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4-Methoxy-*N*′-(4-methoxybenzylidene)-benzohydrazide

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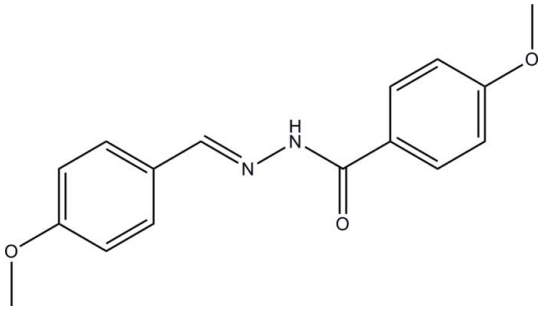
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.011 Å; R factor = 0.059; wR factor = 0.138; data-to-parameter ratio = 7.2.

The title compound, $C_{16}H_{16}N_2O_3$, was prepared by the reaction of 4-methoxybenzaldehyde with 4-methoxybenzohydrazide in methanol. The dihedral angle between the two benzene rings is 3.1 (3)°. In the crystal, intermolecular N—H···O hydrogen bonds link the molecules into $C(4)$ chains along the b axis.

Related literature

For the biological activity of hydrazone compounds, see: Peng (2011); Angelusiu *et al.* (2010); Ajani *et al.* (2010); Horiuchi *et al.* (2009). For related structures, see: Zhang (2011); Lei & Fu (2011); Tang (2011).



Experimental

Crystal data

$C_{16}H_{16}N_2O_3$ M_r = 284.31
Monoclinic, Pc
a = 10.617 (3) Å
b = 4.877 (2) Å
c = 13.632 (3) Å
β = 92.409 (2)°
V = 705.2 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.20 × 0.18 × 0.17 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.982, T_{max} = 0.984
3893 measured reflections
1396 independent reflections
1026 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.138
S = 1.30
1396 reflections
195 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2^{i}	0.90 (1)	1.99 (3)	2.844 (7)	157 (7)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5072).

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supporting information

Acta Cryst. (2011). E**67**, o1182 [doi:10.1107/S1600536811014012]

4-Methoxy-*N*′-(4-methoxybenzylidene)benzohydrazide

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S1. Comment

Hydrazone compounds have attracted much attention due to their biological activities (Peng, 2011; Angelusiu *et al.*, 2010; Ajani *et al.*, 2010; Horiuchi *et al.*, 2009). In this paper, we present the title compound (I), which is a new hydrazone derivative.

In (I) (Fig. 1), all bond lengths and angles are normal and correspond to those observed in the related compounds (Zhang, 2011; Lei & Fu, 2011; Tang, 2011). The dihedral angle between the two benzene rings is 3.1 (3)°. In the crystal structure, intermolecular N—H···O hydrogen bonds (Table 1) link the molecules related by translation along axis *b* into chains (Fig. 2).

S2. Experimental

Equimolar quantities (1.0 mmol each) of 4-methoxybenzaldehyde and 4-methoxybenzohydrazide were mixed in methanol. The mixture was stirred at room temperature for half an hour to give a colorless solution. After keeping the solution in air for a few days, colorless block-shaped crystals were formed.

S3. Refinement

Atom H2A attached to N2 was located on a difference map and refined isotropically, with the N–H distance restrained to 0.90 (1) Å. Other H atoms were placed in calculated positions and constrained to ride on their parent atoms with C–H distances of 0.93-0.96 Å, and with U_{iso}(H) set to 1.2U_{eq}(C) and 1.5U_{eq}(C8 and C16). In the absence of any significant anomalous scatterers in the molecule, 735 Friedel pairs were merged before the final refinement.

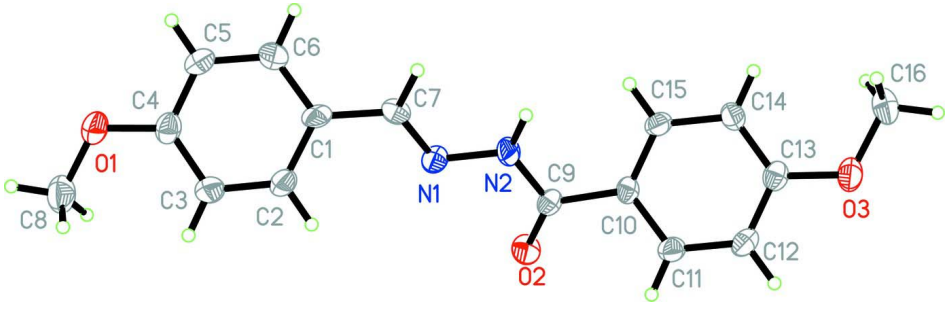

Figure 1

The molecular structure of (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme.

