molecular packing structure of the guest amines was dependent on the structure of the guest amines. Next, we investigated the intercalation behavior of azobenzene derivatives, which were designed based on the intercalation characteristic of several guest amines previously reported. In the present study, azobenzene derivatives containing amino and diamino groups were synthesized and used as the guest for the intercalation. The intercalation of azobenzene derivatives into the interlayer space of poly(muconic acid) crystals was successfully carried out by the dispersion method. We investigated the intercalation and photoisomerization behaviors depending on the structure of the used azobenzene derivatives.

Keywords: intercalation materials, organic crystals, photochemistry

P08.04.22

Fabrication of thin-film organic crystals by vapor deposition and their solid-state polymerization

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The solid-state polymerization of unsaturated monomers is one of the useful methods for the synthesis of polymers with a highly controlled structure. In particular, topochemical polymerization has unique features, such as complete tactility control and the in-situ fabrication of polymer crystals. We previously reported the topochemical polymerization of some derivatives of muconic and sorbic acids as the 1,3-diene monomers in the solid state under photoradiation, which produced stereoregular polymers in the form of polymer crystals. The polymerization reactivity and the structure of the resulting polymers are strictly determined by the monomer crystal structure, that is, the fashion of the molecular arrangement in the monomer crystals. However, the polymorphism often prevents us designing the organic solid materials and controlling their physical properties. In the present study, we have fabricated the organic thin films of bis(3,4-methylenedioxybenzyl) (E,E)-muconate by the vapor deposition method in order to control crystal growth and crystal structures using interaction between the surface of a substrate and the monomer molecules. We have investigated the structure of the obtained thin films of the monomer crystals by AFM observation, IR spectroscopy, and powder X-ray diffraction measurements. The polymerization was carried out in the solid state under UV or gamma-ray radiation. The epitaxial crystal growth on various substrates, the polymerization reactivity of the obtained thin films, and the control of polymer structures are discussed.

Keywords: topochemistry, epitaxial growth, polymer synthesis

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Photocyclization of isopropylbenzophenone derivatives in crystals and the shape changes

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Crystalline state photocyclizations and the morphological changes of isopropylbenzophenone derivatives were investigated. We found diastereospecific photocyclization via single-crystal-to-single-crystal transformation. Absolute asymmetric photocyclization was also achieved. The surface morphological changes of the crystals were traced by atomic force microscopy on photoradiation.

Keywords: photocyclization, isopropylbenzophenone derivatives, morphology change

P08.04.24

Solvent inclusion induces helical molecular assembly in crystals of halobenzoates of myo-inositol

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Reactions in crystals often proceed with high facility, regio- and stereo-selectivity due to topochemical control as compared to those in solution. Earlier, we reported clean solid-state benzyol transfer reactions in crystals of racemic 2,6-di-O-benzyol myo-inositol 1,3,5-orthoesters [1]. Structure correlation studies [2] suggest that pre-organization of the electrophile (El) and nucleophile (Nu) close to tetrahedral angle 110 °C at a distance of about 3 Å is essential for reaction to occur. Structures of reactive orthoesters revealed helical self-assembly of the molecules via O-H···O hydrogen bonds bringing electrophile (-C=O) and nucleophile (-OH) in favourable proximity with weak interactions supporting the migrating group. To investigate molecular organization and solid-state reactivity further, racemic 2,6-di-O-(4-halobenzyol)-myo-inositol 1,3,5-orthofomrate (halo = fluoro, chloro, bromo) were synthesized. Solvent free crystals obtained from methanol and ethyl acetate [3] did not possess the right organization for acyl transfer; however, inclusion crystals from almost all common organic solvents revealed a helical self-assembly of host molecules linked via O-H···O hydrogen bonding with El···Nu geometry close to that observed for reactive orthoesters [1]. One of the inclusion crystals with favorable geometry exhibited neat acyl transfer reaction.


Keywords: solid-state reactions, inositols, inclusion crystals

P08.04.25

Oxide and metal silicide precipitation on structural defects in mc silicon studied by TEM

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