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N′-[1-(4-Fluorophenyl)ethylidene]-acetohydrazide

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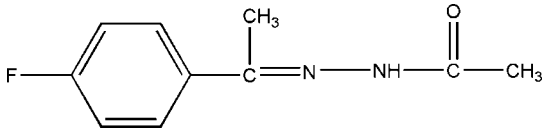
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.054; wR factor = 0.189; data-to-parameter ratio = 13.3.

The title compound, $C_{10}H_{11}FN_2O$, was prepared by the reaction between *p*-fluorohypnone and acetohydrazide. The crystal structure is stabilized by intramolecular C—H···N and intermolecular N—H···O and C—H···O hydrogen-bond interactions.

Related literature

For related literature, see: Cimerman *et al.* (1997); Sutherland & Hoy (1968); Tucker *et al.* (1975).



Experimental

Crystal data

$C_{10}H_{11}FN_2O$
M_r = 194.21
Monoclinic, $P2_1/c$
a = 4.210 (2) Å
b = 12.682 (6) Å
c = 19.016 (9) Å
β = 94.601 (8)°
V = 1012.0 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
0.22 × 0.18 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
4895 measured reflections
1764 independent reflections
1008 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.189
S = 1.07
1764 reflections
133 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.90 (3)	2.20 (3)	3.063 (4)	162 (3)
C1—H1···N1	0.93	2.49	2.803 (4)	100
C8—H8C···O1^{i}	0.96	2.53	3.315 (4)	138
C10—H10B···N1	0.96	2.42	2.816 (4)	104

Symmetry code: (i) $-x+3, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2313).

References

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Tucker, P. A., Hoekstra, A., ten Cate, J. M. & Vos, A. (1975). *Acta Cryst.* B**31**, 733–737.

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supplementary materials

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N'-[1-(4-Fluorophenyl)ethylidene]acetohydrazide

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Comment

Schiff bases are attractive from several points of view, such as the possibility of analytical application (Cimerman, *et al.*, 1997). As part of our search for new schiff base compounds we synthesized the title compound (I), and report its structure here.

In the title molecule (Fig.1), all bond lengths and angles are generally normal. The N1—C7 distance of 1.310 (3) Å is similar to the distance 1.287Å reported by Tucker *et al.* 1975. The O1—C9 distance of 1.244 (3) Å is shorter than the reported distance [1.298 Å] by Sutherland *et al.* 1968.

The crystal structure of the title compound is stabilized by intramolecular C—H···N and intermolecular N—H···O and C—H···O hydrogen bonding interactions.

Experimental

A mixture of the *p*-fluorohypnone (0.1 mol), and acetohydrazide (0.1 mol) was stirred in refluxing ethanol (30 ml) for 5 h to afford the title compound (0.087 mol, yield 87%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Refinement

The H atom bound to N2 atom was found from a difference Fourier map and rwfined freely. The other H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H = 0.93 − 0.98 Å, and with U_{iso}=1.2U_{eq}($C_{aromatic}$) or 1.5U_{eq}(C_{methyl}).

