

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: MU1179). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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*Acta Cryst.* (1995). **C51**, 2289–2292

## (Hexamethylenetetramine)diiodomercury(II), HgI<sub>2</sub>.hmt

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(Received 22 December 1994; accepted 24 April 1995)

## Abstract

The reaction of 1,3,5,7-tetraazatricyclo[3.3.1.1<sup>3,7</sup>]decane, trivial name hexamethylenetetramine (hmt), and HgI<sub>2</sub> (molar ratio 1:1) in ethanol or acetone diiodide (1:1), gives the title compound, *catena*-poly[diiodomercury- $\mu$ -1,3,5,7-tetraazatricyclo[3.3.1.1<sup>3,7</sup>]decane-*N*<sup>1</sup>:*N*<sup>5</sup>], [HgI<sub>2</sub>(C<sub>6</sub>H<sub>12</sub>N<sub>4</sub>)] (HgI<sub>2</sub>.hmt). The crystal and molecular structure of the title compound have been determined by X-ray structure analysis. HgI<sub>2</sub>.hmt belongs to the class of donor–acceptor complexes between hmt and metal salts. Hg is fourfold coordinated by two I and two hmt ligands. hmt acts as a bifunctional bridging ligand forming bent (–Hg–hmt–)<sub>n</sub> chains in the **b** direction of the *Pnma* space group.

## Comment

A large number of hexamethylenetetramine (hmt) complexes were reviewed in 1931 (Alpeter, 1931). Only a few of the complexes have been structurally analysed. hmt has four N-atom lone electron pairs which allow various coordination types in complex chemistry. Five types of hmt coordination in complexes with metal salts can be distinguished:

(1) hmt as a non-metal-coordinated structure element. Compounds of this type are often found in complexes containing water of crystallization, for instance in *MX*<sub>2</sub>.2hmt.10H<sub>2</sub>O, with *MX*<sub>2</sub> = CaBr<sub>2</sub> (Mazzarella, Kovacs, de Santis & Liquori, 1967), CoCl<sub>2</sub> (Ganesh, Seshasayee, Aravamudan, Heijdenrijk & Schenk, 1990), MgCl<sub>2</sub> (Kovacs & Mazzarella, 1966) or Co(NO<sub>3</sub>)<sub>2</sub> (Viostat, Khodadad & Rodier, 1981), in *M*Cr<sub>2</sub>O<sub>7</sub>.2hmt.yH<sub>2</sub>O, with *M* = Ca, *y* = 7 (Dahan, 1975) or *M* = Mg, *y* = 6 (Dahan, 1974), or in hexacyanoferrate complexes *M*<sub>a</sub>[Fe(CN)<sub>6</sub>]<sub>b</sub>.xhmt.yH<sub>2</sub>O of various composition with *M* = Li, Mg, Sr, Ba, *x* = 1–4 and *y* = 4–11 (Meyer & Pickardt, 1988*a,b,c*, 1989; Pickardt, Kahler, Rautenberg & Riedel, 1984). In all these compounds hmt is not part of the metal-coordination sphere.

(2) hmt as a monofunctional ligand. This coordination type has only been found in a few complexes: Mo(CO)<sub>5</sub>.hmt (Hui, Chan & Mak, 1984), (ZnCl<sub>2</sub>)<sub>3</sub>.hmt.12H<sub>2</sub>O (Mak & Huang, 1987), Cd{P(S<sub>2</sub>O-C<sub>2</sub>H<sub>5</sub>)<sub>2</sub>}<sub>2</sub>.2hmt (Shimoi, Ouchi, Aikawa, Sato & Saito, 1982). The structures of these compounds consist of isolated molecular units or networks formed by  $\mu$ -halogeno bridges.

(3) hmt as a bifunctional bridging ligand. This is the most common type of hmt coordination. Depending on coordination number and the shape of the metal, different networks are formed, *e.g.* in (CdCl<sub>2</sub>)<sub>2</sub>.hmt.5H<sub>2</sub>O (Lai & Mak, 1983), Cd(NO<sub>3</sub>)<sub>2</sub>.hmt.2H<sub>2</sub>O (Viostat, Khodadad & Rodier, 1982), (CdI<sub>2</sub>)<sub>3</sub>.2hmt.4H<sub>2</sub>O (Mak, 1982; Pickardt 1981*b*), [Hg(SCN)<sub>2</sub>]<sub>x</sub>.hmt, *x* = 1, 2 (Mak & Wu, 1985, 1986), (CuCN)<sub>3</sub>.2hmt (Pickardt & Rautenberg, 1982) or [Cu(CH<sub>3</sub>COO)<sub>2</sub>]<sub>2</sub>.hmt (Pickardt 1981*a*).

