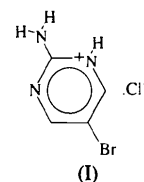


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The bond lengths and angles within the ring (Fig. 1) are, in general, comparable to those of the non-brominated species (Furberg & Groggaard, 1980). The C4—C5—C6 angle is somewhat larger than that of the non-brominated species, and the N3—C4—C5 and C5—C6—N1 angles are correspondingly smaller (all by about 1°). A slight shortening of both the C5—C6 and C4—N3 bonds (0.01–0.02 Å) is observed in comparison with the free base (Watton, Low, Tollin & Howie, 1988).

*Acta Cryst.* (1996). **C52**, 1843–1844

## 2-Amino-5-bromopyrimidinium Chloride

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(Received 7 September 1995; accepted 12 December 1995)

### Abstract

The title compound,  $C_4H_5BrN_3^+.Cl^-$ , crystallized from water as flat plates. The structure is held together by extensive hydrogen bonding between the chloride ions and both the amino and pyrimidinium H atoms. In addition, the pyrimidinium ions are linked *via* hydrogen bonding of one of the amino H atoms and the non-protonated ring N atoms. The molecules packs as sheets, with the sheets at a distance of 3.3 Å from one another.

### Comment

We are interested in the packing of halometallate anions with protonated organic bases, especially aminopyridines and aminopyrimidines. The interactions between the protonated organic molecules, such as  $\pi$  stacking or hydrogen bonding, may make substantial contributions to the formation of the crystal lattice. We have recently begun preparing compounds using 2-amino-5-bromopyrimidine and were therefore interested in what kind of interactions we might expect between the organic groups. Accordingly, we have determined the structure of 2-amino-5-bromopyrimidine as its hydrochloride salt, (I). The structure of 2-amino-pyrimidine has been reported previously (Furberg, Groggaard & Smedsrud, 1979), as well as its hydrochloride hemihydrate (Furberg & Groggaard, 1980). The structure of 2-amino-5-bromopyrimidine has been reported as the free base (Watton, Low, Tollin & Howie, 1988).

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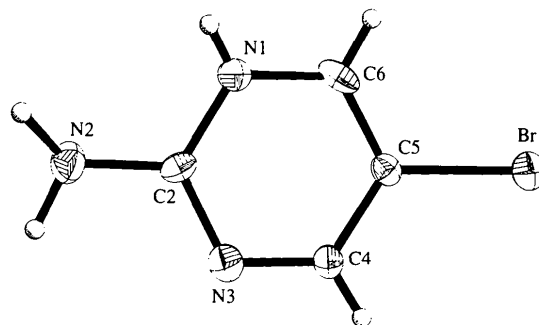


Fig. 1. The molecular structure of 2-amino-5-bromopyrimidinium chloride showing 50% probability ellipsoids.

A slight lengthening of the N2—C2 bond (*ca* 0.02 Å) is also observed. A significant structural difference appears in the packing of the 5-bromo derivative compared with the parent molecule as a result of the large Br atom and the loss of the solvent water molecule. 2-Amino-5-bromopyrimidine packs in sheets (Fig. 2), with an average separation of 3.3 Å. Within the sheets,

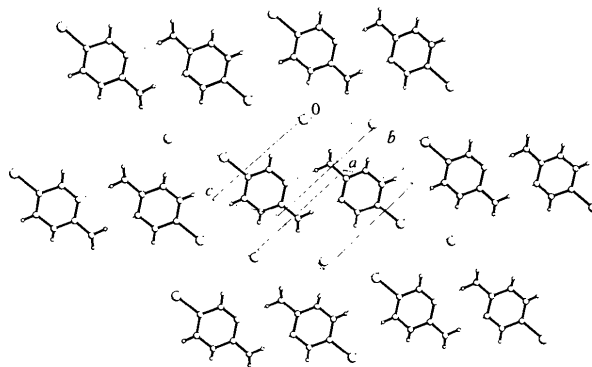


Fig. 2. Packing diagram viewed perpendicular to the planes of the pyrimidinium rings.

the aminopyrimidine rings hydrogen bond in a head-to-tail fashion with an N2—H···N3' distance of 3.0 Å. The chloride ions are hydrogen bonded to both the amino N atom (Cl···H—N2 3.2 Å) and the protonated ring N atom (Cl···H—N1 3.0 Å). Short Cl···Br distances are also observed (3.6–4.0 Å). The largest peak in the final difference density map (1.21 e Å<sup>-3</sup>) lies 0.78 Å from the chloride ion and the largest hole (−1.02 e Å<sup>-3</sup>) lies 1.18 Å from the same ion.

