

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

2-Fluoro-5-(4-fluorophenyl)pyridine

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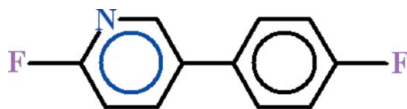
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Received 31 May 2012; accepted 2 June 2012

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.030; wR factor = 0.072; data-to-parameter ratio = 11.6.

In the title compound, $\text{C}_{11}\text{H}_7\text{F}_2\text{N}$, the fluorobenzene and the 2-fluoropyridine rings are oriented at a dihedral angle of $37.93(5)^\circ$. In the crystal, only van der Waals interactions occur.

Related literature

For a related structure, see: Siddle *et al.* (2010).

Experimental

Crystal data

 $\text{C}_{11}\text{H}_7\text{F}_2\text{N}$ $M_r = 191.18$ Orthorhombic, $Pca2_1$ $a = 20.365(2)$ Å $b = 3.8303(3)$ Å $c = 11.4835(14)$ Å $V = 895.74(16)$ Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 0.11$ mm⁻¹ $T = 296$ K $0.26 \times 0.20 \times 0.18$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 2005)

 $T_{\min} = 0.932$, $T_{\max} = 0.950$

3601 measured reflections

1489 independent reflections

1162 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.020$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.030$ $wR(F^2) = 0.072$ $S = 1.03$

1489 reflections

128 parameters

1 restraint

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.11$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.09$ e Å⁻³

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and PLATON (Spek, 2009); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON.

The authors acknowledge the provision of funds for the purchase of a diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan. MA also acknowledges financial support from the World University Service, Germany, for an equipment grant and the Higher Education Commission, Pakistan, for a resource grant.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6833).

References

- Bruker (2005). SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
 Bruker (2007). APEX2 and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Siddle, J. S., Batsanov, A. S., Caldwell, S. T., Cooke, G. & Bryce, M. R. (2010). *Tetrahedron*, **66**, 6138–6149.
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

supporting information

Acta Cryst. (2012). E68, o2070 [https://doi.org/10.1107/S1600536812025160]

2-Fluoro-5-(4-fluorophenyl)pyridine

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S1. Comment

The title compound (I), (Fig. 1) is prepared as a precursor and for the study of biological activities.

The crystal structure of 6-fluoro-3-(4-methoxyphenyl)pyridin-2-ol (Siddle *et al.*, 2010) has been published which is related to (I).

In (I) the fluorophenyl A (C1–C6/F1) and the 2-fluoropyridine B (C7–C11/N1/F2) are almost planar with r. m. s. deviations of 0.0025 Å and 0.0071 Å, respectively. The dihedral angle between A/B is 37.93 (5)°. There does not exist any kind of π -interactions and the molecules must interact due to van Der Waals forces.

S2. Experimental

To a 6 ml solution of 5-bromo-2-fluoropyridine (0.2 g, 1.136 mmol), 4-fluorophenylboronic acid (0.190 g, 1.36 mmol) in Dioxane and K_3PO_4 (0.361 g, 1.5 mmol, in 1 ml H_2O) was added $Pd(PPh_3)_4$ (1.5 mole %) at 373 K under N_2 atmosphere. The reaction mixture was refluxed for 8 h. Then 20 ml of distilled water was added. The aqueous layer was extracted three times with EtOAc (3×15 ml). The organic layer was evaporated *in vacuo* and title compound was obtained as a colourless solid. Yield: 0.185 g, 85%. *M.p.* 350–352 K. Crystallization from a saturated $CHCl_3/CH_3OH$ solution gave colorless rods of (I).

S3. Refinement

The H-atoms were positioned geometrically (C–H = 0.93 Å) and refined as riding with $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.2$ for all H-atoms. The absolute structure of the crystal used in this experiment was indeterminate.

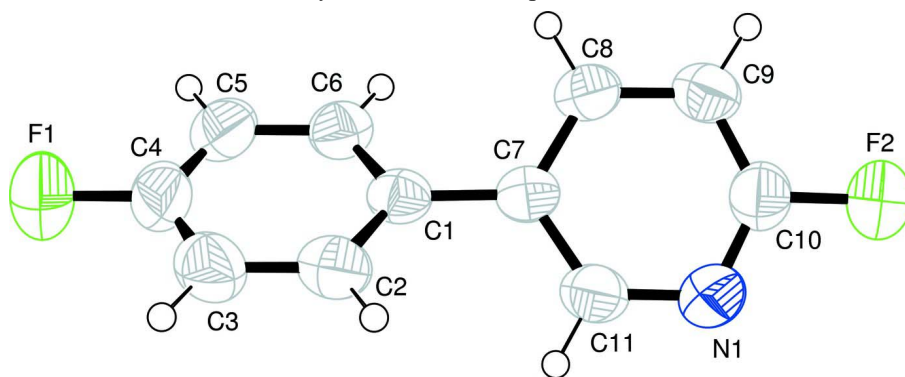


Figure 1

View of the title compound with displacement ellipsoids are drawn at the 50% probability level.

