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5-(2,3-Dichlorophenyl)-2-fluoropyridine

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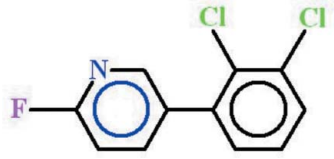
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.028; wR factor = 0.075; data-to-parameter ratio = 13.8.

In the title compound, $C_{11}H_6Cl_2FN$, the dichlorobenzene and the 2-fluoropyridine rings are oriented at a dihedral angle of 47.73 (3)°. In the crystal, pairs of C—H···N interactions link the molecules into dimers with $R_2^2(12)$ motifs. Molecules are arranged in stacks extending along [100] *via* π–π interactions with a centroid–centroid distance of 3.8889 (3) Å.

Related literature

For related structures, see: Adeel *et al.* (2012); Elahi, Adeel & Tahir (2012); Elahi, Adeel, Tahir *et al.* (2012). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{11}H_6Cl_2FN$
M_r = 242.07
Triclinic, $P\overline{1}$
a = 3.8889 (3) Å
b = 11.1006 (11) Å
c = 12.0542 (11) Å
α = 101.526 (5)°
β = 94.930 (4)°
γ = 92.057 (5)°
V = 507.24 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.61 mm^{-1}
T = 296 K
0.34 × 0.18 × 0.16 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.874, T_{max} = 0.898
6978 measured reflections
1874 independent reflections
1625 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.075
S = 1.04
1874 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···N1^{i}	0.93	2.63	3.557 (2)	178

Symmetry code: (i) $-x+1, -y+1, -z$.

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2505).

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supporting information

Acta Cryst. (2012). E**68**, o2180 [https://doi.org/10.1107/S1600536812027833]

5-(2,3-Dichlorophenyl)-2-fluoropyridine

Fazal Elahi, Muhammad Adeel and M. Nawaz Tahir

S1. Comment

We have reported the crystal structure of 5-(4-chlorophenyl)-2-fluoropyridine (Adeel *et al.*, 2012), 4-(2-fluoropyridin-5-yl)phenol (Elahi, Adeel & Tahir, 2012) and 5-(4-fluorophenyl)-2-fluoropyridine (Elahi, Adeel, Tahir *et al.*, 2012)which have common moiety of 2-fluoropyridine as in (I).

In (I) the dichlorobenzene A (C1–C6/CL1/CL2) and the 2-fluoropyridine B (C7—C11/N1/F1) are planar with r.m.s. deviations of 0.0189 Å and 0.0042 Å, respectively. The dihedral angle between A/B is 47.73 (3)°. The molecules are stabilized in the form of dimers with $R_2^2(12)$ ring motif (Bernstein *et al.*, 1995) due to hydrogen bonding of C—H···N type between dichlorophenyl and pyridine groups (Table 1, Fig. 2).

S2. Experimental

To a 6 ml solution of 5-bromo-2-fluoropyridine (0.2 g, 1.136 mmol), 2,3-dichlorophynyl boronic acid (0.260 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 ethyl acetate (3 × 15 ml). The organic layer was evaporated in *vacuo* and the crude product was obtained. Colorless needles of (I) were obtained by the recrystalization of crude product in a saturated $CHCl_3$/CH_3OH (m.p. 350-352 K).

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 aryl H atoms.

