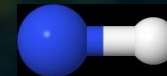
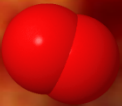
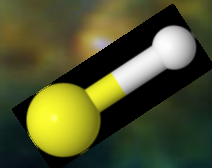
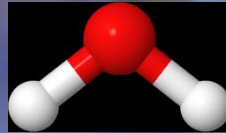
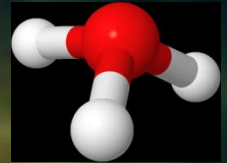
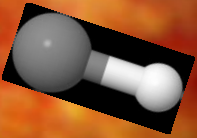


# Astrochemistry

## The promise of Herschel delivered!



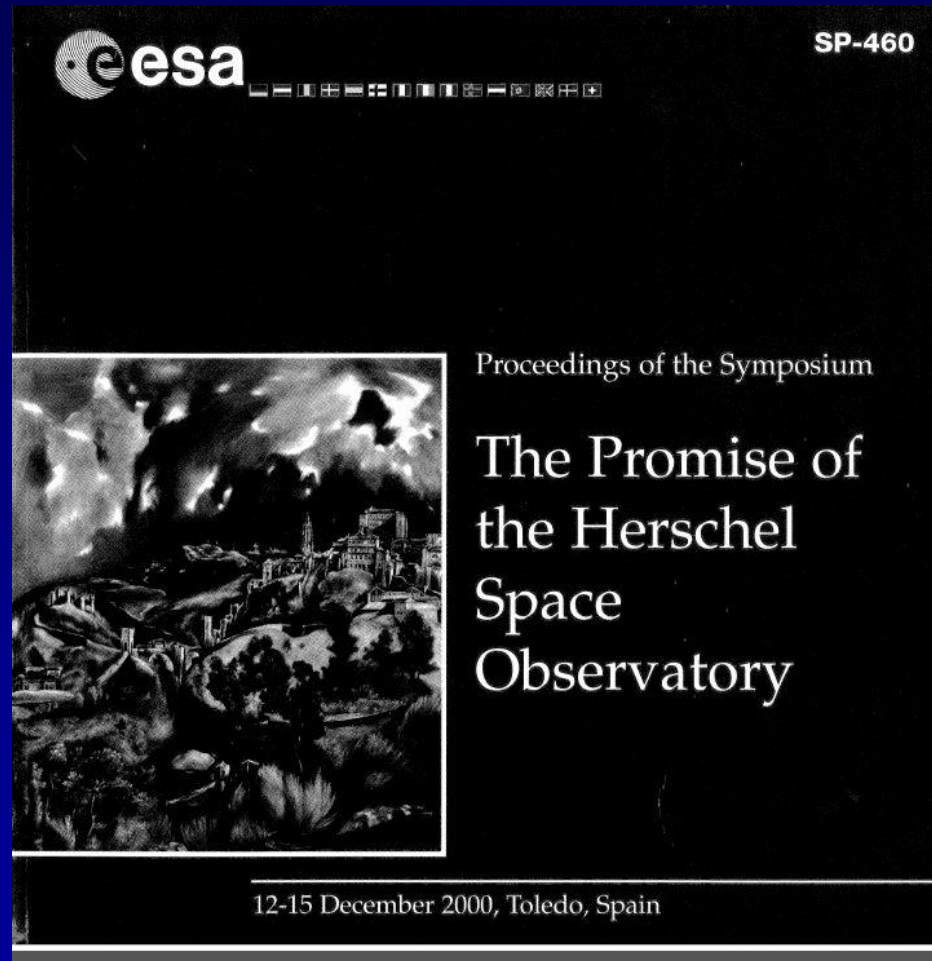
RCW120  
Herschel  
A. Zavagno

**Ewine F. van Dishoeck**  
**Leiden Observatory/MPE**

Thanks to Ted Bergin, Cecilia Ceccarelli, Maryvonne Gerin, Pepe Cernicharo, Feank Helmich, Xander Tielens, Floris van der Tak, Ruud Visser and many other colleagues for input and discussions

*Apologies for not being able to cover all exciting new results*

# Many decades of planning....



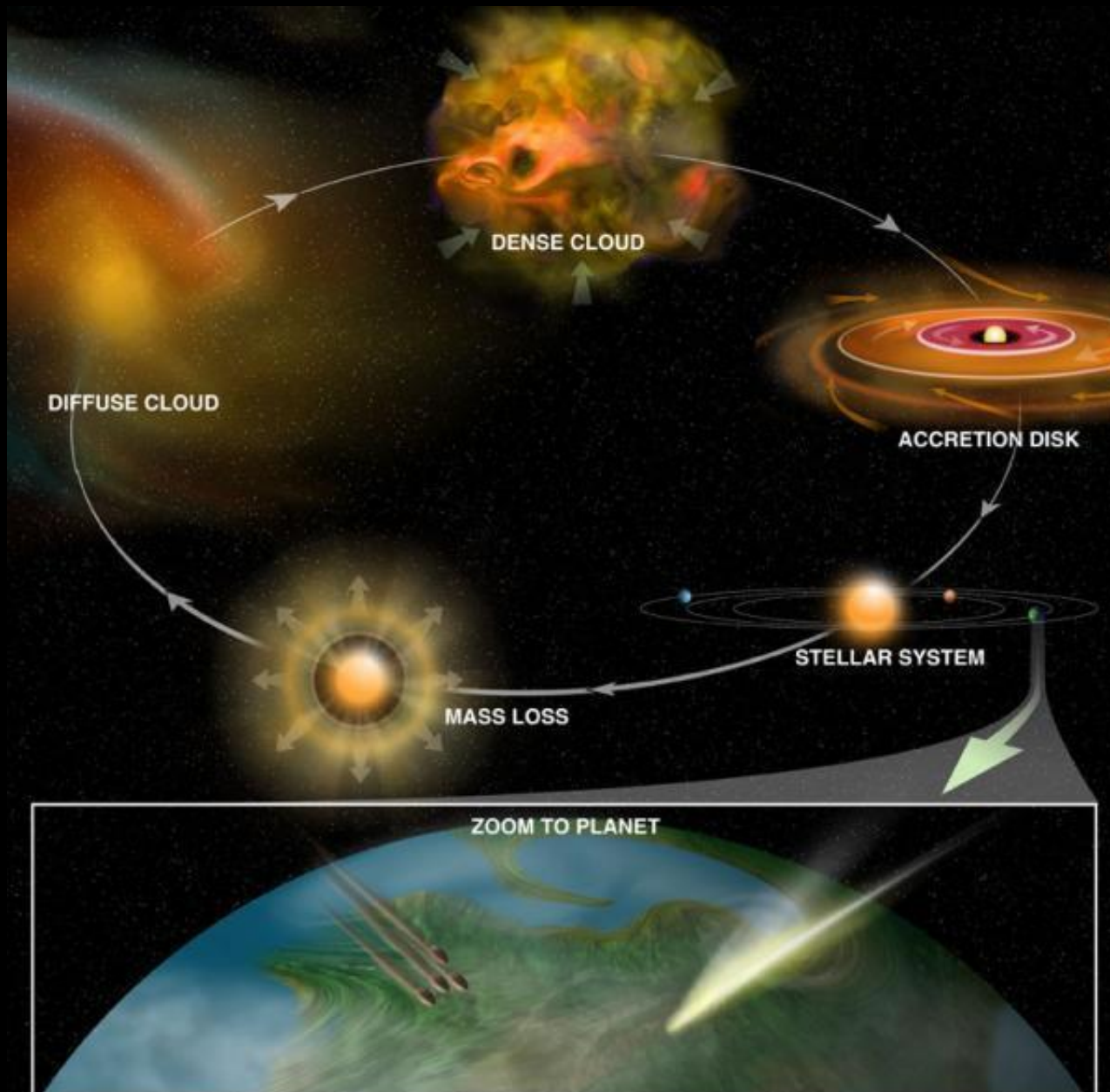
Science cases  
dating back to  
late 1970's  
highlighting  
astrochemistry as  
a major driver

**Thanks to many astrochemists for making the case for Herschel!**

# Herschel astrochemistry drivers

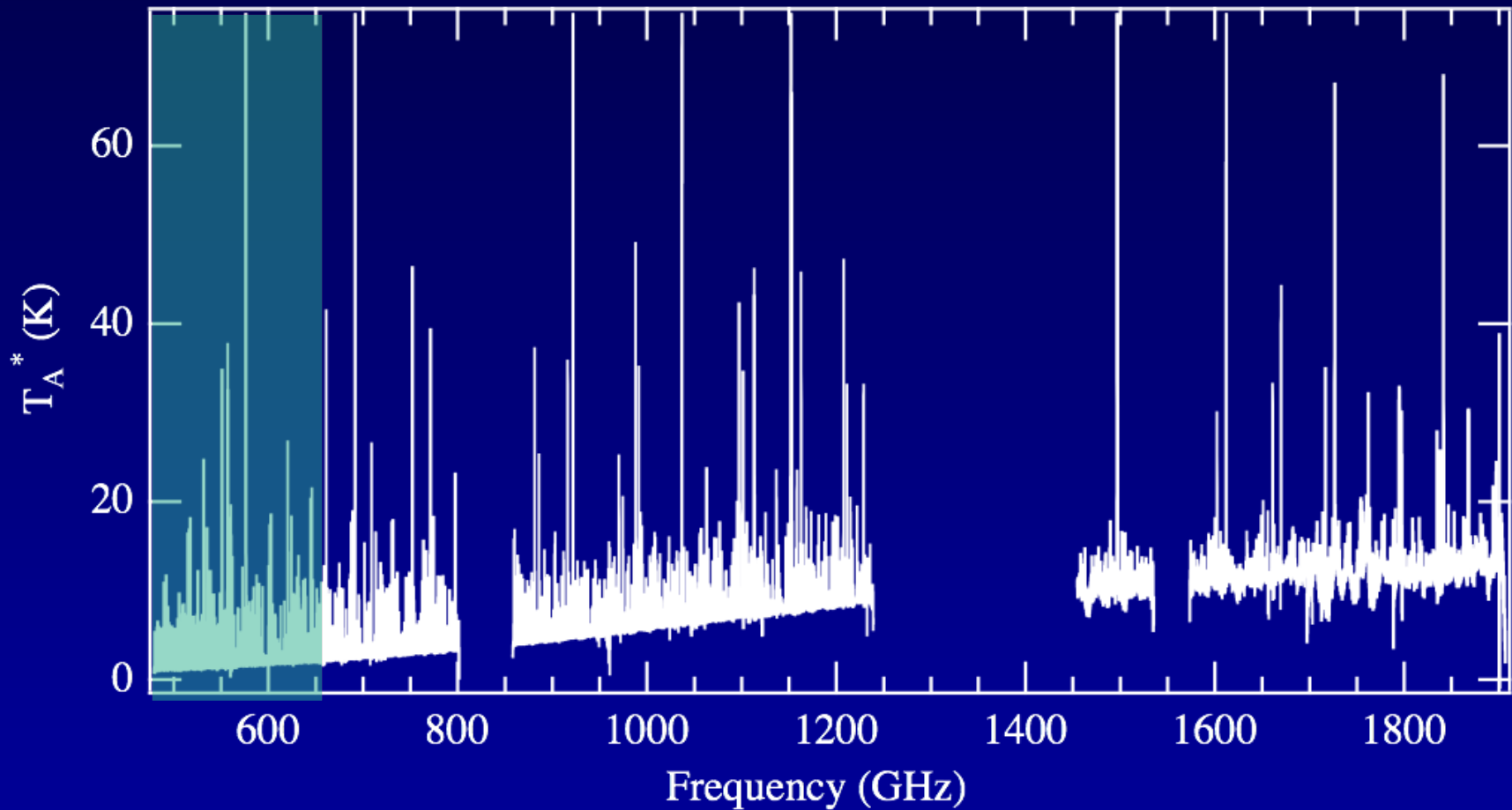
- Hydrides
- Water
- O<sub>2</sub>
- Unbiased spectral surveys

# Cosmic cycle of gas and dust





# The power of Herschel spectroscopy delivered



Bergin, Crockett et al. 2010

Entire spectrum in just tens of hours!



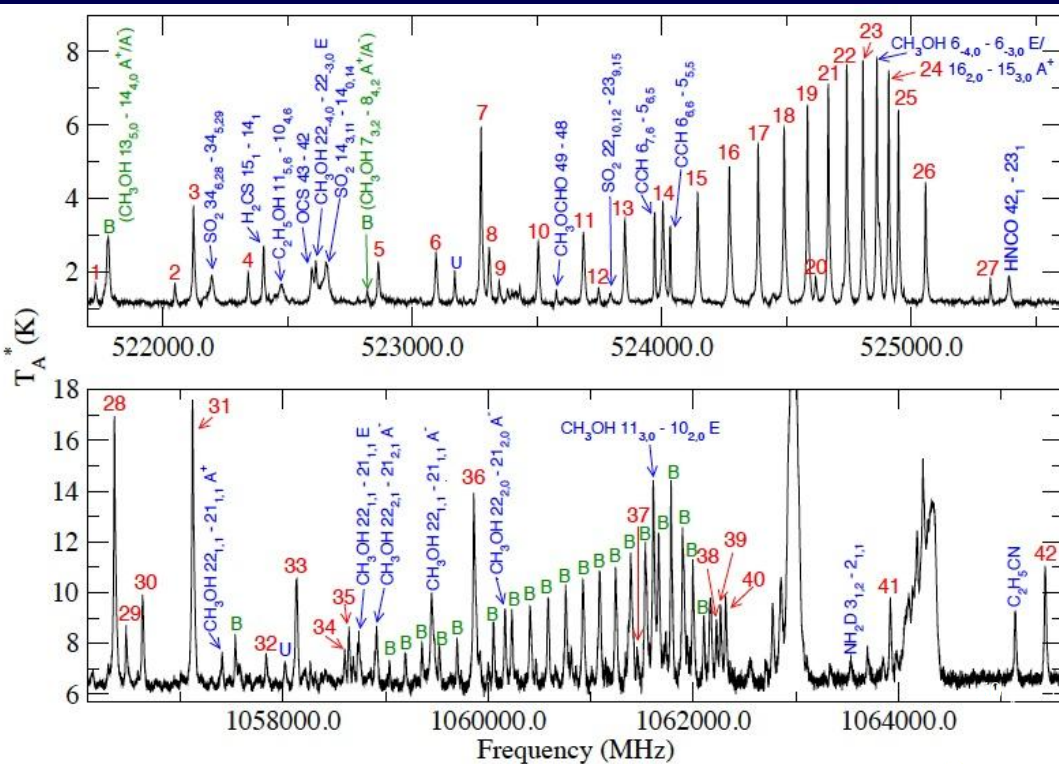
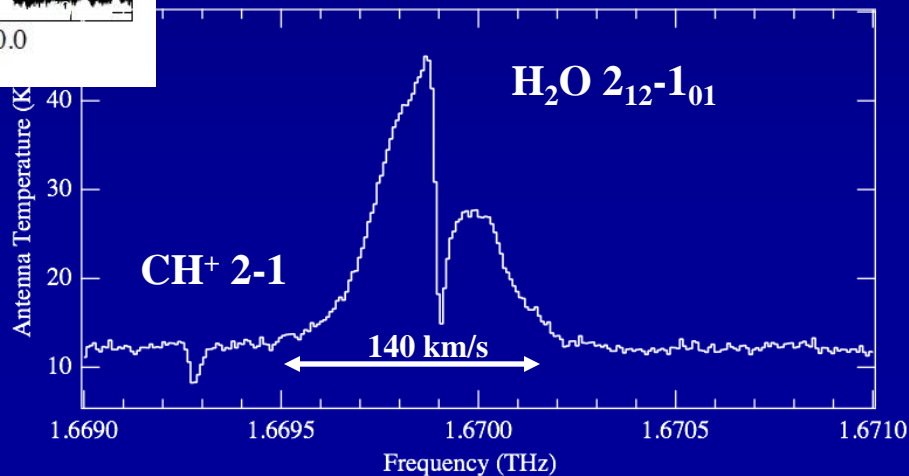
# The power of Herschel spectroscopy

Orion-KL  
HEXOS

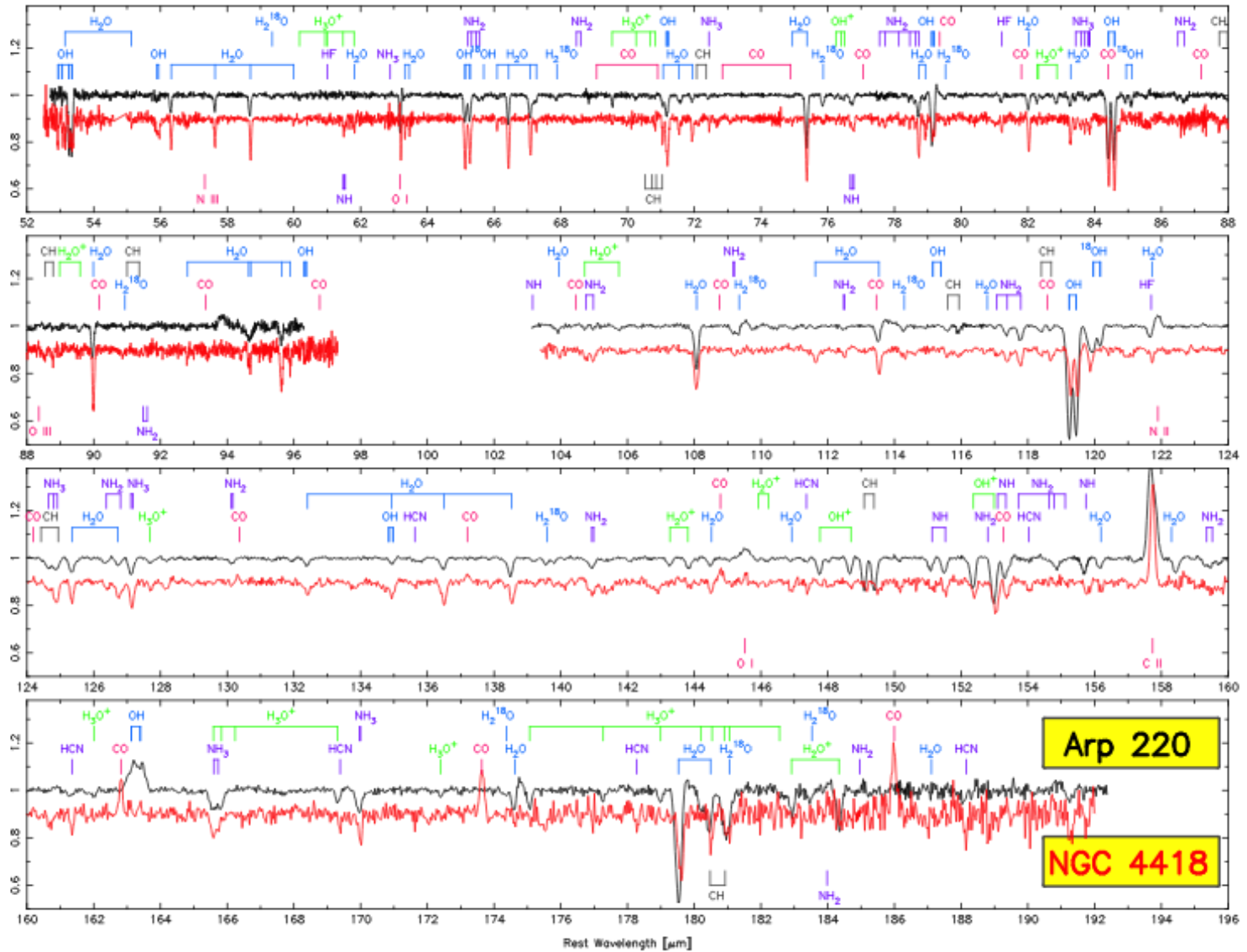
High-quality line profiles,  
even at 1.67 THz!

