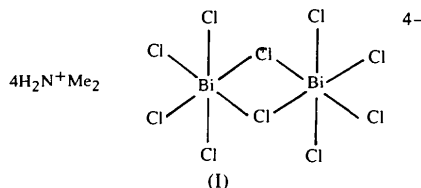


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1993). The coordination sphere of the metal is dominated by a tendency towards hexacoordination. Here we report the structure of the title compound, (I).



Examples of other reported species include  $\text{BiCl}_6^{3-}$  discrete octahedra (Lazarini, 1987),  $\text{Bi}_2\text{Cl}_9^{3-}$  bi-octahedra sharing a face (Aurivillius & Stalhandske, 1978) and  $\text{BiCl}_4^-$  forming infinite chains of edge-sharing octahedra (Blázič & Lazarini, 1985).

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## Dimethylammonium Pentachlorobismuthate(III)

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### Abstract

The structure of  $[\text{NH}_2(\text{CH}_3)_2]_2[\text{BiCl}_5]$  is characterized by hexacoordinate Bi, forming a  $[\text{BiCl}_5]_2^{4-}$  dimer [*i.e.* di- $\mu$ -chloro-bis(tetrachlorobismuth)] with the geometry of two slightly distorted octahedra sharing one edge. The two bridging Cl atoms are connected to the Bi atom by long bonds [2.906 (3) and 2.922 (3) Å]. The other Bi—Cl distances are shorter [2.566 (3)–2.741 (3) Å] and are characteristic of 'free' Cl atoms. The dimethylammonium groups are connected *via* hydrogen bonds to the Cl atoms. The  $\text{NH} \cdots \text{Cl}$  bonds vary in length from 3.22 (1) to 3.280 (9) Å.

### Comment

The present work is part of a study of the interaction between organic cations and heavy-metal halogenides (Jarraya, Ben Salah, Daoud, Rothammel & Burszlauff,

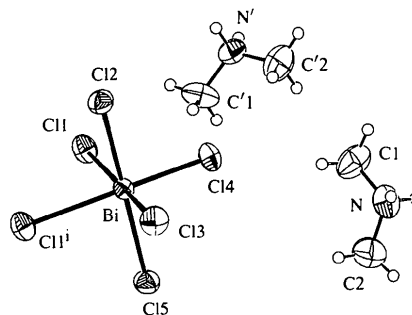


Fig. 1. View of the molecule showing the labelling of the non-H atoms. Displacement ellipsoids are shown at the 50% probability level and H atoms are drawn as small circles of arbitrary radii.

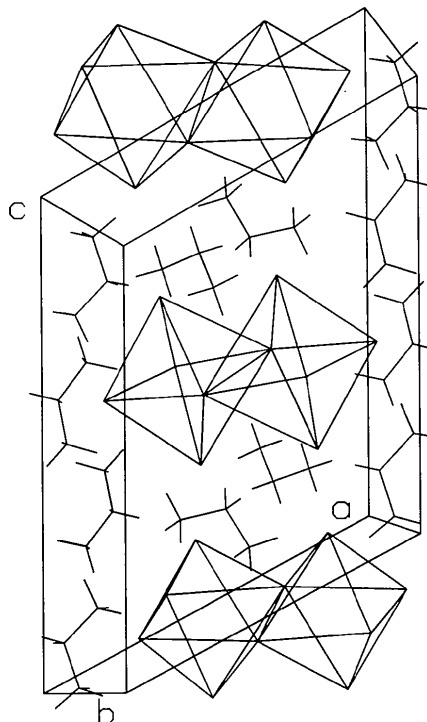


Fig. 2. The packing arrangement.

## Experimental

Crystals of suitable dimensions for X-ray structural analysis were grown by slow evaporation at room temperature of a saturated aqueous solution obtained by dissolving (CH<sub>3</sub>)<sub>2</sub>NH<sub>2</sub>Cl and BiCl<sub>3</sub> (molar ratio 2:1) in 36% HCl.

## Crystal data

(C <sub>2</sub> H <sub>8</sub> N) <sub>2</sub> [BiCl <sub>5</sub> ]	Mo K $\alpha$ radiation
$M_r = 478.42$	$\lambda = 0.71069 \text{ \AA}$
Monoclinic	Cell parameters from 25 reflections
$P2_1/c$	$\theta = 12\text{--}16^\circ$
$a = 10.8234 (9) \text{ \AA}$	$\mu = 13.179 \text{ mm}^{-1}$
$b = 10.3459 (8) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 14.381 (2) \text{ \AA}$	Cubic
$\beta = 63.025 (9)^\circ$	$0.08 \times 0.08 \times 0.08 \text{ mm}$
$V = 1435.2 (2) \text{ \AA}^3$	Colourless
$Z = 4$	
$D_x = 2.214 \text{ Mg m}^{-3}$	

