Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N′-(4-Hydroxybenzylidene)-4-nitrobenzohydrazide

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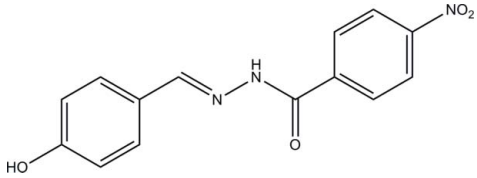
Received 18 October 2010; accepted 19 October 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.119; data-to-parameter ratio = 14.5.

The title compound, $C_{14}H_{11}N_3O_4$, was prepared by the reaction of 4-nitrobenzohydrazide with 4-hydroxybenzaldehyde. The whole molecule of the compound is approximately planar, with a mean deviation from the least-squares plane through all the non-H atoms of 0.050 (2) Å; the dihedral angle between the two benzene rings is 2.0 (2)°. In the crystal, the benzohydrazide molecules are linked through intermolecular O—H···O and N—H···O hydrogen bonds, forming layers in the *bc* plane.

Related literature

For medical applications of hydrazones, see: Ajani *et al.* (2010); Zhang *et al.* (2010); Angelusiu *et al.* (2010). For related structures, see: Huang & Wu (2010); Khaledi *et al.* (2010); Zhou & Yang (2010); Ji & Lu (2010); Singh & Singh (2010); Ahmad *et al.* (2010).



Experimental

Crystal data

$C_{14}H_{11}N_3O_4$
M_r = 285.26
Monoclinic, $P2_1/c$
a = 7.856 (3) Å
b = 13.368 (5) Å
c = 12.527 (5) Å
β = 95.748 (4)°
V = 1309.0 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 K
0.18 × 0.17 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.981, T_{max} = 0.982
7505 measured reflections
2822 independent reflections
1736 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.119
S = 1.04
2822 reflections
194 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 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
O1—H1···O2^{i}	0.82	1.98	2.7841 (18)	166
N2—H2···O4^{ii}	0.90 (1)	2.24 (1)	3.094 (2)	159 (2)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We acknowledge the Jiangsu Provincial Key Laboratory of Coastal Wetland Bioresources and Environmental Protection for financial support (project No. JLCBE07026).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5045).

References

Ahmad, T., Zia-ur-Rehman, M., Siddiqui, H. L., Mahmud, S. & Parvez, M. (2010). *Acta Cryst.* E**66**, o1022.
Ajani, O. O., Obafemi, C. A., Nwinyi, O. C. & Akinpelu, D. A. (2010). *Bioorg. Med. Chem.* **18**, 214–221.
Angelusiu, M. V., Barbuceanu, S. F., Draghici, C. & Almajan, G. L. (2010). *Eur. J. Med. Chem.* **45**, 2055–2062.
Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Huang, H.-T. & Wu, H.-Y. (2010). *Acta Cryst.* E**66**, o2729–o2730.
Ji, X.-H. & Lu, J.-F. (2010). *Acta Cryst.* E**66**, o1514.
Khaledi, H., Alhadi, A. A., Mohd Ali, H., Robinson, W. T. & Abdulla, M. A. (2010). *Acta Cryst.* E**66**, o105–o106.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Singh, V. P. & Singh, S. (2010). *Acta Cryst.* E**66**, o1172.
Zhang, Y.-H., Zhang, L., Liu, L., Guo, J.-X., Wu, D.-L., Xu, G.-C., Wang, X.-H. & Jia, D.-Z. (2010). *Inorg. Chim. Acta*, **363**, 289–293.
Zhou, C.-S. & Yang, T. (2010). *Acta Cryst.* E**66**, o290.

supporting information

Acta Cryst. (2010). E**66**, o2942 [https://doi.org/10.1107/S1600536810042364]

N′-(4-Hydroxybenzylidene)-4-nitrobenzohydrazide

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S1. Comment

Recently, medical applications of a number of hydrazone compounds have been reported (Ajani *et al.*, 2010; Zhang *et al.*, 2010; Angelusiu *et al.*, 2010). Structural investigations of several hydrazone derivatives have also been determined (Huang & Wu, 2010; Khaledi *et al.*, 2010; Zhou & Yang, 2010; Ji & Lu, 2010; Singh & Singh, 2010; Ahmad *et al.*, 2010). In this paper, we report the structure of the new derivative *N*′-(4-Hydroxybenzylidene)-4-nitrobenzohydrazide (I).

The whole molecule of (I) is approximately planar, with a mean deviation from the least squares plane through all 21 non-hydrogen atoms of 0.050 (2) Å; the dihedral angle between the C1···C6 and C9···C14 benzene rings is 2.0 (2)°. The bond lengths and angles are comparable to those found in the hydrazone compounds cited above. In the crystal structure, the hydrazone molecules are linked through intermolecular O1–H1···O2 and N2–H2···O4 hydrogen bonds (Table 1), to form two-dimensional layers in the *bc* plane, as shown in Fig. 2.