Wang, Bergin et al. 2011

Crockett et al.  
2010



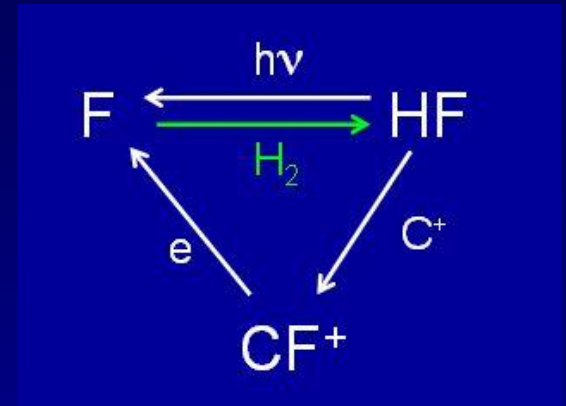
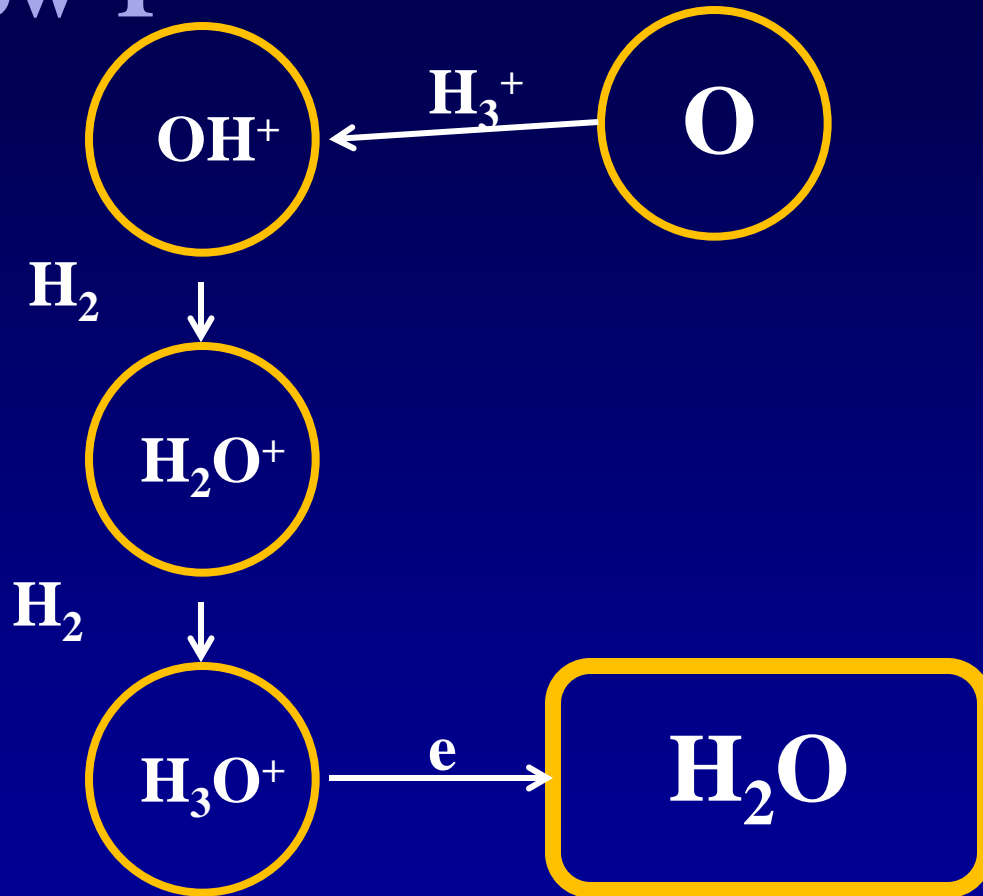
# From galactic to extragalactic astrochemistry!



Gonzalez-Alfonso et al. 2012, Herschel-PACS

# Testing hydride chemistry

Low T

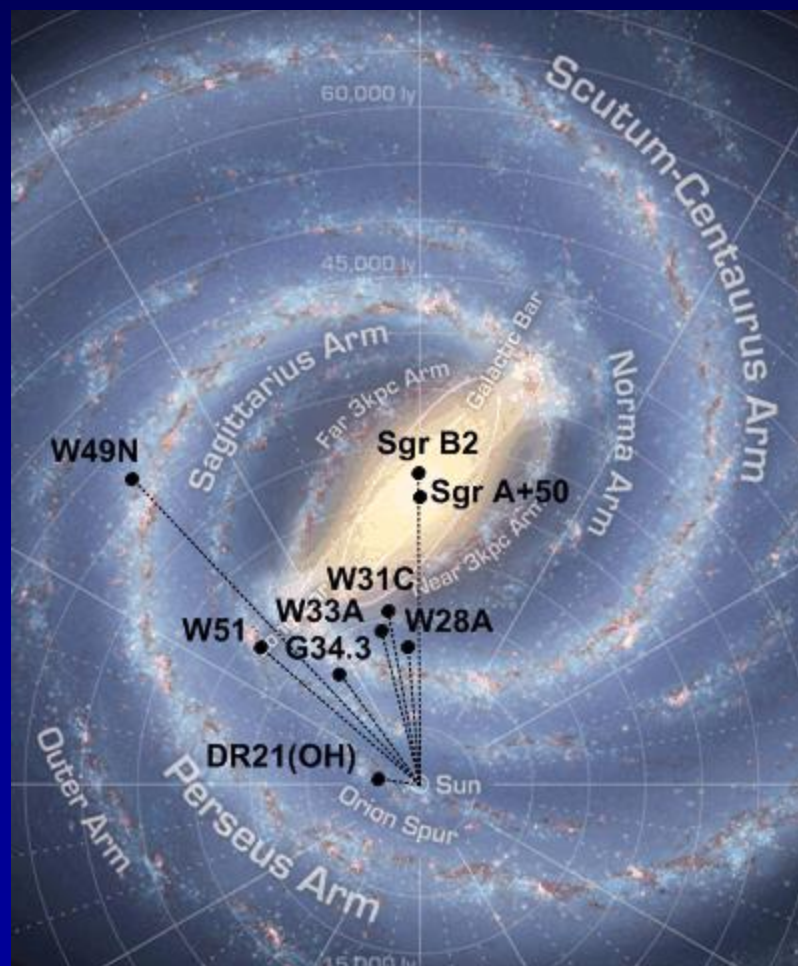


Light molecules  
→ High frequencies

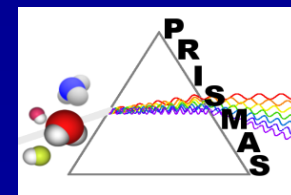
Ion-molecule reaction schemes developed in early 1970's but many of the intermediate building blocks cannot be observed from ground



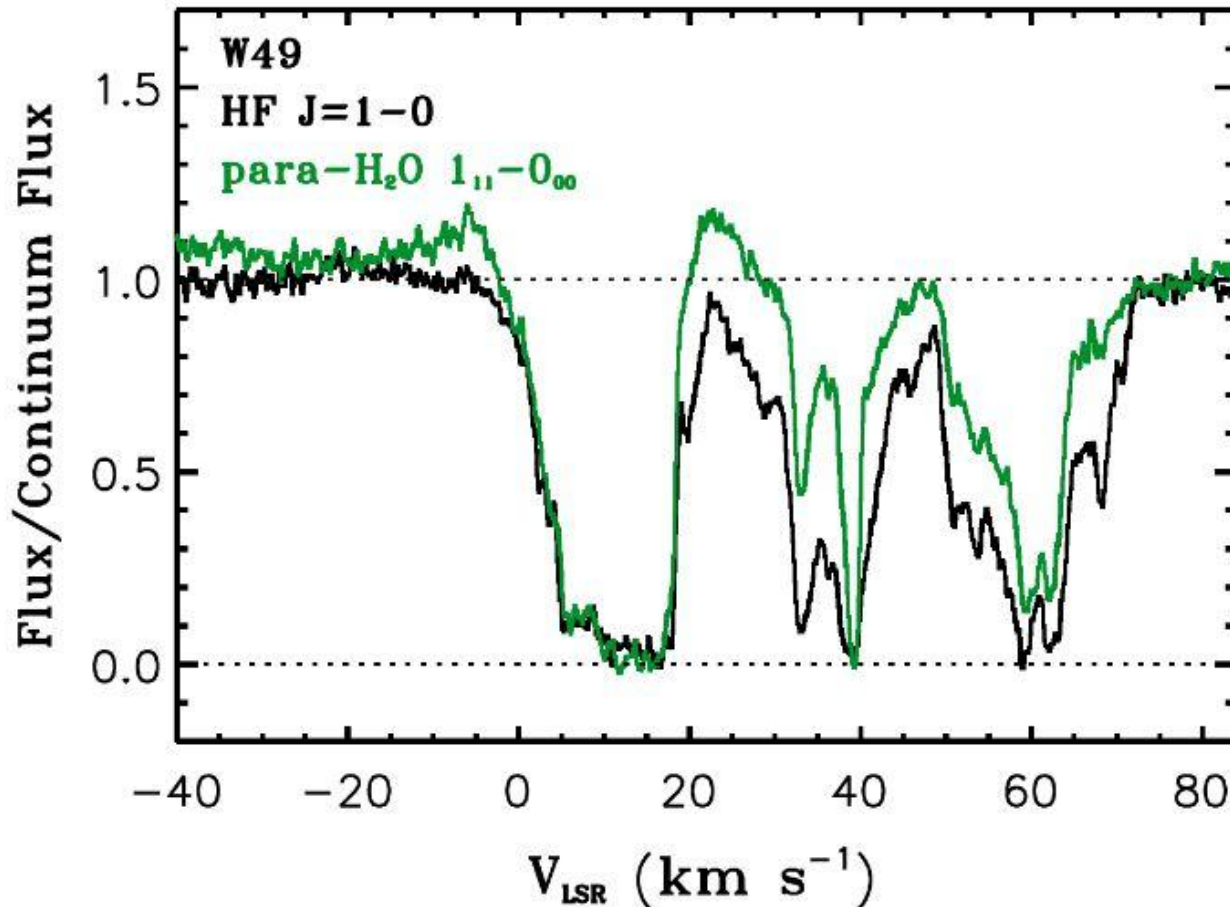
# Testing ion-molecule chemistry



- Absorption against bright far-IR continuum
- Clouds  $A_V \sim \text{few mag}$
- All molecules in ground level  $\rightarrow$  simple analysis
- *Precision astrochemistry* (factor of  $\sim 2$ )



# Absorption lines

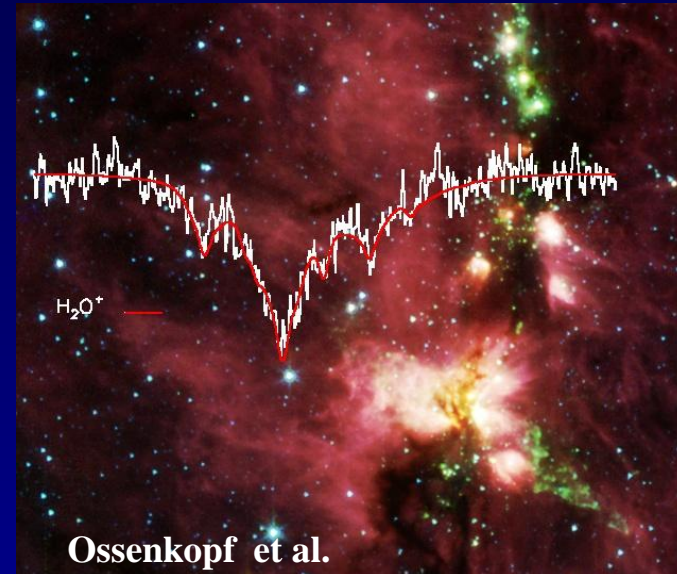
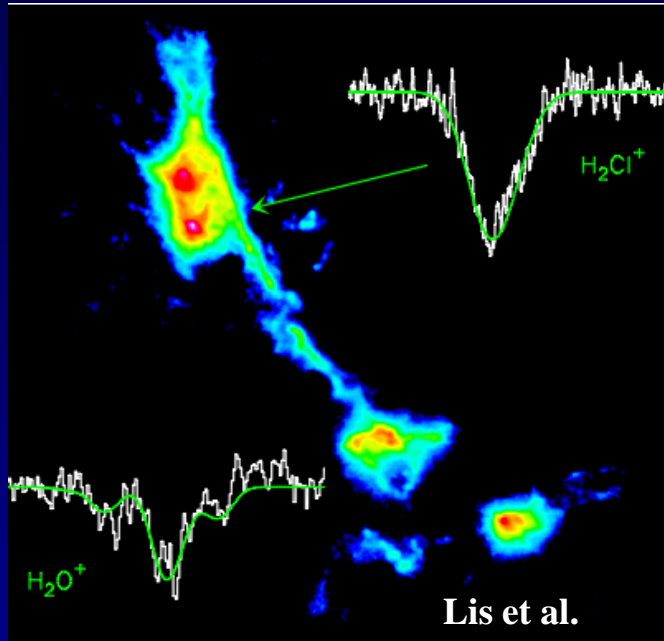


Water  
o/p=3

Neufeld et al. 2010,  
Sonnetrucker et al. 2010  
Godard et al. 2012  
Emprechtinger et al. 2012  
Flagey et al. 2013

- Diffuse and translucent clouds along the line of sight
- HF as tracer of  $\text{H}_2$  column density because of simple chemistry (see  $\text{C}^+$ , GOT-C+)
- Constant  $\text{H}_2\text{O}/\text{H}_2$  abundance of  $5 \times 10^{-8}$  (except GC), consistent with models

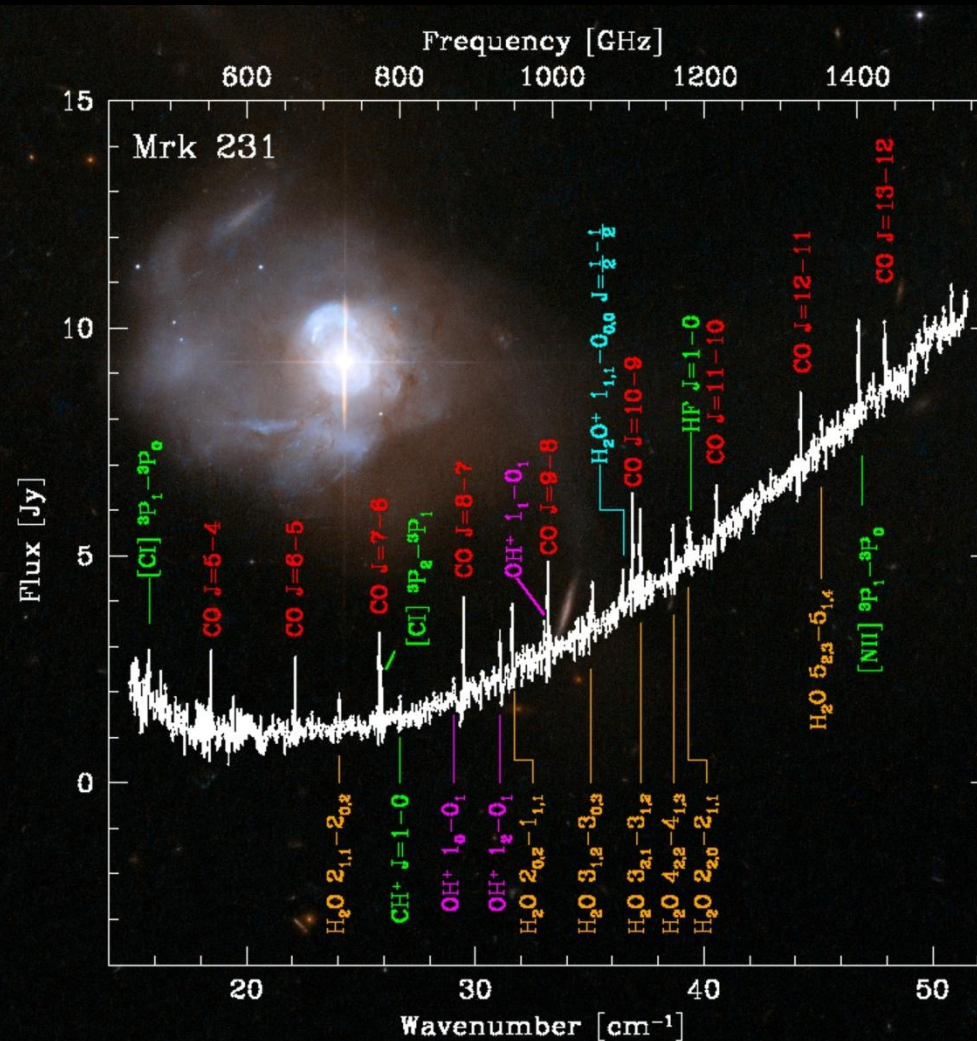
# Detection of $\text{H}_2\text{O}^+$ , $\text{HCl}^+$ and $\text{H}_2\text{Cl}^+$



- $\text{H}_2\text{O}^+$  must arise in  $\text{H}_2$  poor phase ( $\text{H}/\text{H}_2 \sim 10$ )
- $\text{HCl}^+$  and  $\text{H}_2\text{Cl}^+$  detection; chemistry?
- $\text{OH}^+$ ,  $\text{H}_2\text{O}^+$  constrain  $\zeta$

Ossenkopf et al., Benz et al., Bruderer et al., Gerin et al., Wyrowski et al., Gupta et al., Schilke et al., Lis et al. 2010; Neufeld et al. 2012, de Luca et al. 2012, Indriolo et al. 2013, Monje et al. 2013....

