Hydrides in solid phases: physical processes and chemistry

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Hydrides Toolbox, Dec 2016, Paris

Ice party, Cyprus

Outline

Short inventory of clouds & YSOs envelopes ices

Hydrides

- H_2O in disks
- H_2O ice structure, desorption & sputtering
- NH_3 & ice matrix environment
- The related NH_4^+
- CH_4

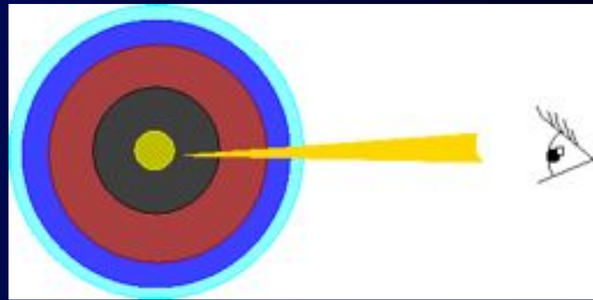
Cosmic abundances & ice detectivity

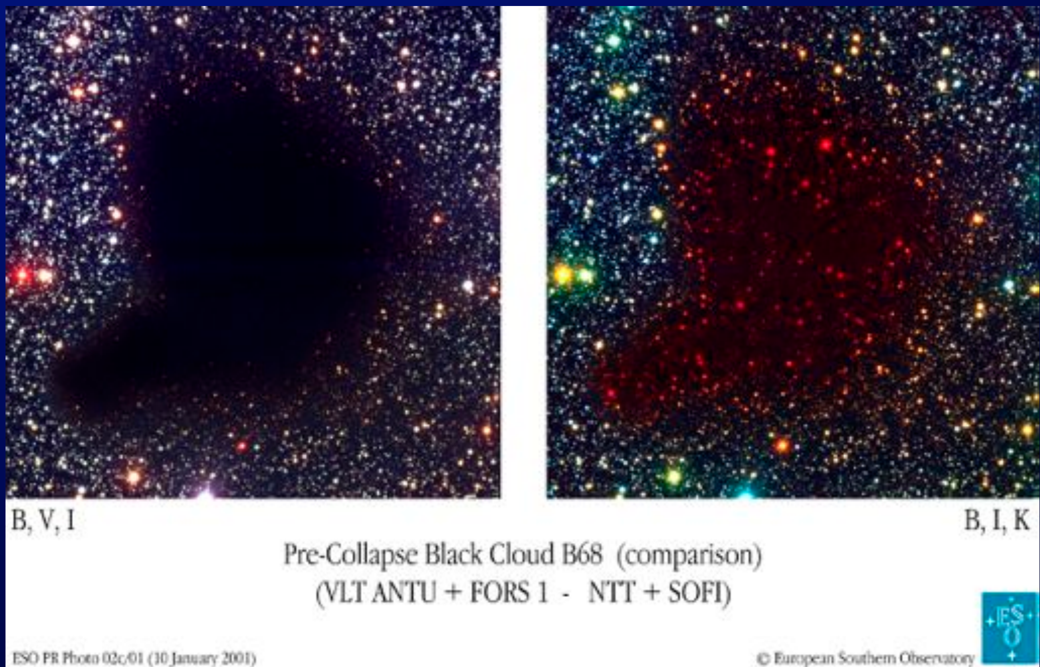
- upper limits (H_2S, NH_2, HF, HCl)

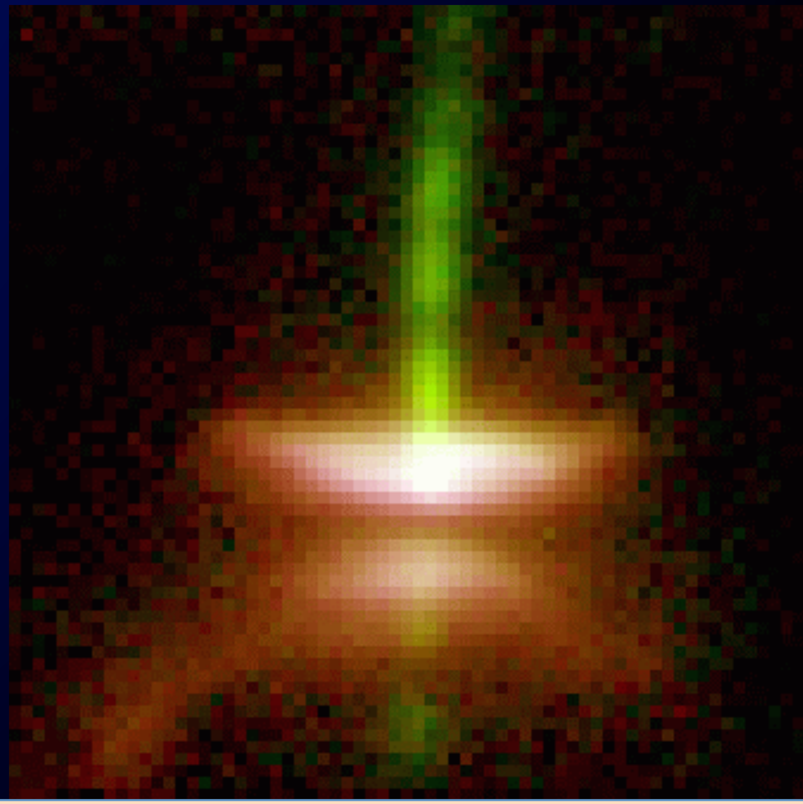
Glossary

Protostars (LYSOs;MYSOs) Disks

Field stars (BG)







HH30 © C. Burrows (STScI & ESA), WFPC 2 Team & NASA

Inventory of ices

Identified and suspected species

	MYSOs	LYSOs	BG Stars[c]
Securely identified species[d]:			
H_2O[e]	100	100	100
CO[e]	7_{4}^{15} (7)	21_{12}^{35} (18)	25_{20}^{43}
	3-26	(<3)-85	9-67
CO_2[e]	19_{12}^{25}	28_{23}^{37}	26_{18}^{39}
	11-27	12-64	14-43
CH_3OH	9_{5}^{23} (5)	6_{5}^{12} (5)	8_{6}^{10} (6)
	(< 3)-31	(< 1)-25	(<1)-12
NH_3		6_{4}^{8} (4)	
	~7[f]	3-10	< 7
CH_4		4.5_{3}^{6} (3)	
	1-3	1-11	< 3
Likely identified species[g]:			
H_2CO	~2-7	~6	
OCN^-	$0.6_{0.3}^{0.7}$	$0.6_{0.4}^{0.8}$ (0.4)	
	0.1-1.9	(< 0.1)-1.1	<0.5
OCS	0.03-0.16	≤1.6	<0.22

The dominant hydride:

$\propto A_V$ past a threshold

$X_{ICE}(H_2O)/X(H) \sim 10^{-5}$-$10^{-4}$

Not easy to observe

Seem contemporary of H_2O phase

Boogert+2015 & ref therein

Inventory of ices

The upper limits (~MYSOs)

Species	X_{H_2O} %
N_2	$< 0.2 - 60$
O_2	< 39
	< 15
H_2	< 68
H_2S	$< 0.3 - 1$
	$< 1 - 3$
H_2O_2	$< 2 - 17$
C_2H_2	$< 1 - 10$
C_2H_6	< 0.3
C_5H_{12}	< 15
C_3O_2	< 5
N_2H_4, $N_2H_5^+$	< 10
HNCO	$< 0.3 - 0.7$
$HCONH_2$	< 1.5
NH_2CH_2OH	$< 3 - 6$
NH_2CH_2COOH[d]	< 0.3

The tentative ice list

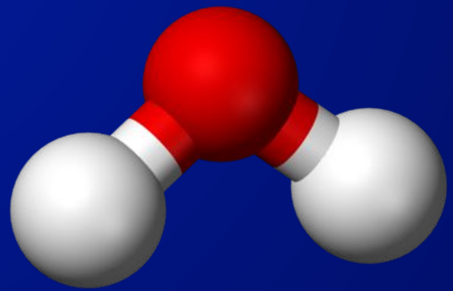
	MYSOs	LYSOs	BGstars
HCOOH[i]	4_3^5 (3)		
	(< 0.5)-6	(< 0.5)-4	<2
C_2H_5OH[i]	$\sim X_{H_2O}(HCOOH)$		
$HCOO^-$[j]	$0.5_{0.5}^{0.7}$ (0.5)		
	0.3-1.0	~0.4	<0.1
C_2H_4O[j]	$X_{H_2O}(HCOO^-)\times 11$		
NH_4^+	11_9^{13}	11_7^{15}	8_6^{11}
	9-34	4-25	4-13
SO_2	(< 0.9)-1.4	~0.2	
PAH[k]	3-20		

Which processing ?

