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2,5-Dibromopyridine

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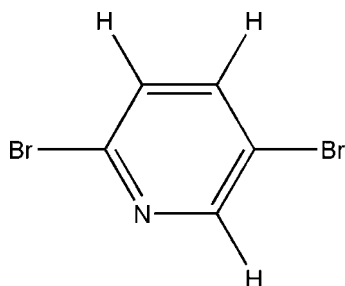
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Key indicators: single-crystal X-ray study; $T = 90$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.021; wR factor = 0.054; data-to-parameter ratio = 20.3.

In the title compound, $\text{C}_5\text{H}_3\text{Br}_2\text{N}$, $\text{C}-\text{H}\cdots\text{N}$ hydrogen-bonding interactions and $\text{Br}\cdots\text{Br}$ interactions [3.9418 (3) and 3.8986 (3) Å] connect the molecules into planar sheets stacked perpendicular to the b axis. In addition, pyridyl-pyridyl intersheet $\pi-\pi$ stacking interactions [centroid-centroid distance = 4.12 (1) Å] result in a three-dimensional network.

Related literature

For hydrogen bonding, see: Desiraju (1997). For related structures, see: Al-Far & Ali (2007, 2008); Ali & Al-Far (2008); Ali *et al.* (2008*a,b*). For bond-length data, see: Allen *et al.* (1987). For theoretical analysis, see: Awwadi *et al.* (2006, 2007).



Experimental

Crystal data

$\text{C}_5\text{H}_3\text{Br}_2\text{N}$
 $M_r = 236.90$

Orthorhombic, $Pnma$
 $a = 6.1063$ (4) Å

$b = 6.5442$ (4) Å
 $c = 15.8196$ (9) Å
 $V = 632.17$ (7) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 12.71$ mm⁻¹
 $T = 90$ K
 $0.46 \times 0.21 \times 0.14$ mm

Data collection

Bruker SMART APEX
diffractometer
Absorption correction: numerical
(*SADABS*; Bruker, 2004)
 $T_{\min} = 0.053$, $T_{\max} = 0.170$

8997 measured reflections
996 independent reflections
887 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.021$
 $wR(F^2) = 0.054$
 $S = 1.05$
996 reflections

49 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.68$ e Å⁻³
 $\Delta\rho_{\min} = -0.77$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C4}-\text{H4A}\cdots\text{N1}^i$	0.95	2.38	3.323 (3)	175

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

Data collection: *SMART* (Bruker, 2006); cell refinement: *SAINT-Plus* (Bruker, 2006); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *XP* (Bruker, 2004) and *SHELXTL*; software used to prepare material for publication: *XCIF* (Bruker, 2004) and *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2146).

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supplementary materials

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2,5-Dibromopyridine

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Comment

Non-covalent interactions play an important role in organizing structural units in both natural and artificial systems (Desiraju, 1997). The interactions governing the crystal organization are expected to affect the packing and specific properties of solids. Intermolecular interactions are the essence of supramolecular chemistry, and the field of crystal supramolecularity seeks to understand intermolecular interactions by analyses of crystal packing. We are presently interested in the synthesis and the structural aspects of halo-metal anion salts containing different organic cations (Al-Far & Ali 2007, 2008; Ali *et al.* 2008*a, b*; Ali & Al-Far 2008). The title compound, (I), arose accidentally when attempting to crystallize CdBr_4^{2-} with 2,5-dibromopyridinium cation. The compound had not been reported previously, thus, the structure of (I) has been characterized crystallographically and is presented here.

The bond distances and angles within the molecule of (I) (Fig. 1) are normal (Allen *et al.*, 1987). There is a non-classical hydrogen bonding interaction of the type C—H \cdots N in the crystal structure which links molecules into one-dimensional chains (Fig. 2) parallel to the *a*-axis. The strength of the hydrogen bonds is represented by relatively short D \cdots A distance and D—H \cdots A angle (H \cdots A = 2.38 Å, D—H \cdots A 175°, Table 1). The resulting chains are further connected through Br \cdots Br interactions in a zig zag arrangement to form sheets in the *ac* plane (Fig. 2); the Br \cdots Br separation being 3.9418 (3) and 3.8986 (3) Å. The sheets are stacked along the *b*-axis with pyridyl \cdots pyridyl $\pi\cdots\pi$ stacking intermolecular interactions with distance between the centroids of the rings being 4.12 (1) Å. It is noteworthy that structural and theoretical results (Awwadi *et al.*, 2006; Awwadi *et al.*, 2007), show the significance of Br \cdots Br bonding synthons in influencing structures of crystalline materials and in use as potential building blocks in crystal engineering *via* supramolecular synthesis.