# OH<sup>+</sup> and H<sub>2</sub>O<sup>+</sup> in other galaxies!



SPIRE-FTS

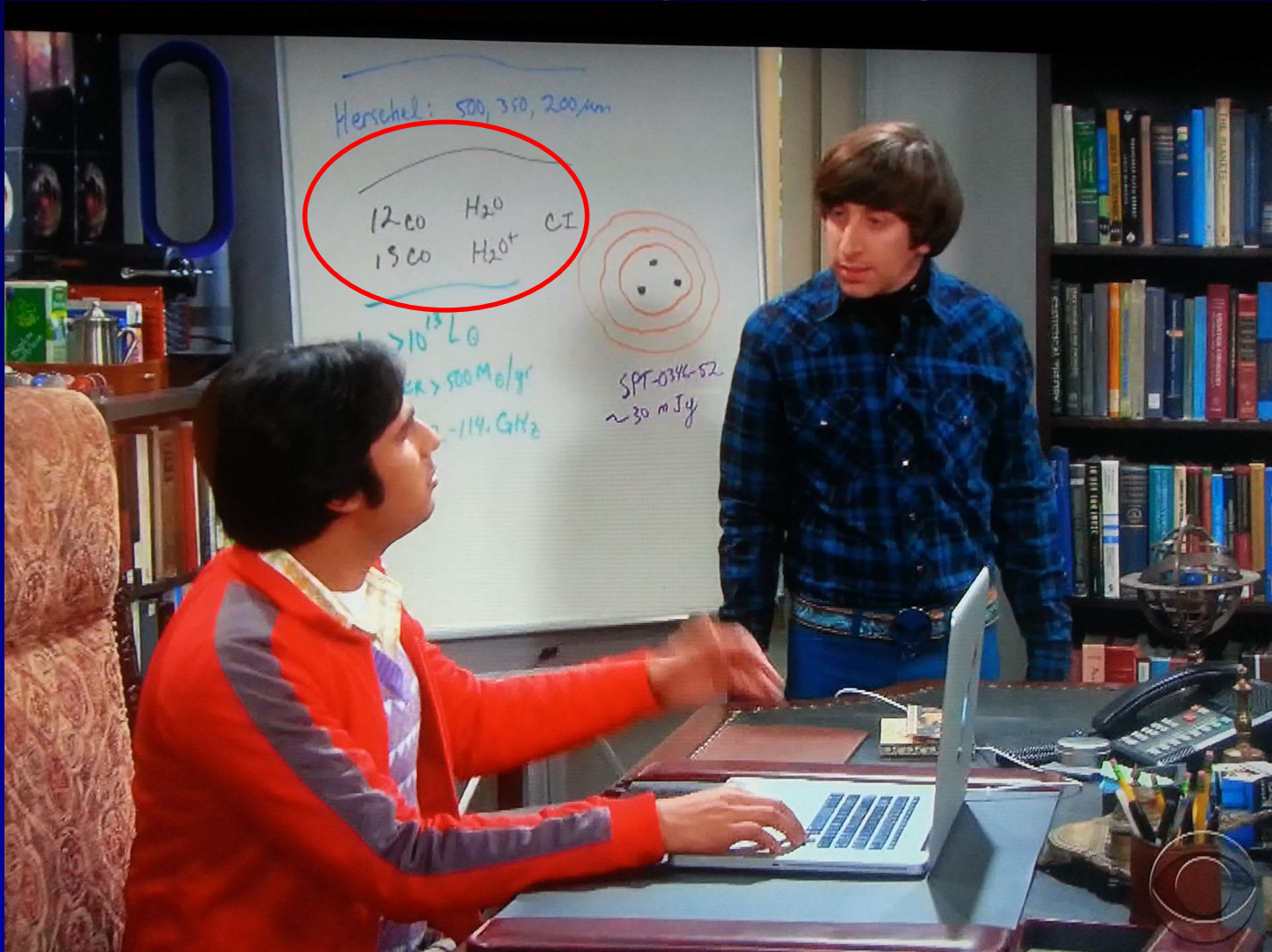
Van der Werf et al. 2010  
Gonzalez-Alfonso et al. 2013

Indriolo et al. 2013

Inferred cosmic ray ionization rates  $\zeta \sim 10^{-13} \text{ s}^{-1}$ ,  $\gg$  galactic  $\zeta$

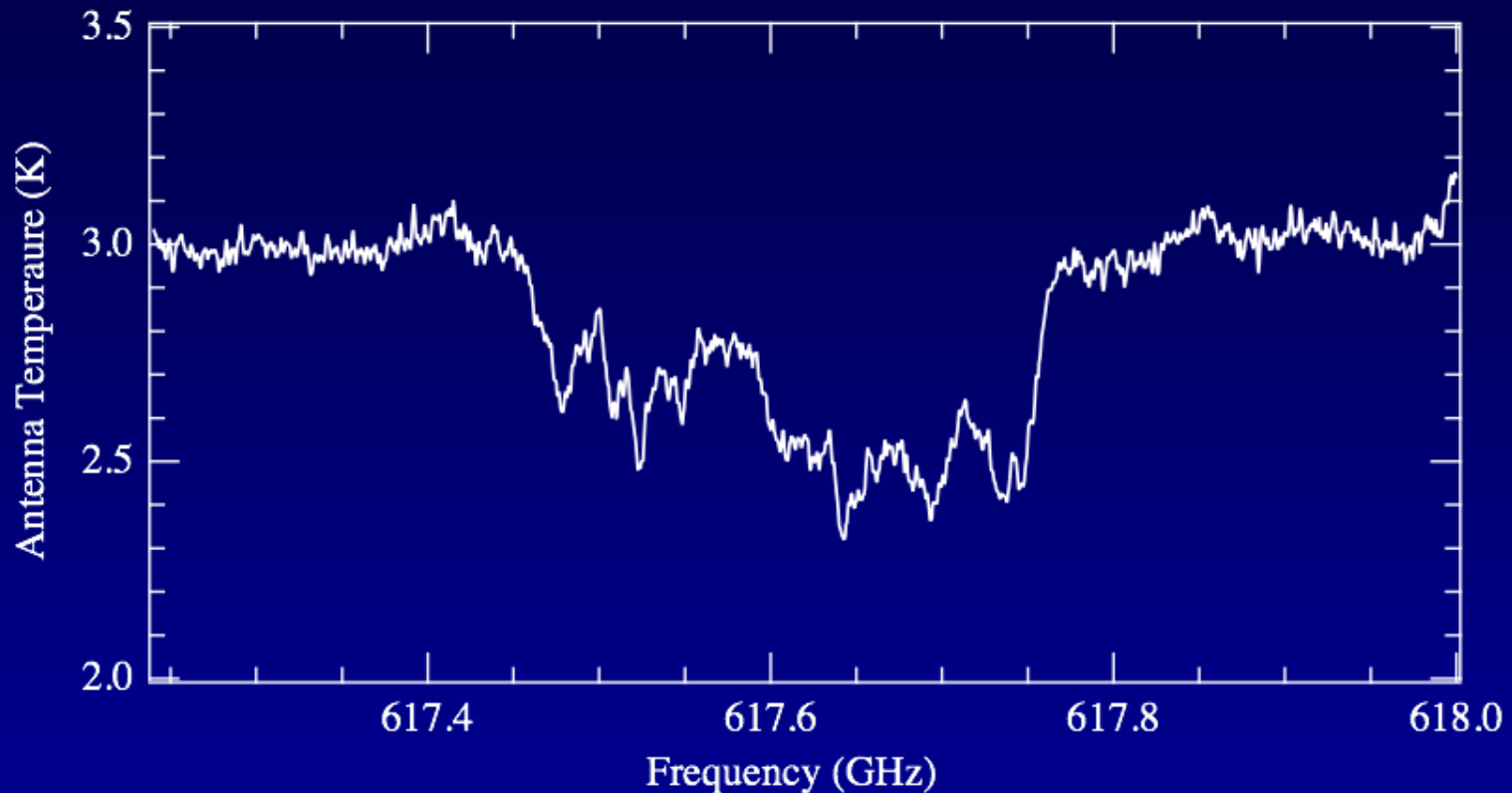


# Even in the Big Bang theory





# U-line SgrB2

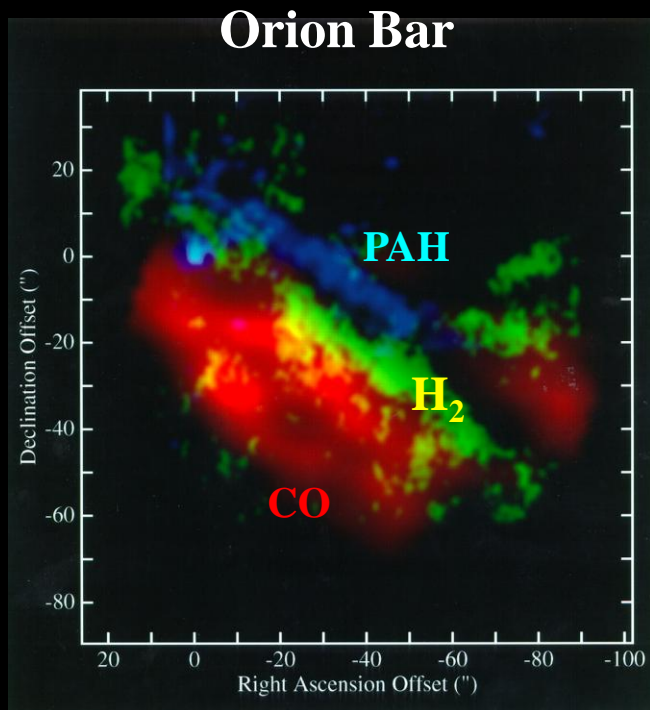


**Molecule present in *all* spiral arm clouds between us and the galactic center**

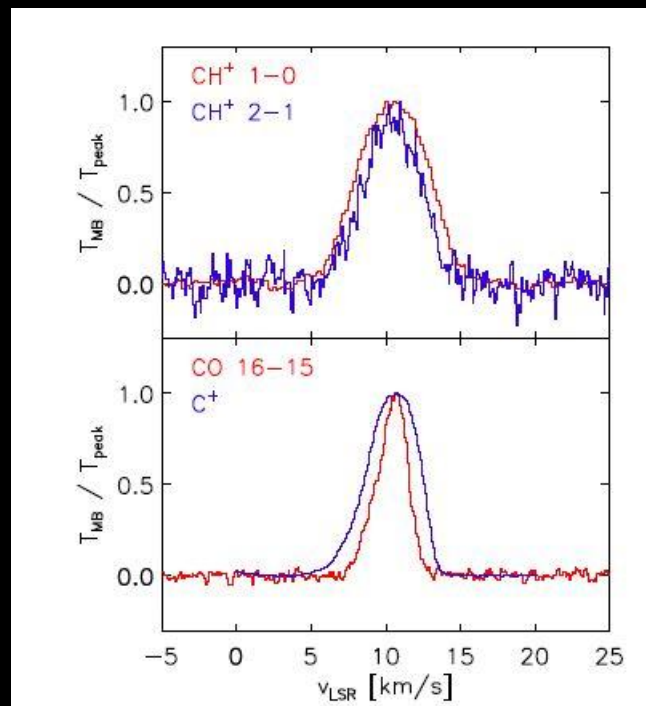
*Post talk comment: feature now identified as  $^{36}\text{ArH}^+$  1-0 absorption, see Mike Barlow talk*



# Dense PDRs: Excitation and formation processes



Tielens et al. 1993, Hogerheijde et al. 1995



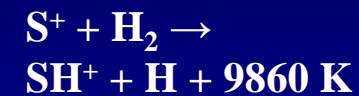
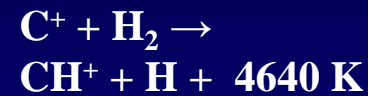
HF: van der Tak et al. 2012, CH<sup>+</sup>: Nagy et al. 2013, J. Black

- Excitation by electrons significant in PDRs
- Formation pumping, e.g.  $C^+ + H_2 \rightarrow CH^+(v, J) + H$
- State specific processes, e.g.  $C^+ + H_2(v, J) \rightarrow CH^+ + H$

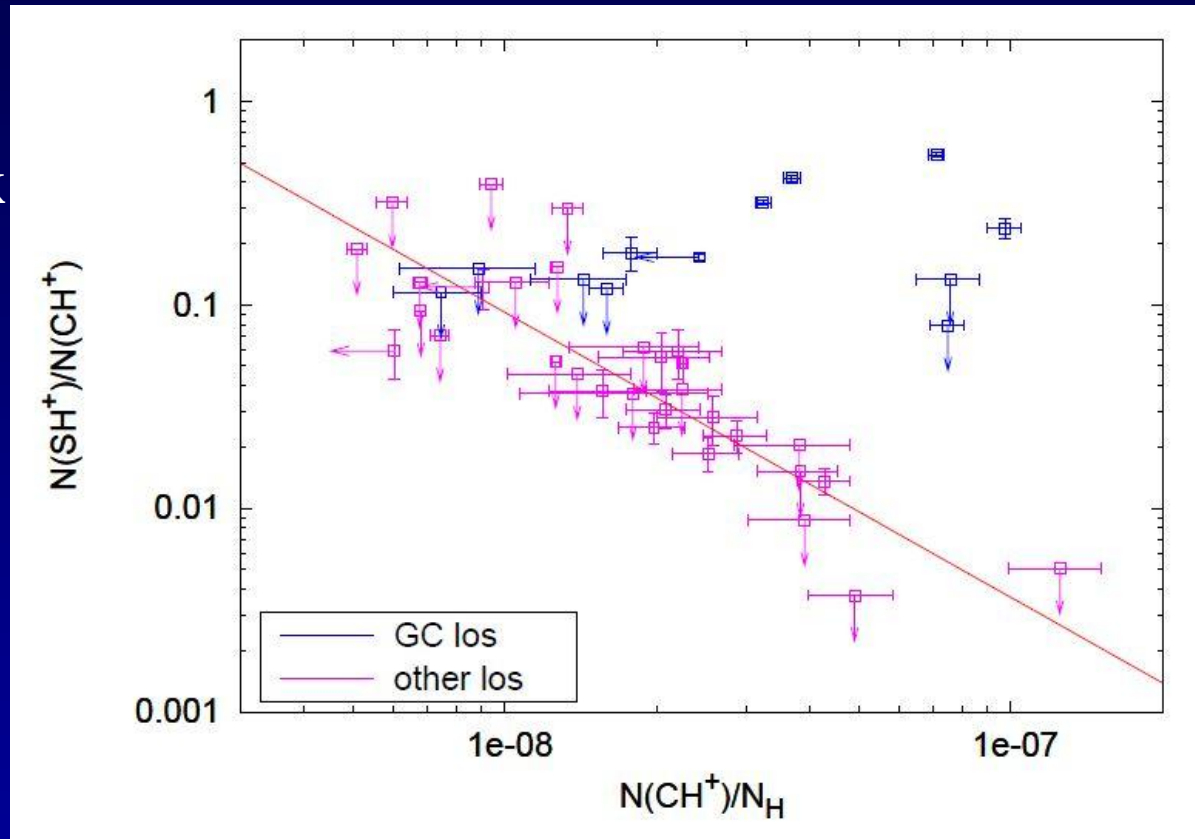
HEXOS,  
WADI

*See case of CH<sup>+</sup>, SH<sup>+</sup> turbulent chemistry, H<sub>3</sub>O<sup>+</sup> excitation later in conference*

