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***N'*-(4-Fluorobenzylidene)acetohydrazide**Huan-mei Guo,^{a*} Li Liu,^a Jie Yang^a and Yang-chun Liu^b^aMicroscale Science Institute, Weifang University, Weifang 261061, People's Republic of China, and ^bDepartment of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China

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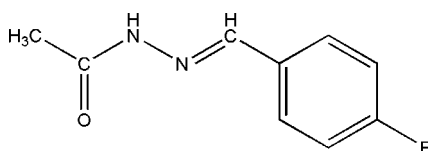
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.052; wR factor = 0.176; data-to-parameter ratio = 17.2.

The title compound, $\text{C}_9\text{H}_9\text{FN}_2\text{O}$, was prepared by the reaction of 4-fluorobenzophenone and acethydrazide. In the molecule, all non-H atoms are essentially coplanar [r.m.s. deviation = 0.065 (2) Å]. In the crystal, molecules are linked into centrosymmetric dimers by pairs of intermolecular N—H \cdots O hydrogen bonds.

Related literature

For general background to Schiff bases, see: Goswami *et al.* (2009); Zhang *et al.* (2010). For related structures, see: Li & Jian (2008); Girgis (2006); Yang *et al.* (2010);



Experimental

Crystal data

$\text{C}_9\text{H}_9\text{FN}_2\text{O}$
 $M_r = 180.18$
 Monoclinic, $P2_1/n$
 $a = 10.443$ (2) Å

$b = 4.0418$ (8) Å
 $c = 21.172$ (4) Å
 $\beta = 96.71$ (3)°
 $V = 887.5$ (3) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.11$ mm⁻¹

$T = 293$ K
 $0.24 \times 0.22 \times 0.22$ mm

Data collection

Bruker SMART CCD
 diffractometer
 7536 measured reflections

2033 independent reflections
 1412 reflections with $I > \sigma(I)$
 $R_{\text{int}} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.176$
 $S = 1.12$
 2033 reflections

118 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.31$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.23$ e Å⁻³

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	2.04	2.899 (2)	176

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; 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: LH5151).

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supporting information

Acta Cryst. (2010). E66, o2952 [https://doi.org/10.1107/S1600536810042765]

N'*-(4-Fluorobenzylidene)acetohydrazide*Huan-mei Guo, Li Liu, Jie Yang and Yang-chun Liu****S1. Comment**

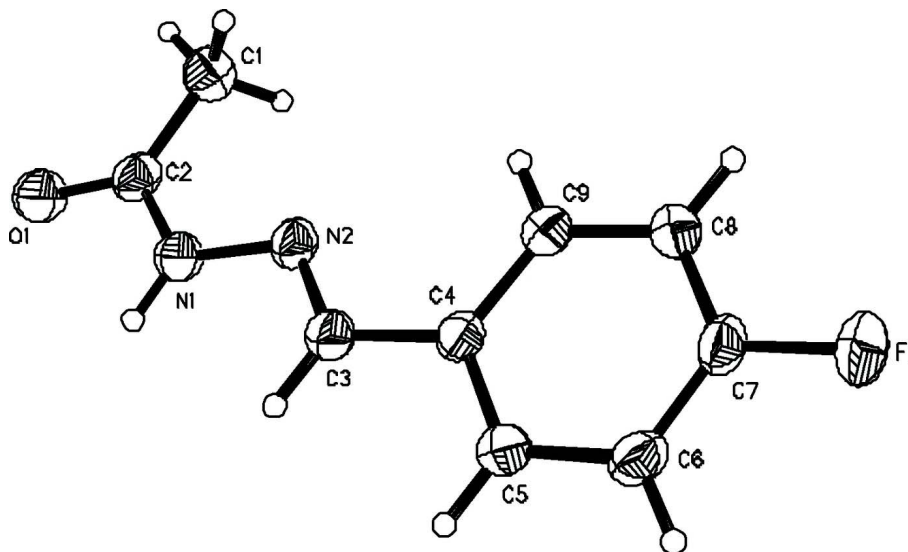
Schiff bases have received considerable attention in the literature (Zhang *et al.*, 2010; Goswami *et al.*, 2009). As part of our search for new schiff base compounds we synthesized the title compound(I) and its crystal structure is reported herein. In the title compound (Fig. 1), the bond lengths and angles are similar to those in related structures (Li & Jian, 2008; Yang *et al.*, 2010). The C3=N2 bond length of 1.269 (2)Å is slight shorter than the C=N double bond [1.281 (2) Å and 1.2732 (18)] reported by Girgis (2006) and Yang *et al.* (2010). In the crystal structure, molecules are linked into centrosymmetric dimers by pairs of intermolecular N—H···O hydrogen bonds (Table 1).