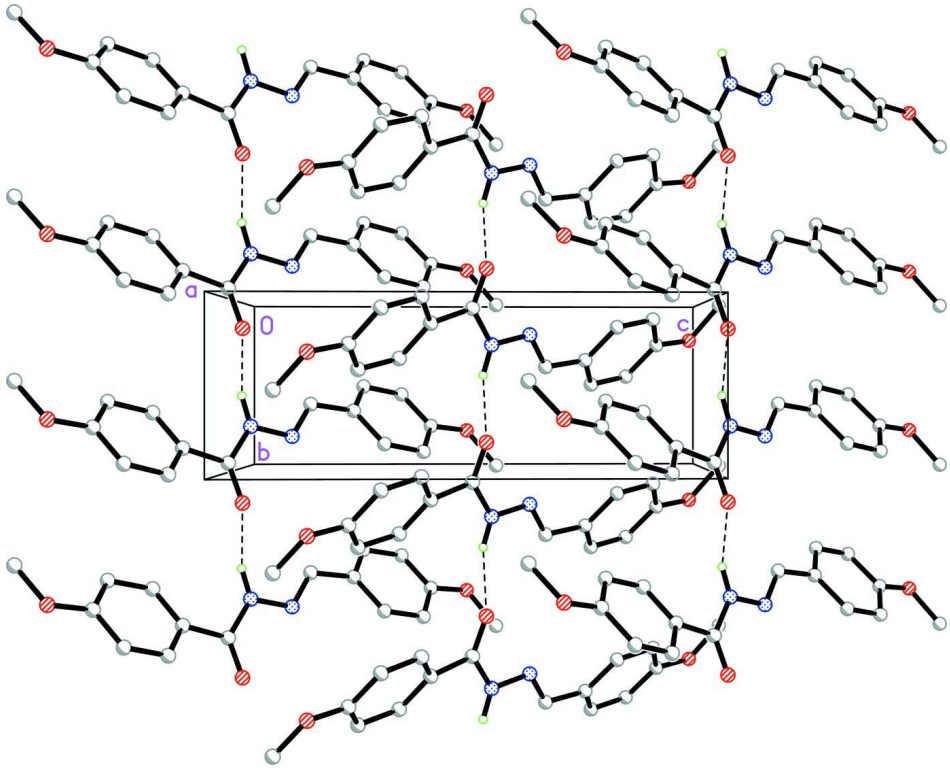

Figure 2

A portion of the crystal packing viewed approximately along the *a* axis. Hydrogen bonds are shown as dashed lines.

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$C_{16}H_{16}N_2O_3$
$M_r = 284.31$
Monoclinic, *Pc*
$a = 10.617\ (3)$ Å
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$c = 13.632\ (3)$ Å
$\beta = 92.409\ (2)°$
$V = 705.2\ (4)$ Å^3
$Z = 2$
$F(000) = 300$
$D_x = 1.339$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1579 reflections
$\theta = 2.9–28.3°$
$\mu = 0.09$ mm^{-1}
$T = 298$ K
Block, colourless
0.20 × 0.18 × 0.17 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
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ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.982$, $T_{max} = 0.984$
3893 measured reflections
1396 independent reflections
1026 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 26.5°$, $\theta_{min} = 3.0°$
$h = -13\rightarrow11$
$k = -6\rightarrow6$
$l = -16\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.138$
$S = 1.30$
1396 reflections
195 parameters
3 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0182P)^2 + 0.6212P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ 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 $F^2 > 2$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}
N1	0.4613 (6)	0.2010 (11)	0.6226 (5)	0.0425 (15)
N2	0.5326 (7)	0.2629 (11)	0.5429 (5)	0.0450 (16)
O1	0.1067 (5)	0.2188 (12)	0.9836 (4)	0.0622 (17)
O2	0.5985 (5)	−0.1728 (8)	0.5324 (4)	0.0565 (13)
O3	0.8991 (5)	0.3171 (14)	0.1869 (4)	0.0609 (16)
C1	0.3252 (7)	0.3481 (14)	0.7438 (6)	0.0426 (19)
C2	0.3588 (7)	0.1499 (17)	0.8117 (6)	0.051 (2)
H2	0.4308	0.0462	0.8022	0.061*
C3	0.2908 (7)	0.0991 (17)	0.8929 (6)	0.056 (2)
H3	0.3165	−0.0343	0.9381	0.067*
C4	0.1832 (8)	0.2503 (16)	0.9059 (6)	0.048 (2)
C5	0.1462 (9)	0.4446 (17)	0.8393 (6)	0.063 (3)
H5	0.0728	0.5442	0.8479	0.076*
C6	0.2175 (9)	0.4938 (16)	0.7594 (7)	0.063 (3)
H6	0.1920	0.6292	0.7148	0.075*
C7	0.3991 (8)	0.3890 (13)	0.6570 (6)	0.046 (2)
H7	0.3992	0.5602	0.6269	0.056*
C8	0.1325 (10)	0.0017 (19)	1.0495 (7)	0.073 (3)
H8A	0.1294	−0.1691	1.0144	0.110*
H8B	0.0708	0.0002	1.0990	0.110*
H8C	0.2150	0.0258	1.0799	0.110*
C9	0.6006 (7)	0.0565 (13)	0.5037 (5)	0.0379 (17)
C10	0.6766 (6)	0.1469 (14)	0.4199 (5)	0.0358 (16)
C11	0.7875 (7)	0.0084 (14)	0.4050 (6)	0.046 (2)