## Data collection

CAD-4 diffractometer	$R_{\text{int}} = 0.0567$
$\omega/2\theta$ scans [width (0.75 + 0.35tan $\theta$ ) $^\circ$ ]	$\theta_{\text{max}} = 24.98^\circ$
Absorption correction:	$h = -12 \rightarrow 12$
$\psi$ scans (North, Phillips & Mathews, 1968)	$k = 0 \rightarrow 12$
$T_{\text{min}} = 0.98$ , $T_{\text{max}} = 0.99$	$l = -17 \rightarrow 17$
3239 measured reflections	2 standard reflections
2525 independent reflections	monitored every 200 reflections
2008 observed reflections	intensity decay: 0.8%
$[I > 2\sigma(I)]$	

## Refinement

Refinement on $F^2$	$\Delta\rho_{\text{max}} = 0.644 \text{ e \AA}^{-3}$
$R[F^2 > 2\sigma(F^2)] = 0.0382$	$\Delta\rho_{\text{min}} = -0.584 \text{ e \AA}^{-3}$
$wR(F^2) = 0.0668$	Extinction correction:
$S = 1.394$	<i>SHELXL93</i> (Sheldrick, 1993)
2525 reflections	Extinction coefficient:
110 parameters	0.0034 (1)
H-atom parameters not refined	Atomic scattering factors
$w = 1/[\sigma^2(F_o^2) + 3.9886P]$	from <i>International Tables for Crystallography</i> (1992), Vol. C, Tables 4.2.6.8 and 6.1.1.4)
where $P = (F_o^2 + 2F_c^2)/3$	
$(\Delta/\sigma)_{\text{max}} = 0.113$	

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	$U_{\text{eq}} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*a_i\cdot a_j$			
	$x$	$y$	$z$	$U_{\text{eq}}$
Bi	0.29825 (4)	0.59322 (4)	0.56499 (3)	0.03285 (14)
Cl1	0.5778 (3)	0.6534 (3)	0.5311 (2)	0.0494 (6)
Cl2	0.2434 (3)	0.5052 (3)	0.7550 (2)	0.0493 (7)
Cl3	0.0508 (3)	0.5295 (3)	0.6026 (2)	0.0565 (7)
Cl4	0.2186 (3)	0.8223 (2)	0.6359 (2)	0.0514 (7)
Cl5	0.3371 (3)	0.6717 (3)	0.3716 (2)	0.0504 (7)
N	0.0137 (9)	0.7246 (9)	0.8915 (7)	0.060 (3)
N'	0.4738 (9)	0.4272 (9)	0.2187 (6)	0.050 (2)

Cl1	-0.086 (1)	0.692 (1)	0.852 (1)	0.081 (4)
Cl2	-0.024 (2)	0.685 (1)	0.997 (1)	0.090 (5)
C'1	0.533 (1)	0.499 (1)	0.1212 (9)	0.077 (4)
C'2	0.342 (1)	0.364 (1)	0.241 (1)	0.086 (5)

Table 2. Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

Bi—Cl3	2.566 (3)	Bi—Cl1'	2.922 (3)
Bi—Cl4	2.569 (3)	N—C2	1.44 (2)
Bi—Cl2	2.679 (2)	N—C1	1.47 (1)
Bi—Cl5	2.741 (3)	N'—C'1	1.45 (1)
Bi—Cl1	2.906 (3)	N'—C'2	1.47 (1)
Cl3—Bi—Cl4	91.31 (9)	Cl5—Bi—Cl1	95.61 (8)
Cl3—Bi—Cl2	88.31 (9)	Cl3—Bi—Cl1'	94.97 (8)
Cl4—Bi—Cl2	91.69 (9)	Cl4—Bi—Cl1'	173.00 (8)
Cl3—Bi—Cl5	87.41 (9)	Cl2—Bi—Cl1'	91.58 (8)
Cl4—Bi—Cl5	89.94 (8)	Cl5—Bi—Cl1'	87.27 (8)
Cl2—Bi—Cl5	175.45 (8)	Cl1—Bi—Cl1'	83.57 (8)
Cl3—Bi—Cl1	176.57 (9)	Bi—Cl1—Bi'	96.43 (8)
Cl4—Bi—Cl1	90.31 (8)	C2—N—C1	116 (1)
Cl2—Bi—Cl1	88.63 (8)	C'1—N'—C'2	113 (1)

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

Table 3. Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ )

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
N—H1N $\cdots$ Cl2	0.900	2.453 (3)	3.280 (9)	152.8 (6)
N—H2N $\cdots$ Cl3'	0.900	2.390 (3)	3.22 (1)	154.1 (6)
N'—H1N' $\cdots$ Cl5	0.900	2.445 (3)	3.236 (9)	146.8 (5)
N'—H2N' $\cdots$ Cl5 <sup>ii</sup>	0.900	2.449 (3)	3.233 (9)	145.7 (5)

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

Diffraction data were corrected for Lorentz-polarization effects. The structure was solved by Patterson method and refined by full-matrix least-squares methods.

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989). Cell refinement: *CAD-4 Software*. Data reduction: *MolEN* (Fair, 1990). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ORTEPII* (Johnson, 1990). Software used to prepare material for publication: *SHELXL93*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: DU1124). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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