Figures

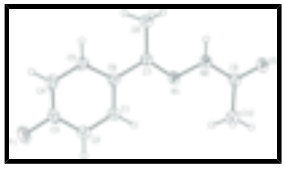

Fig. 1. The structure of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

N'-[1-(4-Fluorophenyl)ethylidene]acetohydrazide

Crystal data

$C_{10}H_{11}FN_2O$	Z = 4
M_r = 194.21	F_{000} = 408

Monoclinic, $P2_1/c$	$D_x = 1.275$ Mg m^{-3}
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 4.210$ (2) Å	$\theta = 1.9$–25.0º
$b = 12.682$ (6) Å	$\mu = 0.10$ mm^{-1}
$c = 19.016$ (9) Å	$T = 294$ (2) K
$\beta = 94.601$ (8)º	Block, colourless
$V = 1012.0$ (8) Å^3	0.22 × 0.18 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer	1008 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.056$
Monochromator: graphite	$\theta_{max} = 25.0$º
$T = 294(2)$ K	$\theta_{min} = 1.9$º
φ and ω scans	$h = -5\rightarrow4$
Absorption correction: none	$k = -13\rightarrow15$
4895 measured reflections	$l = -10\rightarrow22$
1764 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.189$	$w = 1/[\sigma^2(F_o^2) + (0.1007P)^2 + 0.0236P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
1764 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}
133 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2$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}
F1	0.3804 (5)	−0.11853 (14)	0.31178 (11)	0.0743 (7)
O1	1.3986 (5)	0.46938 (17)	0.58653 (11)	0.0580 (7)
N1	1.0628 (5)	0.27734 (18)	0.46623 (12)	0.0422 (7)
N2	1.2235 (6)	0.36871 (19)	0.49241 (12)	0.0449 (7)
C1	0.7895 (7)	0.0838 (2)	0.42358 (16)	0.0500 (9)
H1	0.8530	0.0945	0.4710	0.060*
C2	0.6324 (7)	−0.0104 (2)	0.40306 (17)	0.0555 (9)
H2	0.5929	−0.0618	0.4361	0.067*
C3	0.5375 (8)	−0.0248 (2)	0.33200 (17)	0.0492 (8)
C4	0.5923 (7)	0.0487 (2)	0.28101 (16)	0.0489 (8)
H4	0.5260	0.0367	0.2339	0.059*
C5	0.7524 (7)	0.1431 (2)	0.30238 (14)	0.0450 (8)
H5	0.7920	0.1933	0.2685	0.054*
C6	0.8536 (6)	0.1628 (2)	0.37400 (14)	0.0365 (7)
C7	1.0245 (6)	0.2641 (2)	0.39776 (14)	0.0373 (7)
C8	1.1356 (7)	0.3410 (2)	0.34333 (15)	0.0497 (8)
H8A	0.9908	0.3995	0.3385	0.075*
H8B	1.1410	0.3059	0.2987	0.075*
H8C	1.3450	0.3662	0.3585	0.075*
C9	1.2507 (7)	0.3901 (2)	0.56335 (15)	0.0425 (8)
C10	1.0969 (8)	0.3150 (3)	0.61259 (15)	0.0590 (9)
H10A	1.2212	0.3128	0.6571	0.088*
H10B	1.0867	0.2457	0.5922	0.088*
H10C	0.8854	0.3389	0.6196	0.088*
H2A	1.297 (8)	0.415 (2)	0.4620 (15)	0.081 (12)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0940 (15)	0.0491 (12)	0.0768 (14)	−0.0199 (10)	−0.0125 (11)	−0.0106 (11)
O1	0.0814 (17)	0.0444 (13)	0.0474 (13)	−0.0141 (11)	0.0009 (12)	−0.0075 (10)
N1	0.0534 (15)	0.0325 (13)	0.0401 (15)	−0.0026 (11)	0.0008 (12)	−0.0047 (11)
N2	0.0632 (17)	0.0343 (15)	0.0368 (15)	−0.0052 (12)	0.0021 (12)	−0.0020 (12)
C1	0.067 (2)	0.0436 (18)	0.0384 (17)	−0.0130 (15)	−0.0030 (15)	0.0006 (14)
C2	0.074 (2)	0.044 (2)	0.048 (2)	−0.0139 (17)	0.0020 (17)	0.0042 (15)
C3	0.056 (2)	0.0346 (17)	0.055 (2)	−0.0045 (14)	−0.0041 (16)	−0.0115 (15)
C4	0.065 (2)	0.0395 (18)	0.0407 (17)	0.0065 (15)	−0.0061 (15)	−0.0098 (15)
C5	0.062 (2)	0.0369 (17)	0.0358 (16)	0.0041 (14)	0.0036 (14)	−0.0008 (13)
C6	0.0396 (16)	0.0337 (16)	0.0360 (15)	0.0067 (12)	0.0017 (12)	−0.0021 (12)
C7	0.0401 (16)	0.0321 (16)	0.0392 (17)	0.0036 (12)	0.0005 (13)	−0.0002 (13)
C8	0.064 (2)	0.0421 (18)	0.0432 (17)	−0.0071 (15)	0.0048 (15)	−0.0018 (15)
C9	0.0501 (19)	0.0338 (16)	0.0430 (18)	0.0027 (14)	0.0007 (14)	−0.0012 (14)
C10	0.080 (2)	0.052 (2)	0.0450 (19)	−0.0082 (17)	0.0040 (17)	−0.0003 (16)

