13	120.2 (2)
C2—C3—H3	120.2	C11—C12—H12	119.9
C4—C3—H3	120.2	C13—C12—H12	119.9
O1—C4—C5	118.15 (16)	C12—C13—C14	119.3 (2)
O1—C4—C3	121.59 (15)	C12—C13—H13	120.3
C5—C4—C3	120.26 (15)	C14—C13—H13	120.3
C6—C5—C4	119.83 (16)	C13—C14—C9	120.7 (2)
C6—C5—H5	120.1	C13—C14—H14	119.7
C4—C5—H5	120.1	C9—C14—H14	119.7
C5—C6—C1	120.96 (16)	C10—C15—H15A	109.5
C5—C6—H6	119.5	C10—C15—H15B	109.5
C1—C6—H6	119.5	H15A—C15—H15B	109.5
N1—C7—C1	121.21 (16)	C10—C15—H15C	109.5
N1—C7—H7	119.4	H15A—C15—H15C	109.5
C1—C7—H7	119.4	H15B—C15—H15C	109.5
O2—C8—N2	122.01 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.96	2.7657 (18)	166
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