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N-(6-Bromopyridin-2-yl)pyridin-2-amine

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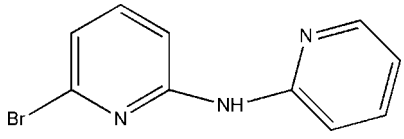
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.032; wR factor = 0.086; data-to-parameter ratio = 13.6.

In the title compound, $C_{10}H_8BrN_3$, the dihedral angle between the pyridine ring planes is 6.10 (15)°. In the crystal structure, the molecules are linked by N—H···N hydrogen bonds, leading to chains.

Related literature

For background, see: Xu *et al.* (2004).



Experimental

Crystal data

$C_{10}H_8BrN_3$
M_r = 250.10
Monoclinic, $C2/c$
a = 22.177 (7) Å
b = 7.551 (2) Å
c = 12.293 (4) Å
β = 109.299 (4)°
V = 1942.9 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 4.19 mm^{-1}
T = 298 (2) K
0.29 × 0.25 × 0.19 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.376, T_{max} = 0.503
(expected range = 0.337–0.451)
5705 measured reflections
1723 independent reflections
1403 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.087
S = 1.06
1723 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···N1^{i}	0.86	2.21	3.052 (3)	168

Symmetry code: (i) $-x+1, y, -z+\frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2598).

References

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supplementary materials

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N-(6-Bromopyridin-2-yl)pyridin-2-amine

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Comment

Here we report the structure of the title compound, (I), which arose as an unexpected product from attempts to prepare a coordination polymer containing zinc(II) ions and *N*-(6-bromopyridin-2-yl)pyridin-2-amine (tpdaH_2Br) (Xu *et al.*, 2004).

The dihedral angle between the pyridine ring planes is 6.10 (15)°. (Fig. 1). In the crystal, molecules are linked by N—H···N hydrogen bonds (Table 1) to result in infinite chains.

Experimental

$ZnSO_4$ (0.016 g, 0.01 mmol), tpdaH_2Br (0.022 g, 0.011 mmol) and NaOH (0.0012 g, 0.003 mmol), were refluxed in acetonitrile for six hours with stirring. The resultant liquor was filtered to give a clear solution which was infiltrated by diethyl ether in a closed vessel. After two weeks, colourless blocks of (I) were recovered.

Refinement

The H atoms were placed in calculated positions (C—H = 0.93 Å, N—H = 0.86 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(carrier).

Figures

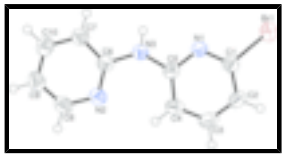

Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids for the non-hydrogen atoms.

N-(6-Bromopyridin-2-yl)pyridin-2-amine

Crystal data

$C_{10}H_8BrN_3$	F_{000} = 992
M_r = 250.10	D_x = 1.710 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 1723 reflections
a = 22.177 (7) Å	θ = 2.0–25.2°
b = 7.551 (2) Å	μ = 4.19 mm^{-1}
c = 12.293 (4) Å	*T* = 298 (2) K
β = 109.299 (4)°	Block, colourless

V = 1942.9 (10) Å^3
Z = 8
0.29 × 0.25 × 0.19 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
Detector resolution: 0 pixels mm^{-1}
T = 298(2) K
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)
T_{min} = 0.376, T_{max} = 0.503
5705 measured reflections
1723 independent reflections
1403 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
θ_{max} = 25.2º
θ_{min} = 2.0º
h = −26→26
k = −8→9
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.087
S = 1.06
1723 reflections
127 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}
Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.348533 (14)	0.03734 (6)	0.56958 (3)	0.06353 (18)
C1	0.41493 (12)	0.1357 (4)	0.5224 (2)	0.0404 (6)

