Poster Presentation

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Effect of high pressure on the crystal structures of sarcosine and betaine

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It is well known that infinite head to tail chains built of zwitterions linked to each other by N-H...O hydrogen bonds are common structural motifs in crystals of amino acids. These chains coincide with directions of the smallest compressibility of a crystal structure on cooling and increasing pressure and can even remain after structural phase transitions. However one should take into account the dual nature of these chains. From the one hand zwitterions of amino acids are linked by N-H...O hydrogen bonds formed from the head, amino group, and the tail, carboxylate group. From the other hand besides hydrogen bonding there is electrostatic interactions which occur between positively charged amino group and negatively charged carboxylate group. Being guided by an idea to distinguish electrostatic contribution from the charge assisted N-H...O hydrogen bonds and to understand their role in the crystal structure distortion on increasing pressure, two crystal structures of N-methyl derivatives of the simplest amino acid glycine are considered as a case study. N-methylglycine or sarcosine has two donors for hydrogen bonding and so forms two infinite head to tail chains in the structure whereas N,N,N-trimethylglycine or betaine has no hydrogen bonds at all, but its zwitterions are lined up resembling head to tail chains. The effect of increasing hydrostatic pressure is different for two crystals. The structure of betaine compresses anisotropically, but sarcosine undergoes a phase transition accompanying crystal fragmentation and changes in N-H...O hydrogen bonds. The phase transition is kinetically controlled and strongly depends on the rate of variation of pressure. Of special interest is distortion of head to tail chains on increasing pressure comparing with those observed in polymorphic modifications of glycine.

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