MOLECULAR ARRANGEMENTS OF ALKYL-AMMONIUM SALTS AND AROMATIC ADDITIVES IN THE COMPLEX CRYSTALS. Keiichi Noguchi, Kultitha Vongbupnimit, Shigehiro Kamitori and Kenji Okuyama, Faculty of Technology, Tokyo University of Agriculture and Technology, Koganei Tokyo 184, Japan.

Recently, it has been found that some amphiphilic molecules such as ammonium salts, phosphonium salts and other onium salts have the specific abilities to form complexes with aromatic molecules. In some cases, the formation of complexes can be prepared simply by mixing both powders of amphiphilic and aromatic molecules in a mortar (Toda, F. Tanaka, K., Okada, T., Boums, S. A. & Nassimbeni, L. R., Supramol. Chem., 1994, 3, 291-298). We have been investigating the crystal structures of various amphiphiles (host) and aromatic molecules (guest) by X-ray diffraction method in order to clarify the structural details and interactions between host and guest molecules (Vongbupnimit, K., Noguchi, K. & Okuyama, K., 1996, Mol. Cryst. Liq. Cryst., in press). In the present work, the molecular arrangements in the complex crystals of dodecylmethylammonium chloride (DTAC) and four aromatic molecules, namely, hydroquinone(1), catechol(2), p-iodophenol(3), and p-phenylphenol(4) will be discussed.

All the four complex crystals show the smectic layer arrangement in which the host amphiphiles are mutually interdigitated and make some space for guest molecules between the parallel alkyl chains. Two types of molecular packings of DTAC and the guest molecules were observed. In the case of complexes 1 and 2, the aromatic ring of the guest molecule is parallel to the zigzag plane of the alkyl chain of the host molecule. Interaction between the guest molecules in these complexes is one-dimensional and very different from those in the guest crystals. On the other hand, the packings of host and guest molecules in the complexes 3 and 4 are found to be some kind of herringbone arrangement. A similar packing has also been observed in the crystal structures of the guest molecules. Also the transition temperature and the shape of the endothermic peak in DTA curves of complexes 3 and 4 are similar to those of their respective guest crystals. These results indicate that the specific interactions between the aromatic molecules in the guest crystals are kept even in the complex crystals. We termed the packing of 1 and 2 as ‘host-dependent packing’, and that of 3 and 4 as ‘guest-dependent packing’.

NOVEL HYDROGEN-BONDED HOST LATTICES IN INCLUSION COMPLEXES OF UREA AND PERALKYLATED AMMONIUM PENTABORATE SALTS. Thomas C.W. MAK* and Qi Li Department of Chemistry, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong, China.

As a sequel to our continuing research program in the rational design of new urea/thiourea-anion host lattices,1,2 two novel inclusion compounds containing hydrogen-bonded host networks constructed from urea and nonplanar pentaborate anions, (n-C5H5)3N[B3O8(OH)4]·2H2O(1) and (n-C5H5)3N[B3O8(OH)4]·3H2O(2), have been prepared and characterized by X-ray crystallography.

Compound 1 has a channel-like host lattice built of urea molecules, pentaborate ions and water molecules in a molar ratio of 4:1:1, and the (n-C5H5)3N+ cations (represented by large circles) are arranged in a zigzag column within each channel (Fig. 1). Compound 2 features a two-dimensional open host network in which two channel systems extend parallel to the [101] and [010] directions, such that the (n-C5H5)3N+ cations are accommodated in a stacked column within each channel of the first type (Fig.2) and in a zigzag column within each channel of the second type (Fig.3).