Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N′-(2-Methoxybenzylidene)acetohydrazide

Tie-Ming Yu and Lu-Ping Lv*

Linjiang College, Hangzhou Vocational and Technical College, Hangzhou 310018, People's Republic of China
Correspondence e-mail: mailofllp@126.com

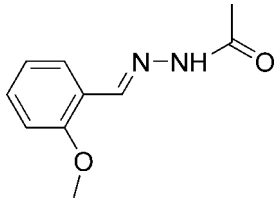
Received 1 September 2010; accepted 24 September 2010

Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.003 Å; R factor = 0.056; wR factor = 0.163; data-to-parameter ratio = 13.2.

In the title molecule, $C_{10}H_{12}N_2O_2$, the acetohydrazide group is almost planar [within 0.0306 (12) Å] and forms a dihedral angle of 12.15 (14)° with the benzene ring. The methoxy group deviates from the attached benzene ring with a C—O—C—C torsion angle of 4.2 (4)°·The molecule adopts a *trans* configuration with respect to the C=N bond. In the crystal, molecules are linked into centrosymmetric dimers by pairs of N—H···O hydrogen bonds and intermolecular C—H···O interactions further stabilize the structure.

Related literature

For general background to Schiff bases, see: Cimerman *et al.* (1997); Offe *et al.* (1952); Richardson *et al.* (1988). For related structures, see: Li & Jian (2008); Tamboura *et al.* (2009).



Experimental

Crystal data

$C_{10}H_{12}N_2O_2$
M_r = 192.22
Triclinic, $P\overline{1}$
a = 5.3865 (7) Å
b = 8.4609 (11) Å
c = 11.3301 (14) Å
α = 77.499 (4)°
β = 76.516 (5)°
γ = 89.101 (5)°
V = 489.90 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 223 K
0.19 × 0.17 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.982, T_{max} = 0.985
4827 measured reflections
1694 independent reflections
1489 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.163
S = 1.06
1694 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 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	2.07	2.899 (2)	163
C6—H6A···O1^{ii}	0.96	2.59	3.491 (3)	157

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

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*.

The authors thank Hangzhou Vocational and Technical College for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2092).

References

Bruker (2002). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cimerman, Z., Galic, N. & Bosner, B. (1997). *Anal. Chim. Acta*, **343**, 145–153.
Li, Y.-F. & Jian, F.-F. (2008). *Acta Cryst.* E**64**, o2409.
Offe, H. A., Siefen, W. & Domagk, G. (1952). *Z. Naturforsch. Teil B*, **7**, 446–447.
Richardson, D., Baker, E., Ponka, P., Wilairat, P., Vitolo, M. L. & Webb, J. (1988). *Thalassemia: Pathophysiology and Management*, Part B, p. 81. New York: Alan R. Liss Inc.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tamboura, F. B., Gaye, M., Sall, A. S., Barry, A. H. & Bah, Y. (2009). *Acta Cryst.* E**65**, m160–m161.

supporting information

Acta Cryst. (2010). E**66**, o2666 [doi:10.1107/S1600536810038092]

N′-(2-Methoxybenzylidene)acetohydrazide

Tie-Ming Yu and Lu-Ping Lv

S1. Comment

Schiff bases have attracted much attention due to the possibility of their analytical applications (Cimerman *et al.*, 1997). They are also important ligands, which have been reported to have mild bacteriostatic activity and are used as potential oral iron-chelating drugs for genetic disorders such as thalassemia (Offe *et al.*, 1952; Richardson *et al.*, 1988). Metal complexes based on Schiff bases have received considerable attention because they can be utilized as model compounds of active centres in various complexes (Tamboura *et al.*, 2009). We report here the crystal structure of the title compound (Fig. 1).

