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# Trimethylphenylammonium trichloromercurate(II), $(Me_3PhN)[HgCl_3]$

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**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.019 Å
*R* factor = 0.023
*wR* factor = 0.058
Data-to-parameter ratio = 17.4

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



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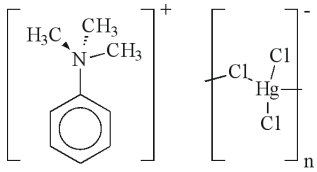
The crystal structure of $(Me_3PhN)[HgCl_3]$ contains $[(CH_3)_3(C_6H_5)N]^+$ cations and chains of distorted vertex-sharing $[HgCl_4]^{2-}$ tetrahedra running parallel to [100]. The tetrahedra around mercury(II) are distorted, exhibiting a [2+2] coordination. Apart from one of the Cl atoms, which is located on a twofold rotation axis, and a pair of symmetry-related methyl C atoms, which are located in general positions, all non H-atoms lie on mirror planes.

## Comment

Coordination polyhedra of chloromercurate(II) anions exhibit a surprisingly wide variety. No less than 252 crystallographically distinct $Hg^{II}$ species were listed in a recent overview (Serezhkin *et al.*, 2001). The trichloromercurate(II) anion, $[HgCl_3]^-$, is only rarely found as an isolated anion. The same is true for the dimeric unit, $[Hg_2Cl_6]^{2-}$, which occurs as two tetrahedra sharing one common edge. In most cases, however, $[3+2]_n$ and $[2+4]_n$ chains are observed, depending upon size and charge of the counter-cation(s) (House *et al.*, 1994).




(I)

The structure of $(Me_3PhN)[HgCl_3]$, (I), consists essentially of $[(CH_3)_3(C_6H_5)N]^+$ cations and chains of distorted vertex-sharing $[HgCl_4]^{2-}$ tetrahedra. The $Hg^{II}$ ion has a distorted tetrahedral coordination, with two chloride ligands with short $Hg^{2+}\cdots Cl^-$ bond lengths of 2.385 (2) and 2.393 (2) Å, and two bridging chloride ligands with considerably longer $Hg^{2+}\cdots Cl^-$ distances of 2.602 (1) Å. These tetrahedra build vertex-sharing chains parallel to [100]. The angle involving the bridging chloride ligands, Cl3—Hg—Cl3$^i$ (symmetry code as in Table 1), and the angle involving the two other Cl ligands, Cl1—Hg—Cl2, show distinct deviations from the ideal tetrahedral geometry, with values of 91.72 (6) and 134.9 (2)°, respectively. The Hg atoms, the Cl1 and Cl2 ligands, and the plane of the phenyl ring lie on a mirror plane perpendicular to the *a* axis.

## Experimental

A solution of 1 mmol (0.1717 g) trimethylphenylammonium chloride, $[(CH_3)_3(C_6H_5)N]Cl$, and 1 mmol (0.2715 g) $HgCl_2$ in a mixture of 20 ml water and 30 ml methanol was stirred at 333 K for 3 h. Colourless single crystals were obtained when the solution was allowed to stand at room temperature for 2 d.

