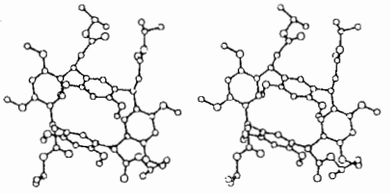
a=11.591, b=12.614, c=16.515, α=97.45, β=101.74 and γ=71.09; isomer D has a=12.483, b=14.022, c=18.123, α=100.59, β=107.40 and γ=71.17. Diffraction data were collected on a CAD4 diffractometer. The structures were solved by direct methods and refined by routine procedures to final R factors of 0.05 and 0.07 for the C and D isomers, respectively. Stereo views of both molecules are given in the Figure.

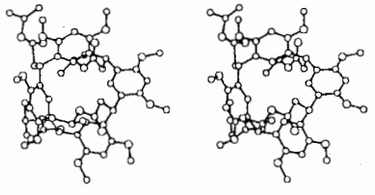
The macrocycle of isomer C can be described as having a 1,3-alternate conformation with an approximate C_{2v} symmetry, in which opposite benzene rings are almost coplanar and successive benzene rings are nearly orthogonal to each other. The C_{2v} symmetry is broken by the four side chain isopropyl ester groups: their relative disposition is cis-cis-cis-cis with different chain conformations.

The macrocycle of isomer D can be grossly described as having 1,2-alternate conformation with an approximate C_s symmetry, generated by an approximate plane of symmetry, bisecting the macrocycle in two halves. The relative disposition of the four isopropyl ester side chain groups is cis-cis-trans-trans and again the chain conformations are different.

The solid state structures of isomers C and D are discussed with relation to NMR results and to molecular mechanics calculations.



Isomer C



Isomer D

References

Botta, B., Iaconacci, P., Di Giovanni, G., Delle Monache, G., Gacs-Baitz, E., Botta, M., Tafi, F., Corelli, F. and Misiti, D. (1992). J. Org. Chem. 57, 230-235.

OPS-07.01.09 HOW METAL ION CHARACTER CONTROLS THE COORDINATION MODE OF POLYETHYLENE GLYCOL. Robin D. Rogers*, Department of Chemistry, Northern Illinois University, DeKalb, IL 60115, USA.

Our work investigating polyethylene glycol (PEG) complexation of the lanthanides and actinides has recently been expanded to Group 1 and 2 cations, as well as to the environmentally toxic heavy metal ions Hg^{2+}, Pb^{2+}, Bi^{3+}, and Cd^{2+}. Ready complexation of the PEGs with the metal ions we have studied has resulted from the flexibility of the acyclic PEG chain and the chelating nature of the donor interactions. In addition, the alcoholic termini of PEGs provide sites for hydrogen bonding which has proven to be an interesting facet of this ligand's coordination chemistry. The supramolecular networks generated by hydrogen bonding to solvent molecules, anions, and other PEG ligands add to the intricacy of the observed structures.

This presentation will survey our structural results for PEG/metal complexes and reveal three primary coordination modes for PEG. Helical wrapping is most commonly observed for the hard oxophilic cations Y^{3+}, La^{3+}, the lanthanides, and Group 1 and 2 cations, while a pseudo-planar template arrangement is commonly observed in Pb^{2+}, Hg^{2+}, and Cd^{2+} complexes. Out-of-cavity pseudo-cyclization closely resembling out-of-cavity crown ether coordination is prominent for the softer Bi^{3+}, and has recently been observed in a single Cd^{2+} structure. We have primarily used chloride or nitrate salts in the preparation of these complexes and the influence of anion will also be discussed.

OPS-07.01.10 NEW CLATHRATE-TYPE STRUCTURES OF TETRALKYLAMMONIUM HALOGENIDE HYDRATES by J.Lipkowski, Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44, 01 224 Warszawa, Poland

Since the pioneer studies of Jeffrey et al. (cf. e.g. review in "Inclusion Compounds", vol.1, Acad. Press) a general structural pattern of clathrate type hydrates of tetralkylammonium fluorides is known as composed of anionic host framework incorporating fluoride ions in the water lattice of hydrogen bonds and tetralkylammonium cations occupying large cavities; the latter being formed by combining polyhedra typical for clathrate hydrates. It is assumed that if an alkylammonium ion does not fit the cavities which may be available, then no solid clathrate can be formed. This is not, in general, true, as recently demonstrated in phase present paper in which data of structural investigations performed on samples prepared by Dyadin's group are reported. In the present paper a series of hydrate structures having water framework structure gradually more and more distorted is given. The series begins with a cage-type structure in which square planar faces of water hydrogen-bonded polyhedra are observed [J.Lipkowski et al., JIPh, 9(1990),275]. Next example represents somewhat more open structure in which guest cations (tetraethylammonium) are arranged along open channels in the water framework. By increasing the molar content of ammonium salt a layered structure was obtained between water molecules is preserved only partially [J.Lipkowski et al. JIPh, 13(1992),295]. And, when going on to increase the clathrated amount of ammonium salt just two-dimensional pattern of the host is observed.

A variety of different structure types and stoichiometries (most part to relate the unpublished yet) will be demonstrated and an attempt to relates the clathrate hydrate structures to hydration patterns of some crown-peptide complexes will be illustrated.

