Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-(2-Fluoropyridin-5-yl)phenol

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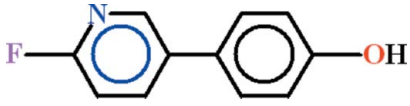
Received 10 June 2012; accepted 11 June 2012

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.051; wR factor = 0.123; data-to-parameter ratio = 13.5.

In the title compound, $C_{11}H_8FNO$, the aromatic rings are oriented at a dihedral angle of 31.93 (6)°. In the crystal, molecules are linked by O—H···N hydrogen bonds, forming $C(9)$ chains propagating along the c-axis direction. There are aromatic π–π stacking interactions between the pyridine rings [centroid–centroid separation = 3.7238 (16) Å].

Related literature

For related structures, see: Adeel *et al.* (2012); Elahi *et al.* (2012).



Experimental

Crystal data

$C_{11}H_8FNO$
M_r = 189.18
Orthorhombic, *Pbca*
a = 12.275 (3) Å
b = 7.4343 (11) Å
c = 19.328 (3) Å
V = 1763.8 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 296 K
0.28 × 0.22 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.975, T_{max} = 0.985
7508 measured reflections
1732 independent reflections
896 reflections with $I > 2\sigma(I)$
R_{int} = 0.064

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.123
S = 1.00
1732 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.82	2.08	2.891 (3)	168

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

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: HB6846).

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supporting information

Acta Cryst. (2012). E**68**, o2124 [https://doi.org/10.1107/S1600536812026499]

4-(2-Fluoropyridin-5-yl)phenol

Fazal Elahi, Muhammad Adeel and M. Nawaz Tahir

S1. Comment

We have reported the crystal structure of 5-(4-fluorophenyl)-2-fluoropyridine (Elahi *et al.*, 2012) and 5-(4-chloro-phenyl)-2-fluoropyridine (Adeel *et al.*, 2012) which are related to (I).

In (I) the 4-hydroxybenzene A (C1–C6/O1) and the 2-fluoropyridine B (C7—C11/N1/F1) are planar with r.m.s. deviations of 0.0222 Å and 0.0154 Å. The dihedral angle between A/B is 31.93 (6)°. There molecules are stabilized in the form of one-dimensional C(9) chains along the *c*-axis due to H-bondings of O—H···N type between hydroxy and pyridine groups (Table 1, Fig. 2). There exist *π*–*π* interaction between *Cg*1···*Cg*1^{i} [i = 1/2 - *x*, -1/2 + *y*, *z*] and *Cg*1···*Cg*1^{ii} [ii = 1/2 - *x*, 1/2 + *y*, *z*] at a distance of 3.7238 (16) Å, where *Cg*1 is the centroid of pyridine ring.

S2. Experimental

To a 6 ml solution of 5-bromo-2-fluoropyridine (0.2 g, 1.136 mmol), 4-hydroxyphenylboronic 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 light brown solid. Yield: 0.191 g, 89%. *M*.p. 350–352 K. Crystallization from a saturated solution of $CHCl_3$ /CH_3OH gave light brown plates.

S3. Refinement

The H-atoms were positioned geometrically (C–H = 0.93, O—H = 0.82 Å) and refined as riding with U_{iso}(H) = xU_{eq}(C, O), where *x* = 1.5 for hydroxy and *x* = 1.2 for other H-atoms.