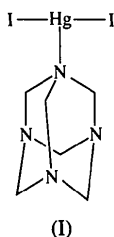
(4) hmt as a trifunctional bridging ligand. To our knowledge, there is only one structure of this type published. AgNO<sub>3</sub>.hmt consists of Ag–hmt–Ag–hmt chains. These chains are linked by additional Ag–hmt bonds. Every hmt ligand thus connects three Ag atoms (Michelet, Viostat, Khodadad & Rodier, 1981).

(5) hmt as a tetrafunctional bridging ligand. This coordination type is known for (AgX)<sub>4</sub>.hmt with X = Cl, Br (Mak, 1984, 1985). All four N-atom lone pairs of each cage molecule serve as ligands, giving rise to octahedral AgX<sub>5</sub>N, tetrahedral AgX<sub>3</sub>N and tetragonal pyramidal AgX<sub>4</sub>N, forming a three-dimensional network.

Alpeter (1931) described the following mercury halide hmt complexes: HgX<sub>2</sub>.hmt with X = Cl, Br, I; 2(HgX<sub>2</sub>)<sub>2</sub>.hmt with X = Cl, Br; (HgX<sub>2</sub>)<sub>3</sub>.2hmt with X = Cl, I. However, no crystal structure of these com-

pounds has yet been published. hmt reacts with HgCl<sub>2</sub> in aqueous solution to form hexamethylenetetrammonium-trichloromercurate (Pickardt & Schendler, 1982). In order to check the results reviewed by Alpeter (1931) the reaction between HgI<sub>2</sub> and hmt in acetone and ethanol solution was studied. HgI<sub>2</sub>.hmt was formed as the main product, in agreement with the theories of Alpeter.

In the title compound, (I), hmt acts as a bifunctional bridging ligand forming well separated bent (—Hg—hmt—)<sub>n</sub> chains in the *b* direction. The compound thus belongs to type (3) (see above). The Hg atom has a distorted tetrahedral environment [101.1 (2) and 98.2 (2)°] formed by two I atoms and two N atoms of different hmt molecules. The two Hg—I bonds [2.625 (2) and 2.638 (2) Å] are significantly shorter than in red HgI<sub>2</sub> (2.78 Å) (Wells, 1986). In pure hmt all C—N distances are 1.476 (2) Å and all N—C—N angles are 113.6 (2)° (Becka & Cruickshank, 1963).



The *T<sub>d</sub>* symmetry of hmt is reduced in HgI<sub>2</sub>.hmt because of the coordination to mercury. If hmt acts as a bifunctional bridging ligand, the symmetry of the free molecule should be reduced from *T<sub>d</sub>* to *C<sub>2v</sub>* and the N—C bonds included in the —Hg—N1—C4—N1\*—Hg— chain should be the longest in the cage. However, in the crystal structure of HgI<sub>2</sub>.hmt the molecular symmetry is further reduced from *C<sub>2v</sub>* to *C<sub>s</sub>* and the longest

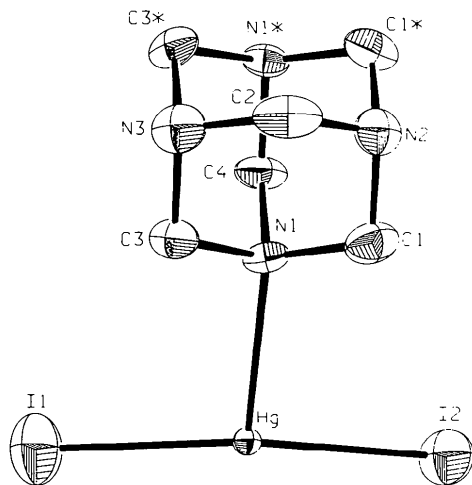


Fig. 1. Molecular structure showing 50% probability displacement ellipsoids. \* Indicates atoms are generated by the mirror plane through N3, C2, N2 and C4.

