Formation, Destruction, and Spectra of Extraterrestrial Molecules

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Some Icy Worlds and Icy Molecules

Charon (Pluto)  Enceladus (Saturn)  Miranda (Uranus)  Triton (Neptune)  Charon (Pluto)

Some Problems and Questions

Expect hydrate formation from some of the known molecules

Data available usually for “high” T and $\geq 1$ atm

Data available usually for samples made from liquids

Our Laboratory Approach

Prepare hydrates - from ices at low T

Characterize hydrates - record IR spectra

Follow hydrate evolution - thermal and radiolytic

Reaction products

Apply results – planetary science, astrobiology, etc.

Laboratory Setup

1 MeV $H^+$

IR Spectrum
Some Ammonia-Containing Ices

<table>
<thead>
<tr>
<th>Component</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>NH₃</td>
<td>ammonia</td>
</tr>
<tr>
<td>NH₃ + H₂O</td>
<td>amorphous mixtures</td>
</tr>
<tr>
<td>NH₄⁺</td>
<td>ammonium</td>
</tr>
<tr>
<td>2 NH₃ • H₂O</td>
<td>hemihydrate</td>
</tr>
<tr>
<td>NH₃ • H₂O</td>
<td>monohydrate</td>
</tr>
<tr>
<td>NH₃ • 2 H₂O</td>
<td>dihydrate</td>
</tr>
</tbody>
</table>

Comparison of 2 NH₃ • H₂O Ices

Thermal Evolution of 2 NH₃ • H₂O

Influence of H₂O on NH₃ Near-IR Bands

Some Ammonia Results

Ices $\xrightarrow{\Delta}$ Hydrates $\xrightarrow{\Delta}$ Deamination

Near-IR bands' positions vary almost linearly with H₂O conc. for $> \sim 25\%$ H₂O

Need more than band positions to identify hydrates
A Space Environment

Some Radiation Results

- Loss of NH₃
- Near-IR band positions hardly change
- Amorphization of hydrate
- NH₄⁺ formation (4527 cm⁻¹, 2.209 μm)
- Timescales

Some Spectral Comparisons

Sulfur-Related Hydrates

Charon data
Cock et al. (2007)

NH₄⁺, NH₃ • H₂O, 2 NH₃ • H₂O, NH₃ + H₂O (1:2)

Band ranges for different NH₃ concentrations

Irradiation gives ions: H₃O⁺, SO₄²⁻, ...

Warm to get hydrate and more

Increasing dose at 86 K
**Some Conclusions**

- Ices can form hydrates on warming.
- Hydrates can change composition on warming.
- Radiation alters molecules and can lead to subsequent hydrate formation.
- These effects appear in IR spectra.
- Need to push experiments out into the near IR!

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- $\Delta$ $\text{SO}_4^{2-}$
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