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5-(4-Chlorophenyl)-2-fluoropyridine

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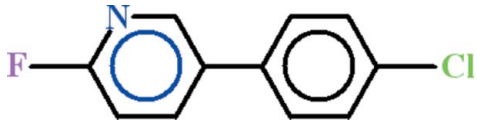
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.032; wR factor = 0.073; data-to-parameter ratio = 15.6.

In the title compound, $C_{11}H_7ClFN$, the chlorobenzene and 2-fluoropyridine rings are oriented at a dihedral angle of 38.83 (5)°. In the crystal, there are no hydrogen-bonding interactions.

Related literature

For a related structure, see: Elahi *et al.* (2012).



Experimental

Crystal data

$C_{11}H_7ClFN$
M_r = 207.63
Orthorhombic, $Pca2_1$
a = 21.1252 (14) Å
b = 3.8763 (3) Å
c = 11.7009 (8) Å
V = 958.16 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 296 K
0.26 × 0.20 × 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
4142 measured reflections
1619 independent reflections
1255 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.073
S = 1.08
1619 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Absolute structure: Flack (1983), 735 Friedel pairs
Flack parameter: −0.09 (8)

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: BQ2365).

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supplementary materials

Acta Cryst. (2012). E**68**, o2043 [doi:10.1107/S1600536812025378]

5-(4-Chlorophenyl)-2-fluoropyridine

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Comment

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

We have reported the crystal structure of 5-(4-fluorophenyl)-2-fluoropyridine previously (Elahi *et al.*, 2012) which is related to (I). In (I) the chlorobenzene A (C1–C6/CL1) and the 2-fluoropyridine B (C7—C11/N1/F1) are planar with r.m.s. deviations of 0.0093 Å and 0.0064 Å. The dihedral angle between A/B is 38.82 (5)°. There does not exist any kind of π-interactions and the molecules must be stabilized due to van Der Wall forces.

Experimental

To a 5 ml solution of 5-bromo-2-fluoropyridine (0.1 g, 0.568 mmol), 4-chlorophenylboronic acid (0.097 g, 0.624 mmol) in dioxane and K_3PO_4 (0.132 g, 0.624 mmol) 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 to the reaction mixture. The aqueous layer was extracted three times with CH_2Cl_2(3 × 15 ml). The organic layer was evaporated *in vacuo* and the title compound (I) was obtained as a colorless crystalline solid. Yield: 0.106 g, 91 %. M.p. 344–347 K. Crystallization from a saturated $CHCl_3$ /CH_3OH solution gave colorless crystals.

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.

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); 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* (Spek, 2009).

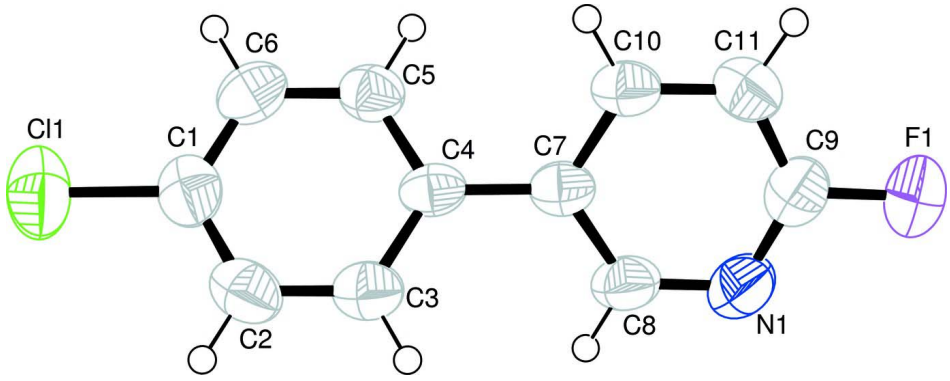

Figure 1

View of the title compound with the atom numbering scheme. The thermal ellipsoids are drawn at the 50% probability level.