N—C bond is found in the mirror plane through N3, C2, N2 and C4 [N3—C2 1.52 (2) Å]. Furthermore, the shortest N—C bond is found in this mirror plane [N2—C2 1.45 (2) Å]. The N—C bonds formed by the Hg-bonded N atom [N1—C1 1.51 (1), N1—C3 1.49 (1) and N1—C4 1.51 (1) Å] are all longer than in free hmt. A comparison of bond distances (Table 3) in four mercury(II) compounds with analogous coordination spheres to that of HgI<sub>2</sub>.hmt indicates that the Hg—I distances are of normal magnitude while the Hg—N distance seems to be significantly longer.

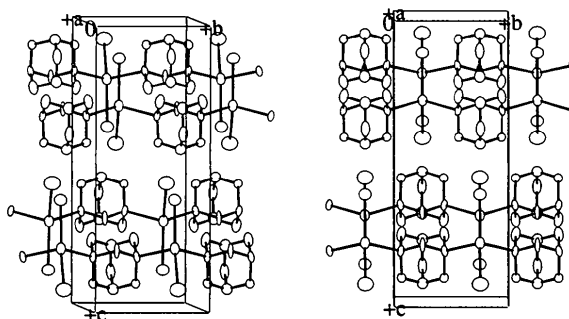


Fig. 2. Stereoview of the crystal packing of HgI<sub>2</sub>.hmt.

## Experimental

HgI<sub>2</sub>.hmt was prepared by reaction of red HgI<sub>2</sub> and hmt (molar ratio 1:1) in ethanol or acetone solution. In order to obtain single crystals, solid HgI<sub>2</sub> was placed in a tube with a G3 glass-filter bottom and a stopper at the top. The tube was inserted into an ethanol solution of hmt. The slow diffusion of the ethanol solution into the tube caused HgI<sub>2</sub> to dissolve. After two weeks, transparent colourless needles of HgI<sub>2</sub>.hmt were formed on the filter bottom.

### Crystal data

[HgI<sub>2</sub>(C<sub>6</sub>H<sub>12</sub>N<sub>4</sub>)]  
*M<sub>r</sub>* = 594.59  
 Orthorhombic  
*Pnma*  
*a* = 12.416 (1) Å  
*b* = 6.391 (1) Å  
*c* = 15.552 (2) Å  
*V* = 1234.1 (2) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 3.20 Mg m<sup>-3</sup>

Mo *Kα* radiation  
 $\lambda$  = 0.71069 Å  
 Cell parameters from 25 reflections  
 $\theta$  = 8.3–13.9°  
 $\mu$  = 17.478 mm<sup>-1</sup>  
*T* = 295 K  
 Needle shaped  
 0.25 × 0.07 × 0.06 mm  
 Colourless

### Data collection

CAD-4 diffractometer  
 $\omega$ -2 $\theta$  scans  
 Absorption correction:  
 analytical  
 $T_{\min}$  = 0.467,  $T_{\max}$  = 0.560  
 1586 measured reflections  
 1586 independent reflections

864 observed reflections  
 $[I > 3\sigma(I)]$   
 $\theta_{\max}$  = 27°  
 $h$  = 0 → 15  
 $k$  = -8 → 0  
 $l$  = -19 → 0  
 1 standard reflection  
 frequency: 60 min  
 intensity decay: 0.66%

## Refinement

Refinement on  $F$  $R = 0.0335$  $wR = 0.0344$  $S = 2.070$ 

864 reflections

71 parameters

H atoms not located

 $w = 1/\sigma^2(F)$  $(\Delta/\sigma)_{\max} < 0.001$  $\Delta\rho_{\max} = 1.79 \text{ e } \text{\AA}^{-3}$  $\Delta\rho_{\min} = -1.25 \text{ e } \text{\AA}^{-3}$ 

Extinction correction:

Zachariasen (1968) type

2, Gaussian isotropic

Extinction coefficient:

2.28353

Atomic scattering factors

from *International Tables*for *X-ray Crystallography*

(1974, Vol. IV)