# Turbulence driven chemistry



Godard et al.  
2012



Menten et al. 2011  
 $\text{SH}^+$

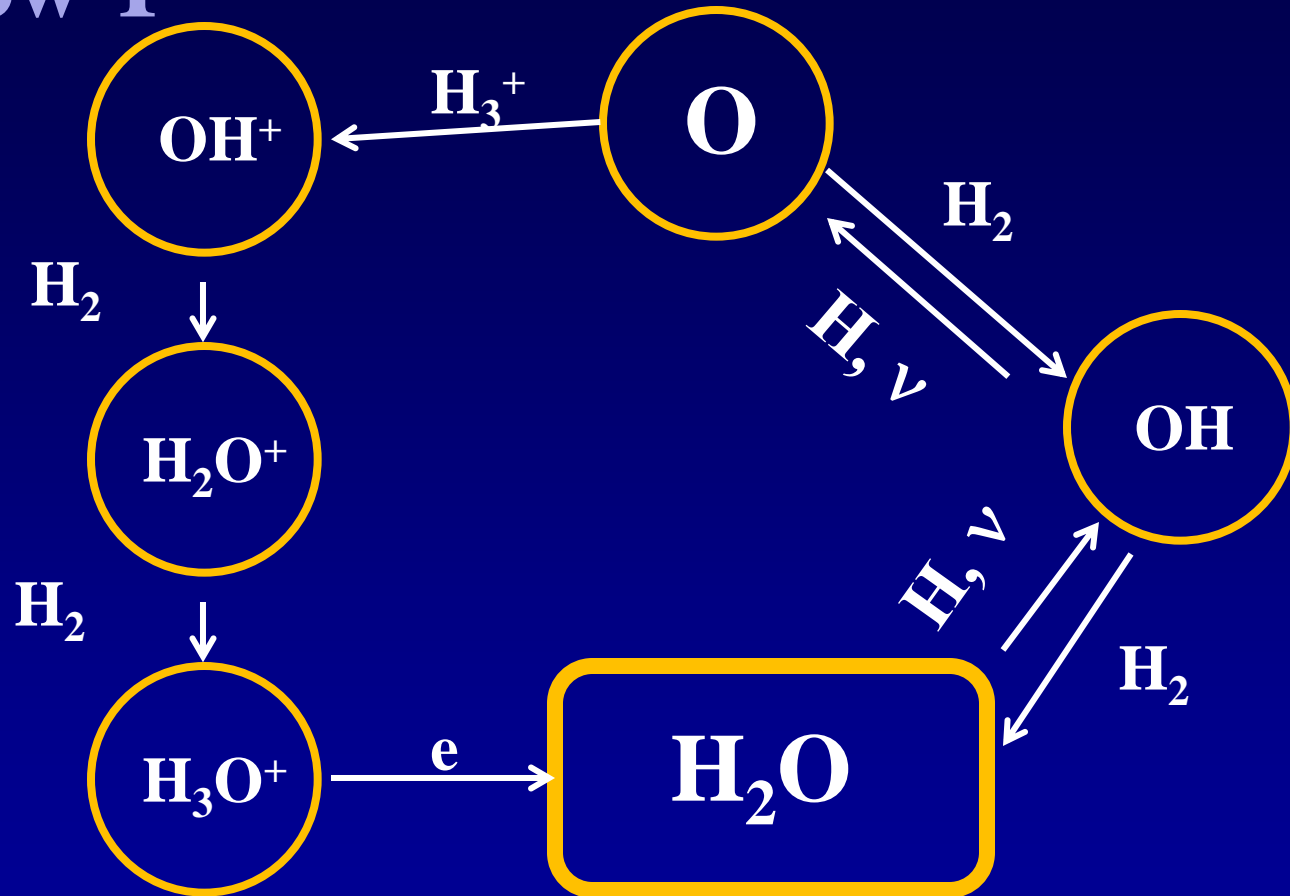
Falgarone et al. 2010  
 $\text{CH}^+$

- Large column densities  $\text{CH}^+$  mystery since its discovery in 1937
- Line widths  $\text{SH}^+$ ,  $\text{CH}^+$  larger than those of CH, CN:  $\sim 4$  vs  $2 \text{ km s}^{-1}$
- Endothermic reactions driven by turbulent dissipation?

# High temperature chemistry: shocks

Low T

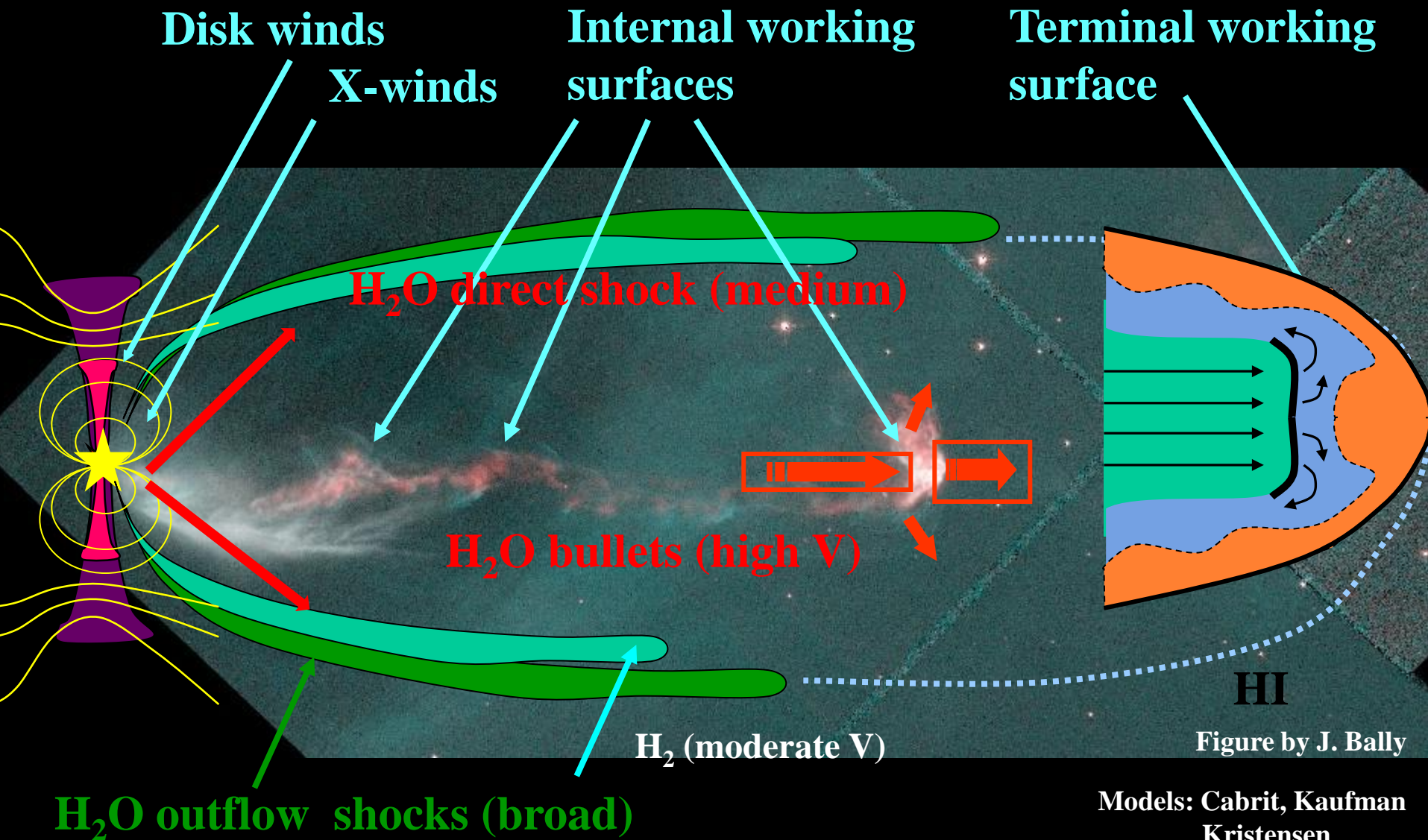
High T



- Need high temperatures ( $> \sim 300$  K) to overcome reaction barriers
- Expect all oxygen to be driven into water:  $\text{H}_2\text{O}/\text{H}_2 \sim 6 \times 10^{-4}$

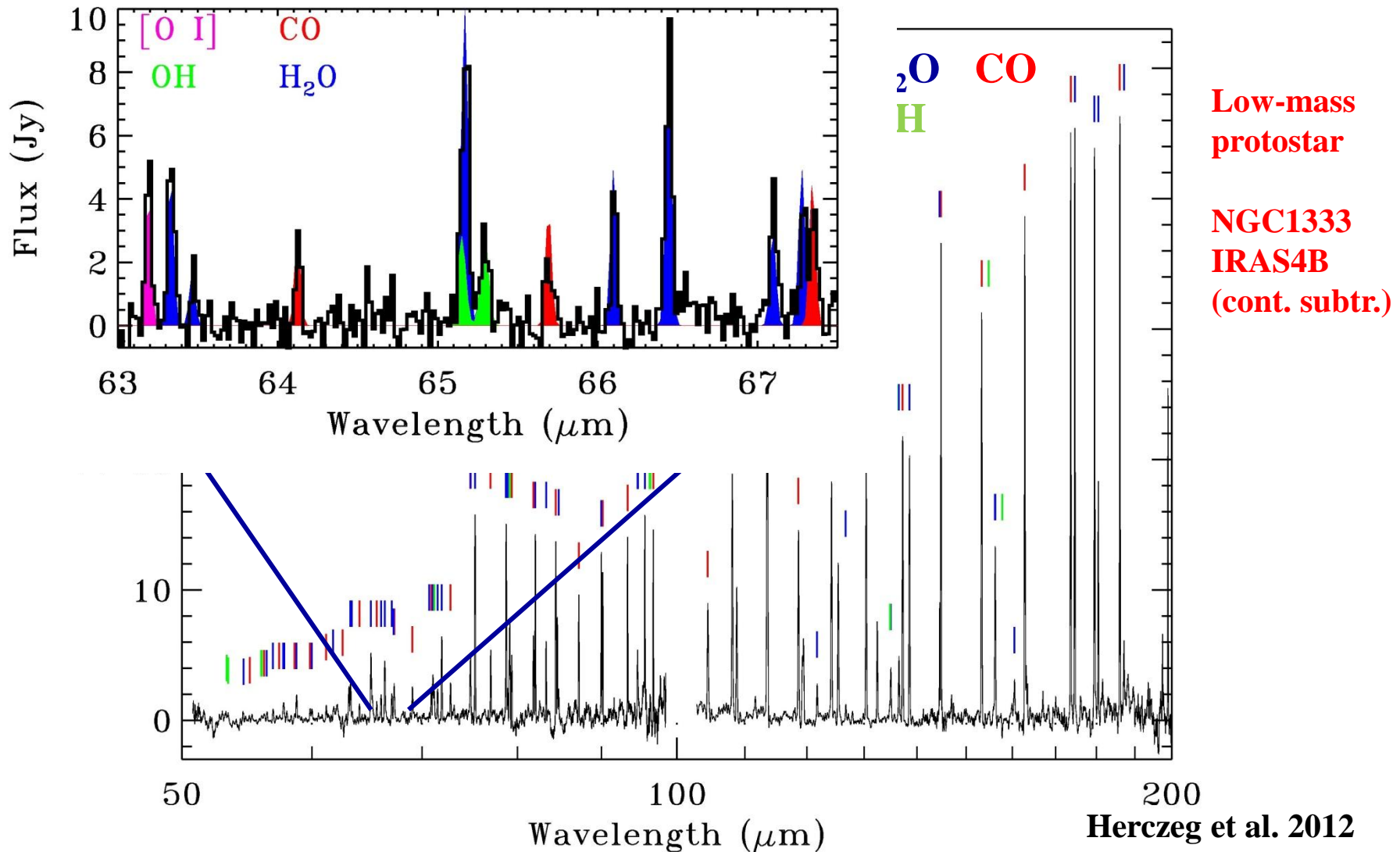
# Physics and chemistry of outflows:

## Jets, winds $\Rightarrow$ wide-angle UV irradiated cavities





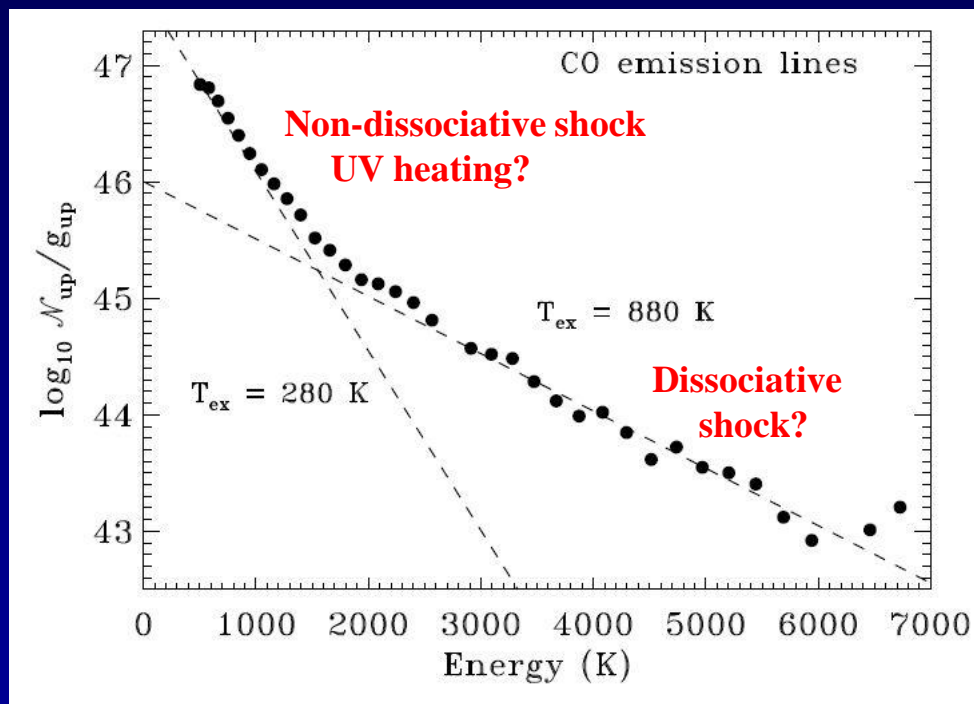
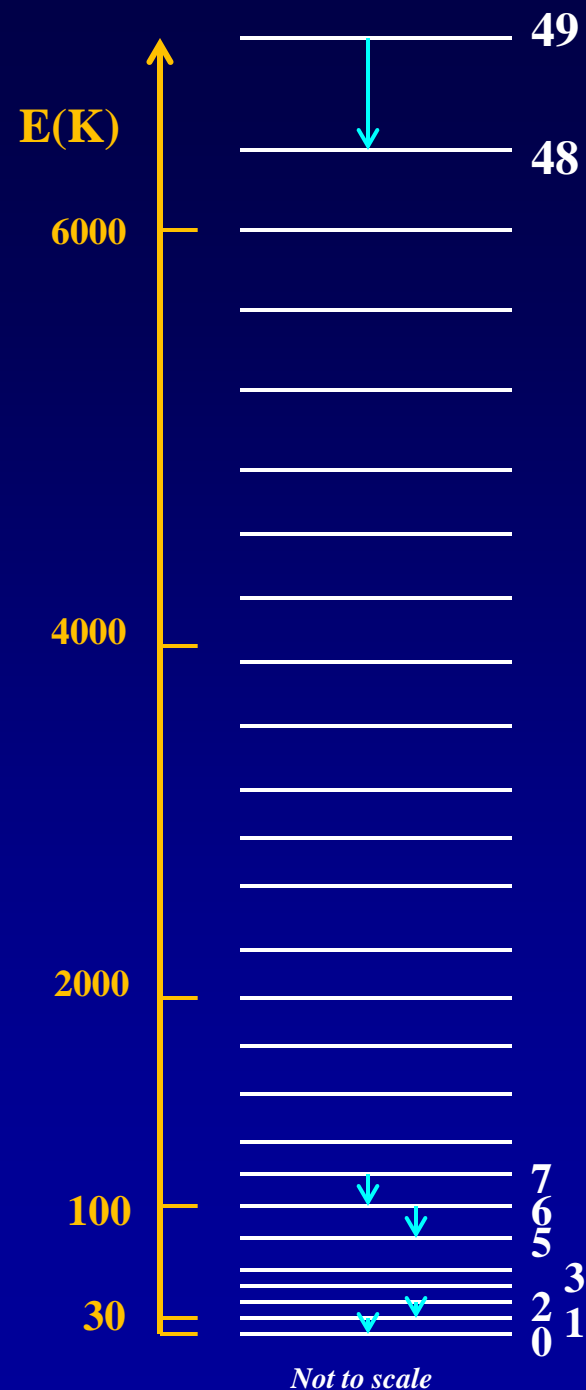
# PACS spectroscopy of shocks: Hot H<sub>2</sub>O, OH and CO



