RADIATIVE TRANSFER MODELING OF GYPSUM-ICE MIXTURES UNDER VARIABLE TEMPERATURES: IMPLICATIONS FOR SPECTRAL MODELING OF ICY BODIES. K.M. Robertson[1], S. Li[2]. [1]Dept. of Earth, Environmental and Planetary Sciences, Brown University, Providence, RI, 02912, [2] Hawai'i Institute of Geophysics and Planetology, University of Hawaii, Honolulu, HI 96822.

Introduction: The unmixing and deriving of quantitative abundances from hyperspectral data is an important component of planetary remote sensing. A fundamental approach is to describe the spectral behavior using the intrinsic scattering properties of the individual components, from which abundances can be extracted [1]. Hapke's radiative transfer model (RTM) has been widely used for deriving modal abundances in airless bodies [2] and icy bodies [3] and is well suited for distinguishing subtle changes in the absorption bands of hydrated minerals [4], thus offering the potential for robust quantitative mineralogical studies of icy bodies.

Optical constants (OC) characterize the wavelength dependent interaction of light with a material, and as such, are required inputs for Hapke's formulation. OC are fundamentally temperature dependent resulting in narrowing and blue shifting of spectral bands with decreasing temperature [5]. Extensive databases of OC exist, however; they need to be expanded to include relevant mineralogy and temperature ranges of icy bodies. While some low temperature OC of hydrated minerals have been derived in the literature [6,7] many relevant mineral systems have yet to be studied which will be invaluable to improving the model outputs.

Here, we describe the spectral changes associated with ice and gypsum under low temperatures (-10°C to -180°C) and derive their OC from a suite of particle size ranges. We use the OC to model a lab derived gypsum-ice particulate mixture under variable temperatures and use these results to discuss the broader implications for quantitative spectral modeling of icy bodies.

Methods: Ice powders were generated by nebulizing water into an LN_2 bath and sieving the resulting slurry to the desired particle size ranges [8]. Gypsum ($CaSO_4 \bullet 2H_20$) was obtained from the White Sands National Monument in New Mexico. Ice and mineral endmembers were ground and sieved to 4 particle size ranges (63-90µm, 90-150µm, 150-180µm, 250-300µm) to allow for the determination of OC. A physical mixture of the gypsum:ice (70:30 wt%) was prepared from the 150-180µm endmembers.

Spectral measurements were taken in the VIS-NIR (300 - 2500 nm) wavelength range using an ASD Fieldspec3 field spectroradiometer, equipped with a QTH fiber optic light source on an optical bench with adjustable goniometers for controlling the viewing geometry (i=30°,e=0°). Samples were loaded into a Linkam Low-T environmental stage purged with N_2 gas and measured at -10°C, -30°C, -50°C, -120°C, and -180°C.

The parameterization of the Hapke model used here is the same as that of [9], where the model inputs are the measured reflectance data, viewing geometry (i, e, g), mineral densities, and endmember optical constants. Endmember optical constants were calculated from the pure mineral spectra using an optimization routine for multiple particle size ranges [4]. Optical constants were calculated for ice and gypsum at -10°C and -180°C.

Results: Fig.1 summarizes the temperature induced spectral changes observed for A) pure ice, B) the 70:30 wt% mixture of gypsum:ice, and C) pure gypsum for the 150-180 µm particle size range. Gypsum (Fig.

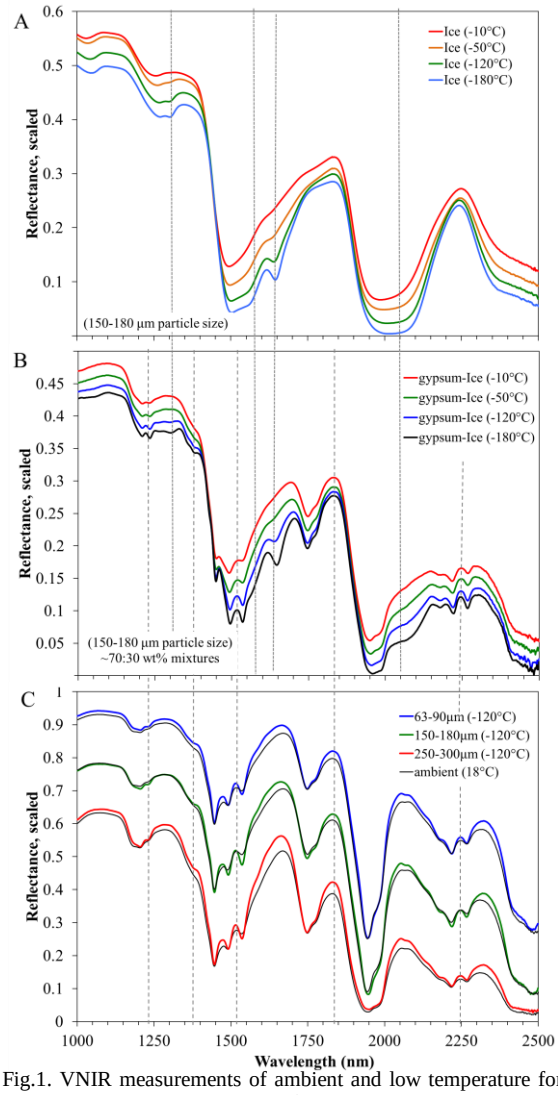

Fig.1. VNIR measurements of ambient and low temperature for A) pure ice, B) a 50:50 mixture of gypsum-ice, and C) pure gypsum. The stippled lines correspond the pure endmembers absorptions to the observed spectral changes in the mixture.

