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# Structure of Ethylene Oxide Oligomer Complexes. I. A 1:1 Complex of Tetraethylene Glycol Dimethyl Ether with Mercuric Chloride

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Molecular and crystal structure of a 1: 1 molecular complex of tetraethylene glycol dimethyl ether $CH_3O(CH_2CH_2O)_4CH_3$ (TGM) with mercuric chloride has been determined by means of X-ray diffraction. The complex has a monoclinic unit cell with $a=14.29$, $b=15.10$, $c=7.84$ Å, and $\beta=97.0°$. The space group is $P2_1/n$. Four molecules of both TGM and mercuric chloride are contained in the unit cell. The structure was determined by the ordinary heavy atom method. The molecular conformation of TGM in the complex is approximately

$$CH_3-O\underset{\mathrm{T}}{-}CH_2\underset{\mathrm{G}}{-}CH_2\underset{\mathrm{T}}{-}O\underset{\mathrm{T}}{-}CH_2\underset{\bar{\mathrm{G}}}{-}CH_2\underset{\mathrm{T}}{-}O\underset{\mathrm{T}}{-}CH_2\underset{\mathrm{G}}{-}CH_2\underset{\mathrm{T}}{-}O\underset{\mathrm{T}}{-}CH_2\underset{\bar{\mathrm{G}}}{-}CH_2\underset{\mathrm{T}}{-}O\underset{\mathrm{T}}{-}CH_2\underset{\mathrm{G}}{-}CH_2\underset{\mathrm{T}}{-}O-CH_3,$$

where T, G, and $\bar{\mathrm{G}}$ indicate *trans*, *gauche*, and minus *gauche* forms, respectively. All the $CH_2$–O bonds are *trans*, while the $CH_2$–$CH_2$ bonds are *gauche* and minus *gauche* in the adjacent chemical units. The conformational unit of

$$O\underset{\mathrm{T}}{-}CH_2\underset{\mathrm{G}}{-}CH_2\underset{\mathrm{T}}{-}O\underset{\mathrm{T}}{-}CH_2\underset{\bar{\mathrm{G}}}{-}CH_2\underset{\mathrm{T}}{-}$$

was found to be very important and favorable for coordination between the O and Hg atoms. The molecule is circular but not closed, and the five oxygen atoms, which are nearly coplanar and located at the inner side of the circular molecule, enclose one $HgCl_2$ molecule with close interatomic distances (2.78—2.96 Å) between the O and Hg atoms.

The molecular complexes of polyethylene oxide (PEO) with $HgCl_2$ were previously investigated,[1,2] and it was found that they have two crystalline forms, one having the composition of $CH_2CH_2O:HgCl_2=$ 4 :1 (type I) and the other that of $CH_2CH_2O:HgCl_2=$ 1: 1 (type II). The conformation of PEO in the complexes is

$$\underset{\mathrm{T}}{-}O\underset{\mathrm{T}}{-}CH_2\underset{\mathrm{T}}{-}CH_2\underset{\mathrm{T}}{-}O\underset{\mathrm{T}}{-}CH_2\underset{\mathrm{G}}{-}CH_2\underset{\mathrm{T}}{-}O\underset{\mathrm{T}}{-}CH_2\underset{\mathrm{T}}{-}CH_2\underset{\mathrm{T}}{-}O\underset{\mathrm{T}}{-}CH_2\underset{\bar{\mathrm{G}}}{-}CH_2-$$

in type I and

$$\underset{\mathrm{T}}{-}O\underset{\mathrm{G}}{-}CH_2\underset{\mathrm{G}}{-}CH_2\underset{\mathrm{T}}{-}O\underset{\mathrm{T}}{-}CH_2\underset{\bar{\mathrm{G}}}{-}CH_2-$$

in type II, where T, G, and $\bar{\mathrm{G}}$ denote *trans*, *gauche*, and minus *gauche*, respectively. These differ significantly from the conformation of PEO in the ordinary PEO,[3] which is helical consisting of a uniform succession of $\underset{\mathrm{T}}{-}O\underset{\mathrm{T}}{-}CH_2\underset{\mathrm{G}}{-}CH_2$. In the type I complex two of the four oxygen atoms in the identity period are coordinated with one Hg atom, while in the type II complex each oxygen atom is coordinated with two Hg atoms. In these complexes the interatomic interactions between the Hg and O atoms cause the complex formation and have important influence on the conformation of PEO.

