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3,5-Dibromo-6-methylpyridin-2-amine

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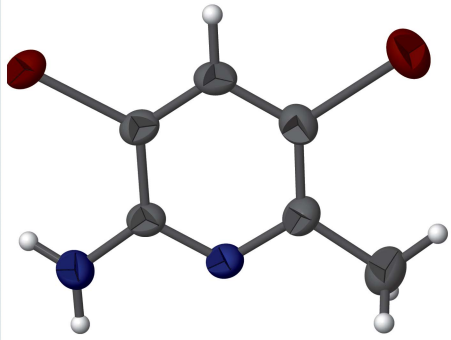
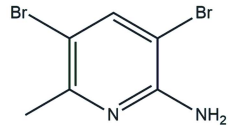
Structural data: full structural data are available from iucrdata.iucr.org

The title molecule, $C_6H_6Br_2N_2$, is almost planar (r.m.s. deviation for the non-H atoms = 0.012 Å). In the crystal, inversion dimers linked by pairs of N—H···N hydrogen bonds generate $R_2^2(8)$ loops.

3D view



Chemical scheme



Structure description

Halogenated organic compounds are known to exhibit diverse biological activities showing anticancer (Nussbaumer *et al.*, 2011), antiviral (De Clercq, 2013), anti-tuberculosis (Beena & Rawat, 2013), anti-malarial (Biamonte *et al.*, 2013), antifungal and anti-diabetic (Hector, 2005) properties. As part of our studies in this area, the crystal structure of the commercially available title compound was determined.

The molecule is almost planar (Fig. 1) with the r.m.s. deviation for the non-H atoms being 0.012 Å. An intramolecular N—H···Br interaction occurs. In the crystal, inversion dimers linked by pairs of N2—H2···N1 hydrogen bonds generate $R_2^2(8)$ loops (Fig. 2, Table 1). The crystal structure does not feature any other interactions, and thus, the supramolecular architecture displayed is zero dimensional.

Synthesis and crystallization

The title compound was purchased from Avra Synthesis Pvt. Ltd, India, and was used as such. Colourless blocks were grown by recrystallization from methanol solution at room temperature.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1···Br1	0.87 (5)	2.68 (5)	3.128 (4)	114 (4)
N2—H2···N1^{i}	0.88 (4)	2.19 (4)	3.070 (6)	173 (3)

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

Refinement

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

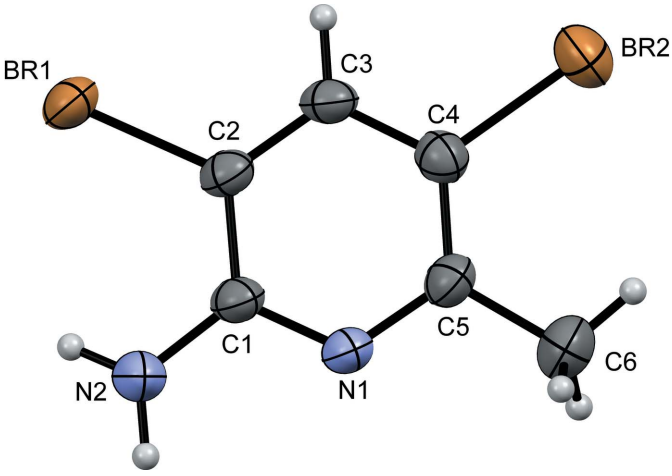


Figure 1
A view of the molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level.

