ESTIMATES OF MOLECULAR WATER ABUNDANCE USING THE 6 MICRON H-O-H BEND. C. I. Honniball[1] P. G. Lucey[1] , S. Li[1], K. Hibbitts[2], [1]Hawaii Institute of Geophysics and Planetology, University of Hawaii at Manoa, 1680 East-West Rd, Honolulu, HI 96822,cih@higp.hawaii.edu, [2]JHU APL, Laurel, MD 20723.

Introduction: The presence of a 3 μm absorption on the lunar surface was reported in 2009, discovered in data collected by three spacecraft [1-3]. This absorption is due to hydroxyl (OH) with a possible addition of molecular water (H_2O): the 3 μm band is a sum of OH and H_2O, termed "total water" (OH + H_2O) in the FTIR community [4]. No methods are available to separate the abundances of OH and H_2O using data near 3 μm.

Data in the 3 μm region also suffer from thermal contamination. In this wavelength region the spectral signal is a mixture of reflected light and thermal emission and these terms require very accurate thermal models to separate. The depth of the 3 μm band varies with temperature, interpreted to be due to diurnal variation in the amount of surface water [2]. But this variation may be entirely due to the competing effects of thermal emission and reflectance [5]. Thus the 3 μm band has important limitations in the study of lunar surface water.

However, the 3 μm region expresses only two of the water molecule's three fundamental features. The third, the H-O-H bend, occurs at ~6.1 μm [6-9]. This absorption is strong and narrow (Fig. 1), well suited for detection of H_2O, and has no influence from OH. At 6.1 μm there is essentially no reflected contamination of the signal, whereas near 3 μm the solar and reflected signal are of similar values, with the reflected signal slightly larger. At 6 μm the ratio of thermal to reflected signal is 1000 times greater than at 3 μm.
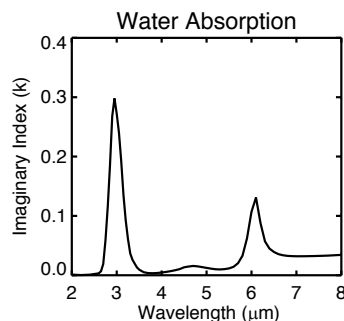

Figure 1: Imaginary index (that controls absorption) of water showing strong peaks at 3 and 6 μm [10].

Utility for lunar surface water studies: The processes that give rise to the remotely sensed lunar surface total water are still only partly understood [11] and uncertainties in the remote sensing results limit the ability to apply constraints. Paramount among questions raised by the lunar 3 μm spacecraft observations is whether the detected diurnal variations reflect a variation in H_2O abundance, a hydration - dehydration cycle. The observed spectral variations, if entirely attributed to abundance variations, imply a significant diurnal supply of H_2O to the lunar atmosphere, an abundance not observed by LADEE [12]. However, because the 3 μm band can be due either to OH or H_2O existing data cannot answer this question.

Observed 6 μm features in existing data: Salisbury et al. 1997 [13] noted a prominent 6.1 μm absorption feature in their diffuse thermal infrared reflectance spectra of lunar soils from several Apollo landing sites, and attributed that to water, probably from terrestrial contamination. We have examined another 17 lunar soils measured at RELAB and each also features a prominent feature at 6 μm.

Li (2016) [14] measured the spectra of a MORB glass in a step-wise heating experiment and these data illustrate the effect of water abundance on the 3 and 6.1 μm bands. In these samples the 6 μm band depth is strongly correlated with the depth of the 3 μm band supporting its use for remote water detection.

Along with the MORB glasses and lunar soils, the 6 μm feature has been detected on Mars using the Thermal Emission Spectrometer on board the Mars Global Surveyor Spacecraft [15] and on multiple asteroids using the Spitzer space telescope [16].

Deriving abundances: Previous studies show that the absorption strength of the 6 μm band correlates with the absolute H_2O content [7,9,10]. Since 1962 the 6 μm band has been used to measure the H_2O content of samples in thin section in chemical and geological literature [6-8,20]. This suggests the 6 μm band can be used to estimate H_2O content from the remote sensing data of the lunar surface. However, little work has been done on deriving the absolute abundance of H_2O from reflectance spectra near 6 μm.