On the other hand, according to Pedersen,[4,5] macrocyclic polyethers especially those containing $CH_2CH_2O$ units form stable crystalline molecular complexes with many metal salts including $HgCl_2$. Investigations have recently been carried out on the crystal structures of some complexes in which an alkali ion is enclosed in a cavity surrounded by oxygen atoms of the molecule.[6,7] This spatial arrangement indicates the existence of strong interactions between oxygen and alkali ions. It was reported that there occurs specific solvation between dimethoxy ethane and $HgCl_2$ in solution.[8] Ethylene oxide oligomers, $CH_3O(CH_2CH_2O)_mCH_3$, have specific solvation with alkali-carbanion ion pairs in solution and the solvation has significant influence on reactivity of the ion pairs, which are the initiators of living polymerization of styrene.[9-11] Dimethoxy ethane has specific interaction with alkali metals, also.[12,13]

These studies indicate that ethers composed of the $CH_2CH_2O$ groups have a specific property to interact with metal salts or ions. In the structural studies of the PEO–$HgCl_2$ complexes,[1,2] it was not possible to determine the precise structure of PEO and to discuss the structure of the complexes in details on account of the small number of reflections and predominant contribution of $HgCl_2$ to the diffraction intensities. Recently it has been found that ethylene oxide oligomers, $RO(CH_2CH_2O)_mR$, form molecular complexes with $HgCl_2$ and some of the complexes give single crystals available for structural investigation by means of X-ray diffraction. It was hoped that the X-ray structure determination of the complexes would give important and more detailed information on the interaction between ethylene oxide groups and mercuric chloride and on the conformational change of the molecules. From this point of view structural studies of a series

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[1] R. Iwamoto, Y. Saito, H. Ishihara, and H. Tadokoro, *J. Polymer. Sci, A-2*, **6**, 1509 (1968).

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[13] S. H. Glarum and J. H. Marshall, *ibid.*, **52**, 5555 (1970).

of the complexes of ethylene oxide oligomers, RO-$(CH_2CH_2O)_mR$, with $HgCl_2$ have been undertaken. The present paper deals with the $CH_3O(CH_2CH_2O)_4$-$CH_3$–$HgCl_2$ complex.

## Experimental

*Samples.* Commercially available sample of tetraethylene glycol dimethyl ether (TGM) was used (Tokyo Kasei Kogyo Co., Ltd.). Crystals of the TGM–$HgCl_2$ complex were prepared by dissolving crystalline powder of $HgCl_2$ into an ethanol-TGM (about 10: 1 volume ratio) mixture to saturation at about 35 °C and cooling the saturated solution to room temperature, single crystals of the complex being precipitated in solution. The crystals are transparent needles grown along the *c* axis. The melting point of the complex is 66 °C as determined microscopically. The density of the crystal was measured by the flotation method by use of a liquid mixture of $CCl_4$ and $CHBr_3$ as the flotation medium. The observed density was 1.96 g/cc. The composition of the complex was found to be TGM: $HgCl_2$ = 1: 1 by elemental analysis (Found: Hg, 40.8%. Calcd for the 1: 1 complex: Hg, 40.6%).

TABLE 1. CRYSTALLOGRAPHIC AND PHYSICAL DATA OF THE TGM–$HgCl_2$ COMPLEX

| | |
|---|---|
| Formula | $CH_3O(CH_2CH_2O)_4CH_3 \cdot HgCl_2$ |
| MW | 493.7 |
| Mp | 66 °C |
| Crystal system | monoclinic |
| Space group | $P2_1/n\text{-}C_{2h}^5$ |
| *a* | 14.29 Å |
| *b* | 15.10 Å |
| *c* | 7.84 Å |
| *β* | 97.0° |
| *Z* | 4 |
| Vol. | 1697.0 Å$^3$ |
| $D_c$ | 1.95 g/cc |
| $D_m$ | 1.96 g/cc |
| $\mu$ (Cu$K\alpha$) | 206.4 cm$^{-1}$ |
| *F*(000) | 944 |

*Unit Cell and Space Group.* The unit cell parameters were determined with a Weissenberg camera and calibrated by silicon powder. Systematic absences were observed with respect to reflections having indices *h*0*l* with $h+l$ odd and 0*k*0 with *k* odd. The space group, thus, is $P2_1/n$. The crystallographic data are given in Table 1 together with some physical constants.