2-Fluoro-5-(4-fluorophenyl)pyridine

Crystal data

C₁₁H₇F₂N $M_r = 191.18$ Orthorhombic, *Pca*2₁

Hall symbol: P 2c -2ac

 $a = 20.365$ (2) Å $b = 3.8303$ (3) Å $c = 11.4835$ (14) Å $V = 895.74$ (16) Å³ $Z = 4$ $F(000) = 392$ $D_x = 1.418$ Mg m⁻³Mo *K*α radiation, $\lambda = 0.71073$ Å

Cell parameters from 1162 reflections

 $\theta = 2.0$ – 25.3° $\mu = 0.11$ mm⁻¹ $T = 296$ K

Rod, colorless

 $0.26 \times 0.20 \times 0.18$ mm

Data collection

Bruker Kappa APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 8.10 pixels mm⁻¹ ω scansAbsorption correction: multi-scan
(*SADABS*; Bruker, 2005) $T_{\min} = 0.932$, $T_{\max} = 0.950$

3601 measured reflections

1489 independent reflections

1162 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.020$ $\theta_{\max} = 25.5^\circ$, $\theta_{\min} = 2.0^\circ$ $h = -21 \rightarrow 24$ $k = -2 \rightarrow 4$ $l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.030$ $wR(F^2) = 0.072$ $S = 1.03$

1489 reflections

128 parameters

1 restraint

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0344P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.11$ e Å⁻³ $\Delta\rho_{\min} = -0.09$ e Å⁻³

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	0.16885 (7)	-0.0787 (5)	0.32200 (16)	0.1219 (8)
F2	0.60621 (6)	0.4445 (4)	0.58901 (13)	0.0984 (6)
N1	0.50519 (9)	0.2455 (5)	0.62465 (14)	0.0695 (7)
C1	0.35628 (9)	0.1391 (5)	0.43374 (16)	0.0497 (7)
C2	0.30232 (10)	0.2088 (6)	0.50519 (18)	0.0635 (9)

C3	0.23904 (11)	0.1346 (7)	0.4674 (2)	0.0767 (10)
C4	0.23116 (11)	-0.0048 (7)	0.3597 (2)	0.0785 (11)
C5	0.28211 (11)	-0.0803 (6)	0.28686 (19)	0.0713 (9)
C6	0.34494 (10)	-0.0045 (5)	0.32527 (18)	0.0586 (8)
C7	0.42374 (9)	0.2219 (5)	0.47208 (15)	0.0468 (7)
C8	0.47047 (9)	0.3501 (6)	0.39465 (17)	0.0560 (8)
C9	0.53273 (10)	0.4268 (5)	0.43285 (19)	0.0609 (8)
C10	0.54517 (11)	0.3685 (6)	0.54736 (19)	0.0636 (9)
C11	0.44444 (10)	0.1735 (5)	0.58562 (18)	0.0603 (8)
H2	0.30881	0.30545	0.57858	0.0761*
H3	0.20297	0.17943	0.51471	0.0918*
H5	0.27490	-0.17911	0.21400	0.0855*
H6	0.38044	-0.05144	0.27678	0.0703*
H8	0.45950	0.38384	0.31684	0.0672*
H9	0.56470	0.51406	0.38289	0.0731*
H11	0.41423	0.08497	0.63868	0.0723*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0663 (9)	0.1613 (16)	0.1380 (14)	-0.0246 (9)	-0.0268 (10)	0.0455 (14)
F2	0.0764 (9)	0.1291 (14)	0.0898 (10)	-0.0286 (8)	-0.0211 (9)	0.0164 (9)
N1	0.0759 (13)	0.0821 (15)	0.0506 (10)	-0.0147 (10)	-0.0079 (10)	0.0035 (9)
C1	0.0565 (12)	0.0413 (12)	0.0512 (11)	0.0046 (9)	0.0032 (9)	0.0085 (9)
C2	0.0662 (15)	0.0613 (17)	0.0629 (13)	0.0067 (11)	0.0106 (11)	0.0089 (10)
C3	0.0576 (15)	0.086 (2)	0.0864 (18)	0.0097 (12)	0.0101 (13)	0.0230 (16)
C4	0.0586 (16)	0.082 (2)	0.095 (2)	-0.0085 (11)	-0.0191 (14)	0.0332 (15)
C5	0.0751 (16)	0.0737 (18)	0.0650 (14)	-0.0054 (12)	-0.0149 (12)	0.0147 (12)
C6	0.0617 (13)	0.0589 (15)	0.0551 (12)	0.0015 (10)	-0.0007 (10)	0.0079 (10)
C7	0.0552 (12)	0.0393 (12)	0.0459 (10)	0.0062 (8)	0.0027 (9)	0.0011 (8)
C8	0.0600 (14)	0.0609 (14)	0.0471 (11)	0.0077 (10)	0.0020 (10)	0.0078 (9)
C9	0.0595 (14)	0.0634 (16)	0.0599 (14)	-0.0003 (10)	0.0094 (10)	0.0089 (10)
C10	0.0596 (15)	0.0635 (16)	0.0678 (14)	-0.0058 (10)	-0.0088 (11)	0.0024 (12)
C11	0.0667 (14)	0.0627 (15)	0.0514 (12)	-0.0080 (10)	0.0065 (10)	0.0050 (10)

