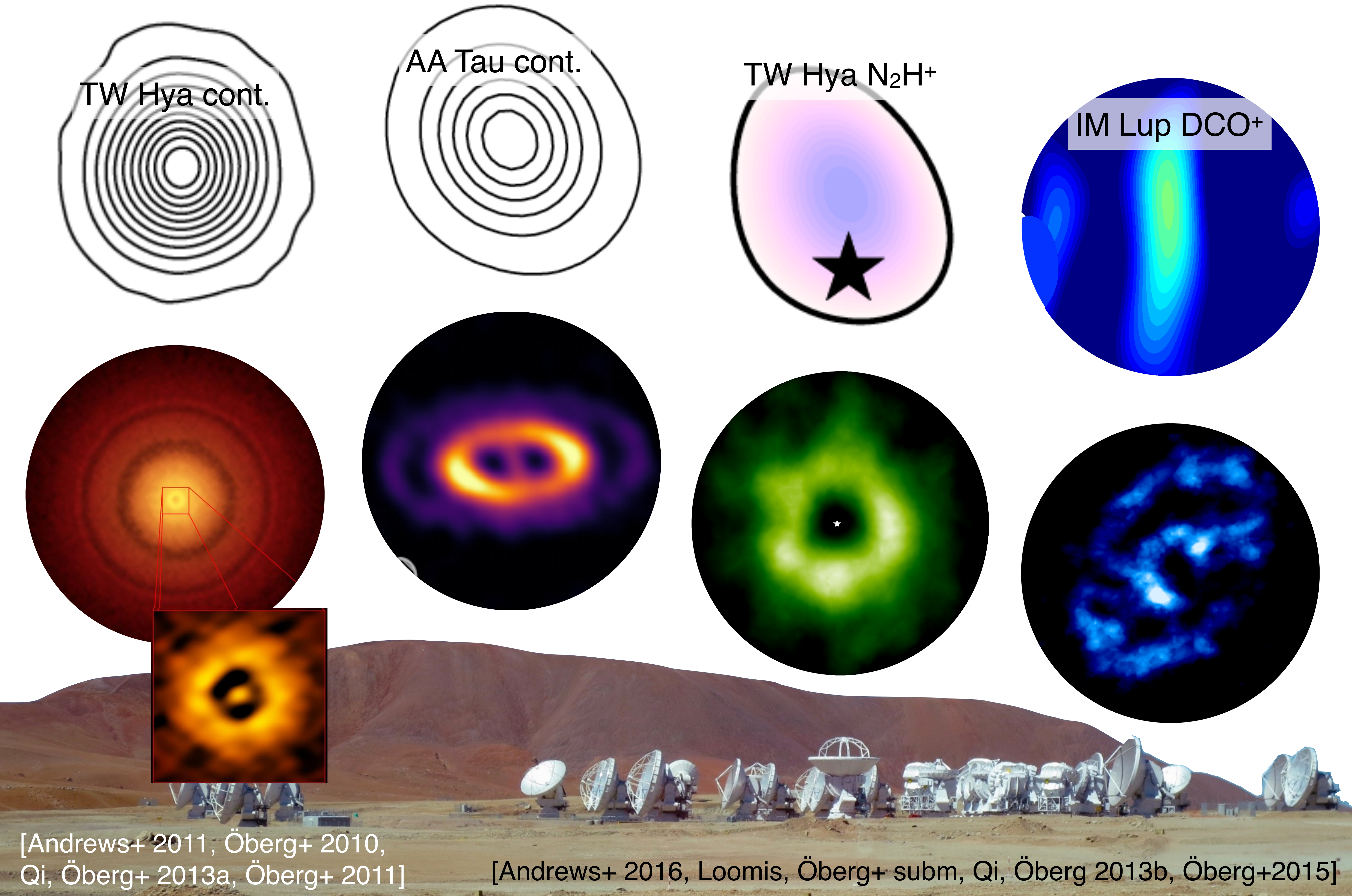
Laboratory astrophysics challenges:

facilitating hydride detections, and constraining hydride chemistry

Karin Öberg

Precision astrochemistry with ALMA (and JWST)



Different flavors of challenges

Identification: Spectroscopy of new species and of isotopologues in gas and solids

Quantification: Accurate excitation of gas-phase hydrides

Gas-phase formation and destruction: (State specific) reaction rates in the gas-phase at low and high temperatures

Surface and ice chemistry: thermal, UV, electron and CR regulated reactions

Sublimation: Thermal and non-thermal sublimation efficiencies and mechanisms

Gas-phase Spectroscopy and Excitation

Line identification:

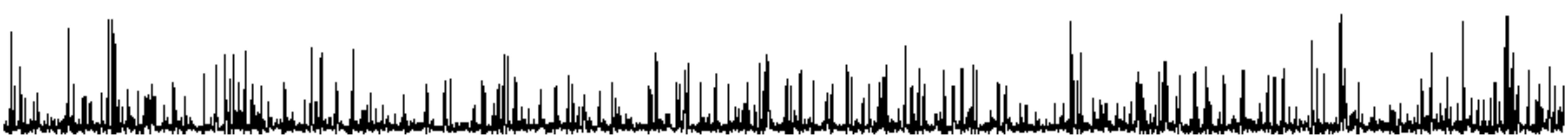
- Missing spectra for unstable species, and for isotopologues of common species

Excitation studies:

- Excited OH as probe of Lyman alpha [Ewine's talk].
- Molecular cloud formation using OH [Poster #9, Yuji+]

Need this data to interpret observations.

Please recommend funding whenever you can!



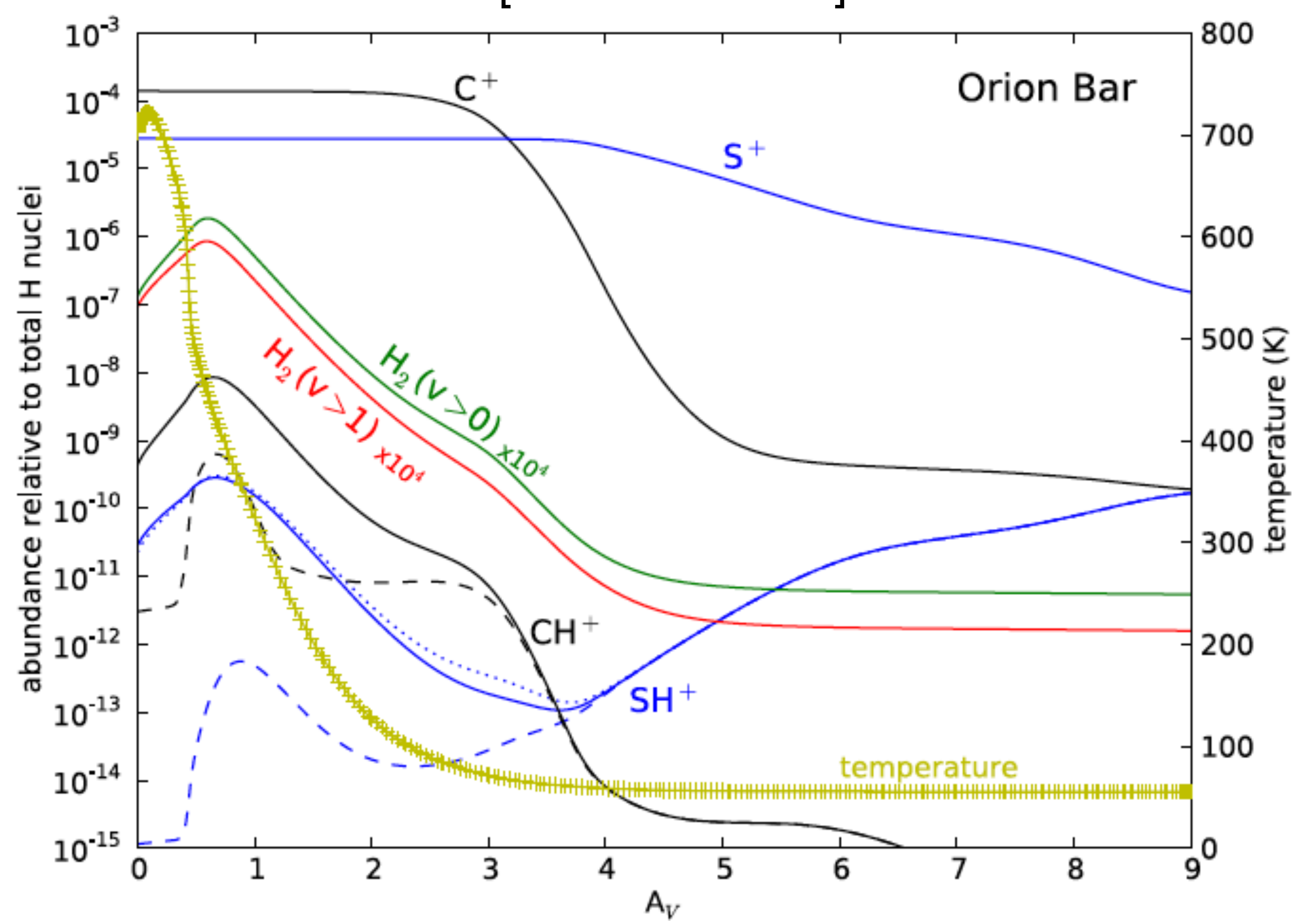
347.5-350.5 GHz spectra toward IRAS 16293-2422 [Jørgensen+ 2016]

State specific gas-phase chemistry

Predicted chemistry in PDRs, diffuse ISM etc. changes dramatically when taking into account reactions with excited H_2

Calculations are advancing knowledge of state-specific reaction rates (e.g. Schneider on H_2^+ recombinations), but experiments are needed to anchor theoretical work

[Zanchet+ 2016]