The acetohydrazide group is planar and it forms a dihedral angle of 12.15 (14)° with the benzene ring. deviates from the attached benzene ring by 4.2 (4)°. [C6—O1—C5—C4 = 4.2 (4)°]. The molecule adopts a *trans* configuration with respect to the C═N bond. Bond lengths and angles are comparable to those observed for *N*′-[1-(4-methoxyphenyl)ethylidene]acetohydrazide (Li & Jian, 2008).

The molecules are linked by N—H···O hydrogen bonds into a centrosymmetric dimer. In addition, an intramolecular C—H···N hydrogen bond is observed.

S2. Experimental

2-Methoxybenzaldehyde (1.36 g, 0.01 mol) and acetohydrazide (0.74 g, 0.01 mol) were dissolved in stirred methanol (25 ml) and left for 2.5 h at room temperature. The resulting solid was filtered off and recrystallized from ethanol to give the title compound in 88% yield. Single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution at room temperature (m.p. 465–467 K).

S3. Refinement

H atoms were positioned geometrically (N-H = 0.86 Å and C-H = 0.93 or 0.96 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C,N) and 1.5U_{eq}(C_{methyl}). A rotating group model was used for the methyl groups.

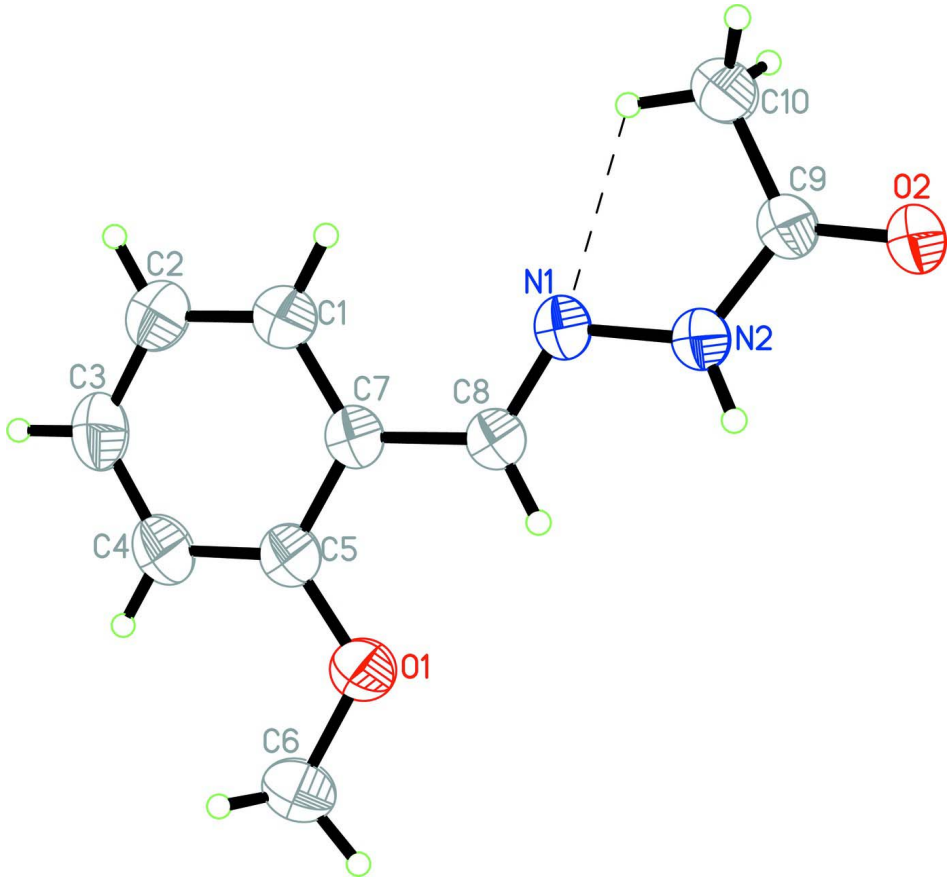


Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

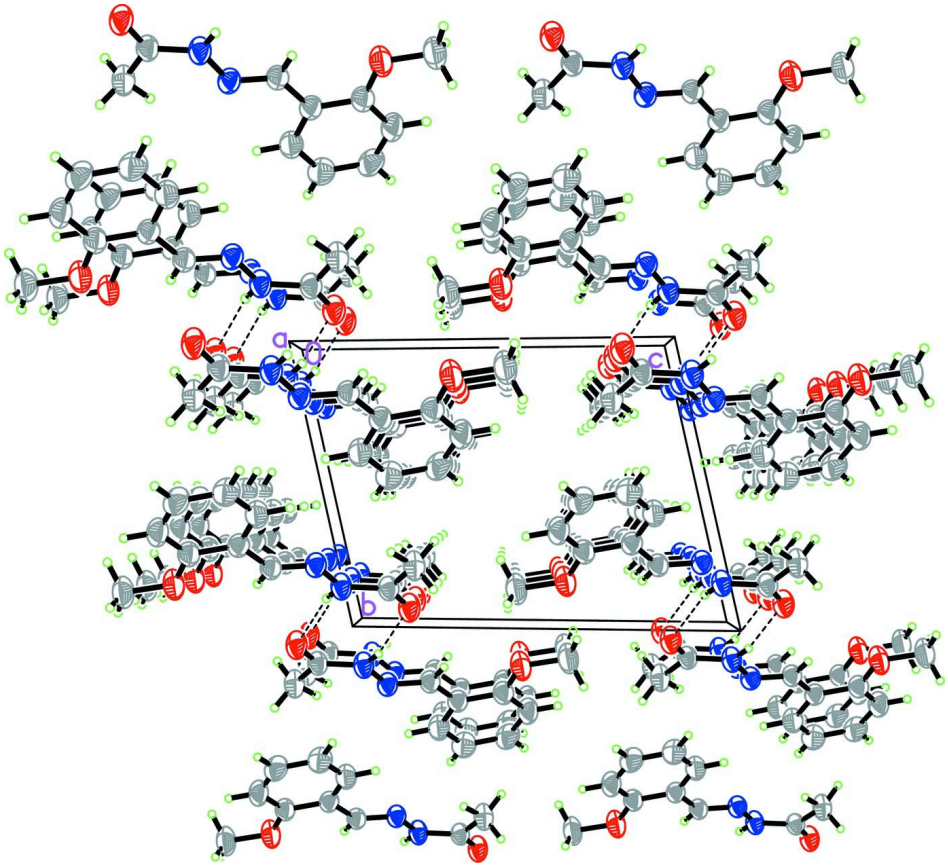


Figure 2

Part of the crystal packing of the title compound. Hydrogen bonds are shown as dashed lines.

N′-(2-Methoxybenzylidene)acetohydrazide

Crystal data

$C_{10}H_{12}N_2O_2$
$M_r = 192.22$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.3865\ (7)$ Å
$b = 8.4609\ (11)$ Å
$c = 11.3301\ (14)$ Å
$\alpha = 77.499\ (4)°$
$\beta = 76.516\ (5)°$
$\gamma = 89.101\ (5)°$
$V = 489.90\ (11)$ Å^3
$Z = 2$
$F(000) = 204$
$D_x = 1.303$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1694 reflections
$\theta = 1.9–25.0°$
$\mu = 0.09$ mm^{-1}
$T = 223$ K
Block, colourless
0.19 × 0.17 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.982$, $T_{max} = 0.985$
4827 measured reflections
1694 independent reflections
1489 reflections with $I > 2\sigma(I)$

