acids is an important challenge. The structure-forming units in the crystals of amino acids are similar to those in the biopolymers: robust head-to-tail chains of molecules linked by hydrogen bonds are preserved even on polymorphic transformations. Packing of the head-to-tail chains can mimic polypeptide structures: helical structures, b-sheets, amiloids. Knowledge about the temperature and pressure-induced changes in these crystals can help to understand better the contributions to the dynamic properties of proteins related to the intrinsic motions of structural fragments. Besides, crystalline amino acids are important materials with non-linear optical and piezoelectric properties. The structures and properties of the chiral and racemic crystals of amino acids are remarkably different. In the present contribution we illustrate this using several selected examples (L- and DL-serine, L- and DL-cysteine, L- and DL-alanine, L- and DL-phenylalanine, L- and DL-phenylglycine) studied at variable temperatures (the range 3-450 K) and variable pressures (up to 1-10 GPa, depending on the compound and the technique) by single-crystal and powder X-ray diffraction, IR-, Raman, inelastic neutron scattering spectroscopy, and calorimetry. The differences in the structural response to variations in temperature and pressure (different values of compressibility and thermal expansion, different strain anisotropy, different stability with respect to phase transitions induced by cooling, heating or increasing pressure). The study was supported by Integration projects #49 and #110 of SB RAS, a grant from RFBR (05-03-32468) and grants from BRHE (NO-008-XI and RUX0-008-NO-06).

Keywords: crystalline amino acids, structure-properties relations, head-to-tail chains

MS.14.3

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Chiroptical properties of *N*-benzoylglycine crystals

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Despite the fact that *N*-benzoylglycine is an achiral molecule, chiral crystal is spontaneously formed. The molecules are helically arranged through the hydrogen bond chains in the crystal. We measured the optical rotatory dispersion by High Accuracy Universal Polarimeter (HAUP). The magnitudes of optical rotation along the helical axes were larger than those perpendicular to the helical axes.

Keywords: chiroptical properties, N-benzoylglycine crytals, chiral crystal

MS.14.4

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A solution to the problem why chiral hydrophobic amino acids form crystals with Z’ = 2

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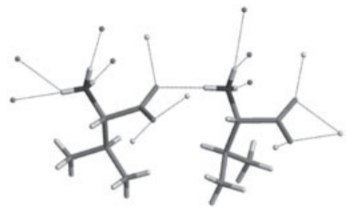
Chiral amino acids that do not have functional groups in their side chains (hydrophobic amino acids) regularly form crystals with two molecules in the asymmetric unit (with different side-chain conformations as shown for L-valine). In contrast, racemates of the same compounds always form crystals with Z’ = 1. What is the origin of the difference between enantiomeric and racemic crystals? No attempts have apparently been made to answer this fundamental question concerning the essential building blocks of life. The present investigation shows that by using a combination of crystallographic, statistical and theoretical methods it is indeed possible to explain the observed behaviour, and furthermore tell why these amino acids do not undergo racemic separation upon crystallization, but rather choose to form racemates in the solid phase.



Keywords: *ab-initio* calculations, amino acids, crystal packing

MS.14.5

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Control of chirality by spontaneous crystallization and absolute asymmetric synthesis in fluid media

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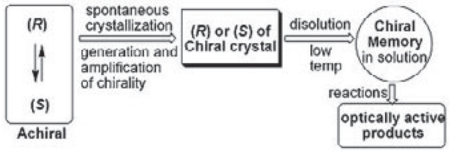
Asymmetric generation influenced by a chiral crystalline environment is considered an attractive methodology for obtaining optically active compounds from achiral compounds. In recent years, the solid-state photochemical reaction using chiral crystals in a variety of new systems has progressed to such an extent that it can now be regarded as an important branch of organic chemistry. Furthermore, a new methodology using molecular chirality in crystal as a source of chiral memory in solution was explored. The chirality can be effectively transferred to optically active products by asymmetric reactions involving a nucleophilic carbonyl addition and intermolecular photochemical reaction. Now we have found that achiral coumarin-3-carboxamide crystallized in a chiral fashion, and the molecular chirality could be transferred to products by intermolecular 2+2 photocycloaddition reactions, cyclopropanation, and the reaction with carbenes in fluid media with high enantiomeric excesses.



Keywords: chiral space groups, asymmetric synthesis, organic synthesis

MS.15.1

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Small beams can play big roles in macromolecular crystallography

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