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4-Fluorobenzaldehyde [(*E*)-4-fluorobenzylidene]hydrazone

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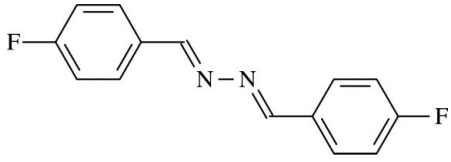
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.143; data-to-parameter ratio = 11.0.

The crystal structure of the title compound, $C_{14}H_{10}F_2N_2$, is stabilized by C—H···F intermolecular hydrogen bonds, which generate edge-fused $R_2^1(6)R_3^2(15)R_2^2(8)R_3^2(17)$ ring motifs. The complete molecule is centrosymmetric and almost planar.

Related literature

For related literature, see: Albayrak *et al.* (2005); Armstrong *et al.* (1998); Duan *et al.* (2005); Ersanlı, Odabaşoğlu *et al.* (2004); Etter (1990); Kazak *et al.* (2004); Kesslen & Euler (1999); Küçükgüzel *et al.* (1999); Kundu *et al.* (2005); Odabaşoğlu *et al.* (2005); Rollas *et al.* (2002); Xu & Hu (2007); Xu *et al.* (1997); Yüce *et al.* (2004); Özek *et al.* (2007); Şahin *et al.* (2005); Zheng *et al.* (2005*a*,*b*).



Experimental

Crystal data

$C_{14}H_{10}F_2N_2$
M_r = 244.24
Monoclinic, $P2_1/c$
a = 3.8488 (18) Å
b = 13.629 (5) Å
c = 11.083 (5) Å
β = 93.17 (4)°
V = 580.5 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 296 K
0.64 × 0.42 × 0.31 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.957, T_{max} = 0.983
2956 measured reflections
1136 independent reflections
804 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.143
S = 1.03
1136 reflections
103 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···F1^{i}	1.04 (2)	2.52 (2)	3.507 (3)	159.36 (1)
C4—H4···F1^{ii}	0.94 (2)	2.63 (2)	3.518 (3)	157.98 (2)
C7—H7···F1^{i}	1.00 (2)	2.79 (3)	3.683 (3)	149.43 (2)

Symmetry codes: (i) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, -y, -z+1$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2402).

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supplementary materials

Acta Cryst. (2007). E**63**, o4145-o4146 [**doi:10.1107/S1600536807045989**]

4-Fluorobenzaldehyde [(*E*)-4-fluorobenzylidene]hydrazone

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Comment

Hydrazones are known to possess antimicrobial, anticonvulsant, analgesic, anti-inflammatory, antiplatelet, antitubercular and antitumoral activities. For example, isonicotinoyl hydrazones are antitubercular; 4-hydroxybenzoic acid [(5-nitro-2-furyl)methylene]-hydrazide (nifuroxazide) is an intestinal antiseptic; 4-fluorobenzoic acid[(5-nitro-2-furyl)methylene]-hydrazide (Rollas *et al.*, 2002) and 2,3,4-pentanetrione-3-[4-[[(5-nitro-2-furyl) methylene]hydrazino]carbonyl]phenyl]-hydrazone (Küçükgüzel *et al.*, 1999) have antibacterial activity. A number of azine compounds containing both a diimine linkage and an N—N bond have been investigated in terms of their crystallography and coordination chemistry (Kundu *et al.*, 2005; Kesslen & Euler, 1999; Armstrong *et al.*, 1998; Xu *et al.*, 1997). The crystal structures of *N*,*N*-bis(4-chlorobenzylidene)hydrazine (Zheng *et al.*, 2005*a*), *N*,*N*'-bis (3-nitrobenzylidene)hydrazine (Zheng *et al.*, 2005*b*), *N*,*N*'-bis(3-hydroxy-4- methoxybenzylidene)hydrazine (Duan *et al.*, 2005), 1,2-bis[4-(trifluoromethyl) benzylidene]hydrazine (Xu & Hu, 2007) have been reported. A new hydrazone, (I), $C_{14}H_{10}F_2N_2$ was synthesized and its crystal structure is reported.

The N1═C1 bond length of 1.266 (2) Å is typical of a double bond and similar to the corresponding bond lengths in our previous works (Odabaşoğlu *et al.*, 2005; Albayrak *et al.*, 2005; Şahin *et al.*, 2005; Kazak *et al.*, 2004; Ersanlı, Odabaşoğlu *et al.*,2004, b; Yüce *et al.*, 2004; Özek *et al.*, 2007). The N—N bond length of 1.410 (3) Å is typical of a N_{sp2}—N_{sp2} single bond.

