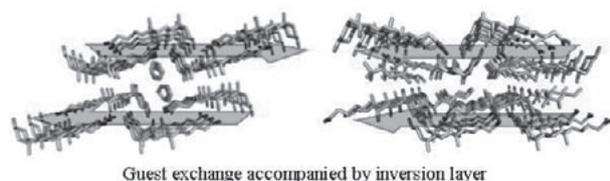


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Solid-state dynamic properties contribute to development of gas sorption and storage materials with microporous coordination polymers. Organic crystals function as dynamic materials due to their flexibility and diversity. We study on steroidal bile acid derivatives which serve as host components and form dynamic inclusion crystals for intercalation and enantioresolution of guest molecules. So far, we reported that cholamide has various types of flexible bilayers where secondary aliphatic alcohols are accommodated. Among them, 2,2-dimethyl-3-hexanol induces a rare bilayer structure which is responsible for high enantioselectivity. Here we present intercalation and enantioresolution of 2,2-dimethyl-3-hexanol by using inclusion crystals of cholamide with 1,4-dioxane. It was found that guest exchanges took place with retention of the crystalline state in appearance. The crystal structures were determined before and after the intercalation by means of powder X-ray diffraction, indicating that the intercalation accompanied layer inversion on the lipophilic sides of the bilayers. Moreover, it was found that the resulting crystals include (*S*)-2,2-dimethyl-3-hexanol in over 95% ee yield.



Keywords: inclusion compound, chiral recognition, intercalation

P06.07.28

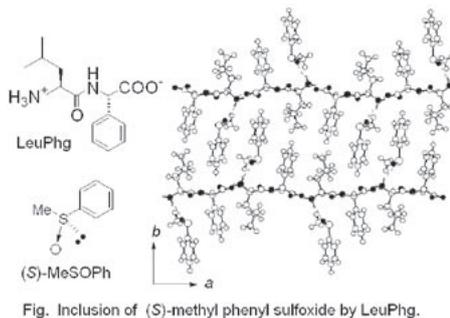
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Enantioselective inclusion of methyl phenyl sulfoxides by (*S*)-alkylglycyl-(*S*)-phenylglycine

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As dipeptide host molecules, (*S*)-alkylglycyl-(*S*)-phenylglycines were examined in terms of enantiomeric inclusion for racemic methyl phenyl sulfoxides. Among them, (*S*)-leucyl-(*S*)-phenylglycines (LeuPhg) and (*S*)-isoleucyl-(*S*)-phenylglycines (IlePhg) mainly included *S*-form of methyl phenyl sulfoxides with high enantioselectivity. By single crystal X-ray analyses of these inclusion compounds, it was elucidated that the dipeptide molecules self-assembled to form layer structures and included the sulfoxides between these layers by hydrogen bonding between the proton of $^+NH_3$ and the oxygen of the sulfoxide. In the cavity, *C*-terminal phenyl group of the dipeptide interacts



with the phenyl group of sulfoxides. In addition to these host-guest interactions, the two homochiral sulfoxides belonging in upper and lower layers make a pair having 2-fold rotation axis or 2-fold screw axis along the channel cavity. In other words, the self-recognition of sulfoxides made a homochiral pair to achieve high enantioselectivity.

Keywords: inclusion compounds, dipeptides, molecular recognition

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Structure and polymorphism of trans mono-unsaturated triacylglycerols

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Trans fats are in a natural way in small quantities present in animal foods. Moreover, unsaturated plant fats are often partially hydrogenated to raise melting temperatures for preparation of foods, and then, as a minor side reaction, a small part of the *cis*-bonds will change into *trans*-configuration. Like saturated fats, fats with *trans* fatty acid residues will have negative effects for human health (1). The presence of the elaidoyl chain, one of the major *trans* fatty-acid chains, is suspected of increasing health risks because it resembles the stearoyl chain. When incorporated in biological membranes elaidoyl chains will be influencing the physical-chemical properties of the membranes. Thus insight in the influence of the differences between the fatty-acid composition of *trans* and saturated triacylglycerols (TAGs) on the conformation and packing, on polymorphic stability, and on phase-transition behavior, will be useful. By combining X-ray powder diffraction (XRPD) techniques a better understanding of *trans* mono-unsaturated TAGs and their related saturated ones can be obtained. Synchrotron and advanced laboratory time- and temperature-resolved XRPD reveal the stability and phase-transition behavior of the important polymorphs like the β and β' . These results can be related to the underlying crystal structure packing that can be obtained from XRPD data using direct-space search techniques. Our recent results will be discussed including novel meta-stable β' polymorphs and the structure of one them, methyl-end plane packing analysis in relation to observed melting points for various subgroups of TAGs, and the difference in β' to β phase-transition behaviour of symmetric versus asymmetric TAGs.

(1) The EFSA Journal, 2004, 81, 1-49

Keywords: *trans* mono-unsaturated triacylglycerols, time-temperature-resolved diffraction, powder structures

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Polymorphism and structure solution from powder data of *N,N'*-1,4-phenylene-bis(3-oxobutanamide)

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N,N'-1,4-Phenylene-bis(3-oxobutanamide) (**1**) is an industrial intermediate which is used as a coupling component in the synthesis