IUCrData
ISSN 2414-3146

2-Fluoro-5-nitroaniline

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Received 21 February 2018
Accepted 13 March 2018

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

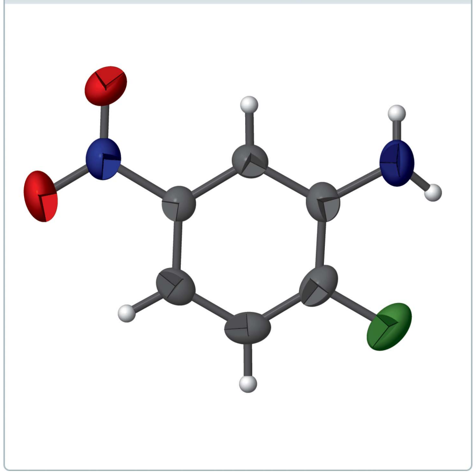
Keywords: crystal structure; aniline; 5-nitroaniline; 2-fluoro-5-nitroaniline; hydrogen bonding.

CCDC reference: 1829279

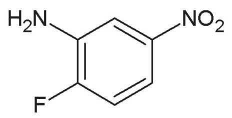
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_6H_5FN_2O_2$, the dihedral angle between the nitro group and the benzene ring is 3.68 (2)°, and an intramolecular N—H···F hydrogen bond is observed. The crystal packing is consolidated by C—H···O and N—H···O hydrogen bonds; together, these generate [110] double chains.

3D view



Chemical scheme



Structure description

The title compound can be utilized to synthesize dyes and pigments (Qi *et al.*, 2009; Hu *et al.*, 2010) but its crystal structure has not yet been determined and is reported here.

The molecular conformation is essentially planar (Fig. 1), with a maximum deviation of 0.062 (2) Å for O2. The dihedral angle between the nitro group and the benzene ring is 3.68 (2)°. The C—N bond distance [1.379 (3) Å] of the NH_2 group is short for a C—N single bond, which may indicate a significant contribution from the imino resonance form to the structure. A weak intramolecular N—H···F hydrogen bond is observed (Table 1).

The crystal packing is consolidated by C—H···O and N—H···O hydrogen bonds (Fig. 2). The aromatic carbon (C6) atom interacts with the nitro group O atom to generate an $R_2^2(10)$ loop. The resulting dimeric units are connected *via* N—H···O hydrogen bonds, forming an $R_4^4(16)$ ring motif. Taken together, [110] double chains arise.

Synthesis and crystallization

2-Fluoro-5-nitroaniline (4 g) was dissolved in the minimum quantity of ethanol and sonicated for 1 h and then placed in an microwave oven for about ten minutes. The resulting paste-like material was dissolved in 10 ml of ethanol and brown blocks were recovered after 48 h as the solvent evaporated.

https://doi.org/10.1107/S241431461800425X

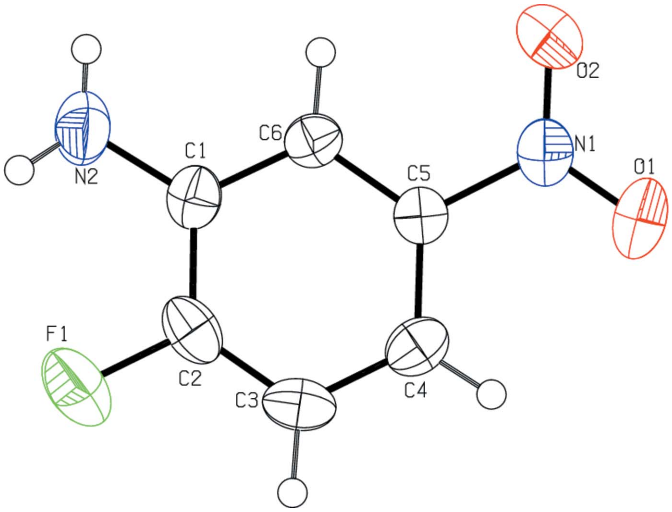


Figure 1
The molecular structure with displacement ellipsoids drawn at the 50% probability level.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors are grateful to the SAIF, IIT, Madras, India, for the data collection.