## Experimental

Crystals of 2-amino-5-bromopyrimidinium chloride were grown by slow evaporation of an aqueous solution of the free base containing one equivalent of HCl.

### Crystal data

C<sub>4</sub>H<sub>5</sub>BrN<sub>3</sub><sup>+</sup>.Cl<sup>-</sup>

*M<sub>r</sub>* = 210.47

Triclinic

*P*1̄

*a* = 5.894 (2) Å

*b* = 7.234 (3) Å

*c* = 8.307 (3) Å

α = 90.68 (3)°

β = 102.81 (3)°

γ = 103.45 (3)°

*V* = 335.1 (2) Å<sup>3</sup>

*Z* = 2

*D<sub>x</sub>* = 2.086 Mg m<sup>-3</sup>

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 16

reflections

θ = 5.07–12.22°

μ = 6.437 mm<sup>-1</sup>

*T* = 158 (2) K

Plate

0.20 × 0.20 × 0.07 mm

Pale yellow

### Data collection

Siemens *P4* diffractometer

ω scans

Absorption correction:

refined from Δ*F*

(*SHELXS86*; Sheldrick, 1990*b*)

*T<sub>min</sub>* = 0.292, *T<sub>max</sub>* =

0.626

1288 measured reflections

1160 independent reflections

847 observed reflections

[*I* > 2σ(*I*)]

*R<sub>int</sub>* = 0.065

θ<sub>max</sub> = 24.99°

*h* = −6 → 0

*k* = −8 → 8

*l* = −9 → 9

3 standard reflections

monitored every 97

reflections

intensity decay: 14.7%

### Refinement

Refinement on *F*<sup>2</sup>

*R*(*F*) = 0.063

*wR*(*F*<sup>2</sup>) = 0.318

*S* = 1.05

1149 reflections

97 parameters

Only coordinates of H atoms

refined

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0514*P*)<sup>2</sup>

+ 7.2909*P*]

where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3

(Δ/σ)<sub>max</sub> = −0.006

Δρ<sub>max</sub> = 1.21 e Å<sup>-3</sup>

Δρ<sub>min</sub> = −1.02 e Å<sup>-3</sup>

Extinction correction: none

Atomic scattering factors

from *International Tables*

for *Crystallography* (1992,

Vol. C, Tables 4.2.6.8 and

6.1.1.4)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å<sup>2</sup>)

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U<sub>eq</sub></i>
Br	0.3136 (2)	0.0096 (2)	0.2871 (2)	0.0247 (4)
Cl	−0.8076 (5)	−0.2901 (4)	−0.1365 (3)	0.0168 (6)
N1	−0.3807 (18)	−0.2832 (13)	0.1425 (12)	0.018 (2)
N2	−0.6476 (18)	−0.4825 (15)	0.2679 (13)	0.025 (2)
N3	−0.2558 (18)	−0.3555 (14)	0.4163 (12)	0.022 (2)
C2	−0.4253 (19)	−0.3732 (15)	0.2757 (14)	0.016 (2)
C4	−0.0438 (21)	−0.2460 (16)	0.4177 (15)	0.017 (2)
C5	0.0094 (19)	−0.1547 (15)	0.2813 (14)	0.017 (2)
C6	−0.1638 (21)	−0.1724 (16)	0.1443 (15)	0.019 (3)

Table 2. Selected geometric parameters (Å, °)

Br—C5	1.897 (11)	N3—C4	1.312 (14)
N1—C2	1.335 (14)	N3—C2	1.341 (14)
N1—C6	1.339 (15)	C4—C5	1.38 (2)
N2—C2	1.351 (14)	C5—C6	1.33 (2)
C2—N1—C6	121.0 (10)	N3—C4—C5	122.7 (11)
C4—N3—C2	117.2 (10)	C6—C5—C4	118.7 (10)
N1—C2—N3	121.5 (10)	C6—C5—Br	118.9 (8)
N1—C2—N2	118.8 (10)	C4—C5—Br	122.2 (9)
N3—C2—N2	119.7 (10)	C5—C6—N1	118.8 (10)

Data collection: *XSCANS* (Siemens, 1994). Cell refinement: *XSCANS*. Data reduction: *SHELXTL-Plus* (Sheldrick, 1990*a*). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990*b*). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *SHELXTL-Plus*. Software used to prepare material for publication: *SHELXTL-Plus*.

The authors are grateful to the New Zealand Lottery Scientific Research Committee for financial support and Professor Ward T. Robinson for many helpful discussions. In addition, MMT is grateful to the Chemistry Department at the University of Canterbury for providing facilities during his sabbatical stay.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: TA1066). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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