Data requirements for interstellar ices

The Open University

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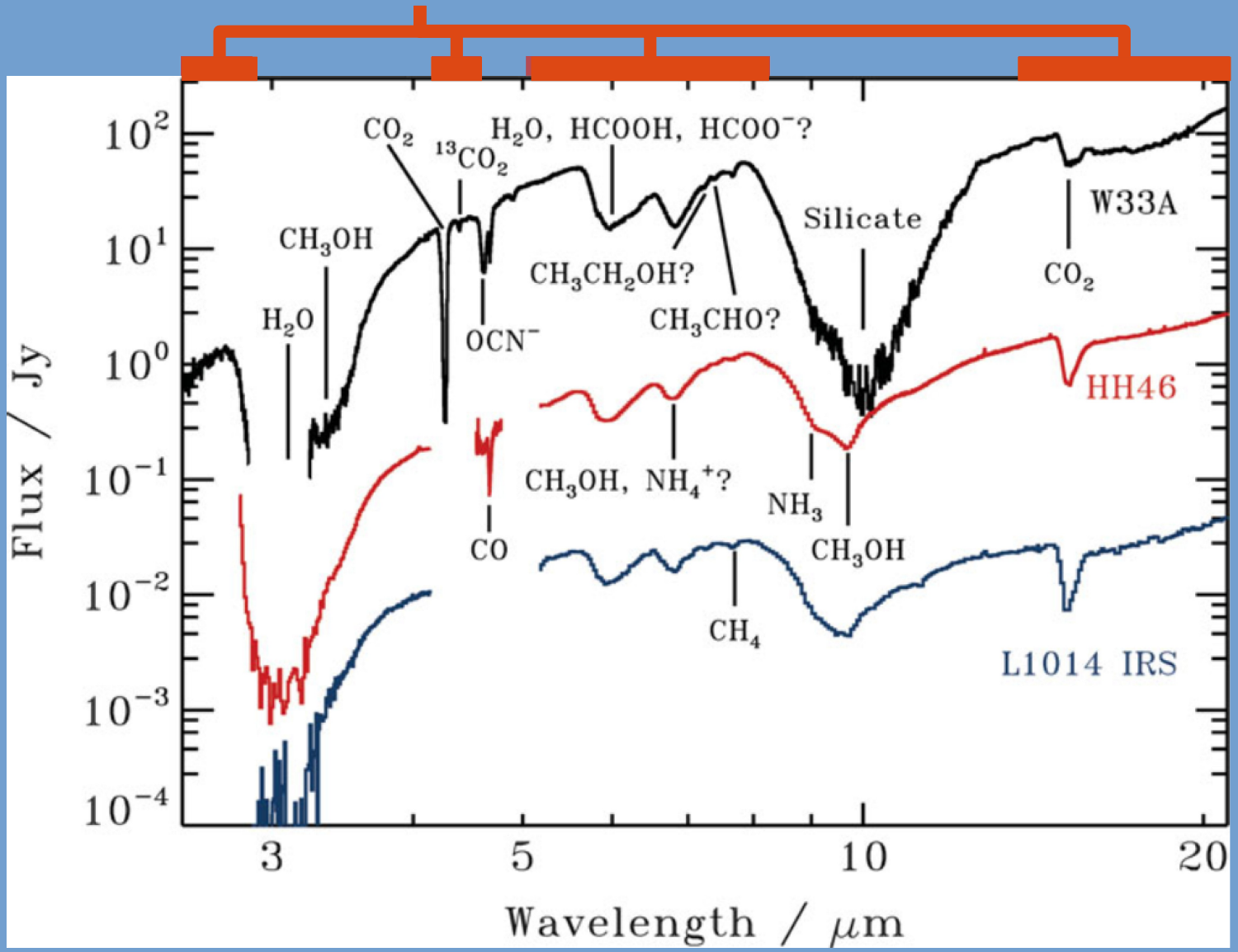
Given at the VAMDC-STFC meeting in Belfast, 17th of April 2015

Interstellar ices in a nutshell



Reproduced from Öberg et al 2011 + references therein

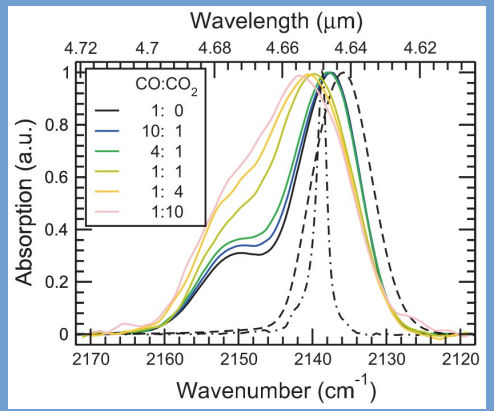
- Ice produce absorption features
- Mostly observable in the near- and mid-IR
- Most of it blocked by Earth's atmosphere
- Column densities are interesting, because science.

