THE STRUCTURAL AND CHEMICAL BEHAVIOR OF HYDROUS COMPONENTS IN MINERALS AT TEMPERATURES UP TO 1000 K

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Water and related proton-bearing species in minerals are of critical importance to many geologic processes, but are poorly understood due to the difficulty of obtaining quantitative information about their speciation, crystallography, and thermodynamic properties. We are using single crystal infrared spectroscopy at temperatures up to 1000 K to study minerals with OH^- (e.g. topaz), minerals with H_2O (e.g. cordierite and beryl), and those with multiple hydrous components (e.g. feldspar and zircon). By observing their thermal behavior, various species may be differentiated and aspects of their bonding, orientation, and thermodynamics determined. An example of the application of this technique is provided by the study of the two types of water in the channels of beryl. From 77 to 1000 K the IR spectrum of both shows line broadening caused by increasing thermal motion of the molecules while still bonded on an IR time scale. A progressive decrease in the integrated intensity of both types occurs due to equilibrium partitioning into a third state, which has the spectroscopic characteristics of a gas, and is not bonded or oriented on an IR time scale. At 1000 K 80% of type II and 90% of type I are in this unbonded state. Both return to ± 10% of their original concentrations upon cooling. From the equilibrium partitioning we calculate that type II is 0.1 kcal more strongly bound than type I. The two types remain chemically distinct to 1000 K; there is no interconversion observed. Minor shifts in absorption maxima in both types may be related to the water's interaction with a lattice of changing size.