

MS15-P04 | EXPERIMENTAL CHARGE DENSITY DISTRIBUTION IN GROSSULAR UNDER HIGH PRESSURE - A FEASIBILITY STUDY

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We will present details of experimental charge density distribution in a natural garnet mineral called grossular, $\text{Ca}_3\text{Al}_2(\text{SiO}_3)_4$ under 1GPa pressure. Single crystal, high resolution X-ray data were collected on the CRISTAL beamline at the SOLEIL synchrotron (Paris, France). Grossular crystallises in the cubic Ia-3d space group. A short wavelength (0.41Å) and a special type of Diamond Anvil Cell (DAC) with the opening angle 110° let us collect data up to 0.35Å (with 100% completeness up to 0.45Å). We compared our results with experimental charge densities obtained for grossular at ambient conditions and those obtained for pyrope - $\text{Mg}_3\text{Al}_2(\text{SiO}_3)_4$ (isostructural with grossular) collected at 30K (Destro at al., 2017) [1]. In the case of grossular, the obtained properties of charge density at the (3, -1) BCPs as well as the net atomic charges are comparable. Our results indicate transfer of charge among ions under high pressure. Up to our knowledge this is the first fully successful determination of quantitative charge distribution in crystal under high pressure accomplished by performing multipole refinement. We will present detailed results of our investigations.

Acknowledgments: This work was supported by the Foundation for Polish Science (FNP) within the “Core Facility for Crystallographic and Biophysical Research to support the development of medicinal products” project.

[1] R. Destro, R. Ruffo, P. Roversi, R. Soave, L. Loconte, LL. Presti, *Acta Cryst.* **B73** (2017) 722-736.