*Intensity Measurement.* X-Ray diffraction photographs of the complex crystal were taken by using Cu$K\alpha$ radiation. The crystals used were about 0.2 mm × 0.2 mm × 0.2 mm in size. Intensity data were recorded on photographs by using equi-inclination Weissenberg multiple film method about the *c* axis from $l=0$ to 6 layers and about the *b* axis for a $k=0$ layer. The number of recorded reflections having non-zero intensities was 2455. The intensities were measured by visual comparison with standard intensity scales. Intensity data were corrected for the Lorentz and polarization factors. Although the absorption coefficient is very large ($\mu$ = 206 cm$^{-1}$ for Cu$K\alpha$ radiation), the intensity data were not corrected for absorption. The smallest possible crystal was used for collecting the intensities. When the crystal was exposed to radiation for longer than 100 hr under operation conditions of 35 kV and 20 mA, it became opaque and light brown, and the diffraction photographs were contaminated with Debye ring reflections due to the decomposed material. The crystal was renewed for each layer line.

## Structure Determination

Since atomic scattering power of a Hg atom is much stronger than that of other atoms contained in the complex, the general feature of reflections can be explained approximately by considering the Hg atom only. The crystal structure has been determined according to the ordinary heavy atom method. Atomic scattering factors were taken from *International Tables of X-Ray Crystallography* (1962). The atomic parameters refined by the block diagonal least squares method[14] were set as the final result. For this, the

TABLE 2. ATOMIC COORDINATES AND TEMPERATURE FACTORS IN THE TGM–$HgCl_2$ COMPLEX

| atom | *x* | *y* | *z* | *B* or $B_{11}$ | $B_{22}$ | $B_{33}$ | $B_{12}$ | $B_{13}$ | $B_{23}$ |
|---|---|---|---|---|---|---|---|---|---|
| Hg | 0.2386 | 0.0598 | −0.0102 | 0.0023 | 0.0017 | 0.0124 | −0.0002 | 0.0005 | 0.0009 |
| $Cl_1$ | 0.3019 | −0.0591 | 0.1500 | 0.0054 | 0.0031 | 0.0218 | 0.0014 | 0.0008 | 0.0051 |
| $Cl_2$ | 0.1614 | 0.1706 | −0.1701 | 0.0050 | 0.0025 | 0.0226 | 0.0013 | −0.0028 | 0.0039 |
| $C_1$ | 0.0461 | −0.0248 | 0.2375 | 4.39A$^2$ | | | | | |
| $O_1$ | 0.0865 | 0.0636 | 0.2140 | 4.31 | | | | | |
| $C_2$ | 0.1131 | 0.1004 | 0.3759 | 4.71 | | | | | |
| $C_3$ | 0.1692 | 0.1851 | 0.3295 | 3.24 | | | | | |
| $O_2$ | 0.2612 | 0.1574 | 0.2928 | 2.76 | | | | | |
| $C_4$ | 0.3259 | 0.2302 | 0.2765 | 3.54 | | | | | |
| $C_5$ | 0.4153 | 0.1952 | 0.2185 | 3.70 | | | | | |
| $O_3$ | 0.3940 | 0.1720 | 0.0490 | 2.95 | | | | | |
| $C_6$ | 0.4748 | 0.1423 | −0.0284 | 3.31 | | | | | |
| $C_7$ | 0.4453 | 0.1197 | −0.2161 | 3.53 | | | | | |
| $O_4$ | 0.3875 | 0.0362 | −0.2108 | 3.44 | | | | | |
| $C_8$ | 0.3594 | 0.0087 | −0.3933 | 5.18 | | | | | |
| $C_9$ | 0.3050 | −0.0813 | −0.3535 | 3.13 | | | | | |
| $O_5$ | 0.2203 | −0.0588 | −0.2968 | 3.29 | | | | | |
| $C_{10}$ | 0.1638 | −0.1345 | −0.2635 | 4.67 | | | | | |

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[14] By the courtesy of Dr. Y. Chatani of Osaka University, the calculation was made at the computer center of the University according to the program programmed by T. Ashida.