S2. Experimental

A mixture of the 4-fluorobenzophenone (0.02 mol) and acethydrazide (0.02 mol) was stirred in refluxing ethanol (30 ml) for 2 h to afford the title compound (yield 65%). Single crystals suitable for X-ray measurements were obtained by recrystallization from a solution of the title compound in ethanol at room temperature.

S3. Refinement

All H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H 0.93–0.96Å, N—H = 0.86 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C},\text{N})$ or $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$

**Figure 1**

The molecular structure of the title compound with the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

N'-(4-Fluorobenzylidene)acetohydrazide*Crystal data*C₉H₉FN₂O $M_r = 180.18$ Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

 $a = 10.443 (2) \text{ \AA}$ $b = 4.0418 (8) \text{ \AA}$ $c = 21.172 (4) \text{ \AA}$ $\beta = 96.71 (3)^\circ$ $V = 887.5 (3) \text{ \AA}^3$ $Z = 4$ $F(000) = 376$ $D_x = 1.349 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2033 reflections

 $\theta = 3.7\text{--}27.5^\circ$ $\mu = 0.11 \text{ mm}^{-1}$ $T = 293 \text{ K}$

Bar, colourless

 $0.24 \times 0.22 \times 0.22 \text{ mm}$ *Data collection*

Bruker SMART CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 φ and ω scans

7536 measured reflections

2033 independent reflections

1412 reflections with $I > \sigma(I)$ $R_{\text{int}} = 0.025$ $\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.3^\circ$ $h = -13 \rightarrow 13$ $k = -5 \rightarrow 5$ $l = -27 \rightarrow 27$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.052$ $wR(F^2) = 0.176$ $S = 1.12$

2033 reflections

118 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

 $w = 1/[\sigma^2(F_o^2) + (0.1001P)^2 + 0.0565P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} < 0.001$ $\Delta\rho_{\text{max}} = 0.31 \text{ e \AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$ *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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N2	0.41309 (13)	0.8047 (4)	0.12439 (6)	0.0506 (4)
C4	0.50404 (14)	0.7947 (4)	0.23307 (7)	0.0448 (4)
C3	0.50479 (15)	0.7172 (4)	0.16566 (7)	0.0517 (4)
H3A	0.5741	0.6012	0.1527	0.062*
N1	0.42670 (14)	0.7124 (4)	0.06305 (6)	0.0574 (4)

