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1,2,4-Triazolium bromide

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The crystal structure of the title compound, $C_2H_4N_3^+\cdot Br^-$, consists of cations and anions linked by N—H···Br hydrogen bonds to form chains running along the [20$\bar{1}$] direction.

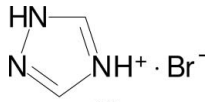
Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(N–C) = 0.003 Å
R factor = 0.016
wR factor = 0.042
Data-to-parameter ratio = 11.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The crystal structure of 1,2,4-triazolium chloride, (II), has previously been reported (Bujak & Zaleski, 2002). The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation and to compare it with that of (II). We report here the crystal structure of (I).



(I)

In (I), the asymmetric unit is composed of one 1,2,4-triazolium cation and one bromide anion (Fig. 1). The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The cations and anions are linked by N—H···Br hydrogen bonds, forming infinite chains running along the [20$\bar{1}$] direction (Fig. 2 and Table 2). In addition, weak C—H···Br interactions are also observed, generating a three-dimensional network.

Salts (I) and (II) are not isostructural. In the crystal structure of (I), adjacent 1,2,4-triazole rings in the chain are twisted with respect to each other with a dihedral angle of 68.91 (8)°, while in the chloride salt, (II), they are coplanar.

Experimental

The title compound, (I), was prepared by reaction of stoichiometric amounts of 1,2,4-triazole and hydrobromic acid (40%). The solution

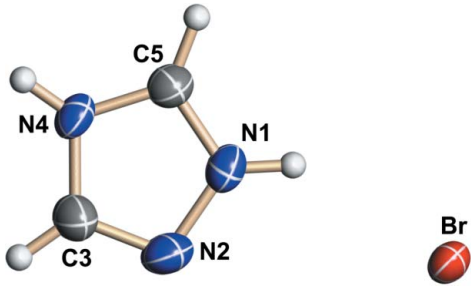


Figure 1
The asymmetric unit of the title compound with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

was allowed to evaporate at room temperature, and crystals formed after a few days.

Crystal data

$C_2H_4N_3^+\cdot Br^-$
M_r = 149.98
Monoclinic, $P2_1/c$
a = 4.9158 (3) Å
b = 10.3166 (6) Å
c = 9.8656 (6) Å
β = 102.411 (7)°
V = 488.64 (5) Å^3
Z = 4
D_x = 2.039 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 8.26 mm^{-1}
T = 291 K
Prism, colorless
0.55 × 0.25 × 0.20 mm

Data collection

Kuma KM-4 CCD diffractometer
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.035, T_{max} = 0.192
3233 measured reflections
851 independent reflections
792 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.042
S = 1.09
851 reflections
72 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0291P)^2 + 0.045P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.0307 (18)

Table 1
Selected geometric parameters (Å, °).

N1—N2	1.361 (3)	N4—C3	1.338 (3)
N1—C5	1.311 (3)	N4—C5	1.321 (3)
N2—C3	1.301 (3)		
N2—N1—C5	111.45 (18)	N2—C3—N4	111.61 (18)
N1—N2—C3	103.29 (17)	N1—C5—N4	106.47 (18)
C3—N4—C5	107.18 (18)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Br	0.89 (3)	2.51 (3)	3.273 (2)	145 (2)
N4—H4···Br^{i}	0.85 (2)	2.49 (2)	3.268 (2)	154 (2)
C3—H3···Br^{ii}	0.90 (2)	2.99 (2)	3.685 (2)	135 (2)
C5—H5···Br^{iii}	0.97 (2)	2.84 (2)	3.515 (2)	127 (2)

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

All H atoms were located in a difference map, and their coordinates and atomic displacement parameters were refined freely (distances are in Table 2).

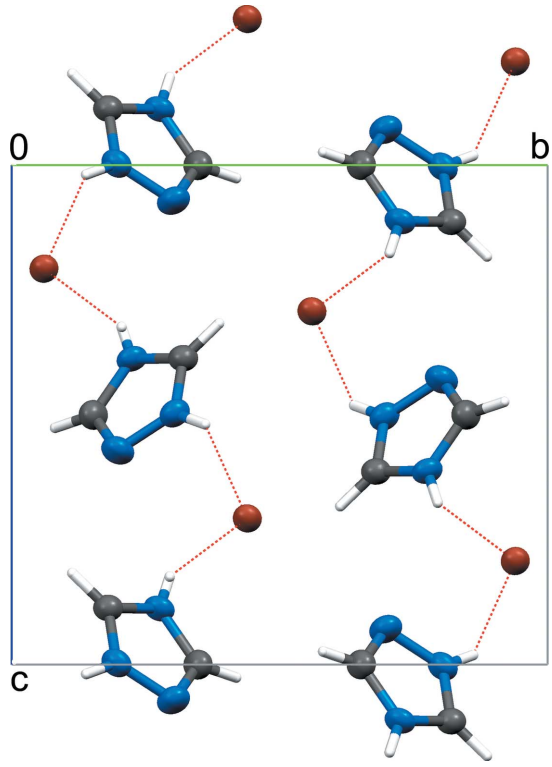


Figure 2
A packing diagram, projected along the *a* axis, showing two chains of hydrogen-bonded (dotted lines) cations and anions running along the [20$\bar{1}$] direction.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2003); molecular graphics: *SHELXTL* and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *PLATON* (Spek, 2003).

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