

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

## N'-(2-Fluorobenzylidene)acetohydrazide

 Jie Yang,<sup>a</sup> Zhao-De Jiang,<sup>b</sup> Fu-Gong Zhang<sup>c</sup> and Fang-Fang Jian<sup>a\*</sup>
<sup>a</sup>Microscale Science Institute, Weifang University, Weifang 261061, People's Republic of China, <sup>b</sup>Yantai Vocational and Technical Institute of Engineering, Yantai 264006, People's Republic of China, and <sup>c</sup>Ministry of Personnel, Weifang University, Weifang 261061, People's Republic of China

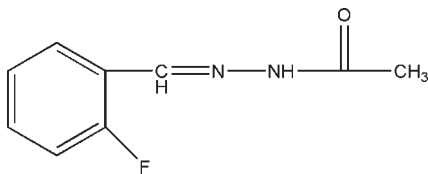
Correspondence e-mail: ffjian2008@163.com

Received 21 March 2010; accepted 22 March 2010

 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.042;  $wR$  factor = 0.128; data-to-parameter ratio = 16.9.

 The title compound,  $\text{C}_9\text{H}_9\text{FN}_2\text{O}$ , was prepared by the reaction between 2-fluorobenzophenone and acetohydrazide. In the crystal structure, inversion dimers linked by pairs of  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds occur, generating  $R_2^2(8)$  loops.

## Related literature

 For background to Schiff bases, see: Cimerman *et al.* (1997); For related structures, see: Girgis (2006); Li & Jian (2008).


## Experimental

## Crystal data

 $\text{C}_9\text{H}_9\text{FN}_2\text{O}$   
 $M_r = 180.18$   
 Monoclinic,  $P2_1/c$ 
 $a = 5.3227$  (11) Å  
 $b = 8.4603$  (17) Å  
 $c = 19.656$  (4) Å

 $\beta = 93.70$  (3)°  
 $V = 883.3$  (3) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation

 $\mu = 0.11$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.30 \times 0.30 \times 0.20$  mm

## Data collection

 Bruker SMART CCD  
 diffractometer  
 7687 measured reflections

 2010 independent reflections  
 1515 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.036$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.128$   
 $S = 1.04$   
 2010 reflections

 119 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.14$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.21$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O1}^i$	0.86	2.08	2.915 (2)	163

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

 Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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 would like to thank the National Natural Science Foundation of Shandong Province (Y2008B29) and Yuandu Scholar of Weifang City for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5371).

## References

- Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Cimerman, Z., Galic, N. & Bosner, B. (1997). *Anal. Chim. Acta*, **343**, 145–153.
- Girgis, A. S. (2006). *J. Chem. Res.* pp. 81–85.
- Li, Y.-F. & Jian, F.-F. (2008). *Acta Cryst. E* **64**, o2409.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.

## supporting information

*Acta Cryst.* (2010). E66, o927 [doi:10.1107/S1600536810010627]

***N'*-(2-Fluorobenzylidene)acetohydrazide**

Jie Yang, Zhao-De Jiang, Fu-Gong Zhang and Fang-Fang Jian

**S1. Comment**

Schiff bases have important applications in analytical chemistry (Cimerman *et al.*, 1997). As part of our search for new Schiff bases with similar applications, we synthesized the title compound, (I), and report its crystal structure herein (Fig. 1).

All the bond lengths and angles in (I) are within normal ranges (Li & Jian, 2008). The C7=N2 bond length of 1.2732 (18) Å is slight shorter than the C=N double bond [1.281 (2) Å] reported (Girgis, 2006) in a related compound.