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

$$B_{\text{eq}} = (8\pi^2/3) \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

|    | $x$         | $y$       | $z$         | $B_{\text{eq}}$ |
|----|-------------|-----------|-------------|-----------------|
| Hg | 0.74589 (6) | 1/4       | 0.21052 (5) | 2.71 (3)        |
| I1 | 0.8707 (1)  | 1/4       | 0.0743 (1)  | 4.80 (8)        |
| I2 | 0.7276 (1)  | 1/4       | 0.37955 (8) | 3.69 (7)        |
| N1 | 0.6251 (7)  | 0.559 (1) | 0.1789 (6)  | 1.9 (4)         |
| N2 | 0.461 (1)   | 3/4       | 0.212 (1)   | 2.7 (7)         |
| N3 | 0.534 (1)   | 3/4       | 0.0651 (9)  | 3.0 (8)         |
| C1 | 0.5240 (9)  | 0.562 (2) | 0.2331 (8)  | 3.0 (7)         |
| C2 | 0.434 (1)   | 3/4       | 0.121 (1)   | 3 (1)           |
| C3 | 0.5977 (9)  | 0.564 (2) | 0.0858 (7)  | 2.4 (6)         |
| C4 | 0.691 (1)   | 3/4       | 0.202 (1)   | 2.5 (8)         |

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

|          |            |          |            |
|----------|------------|----------|------------|
| Hg—I1    | 2.625 (2)  | N1—C4    | 1.51 (1)   |
| Hg—I2    | 2.638 (2)  | N2—C1    | 1.47 (1)   |
| Hg—N1    | 2.530 (9)  | N2—C2    | 1.45 (2)   |
| N1—C1    | 1.51 (1)   | N3—C2    | 1.52 (2)   |
| N1—C3    | 1.49 (1)   | N3—C3    | 1.46 (1)   |
| I1—Hg—I2 | 148.75 (6) | Hg—N1—C3 | 109.9 (7)  |
| I1—Hg—N1 | 101.1 (2)  | Hg—N1—C4 | 105.3 (6)  |
| I2—Hg—N1 | 98.2 (2)   | C1—N2—C2 | 110.2 (10) |
| C1—N1—C3 | 110.7 (9)  | C2—N3—C3 | 108.4 (9)  |
| C1—N1—C4 | 108 (1)    | N1—C1—N2 | 108.9 (10) |
| C3—N1—C4 | 109 (1)    | N2—C2—N3 | 111 (1)    |
| Hg—N1—C1 | 113.2 (7)  | N1—C3—N3 | 110 (1)    |

Table 3. Comparison of bond lengths ( $\text{\AA}$ ) in  $\text{HgI}_2$  complexes with coordination spheres analogous to those of  $\text{HgI}_2 \cdot \text{hmt}$ 

|  | Hg—I      | Hg—N      |
|--|-----------|-----------|
| $\text{HgI}_2(\text{py})_2^a$                                      | 2.7 (1)   | 2.30 (6)  |
|  |           | 2.65 (1)  |
| $\text{HgI}_2(\text{py})_2^b$                                      | 2.668 (1) | 2.424 (9) |
|  | 2.664 (1) |           |
| $o\text{-Me}_2\text{NC}_6\text{H}_4\text{.NMe}_2\text{HgI}_2^c$    | 2.657 (1) | 2.461 (8) |
|  | 2.669 (1) | 2.429 (8) |
| $2\text{Hg}(\text{NH}_3)_2\text{I}_2 \cdot \text{S}_4\text{N}_4^d$ | 2.697 (1) | 2.30 (2)  |
| This work  | 2.625 (2) | 2.530 (9) |
|  |           | 2.638 (2) |

References: (a) Martan & Weiss (1984); (b) Huges, Favas, Skelton & White (1985); (c) Persson, Sandstroem, Goggin & Mosset (1985); (d) Canty, Raston, Skelton & White (1982).

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989). Cell refinement: *CAD-4 Software CELDIM*. Data reduction: *TEXSAN PROCESS* (Molecular Structure Corporation, 1993). Program(s) used to solve structure: *SAPI91* (Fan, 1991). Program(s) used to refine structure: *TEXSAN LS*. Software used to prepare material for publication: *TEXSAN*.

We thank the Deutsche Forschungsgemeinschaft (DFG) and the Swedish Natural Science Research Council (NFR) for financial support.

Lists of structure factors and anisotropic displacement parameters have been deposited with the IUCr (Reference: NA1153). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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unit cell (Tse, Lee & Gabe, 1986). In the title complex the molecule containing Sn2 and C12 has exact threefold symmetry.