5-(4-Chlorophenyl)-2-fluoropyridine

Crystal data

$C_{11}H_7ClFN$
$M_r = 207.63$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 21.1252$ (14) Å
$b = 3.8763$ (3) Å
$c = 11.7009$ (8) Å
$V = 958.16$ (12) Å^3
$Z = 4$
$F(000) = 424$
$D_x = 1.439$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1255 reflections
$\theta = 2.6$–$26.0°$
$\mu = 0.37$ mm^{-1}
$T = 296$ K
Prism, colorless
0.26 × 0.20 × 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 scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.932$, $T_{max} = 0.950$
4142 measured reflections
1619 independent reflections
1255 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.6°$
$h = -18 \rightarrow 26$
$k = -3 \rightarrow 4$
$l = -14 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.073$
$S = 1.08$
1619 reflections
127 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
$w = 1/[\sigma^2(F_o^2) + (0.0344P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.11$ e Å^{-3}
$\Delta\rho_{min} = -0.13$ e Å^{-3}
Absolute structure: Flack (1983), 735 Friedel pairs
Flack parameter: −0.09 (8)

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. 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}
C1	0.25579 (12)	0.5138 (6)	0.1995 (3)	0.0593 (8)
C2	0.24833 (12)	0.3704 (7)	0.3061 (3)	0.0634 (7)
H2	0.2834	0.3347	0.3528	0.076*
C3	0.18888 (12)	0.2798 (7)	0.3435 (2)	0.0571 (7)
H3	0.1840	0.1830	0.4157	0.068*
C4	0.13552 (11)	0.3311 (6)	0.2745 (2)	0.0460 (5)
C5	0.14486 (11)	0.4731 (6)	0.1677 (2)	0.0531 (6)
H5	0.1102	0.5058	0.1199	0.064*
C6	0.20444 (12)	0.5682 (6)	0.1297 (2)	0.0591 (7)
H6	0.2096	0.6673	0.0579	0.071*
C7	0.07137 (11)	0.2343 (6)	0.31377 (19)	0.0464 (6)
C8	0.05152 (13)	0.2866 (7)	0.4246 (2)	0.0607 (7)
H8	0.0804	0.3817	0.4756	0.073*
C9	−0.04479 (14)	0.0724 (8)	0.3900 (3)	0.0646 (8)
C10	0.02695 (11)	0.0942 (6)	0.2397 (2)	0.0521 (6)
H10	0.0374	0.0584	0.1635	0.062*
C11	−0.03221 (12)	0.0085 (7)	0.2783 (3)	0.0595 (7)
H11	−0.0623	−0.0890	0.2301	0.071*
Cl1	0.33061 (3)	0.6376 (2)	0.15406 (9)	0.0880 (3)
F1	−0.10306 (8)	−0.0034 (5)	0.43168 (15)	0.0899 (6)
N1	−0.00621 (11)	0.2107 (6)	0.4643 (2)	0.0696 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0572 (16)	0.0525 (15)	0.068 (2)	0.0040 (12)	0.0070 (13)	−0.0211 (14)
C2	0.0583 (17)	0.0676 (17)	0.064 (2)	0.0100 (14)	−0.0131 (13)	−0.0165 (17)
C3	0.0652 (16)	0.0590 (16)	0.0470 (15)	0.0066 (13)	−0.0051 (12)	−0.0039 (14)
C4	0.0594 (14)	0.0404 (12)	0.0383 (14)	0.0086 (10)	−0.0039 (11)	−0.0043 (11)
C5	0.0569 (13)	0.0544 (14)	0.0479 (16)	0.0071 (11)	−0.0051 (13)	−0.0076 (15)
C6	0.0756 (18)	0.0536 (15)	0.0480 (17)	0.0056 (12)	0.0076 (13)	−0.0061 (13)
C7	0.0550 (14)	0.0421 (13)	0.0423 (16)	0.0082 (11)	−0.0046 (11)	−0.0004 (11)
C8	0.0730 (18)	0.0689 (18)	0.0402 (16)	−0.0056 (14)	−0.0050 (12)	−0.0040 (14)
C9	0.0650 (19)	0.0668 (18)	0.062 (2)	−0.0003 (14)	0.0088 (15)	0.0067 (16)
C10	0.0597 (16)	0.0539 (16)	0.0426 (15)	0.0108 (12)	−0.0054 (12)	−0.0059 (12)
C11	0.0539 (15)	0.0619 (17)	0.063 (2)	0.0036 (13)	−0.0089 (13)	−0.0048 (14)
Cl1	0.0620 (4)	0.0905 (5)	0.1114 (6)	−0.0092 (4)	0.0216 (5)	−0.0273 (6)