$R$ factor ($\sum||F_o|-|F_c||/\sum|F_o|$) for the structure taking the Hg and Cl atoms only into account was 21.5%. Consideration of the C and O atoms of TGM improved the $R$ factor to 15.6%. The atomic parameters are given in Table 2.

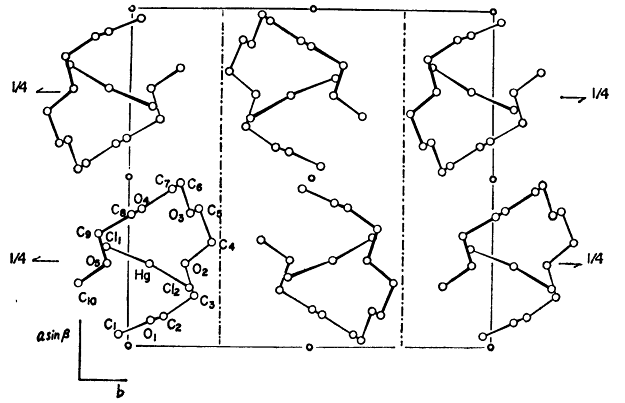

Fig. 1. Crystal structure of the TGM-HgCl$_2$ complex.

Table 3. Bond lengths (Å) and bond angles (°) and their estimated standard deviations in the TGM–HgCl$_2$ complex

| | | | |
|---|---|---|---|
| Hg–Cl$_1$ | 2.311±0.013 | Cl$_1$–Hg–Cl$_2$ | 174.2 |
| Hg–Cl$_2$ | 2.291±0.013 | C$_1$–O$_1$–C$_2$ | 108.3±3.7 |
| C$_1$–O$_1$ | 1.47 ±0.06 | O$_1$–C$_2$–C$_3$ | 101.7±3.8 |
| O$_1$–C$_2$ | 1.40 ±0.06 | C$_2$–C$_3$–O$_2$ | 108.3±3.5 |
| C$_2$–C$_3$ | 1.58 ±0.07 | C$_3$–O$_2$–C$_4$ | 113.9±3.1 |
| C$_3$–O$_2$ | 1.44 ±0.05 | O$_2$–C$_4$–C$_5$ | 109.6±3.5 |
| O$_2$–C$_4$ | 1.45 ±0.05 | C$_4$–C$_5$–O$_3$ | 106.7±3.6 |
| C$_4$–C$_5$ | 1.50 ±0.07 | C$_5$–O$_3$–C$_6$ | 113.2±3.2 |
| C$_5$–O$_3$ | 1.37 ±0.05 | O$_3$–C$_6$–C$_7$ | 109.7±3.5 |
| O$_3$–C$_6$ | 1.44 ±0.05 | C$_6$–C$_7$–O$_4$ | 104.4±3.4 |
| C$_6$–C$_7$ | 1.52 ±0.06 | C$_7$–O$_4$–C$_8$ | 106.8±3.3 |
| C$_7$–O$_4$ | 1.51 ±0.06 | O$_4$–C$_8$–C$_9$ | 97.4±3.7 |
| O$_4$–C$_8$ | 1.50 ±0.06 | C$_8$–C$_9$–O$_5$ | 108.4±3.6 |
| C$_8$–C$_9$ | 1.62 ±0.07 | C$_9$–O$_5$–C$_{10}$ | 113.2±3.4 |
| C$_9$–O$_5$ | 1.38 ±0.05 | | |
| O$_5$–C$_{10}$ | 1.44 ±0.06 | | |

Table 4. Internal rotation angles for the TGM molecule in the complex

| | |
|---|---|
| C$_1$–O$_1$–C$_2$–C$_3$ | 171° |
| O$_1$–C$_2$–C$_3$–O$_2$ | −77 |
| C$_2$–C$_3$–O$_2$–C$_4$ | −170 |
| C$_3$–O$_2$–C$_4$–C$_5$ | −174 |
| O$_2$–C$_4$–C$_5$–O$_3$ | 72 |
| C$_4$–C$_5$–O$_3$–C$_6$ | 176 |
| C$_5$–O$_3$–C$_6$–C$_7$ | −179 |
| O$_3$–C$_6$–C$_7$–O$_4$ | −71 |
| C$_6$–C$_7$–O$_4$–C$_8$ | −178 |
| C$_7$–O$_4$–C$_8$–C$_9$ | 177 |
| O$_4$–C$_8$–C$_9$–O$_5$ | 73 |
| C$_8$–C$_9$–O$_5$–C$_{10}$ | 178 |

