

NEAR INFRARED SPECTRA OF H₂O/HCN MIXTURES. R. M. Mastrapa¹, M. P. Bernstein¹, and S. A. Sandford¹, ¹NASA Ames Research Center (MS 245-5, Moffett Field, CA 94035, rmastrapa@arc.nasa.gov).

Introduction: Cassini's VIMS has already returned exciting results interpreting spectra of Saturn's icy satellites, e. g. [1, 2]. The discovery of unidentified features possibly due to CN compounds [2] inspired the work reported here. We wanted to test HCN as a possibility for explaining these features, and also explore how the features of HCN change when mixed with H₂O. We have previously noted that mixing H₂O and CO₂ produces new spectral features and that those features change with temperature and mixing ratio [3].

The Experiment: All experiments for this project were conducted in the Astrochemistry Laboratory at NASA Ames Research Center. For a description of relevant techniques and equipment please see our studies of H₂O/CO₂ [3].

We conducted a series of experiments mixing H₂O and HCN to determine the effects on the infrared spectrum. Both H₂O and HCN were freeze-pump-thawed at least three times to remove contaminants. Some results include HCN that has not been purified, and some CO₂ features are seen in these samples.

Due to restrictions on beamsplitter/detector combinations, we can collect spectra in the following ranges: 1.25-3.5 μm (8000-2850 cm^{-1}) and 1.33-22.2 μm (7500-450 cm^{-1}). All samples were deposited at 50 K, heated to 160 K at a rate of 1 K/min, and cooled. We assume that the samples are solid solution mixtures at low temperature.

Results: We list the relevant features of pure HCN and mixtures with H₂O in Table 1. These results agree well with previous studies [4-8]. Figure 1 includes spectra of pure HCN and H₂O along with H₂O/HCN. All samples are at 50 K. Most HCN features are at the same center wavelength as in the pure substance. There are some shifts in the HCN features between the pure substance and the mixture, but the strongest features, such as those at 1.91 and 2.10 μm , appear unchanged. However, splitting occurs in some peaks, for example the feature near 2.51 μm . In the mixture, it splits into a doublet with peaks at 2.50 and 2.53 μm . This splitting is temperature dependent. There is also a very strong feature in pure HCN at 2.68 μm that is nearly absent in the mixture. We have yet to identify this feature and do not know why it would be so dramatically reduced in strength in the mixture.

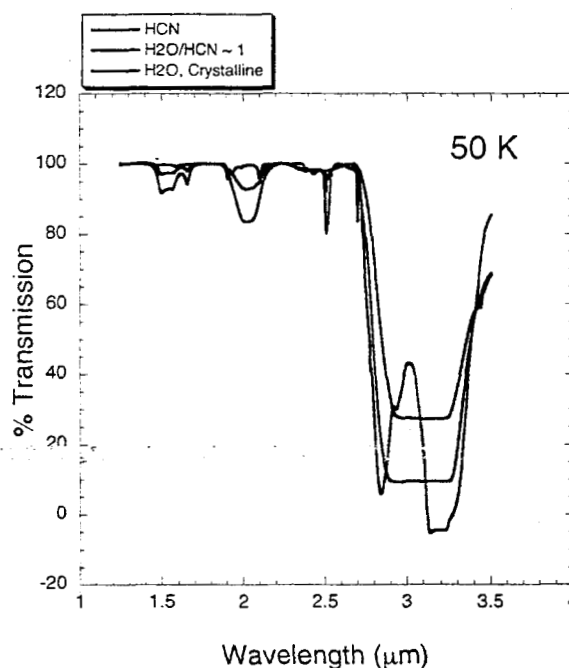


Figure 1. Spectra of Pure HCN (red), pure crystalline H₂O (blue), and H₂O/HCN (black) at 50 K.

To get a good signal in the near infrared, we had to create thick ice samples ($\sim 10 \mu\text{m}$). As a result, the 3 μm H₂O fundamental and the HCN fundamental features appear saturated (Figure 2). The Mid-IR results used thinner samples, so the features are clearer.

The features in HCN mixtures change in strength but not peak center at different concentrations. When warmed to 160 K, some of the HCN escaped from the sample. Because of this, there are more HCN features in the amorphous H₂O samples and those features are much stronger compared to the mixture with warmer crystalline H₂O. The spectra of H₂O/HCN mixtures appear only weakly dependent on temperature. At high temperature, the feature at 2.51 μm is a single peak. The feature splits into a doublet at low temperature. If the splitting is due to grain segregation, then it is unclear why cooling strengthens the splitting, unless segregation is still occurring during cooling.