The crystal structure of (I) is stabilized by three C—H···F intermolecular hydrogen bonds (Table 1). The C—H···F hydrogen bonds generate edge-fussed $R_2^1(6)R_3^2(15)R_2^2(8)R_3^2(17)$ ring motifs (Fig. 2) (Etter, 1990). The molecule is almost planar. There are no C—H···π and π···π interactions in crystal packing.

Experimental

A mixture of 4-fluorobenzaldehyde (2.48 g, 0.02 mol) and hydrazine hydrate (0.5 ml, 0.01 mol) in 15 ml of absolute ethyl alcohol containing 2 drops of 4 *M* sulfuric acid was refluxed for about 3 h. On cooling, the solid separated was filtered and recrystallized from ethyl alcohol [m.p.: 439–441 K]. Analysis for $C_{14}H_{10}F_2N_2$: Found (calculated): C 68.65 (68.85), H 4.18 (4.13), N 11.35% (11.47%).

Refinement

All H atoms were located in Fourier difference map and refined freely.

Figures

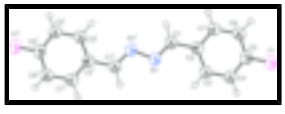

Fig. 1. A view of (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) −*x*, −*y*, −*z*].

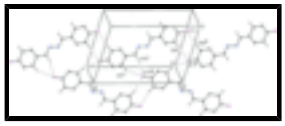

Fig. 2. Part of the crystal structure of (I), showing the formation of $R_2^1(6)R_3^2(15)R_2^2(8)R_3^2(17)$ motifs. [Symmetry codes: (i) $-x, -y, -z$; (ii) $1-x, -y, 1-z$; (iii) $x-1, 1/2-y, z-1/2$].

4-Fluorobenzaldehyde [(*E*)-4-fluorobenzylidene]hydrazone

Crystal data

$C_{14}H_{10}F_2N_2$	$F_{000} = 252$
$M_r = 244.24$	$D_x = 1.397$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2956 reflections
$a = 3.8488$ (18) Å	$\theta = 2.4$–27.8º
$b = 13.629$ (5) Å	$\mu = 0.11$ mm^{-1}
$c = 11.083$ (5) Å	$T = 296$ K
$\beta = 93.17$ (4)º	Prism, light yellow
$V = 580.5$ (4) Å^3	0.64 × 0.42 × 0.31 mm
$Z = 2$	

Data collection

Stoe IPDSII diffractometer	1136 independent reflections
Monochromator: plane graphite	804 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.057$
$T = 296$ K	$\theta_{max} = 26.0$º
ω scans	$\theta_{min} = 2.4$º
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$h = -4 \rightarrow 4$
$T_{min} = 0.957$, $T_{max} = 0.983$	$k = -16 \rightarrow 16$
2956 measured reflections	$l = -9 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.049$	$w = 1/[\sigma^2(F_o^2) + (0.0881P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.143$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.15$ e Å^{-3}
1136 reflections	$\Delta\rho_{min} = -0.19$ e Å^{-3}
103 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.044 (11)

Secondary atom site location: difference Fourier map

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.6680 (5)	0.41276 (12)	0.59066 (17)	0.0559 (5)
C2	0.7183 (4)	0.30733 (12)	0.60689 (16)	0.0499 (5)
C3	0.6028 (5)	0.24038 (13)	0.51855 (18)	0.0561 (5)
C4	0.6501 (5)	0.14112 (12)	0.53589 (19)	0.0620 (5)
C5	0.8109 (5)	0.10995 (12)	0.64283 (18)	0.0605 (5)
C6	0.9276 (5)	0.17279 (14)	0.73247 (19)	0.0618 (5)
C7	0.8812 (5)	0.27196 (13)	0.71346 (18)	0.0587 (5)
N1	0.5085 (4)	0.44837 (9)	0.49769 (14)	0.0590 (5)
F1	0.8551 (4)	0.01213 (8)	0.65970 (13)	0.0915 (6)
H1	0.775 (5)	0.4584 (15)	0.658 (2)	0.073 (6)*
H3	0.485 (5)	0.2631 (13)	0.445 (2)	0.060 (5)*
H4	0.577 (6)	0.0952 (18)	0.476 (2)	0.091 (7)*
H6	1.027 (6)	0.1472 (15)	0.804 (2)	0.083 (7)*
H7	0.965 (6)	0.3201 (19)	0.776 (2)	0.090 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0635 (10)	0.0470 (9)	0.0560 (10)	−0.0012 (7)	−0.0063 (9)	−0.0003 (8)
C2	0.0525 (9)	0.0453 (8)	0.0513 (9)	0.0006 (6)	−0.0031 (7)	0.0005 (7)
C3	0.0645 (10)	0.0492 (9)	0.0530 (10)	0.0010 (7)	−0.0115 (8)	0.0003 (7)
C4	0.0764 (12)	0.0471 (10)	0.0605 (12)	−0.0004 (8)	−0.0141 (10)	−0.0053 (8)
C5	0.0721 (11)	0.0426 (9)	0.0655 (12)	0.0026 (8)	−0.0088 (9)	0.0031 (8)
C6	0.0717 (11)	0.0550 (10)	0.0567 (11)	0.0026 (8)	−0.0150 (9)	0.0046 (8)
C7	0.0682 (11)	0.0507 (10)	0.0554 (11)	−0.0012 (8)	−0.0117 (8)	−0.0039 (8)
N1	0.0733 (10)	0.0393 (7)	0.0630 (10)	0.0023 (6)	−0.0098 (7)	−0.0005 (6)
F1	0.1328 (12)	0.0434 (6)	0.0940 (11)	0.0087 (6)	−0.0326 (8)	0.0052 (6)