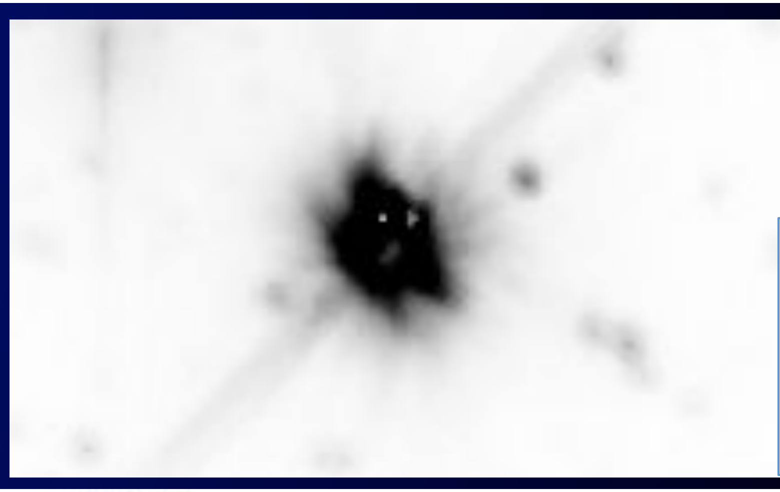
Photolysis
Radiolysis
Surface/thermal

Boogert+ 2015

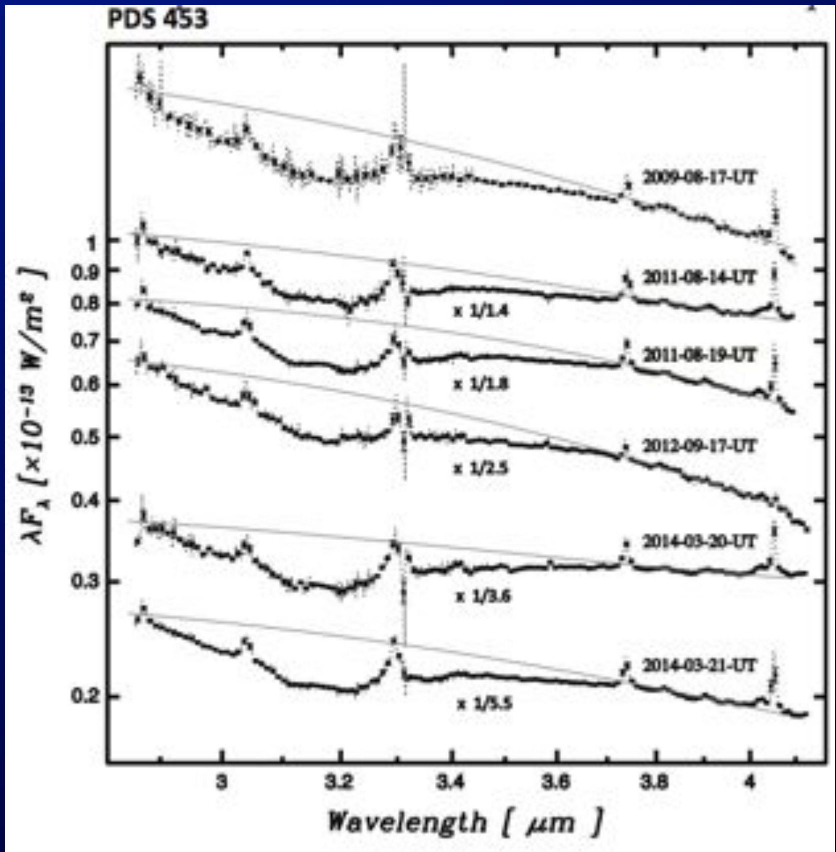
H_2O ice in disks

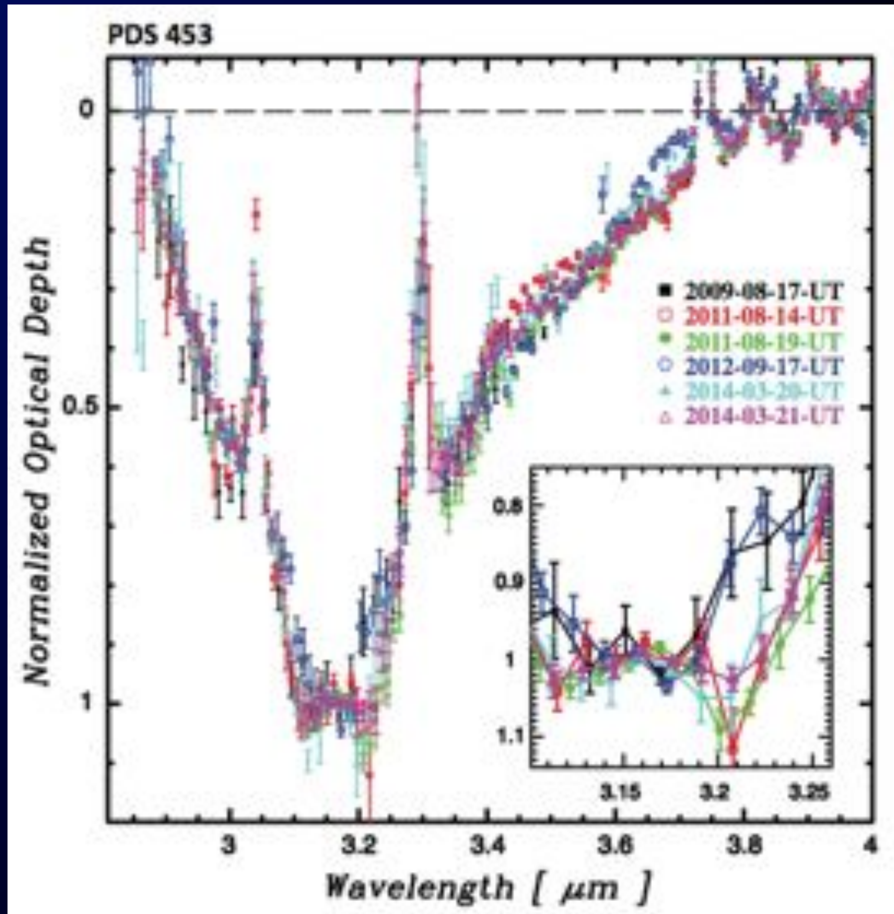


F2V; Herbig Ae d~140pc Incl. ~79deg



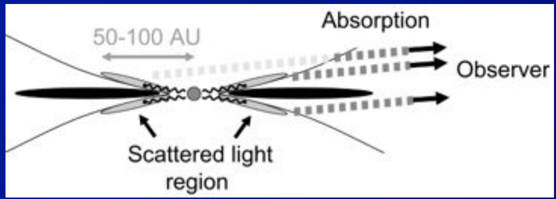
PDS453 / HST





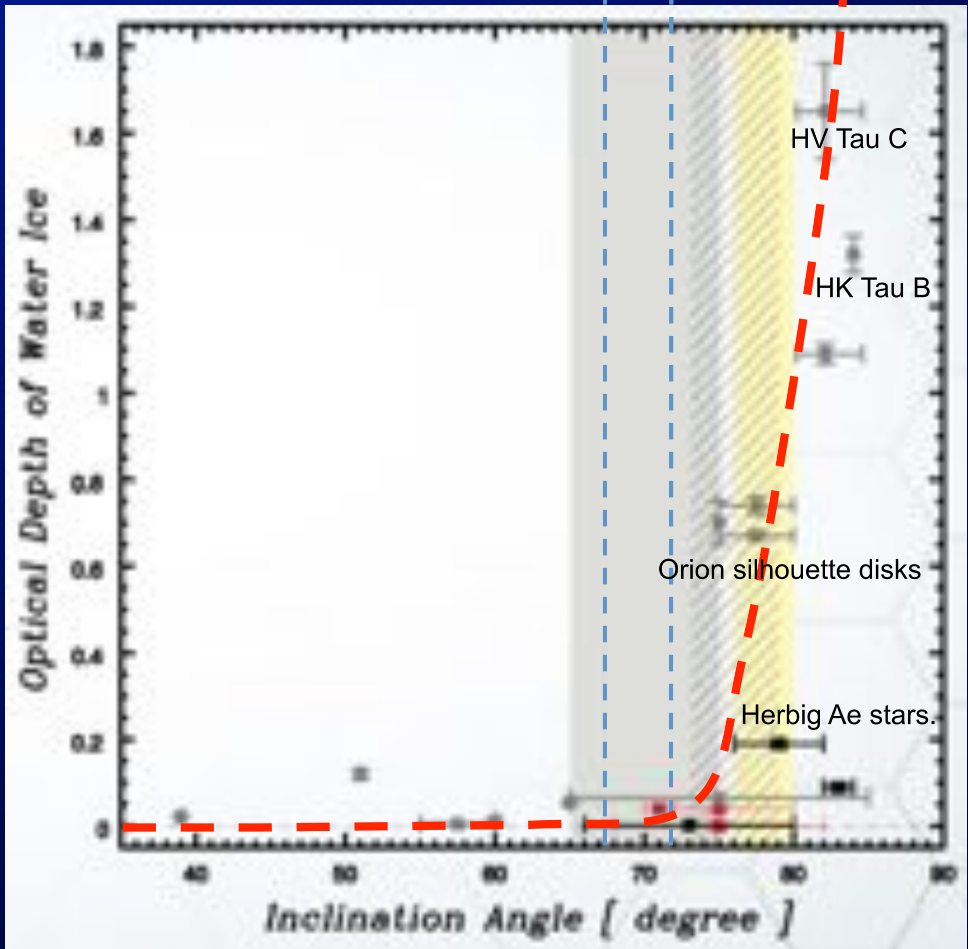
Terada & Tokunaga 2016

Inclination & flaring determines what is probed

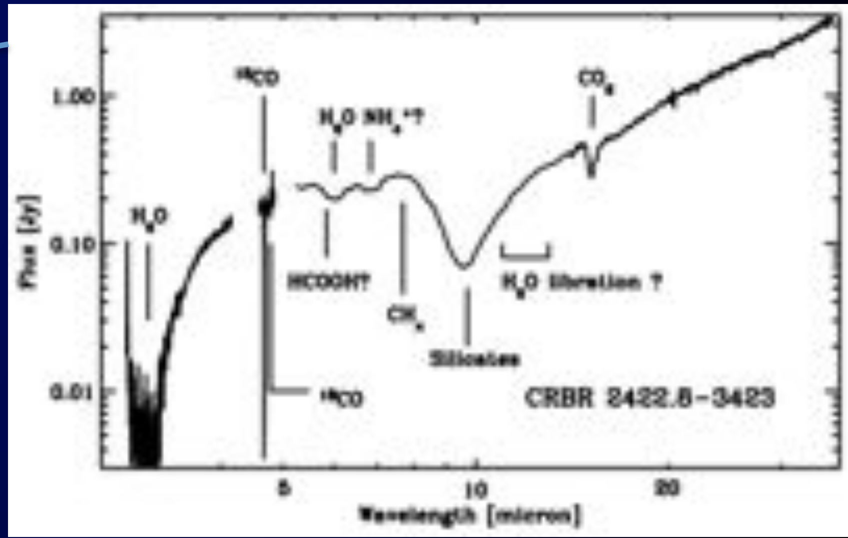


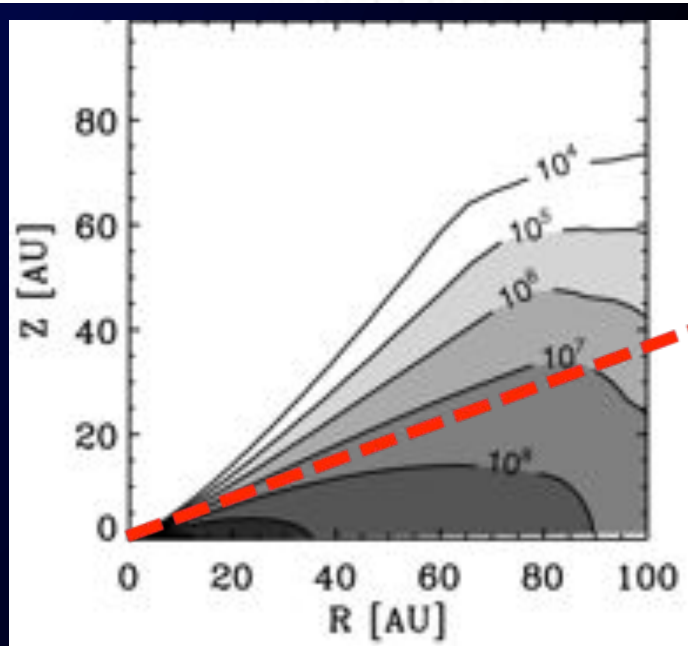
Terada+2007