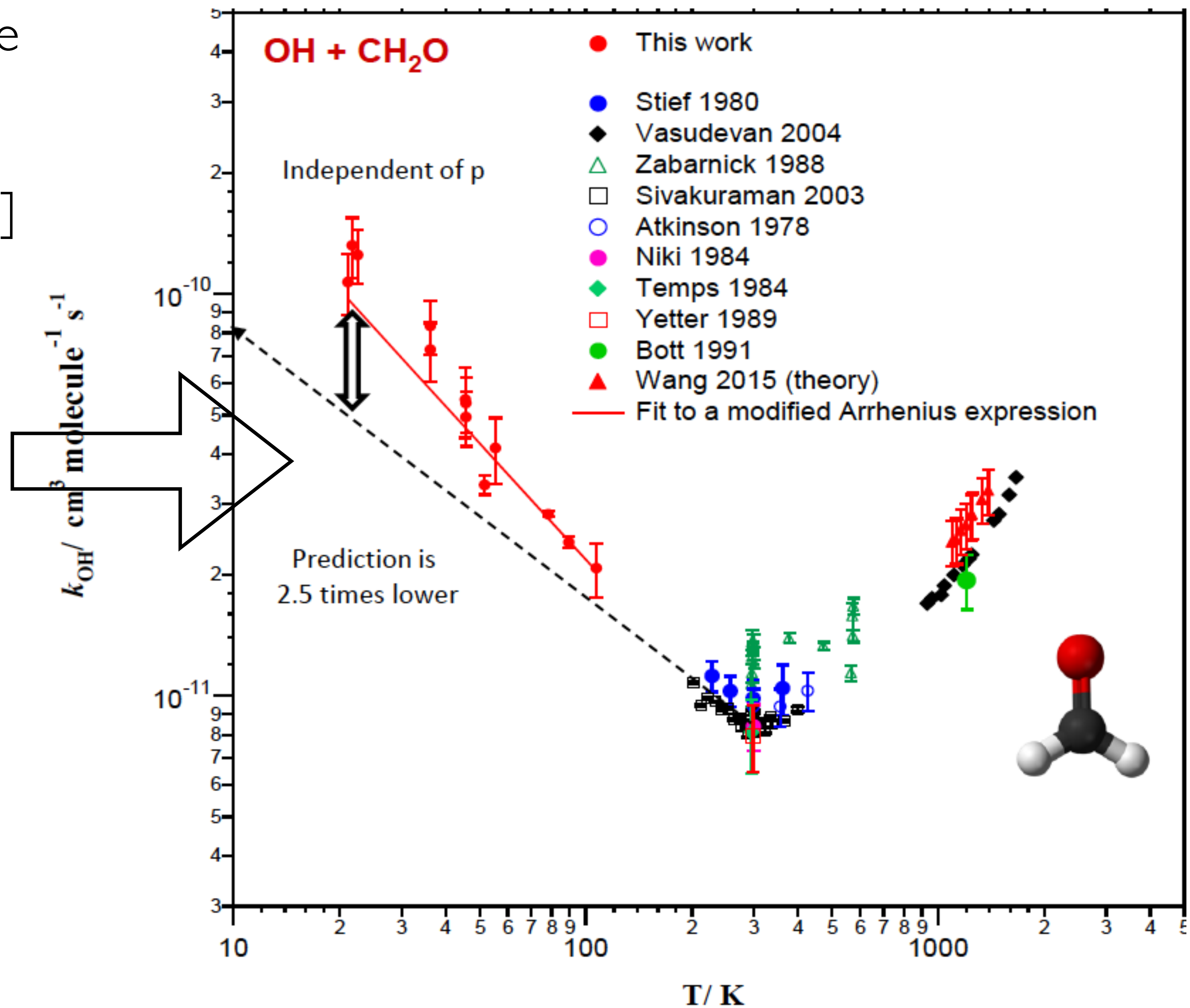


Temperature dependence gas-phase reactions is very difficult to predict

Poster #7: Temperature dependence of H_2D^+ and D_2H^+ recombinations [Petr+]

Poster #11: Temperature dependence of OH reactions with H_2CO [Blázquez Gonzalez+]

Poster #21: Temperature dependence of nitrogen and oxygen hydride ions with H_2 [Rouča+]

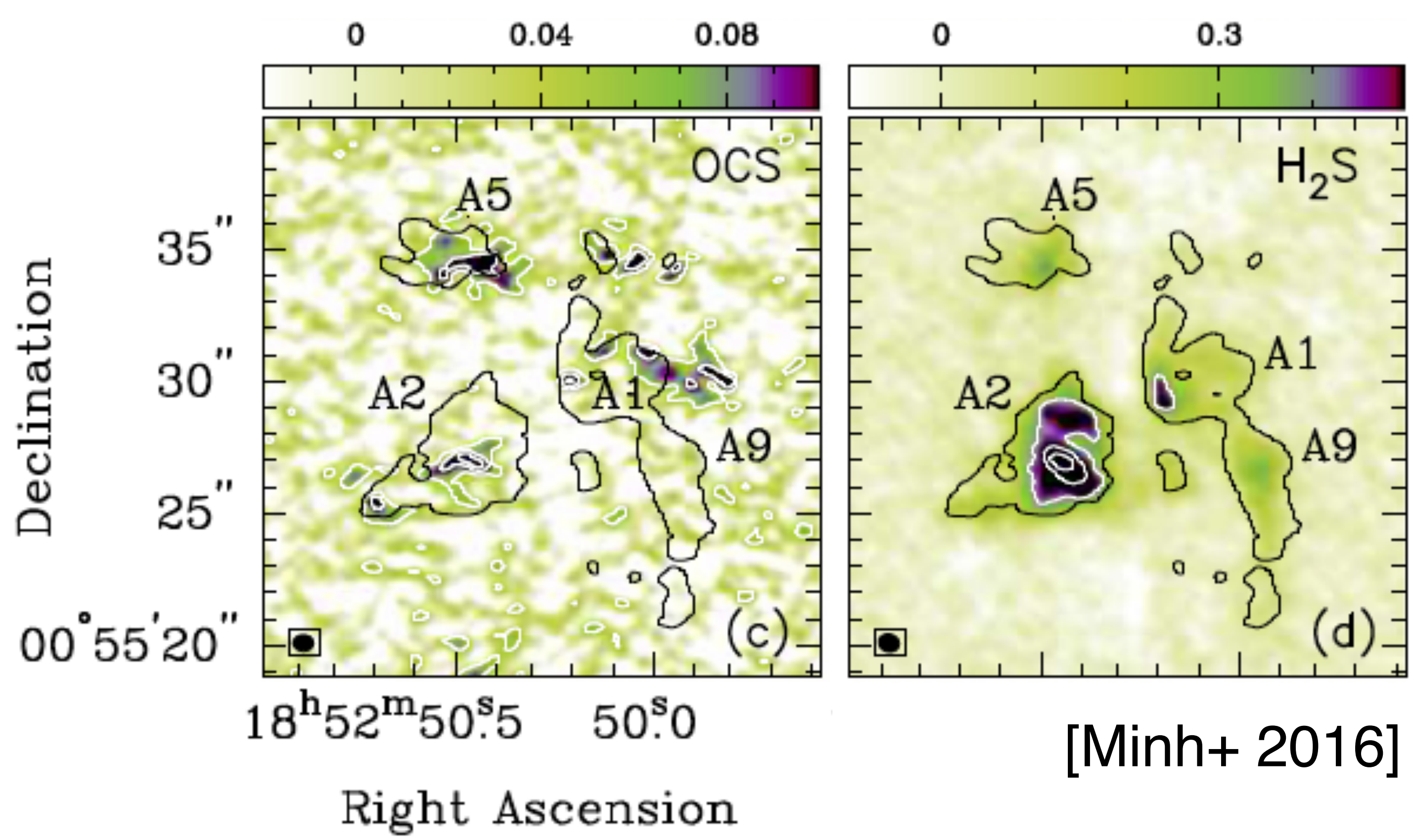


Sulphur chemistry is a big unknown

Sulphur hydrides emerging as empirical new tracers in galactic and extragalactic environments

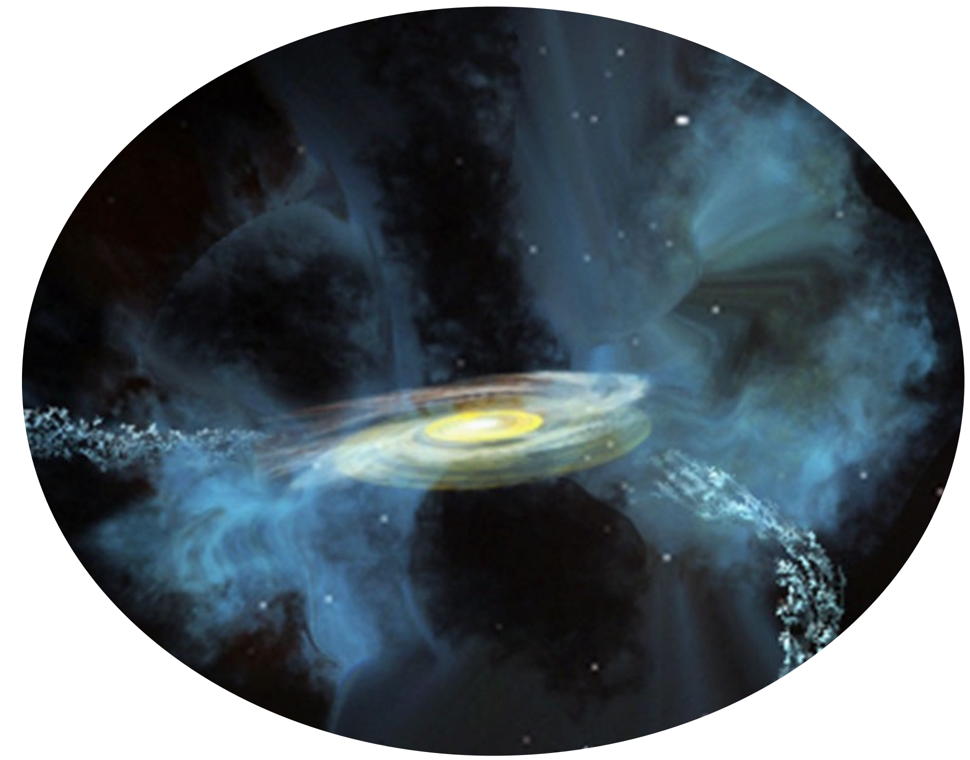
Gas-phase and surface chemistry and sublimation poorly constrained

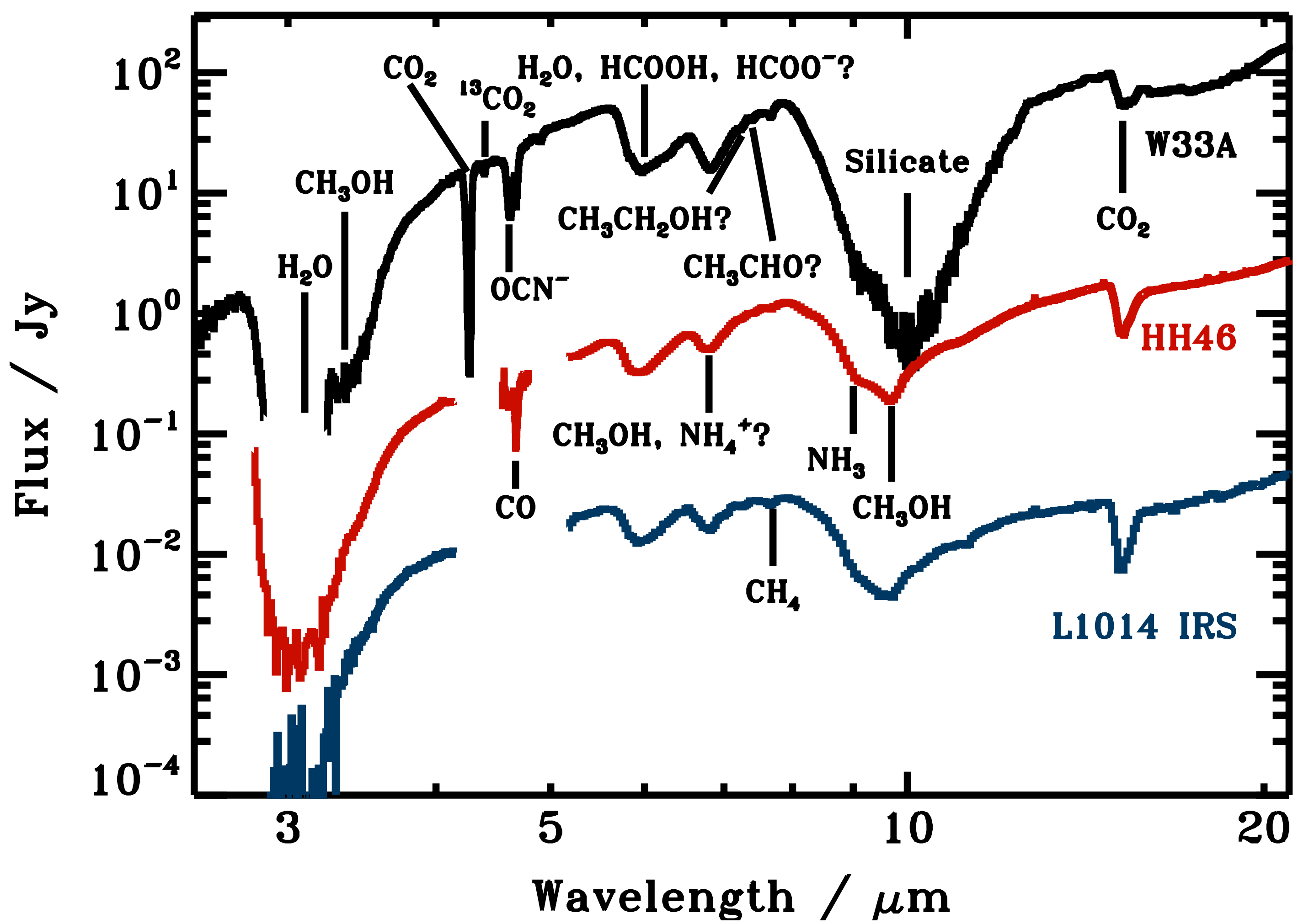
H_2S in dark clouds [Fuente]

