Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-(5-Bromo-2-methoxyphenyl)-2-fluoropyridine

Muhammad Adeel,[a] Fazal Elahi[a] and M. Nawaz Tahir[b]*

[a]Department of Chemistry, Gomal University, Dera Ismail Khan, K.P.K., Pakistan, and [b]Department of Physics, University of Sargodha, Sargodha, Pakistan
Correspondence e-mail: dmntahir_uos@yahoo.com

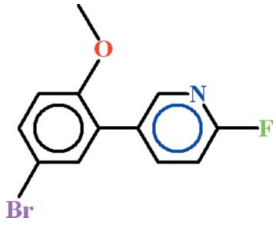
Received 28 July 2012; accepted 2 August 2012

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.035; wR factor = 0.068; data-to-parameter ratio = 13.9.

In the title compound, $C_{12}H_9BrFNO$, the dihedral angle between the aromatic rings is 51.39 (5)°; the C atom of the methoxy group is close to being coplanar with its attached ring (r.m.s. deviation = 0.0172 Å] and is oriented away from the pyridine ring. In the crystal, molecules interact by van der Waals forces.

Related literature

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



Experimental

Crystal data

$C_{12}H_9BrFNO$
M_r = 282.11
Monoclinic, $P2_1/c$
a = 3.9376 (4) Å
b = 20.999 (3) Å
c = 13.2700 (15) Å
β = 95.035 (7)°
V = 1093.0 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.75 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} = 0.674, T_{max} = 0.698
7773 measured reflections
2027 independent reflections
1441 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.068
S = 1.04
2027 reflections
146 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 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 the diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan. MA also acknowledges 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: HB6919).

References

Adeel, M., Elahi, F., Tahir, M. N., Khan, A. & Langer, P. (2012). *Acta Cryst.* E**68**, o2043.
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Elahi, F., Adeel, M. & Tahir, M. N. (2012*a*). *Acta Cryst.* E**68**, o2124.
Elahi, F., Adeel, M. & Tahir, M. N. (2012*b*). *Acta Cryst.* E**68**, o2180.
Elahi, F., Adeel, M., Tahir, M. N., Langer, P. & Ahmad, S. (2012). *Acta Cryst.* E**68**, o2070.
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.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2012). E**68**, o2654 [doi:10.1107/S1600536812034435]

5-(5-Bromo-2-methoxyphenyl)-2-fluoropyridine

Muhammad Adeel, Fazal Elahi 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 *et al.*, 2012*a*), 5-(2,3-dichlorophenyl)-2-fluoropyridine (Elahi *et al.*, 2012*b*) and 2-fluoro-5-(4-fluorophenyl)pyridine (Elahi *et al.*, 2012) which have common moiety of 2-fluoropyridine as in the title compound, (Fig. 1).

In the title compound, the 1-bromo-4-methoxybenzene A (C1–C7/BR1/O1) and the 2-fluoropyridine B (C8—C12/N1/F1) systems are almost planar with r.m.s. deviations of 0.0172 Å and 0.0087 Å, respectively. The dihedral angle between A/B is 51.39 (5)°. There does not exist any kind of H-bonding and the molecules interact by van der Waals forces.

S2. Experimental

To a 6 ml solution of 5-bromo-2-fluoropyridine (0.20 g, 1.13 mmol), 5-bromo-2-methoxyphenylboronic acid (0.314 g, 1.36 mmol) in dioxane and K_3PO_4 (0.361 g, 1.7 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 the crude product was obtained. Colorless needles of (I) were obtained by the recrystalization of crude product in a saturated $CHCl_3/CH_3OH$ solution.

Yield: 0.294 g, 92%. m.p. 345–347 K.

S3. Refinement

The H-atoms were positioned geometrically (C–H = 0.93–0.96 Å) and refined as riding with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for methyl and x = 1.2 for other H-atoms.