1C) does not show significant spectral slope changes that were observed in bloedite or epsomite [6,7], however; it shows a characteristic sharpening and deepening of the diagnostic 'triplet' that is consistent across all particle size ranges and correlated with decreasing temperature. In addition, we observe a deepening of the 1750nm and 1900nm absorptions that substantially increase the height and slope of the corresponding shoulders. The pure ice spectra (Fig.1A) show significant broadening of the 1900 nm hydration feature along with the appearance of the 1650 nm feature which are consistent with the literature [10]. The spectral changes observed in the endmember spectra can be correlated to similar changes in the 70:30 mixture. The most notable changes include the shape of the 'triplet', the appearance of the 1650 nm feature and the change of slope in the 1900nm feature. The diagnostic gypsum features at 1750 nm and 2250 nm remain mostly unchanged.

Modeling results (Fig. 2) for the gypsum-ice mixture (70wt% gypsum) illustrate the importance of using temperature relevant optical constants at low temperatures. Gypsum abundances (Fig.2A) derived from the mixture are shown for the full temperature range using both 'low T' (-180°C) and 'high T' (-10°C) optical constants. Results are compared to the actual measured value (70wt% Gypsum). As expected, the abundances vary widely depending on which set of OC were used. The respective optical constants accurately predicted the modal abundance at their corresponding temperatures but begin to deviate when forced to model the incorrect temperature. The 'high temperature' set of OC showed ~20wt% deviation from the measured abundance value whereas the maximum deviation for the 'low temperature' OC was only 5wt%.

The modeled spectra are compared to the spectra measured spectra taken at -10°C and -180°C (Fig2B). In both cases, the optical constants were able to predict the general shape of the measured spectra with an RMSE error ~10^{-4}. In all cases, the residuals were better when the spectra were modeled using the OC in the appropriate temperature range. There were systematic misfits associated with the ice feature at 2100 nm along with the shoulders between 1500 and 1800nm.

Conclusion: This preliminary work highlights the importance of utilizing optical constants that properly represent the surface conditions of the planetary data sets. The model was able to account for the shape of the spectra for the mixture at all temperatures, but did so at the expense of the modal abundance values resulting in a systematic offset when the inappropriate temperature OC was utilized.

Spectral differences in gypsum began to appear around -30°C and begin to affect the modeling results by –50°C which is relevant to the surface conditions of Mars. The most significant effects however were at the extremely low temperatures ~-120°C and -180°C which is more relevant for the Jovian satellites like Europa, Ganymede, and Callisto. The upcoming Clipper [11] and JUICE [12] missions will offer new insights into the compositional variability of these icy bodies. Our preliminary work highlights the importance of expanding existing OC databases to account for a more varied mineralogy at relevant temperatures in preparation for these missions. Future work will include the derivation and validation of low temperature OC for a wide range of hydrated minerals relevant to planetary spectral data sets from past, current and future missions.

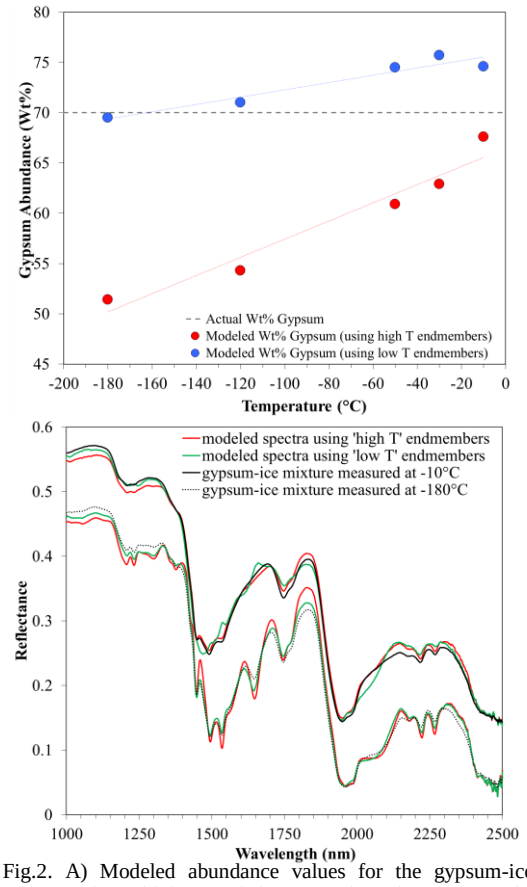

Fig.2. A) Modeled abundance values for the gypsum-ice mixture where 'high T' and 'low T' endmembers refer to the optical constant calculated at -10°C and -180°C respectively. B) Comparison of modeled and measured spectra for the 70:30 wt% mixture of gypsum:ice at -10°C and -180°C.

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