

# **Spectral Properties of Hydrated Sulfate Minerals on Mars**

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## Abstract

The identification of hydrated sulfate minerals on Mars has a number of implications for surface geochemistry and climate evolution, largely due to their involvement in the production of evaporite minerals from ancient lake basins [1,2]. While in-situ identification from surface landers and rovers has advantages in signal fidelity and ground truthing, regional context for now must rely on remote sensing from orbital instruments. Mars Express OMEGA and Mars Reconnaissance Orbiter CRISM observations have identified a number of sulfate mineral deposits based on comparisons with laboratory spectra of these compounds. At the surface temperatures (150 -300K) of Mars, visible to near-infrared (VNIR) spectra of hydrated sulfate minerals exhibit sensitivity to temperature that manifests in shifts of band positions, shapes, and widths [3]. Retrieval of surface mineral abundances from such regional observations may be enhanced by inclusion of temperature-appropriate laboratory reflectance spectra.

### 1. Introduction

Identification of surface minerals from remote sensing observations relies upon comparisons to laboratory reference spectra. Reference spectral libraries must take into account a number of effects that may alter spectral response, including phase angle, grain size, porosity, atmospheric pressure, and temperature. In many cases some of these effects may be safely neglected. However, in the case of hyrated minerals, determination of surface abundances through linear and/or nonlinear spectral mixing algorithms can be significantly impacted by the omission of temperature sensitivities. Many of the sulfate minerals that have been detected recently by VNIR observations at Mars from CRISM and OMEGA have been found to be in a hydrated state.



Figure 3. Spectra of hexahydrite at 150-300K.

In hydrated molecules such as magnesium sulfate hexahydrite,  $MgSO_4$ • $6H_2O$ , the waters of hydration are held in place by hydrogen bonds [4]. As in water ice, the crystal lattice is said to be orientationally disordered: that is, though the host molecules are arranged in a self-consistent repeating lattice, the hydrogen atoms can be oriented toward any of several neighboring atoms. This leads to a situation in which many slightly different configurations can coexist, and consequently multiple absorption features having similar (yet not identical) vibrational frequencies are found together.

At low temperatures, decreased vibrational energy reduces the amount of influence these molecules have on the vibrations of their neighbors. Consequently, the individual bands become more discrete, leading to changes in band center (frequency) positions, strengths, overall band shapes, and in some cases, even band splitting.

### 2. Temperature Dependence

We present here an illustrative example. Hexahydrite grains were ground and sieved to a 100-125  $\mu$ m size fraction and placed in a vacuum environment chamber at the JPL Planetary Ice Characterization Laboratory (PICL). Spectra were acquired with an Analytical Spectral Devices (ASD) FR3 fiber optic spectrometer, and corrected to absolute reflectance using Spectralon<sup>TM</sup> as a calibration standard and a tungsten-halogen light source. A closed-loop helium cryostat was used to control sample temperature to  $\pm 0.5$ K.

Band	300K	250K	200K	150K
1.25 µm				
Center	1.1981	1.2007	1.2061	1.2270
Depth	8.62	12.08	11.45	11.09
Width	106.2	108.6	107.7	105.7
1.5 μm				
Center	1.4697	1.4704	1.4792	1.4800
Depth	53.59	62.64	56.59	56.68
Width	291.3	296.5	270.2	257.3
1.65 µm				
Center	1.6210	1.6139	1.6120	1.6056
Depth	6.98	10.97	8.45	12.65
Width	100.0	100.5	114.9	114.5
2.0 µm				
Center	1.9681	1.9719	1.9766	1.9748
Depth	75.09	80.52	72.34	75.64
Width	214.9	220.9	215.2	214.4

Table 1: Continuum-removed band center positions, band depths (%), and full width at half maximum (nm) for hexahydrite from 150 to 300K.

Temperature-sensitive effects are evident in the VNIR spectra of hexahydrite shown in Figure 1. The room temperature (top curve) spectrum exhibits the major absorption features near 1.25, 1.5, 1.65 and 2.0  $\mu$ m arising from the waters of hydration. Reduction in temperature to 250K produces only subtle changes in band position and depth. However at 200K these become more pronounced, and the 1.5- $\mu$ m absorption feature begins to split into multiple components.

Similar splitting is apparent in the  $2.0-\mu m$  absorption feature at low temperature as well.

Band center positions (in  $\mu$ m), band depths (as a percentage of the continuum reflectance), and full width at half maximum (nm) are given in Table 1. Though each band center shifts monotonically with temperature, not all move to longer wavelengths with decreasing temperature: the 1.65- $\mu$ m feature actually shifts shortward! Generalizations about band behavior are complicated by the band splitting behavior, so that it is not always possible to speak of the same feature at all temperatures.

### 3. Summary and Conclusions

We are working toward providing temperatureappropriate spectra of hydrated sulfate salts to the scientific community. Inclusion of these spectra in spectral unmixing algorithms will enable determination of improved surface abundance estimates for these materials, affecting models of surface-atmosphere exchange, geochemical evolution and the climate history of Mars.

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