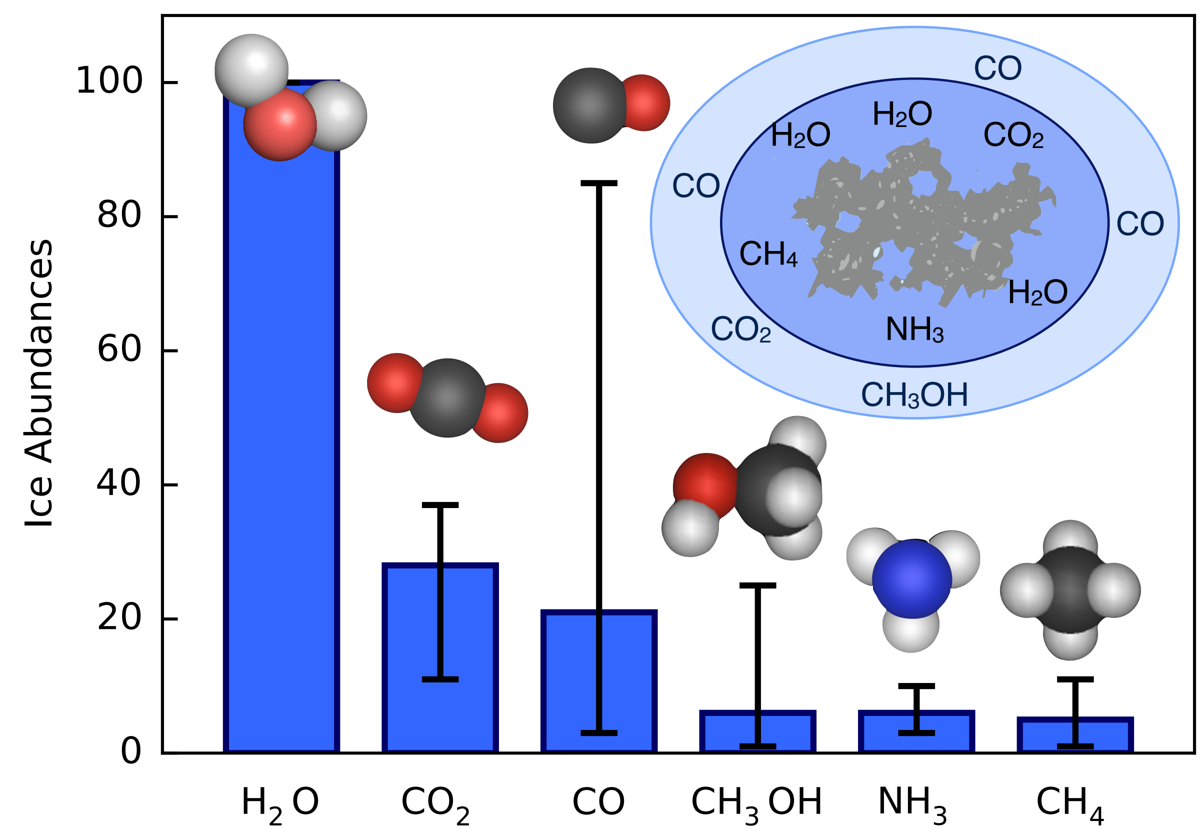


[Minh+ 2016]

Ice spectroscopy needed to constrain main reservoirs of hydrides during star and planet formation

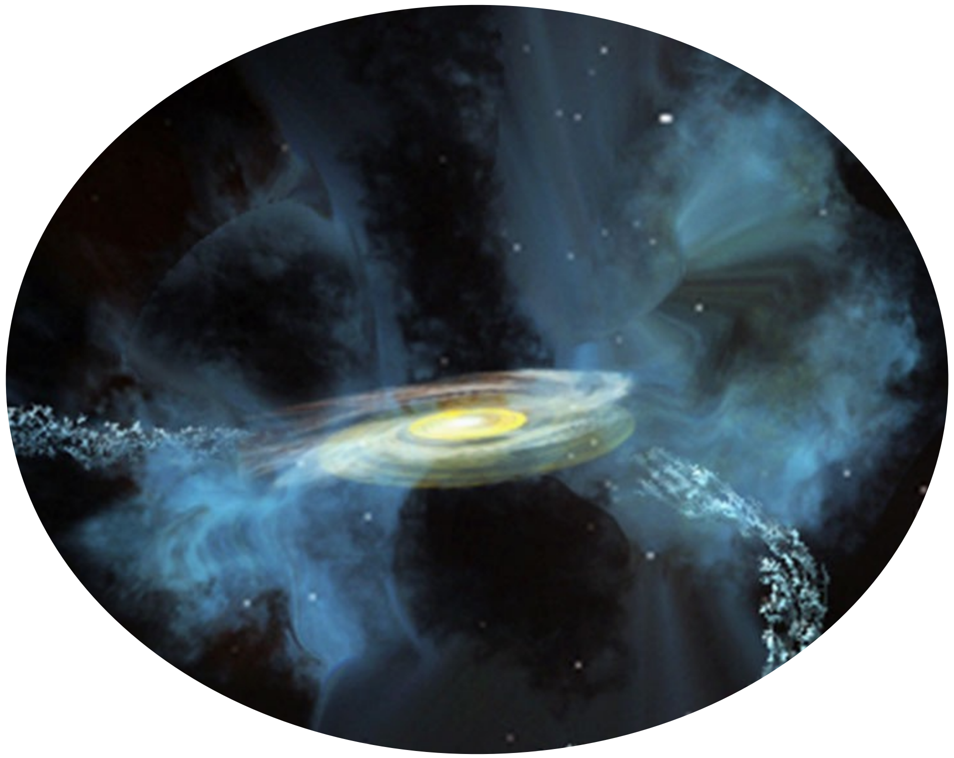




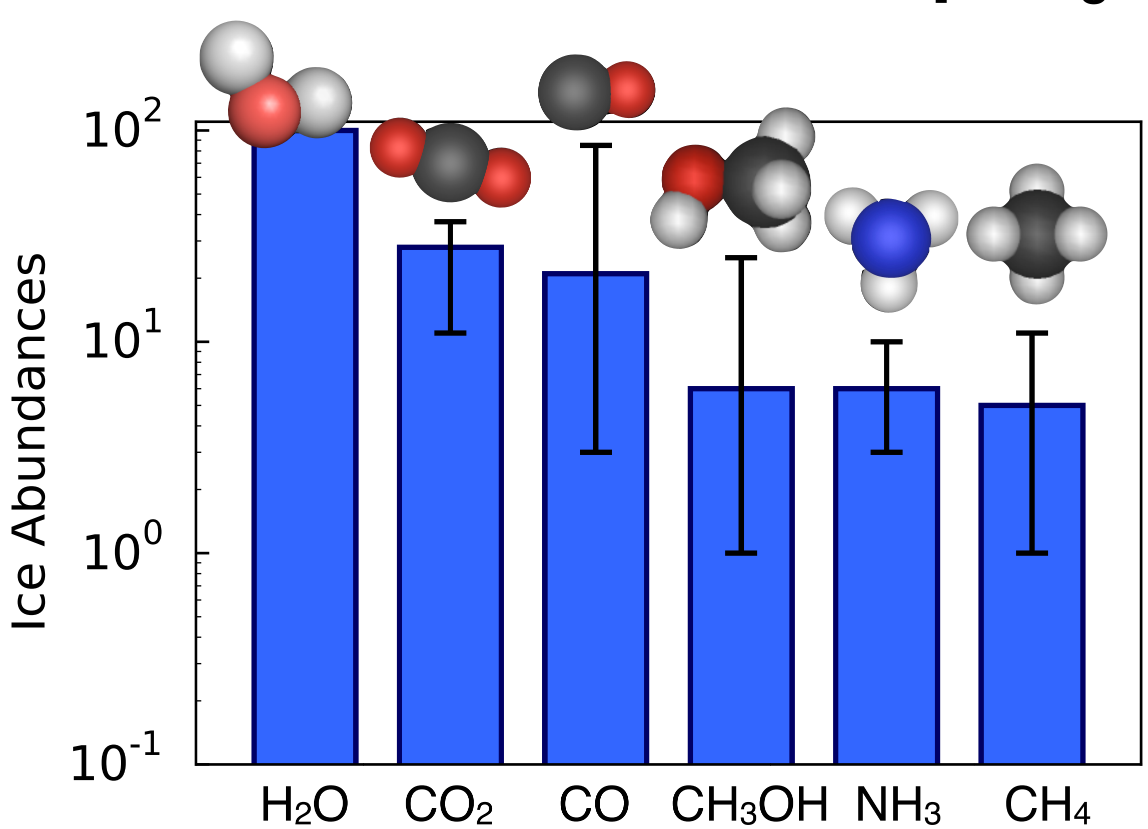


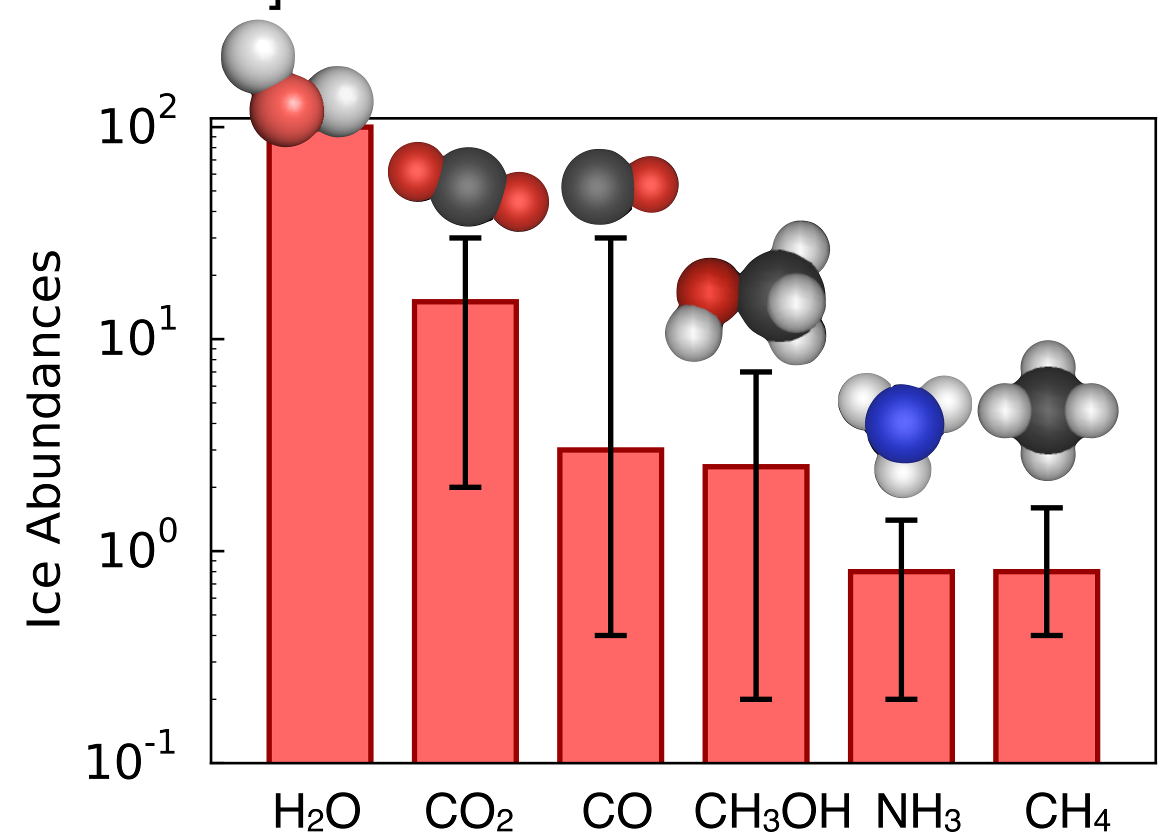
[Öberg+ 2011, Boogert+ 2015]

NH_3 and CH_4 formation and destruction?



