COMBINED X-RAY DIFFRACTION AND RAMAN SPECTROSCOPY STUDIES OF PHASE TRANSITIONS IN CRYSTALLINE AMINO ACIDS AT LOW TEMPERATURES AND HIGH PRESSURES. SELECTED EXAMPLES.

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Crystalline amino acids are interesting as molecular materials (ferroelectrics, piezoelectrics, non-linear optical materials), drugs, and also as biomimetics, which can be used to study the structure and dynamics of molecular fragments of biopolymers [1]. The structure-forming units in the crystals of amino acids – head to tail chains of amino acids linked by hydrogen bonds – are similar to those in peptides [2]. The motions of molecular fragments of the amino acids – either as residues in the peptides, or as zwitter-ions in the crystals – is important for dynamic transitions in these systems (conformational changes related to biological functions in biopolymers; phase transitions in crystalline amino acids). The motions of different groups have different temperature and pressure dependence, what is important for biological functions of biopolymers [3], and manifest themselves differently when spectroscopic or diffraction techniques are used. Diffraction techniques give direct information on the average positions of atoms (first of all –and pressure. Spectroscopic techniques have an obvious advantage, as far as the estimates of the energies of intermolecular interactions and the studies of dynamics of molecular fragments are concerned. In the present contribution the advantage of complementing diffraction and Raman spectroscopy studies will be illustrated at several selected examples: low-temperature [4-6] and high-pressure [7] phase transitions in L- and DL-cysteine, low-temperature [8,9] and high-pressure [10,11] phase transitions in β-glycine, a high-pressure transition in γ-glycine [12-14], a high-pressure phase transition in β-alanine [15], low-temperature [16,17] and high-pressure [18,19] phase transitions in L-serine.

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