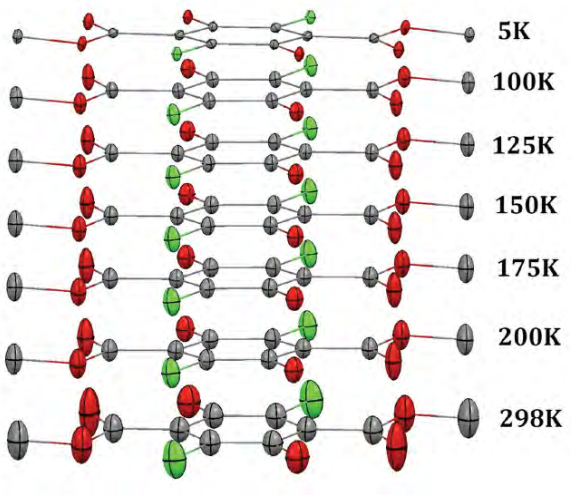

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MS34 Exploring structural dynamics in crystals

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From reactivity of solids to high-pressure crystallography and back: response of molecular crystals to mechanical stress

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The contribution gives a survey of the research that has been carried out through over several decades. Any reaction in a crystal is accompanied by generating stress. The manifestations of this stress are elastic and plastic strain and fragmentation. As a reaction proceeds, the mechanical stress that arises in the crystal can have a significant influence on the subsequent transformation. This phenomenon is termed as feed-back, which can be either positive, or negative. One can introduce the concept on “chemical pressure”, to describe the reaction in the crystal which is stressed by the reaction itself. In selected cases the mechanism of the reaction in relation to the mechanical response of crystals can be studied in detail. I illustrate this, using selected examples of reactions in molecular crystals. The effects of “chemical pressure” can be compared with those of strain imposed by hydrostatic compression. Modern high-pressure crystallography makes it possible to follow even subtle changes in molecular geometry and intermolecular interactions. I discuss structural distortion induced by high pressure and structural transformations, in a comparison with strain and structural transformations accompanying chemical reactions in the same crystal. Eventually, we consider the chemical reactions induced by irradiation or heating if occurring in the hydrostatically compressed crystals.

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