What can be made in the lab can be found out there... and vice-versa (almost)

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Outline:

- Space vs Lab
- CO₂ everywhere
- Biological molecules?
Experimental setup at ISM

Size of ISM cloud 10-100 pc* (1 pc ~ 3 × 10^{16} m = 30,000 billion (UK) Km)
Lifetime ~ 10^6-10^7 years (1 to 10 million years)
Temperature ~ 10-100 K (-263 to -173 ºC) (dense or diffuse medium)
Particle density ~ 1000 to 1 million part cm^{-3} (diffuse or dense medium)

*parsec: parallax of one arc second; 3.26 light years

Experimental setup at IEM-CSIC

Substrate (Au, Si, Ge) on ARS Cryostat (closed cycle helium)
Temperature range 14-300 K; (from -259 °C to room temp)
Deposition pressure ~10^{-6} mbar (~10^{-9} atm: one billionth of atmospheric pressure)
Particle density (in the gas phase) ~10^{11} molec cm^{-3} (100 billions molec cm^{-3})
## Comparison ISM-IEM

<table>
<thead>
<tr>
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<th>ISM</th>
<th>IEM</th>
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</thead>
<tbody>
<tr>
<td>Sample size</td>
<td>$10^{15}$ km</td>
<td>1 cm</td>
</tr>
<tr>
<td>Duration</td>
<td>1 million years</td>
<td>1 day</td>
</tr>
<tr>
<td>Temp</td>
<td>10-100 K</td>
<td>10-100 K</td>
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<tr>
<td>Particle density</td>
<td>1000 per cm$^3$</td>
<td>$10^{11}$ molec per cm$^3$</td>
</tr>
<tr>
<td>Efficiency</td>
<td>$3.6 \times 10^{11}$ particles per day per cm$^3$</td>
<td>$10^{11}$ particles per day per cm$^3$</td>
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</tbody>
</table>
Our aim:

- Study ices (frozen gases at astrophysical temperatures) known or suspected to be out there
- Obtain good laboratory results that can be used to analyze observed data
- Make computer models to compare to experimental results
- Based on our laboratory and computer results, predict and guide future observations
Ice mantles away from stars

100 billion Km

5,000 billion Km
Much closer: Solar System

Space missions to comets: Deep Impact (NASA)

The Deep Impact probe (365 Kg) collides with comet Temple 1 (2005)

Image: NASA/JPL-Caltech/UMD
Deep Impact: spectra of 9P/Tempel1

4 min before impact, 11000 km from nucleus

10 min after impact, 2500 km from nucleus

A’Hearn et al, Science 310, 258 (2005)
Mike A’Hearn: “The variation with time very likely means that there's one particular region on the comet that is enriched in carbon dioxide ice and is actively jetting, and that every time it rotates into the Sun, the outburst flares up”
H₂O/CO₂ ice mixtures

• Part of ongoing project to predict IR spectra of H₂O/CO₂ particles (Mars upper atmosphere, Canadian Space Agency; 2011 Sabbatical at UBC, Vancouver)
• Relaxed structures and prediction of spectra of mixtures
  • H₂O/CO₂ (samples of 32 molecules)
• Always using SIESTA, of course
CO$_2$ in CO$_2$/H$_2$O mixtures

100% H$_2$O

100% CO$_2$

50-50
Measured in the lab, CO$_2$ / H$_2$O mixture

Two peaks!

50 / 50 sample, predicted

Two peaks!
From CO₂ to NH₂CH₂COOH...
Glycine in astrophysical media

- Organic and bio-organic molecules sought in astrophysical media: attempt to clarify history of Solar system, and in particular, origin of life on Earth
- Glycine, simplest aminoacid, confirmed on cometary grains collected by Stardust
- Glycine, alanine and guanine found in the Almahata Sitta Meteorite
- In the lab, glycine formed by UV irradiation of interstellar ice analogs
Motivation and aim

- Comparatively few works on spectra of aminoacids under astrophysically relevant conditions

- Our work: solid mixtures of glycine-water, glycine-CO₂, glycine-CH₄ to compare behaviour of spectra in polar and non-polar environments

- Theoretical calculations and predictions of spectra of solid glycine and gaseous glycine monomer and dimer

B. Mate et al, PCCP (2011)
Experimental modifications

- Retractable oven to generate glycine vapour

Copper body. 50W halogen lamp for heating. Select vaporization temperature to yield desired proportion of neutral glycine

Rotating substrate
Deposition temperature: 25 K
Conclusions

- From astrophysical point of view: glycine could have diverse structures in different media.

- If $\text{CO}_2$ ($\text{CH}_4$) and $\text{H}_2\text{O}$ are present wherever glycine could be found, the neutral form would be favored; therefore search for $1750 \text{ cm}^{-1}$ ($5.71 \mu\text{m}$) band.

- On the other hand, for warmer samples (or material that has undergone warming above the sublimation temperature of those gases), most glycine would be in zwitterionic form; then look for $1326 \text{ cm}^{-1}$ and $1423 \text{ cm}^{-1}$ ($7.54 \mu\text{m}$ and $7.03 \mu\text{m}$, respectively) bands $\rightarrow$ small overlap with water bending vibration ($6.06 \mu\text{m}$).

- A more accurate knowledge of the structure of the solids necessary for better interpretation of all spectral features.
Perspectives

• Further experimental work: ionic species in ice (hyperquenching deposition); interesting to confirm or discard astrophysical observations

• Biological molecules: spectra in astrophysically relevant experimental conditions; alanine, simple aminoacids...

• Theoretical work: further modelling of mixed samples, both to fully explain observed spectra, and to predict spectra of more complex mixtures
Acknowledgments

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Thank you for your attention!