S2. Experimental

The reaction of 4-nitrobenzohydrazide (0.181 g, 1 mmol) with 4-hydroxybenzaldehyde (0.122 g, 1 mmol) in 50 ml methanol at room temperature afforded the title compound. Single crystals were formed by slow evaporation of the clear solution in air.

S3. Refinement

The amino H atom was located in a difference Fourier map and refined with N–H = 0.90 (1) Å, and U_{iso} = 0.08 Å^2. Other H atoms were positioned geometrically (C–H = 0.93 Å, O–H = 0.82 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5 U_{eq}(O).

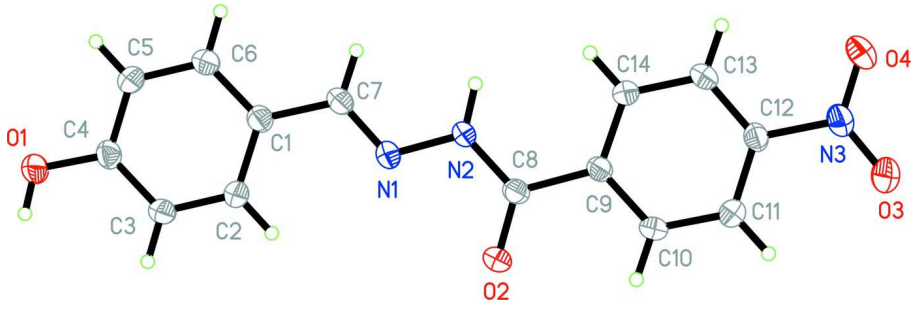

Figure 1

The molecular structure of the title compound showing 30% probability displacement ellipsoids and the atomic numbering.

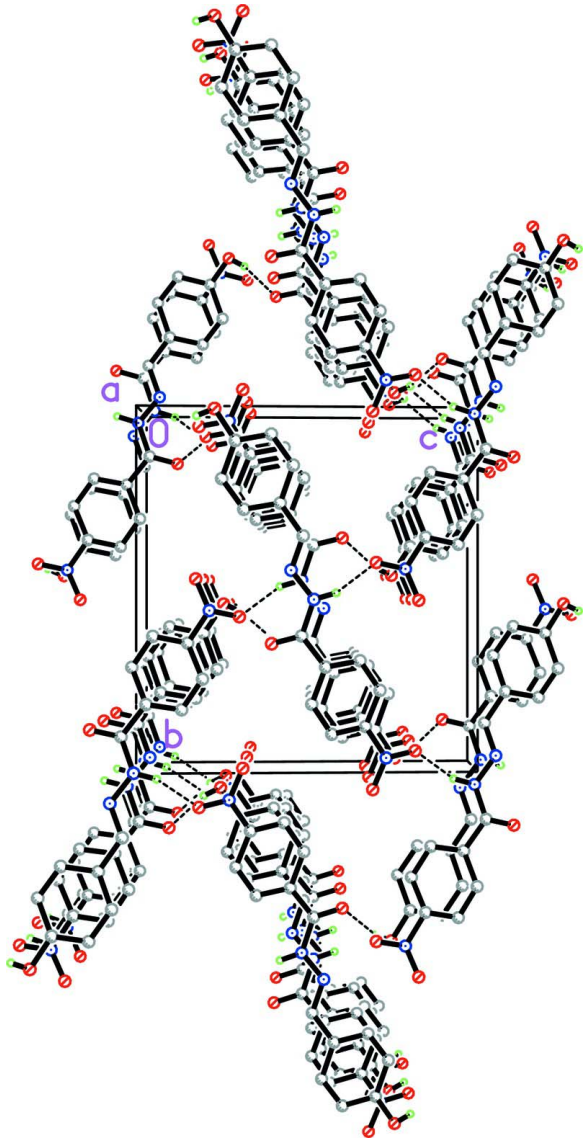

Figure 2

Crystal packing of the title compound, viewed down the *a* axis. Intermolecular interactions are drawn as dashed lines.