CRBR 2422.8- 3423
0.8 Msun



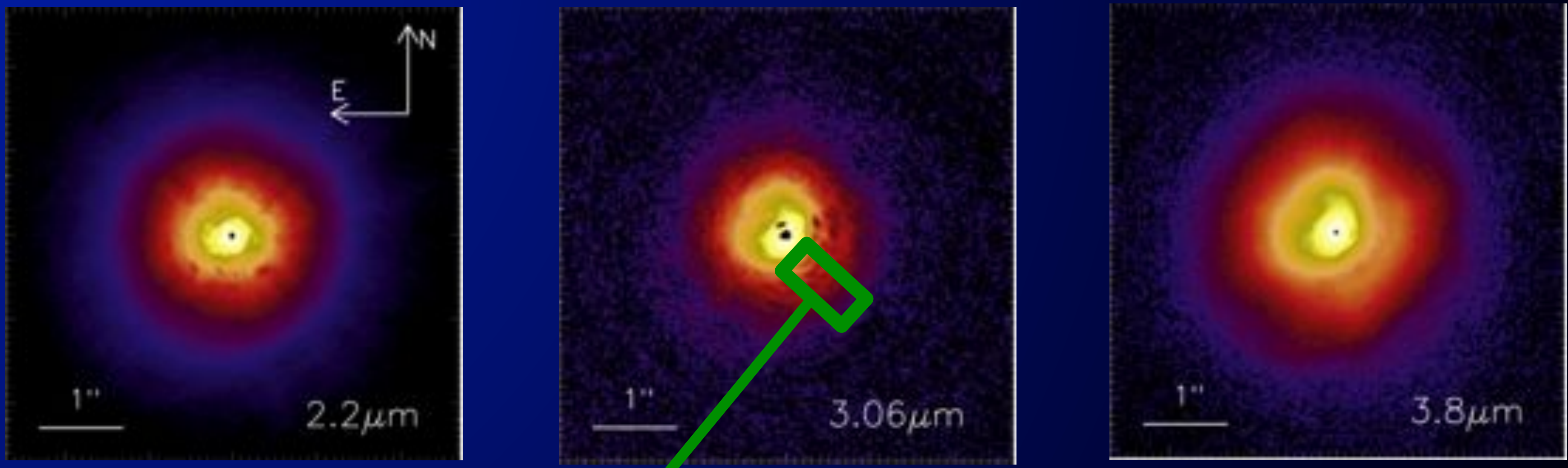
Terada & Tokunaga 2016

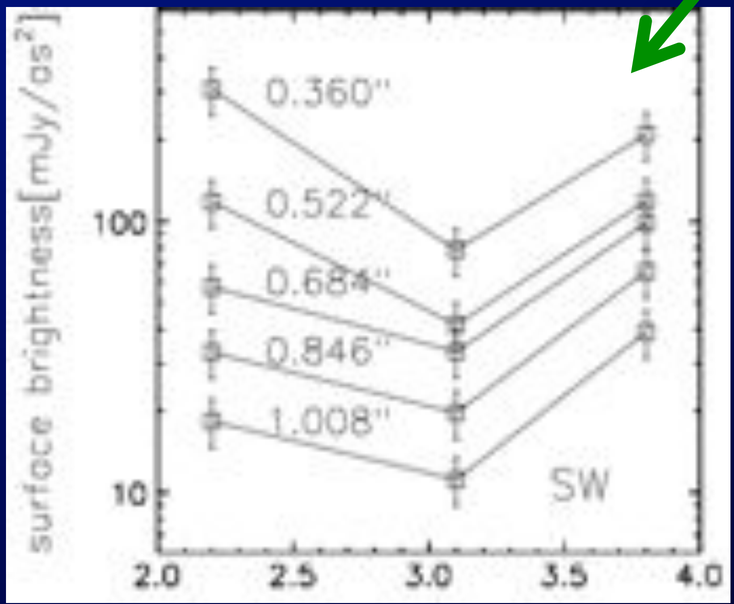


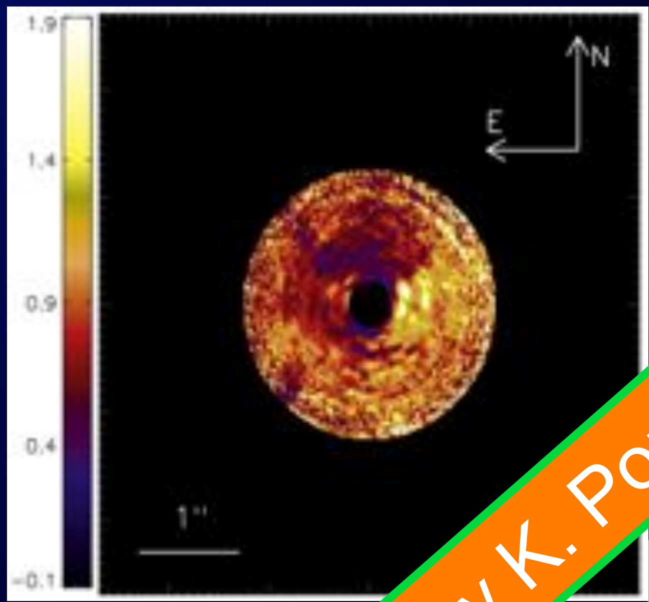


Pontoppidan+2005

Face on disks will observed in scattering







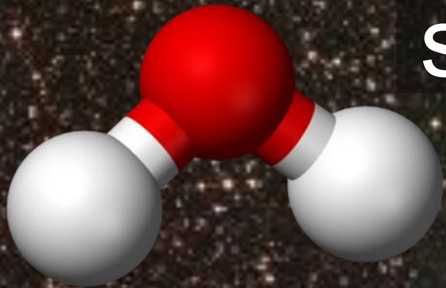
Honda+2016, 2009

Talk by K. Pontoppidan

Water ice observed in emission in the FIR

Ma… …hiang+2001,McLure+2015

A full inventory like in YSOs is long term…

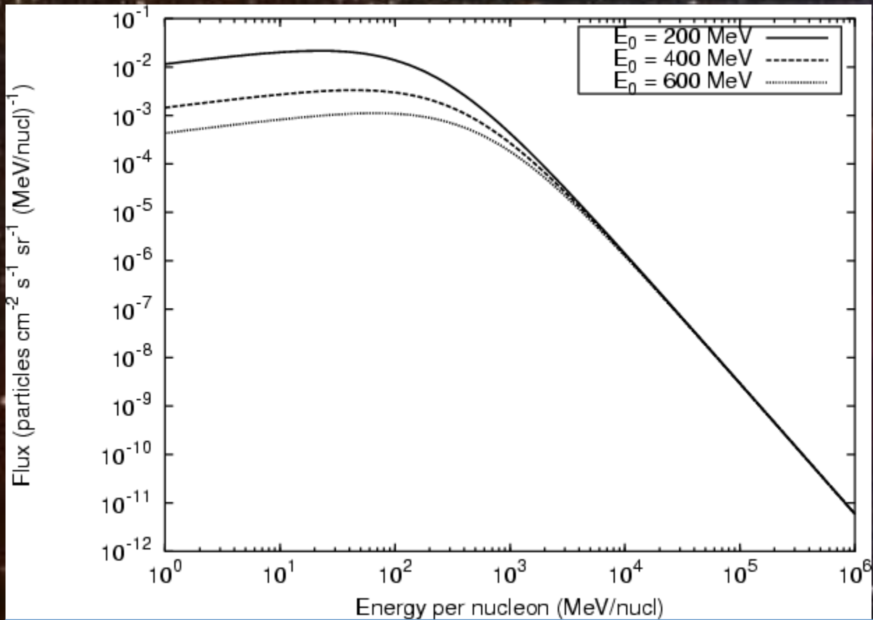


