

EXPLORATION OF WATER IN THE 6 MICRON WAVELENGTH REGION K. M. Taylor^{1,2}, K.A Wilk¹, J. F. Mustard¹, ¹Brown University, Department of Earth, Environmental, and Planetary Sciences, Providence, RI, ²Penn State University, Department of Geosciences, State College, PA.; (kmt5918@psu.edu)

Introduction: Detecting molecular water (H₂O) signatures, distinct from OH⁻, is a persistent challenge for determining volatile processes on the Moon, asteroids, and other airless bodies. In 2009, widespread hydration was detected on the lunar surface, indicated by the presence of an absorption feature at 3 μ m [1–3]. The 3 μ m hydration feature, characterized by H₂O and OH⁻ stretching absorptions between \sim 2.7 – 3.1 μ m, is one of the most widely-used hydration spectral signatures. The 3 μ m feature has been used to quantify water content in the laboratory and remotely sensed data [3], however it is difficult to disentangle hydroxyl (OH⁻) from H₂O signatures.

In contrast, the 6 μ m wavelength fundamental bending vibration of water region contains only signals from H₂O: avoiding the complications of the 3 μ m region and suggesting a promising way to confirm the presence of H₂O on airless bodies. In 2021, telescope observations from SOFIA identified 6 μ m H₂O features on the Lunar surface [4].

However, studies of the 6 μ m H₂O feature are sparse [4,5] and comprehensive studies of the 6 μ m band positions are minimal [6,7]. Here we did a quantitative review of 40 water-bearing crystalline minerals, to characterize and quantify band positions for the 6 μ m fundamental bending vibration of water in minerals.

Methods: 360 spectra of 66 hydrated minerals were downloaded from the Reflectance Experiment Laboratory (RELAB) and USGS Spectral Library [8,9]. 7 of the 66 minerals were common hydrated minerals that do not have H₂O in their formula and acted as confirmation that OH⁻ does not have a signal near 6 μ m.

The spectra's first derivative often emphasizes doublet, triplet, and shoulder features that can be easily missed in visual inspection of spectra. As such, both the spectra and their first derivatives were used to categorize the sample as having a clear singlet, doublet,

or triplet H₂O absorption feature, no discernable feature H₂O feature, or an unclear feature.

Of the 66 minerals, 5 were too saturated near 6 μ m to display a feature, 4 minerals were deemed too complicated for this study, and the 7 non-water-bearing hydrated minerals showed no feature. The band position of the remaining 50 water-bearing minerals were then analyzed. The spectra also were qualitatively evaluated for singlet, doublet, triplet, left shoulder, and right shoulder features (Fig. 2).

To confidently distinguish features from spectrographic variation, the spectra needed a single slope value greater than +0.001 or less than -0.001 between 5.9 and 6.3 μ m (Fig.1). Through this process, 68 out of 252 spectra were removed, which removed all available spectra for 10 minerals.

To prevent the same sample from being overrepresented in our dataset, the spectra file names were cross references with the RELAB sample names. When multiple spectra were available per sample, to avoid spurious spectral behavior for very fine particle sizes [10], the smallest average grain size greater than 5 μ m was chosen as the representative spectra, leaving a remaining 184 spectra.

Of the remaining 184 spectra, locations between 5.75 and 6.30 μ m where the first derivative crossed from a negative to positive value were calculated and marked as the 6 μ m band position. Left shoulder positions were calculated as the average between the local min and local max in the first derivative. Right Shoulder positions were not calculated.

Results: Previous studies primarily analyzed the fundamental bending vibration of water's singlet feature [6,7]. However, this study identified 7 minerals which displayed a doublet feature and 3 which displayed a triplet feature, providing preliminary ranges for these features and highlighting an area of further study.

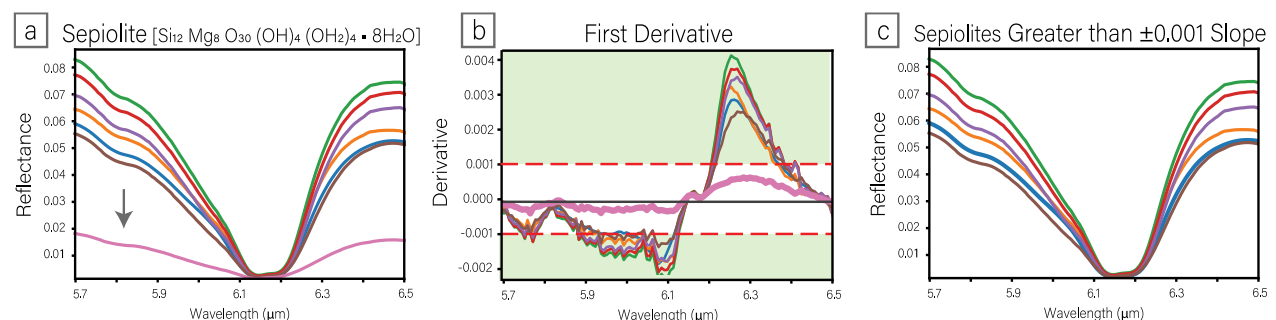


Figure 1: A) Sepiolite spectra that exhibit an absorption feature near 6 μ m before the first derivative spectra test B) The first derivative of sepiolite's spectra, with red dashed horizontal lines indicating the slope cut offs of +0.001 and -0.001. C) Sepiolite spectra that pass the first derivative spectra

Spectral doublet features near 6 μm were found to have band positions ranging between 5.80 – 6.02 μm and 6.05 – 6.29 μm , and triplet band positions ranging between 5.98 – 6.02 μm , 6.04 – 6.09 μm , and 6.27 to 6.29 μm . Left shoulder were found in 11 minerals with shoulder positions ranging from 5.66 to 5.94 μm .