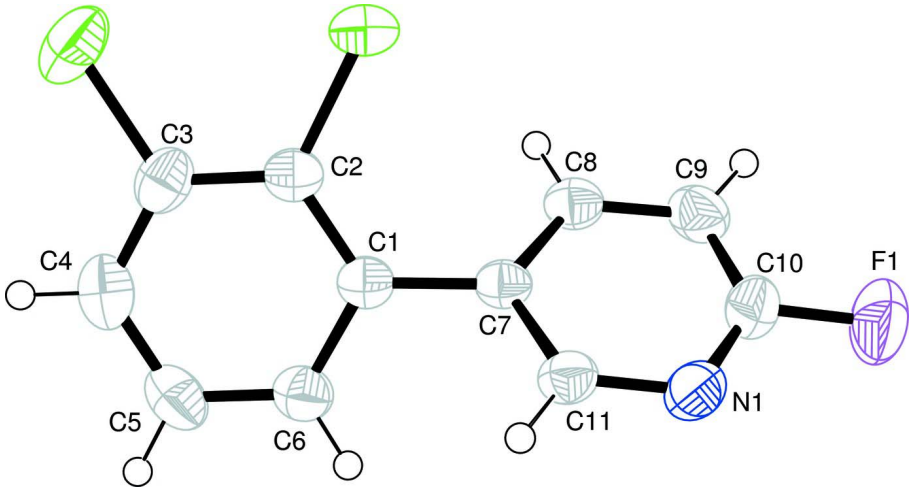

Figure 1

View of the title compound with the atom numbering scheme. Dispalcement ellipsoids are drawn at the 50% probability level. H-atoms are shown by small circles of arbitrary radii.

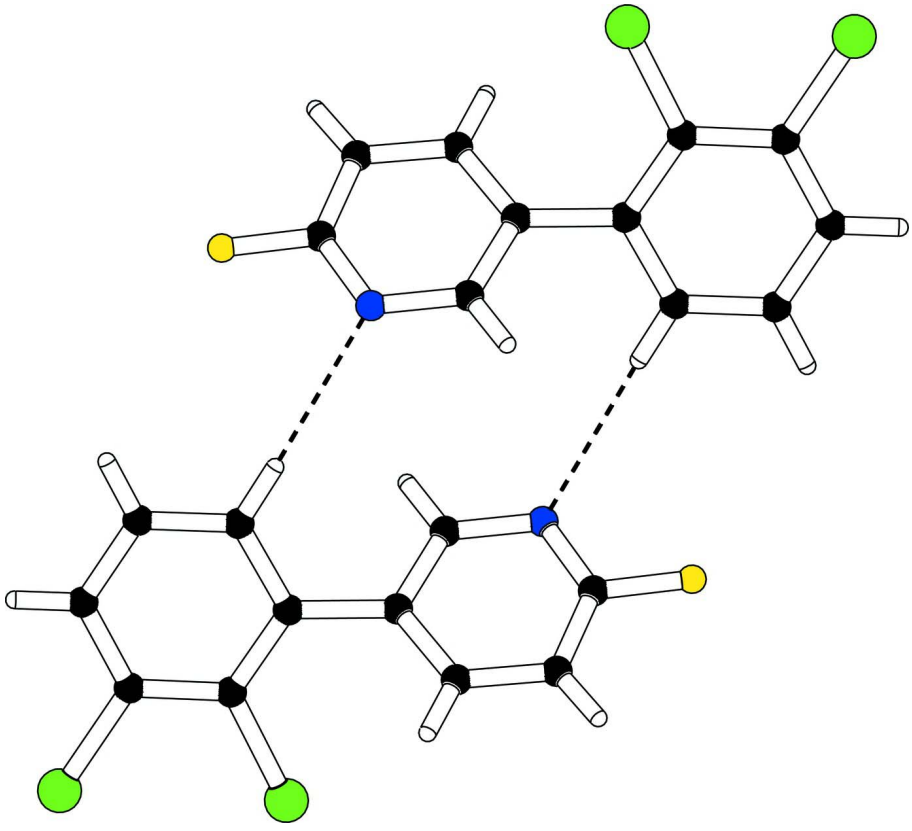

Figure 2

The partial packing (*PLATON*; Spek, 2009) which shows that molecules form dimers via $R_2^2(12)$ motif.

