

**COMPARISON OF CRYSTAL STRUCTURES OF INCLUSION  
COMPLEXES OF DEOXYCHOLIC ACID AND THOSE OF  
APOCHOLIC ACID**

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Deoxycholic acid (DCA) and apocholic acid (ACA), which belong to bile acid, form inclusion complexes of a channel type with a wide variety of organic molecules. Some polymers can be also accommodated into the channel to form the inclusion complexes. The unit cell dimension, *a*, of the DCA complex with ploy(propylene glycol) (PEG) which has methyl side groups is about 0.1 nm longer than that of polytetrahydrofuran (PTHF) which has no side group. However, the values of *a* are similar each other in the complexes of ACA with these polyethers. Though the inclusion complex of DCA with 3-methyl cyclohexanone [1] has large unit cell similarly to PPG, the dimension, *a*, in the ACA complex of this bulky small molecule is comparable to those in the ACA complexes of PPG and PTHF.

## References

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**Keywords: INCLUSION COMPLEX, DEOXYCHOLIC ACID, APOCHOLIC ACID**

**COMPLEXES OF 1,3-ALTERNATE CALIX[4]ARENES WITH  
SILVER CATION**

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Compounds named calixarenes are known more than one century. Various derivatives of calixarenes show very interesting complexing properties towards cations, neutral molecules or anions. These compounds are synthesized in all possible conformations achieving thus higher selectivity [1]. The group of calix[4]arenes derived from 1,3-alternate tetrapropoxycalix[4]arene was studied in the solid state. The derivatives varied only in substitution of the upper rim. All di-substituted derivatives show interesting complexing properties towards silver cation. Single crystals of the complexes of dibromo-, diphenyl-, tert.butyl- derivatives and unsubstituted tetrapropoxycalix[4]arene with silver triflate were prepared. Their structures were determined by single crystal X-ray structure analyses. All these derivatives create complex 1:1 with silver cation. Silver cation is complexed directly inside the cavity in these complexes. In the dependence on the size of the substituent complexes represent dimers or individual molecules in the molecular packing. Tetrapropoxycalix[4]arene is the only exception forming with silver triflate complex 1:2 and creating infinite channel in the molecular packing. The conformation analysis shows that the substituent size does not influence the resulting cavity shape of the calix[4]arene. The cavity shape is the same in all cases. Upper rim substituent affects only the forming of dimers in the molecular packing.

## References

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**SELF-ASSEMBLED CALIX[6]PYRROLE CAPSULES**

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The host-guest chemistry of calixpyrroles has recently become the subject of intensive research due to their ability to complex and recognize anionic guest species. Meso-hexapenyl-calix[6]pyrrole was synthesized and the complex formation with halide ions as well as with trihaloalkanes and electron deficient aromatic systems were studied.

Several inclusion-type molecular complexes of calix[6]pyrrole with molecules of different size and chemical character were obtained and characterized by X-ray diffraction. Preorganized dimeric capsules are found to host different organic molecules.

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**THE MOLECULAR STRUCTURE OF AMPHOTERIC  
THEOPHYLLINE**

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There is considerable interest in the structures of methylxanthines such as theophylline owing to their pharmacological use. This drug and its close relatives are used to treat bronchial asthma, chronic bronchitis, emphysema, cystic fibrosis, etc. Structural study of these compounds can also provide better understanding of their possible genetic role and/or antitumour activity. The solubility of theophylline in water can be increased by either basic or acidic additives. From the solutions prepared with solubility enhancing additives, usually various inclusion compounds of theophylline are crystallised. We prepared four clathrates and determined their crystal structures and made analytic characterisations. Theophyllinate anion is present in the inclusion compounds with ethanalamine (1:1) and 1,4-diamino-butane (2:1). Theophylline is neutral in the complex with ethylenediamine carbamate (1:1). Theophyllinium cation exists in the crystal of theophyllinium salicylic acid 5-sulfonate monohydrate (1:1:1). The ionic character of theophylline and its derivatives in the clathrates is tuneable by the environment. All structures containing theophylline moiety were retrieved from the Cambridge Structural Database and their bonding and conformation compared.

**Keywords: THEOPHYLLINE CLATHRATES CAMBRIDGE STRUCTURAL DATABASE**