[Öberg+ 2011, Mumma+ 2011]



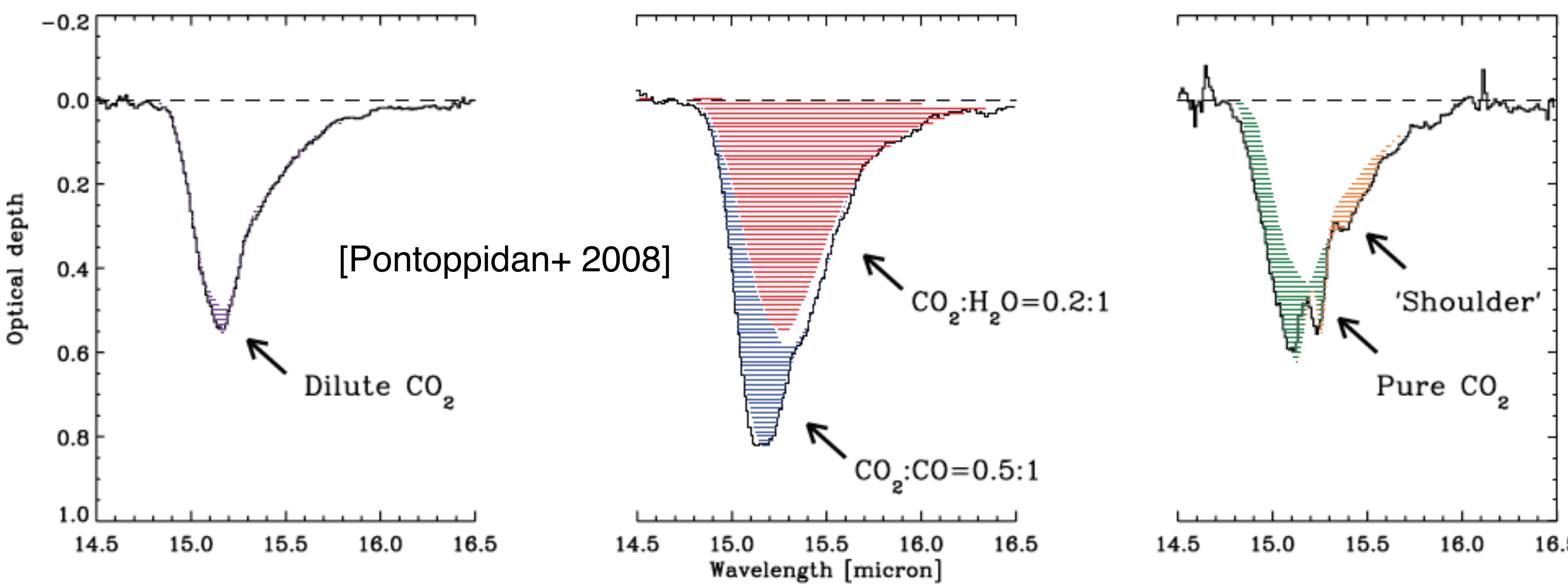


Ice spectroscopy: tracing ice histories

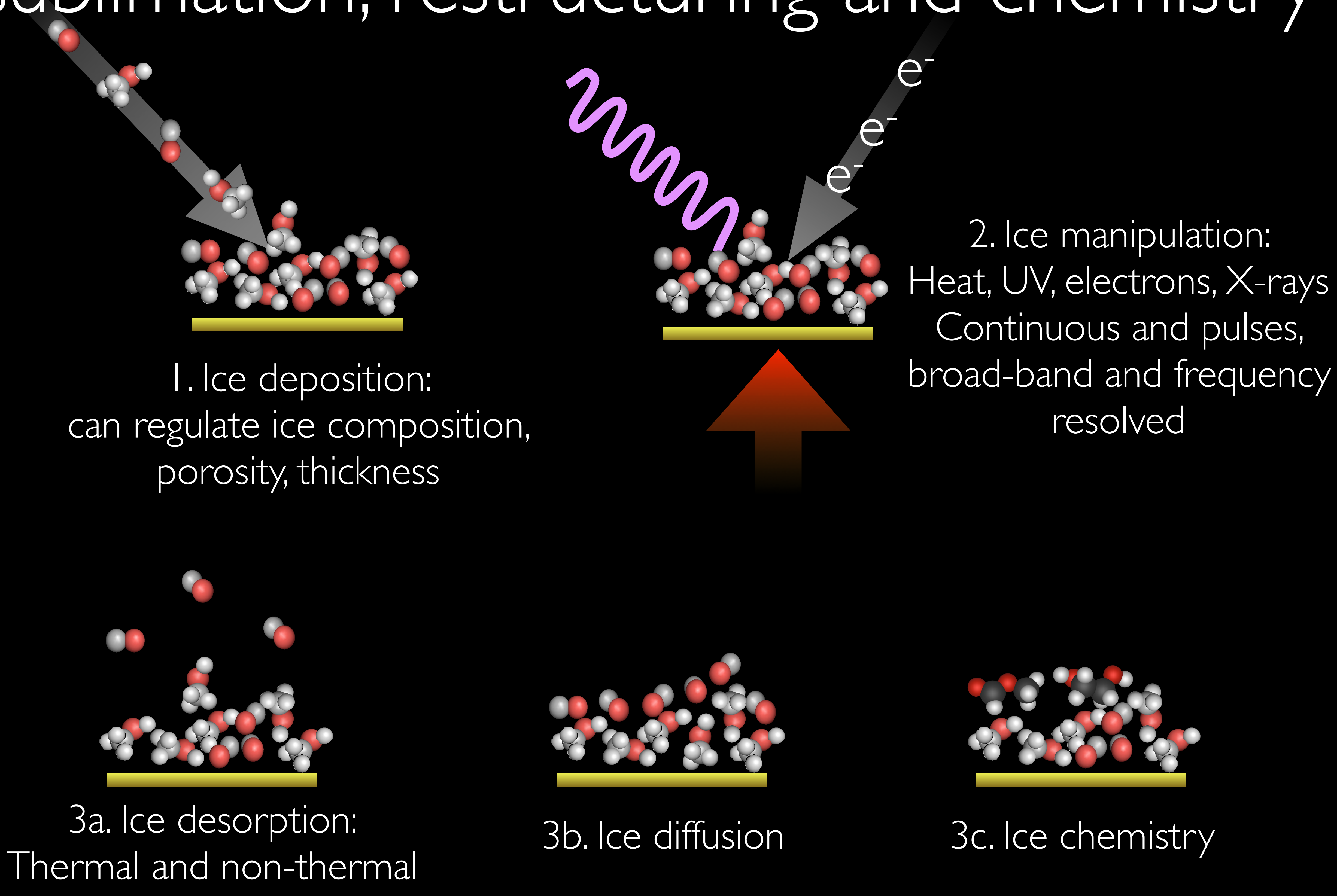
Can use spectral profiles to trace histories of different ice components.

Done successfully for CO_2 with Spitzer and laboratory spectroscopy

Should be possible for CH_4 and NH_3 with JWST: need laboratory spectroscopy studies!

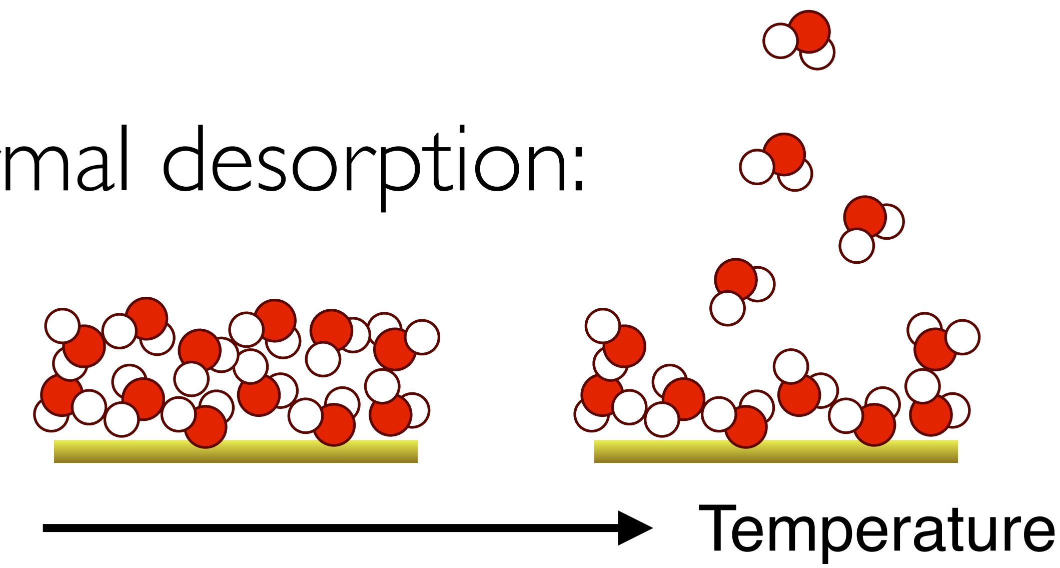


Experimental constraints on ice sublimation, restructuring and chemistry

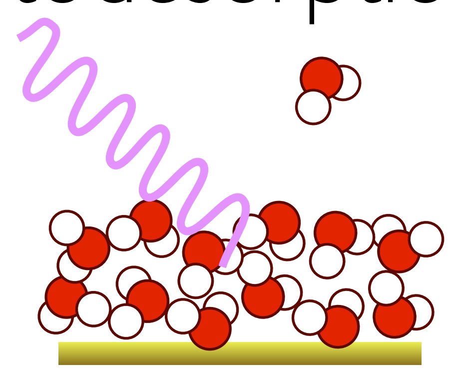


Ice sublimation/desorption

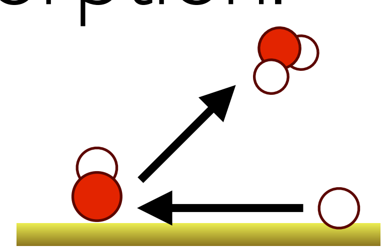
Thermal desorption:



UV + e^- photodesorption:

