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2-Bromo-5-methylpyridine

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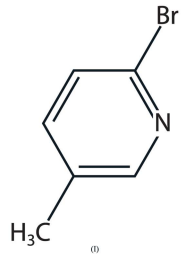
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, C_6H_6BrN, has half of a molecule in the asymmetric unit, as it sits on a crystallographic plane of symmetry. In the crystal, weak C—H···N interactions link the molecules, forming chains along [100]. No π–π interactions are observed.

3D view

Chemical scheme



Structure description

2-Bromopyridine and its derivatives are useful precursors for the formation of bipyridine and terpyridine ligands. Herein, we report the crystal structure of 2-bromo-5-methylpyridine, Fig. 1. The planar molecule lies on a crystallographic plane of symmetry, with a half molecule present in the asymmetric unit. The only intermolecular interactions observed are weak tip-to-tail C3—H3···N1 interactions that form infinite chains along [100]; see Table 1 and Fig. 2. Similar C—H···N interactions have been observed in other 5-substituted 2-bromopyridines (Al-Far & Ali, 2009; Bhasin *et al.*, 2005; Ho & Pascal, 2014), though not in the closely related 2,6-dibromo-3,5-dimethylpyridine (Pugh, 2006). There are no other significant intermolecular interactions present.

Synthesis and crystallization

A commercial sample (Aldrich) of 2-bromo-5-methylpyridine was used for the crystallization. A sample suitable for single-crystal X-ray analysis was grown from the slow evaporation of an ethanol/water solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

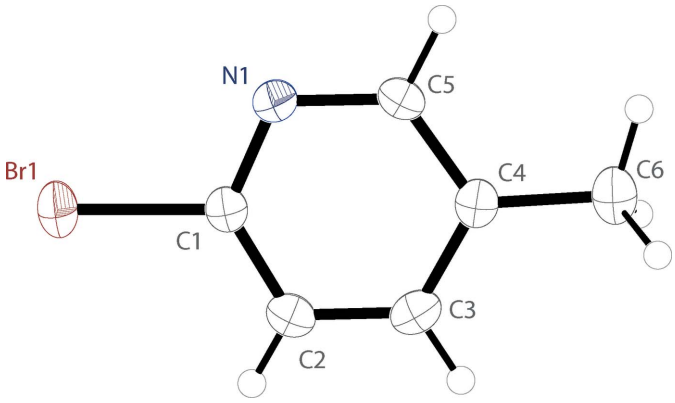


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radius.

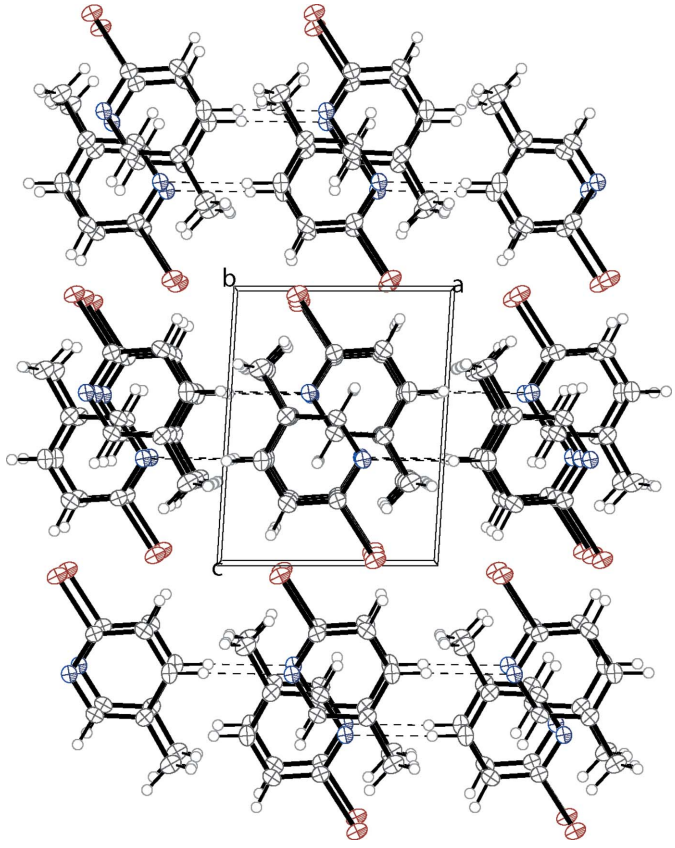


Figure 2
A view along the *b* axis of the crystal packing of the title compound.

Acknowledgements

We greatly acknowledge support from the National Science Foundation (grant No. CHE-1429086).

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···N1^{i}	0.95	2.46	3.409 (5)	179

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

Table 2
Experimental details.

