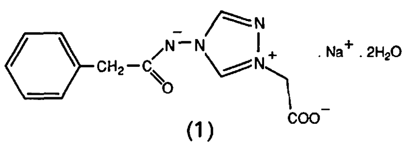
lécules d'eau fixés égaux aux $B_{éq}$ des O auxquels ils sont liés (2,6 Å^2). Facteur R final = 0,049 pour 1704 réflexions non nulles. $wR = 0{,}068$ où $w = 1/(\sigma_F^2 + 0{,}0933F^2)$. Δ/σ des paramètres finals < 0,3. Limites des valeurs $\Delta\rho$ dans la carte de Fourier-différence finale: $-0{,}39$ et $0{,}22$ e Å^{-3}. Les paramètres atomiques finals sont donnés dans le Tableau 1.* La liste des distances et des angles des liaisons se trouve dans le Tableau 2. La Fig. 1 montre une vue en perspective du composé avec la numérotation atomique. La Fig. 2 représente la structure cristalline.

Littérature associée. Le sel sodique du 1-carboxyméthyl-4-phénylacétylimino-1,2,4-triazolium (1) est une molécule originale de synthèse proposée comme un inactivateur potentiel d'enzyme à sérine. Il correspond à la forme déprotonée de la bétaïne du 1-carboxyméthyl-4-phénylacétylamino-1,2,4-triazolium porteur d'une fonction amide à caractère acide exceptionnellement prononcé. La résolution de la structure de cette bétaïne a fait l'objet d'une récente publication (Dupont, Dideberg, Pirotte & Delarge, 1989).



(1)

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* Les listes des facteurs de structures observés et calculés, des positions des atomes H, des paramètres d'agitation thermique anisotrope, des équations des plans moyens et des distances des atomes à ces plans ont été déposées au dépôt d'archives de la British Library Document Supply Centre (Supplementary Publication No. SUP 53703: 8 pp.). On peut en obtenir des copies en s'adressant à: The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, Angleterre.

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Bis(methylammonium) Dibromodichlorocuprate(II)

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Abstract. $2CH_6N^+.CuBr_2Cl_2^{2-}$, $M_r = 358{\cdot}4$, orthorhombic, $Acam$, $a = 7{\cdot}358\,(1)$, $b = 7{\cdot}354\,(1)$, $c = 19{\cdot}209\,(4)$ Å, $V = 1039{\cdot}4\,(4)$ Å^3, $Z = 4$, $T = 295$ K, $D_x = 2{\cdot}29$ Mg m^{-3}, $\lambda(\text{Mo }K\alpha) = 0{\cdot}71069$ Å, $\mu = 102{\cdot}9$ cm^{-1}, $F(000) = 684$, final $R = 0{\cdot}051$ for 556 unique observed $[F \geq 3\sigma(F)]$ reflections. The structure is an antiferro-distortive version of the layer perovskites with two-dimensional networks of corner-sharing octahedra sheathed by the methylammonium ions. The occupancies of the sites for Cl and Br atoms show some statistical disorder, but the dominant occupancies correspond to bridging locations for the Cl atoms and non-bridging locations for the Br atoms. In this space group, the Cl atoms within a layer are constrained to lie in the plane of the Cu atoms, while the Cu—Br bonds are normal to that plane. Thus, the normal puckering associated with the layers in the $(RNH_3)_2MX_4$ systems is apparently absent. However, examination of the thermal ellipsoids of the Cl and Br atoms would indicate the existence of disorder, either static or dynamic, consistent with that puckering.

Experimental. Crystals were grown by slow evaporation of a stoichiometric mixture of CH_3NH_3Cl and $CuBr_2$ in absolute ethanol. A small, square platelet crystal with dimensions of 0·30 × 0·30 × 0·05 mm was selected for data collection on a Syntex $P2_1$ diffractometer, with graphite monochromator, upgraded to Nicolet $P3F$ specifications. Lattice constants from 25 reflections in the range $26 < 2\theta < 30°$. Data were collected with ω scans (1·0°); two check

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reflections monitored every 96 reflections (006 and $\bar{1}\bar{1}7$) show no systematic variations; 1431 total reflections out to $2\theta = 55°$, 622 unique with $R_{\rm int} = 0{\cdot}022$; *hkl* ranges, $0 \le h \le 9$, $0 \le k \le 9$, $0 \le l \le 24$ (Campana, Shepard & Litchman, 1981). Empirical ψ-scan absorption corrections applied assuming an ellipsoidally shaped crystal (Sheldrick, 1985) (relative transmission factors ranged from 0·655 to 0·978). Differential scanning calorimetry (DSC) measurements indicate no phase transition between 103 and 353 K, although a broad region of apparent excess heat capacity appears near 133 K which may be associated with the disappearance of some dynamical disorder in the system.