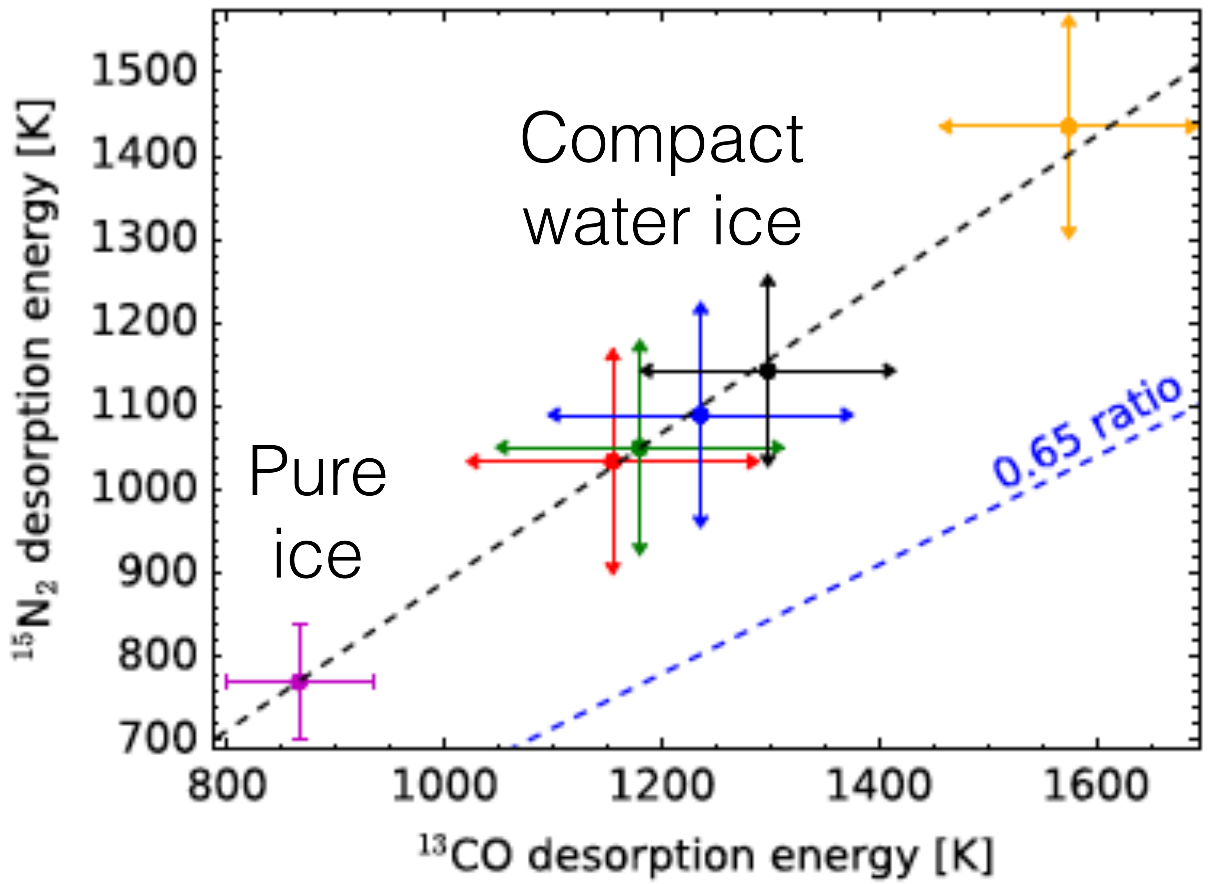


Chemical desorption:

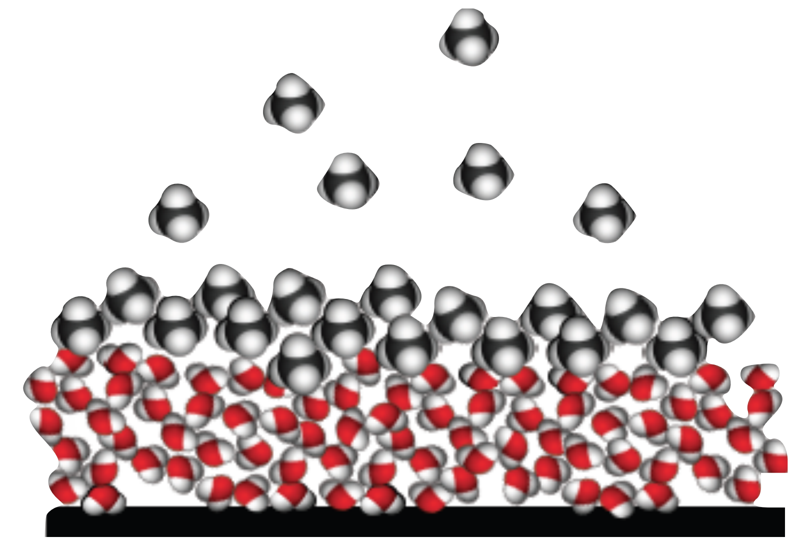


Thermal sublimation

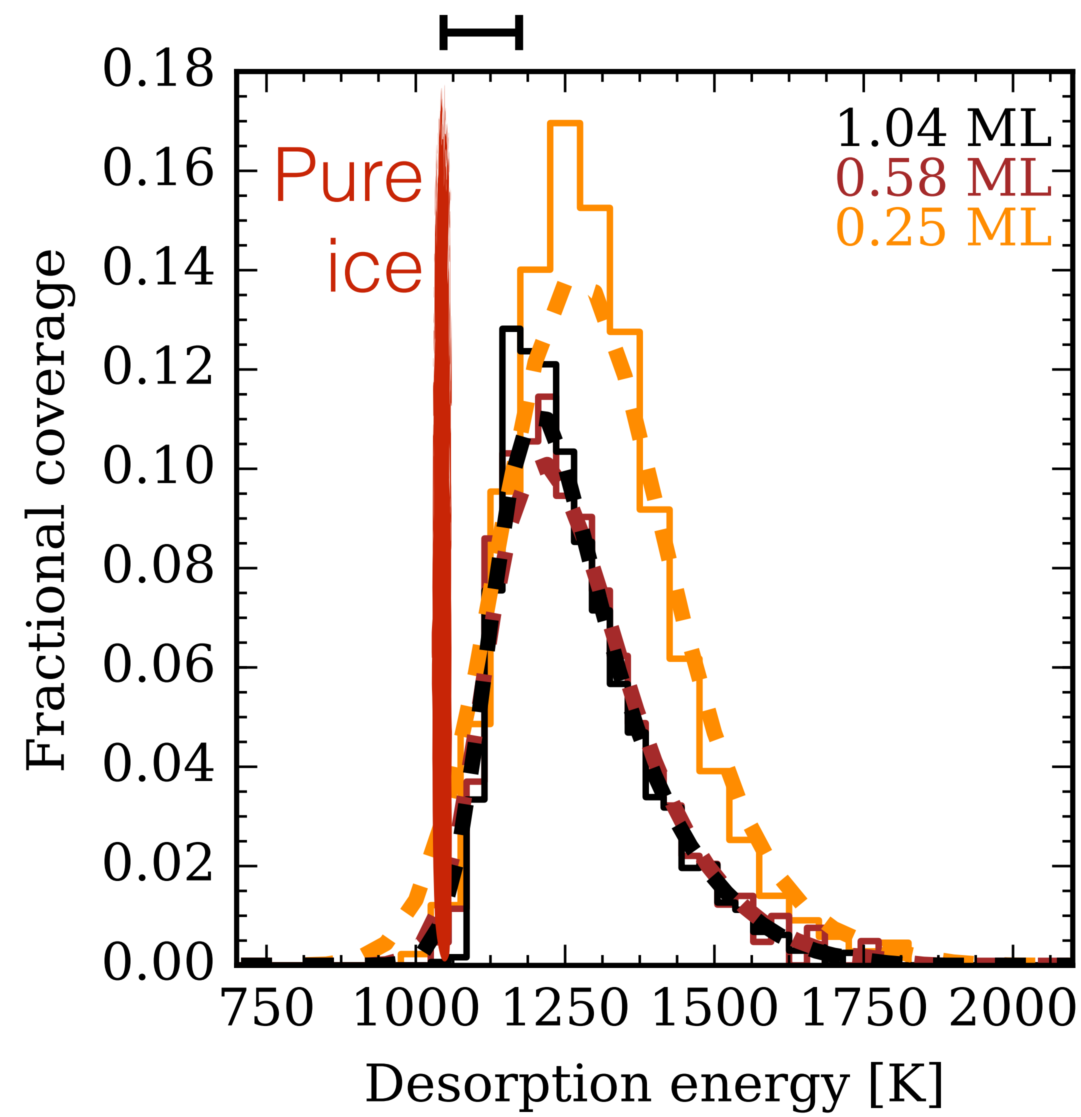
CO and N_2



40-50% increase



10-15% increase



[Fayolle+ 2016, Graninger+ in prep.]

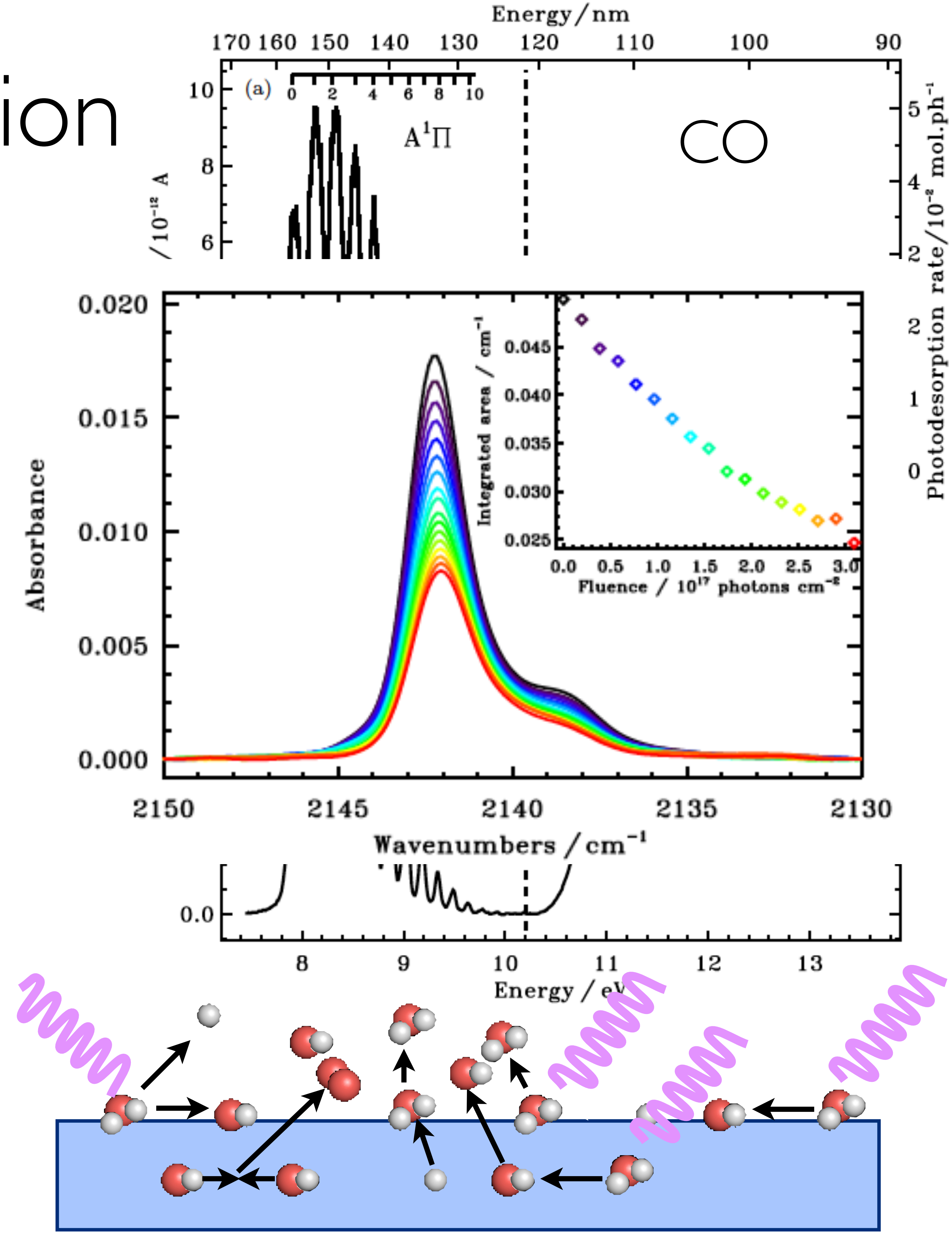
UV photodesorption

Different mechanisms for different molecules:

