Temperature Dependent Selectivity of Inclusion

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Trans-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic acid (DEDA) is a versatile host, capable to form inclusion complexes with both polar and non polar solvents[1]. At the room temperature this compound is crystallized from solutions in acethophenone as a host-guest complex with a ratio 2:3. In the crystal structure DEDA molecules form infinite chains in a direction [01-1] through a pair of centrosymmetric hydrogen bonds. The acethophenone molecules are situated inside different channels formed at stacking of these chains and running along [100] and [0-11] directions.

At decreasing of crystallization temperature until 5°C from the same solution DEDA crystallizes as new complex - hydrate with 1:3 host-guest ratio. In the crystal structure one carboxylic group of DEDA molecules is connected via centrosymmetric H-bonding with the carboxylic group of the other host molecule, while other carboxylic group is deprotonated giving rise to a network of intermolecular H-bonds associating with one ion of hydroxonium (H_3O^+) and two molecules of water. The structure may be described as intercalate type complex with strict separation of the hydrophobic and hydrophilic areas.

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[1] Weber E., Csöregh I., Ahrendt J., Finge S., Czugler M., J. Org. Chem., 1988, 53, 5831-5839.

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