The process of finding frozen molecules

$$\tau(n) = A_1 e^{-2.35\left(\frac{n-A_2}{A_3}\right)^2}$$

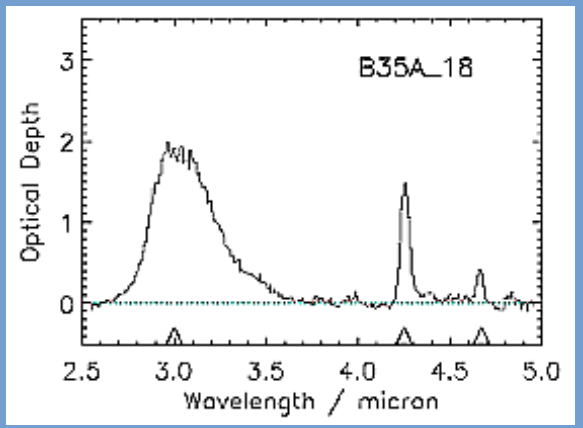
Theoretical models

Laboratory spectra



(Cuppen et al. 2011)

Observed spectra



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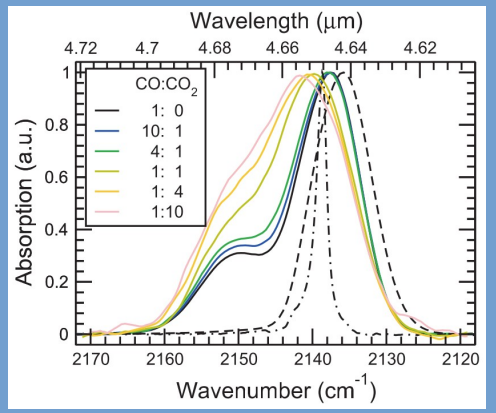
Theoretical models

Lab spectra

Compensate For grain shape



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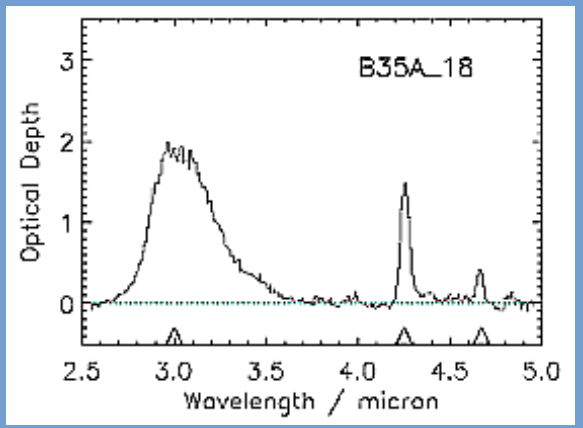

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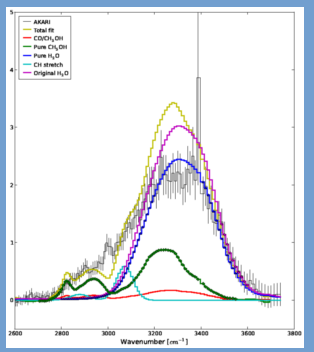
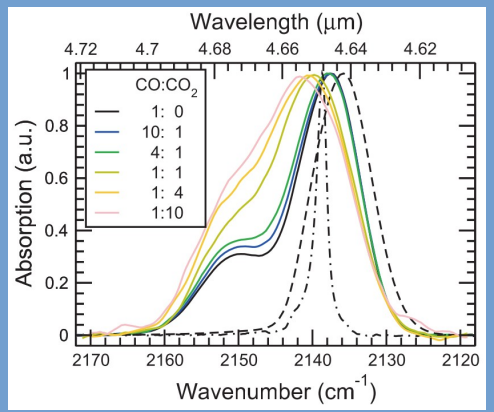
Fit everything together