## Results and Discussion

The crystal structure of the complex as a whole is shown in Fig. 1. Each TGM molecule encloses one HgCl$_2$ molecule in the crystal of the complex. Bond lengths and angles for the TGM molecules are listed in Table 3, together with those for the HgCl$_2$ molecule. These values are reasonable considering the fact that the Hg atoms contribute predominantly to the diffration intensities in the complex. Table 4 gives internal rotation angles around each bond of the TGM molecule in the complex. Internal rotation angles around the CH$_2$–O bonds are approximately *trans* (170—179°), while those around the CH$_2$–CH$_2$ bonds are nearly *gauche* with alternation of *gauche* and minus *gauche* in the succeeding chemical units (71—77°):

$$\underset{T}{-}CH_2\underset{G}{-}CH_2\underset{T}{-}O\underset{T}{-}CH_2\underset{\bar{G}}{-}CH_2\underset{T}{-}O-.$$

The conformation of the whole molecule is, therefore, denoted by

$$CH_3-O\underset{T}{-}CH_2\underset{G}{-}CH_2\underset{T}{-}O\underset{T}{-}CH_2\underset{\bar{G}}{-}CH_2\underset{T}{-}O\underset{T}{-}CH_2\underset{G}{-}CH_2\underset{T}{-}O\underset{T}{-}$$
$$CH_2\underset{\bar{G}}{-}CH_2\underset{T}{-}O-CH_3.$$

**Figure 2** shows the molecular structure of TGM in the complex, where the molecule is projected on the plane formed by the five oxygen atoms. The molecule has an open circular structure and the five oxygen atoms are on the inner side, enclosing one Hg atom in the way shown in Fig. 3. Table 5 gives interatomic distances involving Hg atoms and angles for $O_i\cdots Hg\cdots O_{i+1}$, $Cl_j–Hg\cdots O_i$, and $C_j–O_i\cdots Hg$. Interatomic dis-

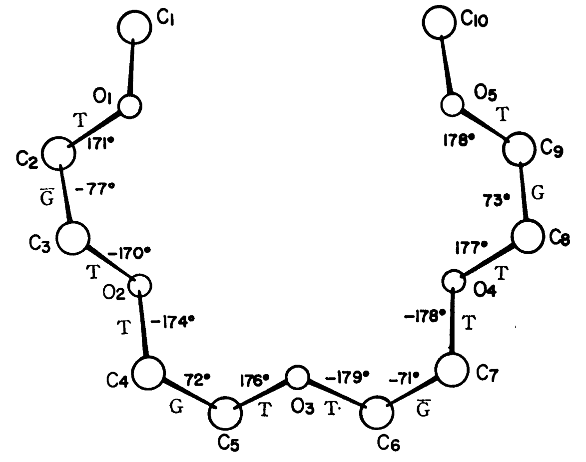

Fig. 2. Molecular conformation of TMG in the complex.

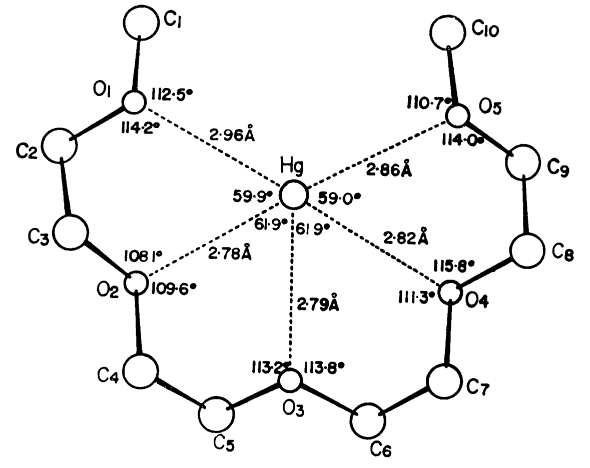

Fig. 3. Interactions between the O and Hg atoms in the TGM-HgCl$_2$ complex.

