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Effect of high-pressure / low temperature on cysteine, its salts and derivatives

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Structure-property investigation of crystalline amino acids is an important challenge since interactions between individual molecular fragments or even structural domains in the structure can simulate interactions in more complicated biological systems such as proteins and peptides. Besides, crystalline amino acids are applied as drugs, as piezoelectric and nonlinear optical materials. Therefore understanding a crystal structure response to variation in temperature and pressure is significant in such applications.

Cysteine is a remarkable amino acid because its side-chain residue contains a sulfhydryl group involved in formation of additional labile hydrogen bonds (S-H…S or S-H…O). The presence of these very weak bonds in the structure allows cysteine to take a peculiar place between hydrophobic (no contribution of side-chains to H-bonds) and hydrophilic amino acids (with that contribution).

In the present contribution we discuss an evolution of chiral and racemic cysteine crystal structures on cooling and on increasing pressure followed by X-ray crystallography and Raman spectroscopy. We also compare their behavior with that of cysteine crystalline salts and derivatives.

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NH···N hydrogen bonds in high-pressure phase of imidazole

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Imidazole is a prototypic compound were molecules in crystal are linked in infinite NH···N bonded chains. At ambient conditions and low temperatures imidazole forms monoclinic structure (space group P21/c) [1-4]. High-pressure of 0.8 GPa transforms imidazole into a new phase, with a planar arrangement of molecules. This structure has been studied by high-pressure X-ray diffraction and infrared spectroscopy. The results have been interpreted in order to explain the structural differences and the formation of polar order.

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Features and development of BEST

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Program BEST for optimal planning of X-ray diffraction measurements from macromolecular crystals is based on modeling the statistical results of data collection taking radiation damage effects into account [1]. Furthermore, tools are provided for automatically characterization of the radiation sensitivity of macromolecular crystals [2] as well as characterization of crystal diffraction quality for the advanced sample evaluation [3]. In recent years, BEST became integrated in automated data collection and on-line data analysis systems (EDNA/MxCuBE, Web-Ice, GDA, CBASS and others) as a standard strategy module. We will present a review on BEST strategy implementations and current applications. Along with the automation and high throughput applications, BEST strategies appear particularly useful for difficult, e.g. small, weakly or very anisotropically diffracting and radiation sensitive crystals. In many experiments, though still with some involvement of human intelligence, the software was helpful in designing an optimal strategy for collecting a data set using small beams and multiple crystal centerings, or multiple crystals. Recent developments in BEST provide the tools for generalization and automation of such experiments, as well as for experiments utilizing ultrafast area detectors and planing of data collection at room temperature.

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Remote access and automation at SSRL

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Complete automation of the macromolecular crystallography experiment has been achieved at SSRL through the combination of