- Quantify excitation, abundances and main coolants of warm gas

Herczeg et al. 2012  
Goicoechea et al. 2012,  
2013

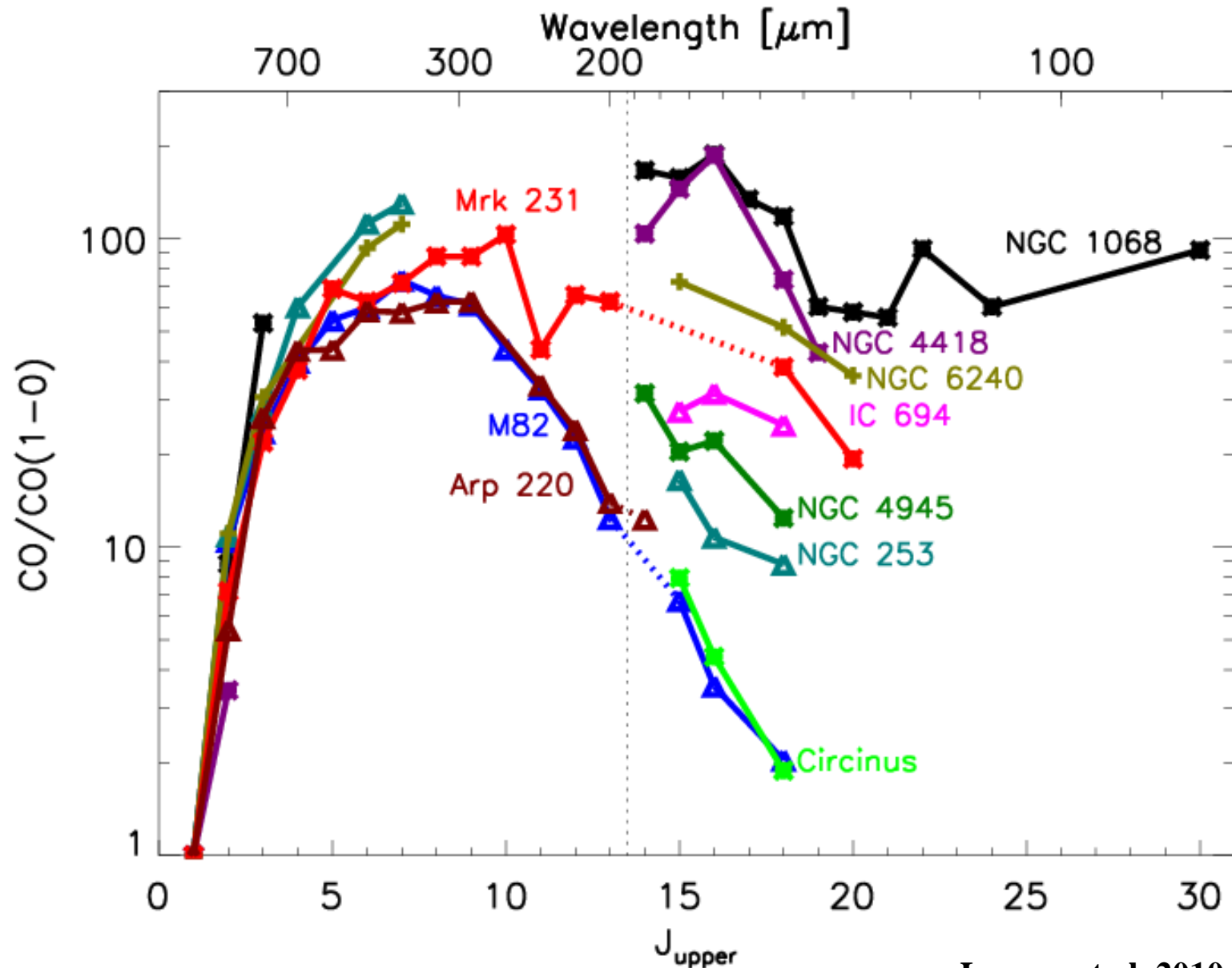
# The CO ladder as a physical probe



WISH, DIGIT,  
HOPS

Herczeg et al. 2012  
 Van Kempen et al. 2010, Benedettini et al. 2012  
 Goicoechea et al. 2012, Karska et al. 2013  
 Manoj et al. 2013, Green et al. 2013  
 Dionatos et al. 2013, Kristensen et al. 2013,  
 Visser et al. 2012

# Extragalactic CO SLEDs



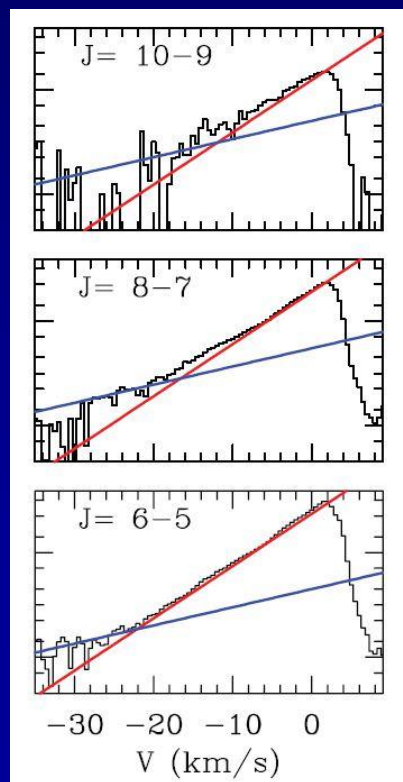
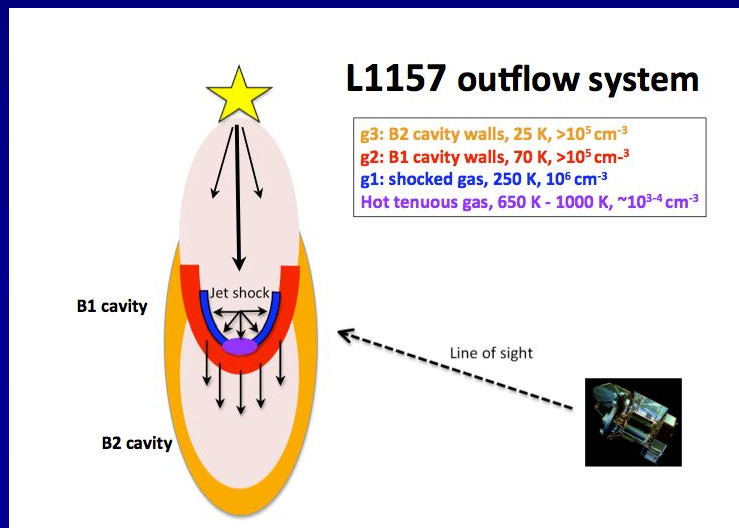
High-J CO PACS lines only prominent for compact AGNs

Loenen et al. 2010

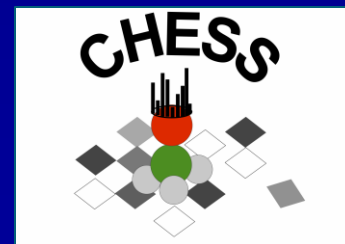
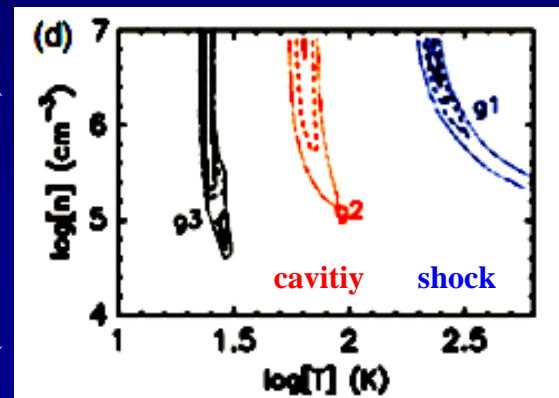
Hailey-Dunsheath et al. 2012

# Multiple shocks revealed by high- $J$ CO

- The jet impact on the cavity (Mach disk) upstream of the bow, associated with a hydrodynamical shock
- The cloud shock (bow), associated with a magnetized shock

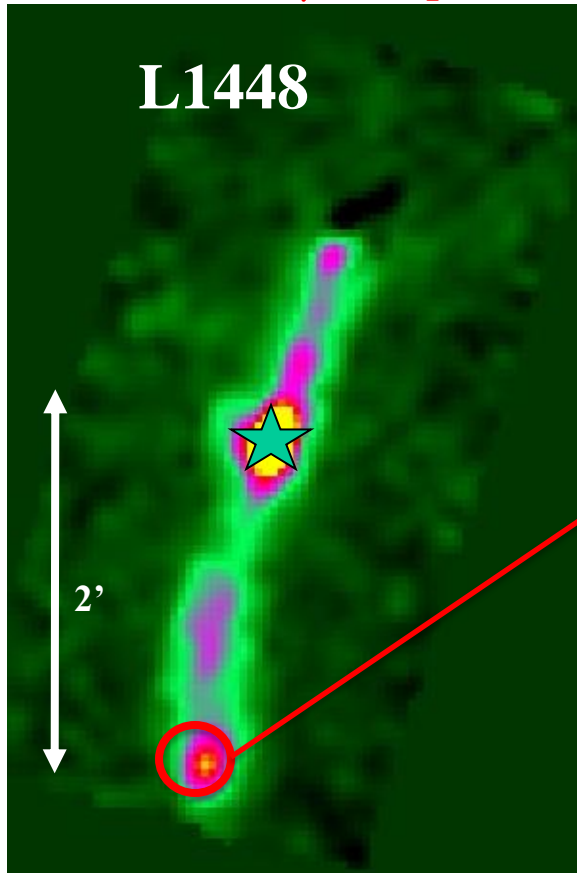


(Lefloch et al. 2012)

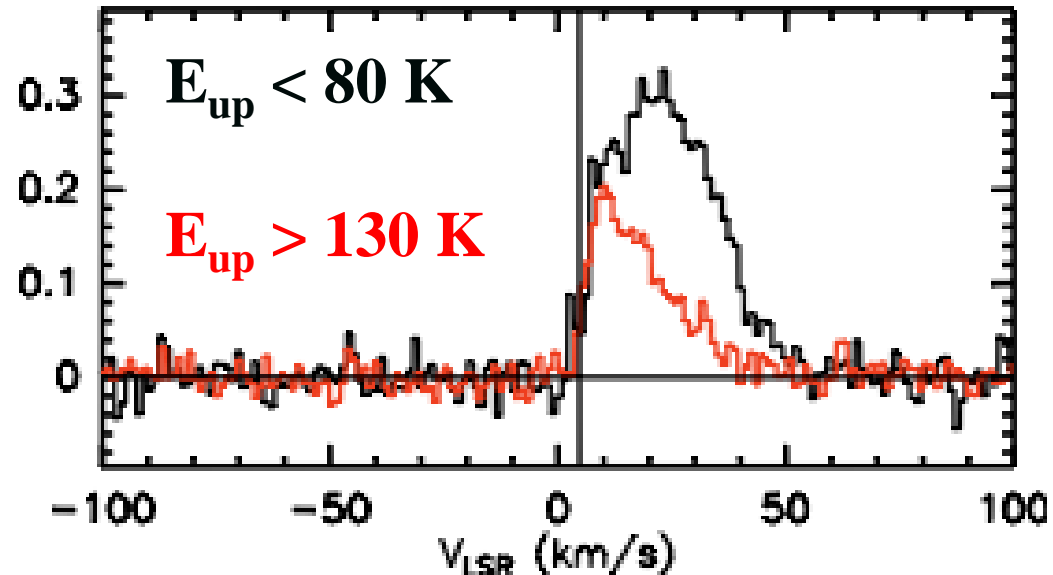


# Shocking water lines

PACS 179  $\mu\text{m}$  map



L1448 R4 Water



Santangelo et al. 2012

Nisini et al. 2010, Tafalla et al. 2013

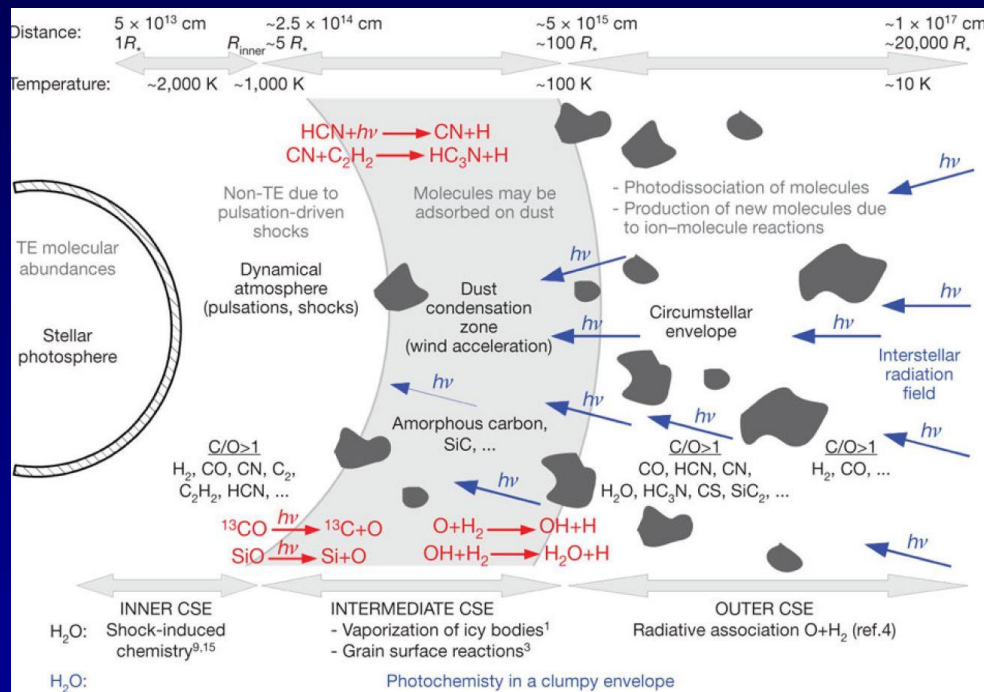
LeFloch et al. 2010, Codella et al. 2010

- High- $J$  CO and  $\text{H}_2\text{O}$  go together, not low- $J$  CO
- Typical  $\text{H}_2\text{O}$  abundances  $10^{-7}$  – few  $\times 10^{-5}$

New type of UV irradiated shocks? See talk Michael Kaufman



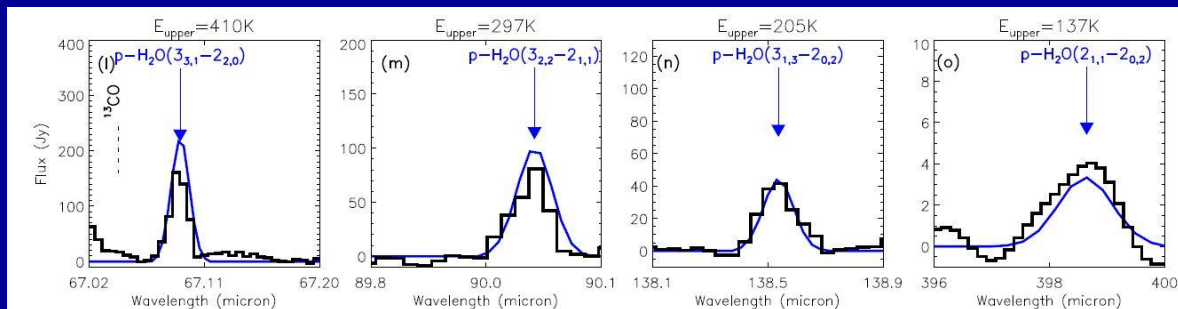
# Hot water in C-rich AGB stars



- Water not due to evaporating comets

- Likely due to photodissociation of CO in clumpy envelope liberating O

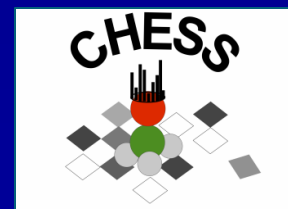
Decin et al. 2010, PACS  
Neufeld et al. 2011, HIFI



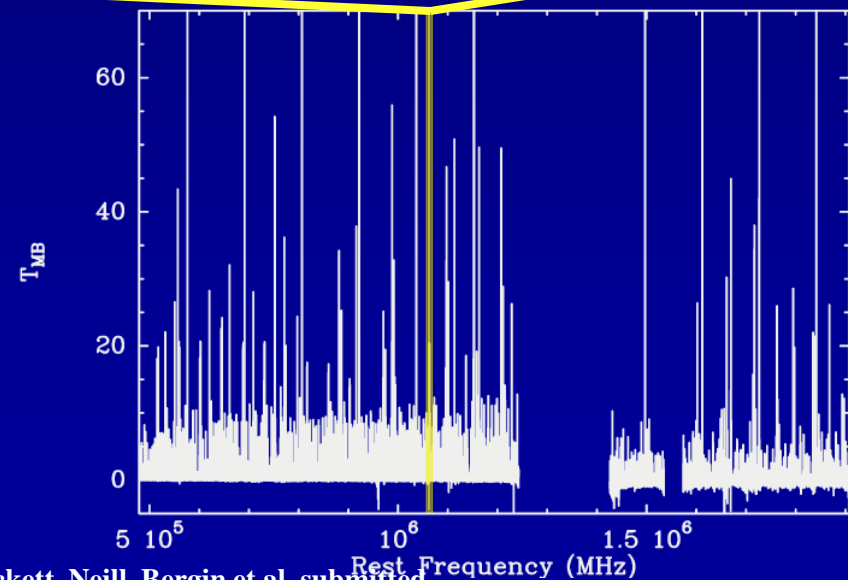
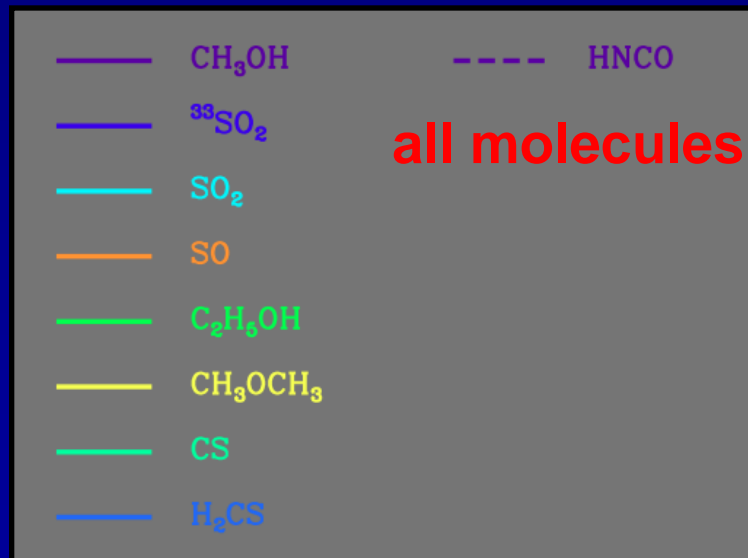
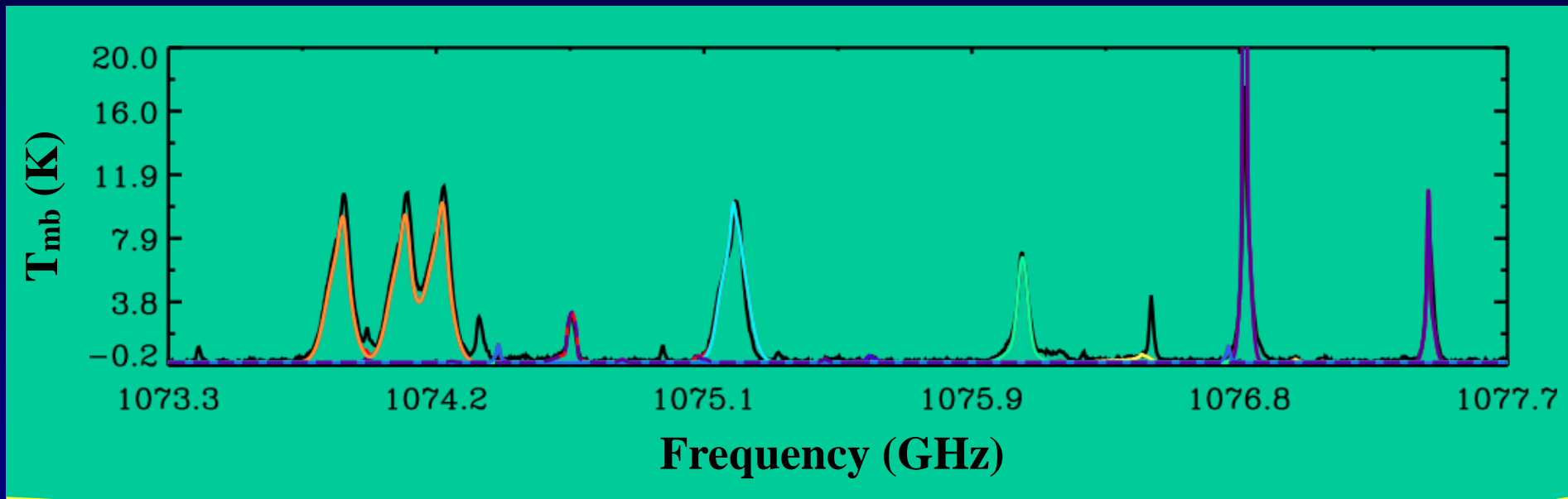
# Full HIFI line surveys

