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(*E*)-*N*′-(2-Methoxybenzylidene)-3-nitrobenzohydrazide

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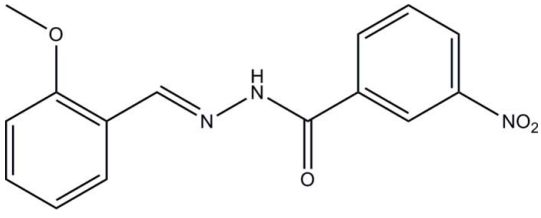
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.067; wR factor = 0.160; data-to-parameter ratio = 15.7.

In the title compound, $C_{15}H_{13}N_3O_4$, the two substituted benzene rings form a dihedral angle of 10.9 (3)°. In the crystal, intermolecular C—H···O and N—H···O hydrogen bonds link molecules into chains running parallel to [101].

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, $P2_1/n$
a = 6.9886 (13) Å
b = 29.543 (3) Å
c = 7.4163 (14) Å
β = 109.229 (2)°
V = 1445.8 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 K
0.20 × 0.17 × 0.13 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.980, T_{max} = 0.987
11773 measured reflections
3140 independent reflections
1547 reflections with $I > 2\sigma(I)$
R_{int} = 0.066

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.160
S = 1.02
3140 reflections
200 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2^{i}	0.86	2.03	2.856 (3)	162
C8—H8···O2^{i}	0.93	2.47	3.231 (3)	139

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2618).

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supplementary materials

Acta Cryst. (2011). E**67**, o1895 [**doi:10.1107/S1600536811025542**]

(*E*)-*N*'-(2-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 comound, (*E*)-*N*'-(2-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 10.9 (3)°. In the crystal, intermolecular C–H···O and N–H···O hydrogen bonds link molecules into one-dimensional chains parallel to the [101] direction (Fig. 2, Table 1).

Experimental

2-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 magnetic stirred at ambient temperature for 10 min until it turns 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

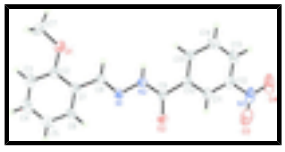

Fig. 1. The molecular structure of the title compound with displacement ellipsoids shown at 30% probability level.

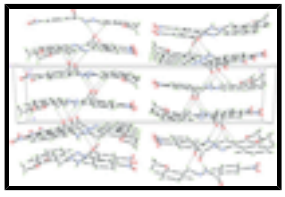

Fig. 2. Packing diagram of the title compound, viewed along the *c* axis. Hydrogen bonds are indicated by dashed lines.