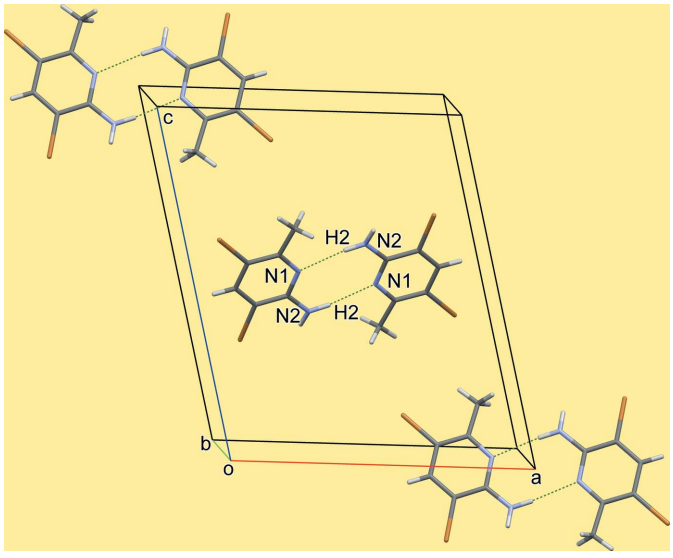


Figure 2
Crystal packing of the title compound, displaying N—H···N hydrogen-bonded $R_2^2(8)$ loops.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_6Br_2N_2$
M_r	265.95
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	13.1047 (16), 4.0310 (4), 15.7631 (18)
β (°)	105.720 (4)
V (Å^3)	801.54 (16)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	10.04
Crystal size (mm)	0.26 × 0.22 × 0.20
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.085, 0.134
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10577, 1670, 1461
R_{int}	0.050
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.631
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.108, 1.09
No. of reflections	1670
No. of parameters	101
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.03, −0.86

Computer programs: *APEX2*, *SAINT-Plus* and *XPREP* (Bruker, 2009), *SHELXT2016* (Sheldrick, 2015a), *SHELXL2016* (Sheldrick, 2015b) and *Mercury* (Macrae *et al.*, 2008).

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full crystallographic data

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Crystal data

$C_6H_6Br_2N_2$
M_r = 265.95
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 13.1047 (16) Å
b = 4.0310 (4) Å
c = 15.7631 (18) Å
β = 105.720 (4)°
V = 801.54 (16) Å^3
Z = 4
$F(000)$ = 504
Prism
D_x = 2.204 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 133 reflections
θ = 2.4–26.7°
μ = 10.04 mm^{-1}
T = 296 K
Block, colourless
0.26 × 0.22 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.085, T_{max} = 0.134
10577 measured reflections
1670 independent reflections
1461 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 26.7°, θ_{min} = 2.4°
h = −16→16
k = −5→4
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.108
S = 1.09
1670 reflections
101 parameters
2 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0701P)^2 + 0.463P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.03 e Å^{-3}
$\Delta\rho_{min}$ = −0.86 e Å^{-3}
Extinction correction: SHELXL2016 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.064 (4)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3237 (3)	0.5000 (10)	0.4445 (2)	0.0352 (8)
C2	0.2125 (3)	0.5194 (10)	0.4153 (2)	0.0343 (8)
C3	0.1522 (3)	0.3994 (10)	0.4668 (2)	0.0360 (8)
H3	0.078637	0.410750	0.448303	0.043*
C4	0.2038 (3)	0.2597 (9)	0.5477 (3)	0.0366 (9)
C5	0.3126 (3)	0.2404 (10)	0.5746 (3)	0.0377 (9)
C6	0.3748 (4)	0.0910 (15)	0.6593 (3)	0.0566 (12)
H6A	0.417884	−0.086130	0.647437	0.085*
H6B	0.327119	0.005584	0.690749	0.085*
H6C	0.419361	0.257416	0.694366	0.085*
N1	0.3710 (3)	0.3633 (9)	0.5226 (2)	0.0385 (8)
N2	0.3883 (3)	0.6093 (13)	0.3955 (3)	0.0517 (10)
BR1	0.14692 (3)	0.70991 (12)	0.30385 (3)	0.0436 (2)
BR2	0.11914 (4)	0.10117 (13)	0.61976 (3)	0.0544 (3)
H1	0.359 (4)	0.736 (12)	0.351 (3)	0.056 (16)*
H2	0.458 (3)	0.609 (15)	0.415 (3)	0.063 (16)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.026 (2)	0.046 (2)	0.0313 (18)	−0.0019 (16)	0.0032 (15)	−0.0038 (16)
C2	0.029 (2)	0.040 (2)	0.0304 (18)	0.0003 (16)	0.0019 (15)	−0.0044 (15)
C3	0.0243 (19)	0.044 (2)	0.038 (2)	−0.0019 (15)	0.0046 (16)	−0.0047 (17)
C4	0.037 (2)	0.040 (2)	0.035 (2)	−0.0040 (16)	0.0123 (17)	−0.0031 (15)
C5	0.036 (2)	0.045 (2)	0.0288 (19)	0.0000 (16)	0.0029 (16)	−0.0006 (15)
C6	0.052 (3)	0.074 (3)	0.040 (2)	−0.001 (2)	0.004 (2)	0.011 (2)
N1	0.0260 (17)	0.056 (2)	0.0308 (16)	−0.0020 (15)	0.0031 (13)	0.0018 (15)
N2	0.032 (2)	0.085 (3)	0.037 (2)	−0.0064 (19)	0.0073 (17)	0.0091 (19)
BR1	0.0351 (3)	0.0561 (3)	0.0337 (3)	0.00406 (17)	−0.00072 (19)	0.00301 (17)
BR2	0.0524 (4)	0.0647 (4)	0.0525 (3)	−0.0082 (2)	0.0248 (2)	0.0056 (2)