5-(2,3-Dichlorophenyl)-2-fluoropyridine

Crystal data

$C_{11}H_6Cl_2FN$
$M_r = 242.07$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 3.8889$ (3) Å
$b = 11.1006$ (11) Å
$c = 12.0542$ (11) Å
$\alpha = 101.526$ (5)°
$\beta = 94.930$ (4)°
$\gamma = 92.057$ (5)°
$V = 507.24$ (8) Å^3
$Z = 2$
$F(000) = 244$
$D_x = 1.585$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 869 reflections
$\theta = 1.7$–25.5°
$\mu = 0.61$ mm^{-1}
$T = 296$ K
Needle, colorless
0.34 × 0.18 × 0.16 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.10 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.874$, $T_{max} = 0.898$
6978 measured reflections
1874 independent reflections
1625 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 25.5$°, $\theta_{min} = 1.7$°
$h = -4 \rightarrow 4$
$k = -13 \rightarrow 13$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.075$
$S = 1.04$
1874 reflections
136 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
$w = 1/[\sigma^2(F_o^2) + (0.0353P)^2 + 0.1351P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.89637 (11)	0.34986 (4)	0.42850 (3)	0.0469 (2)
Cl2	0.69950 (16)	0.07317 (5)	0.40724 (5)	0.0705 (2)
F1	0.8508 (4)	0.81300 (10)	0.19925 (12)	0.0787 (5)
N1	0.8522 (4)	0.61337 (13)	0.12178 (12)	0.0454 (5)

C1	0.5754 (4)	0.32731 (14)	0.21540 (13)	0.0333 (5)
C2	0.6680 (4)	0.26882 (14)	0.30479 (13)	0.0355 (5)
C3	0.5869 (4)	0.14425 (15)	0.29533 (15)	0.0441 (6)
C4	0.4176 (5)	0.07576 (17)	0.19693 (18)	0.0535 (6)
C5	0.3322 (5)	0.13175 (16)	0.10746 (17)	0.0518 (6)
C6	0.4073 (4)	0.25512 (15)	0.11605 (14)	0.0421 (5)
C7	0.6503 (4)	0.46004 (14)	0.21958 (12)	0.0329 (5)
C8	0.5751 (4)	0.55329 (15)	0.30850 (13)	0.0393 (5)
C9	0.6419 (5)	0.67424 (16)	0.30366 (15)	0.0469 (6)
C10	0.7801 (5)	0.69556 (15)	0.20828 (16)	0.0475 (6)
C11	0.7863 (4)	0.49632 (15)	0.12855 (13)	0.0383 (5)
H4	0.36156	−0.00758	0.19106	0.0642*
H5	0.22187	0.08546	0.04010	0.0621*
H6	0.34500	0.29133	0.05456	0.0505*
H8	0.47957	0.53360	0.37117	0.0472*
H9	0.59579	0.73832	0.36209	0.0562*
H11	0.83512	0.43519	0.06797	0.0460*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0512 (3)	0.0576 (3)	0.0312 (2)	0.0030 (2)	−0.0007 (2)	0.0092 (2)
Cl2	0.0884 (4)	0.0636 (3)	0.0719 (4)	0.0107 (3)	0.0127 (3)	0.0404 (3)
F1	0.1164 (11)	0.0382 (6)	0.0853 (9)	−0.0001 (6)	0.0163 (8)	0.0196 (6)
N1	0.0540 (9)	0.0448 (8)	0.0408 (8)	0.0054 (7)	0.0071 (7)	0.0155 (6)
C1	0.0300 (8)	0.0385 (8)	0.0319 (8)	0.0047 (6)	0.0071 (6)	0.0060 (6)
C2	0.0325 (8)	0.0425 (9)	0.0322 (8)	0.0039 (6)	0.0076 (6)	0.0068 (6)
C3	0.0422 (10)	0.0445 (9)	0.0512 (10)	0.0069 (7)	0.0130 (8)	0.0185 (8)
C4	0.0530 (11)	0.0382 (9)	0.0687 (13)	−0.0011 (8)	0.0091 (9)	0.0089 (9)
C5	0.0497 (11)	0.0452 (10)	0.0524 (11)	−0.0033 (8)	−0.0035 (8)	−0.0045 (8)
C6	0.0422 (9)	0.0444 (9)	0.0383 (9)	0.0049 (7)	0.0011 (7)	0.0058 (7)
C7	0.0309 (8)	0.0383 (8)	0.0294 (8)	0.0051 (6)	0.0019 (6)	0.0064 (6)
C8	0.0409 (9)	0.0446 (9)	0.0323 (8)	0.0049 (7)	0.0062 (7)	0.0062 (7)
C9	0.0555 (11)	0.0409 (9)	0.0407 (10)	0.0093 (8)	0.0031 (8)	−0.0007 (7)
C10	0.0558 (11)	0.0360 (9)	0.0519 (10)	0.0019 (8)	−0.0005 (8)	0.0141 (8)
C11	0.0428 (9)	0.0407 (9)	0.0323 (8)	0.0073 (7)	0.0051 (7)	0.0079 (7)