Geometric parameters (Å, °)

F1—C4	1.370 (3)	C7—C8	1.392 (3)
F2—C10	1.363 (3)	C7—C11	1.383 (3)
N1—C10	1.293 (3)	C8—C9	1.374 (3)
N1—C11	1.344 (3)	C9—C10	1.358 (3)
C1—C2	1.397 (3)	C2—H2	0.9300
C1—C6	1.381 (3)	C3—H3	0.9300
C1—C7	1.477 (3)	C5—H5	0.9300
C2—C3	1.389 (3)	C6—H6	0.9300
C3—C4	1.357 (3)	C8—H8	0.9300
C4—C5	1.364 (3)	C9—H9	0.9300
C5—C6	1.384 (3)	C11—H11	0.9300

C10—N1—C11	115.17 (18)	F2—C10—C9	118.35 (19)
C2—C1—C6	118.31 (18)	N1—C10—C9	127.4 (2)
C2—C1—C7	121.03 (17)	N1—C11—C7	124.57 (18)
C6—C1—C7	120.66 (17)	C1—C2—H2	120.00
C1—C2—C3	120.47 (19)	C3—C2—H2	120.00
C2—C3—C4	118.4 (2)	C2—C3—H3	121.00
F1—C4—C3	118.6 (2)	C4—C3—H3	121.00
F1—C4—C5	117.8 (2)	C4—C5—H5	121.00
C3—C4—C5	123.6 (2)	C6—C5—H5	121.00
C4—C5—C6	117.6 (2)	C1—C6—H6	119.00
C1—C6—C5	121.70 (19)	C5—C6—H6	119.00
C1—C7—C8	121.42 (16)	C7—C8—H8	120.00
C1—C7—C11	122.40 (17)	C9—C8—H8	120.00
C8—C7—C11	116.18 (17)	C8—C9—H9	122.00
C7—C8—C9	120.17 (18)	C10—C9—H9	122.00
C8—C9—C10	116.52 (19)	N1—C11—H11	118.00
F2—C10—N1	114.27 (19)	C7—C11—H11	118.00
C11—N1—C10—F2	179.11 (18)	C2—C3—C4—F1	180.0 (2)
C11—N1—C10—C9	-1.0 (3)	C2—C3—C4—C5	0.8 (4)
C10—N1—C11—C7	0.1 (3)	F1—C4—C5—C6	179.9 (2)
C6—C1—C2—C3	0.0 (3)	C3—C4—C5—C6	-1.0 (4)
C7—C1—C2—C3	179.0 (2)	C4—C5—C6—C1	0.7 (3)
C2—C1—C6—C5	-0.2 (3)	C1—C7—C8—C9	179.62 (19)
C7—C1—C6—C5	-179.19 (19)	C11—C7—C8—C9	-1.1 (3)
C2—C1—C7—C8	-142.1 (2)	C1—C7—C11—N1	-179.87 (18)
C2—C1—C7—C11	38.7 (3)	C8—C7—C11—N1	0.9 (3)
C6—C1—C7—C8	36.9 (3)	C7—C8—C9—C10	0.4 (3)
C6—C1—C7—C11	-142.3 (2)	C8—C9—C10—F2	-179.37 (19)
C1—C2—C3—C4	-0.3 (4)	C8—C9—C10—N1	0.7 (3)
