Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-*N*′-(4-Methoxybenzylidene)-3-nitrobenzohydrazide

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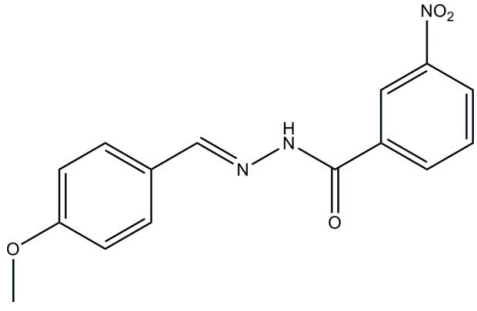
Received 22 June 2011; accepted 28 June 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.063; wR factor = 0.173; data-to-parameter ratio = 14.9.

In the title compound, $C_{15}H_{13}N_3O_4$, the two substituted benzene rings form a dihedral angle of 5.0 (3)°. In the crystal, intermolecular N—H···O hydrogen bonds link molecules into chains along the b axis.

Related literature

For background to the binding properties and biological activity of condensation products of aldehydes with benzohydrazides, see: Sanchez-Lozano *et al.* (2011); Wang (2011); Cui *et al.* (2011); Zhu (2011); Peng (2011). For related structures, see: Hashemian *et al.* (2011); Shalash *et al.* (2010).



Experimental

Crystal data

$C_{15}H_{13}N_3O_4$ M_r = 299.28
Monoclinic, $P2_1/c$
a = 13.667 (4) Å
b = 4.889 (3) Å
c = 22.522 (4) Å
β = 104.113 (3)°
V = 1459.5 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 K
0.30 × 0.28 × 0.27 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.970, T_{max} = 0.973
9043 measured reflections
2981 independent reflections
1493 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.173
S = 1.02
2981 reflections
200 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 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}	0.86	2.13	2.895 (3)	148

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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 Henan University of Science and Technology is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2619).

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supplementary materials

Acta Cryst. (2011). E**67**, o1886 [**doi:10.1107/S1600536811025554**]

(*E*)-*N*'-(4-Methoxybenzylidene)-3-nitrobenzohydrazide

J.-W. Guo, J.-Y. Ma and C.-W. Sun

Comment

The compounds derived from the condensation reaction of aldehydes with benzohydrazides play a vital role in coordination chemistry due to their metal binding property (Sanchez-Lozano *et al.*, 2011; Wang, 2011; Cui *et al.*, 2011). Moreover, most of such compounds possess effective biological activity (Zhu, 2011; Peng, 2011). In recent years, a number of such compounds have been reported (Hashemian *et al.*, 2011; Shalash *et al.*, 2010). In this paper, the title new compound, (*E*)-*N*'-(4-Methoxybenzylidene)-3-nitrobenzohydrazide, (I), is reported.

The molecular structure of (I) is shown in Fig. 1. The bond lengths in (I) are normal and comparable with those observed in the reported structures cited above. The two substituted benzene rings form a dihedral angle of 5.0 (3)°. In the crystal, intermolecular N–H···O hydrogen bonds link molecules into one-dimensional chains along the *b* axis (Fig. 2; Table 1).

Experimental

4-Methoxybenzaldehyde (0.136 g, 1 mmol), 3-nitrobenzohydrazide (0.181 g, 1 mmol), and a few drops of acetic acid were mixed in methanol (30 ml). The solution was magnetically stirred at ambient temperature for 10 min until it turned to yellow. The solution was slowly evaporated in open air to give needle-shaped pale yellow single crystals.

Refinement

H atoms were placed in idealized positions (C–H = 0.93-0.96 Å, N–H = 0.86 Å), and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C, N) or 1.5U_{eq}(C) for methyl H atoms.

Figures

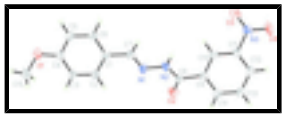

Fig. 1. The molecular structure of the title compound with displacement ellipsoids shown at 30% probability level.