structure, desorption & sputtering

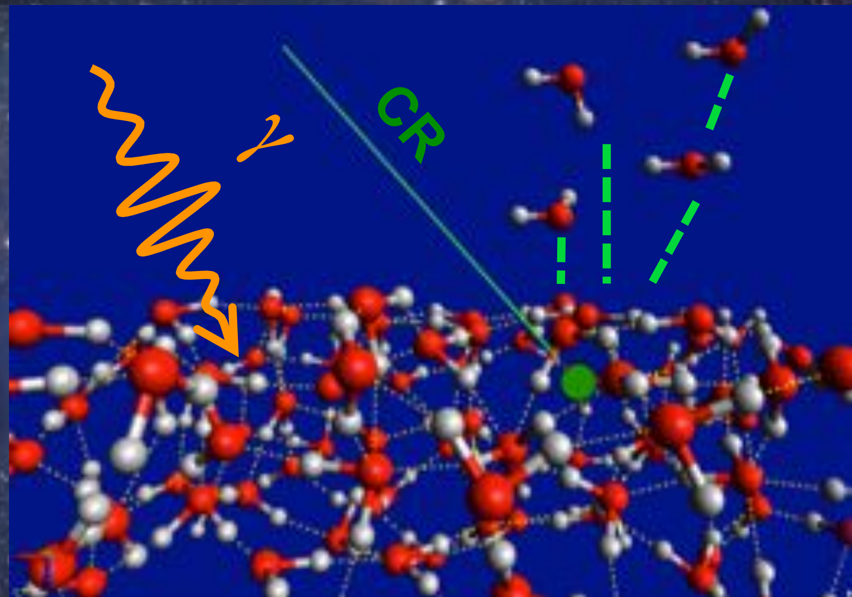
In dense clouds & YSOs envelopes

Gas phase accretion timescale~10^9 years / n_H

➡ everything should condense



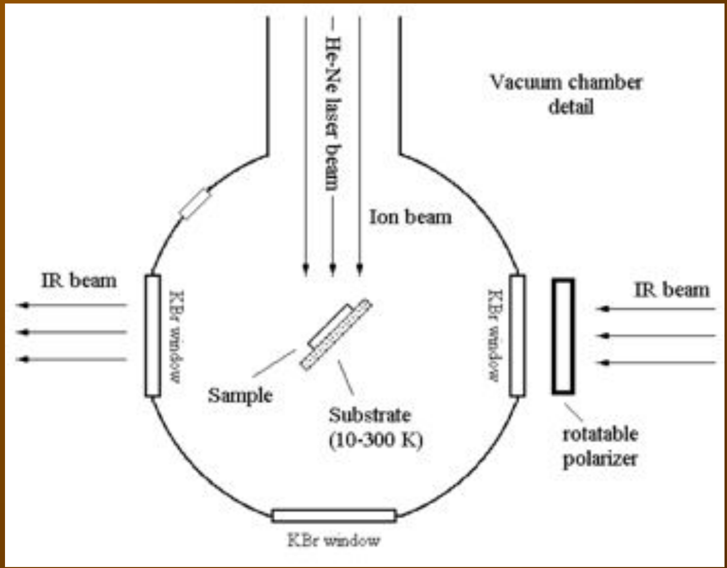
Webber+1983,Shen+2004,Padovani+2015,Chabot+2016



Dartois+2015

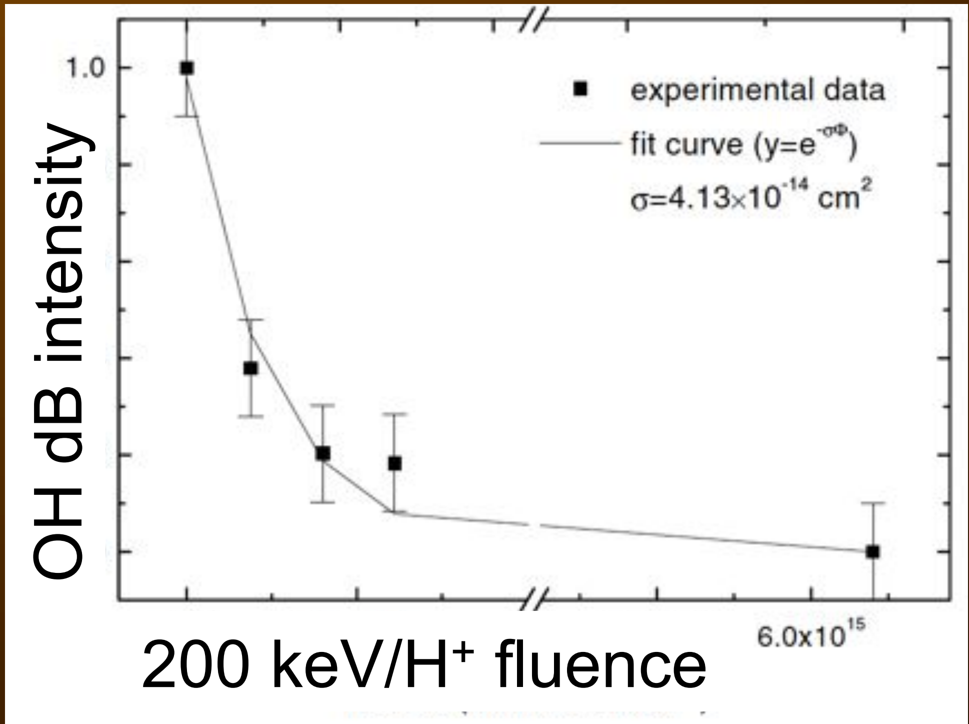
- Sputtering together with stochastic heating and VUV secondary photons (re-)inject species in the gas phase

Lupus 3 dark cloud © ESO/F. Comeron



CR induced ice phase modification ?