The structure solution was obtained *via* the *SOLV* routine in the *SHELXTL* (Sheldrick, 1985) crystallographic program package and refinement also used programs from that set. A difference synthesis based on the Cu-, Br- and Cl-atom positions so obtained yielded the C- and N-atom positions. Refinement at this stage yielded thermal parameters for the Cl and Br atoms which were unrealistically small and large respectively. This indicated disorder of the halide atoms between bridging and non-bridging locations. Thus a Cl and Br atom were introduced at both sites, subject to the constraints (1) that the respective site occupancies sum to unity and (2) assignment of isotropic thermal parameters to the atom with the smaller occupancy factors (labelled Br′ and Cl′ in Table 1). The anisotropic thermal parameters for Br, Cl, Cl and N atoms all gave indication of disorder in which the atoms were displaced away from the respective symmetry element. Such displacements would be consistent with the normal puckering of the metal-halide framework found in $(R\mathrm{NH_3})MX_4$ layer perovskites (Willett & Peterson, 1972). However, no attempt was made to model this disorder. H atoms were constrained to ideal positions (C—H and N—H = 0·96 Å) and assigned isotropic thermal parameters of 0·06 (N) and 0·10 (C) Å^2. The final refinement resulted in $R = 0{\cdot}051$ (3σ data set) and 0·055 (all data), and $wR = 0{\cdot}074$ (3σ data set) and 0·076 (all data) and $w = 1/[\sigma^2(F) + g(F)^2]$, with $g = 0{\cdot}003$. The goodness of fit, S, was 1·118, $|\Delta/\sigma|(\max.) = 0{\cdot}003$. The largest peak on the final difference map was 0·6 e Å^{-3} near the Cu atom, while the most negative excursion was $-1{\cdot}3$ e Å^{-3}. An extinction correction was made. Scattering factors were those supplied by the *SHELXTL* program package. Atomic coordinates are listed in Table 1 and bond distances and angles are given in Table 2.*

Table 1. *Atomic coordinates* ($\times 10^4$) *and isotropic thermal parameters* (Å$^2 \times 10^3$) *and site occupancy factors for* $(\mathrm{CH_3NH_3})_2\mathrm{CuBr_2Cl_2}$

The equivalent isotropic U is defined as one third of the trace of the orthoganalized U_{ij} tensor.

	x	y	z	$U_{\rm eq}$	K*
Cu	5000	2500	2500	37 (1)	
Br	5000	2500	1233 (1)	69 (1)	0·76 (1)
Cl′	5000	2500	1225 (6)	22 (3)	0·24 (1)
Cl	7189	309 (3)	2500	43 (1)	0·88 (1)
Br′	7279 (45)	231 (44)	2500	199 (11)	0·12 (1)
N	0	2500	1384 (3)	51 (2)	
C	0	2500	650 (5)	75 (3)	

* Occupancy factor.

Table 2. *Bond lengths* (Å) *and angles* (°) *for* $(\mathrm{CH_3NH_3})_2\mathrm{CuBr_2Cl_2}$

Cu—Br	2·409 (1)	Cu—Cl(*a*)	2·922 (2)
Cu—Cl′	2·425 (1)	Cu—Br′(*a*)	2·835 (34)
Cu—Cl	2·278 (2)	N—C	1·388 (12)
Cu—Br′	2·365 (34)		
Cu—Br′—Cu(*a*)	179·8 (9)	Cu—Cl—Cu(*a*)	179·7 (1)

The symbol *a* denotes atom translated by the symmetry operation $1{\cdot}5 - x, \frac{1}{2} + y, z$.

Related literature. The structure has the same space group as that of $(\mathrm{NH_4})_2\mathrm{CuCl_4}$ (Willett, 1964), and thus corresponds to the highest symmetry observed for the antiferrodistortive layer perovskite series of $A_2\mathrm{Cu}X_4$ salts (Willett, Place & Middleton, 1988). The structure of the corresponding tetrachloride salt is monoclinic, $P2_1/a$ (Pabst, Fuess & Bats, 1987; Steiger, Frikkee, de Jongh & Huiskamp, 1984).

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* Lists of structure factors, anisotropic thermal parameters, data collection parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53722 (9 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.