

## *N*-(4-Fluorophenyl)acetamide

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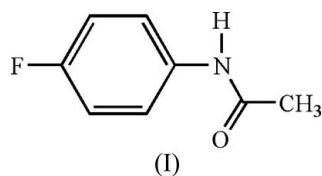
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**Key indicators**Single-crystal X-ray study  
*T* = 294 K  
Mean  $\sigma$ (C–C) = 0.004 Å  
*R* factor = 0.027  
*wR* factor = 0.078  
Data-to-parameter ratio = 7.6For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

The title compound, C<sub>8</sub>H<sub>8</sub>FNO, is an important medicinal intermediate. Intermolecular hydrogen bonds are formed between the NH group and the carbonyl O atom of an adjacent molecule.

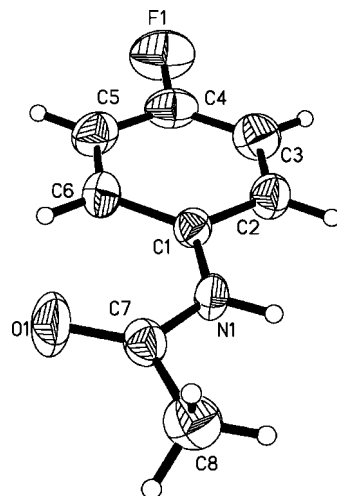
**Comment**

*N*-(4-Fluorophenyl)acetamide is a useful building block for pharmaceuticals. It was prepared by the reaction of acetic anhydride and 4-fluoroaniline in the presence of triethylamine (Goundwater *et al.*, 1996).



The molecular structure of (I) and the atom-numbering scheme are shown in Fig. 1. In the molecular structure of (I), the N1–C7 bond length [1.338 (3) Å] is longer than that (1.32 Å) for a peptide linkage. The N1–C1 bond length [1.414 (3) Å] is shorter than a normal C–N single bond and longer than a normal C=N double bond, probably as a result of electron delocalisation, suggesting that the C1–N1 bond participates in the conjugated system of the benzene ring (Taira *et al.*, 1988).

An intermolecular hydrogen bond is formed between the NH group and the carbonyl O atom of an adjacent molecule (Fig. 2).



**Figure 1**  
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level.

## Experimental

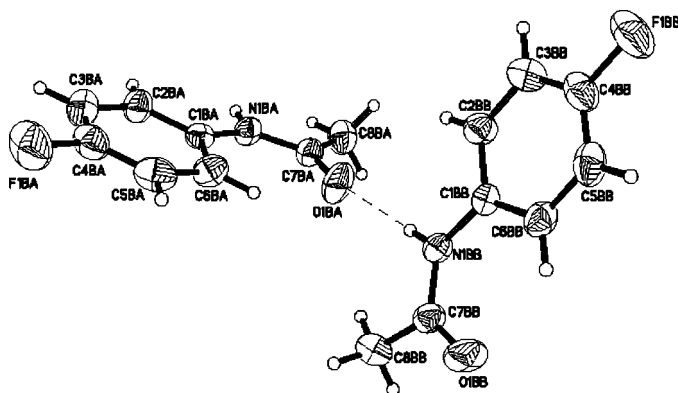
Acetic anhydride (23.2 ml) was added slowly with stirring to a solution of 4-fluoroaniline (25.0 g) in the presence of triethylamine (25.3 g) at 273 K. The mixture was stirred at room temperature for 3 h. The resulting precipitate was filtered off and washed with water three times. A colourless solid (yield 30 g, 86%) was obtained, and single crystals suitable for crystallographic analysis were obtained by slow evaporation of an ethyl acetate solution [m.p. 426 (2) K]. IR (KBr,  $\text{cm}^{-1}$ ):  $\nu$  1702. Analysis required for  $\text{C}_8\text{H}_8\text{FNO}$ : C 62.7, H 5.3, N 9.2%; found: C 63.0, H 5.4, N 9.3%.

### Crystal data

$\text{C}_8\text{H}_8\text{FNO}$	$D_x = 1.310 \text{ Mg m}^{-3}$
$M_r = 153.15$	Mo $K\alpha$ radiation
Monoclinic, $Cc$	Cell parameters from 1238 reflections
$a = 4.7307 (15) \text{ \AA}$	$\theta = 2.4\text{--}25.8^\circ$
$b = 17.067 (5) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$c = 9.634 (3) \text{ \AA}$	$T = 294 (2) \text{ K}$
$\beta = 92.871 (5)^\circ$	Prism, colourless
$V = 776.8 (4) \text{ \AA}^3$	$0.24 \times 0.20 \times 0.14 \text{ mm}$
$Z = 4$	

### Data collection

Bruker SMART CCD area-detector diffractometer	796 independent reflections
$\varphi$ and $\omega$ scans	681 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.018$
$T_{\text{min}} = 0.963$ , $T_{\text{max}} = 0.986$	$\theta_{\text{max}} = 26.4^\circ$
2137 measured reflections	$h = -5 \rightarrow 5$
	$k = -21 \rightarrow 20$
	$l = -12 \rightarrow 9$



**Figure 2**  
The intermolecular  $\text{N—H}\cdots\text{O}$  hydrogen bond, shown as a dashed line. [Symmetry codes: (BB)  $x, y, z$ ; (BA)  $x, y, z - 1$ .]

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0419P)^2 + 0.1195P]$
$R[F^2 > 2\sigma(F^2)] = 0.027$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.078$	$(\Delta/\sigma)_{\text{max}} = 0.002$
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.09 \text{ e \AA}^{-3}$
796 reflections	$\Delta\rho_{\text{min}} = -0.10 \text{ e \AA}^{-3}$
105 parameters	
H atoms treated by a mixture of independent and constrained refinement	

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
$\text{N1—H1}\cdots\text{O1}^i$	0.85 (3)	2.00 (3)	2.835 (3)	167 (3)

Symmetry code: (i)  $x, -y + 1, z + \frac{1}{2}$ .

All C-bound H atoms were positioned geometrically and refined as riding ( $\text{C—H} = 0.93\text{--}0.96 \text{ \AA}$ ). The H atom of the NH group was refined isotropically [ $\text{N—H} = 0.85 (3) \text{ \AA}$ ]. For the CH groups,  $U_{\text{iso}}(\text{H})$  values were set equal to  $1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ . In the absence of anomalous dispersion effects, the Friedel pairs were merged.

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

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