*Acta Cryst.* (1995). **C51**, 2292–2293

## Rhombohedral Chlorotriphenyltin

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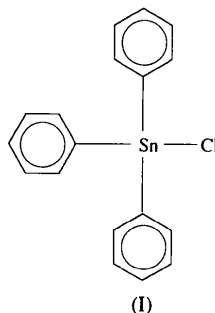
(Received 28 March 1995; accepted 20 April 1995)

### Abstract

The Sn atoms in the two independent molecules of rhombohedral chlorotriphenyltin, [SnCl(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>], both show tetrahedral coordination.

### Comment

This rhombohedral modification of chlorotriphenyltin shows no new or unusual features compared with the monoclinic modification, which also has two independent but structurally similar tetrahedral molecules in the



### Experimental

This modification of triphenyltin chloride was obtained in an unsuccessful attempt at synthesizing the 1/1 complex with 2,2'-bipyridine *N,N'*-dioxide. The reagents in equimolar amounts were heated in a small volume of ethanol; slow cooling of the solution returned the starting organotin halide in the rhombohedral modification.

#### Crystal data

[SnCl(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>]  
*M<sub>r</sub>* = 385.44  
 Trigonal  
*R* $\bar{3}$  (hexagonal axes)  
*a* = 24.4935 (4) Å  
*c* = 19.1219 (6) Å  
*V* = 9934.9 (4) Å<sup>3</sup>  
*Z* = 24  
*D<sub>x</sub>* = 1.546 Mg m<sup>-3</sup>

Mo K $\alpha$  radiation  
 $\lambda$  = 0.71073 Å  
 Cell parameters from 25 reflections  
 $\theta$  = 14–15°  
 $\mu$  = 1.692 mm<sup>-1</sup>  
*T* = 298 K  
 Cube  
 0.44 × 0.44 × 0.44 mm  
 Colourless

#### Data collection

Enraf–Nonius CAD-4 diffractometer  
 $\omega$ -2 $\theta$  scans  
 Absorption correction:  $\psi$  scans (North, Phillips & Mathews, 1968)  
 $T_{\min}$  = 0.91,  $T_{\max}$  = 1.00  
 4189 measured reflections  
 3887 independent reflections

2853 observed reflections  
 $[I > 2\sigma(I)]$   
 $R_{\text{int}}$  = 0.0174  
 $\theta_{\text{max}}$  = 24.97°  
 $h$  = 0 → 25  
 $k$  = 0 → 25  
 $l$  = -22 → 22  
 3 standard reflections  
 frequency: 60 min  
 intensity decay: 0.8%

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)]$  = 0.0344  
 $wR(F^2)$  = 0.0766  
 $S$  = 1.088  
 3887 reflections  
 321 parameters  
 H-atoms were located and refined isotropically  
 $w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 6.3034P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}}$  = 0.001  
 $\Delta\rho_{\text{max}}$  = 0.71 e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}}$  = -0.34 e Å<sup>-3</sup>  
 Extinction correction: none  
 Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

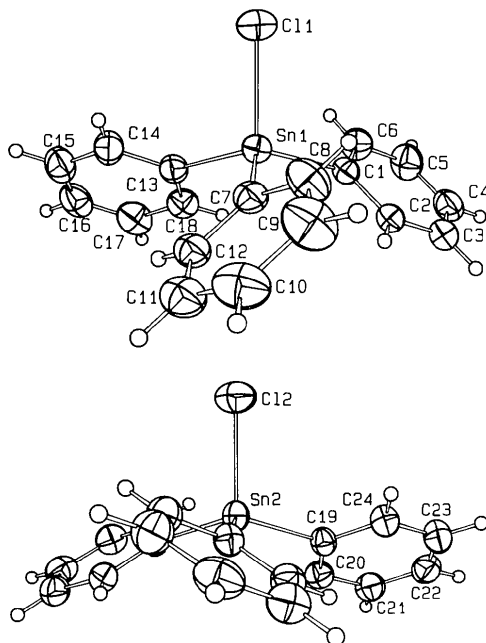


Fig. 1. Atomic labelling scheme for the two crystallographically independent molecules of chlorotriphenyltin. Displacement ellipsoids are plotted at the 30% probability level.