Models+spectra fitted to observations



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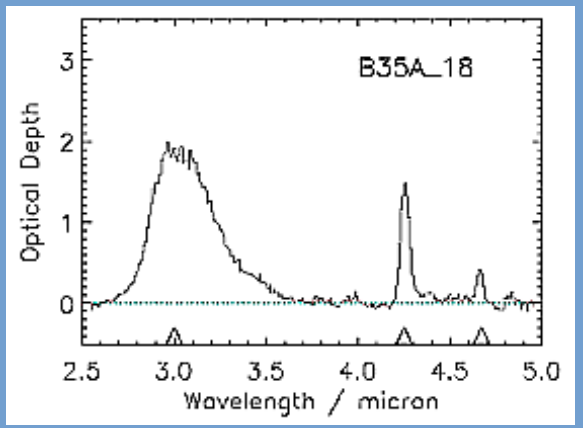

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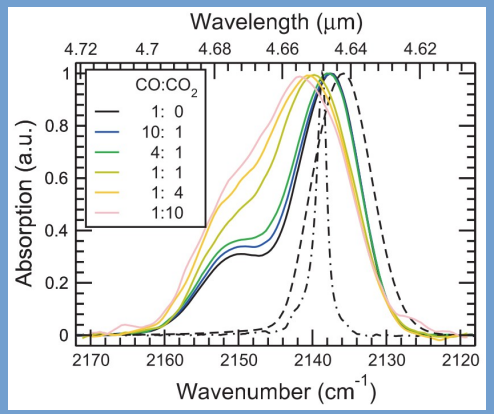

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Fit everything together

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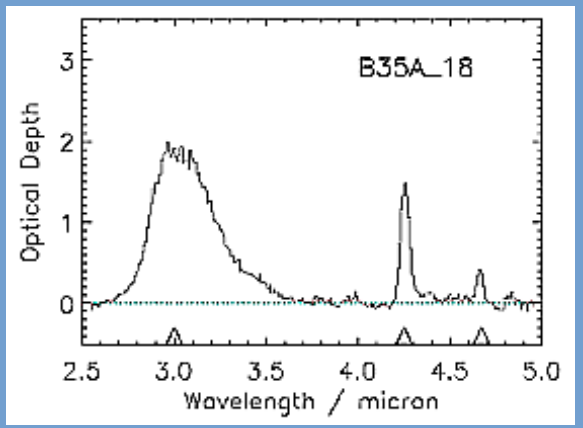

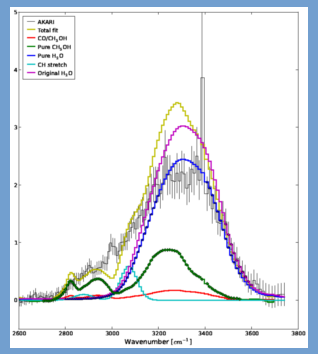

Models+spectra fitted to observations

Calculate column densities

The process of finding frozen molecules

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Theoretical models

Lab spectra

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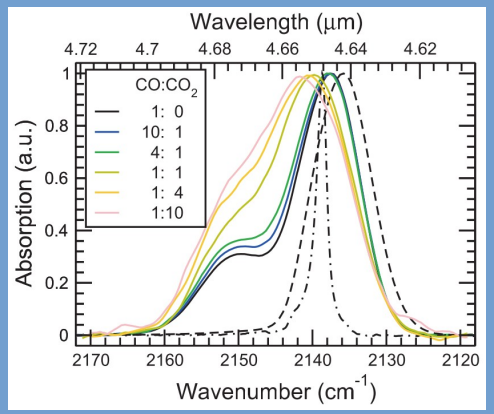

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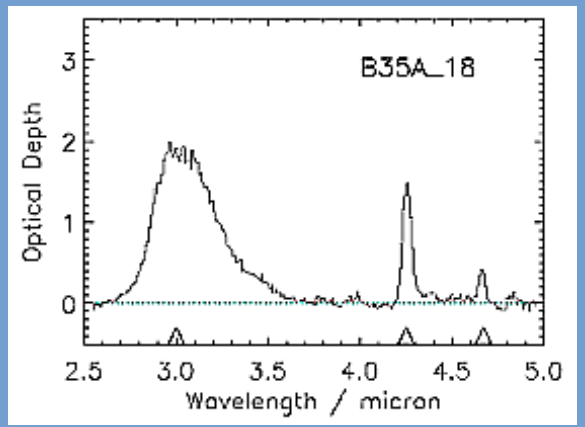
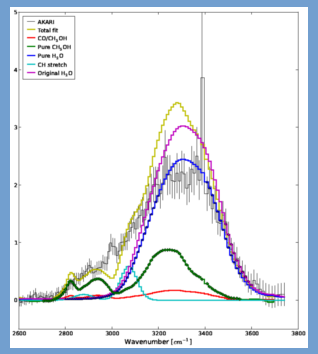
Fit everything together

Observed spectra





Models+spectra fitted to observations

Calculate column densities

SCIENCE!