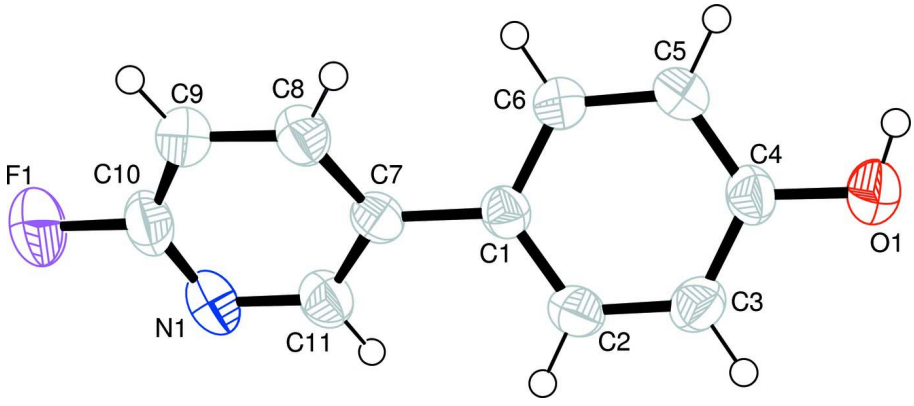

Figure 1

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

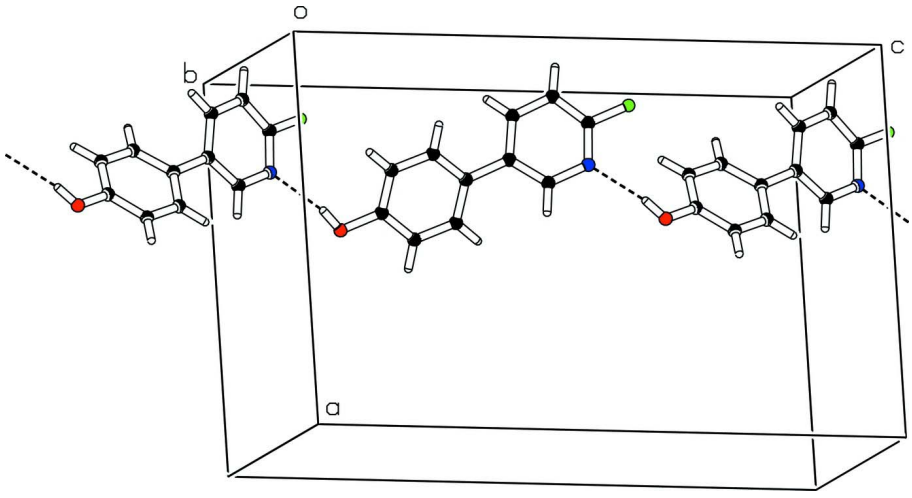

Figure 2

The partial packing, which shows that molecules form C(9) chains extending along [001].

4-(2-Fluoropyridin-5-yl)phenol

Crystal data

$C_{11}H_8FNO$
$M_r = 189.18$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 12.275$ (3) Å
$b = 7.4343$ (11) Å
$c = 19.328$ (3) Å
$V = 1763.8$ (6) Å^3
$Z = 8$
$F(000) = 784$
$D_x = 1.425$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 869 reflections
$\theta = 2.1$–$26.0°$
$\mu = 0.11$ mm^{-1}
$T = 296$ K
Plate, light brown
0.28 × 0.22 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.00 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.975$, $T_{max} = 0.985$
7508 measured reflections
1732 independent reflections
896 reflections with $I > 2\sigma(I)$
$R_{int} = 0.064$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.1°$
$h = -15 \rightarrow 6$
$k = -9 \rightarrow 9$
$l = -17 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.123$
$S = 1.00$
1732 reflections
128 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ 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)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.16138 (14)	0.0574 (2)	0.57218 (6)	0.0807 (7)
O1	0.44529 (15)	0.4234 (3)	0.12632 (8)	0.0611 (8)
N1	0.3071 (2)	0.1137 (3)	0.50603 (9)	0.0532 (9)
C1	0.3319 (2)	0.2565 (3)	0.31870 (11)	0.0361 (9)
C2	0.4308 (2)	0.3444 (3)	0.31099 (12)	0.0414 (9)
C3	0.4687 (2)	0.3971 (3)	0.24670 (12)	0.0439 (10)
C4	0.4071 (2)	0.3622 (3)	0.18829 (12)	0.0416 (9)
C5	0.3108 (2)	0.2682 (3)	0.19463 (11)	0.0449 (10)
C6	0.2736 (2)	0.2170 (3)	0.25895 (10)	0.0419 (9)
C7	0.2856 (2)	0.2081 (3)	0.38699 (11)	0.0367 (9)
C8	0.1738 (2)	0.2085 (3)	0.39711 (12)	0.0462 (10)
C9	0.1293 (2)	0.1575 (3)	0.45939 (12)	0.0520 (11)
C10	0.2008 (3)	0.1116 (3)	0.51007 (12)	0.0524 (10)
C11	0.3492 (2)	0.1610 (3)	0.44353 (11)	0.0470 (10)
H1	0.39877	0.40831	0.09643	0.0916*
H2	0.47273	0.36848	0.34999	0.0497*
H3	0.53530	0.45572	0.24276	0.0527*
H5	0.27072	0.23925	0.15533	0.0540*
H6	0.20815	0.15470	0.26247	0.0503*
H8	0.12817	0.24378	0.36118	0.0555*
H9	0.05436	0.15458	0.46643	0.0624*
H11	0.42453	0.16170	0.43841	0.0565*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0964 (16)	0.1031 (13)	0.0427 (9)	−0.0147 (11)	0.0132 (9)	0.0107 (8)
O1	0.0498 (15)	0.0910 (14)	0.0424 (10)	−0.0135 (11)	0.0072 (9)	0.0057 (10)
N1	0.066 (2)	0.0596 (15)	0.0339 (13)	0.0057 (14)	0.0004 (12)	−0.0012 (10)
C1	0.0395 (18)	0.0352 (13)	0.0335 (14)	0.0013 (12)	0.0020 (12)	−0.0030 (10)
C2	0.0406 (18)	0.0456 (14)	0.0380 (14)	0.0002 (13)	−0.0052 (12)	−0.0044 (10)
C3	0.0363 (18)	0.0471 (16)	0.0484 (16)	−0.0038 (13)	0.0056 (13)	−0.0035 (11)
C4	0.0421 (19)	0.0493 (15)	0.0335 (15)	0.0028 (14)	0.0063 (13)	−0.0012 (11)
C5	0.045 (2)	0.0555 (16)	0.0341 (15)	−0.0048 (14)	−0.0050 (12)	−0.0024 (11)
C6	0.0418 (18)	0.0457 (15)	0.0382 (15)	−0.0071 (13)	0.0006 (13)	−0.0018 (11)
C7	0.0412 (19)	0.0336 (13)	0.0354 (14)	0.0023 (12)	−0.0028 (13)	−0.0028 (10)