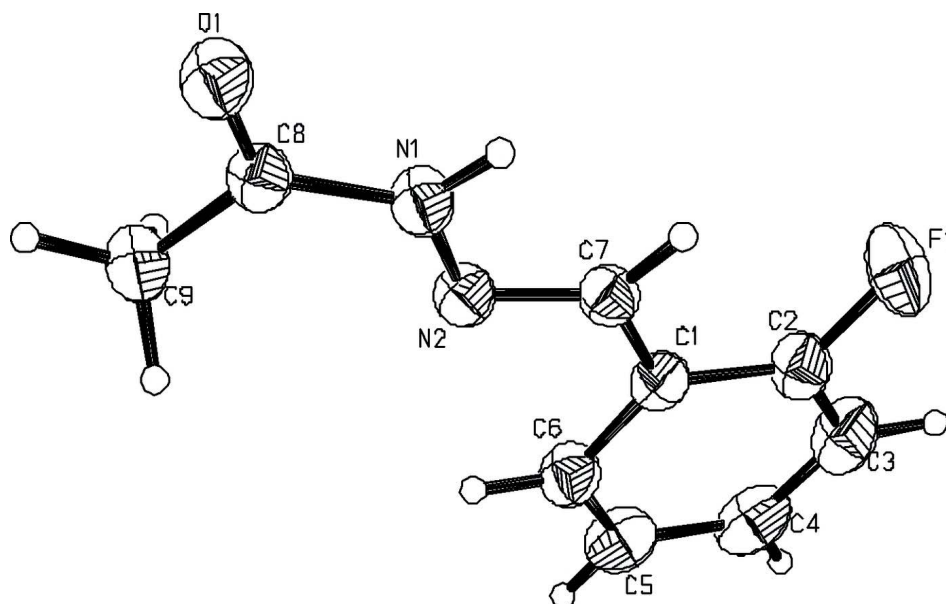
In the crystal structure, adjacent molecules are linked into a centro-symmetric supra-molecular dimer by intermolecular N—H···O hydrogen bonding (Table 1).

**S2. Experimental**

A mixture of 2-fluorobenzophenone (0.05 mol) and acethydrazide (0.05 mol) was stirred in refluxing ethanol(30 ml) for 4 h to afford the title compound (yield 70%). Colourless blocks of (I) were obtained by recrystallization from ethanol at room temperature.

**S3. Refinement**

All H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H and N—H distances in the range 0.93-0.97 Å and 0.86 Å, respectively, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$  of the parent atoms.

**Figure 1**

The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level.

### ***N'*-(2-Fluorobenzylidene)acetohydrazide**

#### *Crystal data*

$C_9H_9FN_2O$

$M_r = 180.18$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2ybc$

$a = 5.3227$  (11) Å

$b = 8.4603$  (17) Å

$c = 19.656$  (4) Å

$\beta = 93.70$  (3)°

$V = 883.3$  (3) Å<sup>3</sup>

$Z = 4$

$F(000) = 376$

$D_x = 1.355$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 1515 reflections

$\theta = 3.2$ – $27.5$ °

$\mu = 0.11$  mm<sup>-1</sup>

$T = 293$  K

Block, colourless

$0.30 \times 0.30 \times 0.20$  mm

#### *Data collection*

Bruker SMART CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega$  scans

7687 measured reflections

2010 independent reflections

1515 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.036$

$\theta_{max} = 27.5$ °,  $\theta_{min} = 3.2$ °

$h = -6 \rightarrow 6$

$k = -9 \rightarrow 10$

$l = -25 \rightarrow 25$

#### *Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.128$

$S = 1.04$

2010 reflections

119 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

$$w = 1/[\sigma^2(F_o^2) + (0.0696P)^2 + 0.0888P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.14 \text{ e } \text{Å}^{-3}$

$$\Delta\rho_{\min} = -0.21 \text{ e } \text{Å}^{-3}$$

Extinction correction: *SHELXL97* (Sheldrick, 2008),  $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.035 (6)

*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  $F^2 > \sigma(F^2)$  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<sup>2</sup>)*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N2	0.4557 (2)	0.26752 (14)	0.01843 (6)	0.0474 (3)
O1	0.04461 (18)	0.48232 (13)	-0.09198 (5)	0.0578 (3)
N1	0.2546 (2)	0.35774 (14)	-0.00633 (6)	0.0505 (3)
H1A	0.1453	0.3885	0.0212	0.061*
C1	0.6693 (3)	0.15209 (16)	0.11622 (7)	0.0479 (3)
C8	0.2245 (2)	0.39930 (17)	-0.07282 (7)	0.0473 (3)
C7	0.4679 (3)	0.24649 (16)	0.08270 (7)	0.0477 (3)
H7A	0.3469	0.2919	0.1086	0.057*
F1	0.5354 (2)	0.23104 (15)	0.22231 (5)	0.0865 (4)
C9	0.4142 (3)	0.3418 (2)	-0.11987 (7)	0.0583 (4)
H9A	0.3699	0.3789	-0.1652	0.087*
H9B	0.4168	0.2284	-0.1197	0.087*
H9C	0.5777	0.3812	-0.1049	0.087*
C6	0.8398 (3)	0.0646 (2)	0.08064 (8)	0.0592 (4)
H6A	0.8267	0.0649	0.0332	0.071*
C2	0.6989 (3)	0.1453 (2)	0.18648 (7)	0.0586 (4)
C5	1.0271 (3)	-0.0222 (2)	0.11457 (10)	0.0708 (5)
H5A	1.1397	-0.0794	0.0900	0.085*
C3	0.8824 (4)	0.0594 (2)	0.22135 (9)	0.0756 (5)
H3A	0.8947	0.0580	0.2688	0.091*
C4	1.0489 (3)	-0.0250 (2)	0.18462 (10)	0.0756 (5)
H4A	1.1760	-0.0839	0.2072	0.091*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N2	0.0448 (6)	0.0508 (6)	0.0460 (6)	0.0032 (5)	-0.0023 (5)	0.0011 (5)
O1	0.0518 (6)	0.0700 (7)	0.0507 (6)	0.0133 (5)	-0.0049 (4)	0.0030 (5)
N1	0.0475 (6)	0.0591 (7)	0.0447 (6)	0.0106 (5)	0.0006 (5)	0.0019 (5)
C1	0.0475 (7)	0.0482 (7)	0.0471 (7)	-0.0069 (6)	-0.0046 (5)	0.0041 (5)
C8	0.0434 (7)	0.0520 (7)	0.0455 (7)	-0.0015 (6)	-0.0035 (5)	-0.0004 (5)