- indirect non-dissociative,
- direct dissociative,
- indirect dissociative,
- thermal desorption following photodissociation

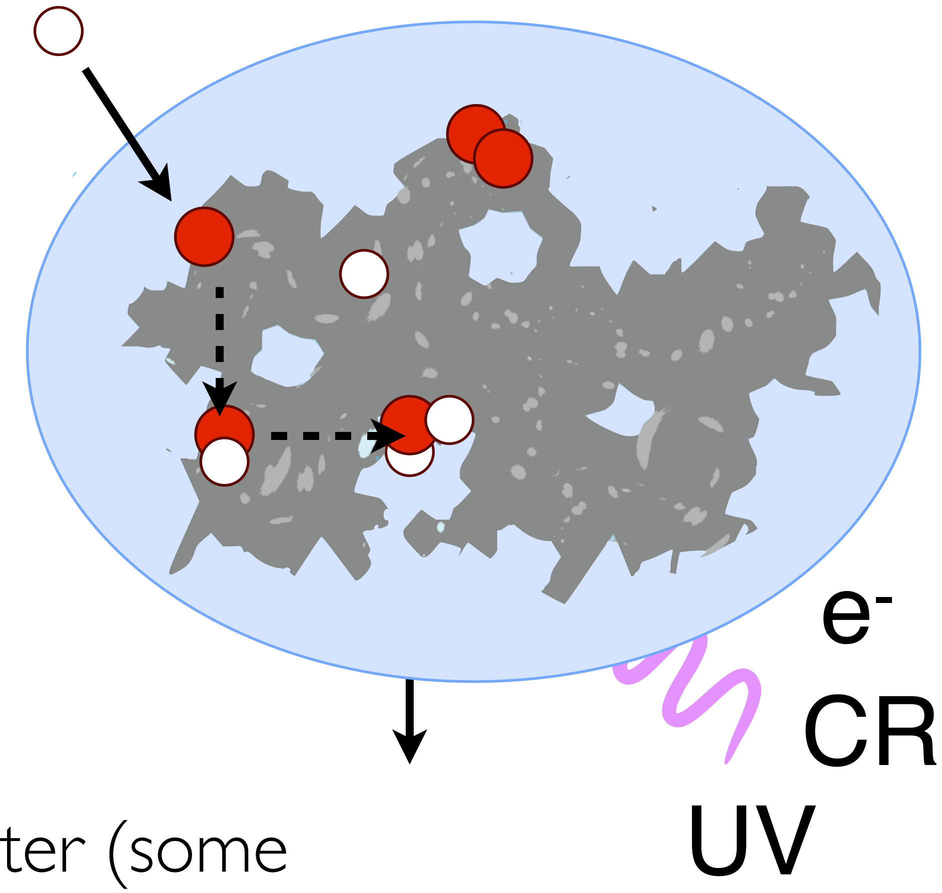
Hydride photodesorption is complicated

Need yields, and an understanding of the precise mechanism to predict rates in interstellar environments



[Öberg+ 2008, 2009ab, Hama+ 2010, Fayolle+ 2011, Bertin+ 2012]

Different non-thermal desorption processes in different environments?



Have:

- Detailed UV photodesorption measurements for water (some inconsistencies between different groups), and CH_4 [P#27, Dupuy]
- Preliminary chemical desorption rates and limits
- Some measurements on electron-induced desorption [P#13, Amlaud+]

Need:

- UV photodesorption yields and mechanisms for all hydrides (including SH_2)
- Chemical desorption measurements from additional groups
- UV vs. electron yields for different kinds of ices to estimate relative importance

Hydride ice chemistry

Hydride formation: H addition reactions

Hydride modification: Salt formation

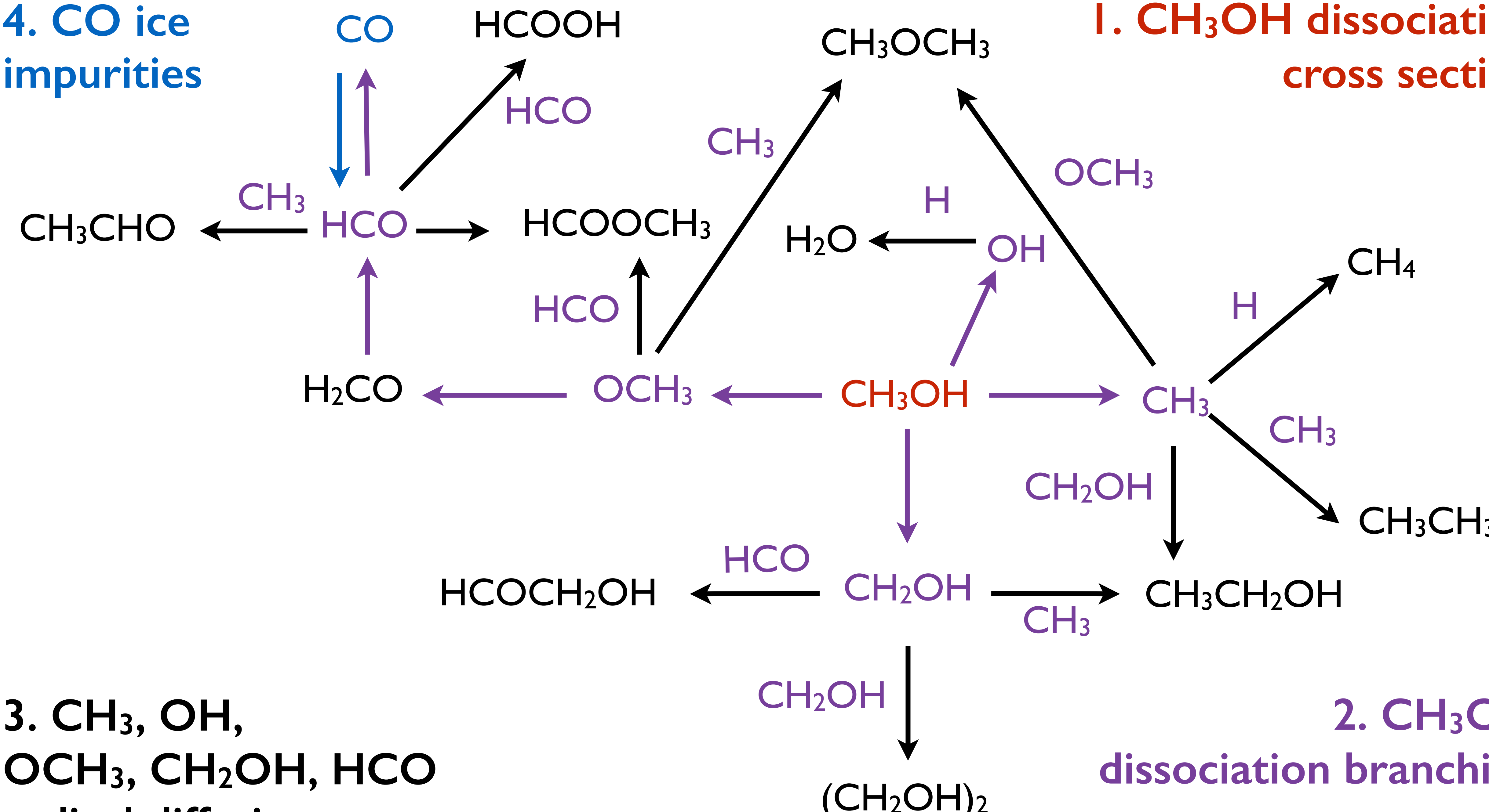
Hydride destruction: Heavy atom addition and UV and electron induced chemistry

In each case the challenge is to obtain quantitative data that can be incorporated into astrochemical models!