Porous ASW -> compact amorphous ice



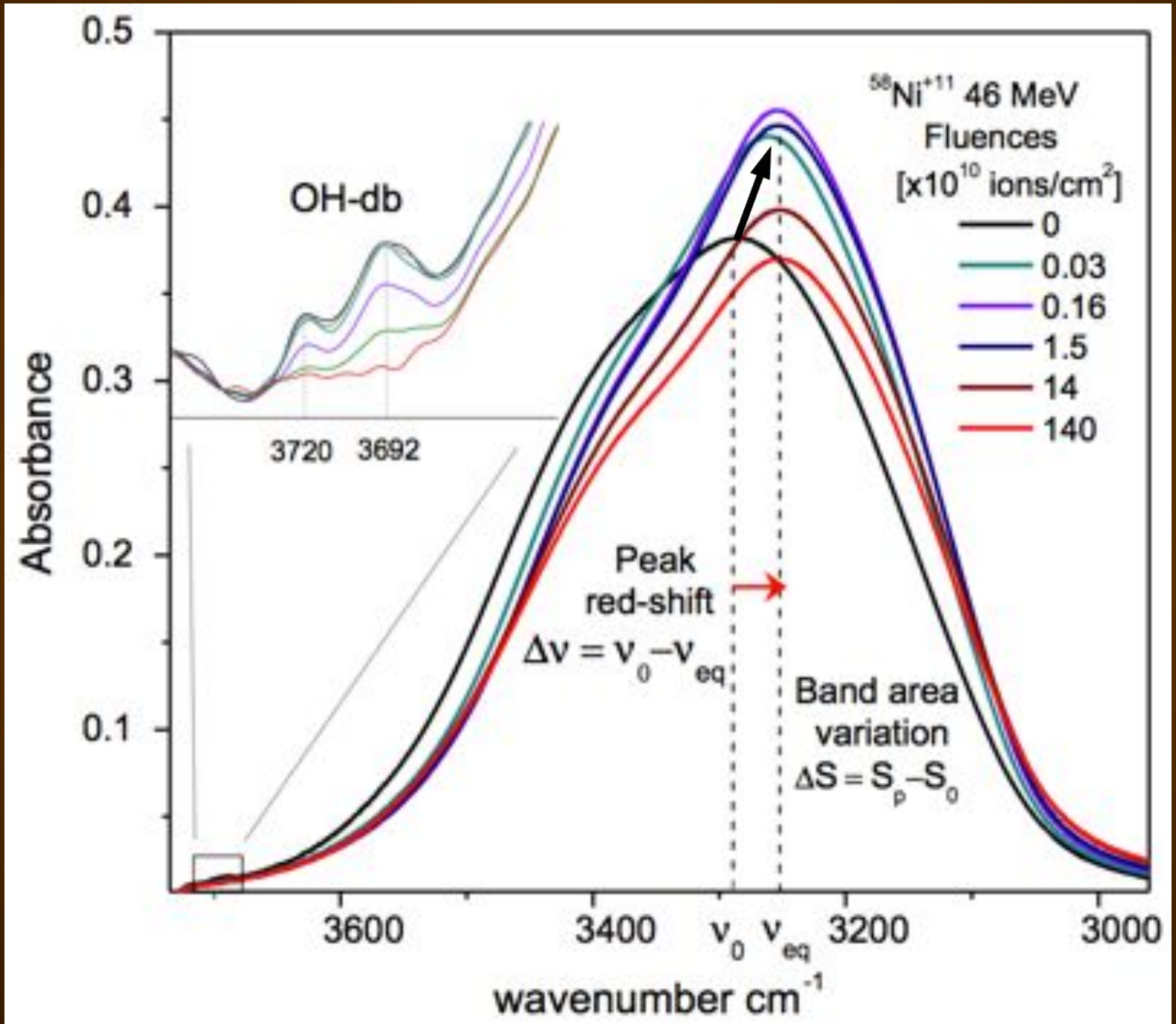
Palumbo et al. 2006

Many work already @ low energies:

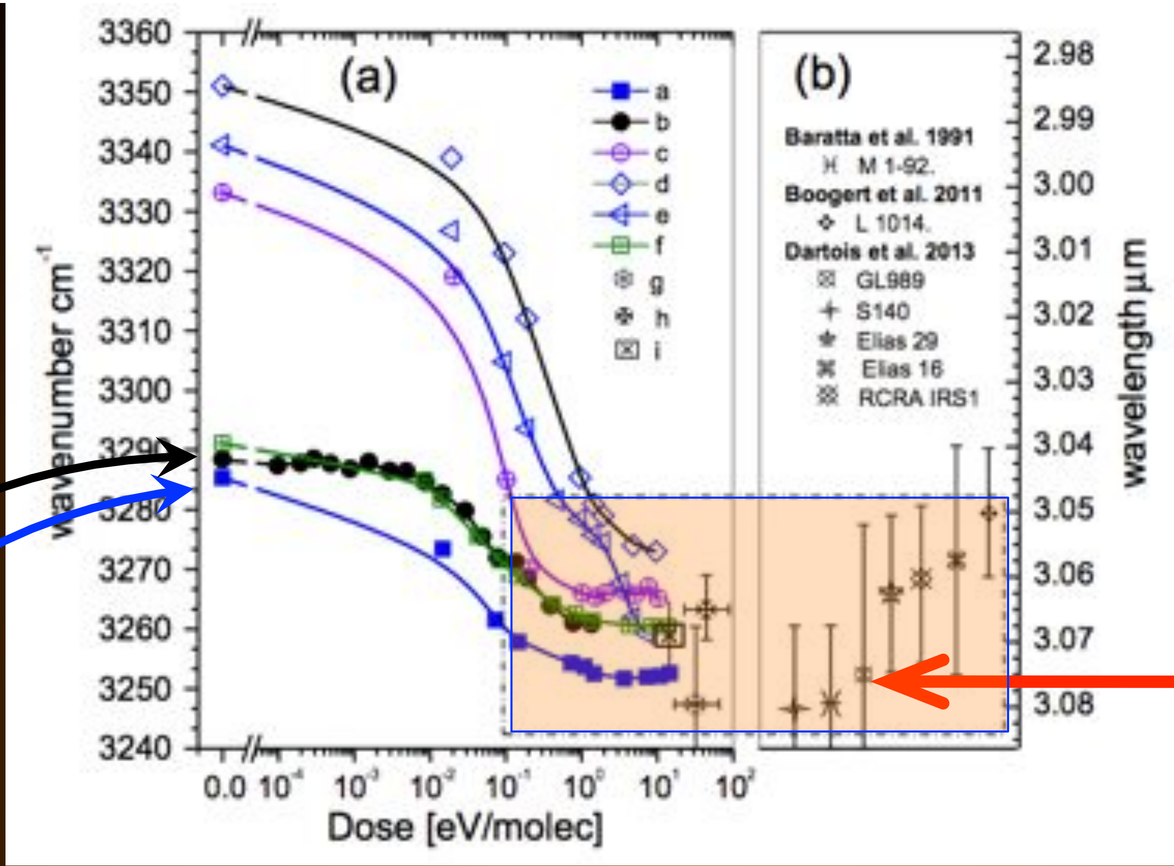
e.g. Baratta et al. 1991; Strazzulla et al. 1992; Moore & Hudson 1992; Leto & Baratta 2003; Baragiola et al. 2005; Mastrapa & Brown 2006; Raut et al. 2007; 2008; Famá et al. 2010…

Change reactivity for surface reactions:
reduce surface available & nature of sites
close the porosity for diffusion

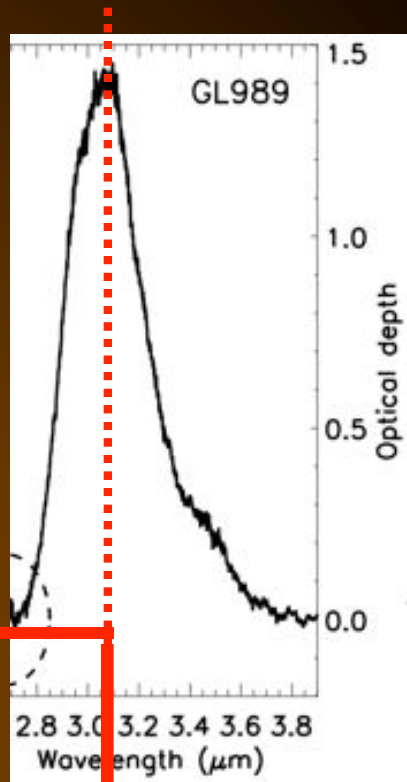
The ice profile contains information on the structural processing