Geometric parameters (Å, °)

C1—N1	1.266 (2)	C4—H4	0.94 (3)
C1—C2	1.460 (2)	C5—F1	1.356 (2)

C1—H1	1.04 (2)	C5—C6	1.368 (3)
C2—C7	1.392 (3)	C6—C7	1.378 (3)
C2—C3	1.393 (3)	C6—H6	0.93 (3)
C3—C4	1.377 (2)	C7—H7	1.00 (3)
C3—H3	0.96 (2)	N1—N1^{i}	1.410 (3)
C4—C5	1.374 (3)		
N1—C1—C2	122.17 (16)	C3—C4—H4	121.5 (16)
N1—C1—H1	120.8 (12)	F1—C5—C6	118.79 (17)
C2—C1—H1	117.0 (12)	F1—C5—C4	118.04 (15)
C7—C2—C3	118.74 (17)	C6—C5—C4	123.16 (17)
C7—C2—C1	119.72 (15)	C5—C6—C7	117.92 (18)
C3—C2—C1	121.54 (16)	C5—C6—H6	119.2 (14)
C4—C3—C2	120.71 (18)	C7—C6—H6	122.9 (14)
C4—C3—H3	119.1 (11)	C6—C7—C2	121.18 (18)
C2—C3—H3	120.2 (11)	C6—C7—H7	120.3 (15)
C5—C4—C3	118.29 (17)	C2—C7—H7	118.5 (15)
C5—C4—H4	120.2 (15)	C1—N1—N1^{i}	111.98 (18)
N1—C1—C2—C7	−176.97 (19)	F1—C5—C6—C7	179.80 (18)
N1—C1—C2—C3	2.2 (3)	C4—C5—C6—C7	−0.2 (3)
C7—C2—C3—C4	−0.3 (3)	C5—C6—C7—C2	0.5 (3)
C1—C2—C3—C4	−179.46 (18)	C3—C2—C7—C6	−0.2 (3)
C2—C3—C4—C5	0.6 (3)	C1—C2—C7—C6	178.91 (18)
C3—C4—C5—F1	179.65 (18)	C2—C1—N1—N1^{i}	179.84 (17)
C3—C4—C5—C6	−0.4 (3)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···F1^{ii}	1.04 (2)	2.52 (2)	3.507 (3)	159.36 (1)
C4—H4···F1^{iii}	0.94 (2)	2.63 (2)	3.518 (3)	157.98 (2)
C7—H7···F1^{ii}	1.00 (2)	2.79 (3)	3.683 (3)	149.43 (2)

Symmetry codes: (ii) −*x*+2, *y*+1/2, −*z*+3/2; (iii) −*x*+1, −*y*, −*z*+1.

Fig. 1

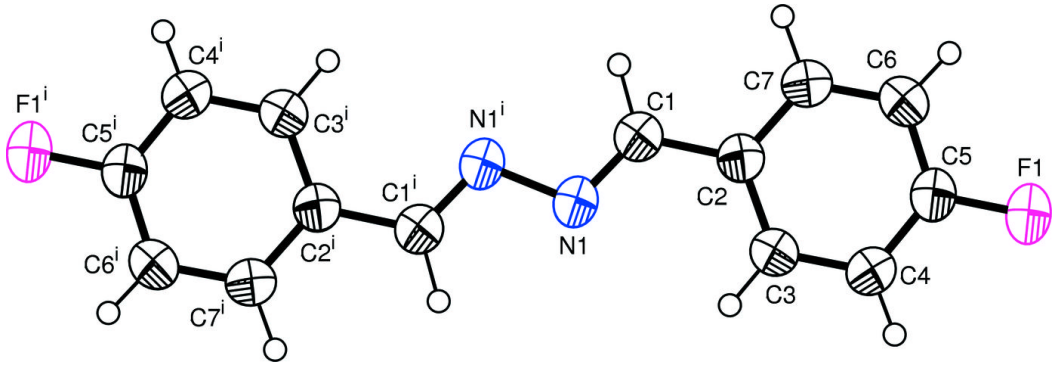

Fig. 2