- Thousands of lines in line-rich sources
- Fraction of U-lines  $\sim 10\%$
- Highly excited lines of (complex) organic molecules and isotopologs
  - No new complex organics molecules
    - OK, complex species better found at lower frequencies
  - Complete inventory of which molecule 'lives' in which type of gas

*HIFIStars*



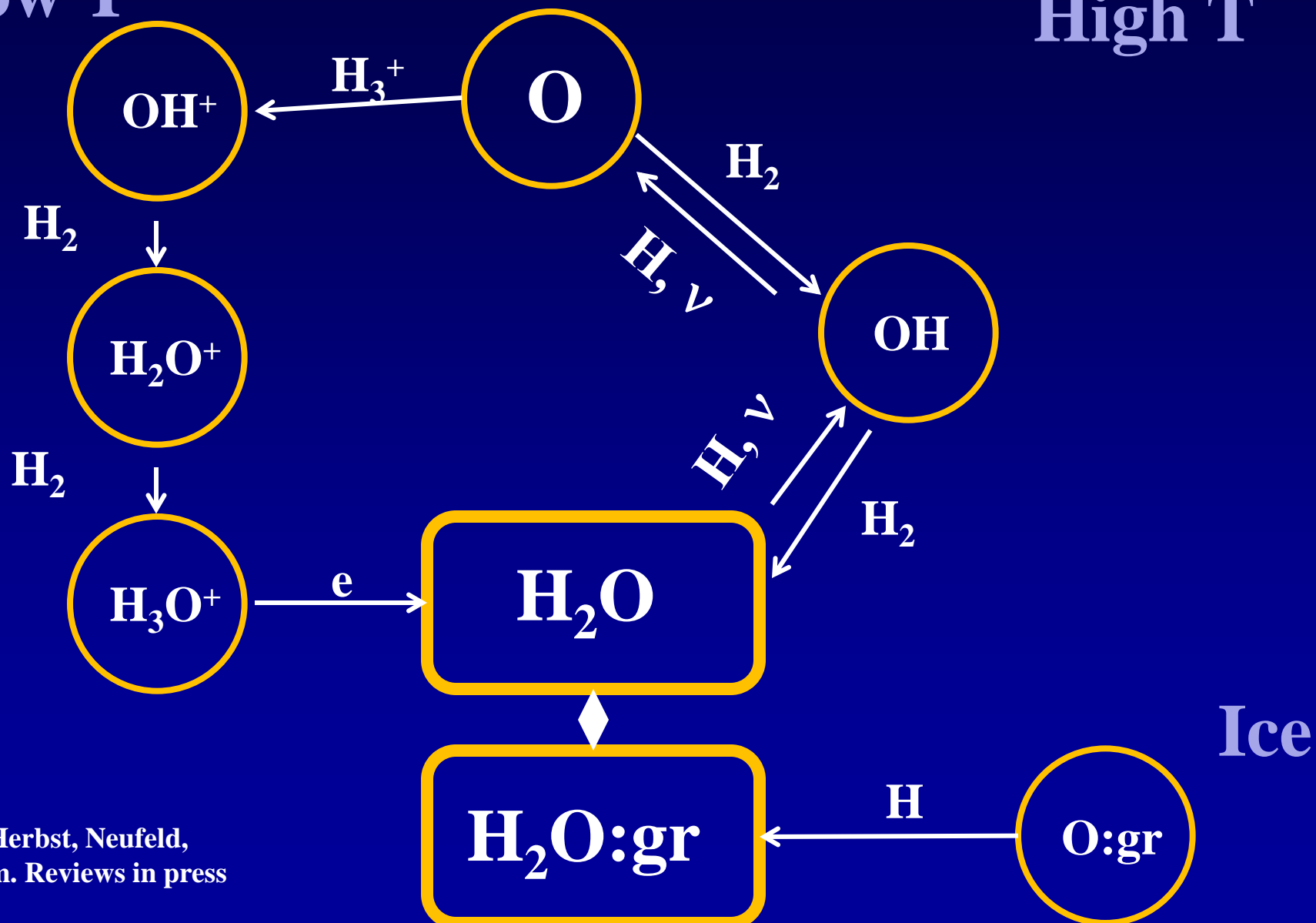
# Identifying and modeling emission



# Ice chemistry

Low T

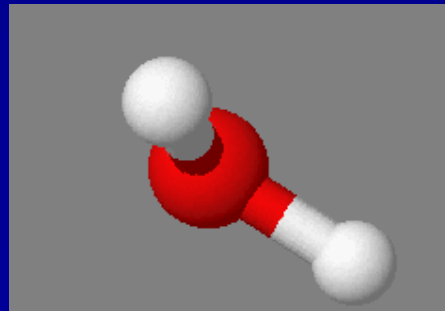
High T



# Water

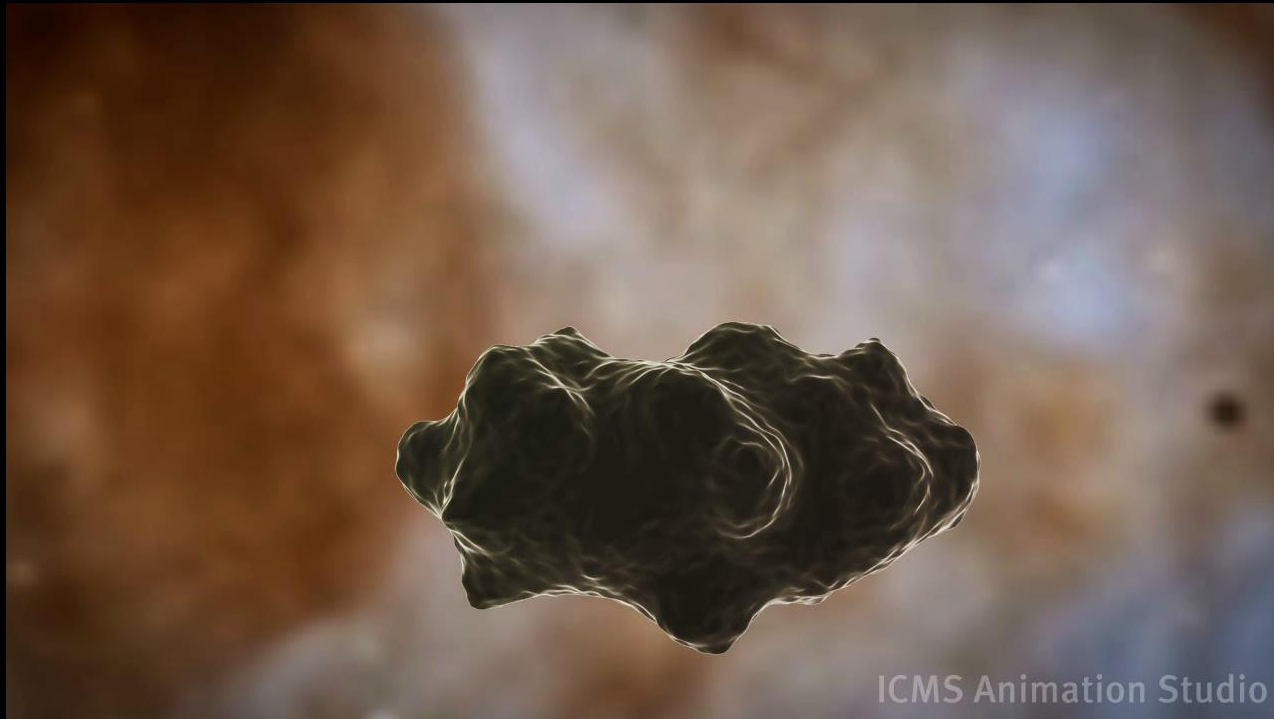


- Where is water formed in space and by which processes?
  - Gas vs grains
- What is the water 'trail' from clouds to planets?
  - Origin of water on Earth





# Formation of water on grains

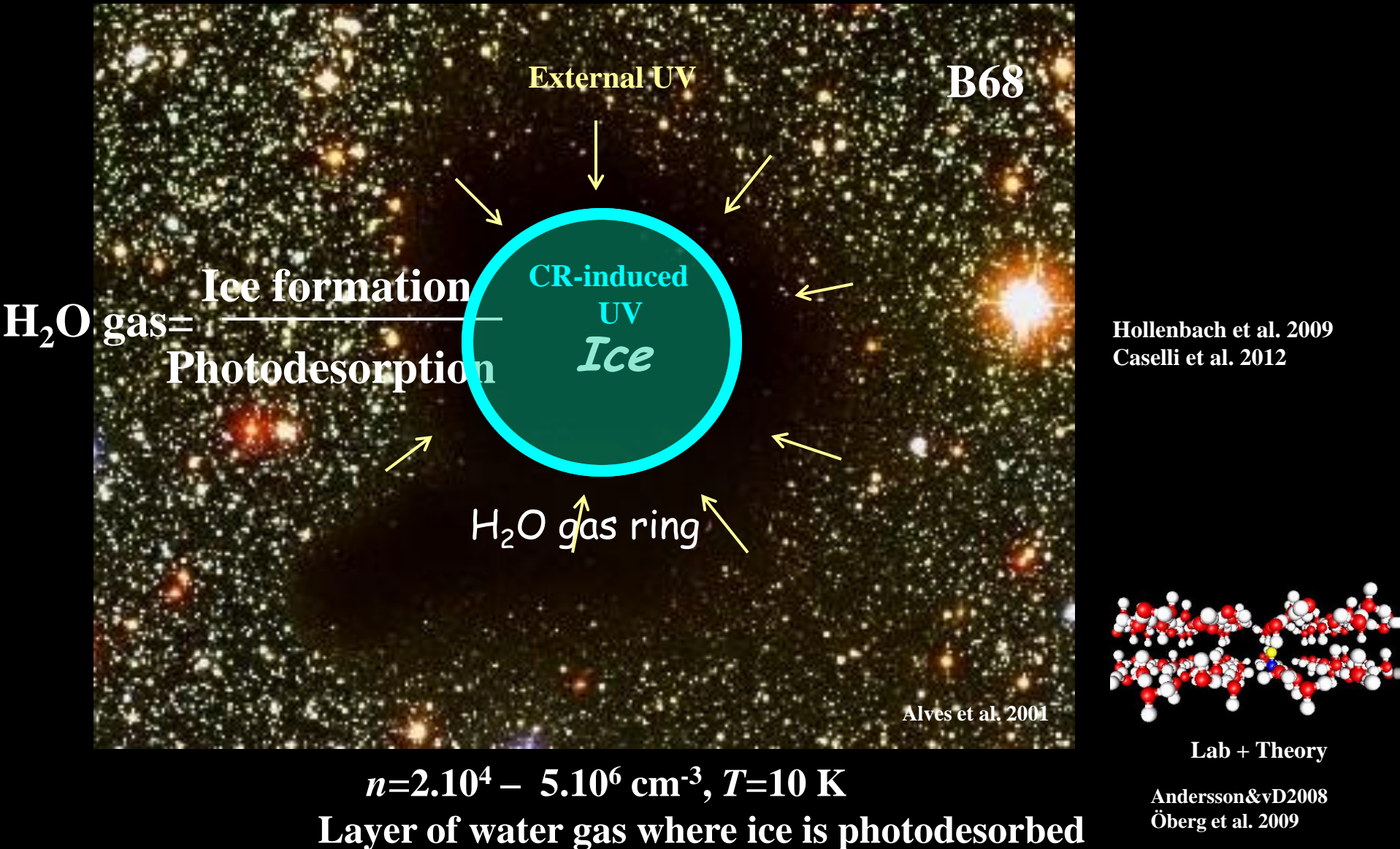


Based on Tielens & Hagen 1982  
Cuppen & Herbst 2007  
Cuppen et al. 2010

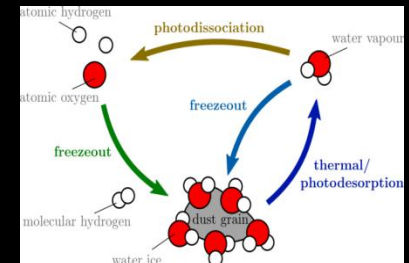
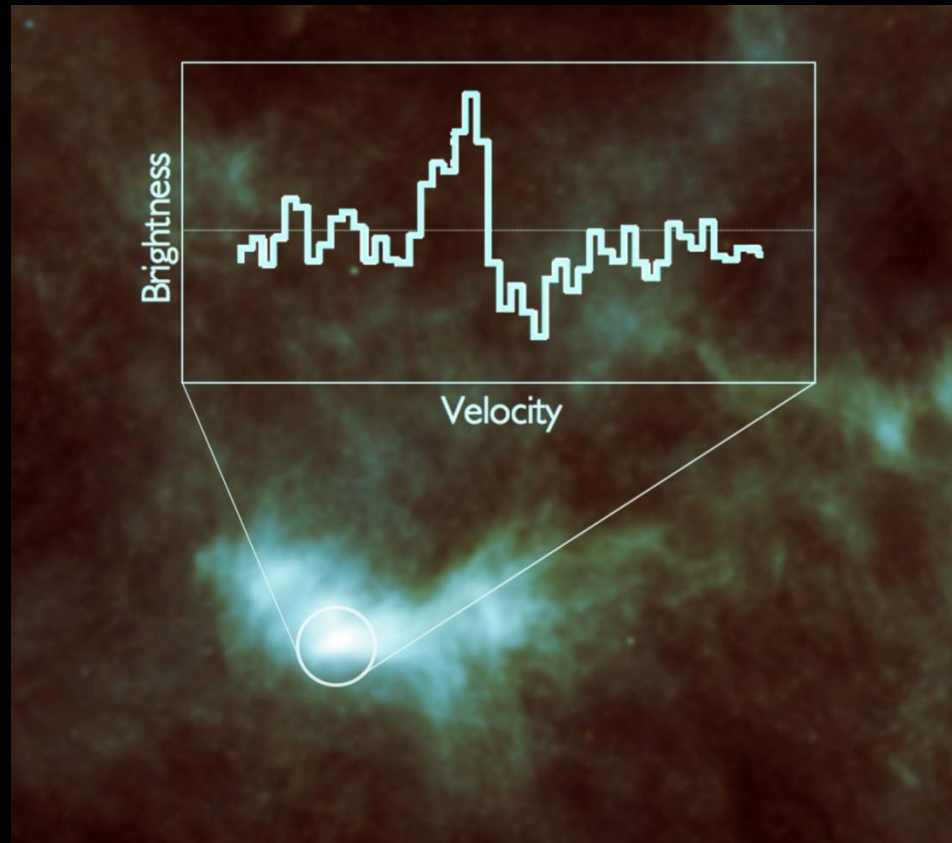
**Based on many laboratory experiments**

*Movie will be posted late 2013 at [www.strw.leidenuniv.nl/~ewine](http://www.strw.leidenuniv.nl/~ewine)*

# Pre-stellar cores: where is gas-phase water?



# Detection of cold water reservoir in pre-stellar cores



Hollenbach et al. 2009  
Keto et al., Schmalzl et al.