(*E*)-*N*'-(2-Methoxybenzylidene)-3-nitrobenzohydrazide

Crystal data

$C_{15}H_{13}N_3O_4$	$F(000) = 624$
$M_r = 299.28$	$D_x = 1.375$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 1029 reflections
$a = 6.9886$ (13) Å	$\theta = 2.7$–$24.6°$
$b = 29.543$ (3) Å	$\mu = 0.10$ mm^{-1}
$c = 7.4163$ (14) Å	$T = 298$ K
$\beta = 109.229$ (2)°	Needle fragment, pale yellow
$V = 1445.8$ (4) Å^3	0.20 × 0.17 × 0.13 mm
$Z = 4$	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3140 independent reflections
Radiation source: fine-focus sealed tube	1547 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.066$
ω scans	$\theta_{max} = 27.0°$, $\theta_{min} = 2.8°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)	$h = -7 \rightarrow 8$
$T_{min} = 0.980$, $T_{max} = 0.987$	$k = -37 \rightarrow 37$
11773 measured reflections	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.067$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.160$	H-atom parameters constrained
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 0.2817P]$ where $P = (F_o^2 + 2F_c^2)/3$
3140 reflections	$(\Delta/\sigma)_{max} < 0.001$
200 parameters	$\Delta\rho_{max} = 0.27$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.20$ 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	0.1106 (3)	0.28532 (7)	0.7046 (3)	0.0472 (6)
N2	0.1501 (3)	0.25598 (7)	0.8592 (3)	0.0484 (6)
H2	0.2305	0.2639	0.9698	0.058*
N3	0.1869 (5)	0.06220 (10)	1.1044 (6)	0.0779 (10)
O1	0.2305 (4)	0.41464 (7)	0.8421 (3)	0.0717 (7)
O2	−0.0564 (3)	0.20220 (6)	0.6790 (3)	0.0594 (6)
O3	0.1521 (5)	0.04907 (9)	0.9404 (5)	0.1073 (11)
O4	0.2330 (5)	0.03803 (9)	1.2447 (5)	0.1236 (12)
C1	0.1507 (4)	0.35973 (8)	0.6012 (4)	0.0422 (7)
C2	0.1822 (4)	0.40543 (9)	0.6509 (5)	0.0521 (8)
C3	0.1630 (5)	0.43806 (11)	0.5128 (6)	0.0696 (10)
H3	0.1813	0.4685	0.5463	0.084*
C4	0.1166 (5)	0.42509 (13)	0.3260 (6)	0.0775 (11)
H4	0.1030	0.4471	0.2329	0.093*
C5	0.0895 (5)	0.38036 (13)	0.2730 (5)	0.0694 (10)
H5	0.0613	0.3720	0.1460	0.083*
C6	0.1050 (4)	0.34806 (10)	0.4110 (4)	0.0534 (8)
H6	0.0843	0.3178	0.3756	0.064*
C7	0.2868 (6)	0.45963 (11)	0.9068 (6)	0.0987 (14)
H7A	0.3885	0.4703	0.8561	0.148*
H7B	0.3399	0.4600	1.0438	0.148*
H7C	0.1701	0.4790	0.8641	0.148*
C8	0.1739 (4)	0.32553 (9)	0.7488 (4)	0.0438 (7)
H8	0.2356	0.3332	0.8765	0.053*
C9	0.0617 (4)	0.21543 (9)	0.8337 (4)	0.0424 (7)
C10	0.1119 (4)	0.18579 (9)	1.0065 (4)	0.0408 (7)
C11	0.1229 (4)	0.13972 (9)	0.9798 (4)	0.0471 (7)
H11	0.1008	0.1281	0.8580	0.057*
C12	0.1664 (4)	0.11134 (10)	1.1332 (5)	0.0555 (8)
C13	0.1935 (5)	0.12710 (13)	1.3129 (5)	0.0705 (10)
H13	0.2224	0.1071	1.4152	0.085*
C14	0.1779 (5)	0.17262 (13)	1.3418 (4)	0.0679 (10)
H14	0.1927	0.1836	1.4632	0.082*
C15	0.1397 (4)	0.20246 (10)	1.1875 (4)	0.0519 (8)
H15	0.1331	0.2335	1.2066	0.062*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0486 (15)	0.0407 (13)	0.0443 (14)	−0.0023 (11)	0.0043 (11)	0.0050 (11)
N2	0.0522 (15)	0.0401 (13)	0.0404 (13)	−0.0071 (11)	−0.0018 (11)	0.0035 (11)
N3	0.058 (2)	0.053 (2)	0.120 (3)	0.0095 (15)	0.026 (2)	0.032 (2)
O1	0.0983 (19)	0.0453 (13)	0.0778 (16)	−0.0138 (12)	0.0374 (14)	−0.0101 (11)
O2	0.0711 (15)	0.0427 (11)	0.0449 (12)	−0.0095 (10)	−0.0074 (10)	0.0009 (9)
O3	0.120 (3)	0.0580 (17)	0.148 (3)	0.0149 (16)	0.051 (2)	0.0044 (18)
O4	0.118 (3)	0.0780 (19)	0.170 (3)	0.0217 (17)	0.040 (2)	0.071 (2)
C1	0.0329 (16)	0.0424 (16)	0.0473 (17)	−0.0009 (12)	0.0080 (13)	0.0055 (13)
C2	0.0479 (19)	0.0468 (18)	0.063 (2)	−0.0025 (14)	0.0205 (16)	0.0043 (15)
C3	0.069 (2)	0.051 (2)	0.092 (3)	0.0039 (17)	0.030 (2)	0.0190 (19)
C4	0.074 (3)	0.078 (3)	0.082 (3)	0.012 (2)	0.026 (2)	0.037 (2)
C5	0.064 (2)	0.089 (3)	0.052 (2)	0.010 (2)	0.0146 (17)	0.0144 (19)
C6	0.0457 (19)	0.0603 (19)	0.0484 (18)	0.0025 (15)	0.0076 (14)	0.0078 (15)
C7	0.132 (4)	0.062 (2)	0.120 (3)	−0.031 (2)	0.065 (3)	−0.037 (2)
C8	0.0397 (17)	0.0452 (17)	0.0424 (16)	0.0018 (13)	0.0081 (13)	0.0014 (13)
C9	0.0427 (18)	0.0387 (15)	0.0400 (16)	0.0026 (13)	0.0056 (14)	−0.0001 (12)
C10	0.0312 (16)	0.0437 (16)	0.0414 (16)	−0.0002 (12)	0.0037 (12)	0.0041 (13)
C11	0.0372 (17)	0.0478 (18)	0.0529 (18)	0.0002 (13)	0.0102 (14)	0.0055 (14)
C12	0.0377 (18)	0.0513 (19)	0.074 (2)	0.0027 (14)	0.0143 (16)	0.0158 (17)
C13	0.053 (2)	0.078 (3)	0.071 (3)	−0.0061 (18)	0.0075 (18)	0.034 (2)
C14	0.059 (2)	0.099 (3)	0.0434 (18)	−0.014 (2)	0.0130 (16)	0.0054 (18)
C15	0.0441 (19)	0.0610 (19)	0.0466 (17)	−0.0066 (14)	0.0096 (14)	−0.0014 (15)

Geometric parameters (Å, °)