C8	0.049 (2)	0.0521 (16)	0.0376 (16)	0.0036 (14)	−0.0005 (14)	0.0011 (11)
C9	0.048 (2)	0.0627 (18)	0.0453 (17)	−0.0060 (15)	0.0049 (15)	−0.0046 (12)
C10	0.069 (2)	0.0544 (17)	0.0339 (17)	−0.0055 (17)	0.0102 (17)	−0.0002 (12)
C11	0.050 (2)	0.0504 (16)	0.0405 (16)	0.0029 (14)	0.0015 (14)	−0.0054 (11)

Geometric parameters (Å, º)

F1—C10	1.356 (3)	C7—C8	1.386 (3)
O1—C4	1.364 (3)	C7—C11	1.388 (3)
O1—H1	0.8200	C8—C9	1.375 (3)
N1—C11	1.360 (3)	C9—C10	1.359 (4)
N1—C10	1.307 (4)	C2—H2	0.9300
C1—C2	1.387 (3)	C3—H3	0.9300
C1—C7	1.481 (3)	C5—H5	0.9300
C1—C6	1.390 (3)	C6—H6	0.9300
C2—C3	1.384 (3)	C8—H8	0.9300
C3—C4	1.383 (3)	C9—H9	0.9300
C4—C5	1.379 (3)	C11—H11	0.9300
C5—C6	1.378 (3)		
C4—O1—H1	109.00	N1—C10—C9	126.8 (2)
C10—N1—C11	115.8 (2)	F1—C10—C9	118.9 (3)
C2—C1—C6	117.5 (2)	N1—C11—C7	123.4 (2)
C6—C1—C7	119.4 (2)	C1—C2—H2	119.00
C2—C1—C7	123.1 (2)	C3—C2—H2	119.00
C1—C2—C3	121.6 (2)	C2—C3—H3	120.00
C2—C3—C4	119.7 (2)	C4—C3—H3	120.00
O1—C4—C5	122.8 (2)	C4—C5—H5	120.00
C3—C4—C5	119.4 (2)	C6—C5—H5	120.00
O1—C4—C3	117.8 (2)	C1—C6—H6	119.00
C4—C5—C6	120.3 (2)	C5—C6—H6	119.00
C1—C6—C5	121.4 (2)	C7—C8—H8	119.00
C1—C7—C8	120.3 (2)	C9—C8—H8	119.00
C1—C7—C11	123.2 (2)	C8—C9—H9	122.00
C8—C7—C11	116.5 (2)	C10—C9—H9	122.00
C7—C8—C9	121.1 (2)	N1—C11—H11	118.00
C8—C9—C10	116.3 (2)	C7—C11—H11	118.00
F1—C10—N1	114.4 (2)		
C11—N1—C10—F1	177.63 (19)	C2—C3—C4—O1	177.2 (2)
C11—N1—C10—C9	−2.5 (4)	C2—C3—C4—C5	−2.8 (3)
C10—N1—C11—C7	1.2 (3)	O1—C4—C5—C6	−176.9 (2)
C6—C1—C2—C3	2.3 (3)	C3—C4—C5—C6	3.1 (3)
C7—C1—C2—C3	−176.1 (2)	C4—C5—C6—C1	−0.7 (4)
C2—C1—C6—C5	−2.0 (3)	C1—C7—C8—C9	177.6 (2)
C7—C1—C6—C5	176.5 (2)	C11—C7—C8—C9	−2.6 (3)
C2—C1—C7—C8	146.8 (2)	C1—C7—C11—N1	−178.9 (2)
C2—C1—C7—C11	−33.1 (3)	C8—C7—C11—N1	1.2 (3)

C6—C1—C7—C8	−31.6 (3)	C7—C8—C9—C10	1.5 (3)
C6—C1—C7—C11	148.5 (2)	C8—C9—C10—F1	−178.9 (2)
C1—C2—C3—C4	0.1 (3)	C8—C9—C10—N1	1.2 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	2.08	2.891 (3)	168

Symmetry code: (i) *x*, −*y*+1/2, *z*−1/2.