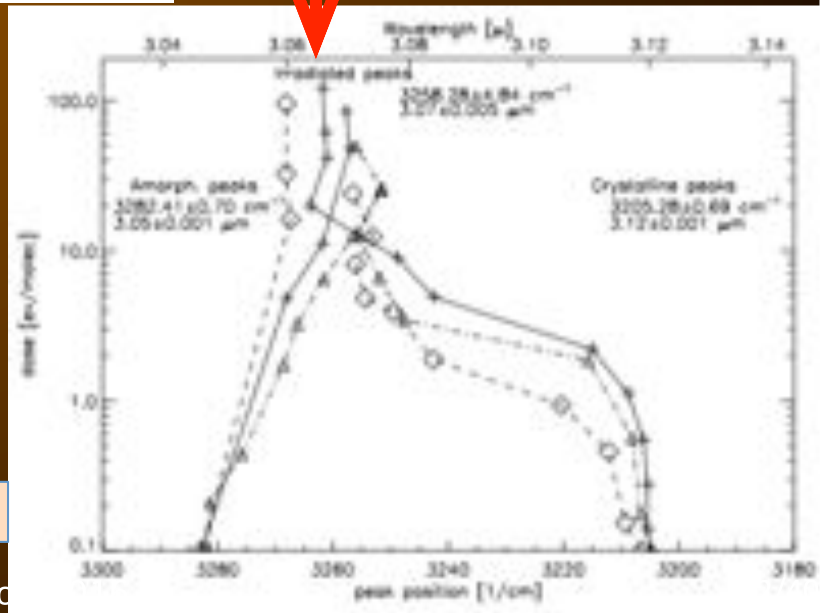
Mejia+2015



ASW



Mejia+2015



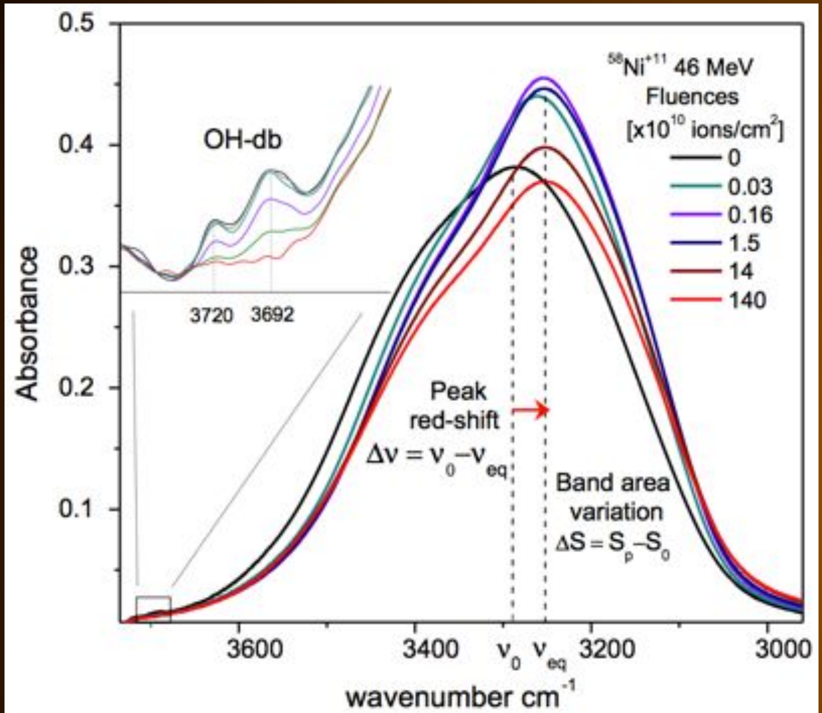
Evolution of the peak position with irradiation

Leto+2003

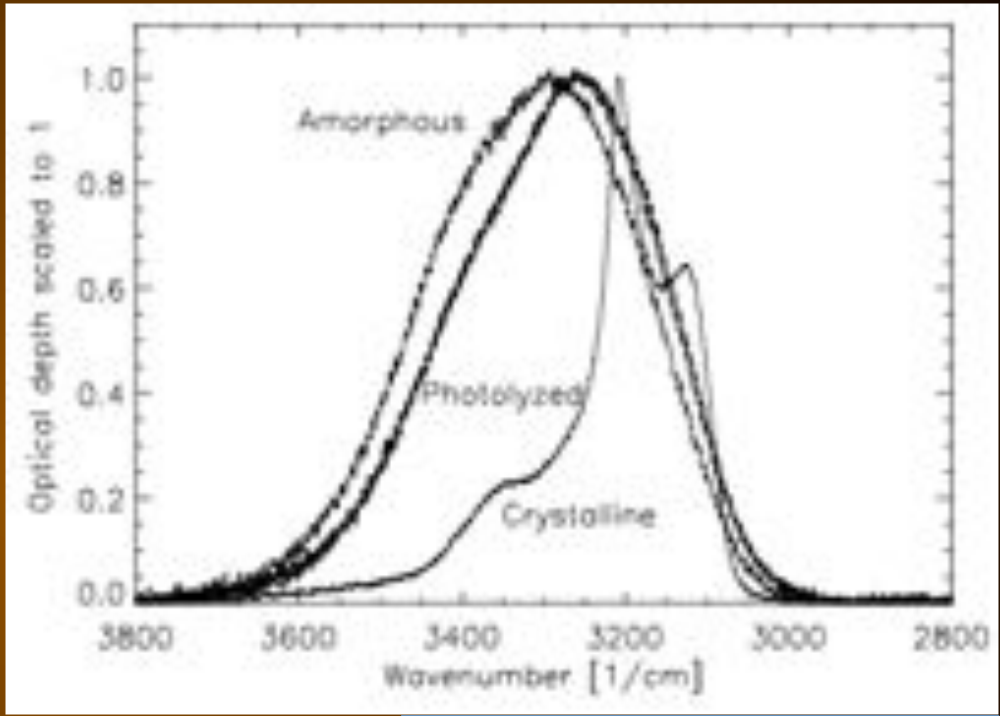
Observational Spectroscopic differences ?

CR

UV photons



Mejia+ 2015, Dartois+2015



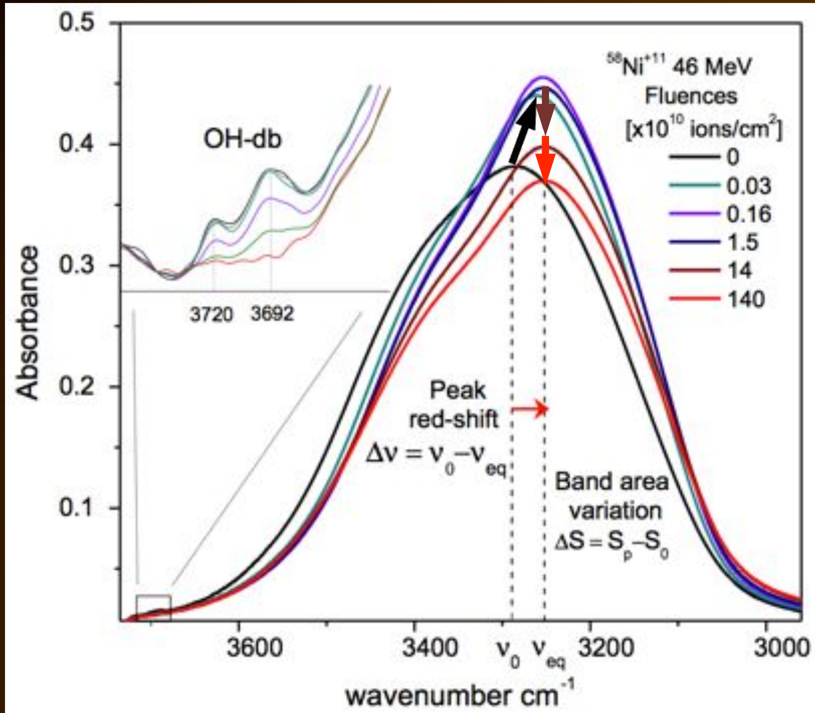
Leto & Baratta 2003, Palumbo+ 2010

Surface reaction formation: also compact ice

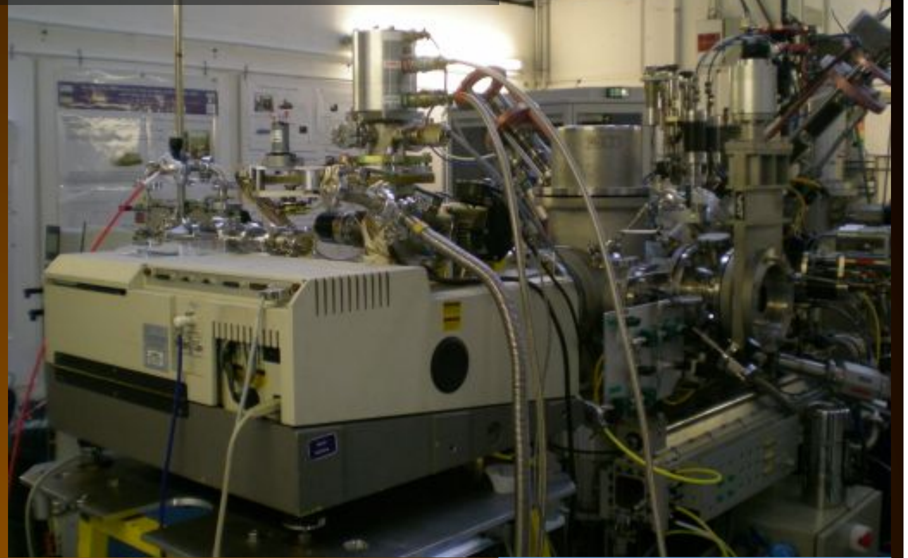
Accolla+2013

Spectroscopically difficult to pinpoint which process is at work,
More based on lab measured efficiencies

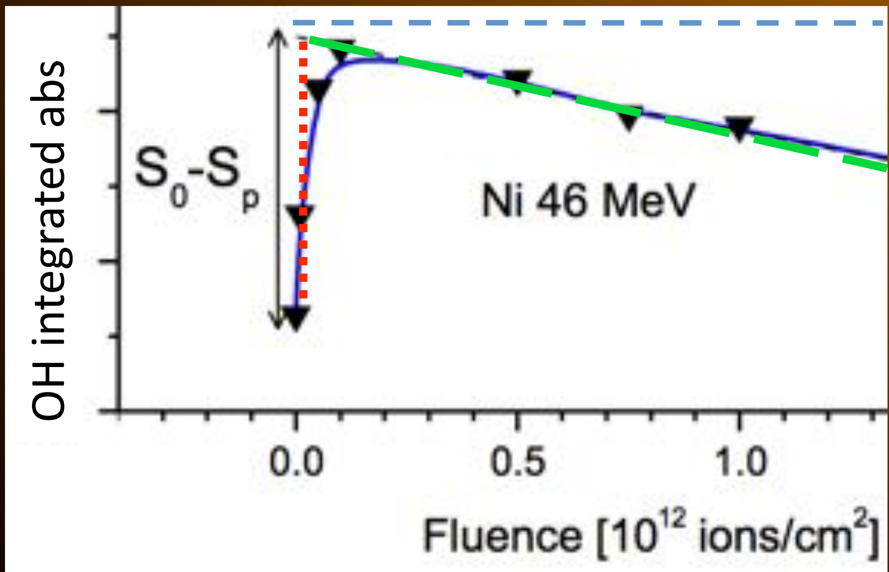
Measuring the CR sputtering yield with IR