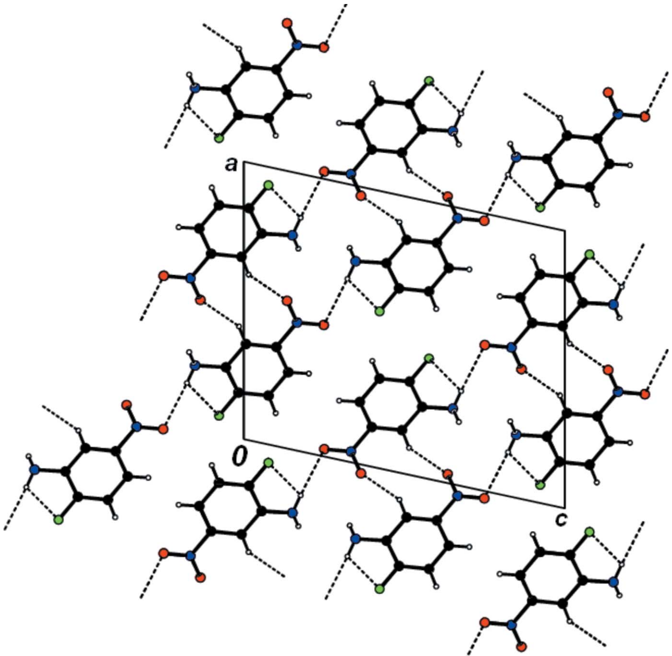


Figure 2
The crystal packing of the title compound, viewed down [010]. The hydrogen bonds are shown as dashed lines.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H2$B\cdots$F1	0.85 (3)	2.37 (3)	2.718 (3)	105 (2)
N2—H2$B\cdots$O1$^{\rm i}$	0.85 (3)	2.45 (3)	3.270 (3)	162 (2)
C6—H6$\cdots$O2$^{\rm ii}$	0.93	2.51	3.348 (3)	150

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{5}{2}, z-\frac{1}{2}$; (ii) $-x+1, -y+3, -z+2$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_5FN_2O_2$
M_r	156.12
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	12.1967 (9), 3.7559 (2), 14.4539 (10)
β (°)	102.143 (3)
V (Å^3)	647.31 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.14
Crystal size (mm)	0.25 × 0.20 × 0.15
Data collection	
Diffractometer	Bruker KappaCCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
$T_{\rm min}$, $T_{\rm max}$	0.666, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7982, 1124, 731
$R_{\rm int}$	0.040
$(\sin \theta/\lambda)_{\rm max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.106, 1.09
No. of reflections	1124
No. of parameters	108
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\rm max}$, $\Delta\rho_{\rm min}$ (e Å^{-3})	0.15, −0.19

Computer programs: *APEX2* (Bruker, 2004), *SAINT* (Bruker, 2004), *SHELXT2014* (Sheldrick, 2015*a*), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008), *SHELXL2014* (Sheldrick, 2015*b*), *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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full crystallographic data

IUCrData (2018). **3**, x180425 [https://doi.org/10.1107/S241431461800425X]

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Crystal data

$C_6H_5FN_2O_2$
$M_r = 156.12$
Monoclinic, $P2_1/n$
$a = 12.1967\ (9)$ Å
$b = 3.7559\ (2)$ Å
$c = 14.4539\ (10)$ Å
$\beta = 102.143\ (3)°$
$V = 647.31\ (7)$ Å^3
$Z = 4$

$F(000) = 320$
$D_x = 1.602$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2057 reflections
$\theta = 2.5–28.0°$
$\mu = 0.14$ mm^{-1}
$T = 296$ K
Block, brown
0.25 × 0.20 × 0.15 mm

Data collection

Bruker KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
$T_{\min} = 0.666$, $T_{\max} = 0.746$