Experimental

The title compound crystallized during a reaction aiming to crystallize the anion $[\text{CuBr}_4]^{2-}$ with 2,5-dibromopyridinium cation. Colorless diamond like crystals of the title compound were obtained from an ethanolic solution of the reaction which involved a sequential addition to excess 2,5-dibromopyridine (2.25 mmole) in ethanol of CdCl_2 (1 mmole) and 60% HBr (1 ml) in ethanol.

Refinement

Hydrogen atoms were positioned geometrically, with C—H = 0.95 Å, and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

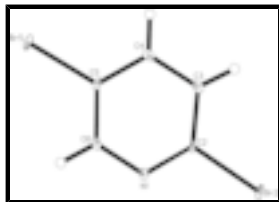


Fig. 1. A molecular drawing of (I) shown with 50% probability ellipsoids.

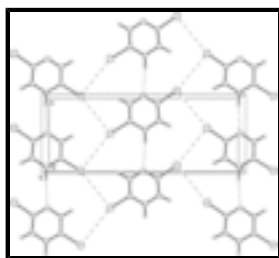


Fig. 2. Packing diagram of (I) down the *b*-axis. Hydrogen bonding and Br...Br interactions are shown as dashed lines.

2,5-dibromopyridine

Crystal data

$C_5H_3Br_2N$

$M_r = 236.90$

Orthorhombic, *Pnma*

Hall symbol: -P 2ac 2n

$a = 6.1063$ (4) Å

$b = 6.5442$ (4) Å

$c = 15.8196$ (9) Å

$V = 632.17$ (7) Å³

$Z = 4$

$F_{000} = 440$

$D_x = 2.489$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 5485 reflections

$\theta = 2.6$ – 30.0°

$\mu = 12.71$ mm⁻¹

$T = 90$ K

Diamond, colourless

$0.46 \times 0.21 \times 0.14$ mm

Data collection

Bruker SMART APEX
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 8.3 pixels mm⁻¹

$T = 90$ K

ω scans

Absorption correction: numerical
(SADABS; Bruker, 2004)

$T_{\min} = 0.053$, $T_{\max} = 0.170$

8997 measured reflections

996 independent reflections

887 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\text{max}} = 30.0^\circ$

$\theta_{\text{min}} = 3.6^\circ$

$h = -8 \rightarrow 8$

$k = -9 \rightarrow 9$

$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.021$	H-atom parameters constrained
$wR(F^2) = 0.054$	$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2 + 0.1337P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
996 reflections	$(\Delta/\sigma)_{\max} < 0.001$
49 parameters	$\Delta\rho_{\max} = 0.68 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.77 \text{ e } \text{\AA}^{-3}$
	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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br2	0.41023 (4)	0.7500	0.171199 (12)	0.01101 (9)
N1	0.4781 (3)	0.7500	-0.00105 (12)	0.0077 (4)
Br5	0.98268 (4)	0.7500	-0.173378 (13)	0.01214 (9)
C2	0.5860 (4)	0.7500	0.07141 (12)	0.0063 (4)
C3	0.8124 (3)	0.7500	0.07962 (13)	0.0089 (4)
H3A	0.8808	0.7500	0.1336	0.011*
C4	0.9342 (4)	0.7500	0.00590 (14)	0.0088 (4)
H4A	1.0897	0.7500	0.0077	0.011*
C5	0.8236 (4)	0.7500	-0.07079 (12)	0.0074 (4)
C6	0.5958 (4)	0.7500	-0.07196 (12)	0.0083 (4)
H6A	0.5221	0.7500	-0.1248	0.010*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br2	0.01285 (15)	0.01709 (15)	0.00310 (12)	0.000	0.00345 (7)	0.000
N1	0.0081 (9)	0.0110 (9)	0.0041 (8)	0.000	0.0000 (6)	0.000
Br5	0.01335 (15)	0.01839 (15)	0.00466 (13)	0.000	0.00480 (7)	0.000

supplementary materials

C2	0.0095 (11)	0.0078 (10)	0.0015 (8)	0.000	0.0012 (7)	0.000
C3	0.0087 (10)	0.0114 (10)	0.0066 (9)	0.000	-0.0024 (8)	0.000
C4	0.0067 (9)	0.0114 (10)	0.0084 (10)	0.000	-0.0018 (8)	0.000
C5	0.0088 (10)	0.0096 (10)	0.0040 (9)	0.000	0.0026 (7)	0.000
C6	0.0100 (11)	0.0100 (11)	0.0048 (9)	0.000	-0.0019 (7)	0.000