F1	0.0695 (10)	0.1191 (15)	0.0811 (12)	−0.0215 (10)	0.0192 (10)	0.0066 (10)
N1	0.0768 (16)	0.0824 (17)	0.0495 (15)	−0.0109 (13)	0.0091 (13)	−0.0003 (13)

Geometric parameters (Å, º)

C1—C2	1.374 (4)	C6—H6	0.9300
C1—C6	1.375 (3)	C7—C8	1.378 (3)
C1—Cl1	1.735 (3)	C7—C10	1.388 (3)
C2—C3	1.376 (4)	C8—N1	1.338 (3)
C2—H2	0.9300	C8—H8	0.9300
C3—C4	1.400 (3)	C9—N1	1.306 (3)
C3—H3	0.9300	C9—F1	1.356 (3)
C4—C5	1.380 (3)	C9—C11	1.357 (4)
C4—C7	1.479 (3)	C10—C11	1.369 (3)
C5—C6	1.385 (3)	C10—H10	0.9300
C5—H5	0.9300	C11—H11	0.9300
C2—C1—C6	120.8 (2)	C5—C6—H6	120.5
C2—C1—Cl1	119.6 (2)	C8—C7—C10	116.1 (2)
C6—C1—Cl1	119.6 (2)	C8—C7—C4	122.2 (2)
C1—C2—C3	119.8 (2)	C10—C7—C4	121.7 (2)
C1—C2—H2	120.1	N1—C8—C7	124.9 (2)
C3—C2—H2	120.1	N1—C8—H8	117.6
C2—C3—C4	121.0 (3)	C7—C8—H8	117.6
C2—C3—H3	119.5	N1—C9—F1	114.6 (3)
C4—C3—H3	119.5	N1—C9—C11	126.4 (3)
C5—C4—C3	117.6 (2)	F1—C9—C11	119.0 (3)
C5—C4—C7	120.9 (2)	C11—C10—C7	120.4 (2)
C3—C4—C7	121.5 (2)	C11—C10—H10	119.8
C4—C5—C6	121.8 (2)	C7—C10—H10	119.8
C4—C5—H5	119.1	C9—C11—C10	116.8 (2)
C6—C5—H5	119.1	C9—C11—H11	121.6
C1—C6—C5	119.0 (3)	C10—C11—H11	121.6
C1—C6—H6	120.5	C9—N1—C8	115.3 (2)
C6—C1—C2—C3	0.0 (4)	C5—C4—C7—C10	37.1 (3)
Cl1—C1—C2—C3	178.4 (2)	C3—C4—C7—C10	−142.3 (2)
C1—C2—C3—C4	0.1 (4)	C10—C7—C8—N1	0.4 (4)
C2—C3—C4—C5	0.5 (4)	C4—C7—C8—N1	178.6 (2)
C2—C3—C4—C7	179.9 (2)	C8—C7—C10—C11	−1.5 (3)
C3—C4—C5—C6	−1.1 (3)	C4—C7—C10—C11	−179.7 (2)
C7—C4—C5—C6	179.5 (2)	N1—C9—C11—C10	0.7 (4)
C2—C1—C6—C5	−0.6 (4)	F1—C9—C11—C10	179.0 (2)
Cl1—C1—C6—C5	−179.00 (17)	C7—C10—C11—C9	1.0 (3)
C4—C5—C6—C1	1.2 (3)	F1—C9—N1—C8	179.9 (2)
C5—C4—C7—C8	−140.9 (3)	C11—C9—N1—C8	−1.7 (4)
C3—C4—C7—C8	39.6 (3)	C7—C8—N1—C9	1.1 (4)