7982 measured reflections
1124 independent reflections
731 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.040$
$\theta_{\max} = 25.0°$, $\theta_{\min} = 2.5°$
$h = -14 \rightarrow 14$
$k = -4 \rightarrow 4$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.106$
$S = 1.09$
1124 reflections
108 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 0.1287P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.15$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The N-bound H atoms were located in a difference Fourier map and refined with distance restraints: N—H = 0.89 (2) Å. The C-bound H atoms were positioned geometrically and refined using a riding model: C—H = 0.93 Å with $U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
C1	0.24514 (17)	1.0767 (5)	0.94448 (14)	0.0370 (5)
C2	0.16370 (17)	0.9076 (5)	0.98328 (16)	0.0423 (6)
C3	0.17626 (19)	0.8268 (5)	1.07728 (16)	0.0430 (6)
H3	0.1187	0.7157	1.0995	0.052*
C4	0.27553 (18)	0.9127 (5)	1.13846 (15)	0.0402 (6)
H4	0.2869	0.8600	1.2026	0.048*
C5	0.35721 (17)	1.0787 (5)	1.10151 (13)	0.0327 (5)
C6	0.34464 (17)	1.1593 (5)	1.00692 (13)	0.0343 (5)
H6	0.4027	1.2687	0.9850	0.041*
N1	0.46159 (16)	1.1836 (4)	1.16606 (12)	0.0439 (5)
N2	0.2278 (2)	1.1426 (7)	0.84863 (14)	0.0563 (6)
O1	0.47362 (16)	1.1064 (6)	1.24921 (11)	0.0826 (7)
O2	0.53201 (14)	1.3472 (5)	1.13505 (11)	0.0627 (5)
F1	0.06598 (11)	0.8233 (4)	0.92311 (10)	0.0660 (5)
H2B	0.158 (2)	1.155 (7)	0.8230 (19)	0.074 (9)*
H2A	0.271 (2)	1.293 (7)	0.830 (2)	0.083 (11)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0376 (13)	0.0370 (12)	0.0353 (11)	0.0103 (11)	0.0055 (10)	−0.0004 (10)
C2	0.0295 (13)	0.0389 (12)	0.0552 (14)	0.0049 (10)	0.0015 (11)	−0.0096 (11)
C3	0.0391 (14)	0.0358 (12)	0.0597 (15)	−0.0010 (11)	0.0231 (12)	−0.0013 (10)
C4	0.0499 (15)	0.0358 (12)	0.0380 (11)	0.0044 (11)	0.0164 (11)	0.0006 (10)
C5	0.0341 (12)	0.0294 (10)	0.0345 (11)	0.0040 (9)	0.0067 (9)	−0.0024 (9)
C6	0.0343 (12)	0.0341 (11)	0.0364 (11)	0.0040 (10)	0.0117 (10)	−0.0001 (9)
N1	0.0433 (12)	0.0475 (11)	0.0387 (11)	0.0041 (10)	0.0035 (9)	−0.0031 (9)
N2	0.0491 (15)	0.0750 (16)	0.0400 (12)	0.0034 (14)	−0.0016 (11)	0.0038 (11)
O1	0.0832 (15)	0.1230 (16)	0.0340 (10)	−0.0218 (12)	−0.0053 (9)	0.0090 (11)
O2	0.0414 (10)	0.0848 (12)	0.0595 (11)	−0.0144 (10)	0.0056 (9)	0.0022 (9)
F1	0.0375 (8)	0.0796 (10)	0.0755 (10)	−0.0046 (7)	−0.0001 (7)	−0.0135 (8)

Geometric parameters (Å, º)

C1—N2	1.379 (3)	C4—H4	0.9300
C1—C6	1.387 (3)	C5—C6	1.377 (3)
C1—C2	1.392 (3)	C5—N1	1.465 (3)
C2—F1	1.357 (2)	C6—H6	0.9300
C2—C3	1.369 (3)	N1—O1	1.215 (2)
C3—C4	1.379 (3)	N1—O2	1.216 (2)
C3—H3	0.9300	N2—H2B	0.85 (3)
C4—C5	1.375 (3)	N2—H2A	0.85 (3)
N2—C1—C6	122.8 (2)	C4—C5—C6	123.2 (2)
N2—C1—C2	121.0 (2)	C4—C5—N1	118.56 (18)

C6—C1—C2	116.15 (19)	C6—C5—N1	118.27 (18)
F1—C2—C3	119.0 (2)	C5—C6—C1	119.77 (19)
F1—C2—C1	116.9 (2)	C5—C6—H6	120.1
C3—C2—C1	124.1 (2)	C1—C6—H6	120.1
C2—C3—C4	119.0 (2)	O1—N1—O2	122.5 (2)
C2—C3—H3	120.5	O1—N1—C5	118.28 (19)
C4—C3—H3	120.5	O2—N1—C5	119.18 (18)
C5—C4—C3	117.85 (19)	C1—N2—H2B	111.9 (18)
C5—C4—H4	121.1	C1—N2—H2A	117 (2)
C3—C4—H4	121.1	H2B—N2—H2A	117 (3)

N2—C1—C2—F1	−2.2 (3)	C4—C5—C6—C1	1.0 (3)
C6—C1—C2—F1	−179.70 (16)	N1—C5—C6—C1	−177.43 (16)
N2—C1—C2—C3	178.47 (19)	N2—C1—C6—C5	−178.51 (18)
C6—C1—C2—C3	1.0 (3)	C2—C1—C6—C5	−1.1 (3)
F1—C2—C3—C4	−179.95 (17)	C4—C5—N1—O1	3.0 (3)
C1—C2—C3—C4	−0.7 (3)	C6—C5—N1—O1	−178.58 (19)
C2—C3—C4—C5	0.4 (3)	C4—C5—N1—O2	−176.16 (18)
C3—C4—C5—C6	−0.6 (3)	C6—C5—N1—O2	2.3 (3)
C3—C4—C5—N1	177.80 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···F1	0.85 (3)	2.37 (3)	2.718 (3)	105 (2)
N2—H2*B*···O1^{i}	0.85 (3)	2.45 (3)	3.270 (3)	162 (2)
C6—H6···O2^{ii}	0.93	2.51	3.348 (3)	150

Symmetry codes: (i) *x*−1/2, −*y*+5/2, *z*−1/2; (ii) −*x*+1, −*y*+3, −*z*+2.