Geometric parameters (Å, °)

Br2—C2	1.909 (2)	C3—H3A	0.9500
N1—C2	1.322 (3)	C4—C5	1.389 (3)
N1—C6	1.332 (3)	C4—H4A	0.9500
Br5—C5	1.891 (2)	C5—C6	1.391 (3)
C2—C3	1.389 (3)	C6—H6A	0.9500
C3—C4	1.383 (3)		
C2—N1—C6	117.43 (19)	C3—C4—H4A	120.8
N1—C2—C3	125.27 (19)	C5—C4—H4A	120.8
N1—C2—Br2	115.88 (16)	C4—C5—C6	119.87 (19)
C3—C2—Br2	118.85 (15)	C4—C5—Br5	119.98 (17)
C4—C3—C2	117.15 (19)	C6—C5—Br5	120.15 (16)
C4—C3—H3A	121.4	N1—C6—C5	121.91 (19)
C2—C3—H3A	121.4	N1—C6—H6A	119.0
C3—C4—C5	118.38 (19)	C5—C6—H6A	119.0
C6—N1—C2—C3	0.0	C3—C4—C5—C6	0.0
C6—N1—C2—Br2	180.0	C3—C4—C5—Br5	180.0
N1—C2—C3—C4	0.0	C2—N1—C6—C5	0.0
Br2—C2—C3—C4	180.0	C4—C5—C6—N1	0.0
C2—C3—C4—C5	0.0	Br5—C5—C6—N1	180.0

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C4—H4A \cdots N1 ⁱ	0.95	2.38	3.323 (3)	175

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

Fig. 1

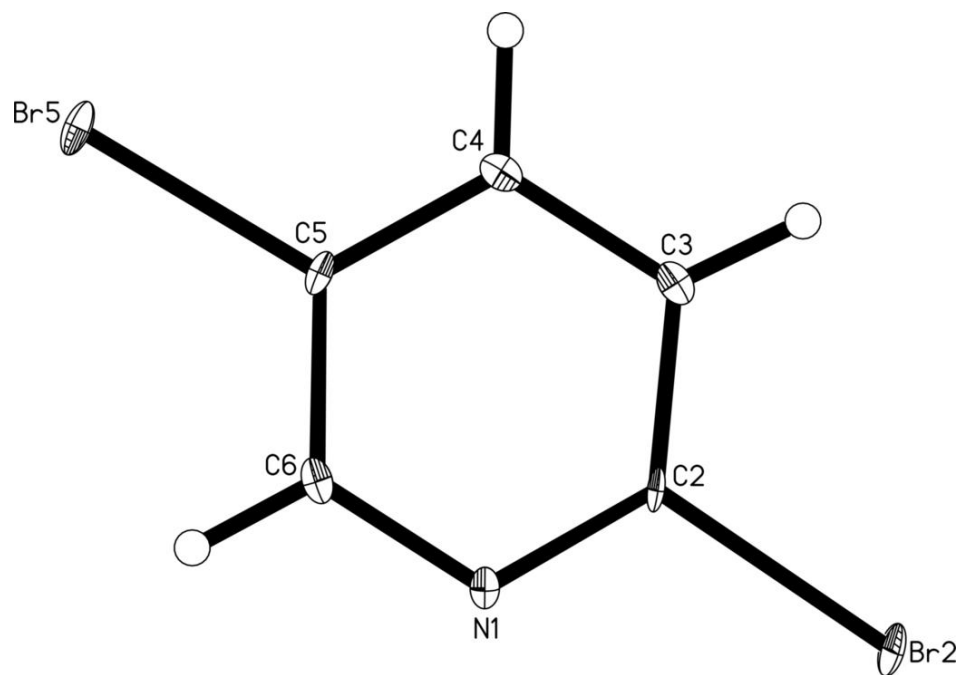


Fig. 2

