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

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“Water” in Silicate Garnet: Hydrogarnet Clusters**
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**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