Quantifying the CH_3OH ice photochemistry

4. CO ice impurities

1. CH_3OH dissociation cross section



3. CH_3, OH, OCH_3, CH_2OH, HCO radical diffusion rates

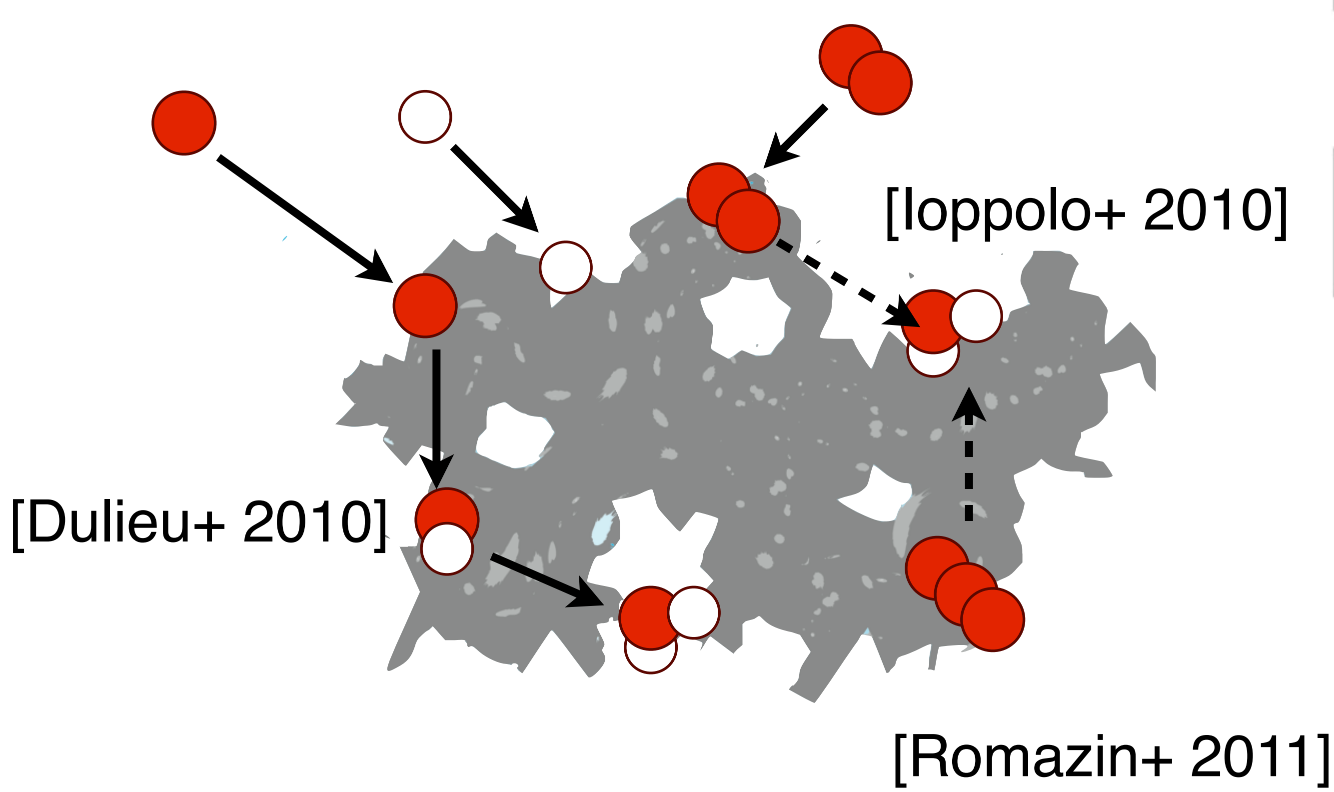
2. CH_3OH dissociation branching ratio

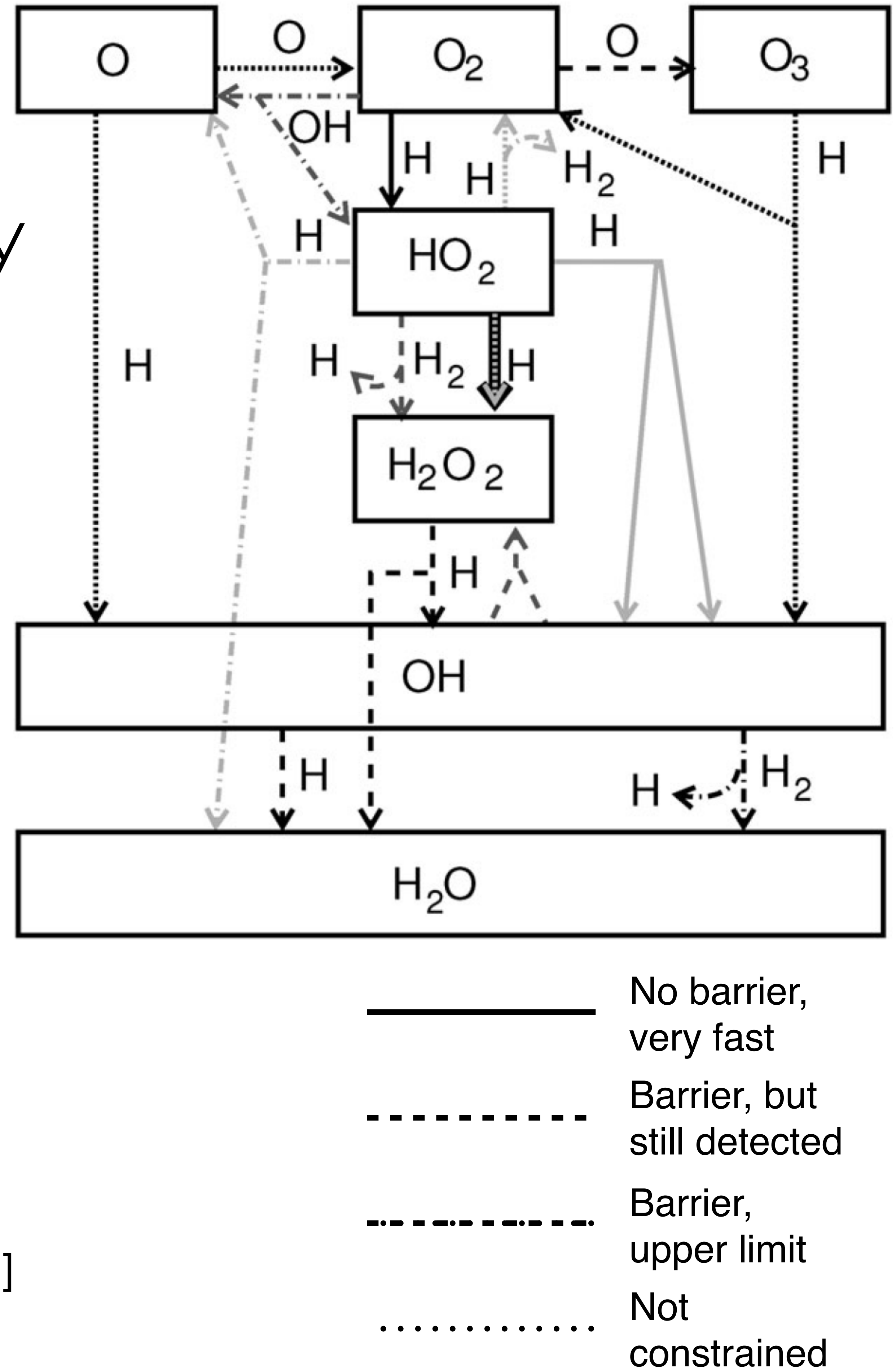
[Öberg, Garrod et al. 2009]

Hydride formation: H addition ice chemistry

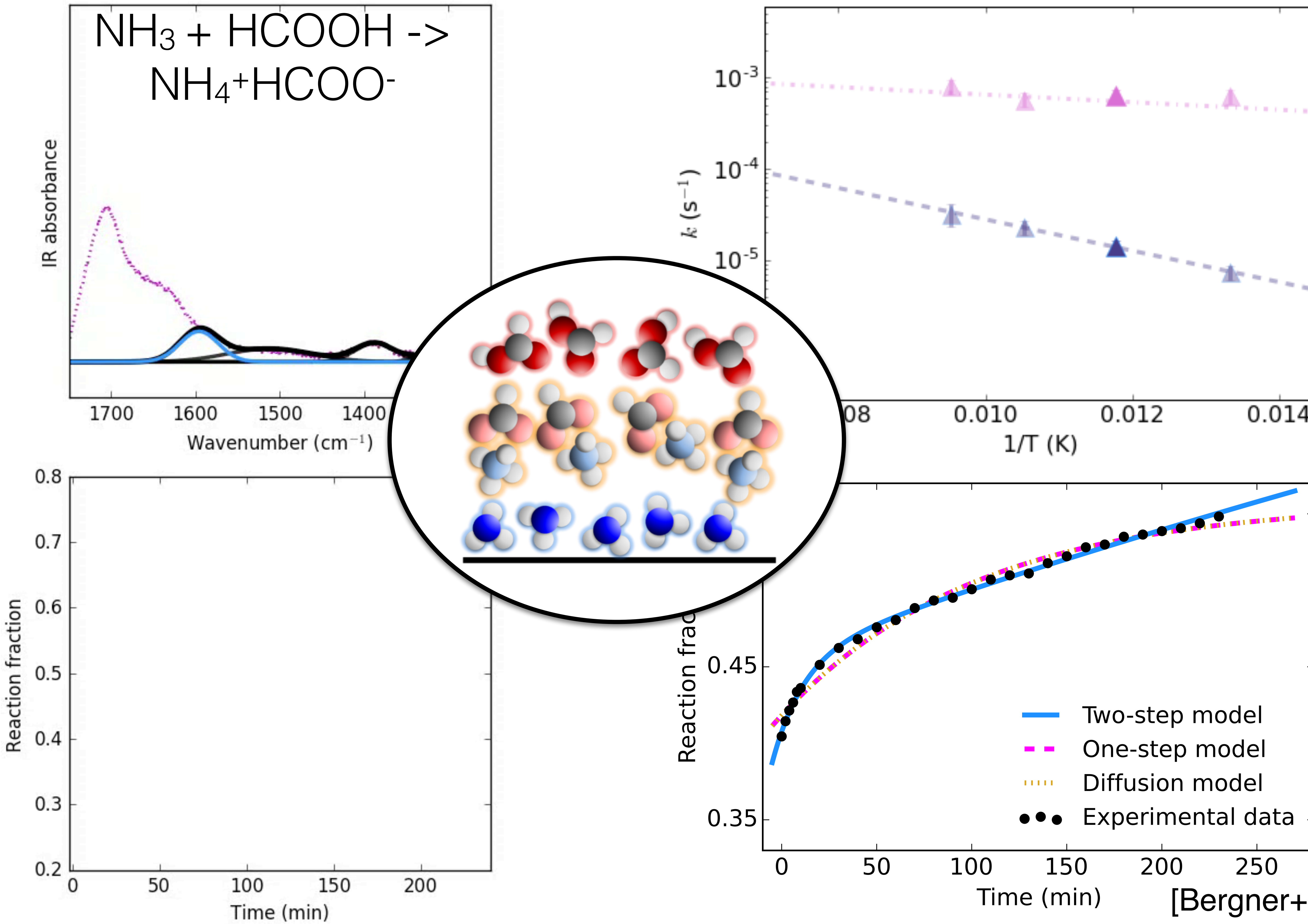
Recent success: resolving H_2O formation

