

METHANOL AND METHANOL IN WATER: EXPLORING THE SPECTRA. J. A. Myszka¹ R. M. Mastrapa² A. S. Curry³, ¹Villanova University (janine.myszka@villanova.edu), ²NASA Ames Research Center, SETI Institute (rachel.m.mastrapa@nasa.gov), ³CSU Pomona (acurry@csupomona.edu).

Introduction: As scientific instruments evolve to allow astronomers to peer deeper into space with a greater resolution, it becomes increasingly relevant to analyze spectra in order to remotely determine the composition of outer solar system objects and parts of the interstellar medium (ISM). Lab produced spectra of suspected components of such objects will allow us to produce optical constants which can be used to simulate what the spectra (reflectance, transmittance, absorbance) from objects on which the components are present might look like. Methanol (CH_3OH) has been identified as a possible component of both Enceladus [1] and the centaur 5145 Pholus [2] and can be formed on irradiated surfaces where methane and water ices are present. To that end, we have deposited methanol and a methanol water mix at low temperatures (15 and 100 K) and have observed the spectra at different temperatures and in the wavelength range from 1 to 20 μm . We will use this data to create a comprehensive table of optical constants for use by the broader astronomical and scientific community.

Methods: Our lab setup and procedure has been describe in depth [3]. The apparatus has the capability of cooling to a temperature of 15 K and attaining a pressure on the order of 10^{-8} Torr. Spectra are collected in the infrared from about 1 to 20 μm . Deposits of methanol or mixtures of methanol and water were made from gas samples and the thickness of the sample was measured using laser interferometry with a photometer. The number of fringes during the course of the deposition was counted manually and, from this, the thickness of the ice was derived. Spectra of the ice were then collected using an Fourier Transform Infrared (FTIR) spectrometer and Resolutions Pro software at various temperatures with the temperature change generally occurring at a rate of about 2 K/min. Each spectrum consists of the average of 1000 spectra of the ice to reduce noise in the signal. In the course of a typical experiment, we would deposit at 15 K, collect spectra at 30, 50, 90, and 130 K and then cool back down to 15 K to determine if any changes in the spectra were reversible or whether the ice went through a phase change.

After collecting the spectra from a single experiment the light scattering continuum is removed from the data by baselining the data. The spectra are then converted to absorbance from transmittance and the major peaks are identified. In order to track changes and trends in the peaks versus temperature, the data is

stored in a Microsoft Excel workbook marking the beginning, end and center of each prominent peak. In our case the center is generally defined as the most extreme point in the given wavelength range for the peak, but in some cases the “center of gravity” method is used. That is, when a peak is located on a curve, occasionally the limit of the peak will have a greater absorbance than the center of the band, and using the “center of gravity” option the program identifies the actual center of the peak. The area of the peak is also recorded. From this data, we can determine general shifting trends, note qualitative changes in peak shape, and track band strength as a function of temperature.

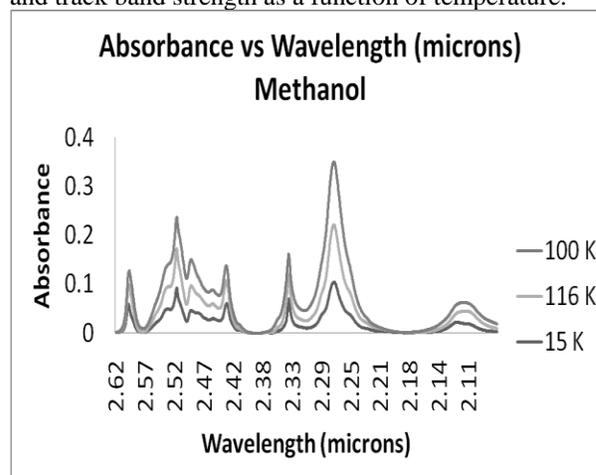


Figure 1: Methanol ice spectra from a single deposition. In chronological order, the spectra were taken at 100, 116 and 15 K. This figure demonstrates methanol’s temperature dependence.