ESA Sci-Tech



- Simple ice chemistry works
- High density required for emission

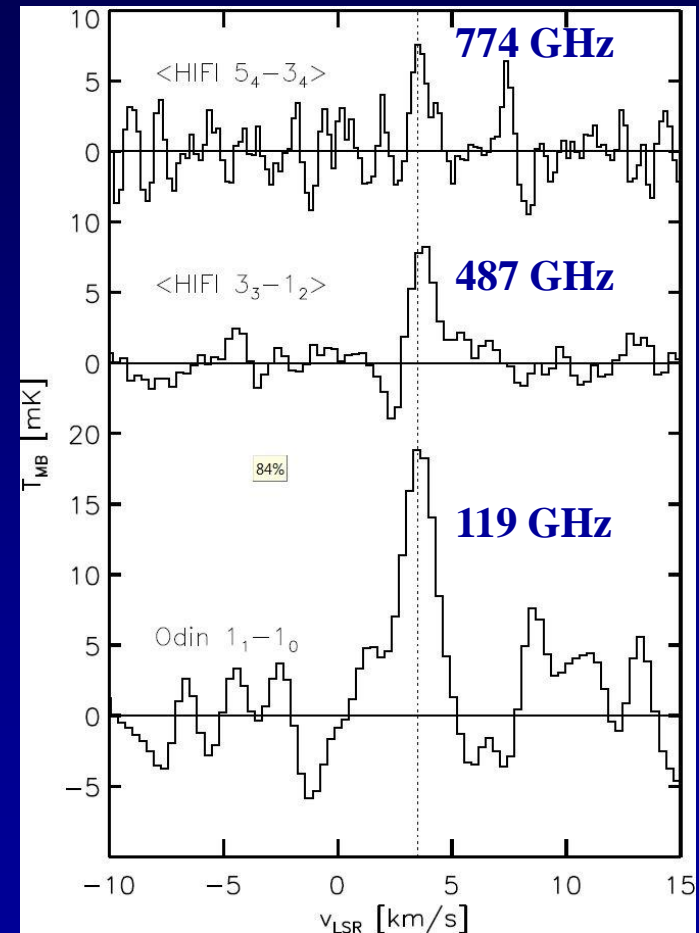
Caselli et al. 2012

# Multiline detection of O<sub>2</sub>



$$\text{O}_2/\text{H}_2 = 5 \times 10^{-8}$$

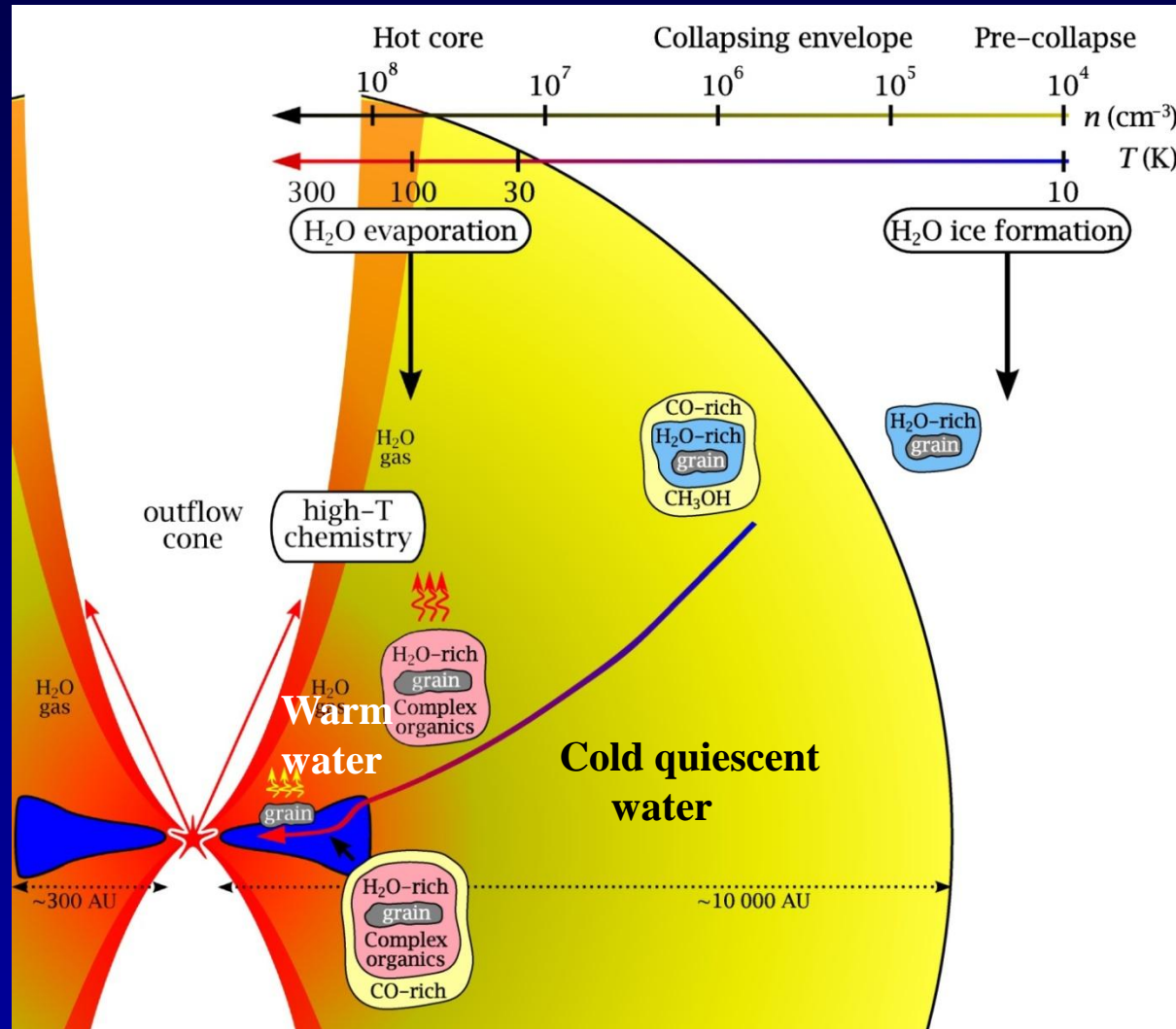
- Most O and O<sub>2</sub> converted to H<sub>2</sub>O
- O<sub>2</sub> only detected when grains warm enough to prevent O freeze-out



Liseau et al. 2012 Oph  
Goldsmith et al. 2011 Orion  
Yildiz et al. 2013 NGC 1333 I4A

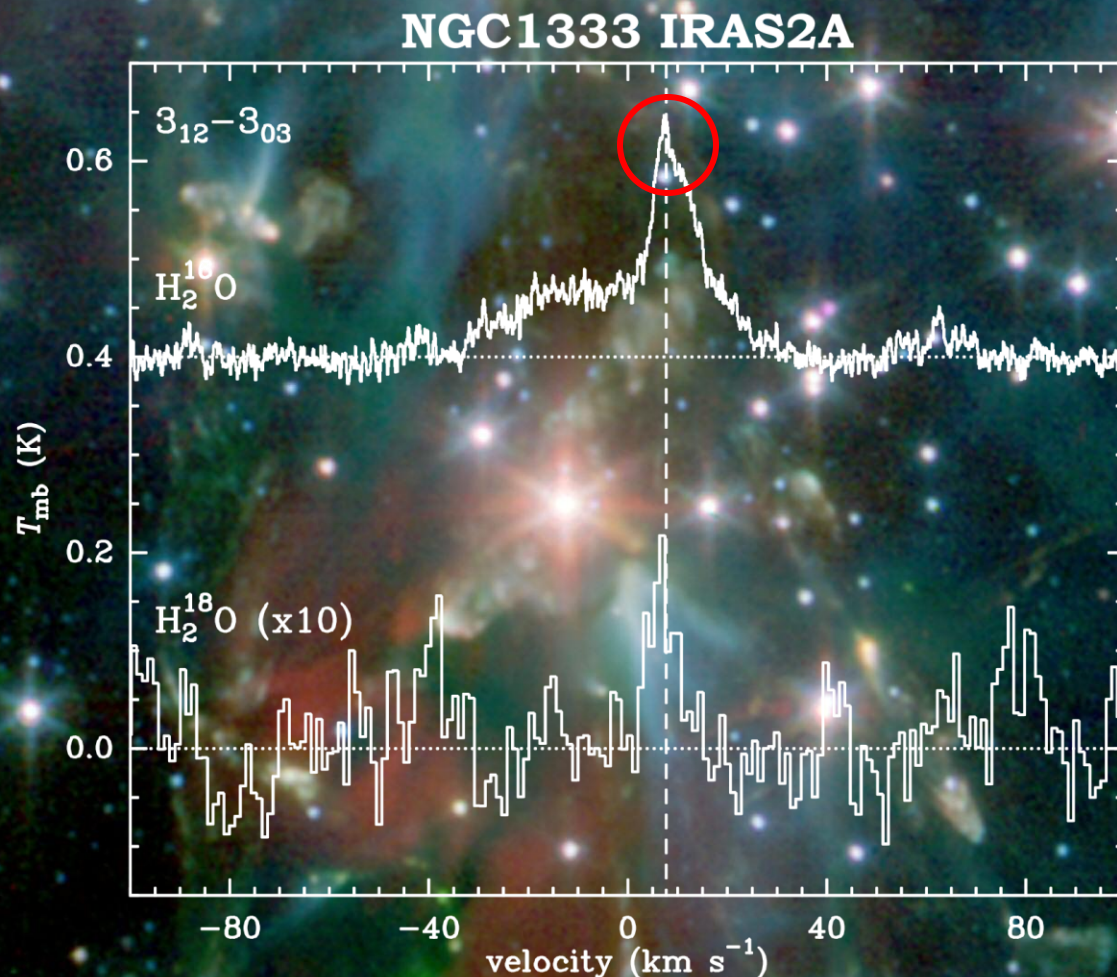


# How much water is where?



Expect high water abundance in 'hot core'

# How 'wet' is the hot core?



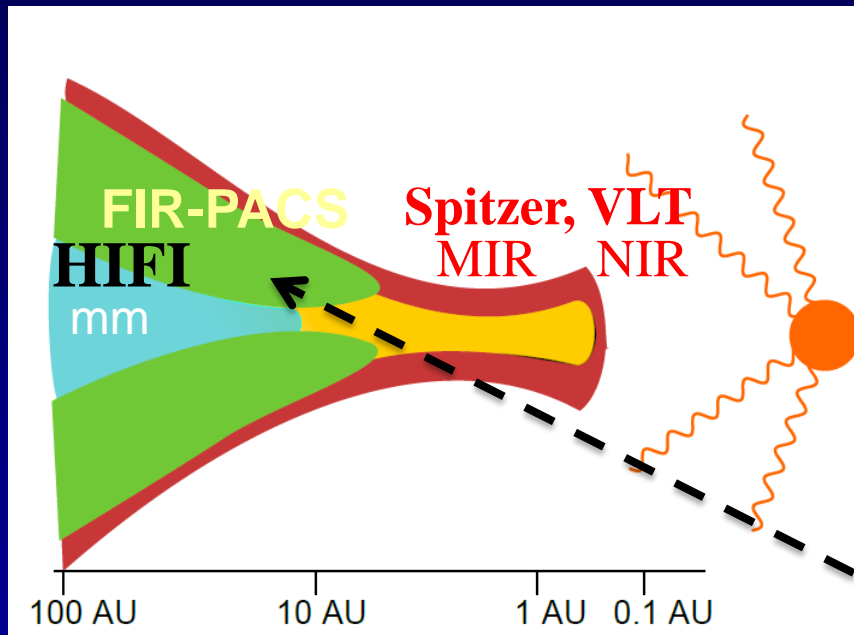
Visser et al. 2013  
Herpin et al. 2012  
Emprechtinger et al. 2013

.....

- Need isotopologs  $\text{H}_2^{18}\text{O}$  to detect *narrow* emission from quiescent hot core
- Inner abundances range from  $10^{-6}$  to  $10^{-4}$  for low and high-mass protostars, not yet understood

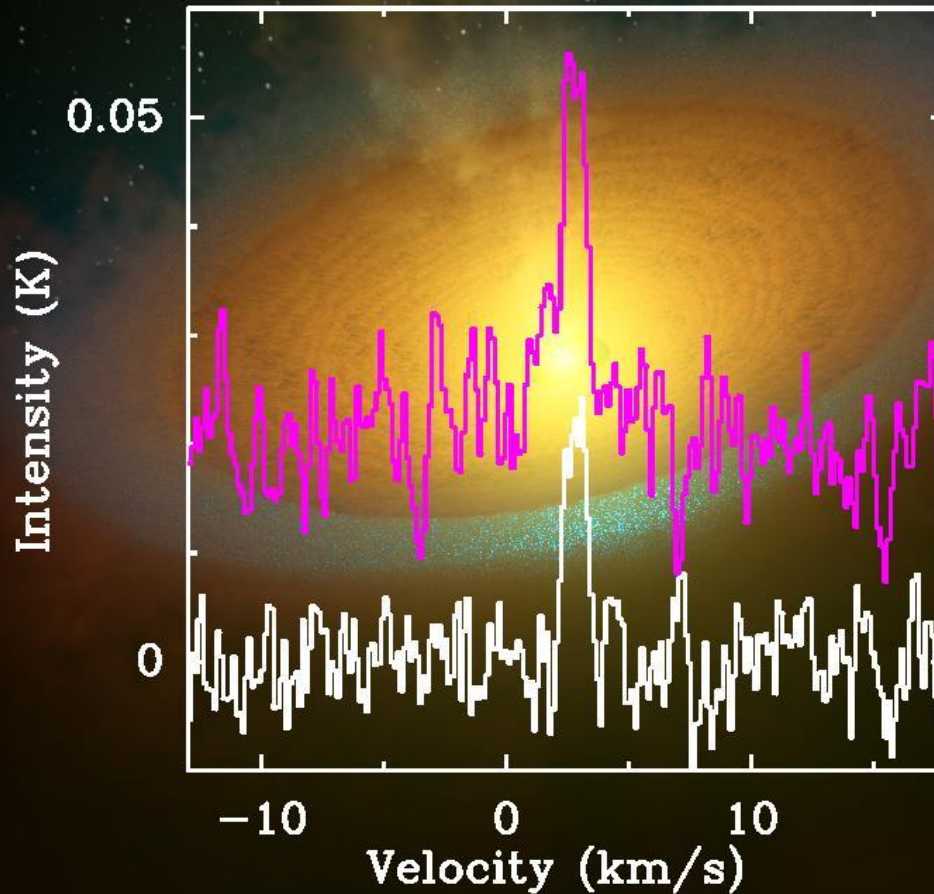


# Probing H<sub>2</sub>O across the entire disk surface



D. Fedele

# Revealing the cold water reservoir in disks



$p\text{-H}_2\text{O } 1_{11}-0_{00}$   
1113 GHz

$o\text{-H}_2\text{O } 1_{10}-1_{01}$   
557 GHz

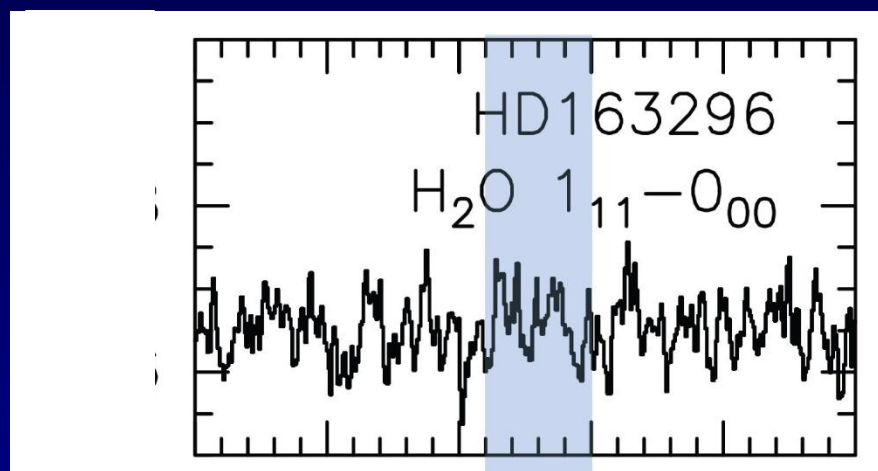
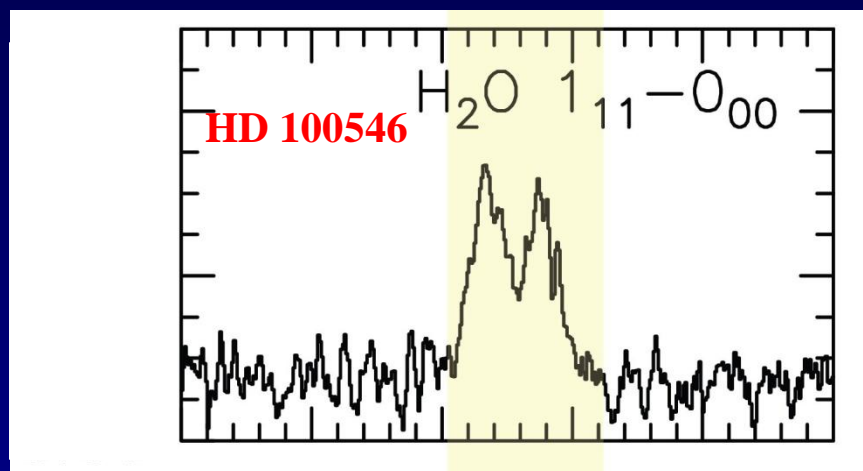
$o/p < 1$

Hogerheijde et al. 2011,  
Science

Detection points to 6000 oceans of water ice



# Water in disks survey



Hogerheijde et al., in prep.

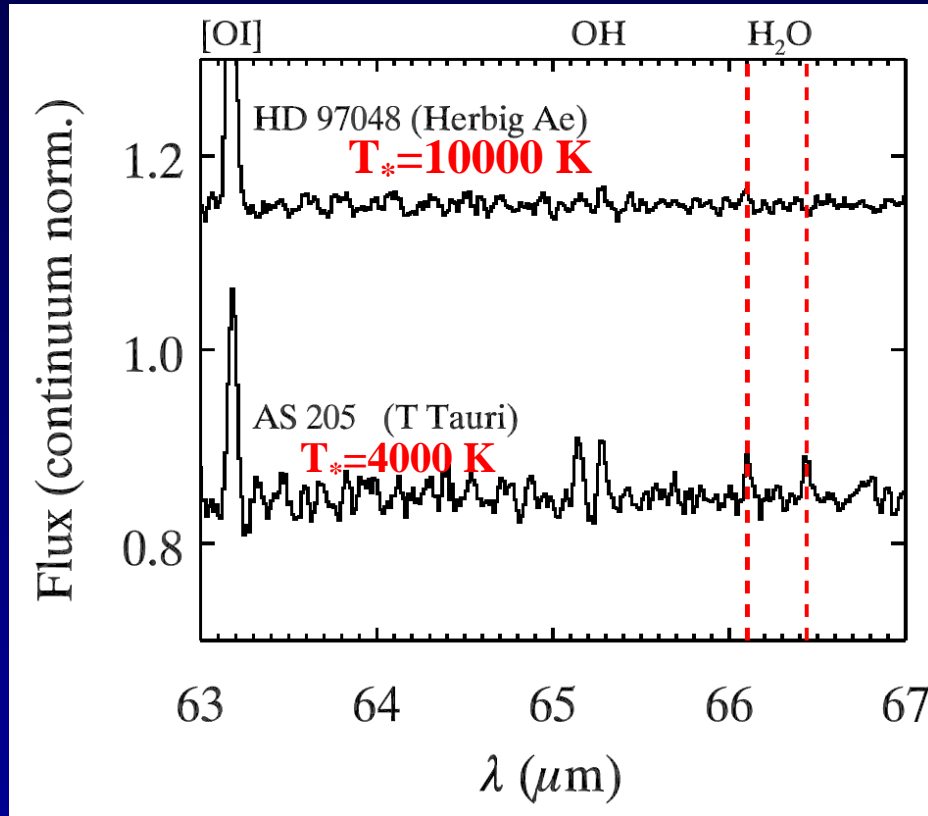
- Firm detections in 2 disks
  - o/p<1 unless gas does not follow dust
  - + DG Tau special case (late Class I, outflow?) Podio et al. 2013
- No detections in other disks in spite of very deep obs

*Absence of cold water emission is common feature*

Models:  
Bergin et al.,  
Woitke et al.  
Kamp et al.