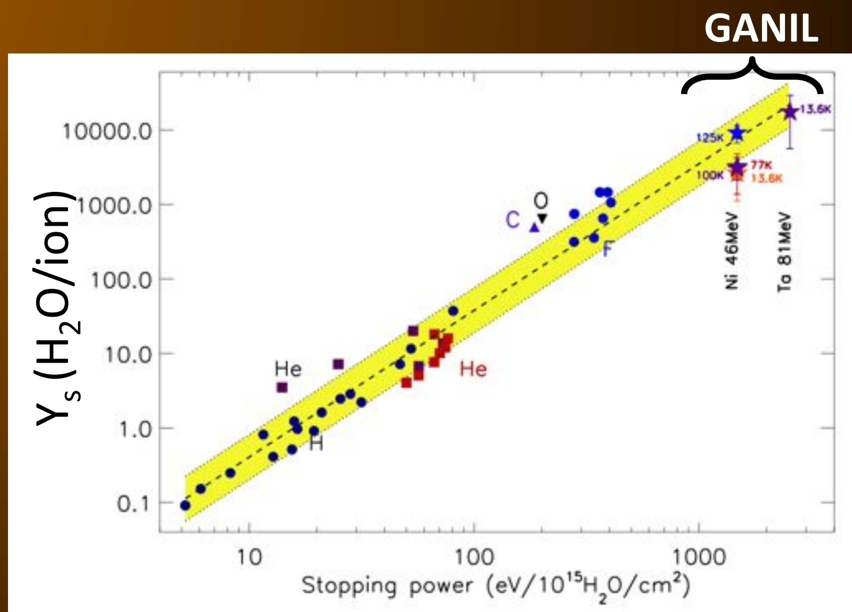


Mejia+2015, Dartois+2015, Rothard+2016



CASIMIR Setup/GANIL

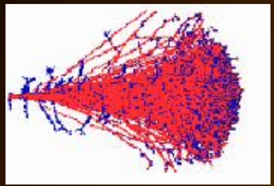




Brown+1984 & ref therein

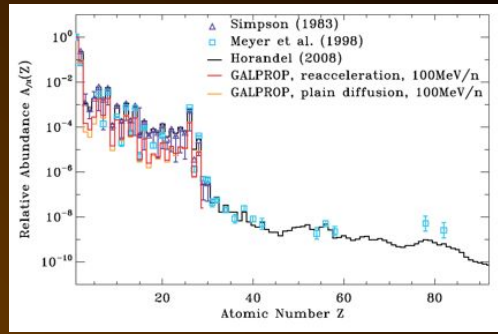
Dartois+2015

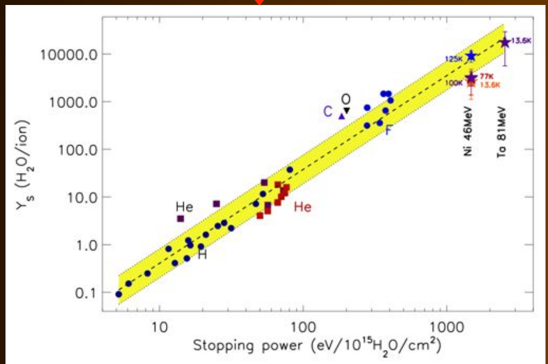
Implementation in astrophysical models



Se(Z,E)

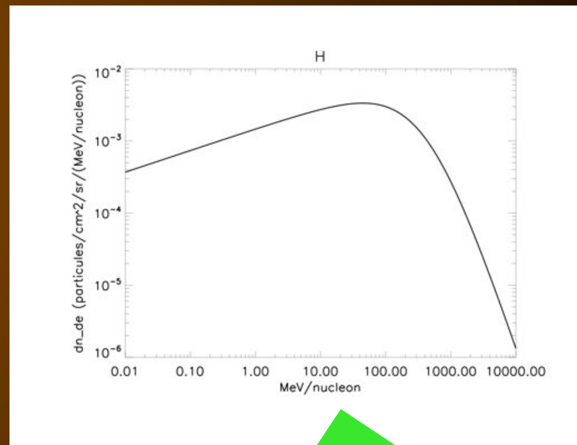
f (Z)





Y(Se)

Φ(Z,E)



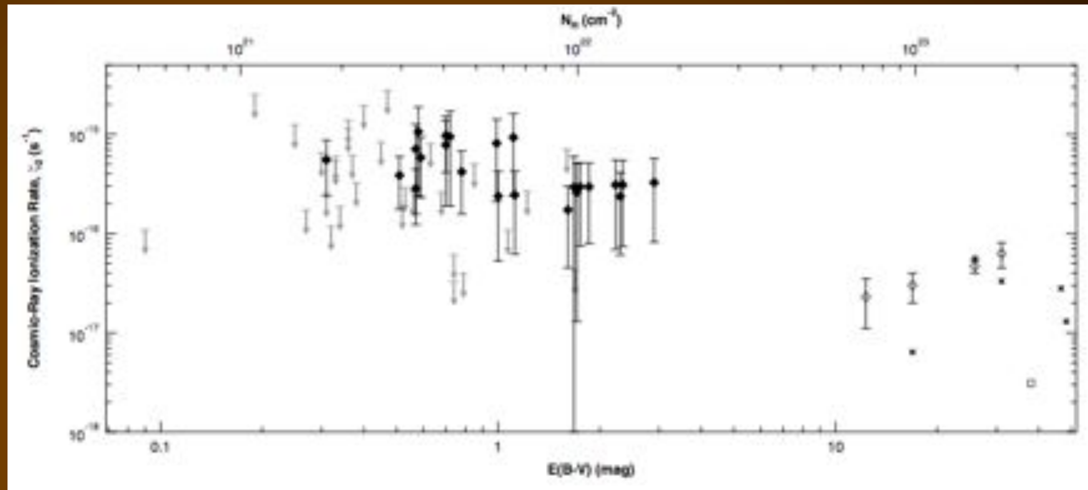
Y(Z,E) = Y(Se(Z,E))

CR desorption rate:

