

Multitemperature X-ray Diffraction Analysis in the Study of Phase Transitions, Molecular Dynamics and Crystal Disorder

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Routine ability to analyze crystal structures of different compounds at many temperatures (including “low” temperatures - up to 100K, and “very low” ones - up to 20-30K or even less) is important in many cases for different applications in the study of phase transitions, the nature of crystal disorder, and the study of dynamics of molecular (atomic) motions in the solid state. In addition, low-temperature data collection allows one to increase dramatically real accuracy of diffraction data and to increase the field of its analytical applications (the study of low-melting and/or unstable compounds). In particular, several methods of low-temperature crystallization techniques were elaborated during last time to analyze crystal structures of compounds which are liquids or even gases at normal conditions. Some new examples of the low/multitemperature X-ray diffraction analysis of molecular crystals will be demonstrated. These examples include the study of strong H-bond dynamics in organic compounds, polymorphism, phase transitions in liquid-crystalline precursors, structural studies of high-energetic and non-linear optical materials.

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