N′-(4-Hydroxybenzylidene)-4-nitrobenzohydrazide

Crystal data

$C_{14}H_{11}N_3O_4$
$M_r = 285.26$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.856\ (3)$ Å
$b = 13.368\ (5)$ Å
$c = 12.527\ (5)$ Å
$\beta = 95.748\ (4)°$
$V = 1309.0\ (9)$ Å^3
$Z = 4$

$F(000) = 592$
$D_x = 1.447$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1632 reflections
$\theta = 2.2–26.0°$
$\mu = 0.11$ mm^{-1}
$T = 298$ K
Block, yellow
0.18 × 0.17 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.981, T_{max} = 0.982
7505 measured reflections
2822 independent reflections
1736 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 27.0°, θ_{min} = 2.2°
h = −9→10
k = −17→14
l = −16→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.119
S = 1.04
2822 reflections
194 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
$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 0.1504P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
N1	0.20526 (19)	−0.05033 (11)	0.04617 (11)	0.0433 (4)
N2	0.2594 (2)	0.02540 (11)	−0.01727 (11)	0.0420 (4)
N3	0.4845 (2)	0.44506 (12)	−0.22229 (13)	0.0510 (4)
O1	0.0039 (2)	−0.46112 (9)	0.25453 (11)	0.0598 (4)
H1	−0.0521	−0.4411	0.3021	0.090*
O2	0.17995 (17)	0.13969 (9)	0.09997 (10)	0.0512 (4)
O3	0.4755 (2)	0.52833 (11)	−0.18407 (13)	0.0872 (6)
O4	0.54671 (18)	0.42836 (10)	−0.30610 (10)	0.0603 (4)
C1	0.1654 (2)	−0.22332 (13)	0.07612 (14)	0.0395 (4)
C2	0.1046 (2)	−0.20626 (13)	0.17594 (14)	0.0433 (5)
H2A	0.1006	−0.1412	0.2020	0.052*
C3	0.0511 (2)	−0.28366 (13)	0.23572 (14)	0.0444 (5)
H3	0.0107	−0.2708	0.3017	0.053*
C4	0.0567 (2)	−0.38146 (13)	0.19834 (14)	0.0424 (5)
C5	0.1185 (2)	−0.39987 (13)	0.10044 (15)	0.0463 (5)

H5	0.1240	−0.4651	0.0753	0.056*
C6	0.1721 (2)	−0.32147 (13)	0.04010 (14)	0.0446 (5)
H6	0.2132	−0.3346	−0.0256	0.053*
C7	0.2197 (2)	−0.13939 (13)	0.01282 (14)	0.0422 (4)
H7	0.2649	−0.1512	−0.0519	0.051*
C8	0.2426 (2)	0.12013 (13)	0.01678 (13)	0.0372 (4)
C9	0.3070 (2)	0.20201 (12)	−0.05002 (13)	0.0352 (4)
C10	0.2986 (2)	0.29875 (13)	−0.01120 (14)	0.0454 (5)
H10	0.2541	0.3099	0.0538	0.055*
C11	0.3552 (2)	0.37861 (13)	−0.06733 (15)	0.0482 (5)
H11	0.3492	0.4435	−0.0411	0.058*
C12	0.4209 (2)	0.36016 (13)	−0.16304 (14)	0.0395 (4)
C13	0.4312 (2)	0.26543 (14)	−0.20412 (14)	0.0449 (5)
H13	0.4760	0.2548	−0.2691	0.054*
C14	0.3738 (2)	0.18647 (13)	−0.14713 (14)	0.0446 (5)
H14	0.3799	0.1219	−0.1740	0.054*
H2	0.299 (3)	0.0083 (16)	−0.0797 (11)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0554 (10)	0.0363 (9)	0.0402 (9)	−0.0019 (7)	0.0149 (7)	0.0061 (7)
N2	0.0593 (10)	0.0337 (8)	0.0360 (8)	−0.0025 (7)	0.0187 (7)	0.0034 (7)
N3	0.0596 (11)	0.0466 (10)	0.0482 (10)	−0.0082 (8)	0.0127 (8)	0.0080 (8)
O1	0.0868 (11)	0.0365 (7)	0.0615 (9)	−0.0022 (7)	0.0338 (8)	0.0061 (7)
O2	0.0688 (9)	0.0451 (8)	0.0442 (8)	0.0005 (7)	0.0273 (6)	−0.0002 (6)
O3	0.1470 (17)	0.0418 (9)	0.0802 (12)	−0.0201 (10)	0.0472 (11)	0.0006 (8)
O4	0.0700 (10)	0.0636 (9)	0.0511 (9)	−0.0088 (7)	0.0247 (7)	0.0110 (7)
C1	0.0415 (10)	0.0392 (10)	0.0385 (10)	0.0004 (8)	0.0075 (8)	0.0030 (8)
C2	0.0554 (11)	0.0332 (10)	0.0429 (10)	−0.0023 (8)	0.0127 (9)	−0.0005 (8)
C3	0.0553 (11)	0.0411 (10)	0.0390 (10)	0.0011 (9)	0.0154 (9)	−0.0003 (9)
C4	0.0467 (11)	0.0362 (10)	0.0453 (11)	0.0007 (8)	0.0100 (9)	0.0077 (9)
C5	0.0585 (12)	0.0326 (9)	0.0495 (11)	0.0012 (9)	0.0135 (9)	−0.0022 (9)
C6	0.0524 (11)	0.0432 (11)	0.0400 (10)	0.0015 (9)	0.0142 (9)	−0.0008 (9)
C7	0.0472 (11)	0.0441 (11)	0.0367 (10)	−0.0006 (9)	0.0123 (8)	0.0042 (9)
C8	0.0394 (10)	0.0405 (10)	0.0327 (9)	0.0025 (8)	0.0084 (8)	0.0015 (8)
C9	0.0367 (9)	0.0369 (9)	0.0330 (9)	0.0032 (7)	0.0083 (7)	0.0026 (8)
C10	0.0589 (12)	0.0430 (11)	0.0373 (10)	−0.0008 (9)	0.0197 (9)	−0.0045 (8)
C11	0.0632 (12)	0.0353 (10)	0.0481 (11)	−0.0029 (9)	0.0159 (10)	−0.0030 (9)
C12	0.0424 (10)	0.0371 (10)	0.0400 (10)	−0.0021 (8)	0.0088 (8)	0.0068 (8)
C13	0.0554 (11)	0.0457 (11)	0.0363 (10)	0.0012 (9)	0.0180 (9)	0.0024 (9)
C14	0.0605 (12)	0.0343 (9)	0.0417 (10)	0.0032 (9)	0.0186 (9)	−0.0013 (8)