Table 5. Interatomic distances and angles for non-bonded atoms in the TGM–$HgCl_2$ complex

| | | | |
|---|---|---|---|
| $O_1..Hg..O_2$ | 59.9° | $Hg..O_1$ | 2.96Å |
| $O_2..Hg..O_3$ | 61.9 | $Hg..O_2$ | 2.78 |
| $O_3..Hg..O_4$ | 61.9 | $Hg..O_3$ | 2.79 |
| $O_4..Hg..O_4$ | 59.0 | $Hg..O_4$ | 2.82 |
| | | $Hg..O_5$ | 2.86 |
| $Cl_1–Hg..O_1$ | 87.7 | | |
| $Cl_2–Hg..O_1$ | 88.4 | $C_1–O_1..Hg$ | 112.5° |
| $Cl_1–Hg..O_2$ | 87.2 | $C_2–O_1..Hg$ | 114.2 |
| $Cl_2–Hg..O_2$ | 94.5 | $C_3–O_2..Hg$ | 108.1 |
| $Cl_1–Hg..O_3$ | 97.5 | $C_4–O_2..Hg$ | 109.6 |
| $Cl_2–Hg..O_3$ | 88.2 | $C_5–O_3..Hg$ | 113.2 |
| $Cl_1–Hg..O_4$ | 86.2 | $C_6–O_3..Hg$ | 113.8 |
| $Cl_2–Hg..O_4$ | 97.6 | $C_7–O_4..Hg$ | 111.3 |
| $Cl_1–Hg..O_5$ | 86.2 | $C_8–O_4..Hg$ | 115.8 |
| $Cl_2–Hg..O_5$ | 92.0 | $C_9–O_5..Hg$ | 114.0 |
| | | $C_{10}–O_5..Hg$ | 110.7 |

tances between the Hg and O atoms range from 2.78 to 2.96 Å. All the angles of $Cl_j$–Hg···$O_i$ are 86—98° and the five oxygen atoms of the TGM molecule enclose one Hg atom in the plane nearly perpendicular to the Cl–Hg–Cl direction and passing through the Hg atom. The angles of $O_i$···Hg···$O_{i+1}$ are 59—62°. The five oxygen atoms are located at the five corners of a hexagon with the remaining one corner empty, the Hg atom being located at the center of the hexagon. Since the $C_j$–$O_i$···Hg angles are 108—116° and nearly of a tetrahedral angle, the Hg atom is located at one of the tetrahedral directions of an oxygen atom with respect to the bonded carbon atoms. The above geometry of the coordination indicates that the circular structure of TGM is very favorable for coordination of the O atoms with the Hg atom. Figure 4 shows the structure of the complexed pair projected along the *a* axis.

The chain conformation of TGM in the complex is very similar to that of PEO[3] with respect to the single chemical unit of O–$CH_2$–$CH_2$–. However, since the $CH_2$–$CH_2$ bonds are alternately *gauche* and minus *gauche* in the adjacent $CH_2CH_2O$ groups, the shape of the molecule as a whole becomes open circular in contrast to the helical conformation of PEO which consists of a uniform succession of $\underset{T}{-}CH_2\underset{G}{-}CH_2\underset{T}{-}O$. It has been shown that when PEO forms molecular complexes with $HgCl_2$, the conformation of the asymmetric unit changes either to $\underset{T}{-}O\underset{T}{-}CH_2\underset{T}{-}CH_2\underset{T}{-}O\underset{T}{-}CH_2\underset{G}{-}CH_2-$ (type I)[1] or to $\underset{T}{-}O\underset{G}{-}CH_2\underset{G}{-}CH_2-$ (type II).[2] It might be of interest to compare these conformations with that found in the complex $\underset{T}{-}CH_2\underset{G}{-}CH_2\underset{T}{-}O\underset{T}{-}CH_2\underset{\bar{G}}{-}CH_2\underset{T}{-}O-$. The stability of these conformations will be considered next. With respect to the $CH_2$–$CH_2$ bonds, the *gauche* form may be more stable by about 400 cal/mol than the *trans* form,[15] while for the $CH_2$–O bonds the *trans* form is more stable by 1.2 kcal/mol than the *gauche* one.[16] Consequently, the conformation of TGM in the present complex must be stable as an isolated molecule. The conformational stability of PEO in the type I complex,[1] which contains equal number of *gauche* and *trans* forms of the $CH_2$–$CH_2$ bond, must be next to the most stable form of $\underset{T}{-}CH_2\underset{G}{-}CH_2\underset{T}{-}O\underset{T}{-}CH_2\underset{\bar{G}}{-}CH_2\underset{T}{-}O-$. In contrast to this, the conformation of PEO in the type II complex is less stable as a single chain, since one half of the $CH_2$–O bonds is gauche. This may be clearly understood from Fig. 5, where the five possible conformations of O–$CH_2$–$CH_2$–O–$CH_2$–$CH_2$– are given in the order of decreasing stability from the top to the bottom. The conformations of TGM and ordinary PEO correspond to A, the most stable one. PEO of type I complex corresponds to B, and PEO of type II complex to E.