Some initial constraints on CH_4 and NH_3 formation



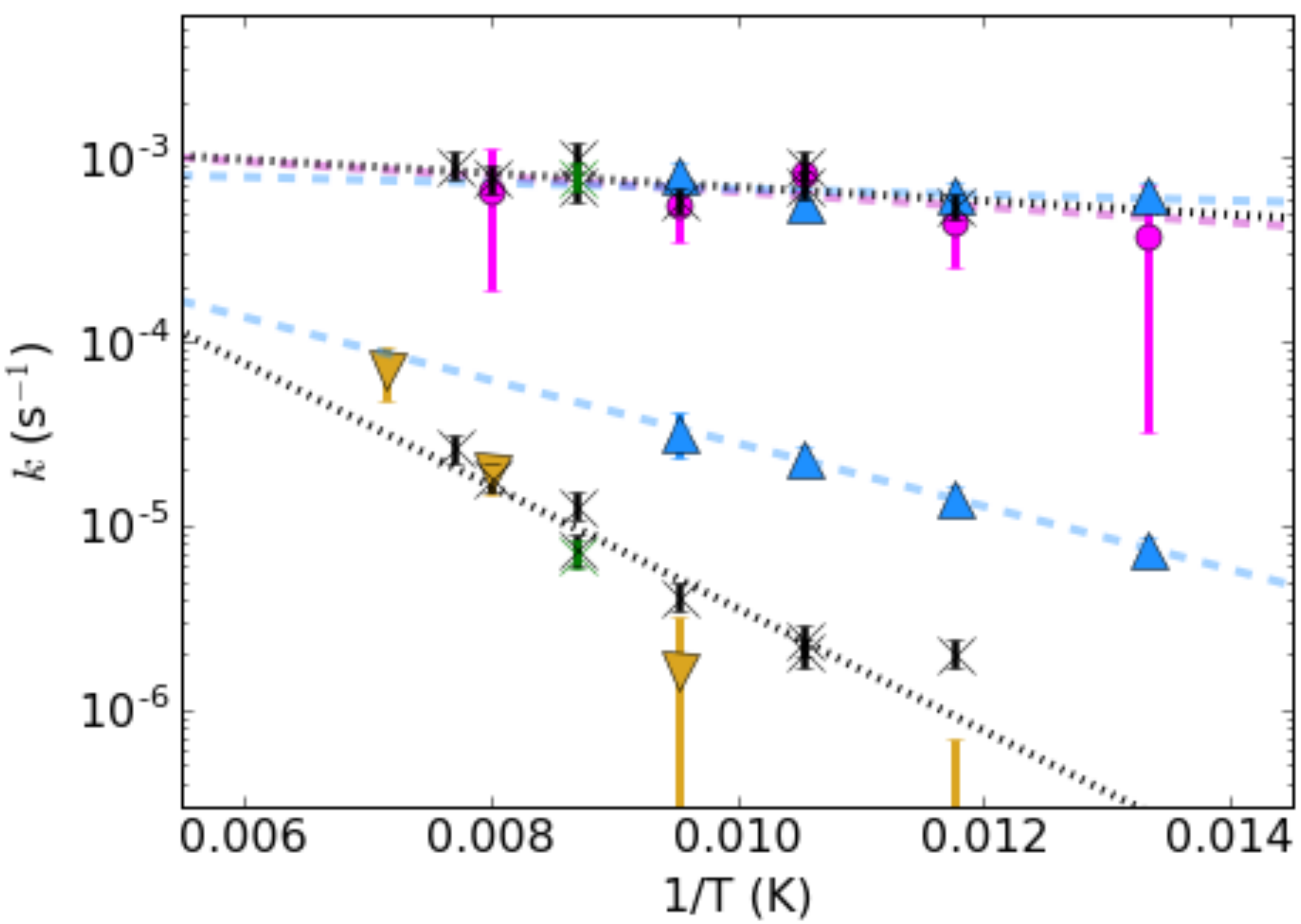


Hydride modification: NH_3 to NH_4^+

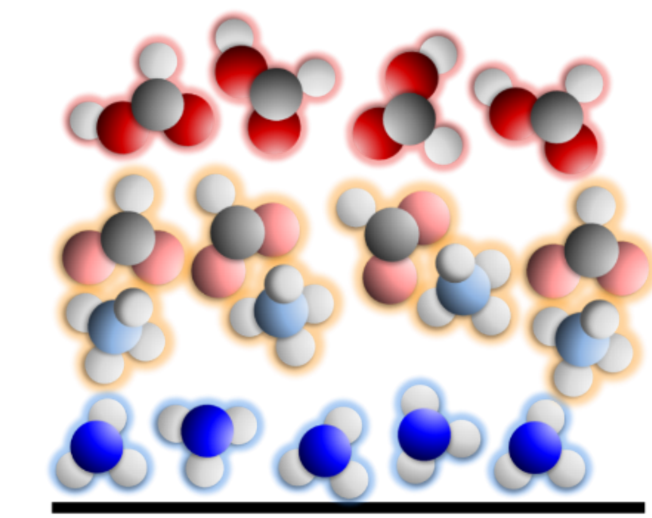


[Bergner+ 2016]

Quantifying salt formation in ices

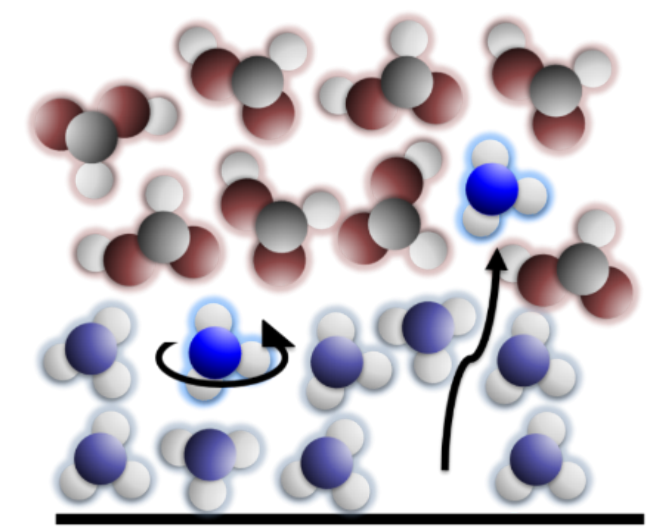


Proton transfer reaction



Re-orientation

Diffusion

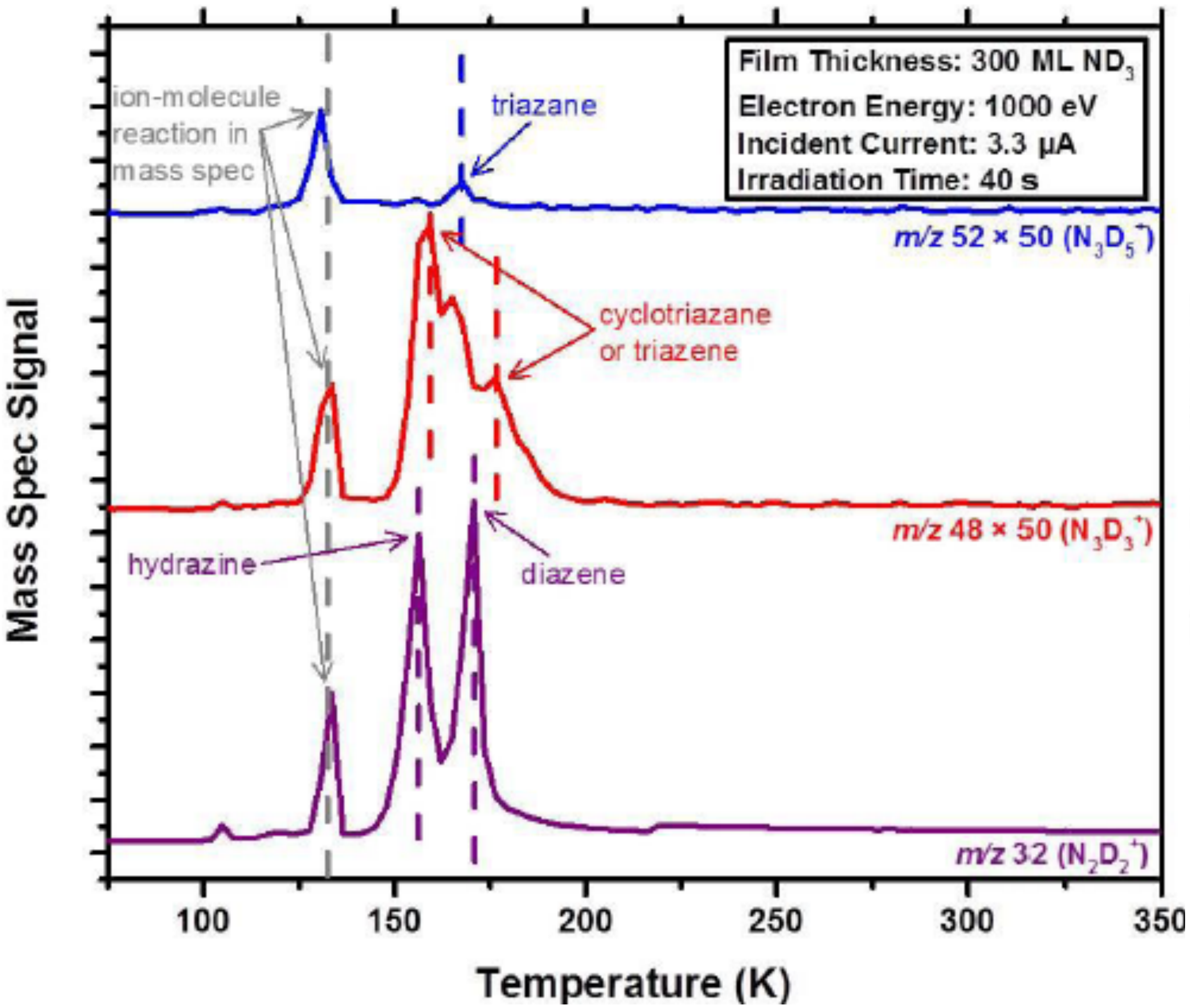


Reaction barrier: 70+/-30 K
Re-orientation barrier: 400+/-10 K
Diffusion barrier: 770+/-110 K

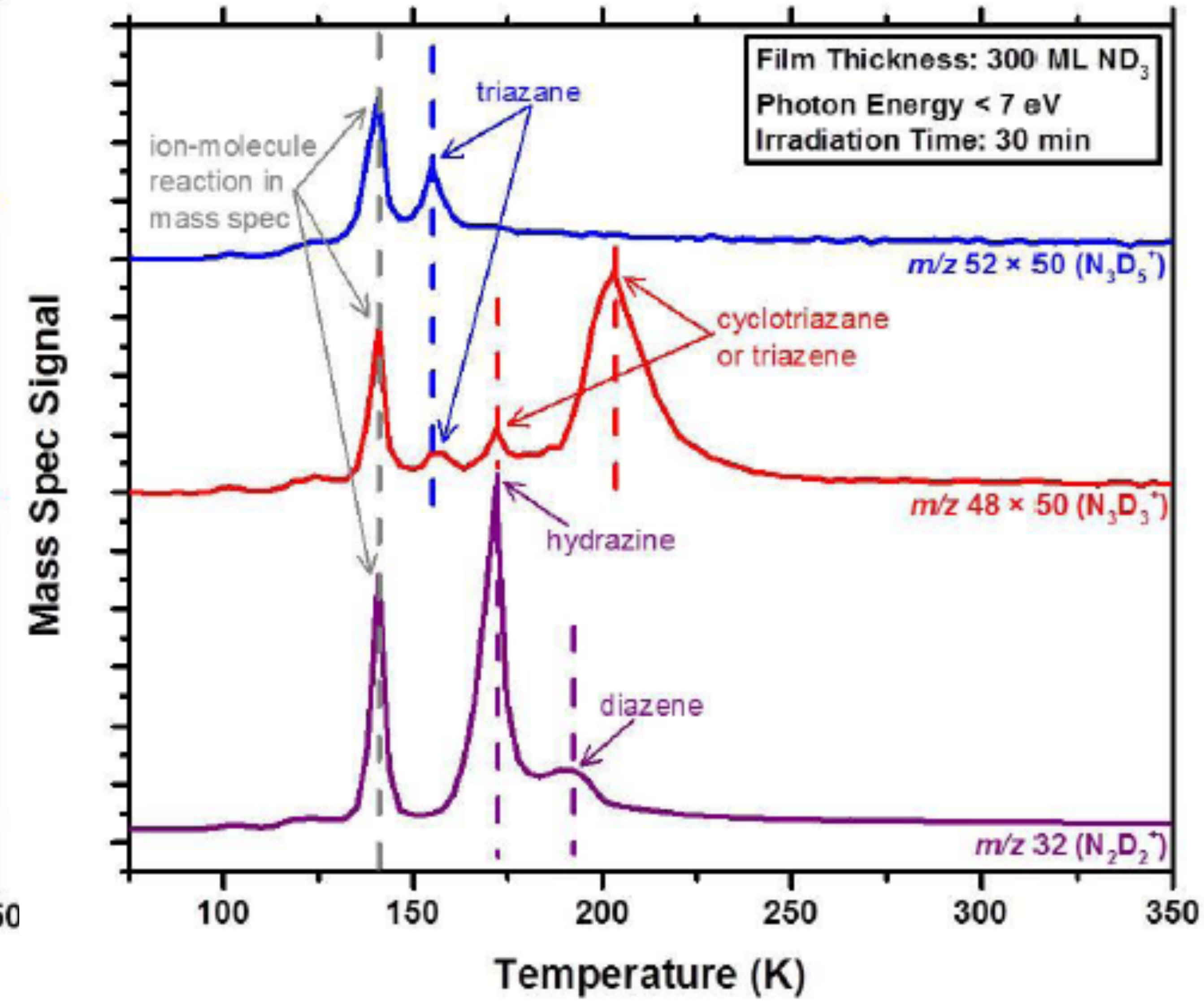
[Bergner+ 2016]

UV vs. electron induced chemistry

Electrons



UV photons



[Campbell's poster]

Recent successes and upcoming challenges in laboratory astrophysics

Spectroscopy and excitation studies essential to extract molecular identifications and abundances in gas

Gas phase ISM chemistry studies are in an advanced stated, but state-to-state reaction data and low temperature experiments still lacking for many key systems

Ice spectra of the minor hydrides needed to trace their chemical history

Many uncertainties remain on how ice chemistry couples with the gas-phase. Knowing mechanisms as well as yields are key to predict this behavior in different interstellar regions.

Surface and ice chemistry are still largely terra incognita. Need intuition building studies, as well as experiments that enables quantification of the basic reaction steps.