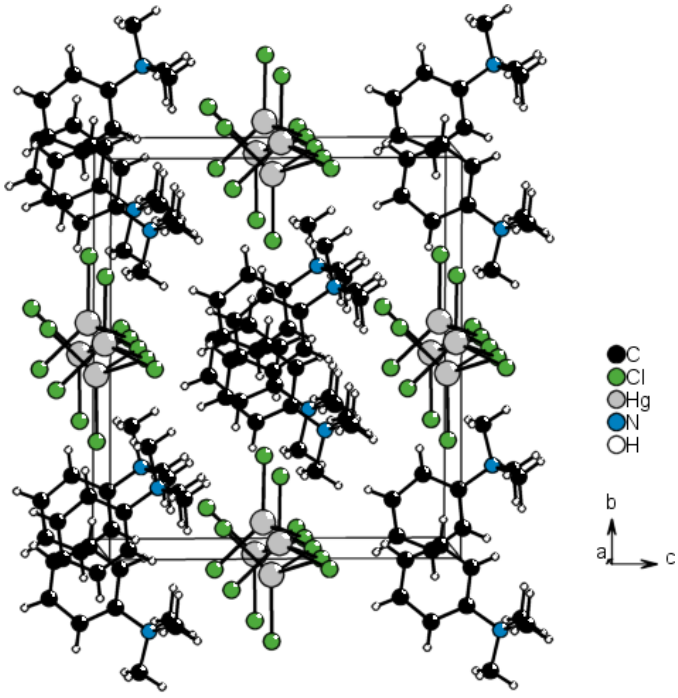



**Figure 1**
Packing diagram viewed down the *a* axis.

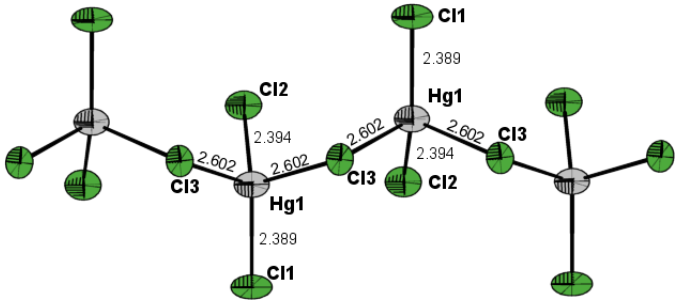



**Figure 2**
Part of the vertex-sharing chain of $[HgCl_4]^{2-}$ tetrahedra. Displacement ellipsoids are at the 50% probability level.

*Crystal data*

$(C_9H_{14}N)[HgCl_3]$
$M_r$ = 443.15
Orthorhombic, *Ama*2
*a* = 7.4699 (19) Å
*b* = 14.379 (2) Å
*c* = 12.5687 (10) Å
*V* = 1350.0 (4) Å$^3$
*Z* = 4
$D_x$ = 2.180 Mg m$^{-3}$

Mo *Kα* radiation
Cell parameters from 7398 reflections
$\theta$ = 2.2–32.3°
$\mu$ = 11.96 mm$^{-1}$
*T* = 293 (2) K
Prism, colourless
0.4 × 0.3 × 0.2 mm

*Data collection*

Stoe Imaging Plate Diffraction System (IPDS-I)
$\varphi$ scans
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1998)
$T_{min}$ = 0.034, $T_{max}$ = 0.585
7398 measured reflections

1426 independent reflections
1249 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.086
$\theta_{max}$ = 26.0°
*h* = −9 → 7
*k* = −17 → 17
*l* = −15 → 15

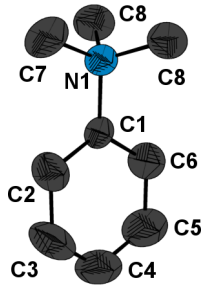



**Figure 3**
The $[Me_3PhN]^+$ cation. Displacement ellipsoids are at the 50% probability level.

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.058
*S* = 1.00
1426 reflections
82 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0241P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.98 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.08 e Å$^{-3}$
Extinction correction: *SHELXL*97
Extinction coefficient: 0.00312 (19)
Absolute structure: Flack (1983), 0000 Friedel pairs
Flack parameter = −0.015 (12)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Hg1—Cl1 | 2.385 (2) | C1—C2 | 1.379 (13) |
| Hg1—Cl2 | 2.393 (2) | C1—C6 | 1.385 (14) |
| Hg1—Cl3 | 2.6022 (14) | C2—C3 | 1.41 (2) |
| N1—C1 | 1.466 (14) | C3—C4 | 1.34 (2) |
| N1—C7 | 1.510 (13) | C4—C5 | 1.33 (2) |
| N1—C8 | 1.508 (9) | C5—C6 | 1.37 (2) |
| | | | |
| Cl1—Hg1—Cl2 | 134.88 (18) | C8$^{i}$—N1—C8 | 107.8 (7) |
| Cl1—Hg1—Cl3$^{i}$ | 106.36 (11) | C2—C1—C6 | 119.1 (11) |
| Cl2—Hg1—Cl3$^{i}$ | 104.64 (5) | C2—C1—N1 | 121.7 (9) |
| Cl1—Hg1—Cl3 | 106.36 (11) | C6—C1—N1 | 119.2 (10) |
| Cl2—Hg1—Cl3 | 104.64 (5) | C1—C2—C3 | 118.6 (14) |
| Cl3—Hg1—Cl3$^{i}$ | 91.72 (6) | C4—C3—C2 | 120.9 (13) |
| Hg1$^{ii}$—Cl3—Hg1 | 101.40 (7) | C3—C4—C5 | 119.7 (14) |
| C1—N1—C7 | 112.8 (9) | C4—C5—C6 | 122.3 (15) |
| C1—N1—C8 | 110.2 (5) | C5—C6—C1 | 119.4 (12) |
| C7—N1—C8 | 107.9 (6) | | |

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-STEP*32 (Stoe & Cie, 2000); data reduction: *X-RED* (Stoe & Cie, 2001); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999).

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