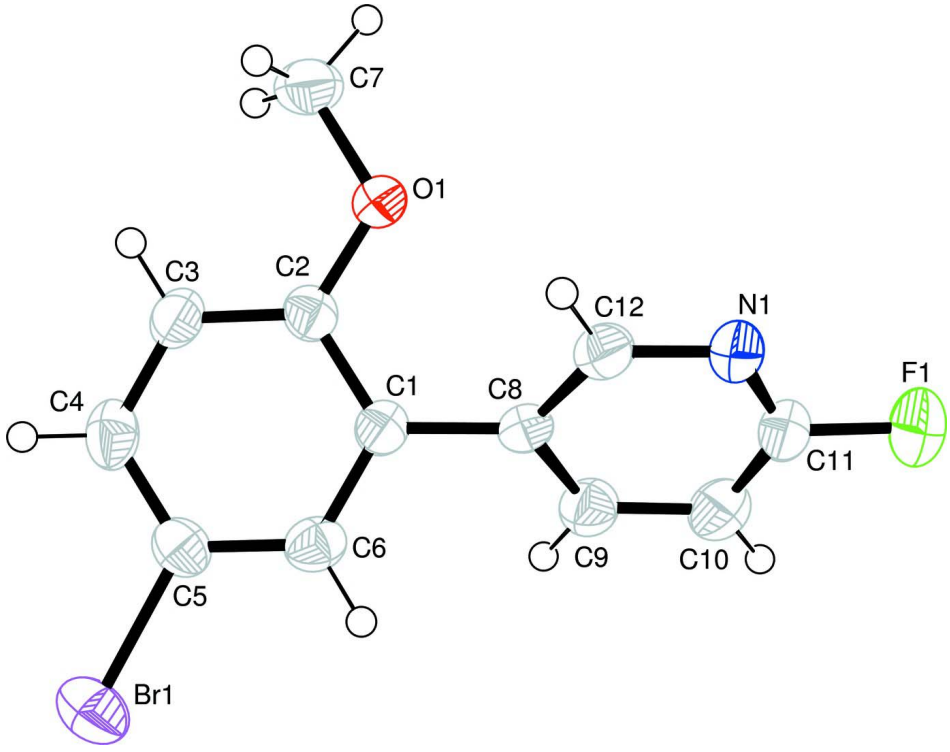


Figure 1

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

5-(5-Bromo-2-methoxyphenyl)-2-fluoropyridine

Crystal data

$C_{12}H_9BrFNO$
$M_r = 282.11$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 3.9376$ (4) Å
$b = 20.999$ (3) Å
$c = 13.2700$ (15) Å
$\beta = 95.035$ (7)°
$V = 1093.0$ (2) Å^3
$Z = 4$

$F(000) = 560$
$D_x = 1.714$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1441 reflections
$\theta = 1.8$–25.5°
$\mu = 3.75$ 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)
$T_{min} = 0.674$, $T_{max} = 0.698$

