Abstract Submission  
OL28\_2

***T4 - The dynamical world of minerals  
Spectroscopic methods applied to mineralogy***

**IMA2022-1432  
“Water” in Silicate Garnet: Hydrogarnet Clusters**  
Charles A. Geiger\* 1, 2, George R. Rossman3  
1Dept. of Physics and Chemistry of Materials, University of Salzburg, Salzburg, 2Institute of Mineralogy and Crystallography, University of Vienna, Vienna, Austria, 3Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, United States

**Please designate the presenter/contributor author(s)?:** Charles A. Geiger  
**Abstract Content:** Nominally anhydrous garnets, X3(Al, Fe3+)2Si3O12 with X = Ca and Mg, for example, can incorporate various amounts of structural OH-. Many various mineralogical and petrological investigations have been made on them. IR spectroscopy has been the main method to study OH-. However, it was not understood how to interpret the spectra and how OH- is incorporated crystal chemically in garnet.

The IR spectra of a number of grossular, andradite, and pyrope single crystals were recorded at room temperature and 80 K between 3000 and 4000 cm-1. The various spectra show a number of different wavenumber OH- stretching modes. The data were analyzed and the modes assigned by considering atomic-vibrational and crystal-chemical behavior to explain the energy of the OH- dipole and the structural incorporation mechanism of OH-. It is argued that OH- is located in various local hydrogarnet-like clusters with sizes between 3 and 15 Å. The basic substitution mechanism is (H4O4)4- = (SiO4)4-, and various local configurations containing different numbers of (H4O4)4- groups define the cluster type. Published proposals invoking purely hypothetical “defect” (e.g., Al3+ = 3H+, Ca2+ = 2H+) and coupled-substitution mechanisms (e.g., H+ + Al3+ = Si4+, H+ + Na+ = Ca2+) are not needed to interpret the OH- modes above about 3560 cm-1.

New understanding at the atomic level of published dehydration and H-species diffusion studies is now possible for the first time. This is also the case for H2O-concentration and IR absorption-coefficient investigations. Hydrogarnet-cluster types could potentially be used to decipher petrologic conditions (i.e., P-T-X) under which a garnet crystal formed.

**Disclosure of Interest:** None Declared