Geometric parameters (Å, º)

N1—C7	1.271 (2)	C4—C5	1.386 (2)
N1—N2	1.3803 (19)	C5—C6	1.382 (2)
N2—C8	1.347 (2)	C5—H5	0.9300

N2—H2	0.899 (9)	C6—H6	0.9300
N3—O3	1.217 (2)	C7—H7	0.9300
N3—O4	1.2220 (19)	C8—C9	1.496 (2)
N3—C12	1.471 (2)	C9—C10	1.386 (2)
O1—C4	1.364 (2)	C9—C14	1.388 (2)
O1—H1	0.8200	C10—C11	1.376 (2)
O2—C8	1.2247 (19)	C10—H10	0.9300
C1—C6	1.390 (2)	C11—C12	1.374 (2)
C1—C2	1.401 (2)	C11—H11	0.9300
C1—C7	1.462 (2)	C12—C13	1.372 (2)
C2—C3	1.368 (2)	C13—C14	1.375 (2)
C2—H2A	0.9300	C13—H13	0.9300
C3—C4	1.391 (2)	C14—H14	0.9300
C3—H3	0.9300		

C7—N1—N2	117.08 (14)	C1—C6—H6	119.5
C8—N2—N1	117.50 (13)	N1—C7—C1	120.02 (15)
C8—N2—H2	124.6 (15)	N1—C7—H7	120.0
N1—N2—H2	117.9 (15)	C1—C7—H7	120.0
O3—N3—O4	123.30 (16)	O2—C8—N2	122.05 (15)
O3—N3—C12	118.13 (16)	O2—C8—C9	120.45 (15)
O4—N3—C12	118.55 (16)	N2—C8—C9	117.49 (14)
C4—O1—H1	109.5	C10—C9—C14	118.85 (15)
C6—C1—C2	118.08 (16)	C10—C9—C8	117.14 (14)
C6—C1—C7	121.71 (15)	C14—C9—C8	124.01 (15)
C2—C1—C7	120.20 (16)	C11—C10—C9	121.04 (16)
C3—C2—C1	121.08 (16)	C11—C10—H10	119.5
C3—C2—H2A	119.5	C9—C10—H10	119.5
C1—C2—H2A	119.5	C12—C11—C10	118.37 (17)
C2—C3—C4	120.32 (16)	C12—C11—H11	120.8
C2—C3—H3	119.8	C10—C11—H11	120.8
C4—C3—H3	119.8	C13—C12—C11	122.28 (16)
O1—C4—C5	118.02 (16)	C13—C12—N3	119.15 (15)
O1—C4—C3	122.60 (15)	C11—C12—N3	118.56 (16)
C5—C4—C3	119.38 (16)	C12—C13—C14	118.62 (15)
C6—C5—C4	120.15 (17)	C12—C13—H13	120.7
C6—C5—H5	119.9	C14—C13—H13	120.7
C4—C5—H5	119.9	C13—C14—C9	120.83 (16)
C5—C6—C1	120.97 (16)	C13—C14—H14	119.6
C5—C6—H6	119.5	C9—C14—H14	119.6

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.98	2.7841 (18)	166
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