Data: Figure 1 demonstrates the effect temperature has on the position and strength of bands, the sample was heated up to 100 and 116 K and then cooled down to 15 K. In this way, it can be determined whether an alteration in feature is purely temperature dependent or if, in fact, the substance has gone through a phase change. In terms of temperature dependent changes, a feature such as the one at 2.11 μm is a good example. At 15 K, this feature is double peaked, but this is not the case at 100 or 116 K. We can tell that methanol changes phase at about 116 K and this is best illustrated by the shoulders that appear on the features near 2.27, 2.47, and 2.55 μm . These features are not strong on the 100 K spectrum, but are prominent on both the 116 K and 15 K spectra. Therefore, it is the case that these features are a result of a phase change and, if

observed in other unknown spectra, would indicate that the surface had at one point been warmer than 116 K.

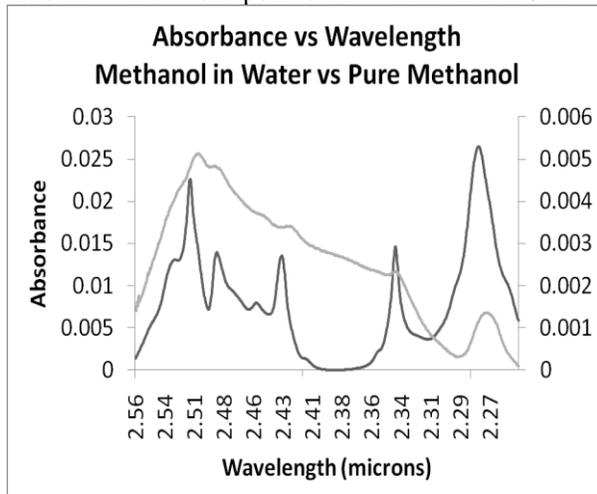


Figure 2: This figure demonstrates the difference in peak location between methanol ice and methanol in water ice. The darker line with more apparent peaks is methanol ice, and the lighter line with more indistinct features shifted to the right is the ice of methanol in water.

In the Figure 2, methanol in water is the lighter gray, more broadly featured spectrum whereas pure methanol is the darker lined, distinctly peaked spectrum. In the methanol and water mix, there were twenty parts water to every one part methanol. Water is responsible for the broad feature and, since methanol and water both have an OH component, the lines produced by this bond appear at similar wavelengths. Of note in Figure 2 is the fact that the methanol peaks are shifted toward the shorter wavelengths in the presence of water, and are also much fainter features. There is still a temperature dependency of methanol in water with respect to temperature, with certain features shifting or becoming stronger depending on temperature. The most significant methanol peak to note is the feature at 2.27 μm . This feature is not overwhelmed by the presence of water, so if a methanol detection in a spectrum where water was present were to be made, the feature at 2.27 μm is the strongest feature that remains distinguishable once water ice is introduced.

Conclusions: We have observed spectra of methanol and methanol in water ices at high (100 K) and low (15 K) temperature deposits in the near to mid infrared wavelength range (1-20 microns). We present here data of the most prominent methanol features in the wavelength range of ~ 2.0 - $2.6 \mu\text{m}$, a range in which observations of objects containing ices of methanol or methanol in water are generally taken. Our data suggest that methanol peaks do shift with temperature and methanol

undergoes a phase change, or reordering of the lattice structure, near 116 K.

In the presence of water, prominent methanol peaks can become difficult to distinguish due to the OH stretch present in both methanol and water molecules. There is also a consistently observed shift towards shorter wavelengths when methanol is in the presence of water. There is one methanol peak near 2.27 μm which is not drowned out by the water features, and would probably be the most useful peak to identify the presence of methanol when it is mixed with water.

Future Work: This work will be continued with a different ratio of water to methanol mix, that is, ten parts water to every one part methanol, so that the methanol lines are stronger in the spectra. The investigation will also continue with different, in some cases more complex, molecules and mixtures. The wealth of potential knowledge that can be gleaned from this study is indispensable for spectral identification purposes.

References:

- [1] Hodyss, R., et al., (2009) *Geophysical Research Letters*, 36, 17103.
- [2] Cruikshank, D.P., et al., (1998) *Icarus*, 135, 389-407.
- [3] Mastrapa, R.M., et al., (2008) *Icarus*, 197, 307-320.