Geometric parameters (Å, °)

F1—C3	1.399 (3)	C4—H4	0.9300
O1—C9	1.244 (3)	C5—C6	1.416 (4)
N1—C7	1.310 (3)	C5—H5	0.9300
N1—N2	1.412 (3)	C6—C7	1.523 (4)
N2—C9	1.372 (4)	C7—C8	1.523 (4)
N2—H2A	0.900 (10)	C8—H8A	0.9600
C1—C2	1.405 (4)	C8—H8B	0.9600
C1—C6	1.417 (4)	C8—H8C	0.9600
C1—H1	0.9300	C9—C10	1.517 (4)
C2—C3	1.390 (4)	C10—H10A	0.9600
C2—H2	0.9300	C10—H10B	0.9600
C3—C4	1.377 (4)	C10—H10C	0.9600
C4—C5	1.417 (4)		
C7—N1—N2	118.2 (2)	C5—C6—C7	122.2 (3)
C9—N2—N1	120.6 (2)	C1—C6—C7	120.7 (2)
C9—N2—H2A	120 (2)	N1—C7—C6	114.9 (2)
N1—N2—H2A	120 (2)	N1—C7—C8	125.0 (2)
C2—C1—C6	121.8 (3)	C6—C7—C8	120.2 (2)
C2—C1—H1	119.1	C7—C8—H8A	109.5
C6—C1—H1	119.1	C7—C8—H8B	109.5
C3—C2—C1	118.3 (3)	H8A—C8—H8B	109.5
C3—C2—H2	120.9	C7—C8—H8C	109.5
C1—C2—H2	120.9	H8A—C8—H8C	109.5
C4—C3—C2	123.0 (3)	H8B—C8—H8C	109.5
C4—C3—F1	118.9 (3)	O1—C9—N2	120.5 (3)
C2—C3—F1	118.1 (3)	O1—C9—C10	121.0 (3)
C3—C4—C5	118.2 (3)	N2—C9—C10	118.5 (3)
C3—C4—H4	120.9	C9—C10—H10A	109.5
C5—C4—H4	120.9	C9—C10—H10B	109.5
C6—C5—C4	121.6 (3)	H10A—C10—H10B	109.5
C6—C5—H5	119.2	C9—C10—H10C	109.5
C4—C5—H5	119.2	H10A—C10—H10C	109.5
C5—C6—C1	117.2 (3)	H10B—C10—H10C	109.5
C7—N1—N2—C9	175.5 (2)	C2—C1—C6—C7	−180.0 (3)
C6—C1—C2—C3	−0.4 (5)	N2—N1—C7—C6	179.1 (2)
C1—C2—C3—C4	0.4 (5)	N2—N1—C7—C8	−1.1 (4)
C1—C2—C3—F1	−179.8 (3)	C5—C6—C7—N1	170.8 (2)
C2—C3—C4—C5	−0.1 (5)	C1—C6—C7—N1	−9.2 (4)
F1—C3—C4—C5	−179.8 (2)	C5—C6—C7—C8	−9.0 (4)
C3—C4—C5—C6	−0.3 (4)	C1—C6—C7—C8	171.0 (3)
C4—C5—C6—C1	0.3 (4)	N1—N2—C9—O1	178.3 (2)
C4—C5—C6—C7	−179.7 (2)	N1—N2—C9—C10	−1.6 (4)
C2—C1—C6—C5	0.0 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O1^{i}	0.90 (3)	2.20 (3)	3.063 (4)	162 (3)
C1—H1···N1	0.93	2.49	2.803 (4)	100
C8—H8C···O1^{i}	0.96	2.53	3.315 (4)	138
C10—H10B···N1	0.96	2.42	2.816 (4)	104

Symmetry codes: (i) −*x*+3, −*y*+1, −*z*+1.

Fig. 1