

Integrating Crystal Chemistry with Laboratory Analysis to Model Bound and Adsorbed OH⁻ and H₂O

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Investigating the specific characteristics of the H₂O/OH⁻ absorption bands near 3 microns is critical for understanding how these molecules are adhered to a remotely observed surface and for assessing their abundance. Current methods for analyzing the form and amount of water in or on rocks range from precise laboratory measurements of oriented single crystals and glasses in transmission, where individual absorptions can be modeled and examined, through more generalized band-depth analysis where a 3-micron band, observed in reflectance spectra of powdered samples in the lab or remote measurements, is treated as a single integrated absorption and compared to empirically calibrated water abundances. Understanding the relationship between the component band strengths and shapes and the bonding to the mineral also has the potential to provide a method to mathematically model terrestrial adsorbed water out of spectral measurements that were not obtained under vacuum conditions, increasing the number of laboratory spectra available for spectral analysis dramatically.

As part of the VORTICES SSERVI team, we are working to spectrally and mathematically characterize the distribution of energies for absorption bands caused by bound and adsorbed hydroxyl and water. To increase the amount of information that can be derived from spectra of hydrated terrains throughout the solar system, we are working to combine both transmission and reflectance spectra of a series of samples to develop a methodology for reliably separating out the specific component absorptions in the 3 micron region of reflectance spectra. For a suite of nominally anhydrous minerals, we are currently obtaining combined transmission measurements of thin sections and powdered rock measurements in ambient air and in ultra-high vacuum. Samples are dehydrated in vacuum, resulting in a suite of spectra with a decreasing amount of adsorbed water. Transmission measurements, which are dominated by internal water/hydroxyl absorptions, are used to characterize absorption bands of any internal water present. The thin sections are then also dehydrated enabling the baseline absorption to be characterized. We will present new modeling results for analog and meteorite materials.

For our preliminary analysis, we have selected two ordinary chondrites (H and LL) as well as 8 Stillwater complex samples as analogs of lunar material. Stillwater samples include harzburgite, norite, anorthite, gabbro and orthopyroxenite. Each sample is being prepared as a double polished thin section for transmission analysis of internal water, powdered for UHV measurements, and characterized in a Hitachi Desktop SEM with a Bruker EDS attachment. Terrestrial samples have been prepared first to test our methods and to ensure that the chondrites can be handled in a way that uses the minimum amount of sample.

Spectra of each sample are being measured in transmission to characterize the shapes and relative strengths of internal water bands. Powdered samples, with water adsorbed from the atmosphere at ambient temperature and pressure, are then measured, taken to UHV and measured again before being heated to drive the adsorbed water off. Samples are measured at progressively warmer temperatures to monitor the shapes and strengths of the absorption bands at each step. Spectra are then modeled using Gaussian curves in energy space. The current objective is not to explicitly quantify the amount of water through modeling, but to determine whether the positions and shapes of bands resulting from adsorbed

water are distinct enough from the water and/or hydroxyl bands in each mineral or rock type to be spectrally distinguished.

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