

MS17-05 | PRESSURE-INDUCED POLYMERIZATION AND ELECTRICAL CONDUCTIVITY OF A POLYIODIDE

Macchi, Piero (University of Bern, Bern, CH); Poreba, Tomasz (Paul Scherrer institute, Villigen, CH); Ernst, Michelle (University of Bern, Bern, CH); Casati, Nicola (Paul Scherrer institute, Villigen, CH)

The tetra-ethyl ammonium di-iodo triiodide $[\text{C}_8\text{H}_{20}\text{N}][\text{I}_3](\text{I}_2)_2$ is an organic polyiodide salt in which a progressive addition of the electrophilic iodine molecules to the nucleophilic triiodide anion occurs.¹ Compression leads initially to mono-anionic hepta-iodide units and eventually to the polymerization which forms a 3D anionic network. Although the structural changes appear to be continuous, the electrical conductivity changes dramatically above 10 GPa, as the system displays a semiconductive behaviour, whereas at ambient pressure it is a dielectric. The electronic features of the “pre-reactive state” and the polymerized state are revealed by the computed electron and energy density distributions. The formation of the new bonds of course triggers the conductivity, however it is interesting that this occurs only when specific features of electron density and energy densities are observed.

[1] T. Poreba, M. Ernst, D. Zimmer, P. Macchi, N. Casati *Angew. Chem., Int. Ed. Engl.*, **2019**, in the press.