In previous work, we performed a suite of experiments to examine how the 3 μm band strength varies with the total water content [17]. The reflectance spectra collected of those samples feature both 3 and 6 μm bands (Fig. 2a). we use these data (Fig. 2a,b) to develop an empirical model for estimating the absolute abundance of H_2O from the 6.1 μm band. Our previous study showed that the total water content linearly correlates with Hapke's Effective Single Particle Absorption Thickness (ESPAT) parameter [19] at the 3 μm water band [17]. Here we use the same ESPAT parameter to estimate the abundance of H_2O at 6.1 μm. ESPAT is calculated from spectra converted to single scattering albedo. The empirical relation between the ESPAT parameter at 6.1 μm and the abundance of H_2O is:

$$H_2O \ (ppm) = 9244 * ESPAT_{6.1 \ \mu m}$$

and is shown in Fig. 2c as black points. The particle size of this group of samples is 63 - 75 μm which is within the mean particle size range of 60 – 80 μm measured from Apollo samples [18].

In addition, we carried out radiative transfer modeling based on the molecular extinction coefficient (ε) of H_2O reported in literatures to cross-validate our empirical model. Using single scattering albedo and absorbance we can derive a relationship between single scattering albedo and total water content. We used ε values from ~41 (andesite) to ~55 (basalt) L·mol^{-1}·cm^{-1} [20] as the absorption coefficient that has been shown to vary with composition of the host material. We then calculated how the ESPAT parameter at 6.1 μm varies with the absolute H_2O content and plot it in Fig. 2c.

Results: We found that our experiments are consistent with the radiative transfer modeling, confirming that the ESPAT parameter can be used to estimate the absolute abundance of H_2O from the 6.1 μm band for anorthositic and basaltic materials with a particle size ~75 μm that typify the lunar surface.

Summary: Spectroscopic observations at 6 μm offers a powerful unambiguous view of H_2O on the lunar surface enabling testing of the hypothesis that H_2O may be mobile, and determining the phase of water responsible for the 3 μm absorption feature. Using the ESPAT parameter we can estimate the abundance of H_2O present at 6.1 μm. A recent flight on the Stratospheric Observatory For Infrared Astronomy (SOFIA) has provided the first 6 μm observations of the lunar surface. Data is currently being processed but the methods described above will be applied to the data to estimate or put an upper limit on the abundance of H_2O on the lunar surface.

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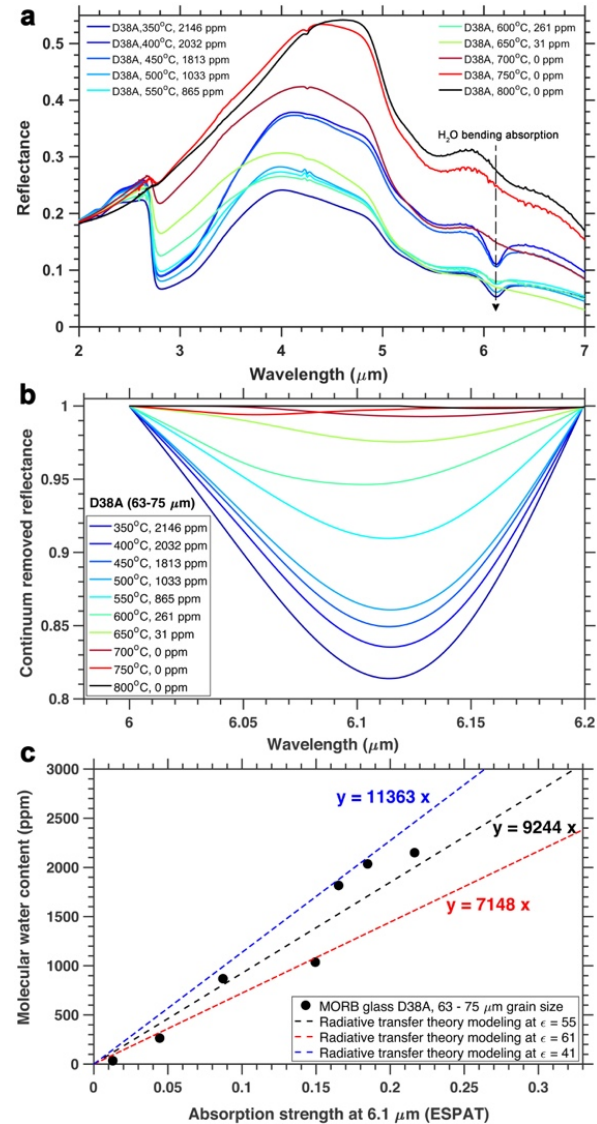

Fig. 2. a. The reflectance spectra and their respective total water content of MORB glasses from 2 μm to 7 μm; b. the continuum-removed reflectance spectra of the MORB glass D38A and the retained H_2O content heated to different temperatures; c. the correlation between the H_2O content and respective ESPAT parameter at 6.1 μm for lab experiments (black points) and radiative transfer modeling results at different molecular extinction coefficient values (black, blue, and red dashed lines).

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