.....

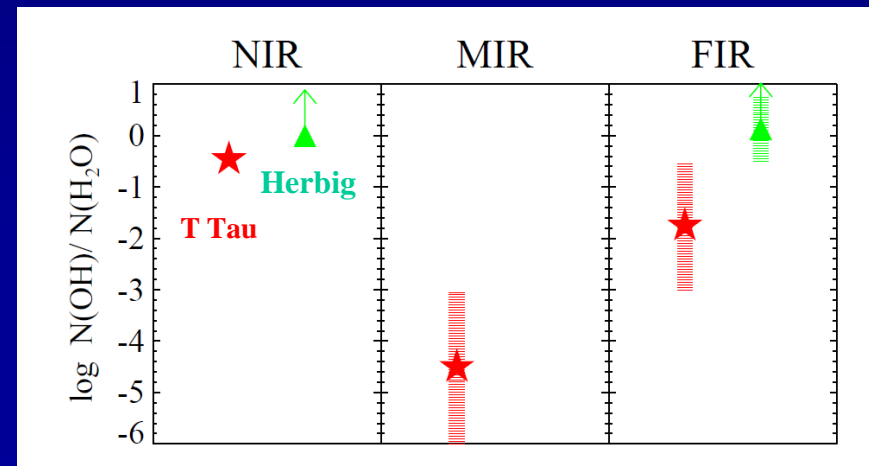
# PACS survey H<sub>2</sub>O



- Far-IR H<sub>2</sub>O detected in T Tau disks,  
but hardly in Herbig disks

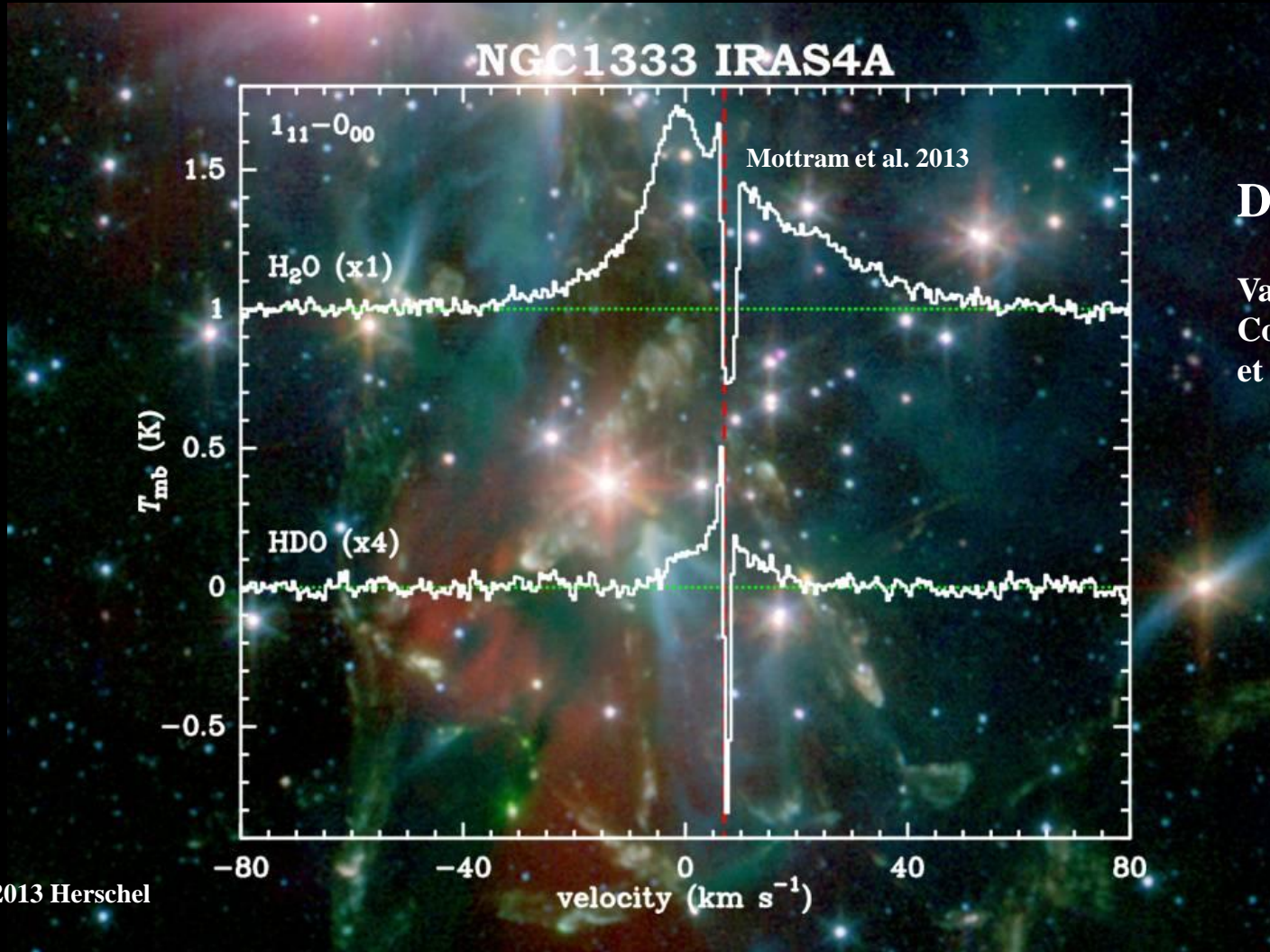


Fedele, Meeus et al. 2012, 2013  
Salyk et al. in prep.  
Riviere-Marichalar et al. 2012, GASPS  
Zhang et al. 2013





# HDO/H<sub>2</sub>O: high or low?



D<sub>2</sub>O

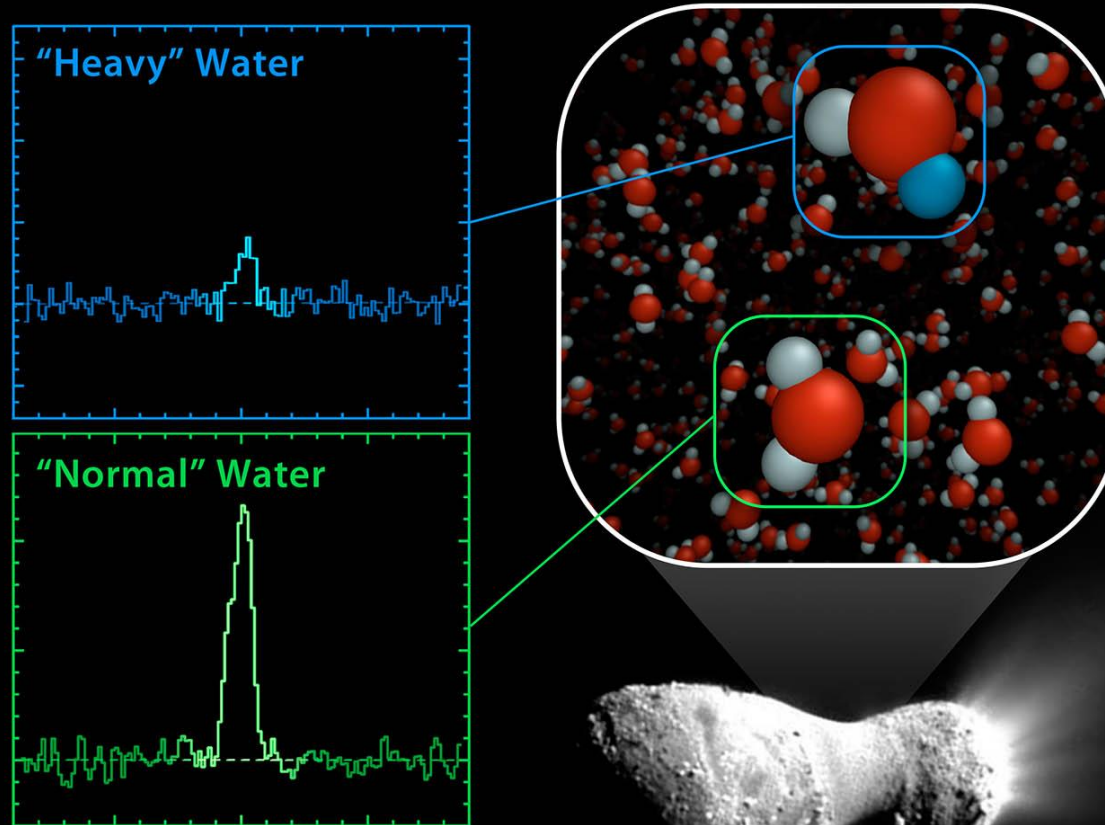
Vastel,  
Coutens  
et al.

Coutens et al. 2012, 2013 Herschel  
Visser et al. 2013

Persson et al. 2012, 2013 IRAM/ALMA

Optical depth H<sub>2</sub><sup>18</sup>O lines higher than thought before  
Recent analyses agree on warm HDO/H<sub>2</sub>O = (0.5-1)x10<sup>-3</sup>

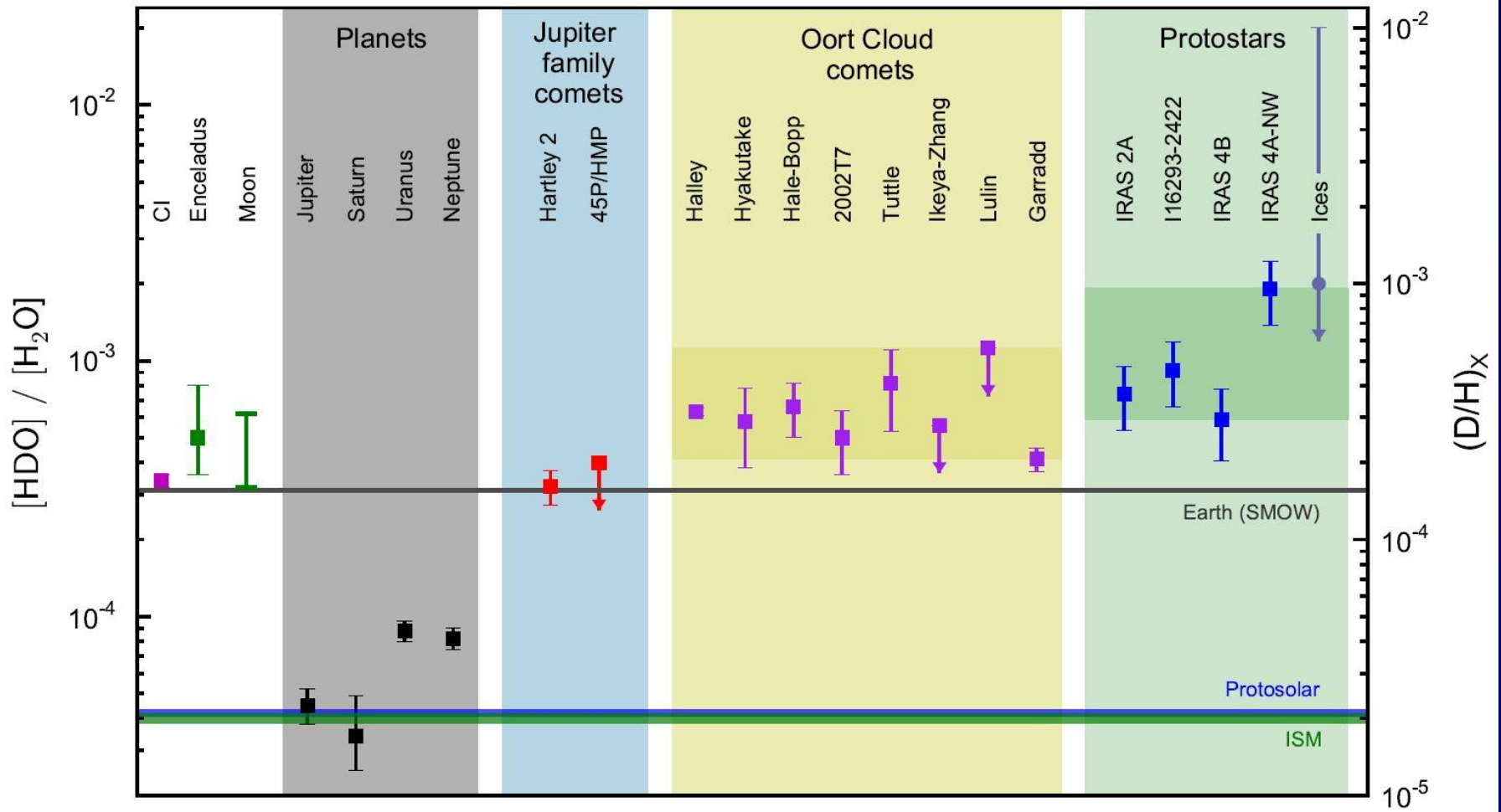
# HDO/H<sub>2</sub>O in Jupiter family comet



$\text{HDO}/\text{H}_2\text{O} = 3 \times 10^{-4}$ , same as Earth oceans



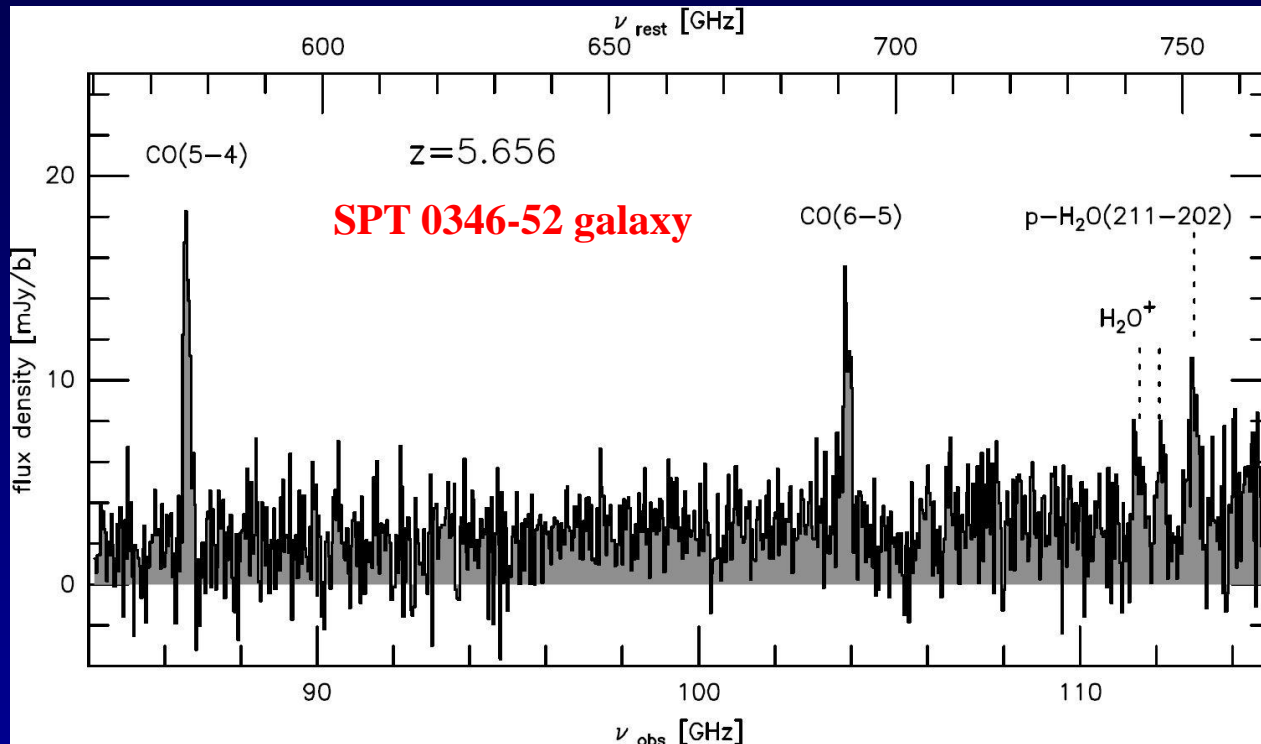
# HDO/H<sub>2</sub>O as tracer of origin of Earth's water



# Summary

- **Hydrides**
  - Precision astrochemistry
  - Diagnostics of  $\text{H}_2$ ,  $\zeta$ , turbulence, ....
  - State specific chemistry and excitation
- **Line surveys**
  - Origin complex organic molecules
  - Legacy
- **High temperature chemistry**
  - Hot CO and  $\text{H}_2\text{O}$  in shocks, CO ladder
  - Importance of irradiated shocks
- **Water and  $\text{O}_2$** 
  - Trail from cores to disks
- **Setting the scene for extragalactic chemistry, out to high  $z$**

# From Herschel to ALMA



Weiss et al. 2013  
ALMA

**Astrochemistry is everywhere throughout the Universe!**

*The promise of Herschel is being delivered  
Thanks to instrument teams for making this possible!*