THE HYDROUS COMPONENT IN GARNETS

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We have studied the IR spectra of garnets representing common occurrences and chemistries. Of 43 garnets, 39 show patterns that are consistent with our predictions for tetrahedral (OH)₄ groups substituting for SiO₄. The consistent spectral behavior over a wide range of chemistry, crystallinity, occurrence, and visible inclusion content, coupled with the lack of absorption at 5200 cm⁻¹ arising from molecular H₂O, demonstrates that the peaks arise from structural OH⁻ and not impurities. Concentrations are commonly in the range of 0.01–0.2 wt.% H₂O. Mantle derived pyrope from the Colorado Plateau diatremes contains 0.08% H₂O. A similar amount is found in mantle pyrope from the Roberts Victor kimberlite, S. Africa. The only anhydrous garnets were from a basalt and a serpentinitized peridotite. The hydrogarnet substitution is commonplace at these concentrations.

The characteristic absorption pattern of end member garnets consists of 3 peaks (in grossular these occur at 3687, 3663, and 3625 cm⁻¹). The positions and intensities depend on the chemistry. The position correlates with the length of the unshared tetrahedral edge. Spectra of intermediate composition garnets show the end member patterns, plus patterns representing tetrahedra in mixed environments. In synthetic Ca₃Al₂(H₄O₄)₃, and in a natural grossular with 2 wt % H₂O, only two peaks are observed. This occurs when there is more than one (OH)₄ group per unit cell. Under these circumstances, the O-H vibrations must conform to the full symmetry of the lattice; factor group analysis predicts two peaks, as we observe. In garnets with less than one (OH)₄ group per unit cell, the vibrations must only conform to the S₄ site symmetry; group theory predicts three peaks, as observed.