H11	0.8132	−0.1311	0.4478	0.055*
C12	0.8599 (8)	0.0742 (16)	0.3281 (6)	0.051 (2)
H12	0.9361	−0.0157	0.3203	0.061*
C13	0.8211 (8)	0.2711 (15)	0.2624 (6)	0.0434 (18)
C14	0.7112 (7)	0.4090 (14)	0.2749 (5)	0.046 (2)
H14	0.6848	0.5440	0.2305	0.055*
C15	0.6390 (7)	0.3463 (15)	0.3546 (5)	0.0427 (18)
H15	0.5644	0.4409	0.3635	0.051*
C16	0.8644 (10)	0.5240 (18)	0.1176 (6)	0.062 (3)
H16A	0.7837	0.4805	0.0870	0.093*
H16B	0.9263	0.5338	0.0684	0.093*
H16C	0.8596	0.6976	0.1504	0.093*
H2A	0.539 (8)	0.440 (5)	0.525 (6)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.047 (4)	0.024 (3)	0.058 (4)	−0.002 (3)	0.015 (3)	−0.002 (3)
N2	0.045 (4)	0.040 (3)	0.052 (4)	−0.006 (3)	0.017 (3)	0.010 (3)
O1	0.055 (4)	0.071 (4)	0.062 (4)	0.008 (3)	0.025 (3)	0.005 (3)
O2	0.077 (3)	0.018 (2)	0.077 (3)	−0.002 (2)	0.027 (3)	0.007 (2)
O3	0.049 (4)	0.081 (4)	0.054 (3)	−0.001 (3)	0.016 (3)	0.008 (3)
C1	0.049 (5)	0.019 (3)	0.060 (5)	0.006 (3)	0.006 (4)	−0.002 (3)
C2	0.040 (5)	0.053 (5)	0.061 (5)	0.009 (4)	0.014 (4)	0.008 (4)
C3	0.043 (5)	0.066 (5)	0.060 (6)	0.012 (5)	0.005 (5)	0.013 (4)
C4	0.037 (4)	0.061 (5)	0.047 (5)	−0.004 (4)	0.006 (4)	−0.004 (4)
C5	0.056 (6)	0.063 (6)	0.071 (7)	0.026 (5)	0.017 (5)	0.009 (5)
C6	0.080 (7)	0.047 (5)	0.063 (6)	0.017 (5)	0.019 (6)	0.017 (4)
C7	0.061 (5)	0.016 (3)	0.063 (5)	−0.003 (3)	0.014 (4)	0.012 (3)
C8	0.085 (8)	0.072 (6)	0.066 (7)	−0.002 (5)	0.030 (6)	0.004 (5)
C9	0.031 (4)	0.038 (4)	0.045 (4)	−0.004 (3)	0.004 (3)	−0.007 (3)
C10	0.031 (4)	0.034 (3)	0.043 (4)	−0.010 (3)	0.006 (3)	0.000 (3)
C11	0.040 (5)	0.039 (4)	0.060 (6)	0.004 (3)	0.006 (4)	0.007 (4)
C12	0.038 (5)	0.058 (5)	0.057 (6)	0.010 (4)	0.009 (4)	−0.002 (4)
C13	0.039 (4)	0.042 (4)	0.050 (5)	−0.007 (3)	0.007 (4)	−0.007 (3)
C14	0.054 (5)	0.042 (4)	0.043 (5)	0.001 (4)	0.012 (4)	0.007 (3)
C15	0.037 (4)	0.038 (4)	0.054 (5)	0.007 (4)	0.005 (4)	0.001 (4)
C16	0.072 (7)	0.067 (5)	0.049 (5)	−0.011 (5)	0.017 (5)	0.003 (4)