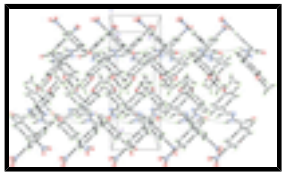

Fig. 2. Packing diagram of the title compound, viewed along the *c* axis. Hydrogen bonds are indicated by dashed lines.

(*E*)-*N*'-(4-Methoxybenzylidene)-3-nitrobenzohydrazide

Crystal data

$C_{15}H_{13}N_3O_4$	$F(000) = 624$
$M_r = 299.28$	$D_x = 1.362$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 762 reflections
$a = 13.667$ (4) Å	$\theta = 2.6$–$24.3°$
$b = 4.889$ (3) Å	$\mu = 0.10$ mm^{-1}
$c = 22.522$ (4) Å	$T = 298$ K
$\beta = 104.113$ (3)°	Needle fragment, pale yellow
$V = 1459.5$ (10) Å^3	0.30 × 0.28 × 0.27 mm
$Z = 4$	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2981 independent reflections
Radiation source: fine-focus sealed tube	1493 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.073$
ω scans	$\theta_{max} = 26.5°$, $\theta_{min} = 2.1°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)	$h = -16 \rightarrow 16$
$T_{min} = 0.970$, $T_{max} = 0.973$	$k = -6 \rightarrow 6$
9043 measured reflections	$l = -28 \rightarrow 28$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.063$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.173$	H-atom parameters constrained
$S = 1.02$	$w = 1/[\sigma^2(F_o^2)]$ where $P = (F_o^2 + 2F_c^2)/3$
2981 reflections	$(\Delta/\sigma)_{max} < 0.001$
200 parameters	$\Delta\rho_{max} = 0.19$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.26$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.26856 (19)	0.4077 (5)	0.12291 (10)	0.0478 (7)
N2	0.22236 (19)	0.4793 (4)	0.06262 (10)	0.0481 (7)
H2A	0.2022	0.6443	0.0537	0.058*
N3	−0.03766 (19)	0.8680 (5)	−0.13175 (12)	0.0519 (7)
O1	0.44934 (18)	0.4662 (5)	0.41484 (9)	0.0673 (7)
O2	0.23532 (17)	0.0453 (4)	0.02765 (9)	0.0572 (6)
O3	−0.05412 (17)	0.9975 (4)	−0.08818 (10)	0.0658 (7)
O4	−0.08122 (19)	0.9108 (5)	−0.18561 (10)	0.0813 (8)
C1	0.3188 (2)	0.5554 (6)	0.22758 (11)	0.0425 (7)
C2	0.3912 (2)	0.3558 (6)	0.24755 (12)	0.0486 (8)
H2	0.4092	0.2423	0.2188	0.058*
C3	0.4377 (2)	0.3199 (6)	0.30896 (12)	0.0501 (8)
H3A	0.4870	0.1862	0.3210	0.060*
C4	0.4100 (2)	0.4862 (6)	0.35258 (12)	0.0467 (8)
C5	0.3381 (3)	0.6875 (6)	0.33375 (13)	0.0543 (9)
H5	0.3197	0.7990	0.3627	0.065*
C6	0.2933 (2)	0.7246 (6)	0.27212 (12)	0.0510 (8)
H6	0.2459	0.8628	0.2600	0.061*
C7	0.2695 (2)	0.5983 (6)	0.16229 (12)	0.0470 (8)
H7	0.2388	0.7651	0.1495	0.056*