Geometric parameters (Å, º)

Cl1—C2	1.7323 (16)	C5—C6	1.372 (2)
Cl2—C3	1.7271 (18)	C7—C8	1.392 (2)
F1—C10	1.350 (2)	C7—C11	1.381 (2)
N1—C10	1.299 (2)	C8—C9	1.372 (2)
N1—C11	1.335 (2)	C9—C10	1.368 (3)
C1—C2	1.394 (2)	C4—H4	0.9300
C1—C6	1.396 (2)	C5—H5	0.9300
C1—C7	1.482 (2)	C6—H6	0.9300
C2—C3	1.387 (2)	C8—H8	0.9300

C3—C4	1.374 (3)	C9—H9	0.9300
C4—C5	1.371 (3)	C11—H11	0.9300
C10—N1—C11	115.72 (15)	C8—C9—C10	116.44 (16)
C2—C1—C6	117.42 (15)	F1—C10—N1	114.38 (16)
C2—C1—C7	123.81 (14)	F1—C10—C9	118.82 (16)
C6—C1—C7	118.76 (14)	N1—C10—C9	126.79 (17)
Cl1—C2—C1	120.44 (12)	N1—C11—C7	124.31 (15)
Cl1—C2—C3	118.82 (12)	C3—C4—H4	120.00
C1—C2—C3	120.72 (15)	C5—C4—H4	120.00
Cl2—C3—C2	120.27 (13)	C4—C5—H5	120.00
Cl2—C3—C4	119.16 (14)	C6—C5—H5	120.00
C2—C3—C4	120.57 (16)	C1—C6—H6	119.00
C3—C4—C5	119.21 (18)	C5—C6—H6	119.00
C4—C5—C6	120.85 (18)	C7—C8—H8	120.00
C1—C6—C5	121.20 (16)	C9—C8—H8	120.00
C1—C7—C8	123.79 (14)	C8—C9—H9	122.00
C1—C7—C11	119.39 (14)	C10—C9—H9	122.00
C8—C7—C11	116.74 (15)	N1—C11—H11	118.00
C7—C8—C9	119.99 (15)	C7—C11—H11	118.00
C11—N1—C10—F1	179.73 (16)	Cl1—C2—C3—C4	−177.52 (14)
C11—N1—C10—C9	−0.7 (3)	C1—C2—C3—Cl2	−179.38 (12)
C10—N1—C11—C7	0.0 (2)	C1—C2—C3—C4	0.9 (2)
C6—C1—C2—Cl1	176.78 (12)	Cl2—C3—C4—C5	−179.13 (15)
C6—C1—C2—C3	−1.6 (2)	C2—C3—C4—C5	0.6 (3)
C7—C1—C2—Cl1	−2.2 (2)	C3—C4—C5—C6	−1.4 (3)
C7—C1—C2—C3	179.45 (15)	C4—C5—C6—C1	0.6 (3)
C2—C1—C6—C5	0.9 (2)	C1—C7—C8—C9	−177.67 (16)
C7—C1—C6—C5	179.88 (16)	C11—C7—C8—C9	−1.0 (2)
C2—C1—C7—C8	−49.6 (2)	C1—C7—C11—N1	177.60 (15)
C2—C1—C7—C11	133.83 (17)	C8—C7—C11—N1	0.8 (2)
C6—C1—C7—C8	131.43 (17)	C7—C8—C9—C10	0.5 (3)
C6—C1—C7—C11	−45.1 (2)	C8—C9—C10—F1	−179.97 (19)
Cl1—C2—C3—Cl2	2.22 (19)	C8—C9—C10—N1	0.5 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···N1^{i}	0.93	2.63	3.557 (2)	178

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