H1A	0.4921	0.5941	0.0561	0.069*
O1	0.35986 (12)	0.7130 (4)	-0.04043 (5)	0.0692 (4)
F1	0.50984 (11)	0.9900 (3)	0.42320 (4)	0.0807 (4)
C2	0.34069 (16)	0.8017 (4)	0.01332 (7)	0.0533 (4)
C8	0.40253 (16)	1.0213 (4)	0.31985 (7)	0.0545 (4)
H8A	0.3333	1.1268	0.3352	0.065*
C7	0.50862 (17)	0.9235 (4)	0.36057 (7)	0.0536 (4)
C5	0.60833 (15)	0.6986 (4)	0.27603 (7)	0.0518 (4)
H5A	0.6772	0.5882	0.2613	0.062*
C9	0.40169 (14)	0.9588 (4)	0.25596 (7)	0.0497 (4)
H9A	0.3318	1.0270	0.2277	0.060*
C6	0.61129 (16)	0.7648 (4)	0.34044 (7)	0.0557 (4)
H6A	0.6815	0.7025	0.3691	0.067*
C1	0.22542 (17)	0.9959 (4)	0.02534 (8)	0.0631 (5)
H1B	0.1738	1.0404	-0.0143	0.095*
H1C	0.2522	1.2011	0.0456	0.095*
H1D	0.1757	0.8720	0.0525	0.095*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.0517 (8)	0.0632 (8)	0.0366 (7)	-0.0062 (6)	0.0045 (5)	-0.0048 (5)
C4	0.0445 (8)	0.0502 (8)	0.0393 (8)	-0.0073 (6)	0.0030 (6)	-0.0030 (6)
C3	0.0471 (8)	0.0647 (10)	0.0433 (8)	-0.0038 (7)	0.0058 (6)	-0.0067 (7)
N1	0.0497 (8)	0.0851 (10)	0.0374 (7)	0.0001 (7)	0.0045 (5)	-0.0076 (6)
O1	0.0619 (7)	0.1067 (11)	0.0384 (6)	-0.0006 (7)	0.0029 (5)	-0.0048 (6)
F1	0.0863 (8)	0.1149 (10)	0.0392 (6)	0.0063 (7)	0.0000 (5)	-0.0137 (5)
C2	0.0511 (9)	0.0682 (10)	0.0400 (8)	-0.0107 (8)	0.0033 (6)	-0.0005 (7)
C8	0.0513 (9)	0.0650 (10)	0.0472 (9)	0.0041 (7)	0.0059 (6)	-0.0074 (7)
C7	0.0600 (9)	0.0648 (10)	0.0350 (7)	-0.0067 (8)	0.0017 (6)	-0.0056 (7)
C5	0.0432 (8)	0.0635 (10)	0.0484 (8)	0.0001 (7)	0.0035 (6)	-0.0029 (7)
C9	0.0451 (8)	0.0584 (9)	0.0441 (8)	-0.0002 (7)	-0.0011 (6)	-0.0030 (6)
C6	0.0488 (9)	0.0697 (10)	0.0458 (8)	-0.0026 (7)	-0.0061 (6)	0.0018 (7)
C1	0.0681 (11)	0.0673 (11)	0.0533 (9)	0.0041 (9)	0.0043 (7)	0.0044 (8)

Geometric parameters (Å, °)

N2—C3	1.269 (2)	C8—C9	1.375 (2)
N2—N1	1.3744 (17)	C8—C7	1.380 (2)
C4—C5	1.390 (2)	C8—H8A	0.9300
C4—C9	1.392 (2)	C7—C6	1.360 (2)
C4—C3	1.462 (2)	C5—C6	1.386 (2)
C3—H3A	0.9300	C5—H5A	0.9300
N1—C2	1.351 (2)	C9—H9A	0.9300
N1—H1A	0.8600	C6—H6A	0.9300
O1—C2	1.2317 (17)	C1—H1B	0.9600
F1—C7	1.3516 (17)	C1—H1C	0.9600
C2—C1	1.484 (2)	C1—H1D	0.9600

C3—N2—N1	114.97 (14)	F1—C7—C8	118.09 (15)
C5—C4—C9	118.69 (14)	C6—C7—C8	122.96 (14)
C5—C4—C3	119.05 (15)	C6—C5—C4	121.01 (15)
C9—C4—C3	122.25 (14)	C6—C5—H5A	119.5
N2—C3—C4	121.53 (15)	C4—C5—H5A	119.5
N2—C3—H3A	119.2	C8—C9—C4	120.87 (14)
C4—C3—H3A	119.2	C8—C9—H9A	119.6
C2—N1—N2	122.09 (15)	C4—C9—H9A	119.6
C2—N1—H1A	119.0	C7—C6—C5	118.13 (15)
N2—N1—H1A	119.0	C7—C6—H6A	120.9
O1—C2—N1	118.51 (16)	C5—C6—H6A	120.9
O1—C2—C1	122.36 (15)	C2—C1—H1B	109.5
N1—C2—C1	119.12 (14)	C2—C1—H1C	109.5
C9—C8—C7	118.32 (15)	H1B—C1—H1C	109.5
C9—C8—H8A	120.8	C2—C1—H1D	109.5
C7—C8—H8A	120.8	H1B—C1—H1D	109.5
F1—C7—C6	118.94 (15)	H1C—C1—H1D	109.5

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 ⁱ	0.86	2.04	2.899 (2)	176

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