In the mid-IR we made solid solution ice samples (Figure 2), but also attempted to simulate grain segregation by layering H₂O on top of HCN. The layered sample looks very different from the mixture, but it could be that we did not deposit enough H₂O.

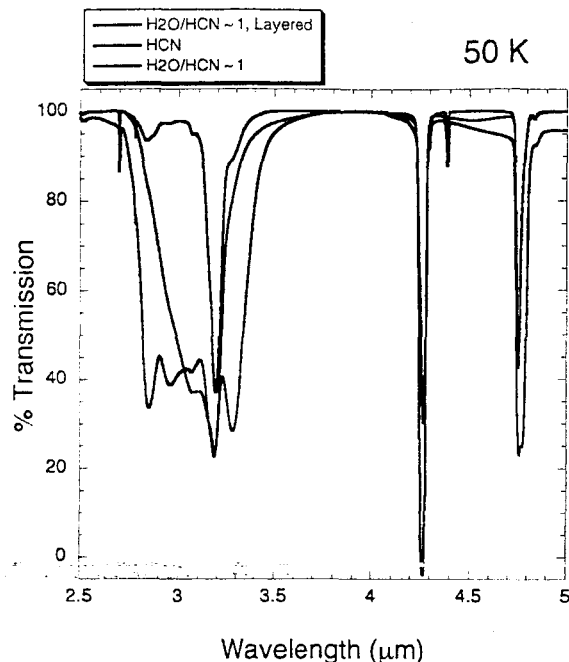


Figure 2. Spectra of pure HCN (red), H₂O/HCN (black), and a layered sample of H₂O and HCN (purple).

To prevent the saturation of the 3 μm fundamental of H₂O, we made thinner samples in the mid-IR. Because the samples were thin, all the HCN was released during warm-up. We also created thick samples of H₂O/HCN and we were able to crystallize the H₂O without losing all of the HCN. The thin samples are useful for identifying features, but not realistic for planetary applications. The spectra of Phoebe are clearly saturated near 3 μm, making the thicker samples more appropriate.

Conclusions: The strongest features of either HCN or H₂O/HCN are not seen in the spectrum of Phoebe, with the exception of a possible fundamental at 4.8 μm. However, the peak strength in our experiment was at a shorter wavelength than the 4.8-5.0 μm given in Table 1. This could be due to the fact that H₂O is in the crystalline phase on Phoebe, while our samples are in amorphous H₂O at that wavelength. However, the peak centers for most features do not seem to change with phase except for the splitting seen in the crystalline phase. However, the HCN fundamental will not be shifted beyond 4.85 μm, so features found at longer wavelengths must be due to a different compound.

We used very high concentrations of HCN in H₂O, higher than would be expected in the Solar System, in order to identify the strongest features. Due to the change in strength of the near-IR features with concentration, it is unlikely that one could identify trace amount of HCN in this wavelength

range. It would be safest to focus on detection of the feature at 4.78 μm.

References: [1] Buratti B.J. *et al.* (2005) *Ap. J.* 622: p. L149-L152. [2] Clark R.N. *et al.* (2005) *Nature.* 435: p. 66-69. [3] Bernstein M.P. *et al.* (2005) *Icarus.* 179: p. 527-534. [4] Bernstein M.P. *et al.* (1997) *Ap. J.* 476: p. 932. [5] dello Russo N. and Khanna R.K. (1996) *Icarus.* 123: p. 366-395. [6] Gerakines P.A. *et al.* (2004) *Icarus.* 170: p. 202-213. [7] Masterson C.M. and Khanna R.K. (1990) *Icarus.* 83: p. 83-92. [8] Moore M.H. and Hudson R.L. (2003) *Icarus.* 161: p. 486-500.

Table 1. H₂O/HCN Peak Maxima.

HCN (mm)	H ₂ O/HCN (mm)
1.91	1.91
1.92	
	1.94
	1.97
	1.99
	2.01
2.09	
	2.1
2.1	
2.12	
2.38	2.38
2.42	
	2.43
2.45	
2.51	2.51
2.53	
	2.68
2.69	
	2.7
2.71	
2.78	2.78
	2.84
2.85	
	2.94
2.96	
3.07	3.07
	3.14
3.19	
	3.2
	3.24
3.29	
4.76	4.76
4.78	