R_{int} = 0.018
θ_{max} = 25.0°, θ_{min} = 1.9°
h = −6→6
k = −10→9
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.163
S = 1.06
1694 reflections
128 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0812P)^2 + 0.265P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 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}
O1	0.3030 (3)	0.1576 (2)	0.41553 (14)	0.0617 (5)
C10	0.6401 (4)	0.2210 (3)	−0.2060 (2)	0.0533 (6)
H10A	0.5000	0.2686	−0.1579	0.080*
H10B	0.5753	0.1429	−0.2424	0.080*
H10C	0.7390	0.3041	−0.2707	0.080*
N1	0.5212 (3)	0.2232 (2)	0.04470 (16)	0.0430 (5)
N2	0.7383 (3)	0.1459 (2)	−0.00176 (16)	0.0461 (5)
H2	0.8319	0.1014	0.0474	0.055*
C1	0.1048 (5)	0.3982 (3)	0.1500 (2)	0.0522 (6)
H1	0.1575	0.4195	0.0637	0.063*
C2	−0.1084 (5)	0.4724 (3)	0.2049 (2)	0.0576 (6)
H2A	−0.1987	0.5420	0.1560	0.069*
C3	−0.1852 (5)	0.4423 (3)	0.3321 (2)	0.0572 (6)
H3	−0.3285	0.4917	0.3696	0.069*
C4	−0.0514 (5)	0.3388 (3)	0.4053 (2)	0.0562 (6)
H4	−0.1048	0.3197	0.4915	0.067*
C5	0.1626 (4)	0.2634 (3)	0.3506 (2)	0.0462 (5)
C6	0.2348 (6)	0.1311 (4)	0.5483 (2)	0.0720 (8)
H6A	0.3527	0.0593	0.5823	0.108*
H6B	0.0651	0.0835	0.5791	0.108*
H6C	0.2408	0.2326	0.5725	0.108*
C7	0.2427 (4)	0.2924 (3)	0.22085 (19)	0.0418 (5)

C8	0.4680 (4)	0.2133 (3)	0.16151 (19)	0.0421 (5)
H8	0.5719	0.1559	0.2096	0.050*
C9	0.8059 (4)	0.1389 (3)	−0.12303 (19)	0.0424 (5)
O2	0.9982 (3)	0.0679 (2)	−0.16141 (14)	0.0528 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0686 (11)	0.0756 (12)	0.0348 (8)	0.0287 (9)	−0.0062 (7)	−0.0076 (8)
C10	0.0497 (13)	0.0723 (16)	0.0378 (12)	0.0158 (11)	−0.0097 (10)	−0.0134 (11)
N1	0.0414 (9)	0.0489 (11)	0.0373 (9)	0.0120 (7)	−0.0048 (7)	−0.0116 (8)
N2	0.0431 (10)	0.0589 (12)	0.0350 (9)	0.0181 (8)	−0.0073 (7)	−0.0107 (8)
C1	0.0573 (13)	0.0584 (14)	0.0412 (12)	0.0157 (11)	−0.0123 (10)	−0.0118 (10)
C2	0.0562 (14)	0.0611 (15)	0.0585 (15)	0.0213 (11)	−0.0178 (11)	−0.0166 (12)
C3	0.0508 (13)	0.0610 (15)	0.0602 (15)	0.0174 (11)	−0.0046 (11)	−0.0242 (12)
C4	0.0582 (14)	0.0650 (15)	0.0409 (12)	0.0131 (11)	0.0008 (10)	−0.0162 (11)
C5	0.0486 (12)	0.0489 (12)	0.0391 (11)	0.0084 (9)	−0.0070 (9)	−0.0098 (9)
C6	0.094 (2)	0.083 (2)	0.0359 (13)	0.0288 (16)	−0.0138 (13)	−0.0109 (12)
C7	0.0422 (11)	0.0440 (12)	0.0387 (11)	0.0064 (9)	−0.0070 (9)	−0.0114 (9)
C8	0.0447 (11)	0.0444 (11)	0.0360 (11)	0.0088 (9)	−0.0078 (9)	−0.0088 (9)
C9	0.0394 (11)	0.0494 (12)	0.0357 (11)	0.0065 (9)	−0.0039 (8)	−0.0091 (9)
O2	0.0479 (9)	0.0689 (11)	0.0396 (8)	0.0221 (7)	−0.0051 (7)	−0.0143 (7)