While the doublet and triplet features report a broad range of band positions, 5.80 – 6.29 μm , it is unclear whether all these absorption features are due to molecular water. Future dehydration experiments can be used to determine clarify this ambiguity.

In contrast, the 36 singlet minerals, with band positions ranging from 6.04 – 6.20 μm and an average of 6.12 μm , displayed more constrained characteristics.

Discussion: Previous analyses determined that a singlet fundamental bending vibration of water occurs between 5.81 – 6.32 μm , with a mean band position of 6.11 μm [7] (Fig.3). That study included inorganic compounds and minerals not available in the RELAB or USGS spectral libraries [11] and therefore were not included in our analysis. Our analysis of 36 common water-bearing minerals displaying a single absorption feature, however, showed no evidence of a singlet water absorption below 6.0 μm or above 6.2 μm .

Our study is more consistent with the previously proposed range of 6.06 μm to 6.25 μm [11]. Future studies should include additional water-bearing crystalline hydrates, as well as further investigation into the nature of the doublet and triplet features.

SOFIA measurements of a 6 μm feature on the lunar surface were attributed to H_2O in silicate impact glass or crystalline minerals [12]. Our proposed 6 μm H_2O band range is still consistent with lunar water signals (Fig.3). While this study is not a perfect lunar analog, properly constraining the 6 μm fundamental bending vibration of water will allow for more accurate identification of H_2O .

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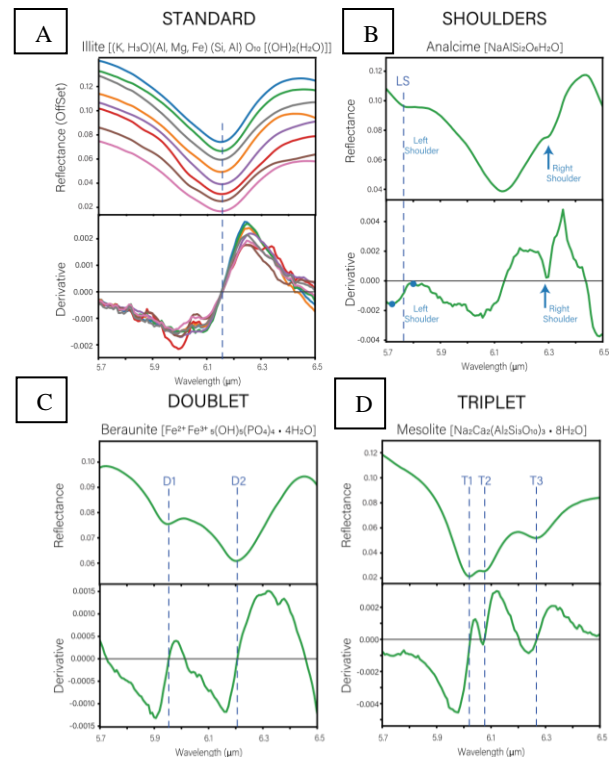


Figure 2: Representative spectra of the four categories of spectral features and their first derivatives observed in the 6 μm region. A) Standard single absorption feature B) Left and right shoulders C) Spectral doublets with D1 and D2 denoting the first and second band position and D) Spectral triplets with T1, T2, and T3 denoting the first, second, and third absorption feature respectively.

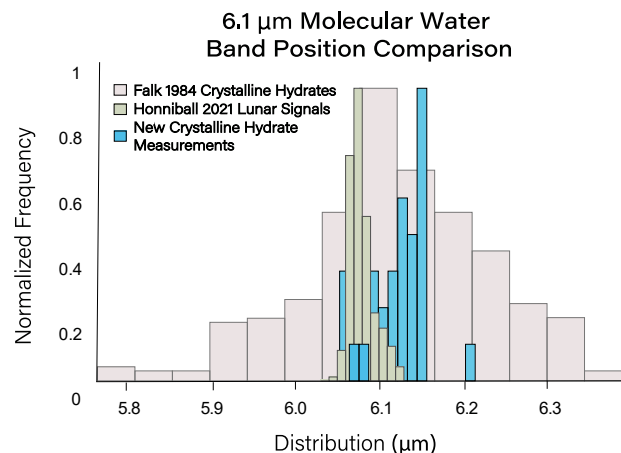


Figure 3: 6 μm H_2O band positions from Falk 1984 (gray), Honniball 2021 (green), and this study (blue).

Acknowledgments: This research was conducted with NSF REU Funding. This research utilizes spectra from the NASA RELAB through the PDS data repository and USGS Spectral Library. RELAB file IDs are available on request.