C8	0.2095 (2)	0.2863 (6)	0.01832 (12)	0.0417 (7)
C9	0.1590 (2)	0.3825 (5)	−0.04553 (11)	0.0399 (7)
C10	0.0857 (2)	0.5890 (5)	−0.05782 (12)	0.0410 (7)
H10	0.0681	0.6832	−0.0261	0.049*
C11	0.0400 (2)	0.6497 (6)	−0.11841 (12)	0.0421 (7)
C12	0.0651 (3)	0.5157 (6)	−0.16723 (13)	0.0523 (8)
H12	0.0331	0.5608	−0.2074	0.063*
C13	0.1384 (2)	0.3145 (6)	−0.15503 (12)	0.0541 (9)
H13	0.1569	0.2247	−0.1870	0.065*
C14	0.1841 (2)	0.2474 (6)	−0.09470 (12)	0.0492 (8)
H14	0.2324	0.1096	−0.0868	0.059*
C15	0.5296 (3)	0.2752 (9)	0.43634 (14)	0.0875 (12)
H15A	0.5063	0.0935	0.4243	0.131*
H15B	0.5512	0.2849	0.4802	0.131*
H15C	0.5852	0.3190	0.4189	0.131*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0634 (18)	0.0364 (15)	0.0395 (13)	0.0020 (13)	0.0045 (12)	0.0084 (11)
N2	0.0673 (19)	0.0320 (14)	0.0397 (14)	0.0072 (13)	0.0030 (12)	0.0094 (10)
N3	0.0450 (17)	0.0560 (18)	0.0523 (17)	−0.0011 (14)	0.0073 (13)	0.0085 (13)
O1	0.0695 (17)	0.0890 (18)	0.0390 (12)	0.0124 (14)	0.0046 (11)	−0.0008 (11)
O2	0.0809 (17)	0.0307 (12)	0.0582 (13)	0.0075 (11)	0.0133 (12)	0.0063 (9)
O3	0.0615 (16)	0.0655 (16)	0.0698 (15)	0.0145 (12)	0.0146 (13)	0.0037 (12)
O4	0.0762 (19)	0.105 (2)	0.0522 (14)	0.0205 (15)	−0.0048 (13)	0.0249 (13)
C1	0.050 (2)	0.0380 (18)	0.0387 (16)	−0.0020 (15)	0.0093 (14)	0.0047 (12)
C2	0.062 (2)	0.0399 (18)	0.0441 (17)	0.0041 (16)	0.0133 (15)	−0.0018 (13)
C3	0.055 (2)	0.052 (2)	0.0405 (16)	0.0077 (16)	0.0058 (14)	0.0046 (14)
C4	0.047 (2)	0.051 (2)	0.0394 (17)	−0.0044 (16)	0.0072 (14)	0.0016 (13)
C5	0.068 (2)	0.054 (2)	0.0424 (17)	0.0057 (18)	0.0169 (16)	−0.0048 (14)
C6	0.054 (2)	0.0454 (19)	0.0536 (18)	0.0073 (16)	0.0128 (15)	0.0032 (14)
C7	0.059 (2)	0.0365 (18)	0.0443 (17)	0.0038 (16)	0.0107 (15)	0.0060 (13)
C8	0.0498 (19)	0.0344 (18)	0.0416 (15)	0.0004 (15)	0.0123 (14)	0.0039 (13)
C9	0.0529 (19)	0.0271 (15)	0.0400 (15)	−0.0051 (14)	0.0118 (14)	0.0011 (12)
C10	0.0461 (19)	0.0353 (17)	0.0417 (16)	−0.0040 (14)	0.0109 (14)	0.0007 (12)
C11	0.0452 (19)	0.0382 (17)	0.0411 (16)	−0.0049 (15)	0.0070 (14)	0.0064 (12)
C12	0.060 (2)	0.057 (2)	0.0356 (16)	−0.0111 (18)	0.0034 (15)	0.0027 (14)
C13	0.070 (2)	0.053 (2)	0.0422 (17)	−0.0027 (18)	0.0203 (16)	−0.0022 (15)
C14	0.057 (2)	0.0402 (19)	0.0511 (18)	−0.0007 (16)	0.0152 (15)	0.0005 (14)
C15	0.093 (3)	0.105 (3)	0.049 (2)	0.024 (3)	−0.013 (2)	0.001 (2)