N1—C8	1.272 (3)	C5—C6	1.377 (4)
N1—N2	1.390 (3)	C5—H5	0.9300
N2—C9	1.332 (3)	C6—H6	0.9300
N2—H2	0.8600	C7—H7A	0.9600
N3—O4	1.215 (4)	C7—H7B	0.9600
N3—O3	1.223 (4)	C7—H7C	0.9600
N3—C12	1.481 (4)	C8—H8	0.9300
O1—C2	1.373 (3)	C9—C10	1.496 (3)
O1—C7	1.424 (3)	C10—C11	1.381 (4)
O2—C9	1.235 (3)	C10—C15	1.382 (4)
C1—C6	1.384 (4)	C11—C12	1.364 (4)
C1—C2	1.397 (4)	C11—H11	0.9300
C1—C8	1.459 (3)	C12—C13	1.365 (4)
C2—C3	1.380 (4)	C13—C14	1.372 (4)
C3—C4	1.369 (5)	C13—H13	0.9300
C3—H3	0.9300	C14—C15	1.399 (4)
C4—C5	1.374 (4)	C14—H14	0.9300
C4—H4	0.9300	C15—H15	0.9300
C8—N1—N2	114.3 (2)	H7A—C7—H7B	109.5

C9—N2—N1	119.1 (2)	O1—C7—H7C	109.5
C9—N2—H2	120.4	H7A—C7—H7C	109.5
N1—N2—H2	120.4	H7B—C7—H7C	109.5
O4—N3—O3	125.1 (4)	N1—C8—C1	120.7 (2)
O4—N3—C12	117.6 (4)	N1—C8—H8	119.7
O3—N3—C12	117.2 (3)	C1—C8—H8	119.7
C2—O1—C7	118.7 (3)	O2—C9—N2	123.6 (2)
C6—C1—C2	118.2 (3)	O2—C9—C10	120.4 (2)
C6—C1—C8	121.6 (2)	N2—C9—C10	116.0 (2)
C2—C1—C8	120.2 (3)	C11—C10—C15	119.6 (3)
O1—C2—C3	124.0 (3)	C11—C10—C9	117.6 (2)
O1—C2—C1	115.3 (2)	C15—C10—C9	122.8 (2)
C3—C2—C1	120.7 (3)	C12—C11—C10	119.6 (3)
C4—C3—C2	119.2 (3)	C12—C11—H11	120.2
C4—C3—H3	120.4	C10—C11—H11	120.2
C2—C3—H3	120.4	C11—C12—C13	121.7 (3)
C3—C4—C5	121.5 (3)	C11—C12—N3	119.2 (3)
C3—C4—H4	119.2	C13—C12—N3	119.1 (3)
C5—C4—H4	119.2	C12—C13—C14	119.6 (3)
C4—C5—C6	119.0 (3)	C12—C13—H13	120.2
C4—C5—H5	120.5	C14—C13—H13	120.2
C6—C5—H5	120.5	C13—C14—C15	119.6 (3)
C5—C6—C1	121.3 (3)	C13—C14—H14	120.2
C5—C6—H6	119.3	C15—C14—H14	120.2
C1—C6—H6	119.3	C10—C15—C14	119.9 (3)
O1—C7—H7A	109.5	C10—C15—H15	120.1
O1—C7—H7B	109.5	C14—C15—H15	120.1

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{i}	0.86	2.03	2.856 (3)	162
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Fig. 1

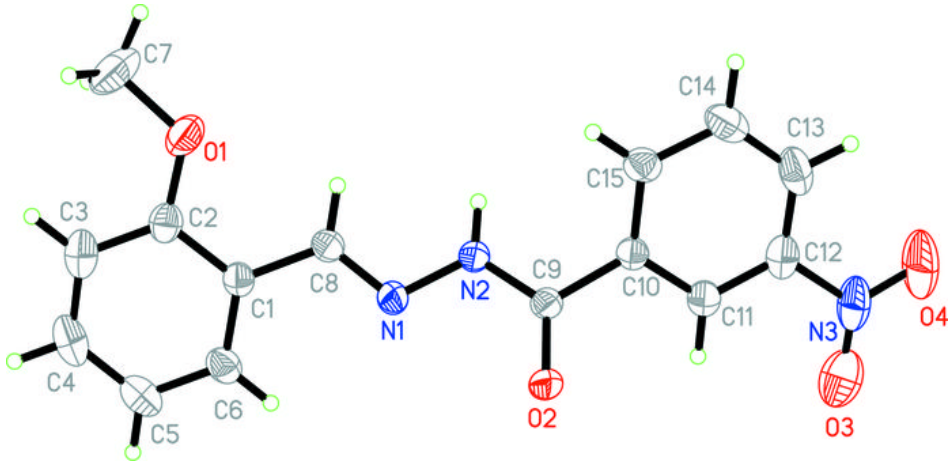
C7
O1
C3
C2
C1
C8
N1
N2
C9
O2
C10
C15
C14
C13
C12
C11
N3
O4
O3
C4
C5
C6

Fig. 2