Geometric parameters (Å, º)

C1—N1	1.338 (5)	C4—BR2	1.900 (4)
C1—N2	1.364 (5)	C5—N1	1.358 (5)
C1—C2	1.407 (5)	C5—C6	1.491 (6)
C2—C3	1.366 (6)	C6—H6A	0.9600
C2—BR1	1.896 (4)	C6—H6B	0.9600
C3—C4	1.390 (6)	C6—H6C	0.9600
C3—H3	0.9300	N2—H1	0.87 (3)
C4—C5	1.375 (6)	N2—H2	0.88 (3)
N1—C1—N2	116.7 (4)	N1—C5—C6	115.3 (4)
N1—C1—C2	120.3 (3)	C4—C5—C6	124.6 (4)
N2—C1—C2	123.0 (4)	C5—C6—H6A	109.5

C3—C2—C1	120.1 (3)	C5—C6—H6B	109.5
C3—C2—BR1	120.3 (3)	H6A—C6—H6B	109.5
C1—C2—BR1	119.7 (3)	C5—C6—H6C	109.5
C2—C3—C4	118.2 (4)	H6A—C6—H6C	109.5
C2—C3—H3	120.9	H6B—C6—H6C	109.5
C4—C3—H3	120.9	C1—N1—C5	120.6 (3)
C5—C4—C3	120.7 (4)	C1—N2—H1	117 (4)
C5—C4—BR2	121.5 (3)	C1—N2—H2	123 (4)
C3—C4—BR2	117.8 (3)	H1—N2—H2	118 (5)
N1—C5—C4	120.1 (4)		

N1—C1—C2—C3	0.2 (6)	C3—C4—C5—N1	1.1 (6)
N2—C1—C2—C3	178.7 (4)	BR2—C4—C5—N1	−178.4 (3)
N1—C1—C2—BR1	−179.4 (3)	C3—C4—C5—C6	−179.1 (4)
N2—C1—C2—BR1	−0.8 (6)	BR2—C4—C5—C6	1.4 (6)
C1—C2—C3—C4	0.0 (6)	N2—C1—N1—C5	−178.3 (4)
BR1—C2—C3—C4	179.5 (3)	C2—C1—N1—C5	0.3 (6)
C2—C3—C4—C5	−0.6 (6)	C4—C5—N1—C1	−0.9 (6)
C2—C3—C4—BR2	178.9 (3)	C6—C5—N1—C1	179.3 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1···Br1	0.87 (5)	2.68 (5)	3.128 (4)	114 (4)
N2—H2···N1^{i}	0.88 (4)	2.19 (4)	3.070 (6)	173 (3)

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