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4′-Fluoro-2′-nitroacetanilide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
R factor = 0.050
wR factor = 0.168
Data-to-parameter ratio = 15.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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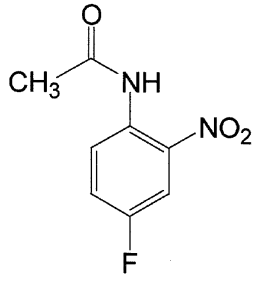
The crystal structure of the title compound, $C_8H_7FN_2O_3$, shows that the amide and nitro groups are rotated slightly out of the aromatic plane, with dihedral angles of 16.30 (6) and 29.60 (10)°, respectively. The overall molecular organization is stabilized by well defined intermolecular hydrogen bonds that lead to the formation of infinite chains.

Comment

One of the structural characteristics of 4′-fluoro-2′-nitroacetanilide, (I), is the presence of a pair of electron-donating ($-NH_2$) and electron-withdrawing ($-NO_2$) groups, a feature which enhances the dipole moment of this molecule through both inductive and resonance effects (Fletton *et al.*, 1986). In addition, molecule (I) contains a single fluoro substituent on its aromatic ring, the signal of which can be easily detected *via* ^{19}F NMR methods. A molecule possessing such structural characteristics in crystalline form is deemed to be an ideal candidate for examination of the hypothesis of time-reversal symmetry violation, a physics theory postulated in the recent years (Li & Nadin, 1995, 1998). As part of our efforts investigating this theory, we present the crystal structure of (I).



(I)

The amide group in (I) (Fig. 1) is rotated out of the ring plane, with a dihedral angle of 16.30 (6)°. Similarly, the nitro group is slightly twisted out of the aromatic ring plane by 29.60 (10)°. The amide N atom approaches the amide O atom of an adjacent molecule at a distance of 2.9536 (16) Å, indicating intermolecular hydrogen bonding. It is also noted that (I) crystallizes in a centrosymmetric space group.

According to the theory of time-reversal symmetry violation (Li & Nadin, 1995, 1998), the magnitudes of the two electric currents operating in opposite directions along the same aromatic ring of (I) will be different, thus resulting in two different signals for the chemical shifts of the F atom in (I). Studies into this effect are underway.

Experimental

The title compound was acquired from a commercial source (Aldrich). The crystal used for the data collection was obtained by slow evaporation from acetone–water (2:1) saturated solution at room temperature.

Crystal data

$C_8H_7FN_2O_3$	D_x = 1.531 Mg m^{-3}
M_r = 198.16	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2891 reflections
a = 3.9758 (7) Å	θ = 1–27.5°
b = 22.489 (4) Å	μ = 0.13 mm^{-1}
c = 9.7419 (16) Å	T = 294 (2) K
β = 99.255 (3)°	Prism, colorless
V = 859.7 (3) Å^3	0.20 × 0.18 × 0.16 mm
Z = 4	

Data collection

CCD area-detector diffractometer	1284 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.024
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)	θ_{max} = 27.6°
T_{min} = 0.974, T_{max} = 0.979	$h = -3 \rightarrow 5$
5833 measured reflections	$k = -28 \rightarrow 29$
1984 independent reflections	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.050	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.168	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.06	$\Delta\rho_{max}$ = 0.36 e Å^{-3}
1978 reflections	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
128 parameters	

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O3^{i}	0.86	2.10	2.9536 (16)	170

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

The C-bound H atoms were placed in their geometrically calculated positions and included in the final refinement in the riding-model approximation.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SHELXTL-NT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-NT*; software used to prepare material for publication: *SHELXTL-NT*.

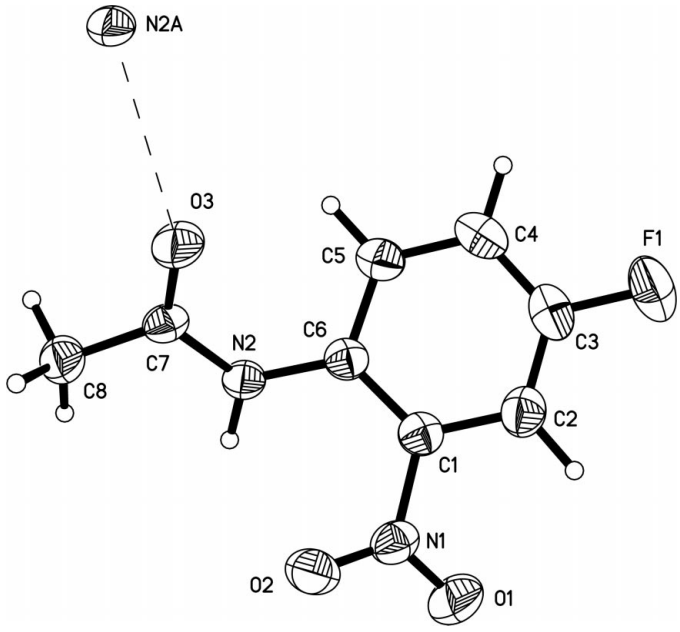


Figure 1
The molecular structure of (I) with ellipsoids at the 30% probability level (Bruker, 1995).

We thank Dr Tianhu Li for his helpful discussion on the topic of time-reversal symmetry violation.

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