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catena-Poly[(2-phenylethyl)ammonium [dichloromercurate(II)-μ_3-chloro]]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.024 Å
R factor = 0.065
wR factor = 0.171
Data-to-parameter ratio = 24.5

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

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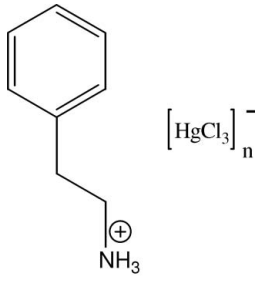
The crystal structure of the title compound, $\{(C_8H_{12}N)[HgCl_3]\}_n$, exhibits alternating organic and inorganic layers, which interact *via* N—H···Cl hydrogen bonding. In the inorganic layer, an infinite one-dimensional anion chain is formed by $[HgCl_3]^-$ subunits.

Comment

The structure of *catena*-poly[(2-phenylethyl)ammonium trichloromercurate(II)] was determined as part of an ongoing investigation of the structures of self-assembling organic–inorganic hybrid materials consisting of an organic molecular cation and a perhalometallate anion, with specific focus on the anion stoichiometry and geometry. Halomercurate(II) anions, $[Hg_nX_m]^{y-}$, display a variety of anionic structures (Linden *et al.*, 1999; Serezhkin *et al.*, 2001). More specifically, chloromercurate(II) anions include zero-dimensional isolated anions such as the commonly found $[HgCl_4]^{2-}$ and the rare anions $[HgCl_3]^-$ and $[HgCl_5]^{2-}$. Isolated blocks of polymeric anions are also observed, for example $[Hg_2Cl_6]^{2-}$ and $[Hg_4Cl_{10}]^{2-}$. A number of different one-dimensional polymeric anionic chains have been reported, including $[HgCl_3]_n^-$ (Authier-Martin & Beauchamp, 1975) and $[Hg_2Cl_3]_n^{3-}$ (House *et al.*, 1989), as well as a two-dimensional perovskite anionic sheet (Amami *et al.*, 2002). Currently the dictating effect of the cation on the chloromercurate(II) anion formed is not fully understood.



(I)

In the structure of the title compound, (I), a one-dimensional anionic chain that has only been reported once before for a chloromercurate(II) anion, in the structure of *catena*-poly[bis(L-tryptophanium) trichloromercurate(II)], (II) (Book *et al.*, 1981), is observed.

The asymmetric unit of (I) contains one 2-phenylethylammonium cation and one $[HgCl_3]^-$ anion, with four units in the unit cell. The asymmetric unit and atomic labelling scheme are shown in Fig. 1.

The crystal structure is composed of alternating organic and inorganic layers, as illustrated in Fig. 2. In the organic layer the

cations are interdigitated, with the aromatic groups packing in a single layer. Despite this packing there is no evidence of aromatic interactions, with the shortest centroid-to-centroid distance between aromatic groups equal to 4.911 (11) Å.

In the inorganic layer one-dimensional $[HgCl_3]_n^-$ polymeric anions extend in the *a*-axis direction. These chains are formed by distorted trigonal–bipyramidal $[HgCl_5]^{3-}$ units sharing three equatorial chloro ligands with four other metals, to form a ladder-like anion, as illustrated in Fig. 3.

The Hg—Cl bond lengths of the two axial ligands are shorter [2.339 (3) Å and 2.355 (3) Å] than the Hg—Cl bond lengths of the shared ligands [bond lengths range from 2.702 (3) Å to 2.984 (3) Å]. This difference in Hg—Cl bond lengths between axial and equatorial ligands was also observed in the structure of (II).

Hydrogen-bonding interactions are present between the ammonium groups and polymeric anions in the inorganic layer. Interaction parameters are listed in Table 1. Each of the H atoms on the ammonium group forms a bifurcated hydrogen bond to two different acceptor chloro ligands. A complex two-dimensional hydrogen-bonding network results parallel to the *ab* plane, in which ammonium groups connect neighbouring one-dimensional polymeric $[HgCl_3]_n^-$ chains, as illustrated in Fig. 4.

Experimental

2-Phenylethylammonium chloride was prepared by the dropwise addition of concentrated HCl (37%, Aldrich) to a solution of 2-phenylethylamine (Aldrich, 99%) in chloroform. The resulting precipitate was filtered. The title compound was prepared by dissolving 2-phenylethylammonium chloride (1.004 g) and $HgCl_2$ (PAL Chemicals, 99%) (0.316 g) (2:1 molar ratio) in distilled water. Colourless crystals formed on evaporation of the solvent at room temperature.

Crystal data

$(C_8H_{12}N)[HgCl_3]$
M_r = 429.13
Monoclinic, $P2_1/n$
a = 5.9927 (9) Å
b = 7.8267 (12) Å
c = 25.971 (4) Å
β = 96.184 (4)°
V = 1211.0 (3) Å^3
Z = 4
D_x = 2.354 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 13.33 mm^{-1}
T = 293 (2) K
Rectangular plate, colourless
0.30 × 0.16 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: integration (*XPREP*; Bruker, 1999)
T_{min} = 0.064, T_{max} = 0.517
8508 measured reflections
2896 independent reflections
2209 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 28.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.171
S = 1.38
2896 reflections
118 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2 + 17.3236P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −2.73 e Å^{-3}