Crystal data	
Chemical formula	C_6H_6BrN
M_r	172.02
Crystal system, space group	Monoclinic, $P2_1/m$
Temperature (K)	120
a, b, c (Å)	6.1889 (18), 6.614 (2), 7.835 (2)
β (°)	93.503 (9)
V (Å^3)	320.12 (17)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	6.31
Crystal size (mm)	0.19 × 0.12 × 0.1
Data collection	
Diffractometer	Bruker D8 Venture CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.208, 0.259
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4211, 639, 586
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.603
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.023, 0.060, 1.10
No. of reflections	639
No. of parameters	53
No. of restraints	7
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.53, −0.50

Computer programs: *APEX2* (Bruker, 2014), *SAINT* (Bruker, 2014), *SHELXS97* (Sheldrick, 2008), *olex2.refine* (Bourhis *et al.*, 2015), *SHELXL2014* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009), *publCIF* (Westrip, 2010).

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full crystallographic data

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Crystal data

C_6H_6BrN
M_r = 172.02
Monoclinic, $P2_1/m$
a = 6.1889 (18) Å
b = 6.614 (2) Å
c = 7.835 (2) Å
β = 93.503 (9)°
V = 320.12 (17) Å^3
Z = 2
$F(000)$ = 167.5322
D_x = 1.785 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2547 reflections
θ = 3.3–25.4°
μ = 6.31 mm^{-1}
T = 120 K
Block, colourless
0.19 × 0.12 × 0.1 mm

Data collection

Bruker D8 Venture CMOS diffractometer
TRIUMPH monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)
T_{min} = 0.208, T_{max} = 0.259
4211 measured reflections
639 independent reflections
586 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.4°, θ_{min} = 3.3°
h = −6→7
k = −7→7
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.060
S = 1.10
639 reflections
53 parameters
7 restraints
8 constraints
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2 + 0.1977P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.28961 (6)	0.25	0.03206 (4)	0.03579 (17)
N1	0.3705 (5)	0.25	0.3819 (4)	0.0249 (6)
C1	0.4724 (6)	0.25	0.2391 (4)	0.0241 (7)
C2	0.6941 (6)	0.25	0.2276 (5)	0.0292 (8)
H2	0.7573 (6)	0.25	0.1201 (5)	0.0350 (9)*
C3	0.8195 (6)	0.25	0.3790 (5)	0.0276 (8)

H3	0.9729 (6)	0.25	0.3775 (5)	0.0331 (9)*
C4	0.7211 (6)	0.25	0.5348 (5)	0.0240 (7)
C5	0.4962 (6)	0.25	0.5274 (4)	0.0252 (7)
H5	0.4270 (6)	0.25	0.6323 (4)	0.0303 (9)*
C6	0.8515 (7)	0.25	0.7021 (5)	0.0341 (9)
H6a	0.751 (5)	0.25	0.794 (3)	0.0409 (11)*
H6b	0.944 (4)	0.130 (3)	0.714 (3)	0.0409 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0341 (3)	0.0495 (3)	0.0228 (2)	−0.000000	−0.00615 (15)	0.000000
N1	0.0209 (16)	0.0293 (15)	0.0245 (15)	−0.000000	0.0022 (12)	0.000000
C1	0.0244 (19)	0.0262 (18)	0.0215 (16)	−0.000000	−0.0001 (13)	0.000000
C2	0.028 (2)	0.036 (2)	0.0236 (18)	−0.000000	0.0062 (14)	0.000000
C3	0.0206 (18)	0.0278 (18)	0.0345 (19)	−0.000000	0.0030 (14)	0.000000
C4	0.0262 (19)	0.0198 (16)	0.0257 (18)	−0.000000	−0.0020 (13)	0.000000
C5	0.0269 (19)	0.0286 (18)	0.0207 (17)	−0.000000	0.0057 (14)	0.000000
C6	0.036 (2)	0.038 (2)	0.028 (2)	−0.000000	−0.0056 (16)	0.000000

Geometric parameters (Å, º)

Br1—C1	1.920 (4)	C3—C4	1.397 (5)
N1—C1	1.317 (5)	C4—C5	1.390 (5)
N1—C5	1.340 (5)	C4—C6	1.496 (5)
C1—C2	1.380 (5)	C5—H5	0.9500
C2—H2	0.9500	C6—H6a	0.979 (5)
C2—C3	1.378 (5)	C6—H6b^{i}	0.979 (5)
C3—H3	0.9500	C6—H6b	0.979 (5)
C5—N1—C1	116.1 (3)	C6—C4—C3	121.6 (3)
N1—C1—Br1	115.5 (3)	C6—C4—C5	121.5 (3)
C2—C1—Br1	118.8 (3)	C4—C5—N1	124.3 (3)
C2—C1—N1	125.8 (3)	H5—C5—N1	117.85 (19)
H2—C2—C1	121.5 (2)	H5—C5—C4	117.8 (2)
C3—C2—C1	117.0 (3)	H6a—C6—C4	108 (2)
C3—C2—H2	121.5 (2)	H6b—C6—C4	111.3 (17)
H3—C3—C2	120.0 (2)	H6b^{i}—C6—C4	111.3 (17)
C4—C3—C2	120.0 (3)	H6b—C6—H6a	109.1 (5)
C4—C3—H3	120.0 (2)	H6b^{i}—C6—H6a	109.1 (5)
C5—C4—C3	116.9 (3)	H6b^{i}—C6—H6b	108 (3)

Symmetry code: (i) x, $-y+1/2$, z.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

C3—H3···N1^{ii}	0.95	2.46	3.409 (5)	179

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