

# **Accurate structure determination of molecular crystals en route to nonmolecular states at high pressures**

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Here I overview our recent experimental and theoretical investigation of simple molecular crystals at very high pressures approaching and reaching the molecular dissociation and transformations to polymeric and monatomic structures. On compression, molecular crystals demonstrate similarities in the most general phenomena, however, the pathway into a nonmolecular state grossly varies depending on the molecular geometry and electronic structure. Here, I present the results of combined synchrotron single crystal X-ray diffraction, Raman spectroscopy, and first-principles theoretical calculations in  $N_2$ ,  $CO_2$ , and  $I_2$ , which allow to determine definitively the structure of molecular and nonmolecular phases in the vicinity of the transition. These investigations address the stability limits of molecular vs nonmolecular phases and the change in the electronic properties across the transition.