C7	0.0482 (7)	0.0490 (7)	0.0455 (7)	-0.0010 (6)	0.0006 (5)	-0.0021 (5)
F1	0.0899 (8)	0.1230 (10)	0.0462 (5)	0.0075 (6)	0.0006 (5)	-0.0129 (5)
C9	0.0538 (8)	0.0733 (10)	0.0478 (7)	0.0058 (7)	0.0039 (6)	0.0000 (7)
C6	0.0601 (9)	0.0623 (9)	0.0545 (8)	0.0069 (7)	-0.0007 (6)	0.0061 (7)
C2	0.0588 (9)	0.0683 (10)	0.0475 (7)	-0.0101 (7)	-0.0058 (6)	0.0002 (6)
C5	0.0599 (10)	0.0664 (11)	0.0850 (12)	0.0100 (8)	-0.0034 (8)	0.0118 (9)
C3	0.0764 (11)	0.0912 (13)	0.0558 (9)	-0.0153 (10)	-0.0222 (8)	0.0153 (8)
C4	0.0619 (10)	0.0734 (12)	0.0880 (12)	-0.0051 (8)	-0.0233 (9)	0.0253 (10)

*Geometric parameters (Å, °)*

N2—C7	1.2732 (18)	C9—H9A	0.9600
N2—N1	1.3775 (16)	C9—H9B	0.9600
O1—C8	1.2269 (17)	C9—H9C	0.9600
N1—C8	1.3529 (17)	C6—C5	1.376 (2)
N1—H1A	0.8600	C6—H6A	0.9300
C1—C2	1.3809 (19)	C2—C3	1.366 (2)
C1—C6	1.394 (2)	C5—C4	1.375 (3)
C1—C7	1.4595 (19)	C5—H5A	0.9300
C8—C9	1.494 (2)	C3—C4	1.379 (3)
C7—H7A	0.9300	C3—H3A	0.9300
F1—C2	1.363 (2)	C4—H4A	0.9300
C7—N2—N1	114.63 (11)	H9A—C9—H9C	109.5
C8—N1—N2	121.75 (11)	H9B—C9—H9C	109.5
C8—N1—H1A	119.1	C5—C6—C1	121.01 (15)
N2—N1—H1A	119.1	C5—C6—H6A	119.5
C2—C1—C6	116.37 (14)	C1—C6—H6A	119.5
C2—C1—C7	120.46 (13)	F1—C2—C3	118.90 (14)
C6—C1—C7	123.17 (12)	F1—C2—C1	117.35 (14)
O1—C8—N1	119.12 (13)	C3—C2—C1	123.74 (16)
O1—C8—C9	122.79 (13)	C4—C5—C6	120.45 (17)
N1—C8—C9	118.08 (12)	C4—C5—H5A	119.8
N2—C7—C1	120.89 (13)	C6—C5—H5A	119.8
N2—C7—H7A	119.6	C2—C3—C4	118.43 (16)
C1—C7—H7A	119.6	C2—C3—H3A	120.8
C8—C9—H9A	109.5	C4—C3—H3A	120.8
C8—C9—H9B	109.5	C5—C4—C3	120.00 (16)
H9A—C9—H9B	109.5	C5—C4—H4A	120.0
C8—C9—H9C	109.5	C3—C4—H4A	120.0

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1A...O1 <sup>i</sup>	0.86	2.08	2.915 (2)	163

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