7773 measured reflections
2027 independent reflections
1441 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 25.5°$, $\theta_{min} = 1.8°$
$h = -4 \rightarrow 4$
$k = -25 \rightarrow 15$
$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.068$
$S = 1.04$
2027 reflections
146 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
$w = 1/[\sigma^2(F_o^2) + (0.027P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ 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}
Br1	0.56028 (8)	0.42649 (2)	0.65535 (3)	0.0533 (1)
F1	0.6238 (6)	0.43194 (10)	−0.01878 (15)	0.0815 (9)
O1	1.0021 (5)	0.25300 (10)	0.32894 (14)	0.0422 (7)
N1	0.5368 (7)	0.35827 (13)	0.0979 (2)	0.0501 (11)
C1	0.7736 (7)	0.35084 (13)	0.3789 (2)	0.0326 (10)
C2	0.9046 (7)	0.29045 (14)	0.4060 (2)	0.0337 (10)
C3	0.9321 (7)	0.27195 (15)	0.5063 (2)	0.0407 (11)
C4	0.8285 (7)	0.31185 (16)	0.5803 (3)	0.0439 (11)
C5	0.7032 (7)	0.37101 (14)	0.5544 (2)	0.0377 (11)
C6	0.6760 (7)	0.39044 (14)	0.4547 (2)	0.0378 (10)
C7	1.1517 (8)	0.19256 (15)	0.3560 (3)	0.0511 (12)
C8	0.7416 (7)	0.37357 (13)	0.2724 (2)	0.0333 (10)
C9	0.8664 (7)	0.43295 (15)	0.2473 (2)	0.0429 (11)
C10	0.8273 (8)	0.45436 (16)	0.1482 (3)	0.0510 (11)
C11	0.6638 (9)	0.41379 (17)	0.0803 (3)	0.0516 (12)
C12	0.5761 (7)	0.33878 (15)	0.1936 (2)	0.0418 (11)
H3	1.02142	0.23212	0.52415	0.0488*
H4	0.84380	0.29866	0.64746	0.0525*
H6	0.59073	0.43076	0.43811	0.0454*
H7A	1.23508	0.17326	0.29741	0.0763*
H7B	0.98311	0.16542	0.38171	0.0763*
H7C	1.33727	0.19847	0.40709	0.0763*
H9	0.97674	0.45841	0.29733	0.0514*
H10	0.90758	0.49388	0.12940	0.0611*
H12	0.48683	0.29927	0.20876	0.0503*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0574 (2)	0.0553 (2)	0.0484 (2)	−0.0061 (2)	0.0108 (2)	−0.0154 (2)
F1	0.138 (2)	0.0654 (14)	0.0405 (13)	0.0176 (14)	0.0042 (12)	0.0153 (12)
O1	0.0590 (13)	0.0327 (12)	0.0339 (13)	0.0100 (11)	−0.0007 (10)	0.0006 (11)
N1	0.0724 (19)	0.0421 (18)	0.0340 (18)	0.0103 (16)	−0.0060 (14)	0.0015 (15)
C1	0.0329 (16)	0.0309 (17)	0.0330 (19)	−0.0033 (14)	−0.0023 (14)	0.0005 (15)
C2	0.0343 (16)	0.0343 (17)	0.0316 (19)	−0.0043 (15)	−0.0022 (14)	−0.0027 (16)
C3	0.0501 (18)	0.0339 (18)	0.037 (2)	−0.0014 (16)	−0.0026 (15)	0.0062 (16)
C4	0.0507 (19)	0.048 (2)	0.0316 (19)	−0.0100 (17)	−0.0040 (15)	0.0046 (17)
C5	0.0379 (17)	0.0410 (19)	0.034 (2)	−0.0041 (15)	0.0014 (14)	−0.0062 (16)
C6	0.0371 (17)	0.0322 (17)	0.043 (2)	−0.0003 (15)	−0.0025 (14)	−0.0026 (17)
C7	0.059 (2)	0.040 (2)	0.053 (2)	0.0107 (17)	−0.0028 (17)	−0.0056 (18)
C8	0.0343 (16)	0.0294 (17)	0.0362 (19)	0.0064 (14)	0.0028 (14)	0.0004 (15)
C9	0.0474 (18)	0.0372 (19)	0.043 (2)	−0.0009 (16)	−0.0016 (15)	−0.0009 (18)
C10	0.065 (2)	0.0376 (19)	0.051 (2)	0.0003 (18)	0.0087 (18)	0.0078 (19)
C11	0.071 (2)	0.050 (2)	0.034 (2)	0.021 (2)	0.0063 (17)	0.0084 (19)
C12	0.0521 (19)	0.0320 (18)	0.040 (2)	0.0030 (16)	−0.0033 (16)	−0.0003 (17)

Geometric parameters (Å, º)