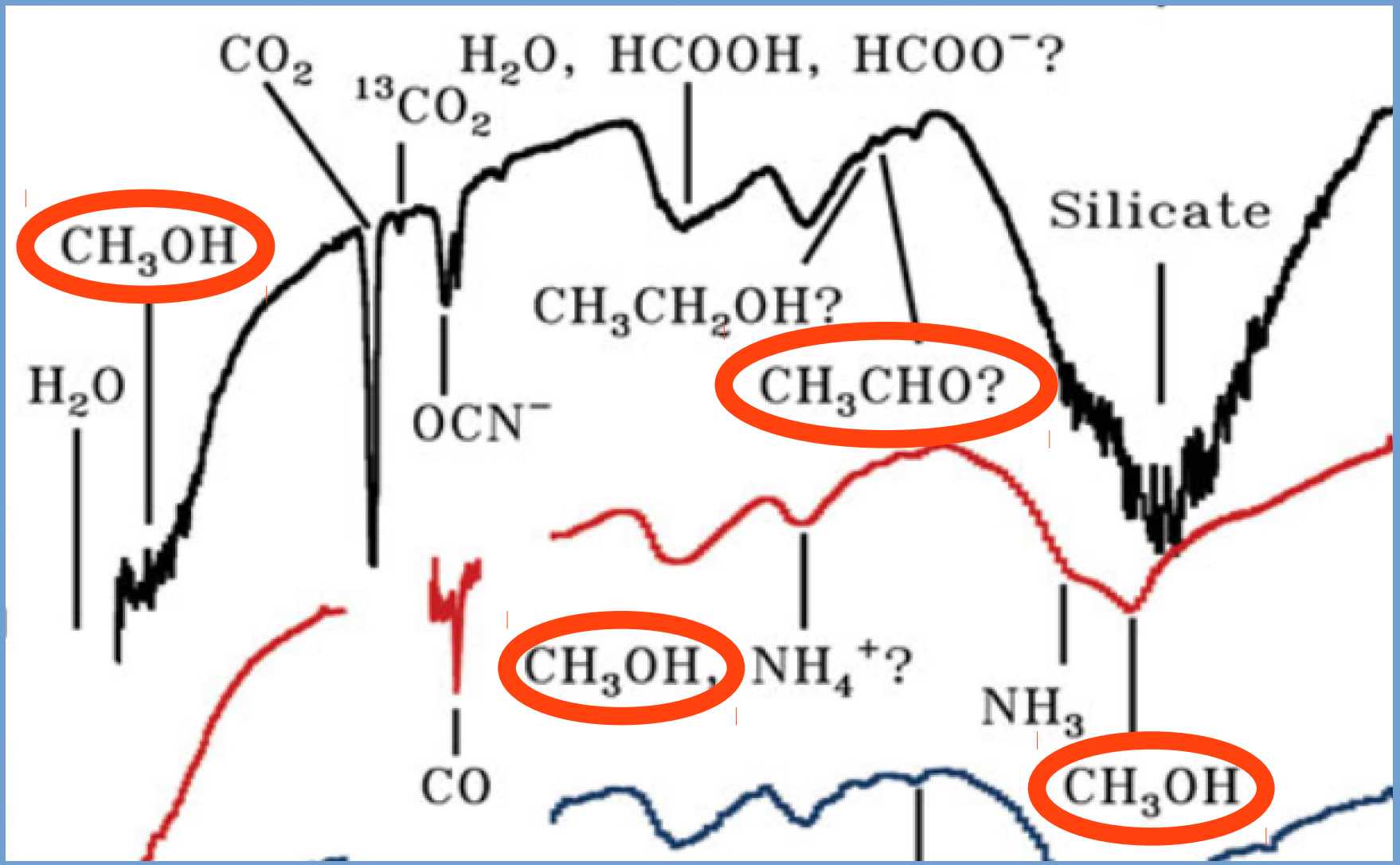
What's needed for this?

