

Study of the Pseudopolymorphism in the Host-Guest Systems

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A specific feature of versatile host compounds is their ability to form various host-guest complexes with the same guest species (pseudopolymorphism). The conventional way for pseudopolymorphism detection and preparation is to carry out crystallization under various conditions (pressure, supersaturation, temperature, etc.). The clathrate formation was used at different temperatures keeping other parameters of the crystallization medium the same. In order to study the host versatility and pseudopolymorphism phenomenon the corresponding host compound was dissolved in the respective guest solvent and kept under definite temperatures for crystallization. Host-guest ratio was determined by NMR-integration and in some cases by thermogravimetry. Stability of the crystals was assessed using Kofler thermomicroscopy. The pseudopolymorphism have been found in the clathrates between 1,1'-binaphthyl-2,2'-dicarboxylic acid (BNDA) with dimethyl formamide (DMF) and 2,2'-bis(9-hydroxy-9-fluorenyl)biphenyl (BHFB) with acetone (AC). The compounds of BNDA and BHFB exist in the α , β , γ and α , β , γ , δ temperature modifications, respectively. In order to analyse the crystal packing of given molecules the special method based on the point representation of molecules has been developed. The conformational search has been carried out for given compounds as a tool for finding the stable structures of molecules, using stochastic approaches based on modification of torsion angles in the framework of the program SPARTAN 5.1.3. The rotation of molecules' fragments performed around the ordinary bonds connecting them. The molecular dynamic simulation has been performed in order to investigate the behaviour of studied compounds under the crystallization temperatures with the aid of the SYBYL 6.5 program. The calculation of molecular interaction energy within of studied crystals has been applied using the attachment energy technique based on CVFF force field. It is shown that fragments of BNDA and BHFB molecules possess the significant dipole moments therefore the small modifications in the conformation of the molecule caused by rotation of these moieties lead to significant variations of the whole molecular dipole moment. This peculiarity may be responsible for the unique

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