Br1—C5	1.898 (3)	C8—C9	1.391 (4)
F1—C11	1.365 (4)	C8—C12	1.390 (4)
O1—C2	1.371 (3)	C9—C10	1.386 (5)
O1—C7	1.432 (4)	C10—C11	1.360 (5)
N1—C11	1.298 (5)	C3—H3	0.9300
N1—C12	1.330 (4)	C4—H4	0.9300
C1—C2	1.404 (4)	C6—H6	0.9300
C1—C6	1.385 (4)	C7—H7A	0.9600
C1—C8	1.487 (4)	C7—H7B	0.9600
C2—C3	1.382 (4)	C7—H7C	0.9600
C3—C4	1.380 (5)	C9—H9	0.9300
C4—C5	1.369 (4)	C10—H10	0.9300
C5—C6	1.380 (4)	C12—H12	0.9300
C2—O1—C7	117.2 (2)	N1—C11—C10	127.7 (4)
C11—N1—C12	115.7 (3)	N1—C12—C8	124.3 (3)
C2—C1—C6	118.4 (2)	C2—C3—H3	120.00
C2—C1—C8	122.2 (2)	C4—C3—H3	120.00
C6—C1—C8	119.5 (2)	C3—C4—H4	120.00
O1—C2—C1	116.6 (2)	C5—C4—H4	120.00
O1—C2—C3	123.6 (3)	C1—C6—H6	119.00
C1—C2—C3	119.8 (3)	C5—C6—H6	119.00
C2—C3—C4	120.8 (3)	O1—C7—H7A	109.00
C3—C4—C5	119.7 (3)	O1—C7—H7B	109.00
Br1—C5—C4	120.2 (2)	O1—C7—H7C	109.00
Br1—C5—C6	119.5 (2)	H7A—C7—H7B	109.00

C4—C5—C6	120.3 (3)	H7A—C7—H7C	109.00
C1—C6—C5	121.0 (3)	H7B—C7—H7C	109.00
C1—C8—C9	120.9 (2)	C8—C9—H9	120.00
C1—C8—C12	122.8 (2)	C10—C9—H9	120.00
C9—C8—C12	116.3 (2)	C9—C10—H10	122.00
C8—C9—C10	120.4 (3)	C11—C10—H10	122.00
C9—C10—C11	115.6 (3)	N1—C12—H12	118.00
F1—C11—N1	114.2 (3)	C8—C12—H12	118.00
F1—C11—C10	118.1 (3)		

C7—O1—C2—C1	177.0 (2)	O1—C2—C3—C4	−179.8 (3)
C7—O1—C2—C3	−2.4 (4)	C1—C2—C3—C4	0.8 (4)
C12—N1—C11—F1	179.1 (3)	C2—C3—C4—C5	−1.3 (4)
C12—N1—C11—C10	−0.9 (5)	C3—C4—C5—Br1	−179.9 (2)
C11—N1—C12—C8	−0.3 (5)	C3—C4—C5—C6	0.9 (4)
C6—C1—C2—O1	−179.2 (2)	Br1—C5—C6—C1	−179.1 (2)
C6—C1—C2—C3	0.2 (4)	C4—C5—C6—C1	0.1 (4)
C8—C1—C2—O1	−0.1 (4)	C1—C8—C9—C10	−178.3 (3)
C8—C1—C2—C3	179.3 (3)	C12—C8—C9—C10	−0.8 (4)
C2—C1—C6—C5	−0.6 (4)	C1—C8—C12—N1	178.6 (3)
C8—C1—C6—C5	−179.8 (3)	C9—C8—C12—N1	1.1 (4)
C2—C1—C8—C9	−130.1 (3)	C8—C9—C10—C11	−0.2 (4)
C2—C1—C8—C12	52.6 (4)	C9—C10—C11—F1	−178.8 (3)
C6—C1—C8—C9	49.0 (4)	C9—C10—C11—N1	1.2 (5)
C6—C1—C8—C12	−128.3 (3)		