Geometric parameters (Å, º)

N1—C7	1.234 (9)	C6—H6	0.9300
N1—N2	1.383 (6)	C7—H7	0.9300
N2—C9	1.361 (9)	C8—H8A	0.9600
N2—H2A	0.900 (11)	C8—H8B	0.9600
O1—C4	1.371 (10)	C8—H8C	0.9600
O1—C8	1.408 (10)	C9—C10	1.492 (9)
O2—C9	1.186 (7)	C10—C15	1.367 (9)

O3—C13	1.366 (10)	C10—C11	1.380 (10)
O3—C16	1.421 (10)	C11—C12	1.364 (10)
C1—C6	1.370 (11)	C11—H11	0.9300
C1—C2	1.375 (10)	C12—C13	1.365 (11)
C1—C7	1.462 (10)	C12—H12	0.9300
C2—C3	1.369 (11)	C13—C14	1.364 (11)
C2—H2	0.9300	C14—C15	1.390 (10)
C3—C4	1.377 (11)	C14—H14	0.9300
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.359 (11)	C16—H16A	0.9600
C5—C6	1.373 (11)	C16—H16B	0.9600
C5—H5	0.9300	C16—H16C	0.9600

C7—N1—N2	117.1 (6)	O1—C8—H8C	109.5
C9—N2—N1	117.6 (5)	H8A—C8—H8C	109.5
C9—N2—H2A	124 (5)	H8B—C8—H8C	109.5
N1—N2—H2A	118 (5)	O2—C9—N2	123.4 (7)
C4—O1—C8	118.1 (7)	O2—C9—C10	123.4 (7)
C13—O3—C16	118.0 (7)	N2—C9—C10	113.2 (6)
C6—C1—C2	117.1 (8)	C15—C10—C11	118.6 (7)
C6—C1—C7	122.3 (7)	C15—C10—C9	123.9 (6)
C2—C1—C7	120.5 (7)	C11—C10—C9	117.4 (7)
C3—C2—C1	122.7 (7)	C12—C11—C10	120.6 (7)
C3—C2—H2	118.7	C12—C11—H11	119.7
C1—C2—H2	118.7	C10—C11—H11	119.7
C2—C3—C4	118.4 (8)	C11—C12—C13	120.4 (8)
C2—C3—H3	120.8	C11—C12—H12	119.8
C4—C3—H3	120.8	C13—C12—H12	119.8
C5—C4—O1	115.5 (8)	C14—C13—C12	120.0 (8)
C5—C4—C3	120.4 (9)	C14—C13—O3	124.2 (7)
O1—C4—C3	124.1 (8)	C12—C13—O3	115.7 (8)
C4—C5—C6	119.9 (8)	C13—C14—C15	119.5 (7)
C4—C5—H5	120.1	C13—C14—H14	120.3
C6—C5—H5	120.1	C15—C14—H14	120.3
C1—C6—C5	121.6 (8)	C10—C15—C14	120.7 (7)
C1—C6—H6	119.2	C10—C15—H15	119.6
C5—C6—H6	119.2	C14—C15—H15	119.6
N1—C7—C1	121.4 (6)	O3—C16—H16A	109.5
N1—C7—H7	119.3	O3—C16—H16B	109.5
C1—C7—H7	119.3	H16A—C16—H16B	109.5
O1—C8—H8A	109.5	O3—C16—H16C	109.5
O1—C8—H8B	109.5	H16A—C16—H16C	109.5
H8A—C8—H8B	109.5	H16B—C16—H16C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N2—H2*A*···O2^{i}	0.90 (1)	1.99 (3)	2.844 (7)	157 (7)

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