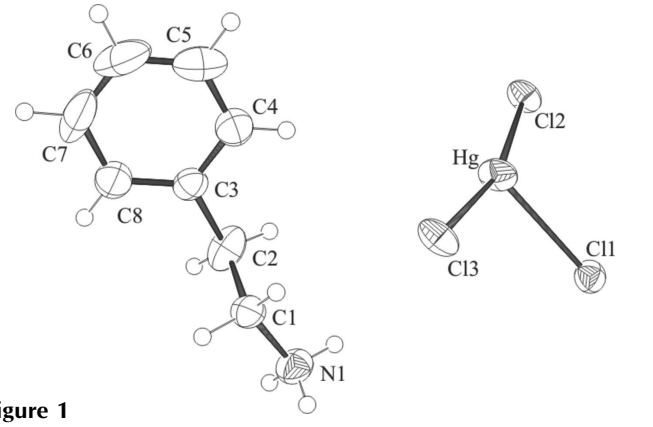


Figure 1
The asymmetric unit of (I), showing the atomic numbering scheme and ellipsoids at the 50% probability level (*ORTEP-3*; Farrugia, 1997).

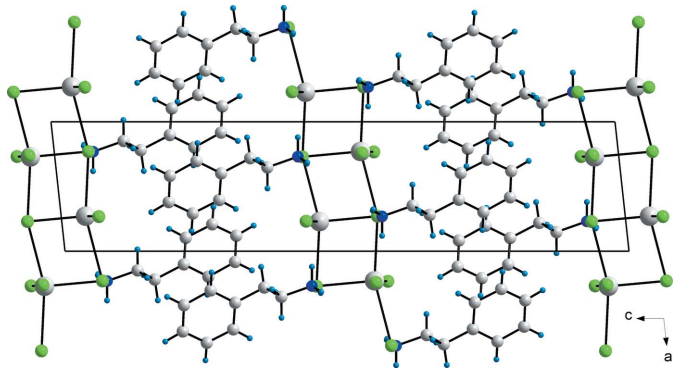


Figure 2
Packing viewed along the *b* axis (*DIAMOND*; Brandenburg, 1999).

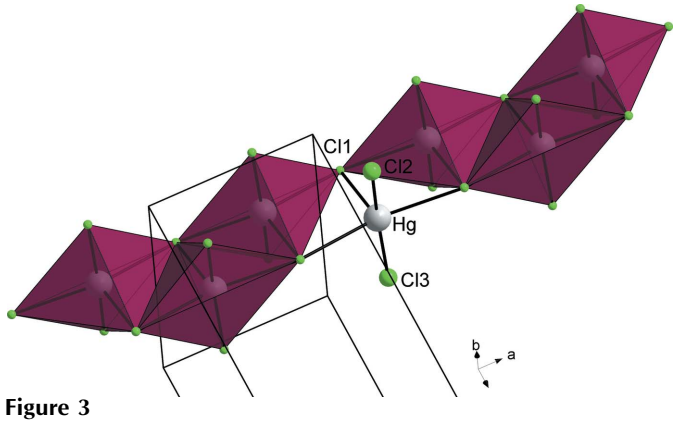


Figure 3
Anion chain geometry (*DIAMOND*; Brandenburg, 1999).

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1C···Cl1^{i}	0.89	2.74	3.459 (14)	139
N1—H1C···Cl2^{ii}	0.89	2.76	3.332 (13)	123
N1—H1D···Cl2^{iii}	0.89	2.77	3.410 (13)	130
N1—H1D···Cl3	0.89	2.91	3.565 (13)	132
N1—H1E···Cl2^{iv}	0.89	2.53	3.303 (13)	146
N1—H1E···Cl3^{v}	0.89	2.84	3.563 (13)	140

Symmetry codes: (i) $-x+2, -y, -z$; (ii) $x, y-1, z$; (iii) $-x+2, -y+1, -z$; (iv) $x-1, y-1, z$; (v) $x-1, y, z$.

All H atoms were placed in calculated positions, with aromatic C—H distances of 0.93 Å, methylene C—H distances of 0.97 Å and N—H distances of 0.89 Å, and were refined using a riding model, with U_{iso}(H) values of 1.2U_{eq} (1.5U_{eq} for ammonium) of the parent atom. The deepest electron-density hole is located 1.65 Å from atom H7.

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *PLATON* (Spek, 2003).

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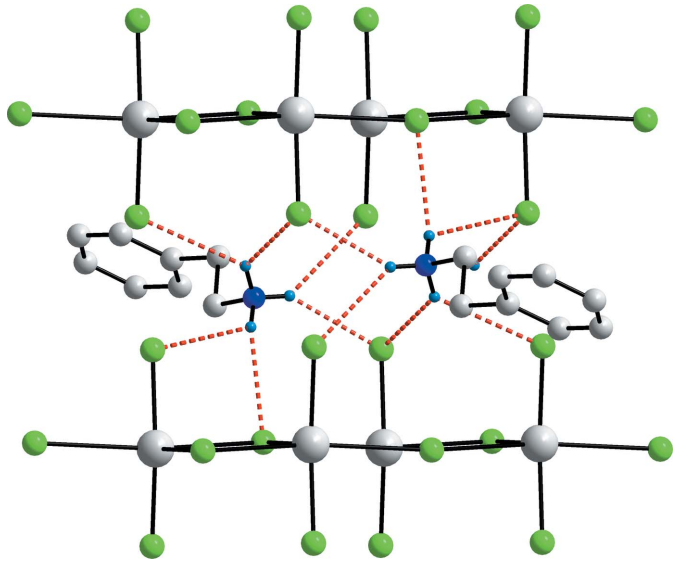

Figure 4
Hydrogen bonding interactions (dashed lines) (*DIAMOND*; Brandenburg, 1999). C-bound H atoms have been omitted.

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