C2	0.41213 (13)	0.1193 (4)	0.4089 (2)	0.0450 (7)
H2	0.3782	0.0637	0.3537	0.054*
C3	0.46233 (13)	0.1898 (4)	0.3832 (2)	0.0475 (7)
H3	0.4623	0.1853	0.3076	0.057*
C4	0.51341 (13)	0.2679 (4)	0.4666 (2)	0.0431 (7)
H4	0.5476	0.3156	0.4485	0.052*
C5	0.51153 (11)	0.2723 (4)	0.5782 (2)	0.0367 (6)
C6	0.61548 (12)	0.4275 (4)	0.6853 (2)	0.0381 (6)
C7	0.64667 (14)	0.5036 (4)	0.7932 (2)	0.0449 (7)
H7	0.6301	0.4932	0.8533	0.054*
C8	0.69133 (15)	0.5299 (4)	0.6151 (3)	0.0526 (8)
H8	0.7069	0.5397	0.5538	0.063*
C9	0.72529 (13)	0.6080 (5)	0.7165 (3)	0.0525 (8)
H9	0.7629	0.6692	0.7241	0.063*
C10	0.70248 (13)	0.5941 (5)	0.8077 (3)	0.0510 (8)
H10	0.7247	0.6455	0.8784	0.061*
N1	0.46154 (9)	0.2106 (3)	0.60504 (16)	0.0381 (5)
N2	0.63662 (11)	0.4391 (3)	0.5976 (2)	0.0465 (6)
N3	0.55897 (10)	0.3372 (3)	0.67403 (17)	0.0438 (6)
H3A	0.5523	0.3185	0.7382	0.053*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0490 (2)	0.0850 (3)	0.0585 (3)	−0.02186 (15)	0.02024 (17)	−0.00919 (16)
C1	0.0378 (13)	0.0412 (18)	0.0436 (15)	0.0047 (12)	0.0153 (12)	0.0020 (12)
C2	0.0442 (15)	0.0518 (19)	0.0350 (14)	0.0043 (13)	0.0077 (12)	−0.0079 (13)
C3	0.0497 (16)	0.062 (2)	0.0308 (13)	0.0095 (14)	0.0126 (12)	−0.0004 (13)
C4	0.0457 (14)	0.0493 (19)	0.0388 (14)	0.0059 (12)	0.0200 (13)	0.0036 (13)
C5	0.0344 (13)	0.0395 (16)	0.0353 (13)	0.0053 (11)	0.0103 (11)	0.0022 (12)
C6	0.0332 (13)	0.0424 (18)	0.0376 (14)	0.0059 (11)	0.0103 (11)	0.0052 (12)
C7	0.0426 (15)	0.053 (2)	0.0386 (15)	0.0000 (12)	0.0128 (13)	0.0025 (13)
C8	0.0430 (16)	0.070 (2)	0.0493 (17)	−0.0016 (14)	0.0218 (14)	0.0038 (16)
C9	0.0371 (14)	0.058 (2)	0.0602 (19)	−0.0044 (14)	0.0131 (14)	0.0058 (16)
C10	0.0442 (16)	0.056 (2)	0.0454 (16)	−0.0016 (14)	0.0054 (13)	−0.0014 (14)
N1	0.0370 (11)	0.0448 (14)	0.0325 (11)	0.0009 (10)	0.0113 (9)	−0.0016 (10)
N2	0.0411 (13)	0.0582 (19)	0.0439 (13)	−0.0025 (11)	0.0189 (11)	−0.0007 (11)
N3	0.0394 (11)	0.0616 (18)	0.0312 (11)	−0.0077 (11)	0.0126 (10)	0.0019 (10)

Geometric parameters (Å, °)

Br1—C1	1.903 (3)	C6—N3	1.392 (3)
C1—N1	1.314 (3)	C6—C7	1.401 (4)
C1—C2	1.381 (4)	C7—C10	1.373 (4)
C2—C3	1.362 (4)	C7—H7	0.9300
C2—H2	0.9300	C8—N2	1.348 (4)
C3—C4	1.384 (4)	C8—C9	1.359 (5)
C3—H3	0.9300	C8—H8	0.9300
C4—C5	1.387 (4)	C9—C10	1.378 (4)

C4—H4	0.9300	C9—H9	0.9300
C5—N1	1.340 (3)	C10—H10	0.9300
C5—N3	1.384 (3)	N3—H3A	0.8600
C6—N2	1.313 (4)		
N1—C1—C2	125.5 (3)	C10—C7—C6	117.9 (3)
N1—C1—Br1	115.00 (19)	C10—C7—H7	121.0
C2—C1—Br1	119.5 (2)	C6—C7—H7	121.0
C3—C2—C1	115.6 (3)	N2—C8—C9	124.3 (3)
C3—C2—H2	122.2	N2—C8—H8	117.8
C1—C2—H2	122.2	C9—C8—H8	117.8
C2—C3—C4	121.8 (3)	C8—C9—C10	118.1 (3)
C2—C3—H3	119.1	C8—C9—H9	120.9
C4—C3—H3	119.1	C10—C9—H9	120.9
C3—C4—C5	117.3 (3)	C7—C10—C9	119.4 (3)
C3—C4—H4	121.4	C7—C10—H10	120.3
C5—C4—H4	121.4	C9—C10—H10	120.3
N1—C5—N3	111.8 (2)	C1—N1—C5	117.6 (2)
N1—C5—C4	122.2 (2)	C6—N2—C8	116.7 (2)
N3—C5—C4	126.0 (2)	C5—N3—C6	131.6 (2)
N2—C6—N3	120.3 (2)	C5—N3—H3A	114.2
N2—C6—C7	123.5 (3)	C6—N3—H3A	114.2
N3—C6—C7	116.2 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···N1^{i}	0.86	2.21	3.052 (3)	168

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2.

Fig. 1