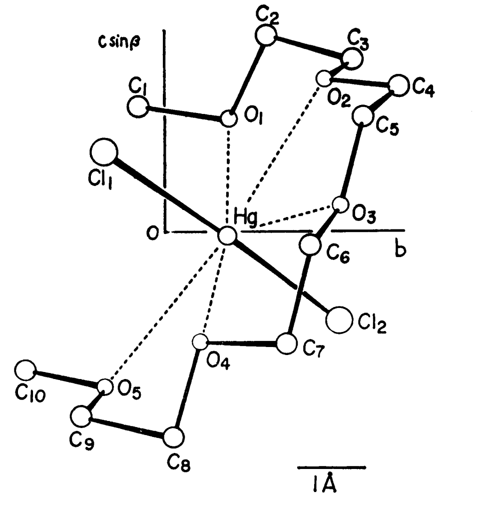

Fig. 4. Structure of one pair of the TGM-$HgCl_2$ complex projected along the *a* axis.

| | | | | | | |
|---|---|---|---|---|---|---|
| | O—C—C—O—C—C— | | | | | |
| A | T | G | T | T | G($\bar{G}$) | T |
| B | T | G | T | T | T | T |
| C | T | T | T | T | T | T |
| D | T | G | T | T | G | G |
| E | T | G | G | T | G($\bar{G}$) | G($\bar{G}$) |

Fig. 5. Possible five conformations for the O–$CH_2$–$CH_2$–O–$CH_2$–$CH_2$– unit. $\bar{G}$ in parentheses indicates alternative possibility for G. A is the most stable and *E* is the least stable conformation.

It is interesting to compare the spatial configuration of the TGM–$HgCl_2$ complex with that of the complex of a cyclic ether with Rb and Na isothiocyanate.[6] In the latter complex, two kinds of molecules are contained in the crystal. One is complexed with the metal ion and the other is free. For the complexed molecule, a Rb or Na ion is enclosed by six oxygen atoms of the cyclic ether molecule, the six oxygen atoms being coplanar. The interatomic distances are 2.73—2.88 Å for Na···O and 2.86—2.93 for Rb···O. Thus, the

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15) J. E. Mark and P. J. Flory, *J. Amer. Chem. Soc.*, **88**, 3702 (1966).

16) H. Wieser, W. G. Lailaw, P. T. Krueger, and H. Fuhrer, *Spectrochim. Acta*, **24** *A*, 1055 (1968).

way of coordination between the cyclic ether molecule and the metal ion is very similar to that found in the TGM–$HgCl_2$ complex.

The fact that the ethers composed of $CH_2CH_2O$, linear or cyclic, form complexes not only with $HgCl_2$ but also with many other metal salts[4] and that a metal ion is coordinated to coplanar five or six oxygen atoms might suggest that the complex is formed by electrostatic forces acting between positively charged metal atom or ion and the negatively charged O atoms, although the tetrahedral arrangement of Hg and O may indicate that some other factors contribute to the coordination.

The angle Cl–Hg–Cl is distorted to 174° from the complete linear form as in the case of the PEO–$HgCl_2$ complexes.[1,2]

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