- Laboratory spectra usually need post-processing before they can be fitted to observations.
  - Grain-shape effect corrections need the complex refractive index as a function of wavelength/frequency.
  - You can either publish your spectra so it includes the complex refractive index...
  - ...or you let us calculate it from some extra information you give us.

The Kramers-Kronig relation

- The Kramers-Kronig relation can be used to convert absorption spectra into spectra of the complex refractive index
- The KK relation requires a few extra things
  - **The thickness of the ice you grew in the lab**
  - **The real part of the refractive index at high frequencies** (relative to the near/mid-IR)
- These are rarely provided with the data, but are necessary for high-quality fits especially to low-wavelength regimes

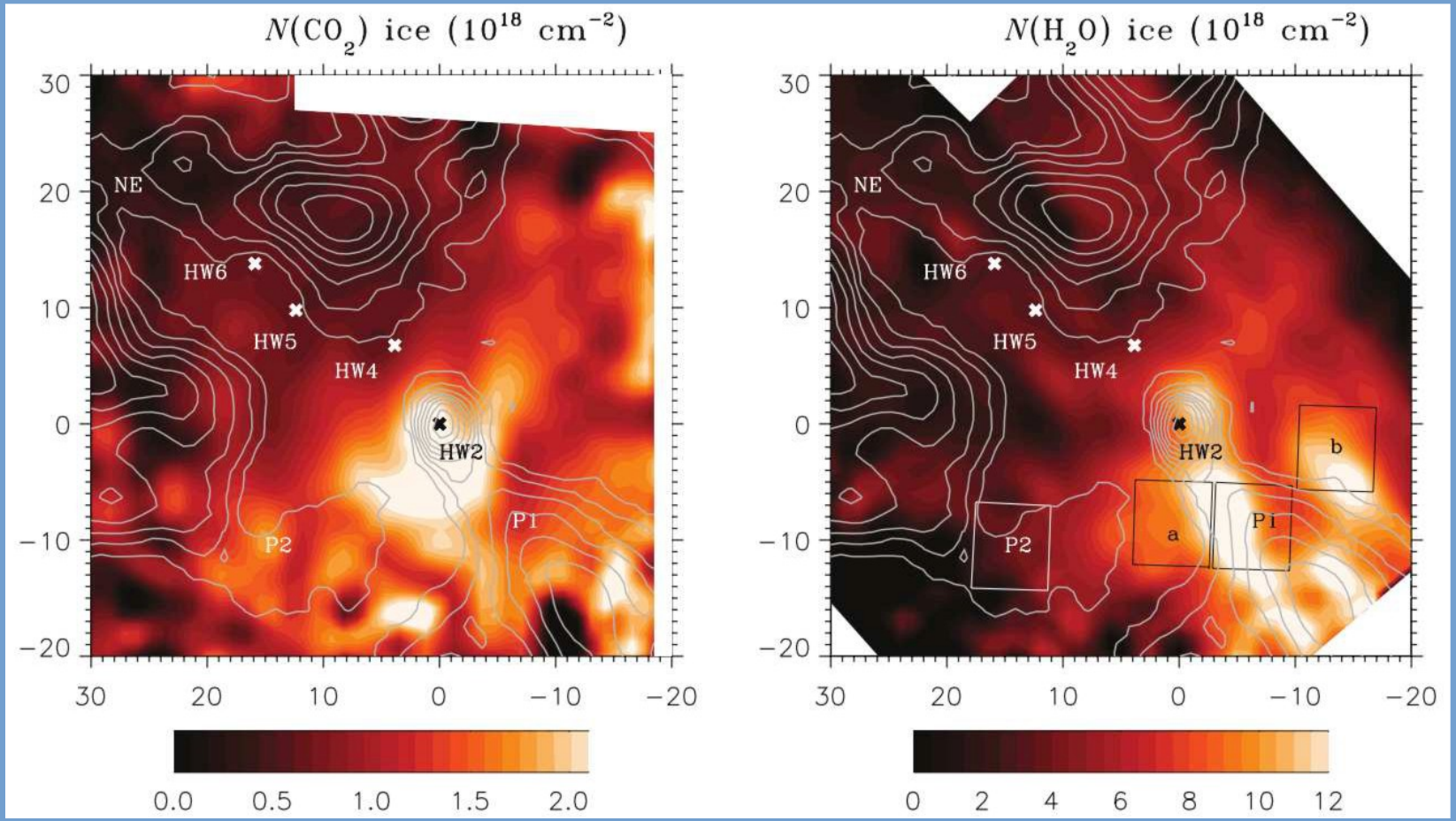
The importance of wavelength coverage



