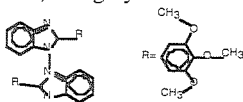


PS06.06.08 INCLUSION INDUCED RESOLUTION OF A BIS-BENZIMIDAZOLE DERIVATIVE BY ACHIRAL ACIDS. By Petra Bombicz and Mátyás Czugler, Central Research Institute for Chemistry, Hungarian Academy of Sciences, H-1525 Budapest 114, POB 17, Hungary.



Crystallization of 2,2'-bis-(3,4,5-trimethoxyphenyl)-1,1'-bibenzimidazole (1) with simple acids such as formic (a), acetic (b), propionic (c), butyric (d) and trimethyl-acetic (e) acid yields to spontaneous resolution in the case of acetic and propionic acids due to inclusion formation (Table) with stoichiometry always 1:2 only. X-ray diffraction structure analyses of these solid associates offer a rationale for this behavior of these five cases.

Analysis of the packing motifs enlightens a possible reason for enantiomer resolution. There are helices of host molecules close packed through inversion centers. The enantiomerically opposite molecules crystallize in different columns placement of which are governed by steric and a multiple of other weak electronic effects. The central methoxy group is the very place which is influenced by the presence and size of an additional acid component. Molecular graphics analyses reveal that the host conformation is hardly changed (1a, 1b, 1c, 1d) thus crystal building is the subject of the interactions of a steady host molecule with the varying guests.

Inclusion	1 ⁽¹⁾	1a	1b	1c	1d	1e
Space group	C 2/c	C 2/c	P3 ₁ ,21	P3 ₂ ,21	C 2/c	C 2/c
L.S. fit [Å]	0	0.096	0.070	0.054	0.046	0.704

* Least Square fit of the host molecule in the asymmetric unit.
 [1] Speier, G.; Párkányi, L.: *J.Org.Chem.* 51, 218, 1986.

PS06.06.10 POLYMORPHISM OF THE GOSSYPOL INCLUSION COMPLEXES. B.T.Ibragimov, Z.G.Tiljakov, S.A.Talipov, K.M.Beketov. Institute of Bioorganic Chemistry, H.Abdullaev str., 83, Tashkent, 700143, Uzbekistan
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The inclusion compound formation by gossypol, biologically active substance of cotton, was studied at different thermodynamic conditions. Most of investigated guests form with gossypol more than one inclusion compound. Very often occurred polymorphism of the gossypol host-guest formation with the same guest is dimorphism and thrimorphism. Several examples of such polymorphism will be given. In the case of dichloromethane host-guest complexes of gossypol at different temperatures has been investigated for the same pressure and concentration. Gossypol forms 3 different clathrates within temperature interval 22-36 C. Single crystals of these three modifications (phases) were obtained. The structure of alpha-phase was earlier determined and gamma-phase is isostructural to the inclusion complexes of gossypol with benzene. The structure of a beta-phase have been solved now and will be discussed. At ambient conditions gossypol forms unstable tubulates of an alpha-phase; high temperature gamma-phase is stable cage type clathrate and host-guest complex of a beta-phase is a clathrate of intermediate tubulato-cryptate type.

PS06.06.11 PHOTODIMERIZATION REACTION OF COUMARIN IN COMPLEX CRYSTALS WITH CHIRAL HOST DERIVED FROM TARTARIC ACID. Ikuko Miyahara*, Yoshitaka Nakajima*, Ken Hirotsu*, Koichi Tanaka**, and Fumio Toda** Faculty of Science, Osaka City University*, Faculty of Engineering, Ehime University**

The chiral hosts molecules derived from tartaric acid have been reported to make the inclusion complexes with various kinds of guest molecules and used as chiral handles to control the stereospecificity of the reaction on the basis of the asymmetric environment around the guest molecules in solid state. Photodimerization of coumarin (2H-1benzopyran-2-one) in solution does not proceed stereospecifically. On the other hand, the inclusion crystals between the chiral hosts (-)- bis (hydroxydiphenylmethyl)-2,2-dimethyl-1,3-dioxacyclopentane (1) and coumarin were irradiated to give the products in a stereocontrolled manner. In order to elucidate the relationship between the reactivity, arrangements of guest molecules, and intermolecular interactions, X-ray studies of these complex crystals were undertaken.

The complex of (-)-(1) and coumarin crystallized as monoclinic (C2) and triclinic (P1) forms from ethylacetate and toluene, respectively. On the irradiation of these crystals, the chiral dimer was obtained from the monoclinic form and the achiral dimer from the triclinic forms. The racemic complex crystal (P1) between (+)-(1) and coumarin was also irradiated, but no photoproduct was detected. The mechanism of reactivity and stereochemical control will be presented.