Geometric parameters (Å, °)

N1—C7	1.284 (3)	C5—C6	1.386 (4)
N1—N2	1.395 (3)	C5—H5	0.9300
N2—C8	1.353 (3)	C6—H6	0.9300
N2—H2A	0.8600	C7—H7	0.9300
N3—O4	1.232 (3)	C8—C9	1.510 (4)
N3—O3	1.234 (3)	C9—C14	1.402 (3)
N3—C11	1.483 (4)	C9—C10	1.402 (4)
O1—C4	1.377 (3)	C10—C11	1.387 (3)
O1—C15	1.432 (4)	C10—H10	0.9300
O2—C8	1.233 (3)	C11—C12	1.393 (4)
C1—C2	1.385 (4)	C12—C13	1.383 (4)
C1—C6	1.408 (4)	C12—H12	0.9300
C1—C7	1.475 (4)	C13—C14	1.389 (4)
C2—C3	1.385 (4)	C13—H13	0.9300
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.397 (4)	C15—H15A	0.9600
C3—H3A	0.9300	C15—H15B	0.9600
C4—C5	1.382 (4)	C15—H15C	0.9600
C7—N1—N2	114.6 (2)	C1—C7—H7	119.7

C8—N2—N1	119.3 (2)	O2—C8—N2	124.1 (2)
C8—N2—H2A	120.4	O2—C8—C9	120.3 (2)
N1—N2—H2A	120.4	N2—C8—C9	115.6 (2)
O4—N3—O3	123.9 (3)	C14—C9—C10	118.9 (2)
O4—N3—C11	118.1 (3)	C14—C9—C8	117.6 (3)
O3—N3—C11	117.9 (2)	C10—C9—C8	123.4 (2)
C4—O1—C15	117.8 (2)	C11—C10—C9	118.5 (3)
C2—C1—C6	117.6 (2)	C11—C10—H10	120.8
C2—C1—C7	122.7 (3)	C9—C10—H10	120.8
C6—C1—C7	119.6 (3)	C10—C11—C12	122.5 (3)
C1—C2—C3	122.1 (3)	C10—C11—N3	118.8 (3)
C1—C2—H2	119.0	C12—C11—N3	118.7 (3)
C3—C2—H2	119.0	C13—C12—C11	118.9 (3)
C2—C3—C4	119.4 (3)	C13—C12—H12	120.5
C2—C3—H3A	120.3	C11—C12—H12	120.5
C4—C3—H3A	120.3	C12—C13—C14	119.6 (3)
O1—C4—C5	115.8 (3)	C12—C13—H13	120.2
O1—C4—C3	124.7 (3)	C14—C13—H13	120.2
C5—C4—C3	119.5 (3)	C13—C14—C9	121.5 (3)
C4—C5—C6	120.5 (3)	C13—C14—H14	119.2
C4—C5—H5	119.7	C9—C14—H14	119.2
C6—C5—H5	119.7	O1—C15—H15A	109.5
C5—C6—C1	120.7 (3)	O1—C15—H15B	109.5
C5—C6—H6	119.6	H15A—C15—H15B	109.5
C1—C6—H6	119.6	O1—C15—H15C	109.5
N1—C7—C1	120.7 (3)	H15A—C15—H15C	109.5
N1—C7—H7	119.7	H15B—C15—H15C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O2^{i}	0.86	2.13	2.895 (3)	148

Symmetry codes: (i) *x*, *y*+1, *z*.

Fig. 1

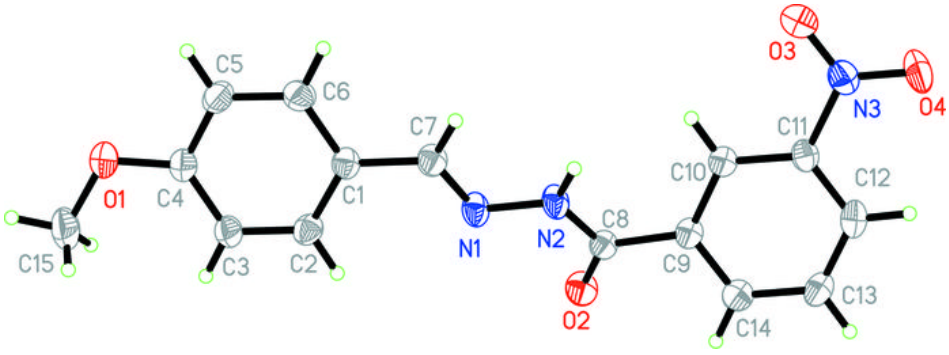
O3
N3
O4
C5
C6
C7
C11
C10
C12
O1
C4
C1
N1
N2
C8
C9
C15
C3
C2
O2
C13
C14

Fig. 2