Other things that I wish was done with published spectra

- **Make them easy to cite!**
- Provide information about the physical conditions
  - Deposition method
  - Ice temperature
  - Unambiguous mixing ratios for mixtures
  - Accurate column density estimates
- The wavelength resolution should be at least as high as what the telescopes are capable of
  - JWST/MIRI can do up to R≈2000 spectroscopy
  - JWST/NIRSPEC does up to R≈1000
  - VLT/ISAAC could do R≈3000

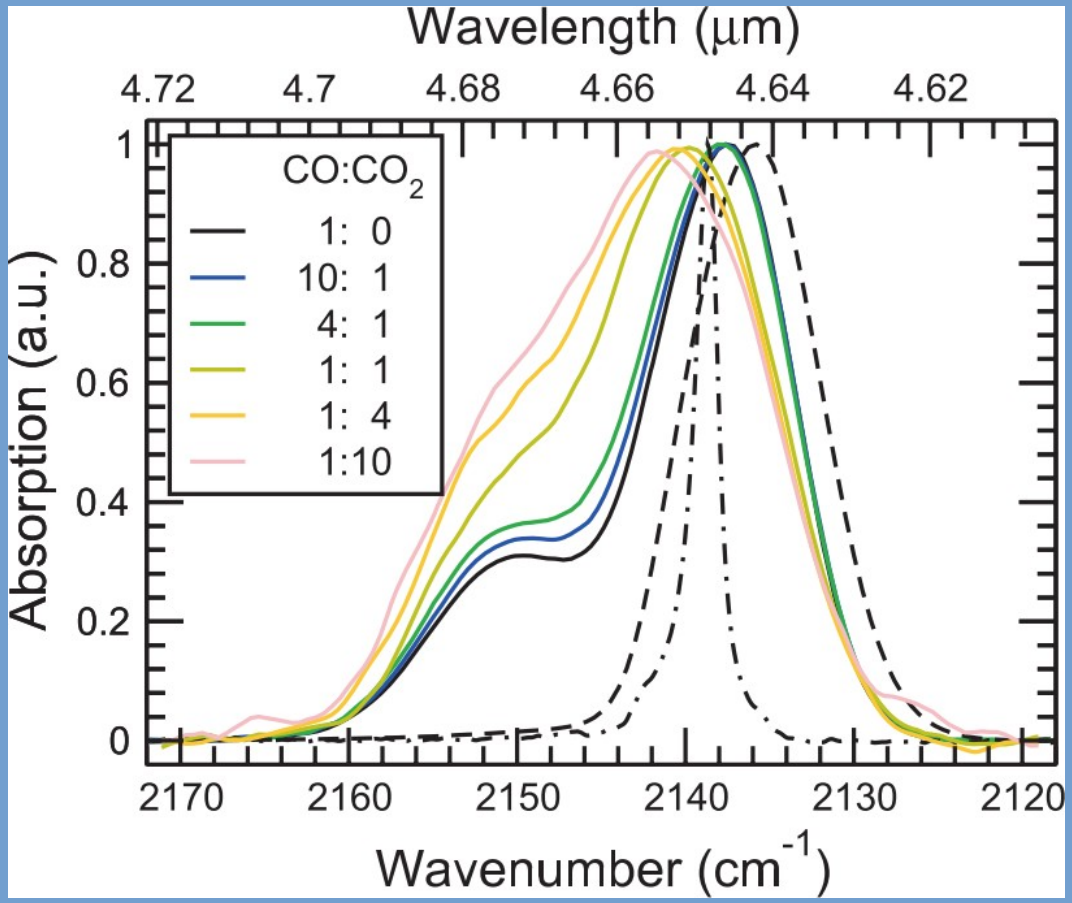
From ice+gas mapping to more accurate chemical evolution models?



Colour gradient: ice column density
Contours: gas-phase NH_3 (1,1) emission

From Sonnentrucker et al. 2008

Physical conditions as free parameters?



From Cuppen et al. 2011

- Fitting ices always makes assumptions about the ice mixing ratios etc. being fixed
- If it was possible to un-fix these into free parameters, that might be interesting.