

m27.p06

Formation of resorcinarene complex in binary solvent systems. X-ray structure of resorcinarene-acetone-hexane solid solution

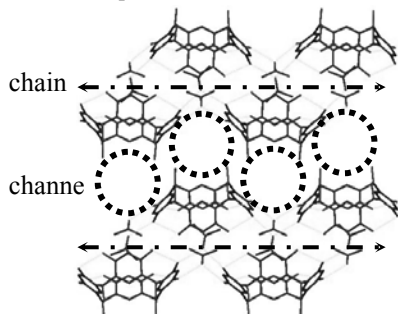
Dariusz Swierczynski^a, Vitaly I. Kalchenko^b, Janusz Lipkowski^a

^a *Institute of Physical Chemistry, PAS, Warsaw, Poland,* ^b *Institute of Organic Chemistry, NASU, Kiev, Ukraine*

Keywords: resorcinarene, solvate, channel

Majority of chemical processes associated inter alia with supramolecular chemistry is carried out in the environment of chosen pure solvent or component solvent systems. So that knowledge of the structure of aggregates formed by investigated compound with solvent molecules is essential. This fact is especially important in the case of complex compounds-host applied in supramolecular chemistry.

In this paper we present the crystal structure of solid solution of resorcinarene in acetone-hexane binary solvent system. The crystallization process lead to colorless crystals of [C-methyl resorc[4]arene • acetone] • acetone • n-hexane solvate with well formed natural faces ($a=9.9529$, $b=13.7824$, $c=29.2534$, $\beta=99.482$, P21/c). Acetone molecule is slipped into the macromolecular cavity of resorcinarene host possessing flattened cone conformation. Nonetheless the acetone molecule is obliquely positioned and included inside the cavity not as deep as it is observed for typical C-methylresorcinarene-acetone inclusion complexes. Discussed guest molecule takes part in formation of acceptor bifurcated hydrogen bond with two resorcinarene molecules placed above the complex moiety. The second not complexed acetone molecule participates in formation of acceptor bifurcated hydrogen bonds with resorcinarene as well. As a consequence infinitive chains consisting of two acetone molecules per calixarene unit are formed. Chains pack parallel in the crystal lattice along b axis in the fashion of Atwood's organic clays. Packing of the chains of a complex topology into layered mode lead to the formation of semi-channels along a crystallographic axis enclosed by the alkyl groups of the resorcinarene host and carbonyl group of acetone molecule. The channels are filled by the acetone and n-hexane molecules, which occupy well-defined positions in close proximity of four alkyl groups of resorcinarene molecule (and in the depression of the acetone-resorcinarene chain on the other side). The molecules taking up the position inside the channel are disordered with occupancy factor of value 63.5% for n-hexane and 36.5% for acetone. That indicates that these molecules fill channel in random manner with the preference of n-hexane.



(molecules filling channels removed for clarity)