Geometric parameters (Å, º)

O1—C5	1.367 (3)	C2—C3	1.371 (3)
O1—C6	1.430 (3)	C2—H2A	0.9300
C10—C9	1.501 (3)	C3—C4	1.385 (4)
C10—H10A	0.9600	C3—H3	0.9300
C10—H10B	0.9600	C4—C5	1.391 (3)
C10—H10C	0.9600	C4—H4	0.9300
N1—C8	1.272 (3)	C5—C7	1.399 (3)
N1—N2	1.382 (2)	C6—H6A	0.9600
N2—C9	1.351 (3)	C6—H6B	0.9600
N2—H2	0.8600	C6—H6C	0.9600
C1—C2	1.383 (3)	C7—C8	1.470 (3)
C1—C7	1.394 (3)	C8—H8	0.9300
C1—H1	0.9300	C9—O2	1.227 (2)
C5—O1—C6	117.66 (19)	C3—C4—H4	119.8
C9—C10—H10A	109.5	C5—C4—H4	119.8
C9—C10—H10B	109.5	O1—C5—C4	124.3 (2)
H10A—C10—H10B	109.5	O1—C5—C7	116.03 (19)
C9—C10—H10C	109.5	C4—C5—C7	119.7 (2)
H10A—C10—H10C	109.5	O1—C6—H6A	109.5
H10B—C10—H10C	109.5	O1—C6—H6B	109.5
C8—N1—N2	115.56 (18)	H6A—C6—H6B	109.5
C9—N2—N1	121.13 (17)	O1—C6—H6C	109.5

C9—N2—H2	119.4	H6A—C6—H6C	109.5
N1—N2—H2	119.4	H6B—C6—H6C	109.5
C2—C1—C7	121.7 (2)	C1—C7—C5	118.4 (2)
C2—C1—H1	119.2	C1—C7—C8	121.2 (2)
C7—C1—H1	119.2	C5—C7—C8	120.42 (19)
C3—C2—C1	119.2 (2)	N1—C8—C7	120.22 (19)
C3—C2—H2A	120.4	N1—C8—H8	119.9
C1—C2—H2A	120.4	C7—C8—H8	119.9
C2—C3—C4	120.6 (2)	O2—C9—N2	119.71 (19)
C2—C3—H3	119.7	O2—C9—C10	122.64 (19)
C4—C3—H3	119.7	N2—C9—C10	117.65 (18)
C3—C4—C5	120.4 (2)		

C8—N1—N2—C9	175.77 (19)	O1—C5—C7—C1	179.4 (2)
C7—C1—C2—C3	0.5 (4)	C4—C5—C7—C1	0.5 (4)
C1—C2—C3—C4	0.0 (4)	O1—C5—C7—C8	−0.9 (3)
C2—C3—C4—C5	−0.3 (4)	C4—C5—C7—C8	−179.8 (2)
C6—O1—C5—C4	−4.2 (4)	N2—N1—C8—C7	179.40 (17)
C6—O1—C5—C7	176.9 (2)	C1—C7—C8—N1	−9.4 (3)
C3—C4—C5—O1	−178.8 (2)	C5—C7—C8—N1	171.0 (2)
C3—C4—C5—C7	0.0 (4)	N1—N2—C9—O2	−179.23 (19)
C2—C1—C7—C5	−0.8 (4)	N1—N2—C9—C10	1.3 (3)
C2—C1—C7—C8	179.6 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*A*···N1	0.96	2.27	2.766 (3)	111
N2—H2···O2^{i}	0.86	2.07	2.899 (2)	163
C6—H6*A*···O1^{ii}	0.96	2.59	3.491 (3)	157

Symmetry codes: (i) −*x*+2, −*y*, −*z*; (ii) −*x*+1, −*y*, −*z*+1.