$$\eta(H_2O/cm^2/s) = 4\pi \sum_Z \int_E Y(Z,E)\, f(Z)\, \Phi(Z,E)\, dE$$

H_2O CR sputtering rate

$\eta_{CR\ sputtering} \approx 8\ H_2O/cm^2/s$ for $\zeta = 10^{-16} s^{-1}$



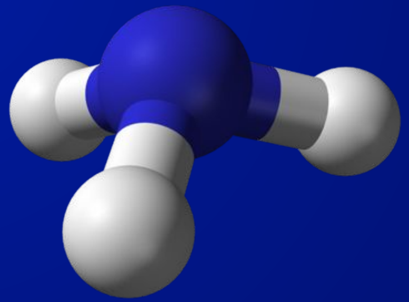
Indriolo+2012

Under implementation in the Meudon PDR code

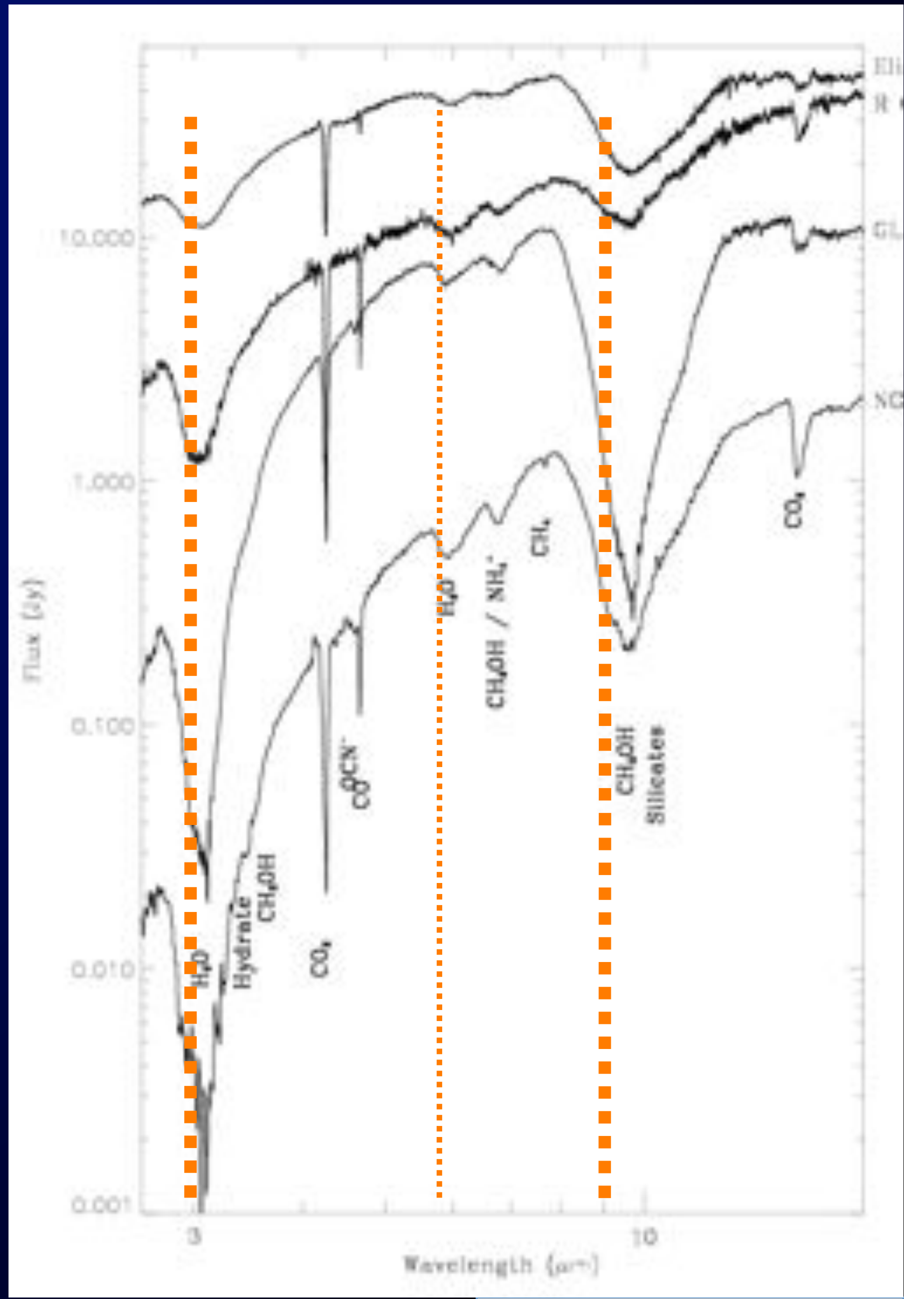
Le Petit, Bron, …, in preparation

A mechanism to add to UV photons photodesorption

Talk by R. Martin-Doménech
Visit p27(R. Dupuy) & p28(T. Putaud)

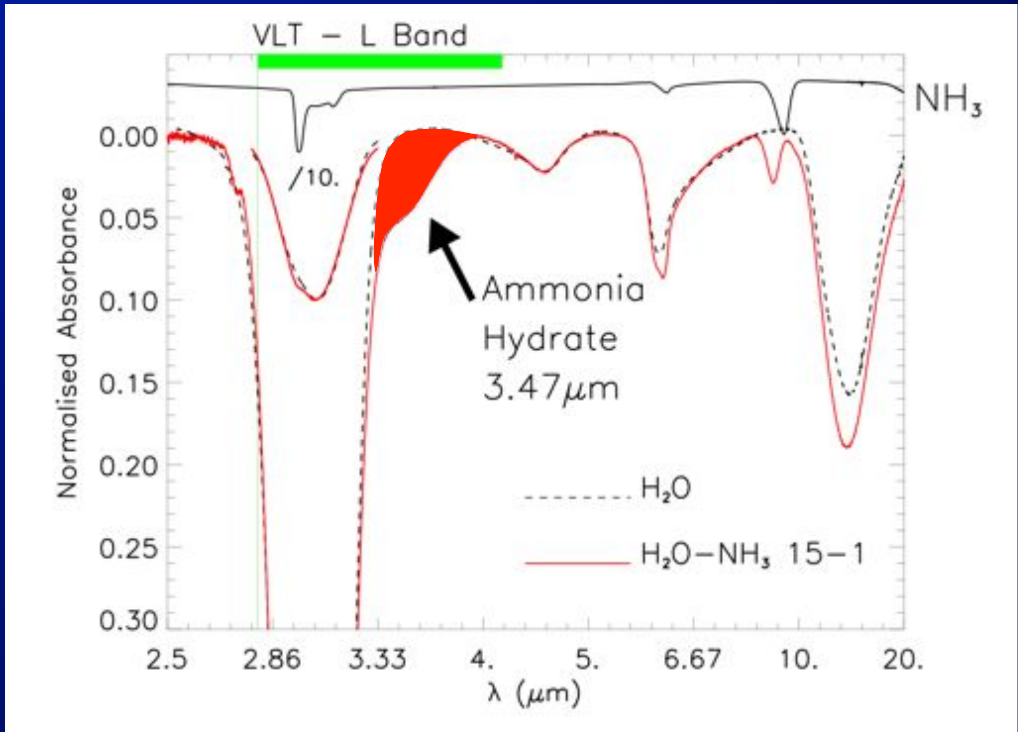


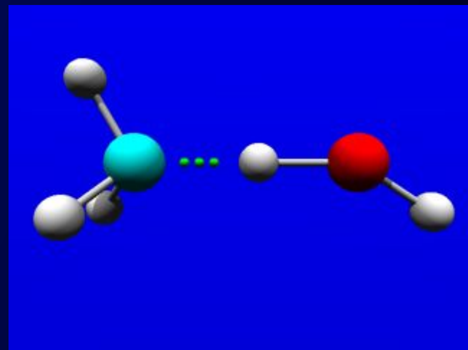
- Ammonia IR active modes, if pure, fall in strong absorption of ice and silicates



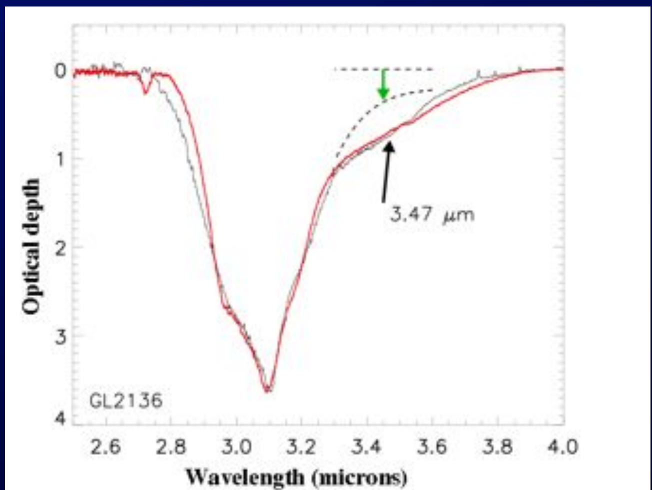
ISO database extract

Band profiles – hydrate (NH_3 abundance limit)



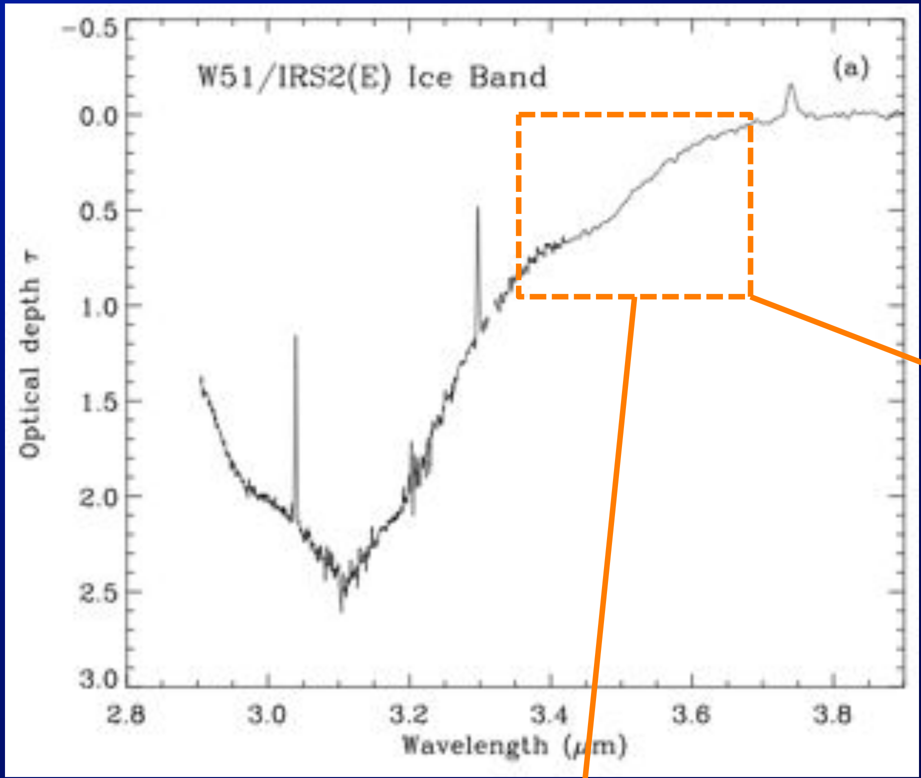


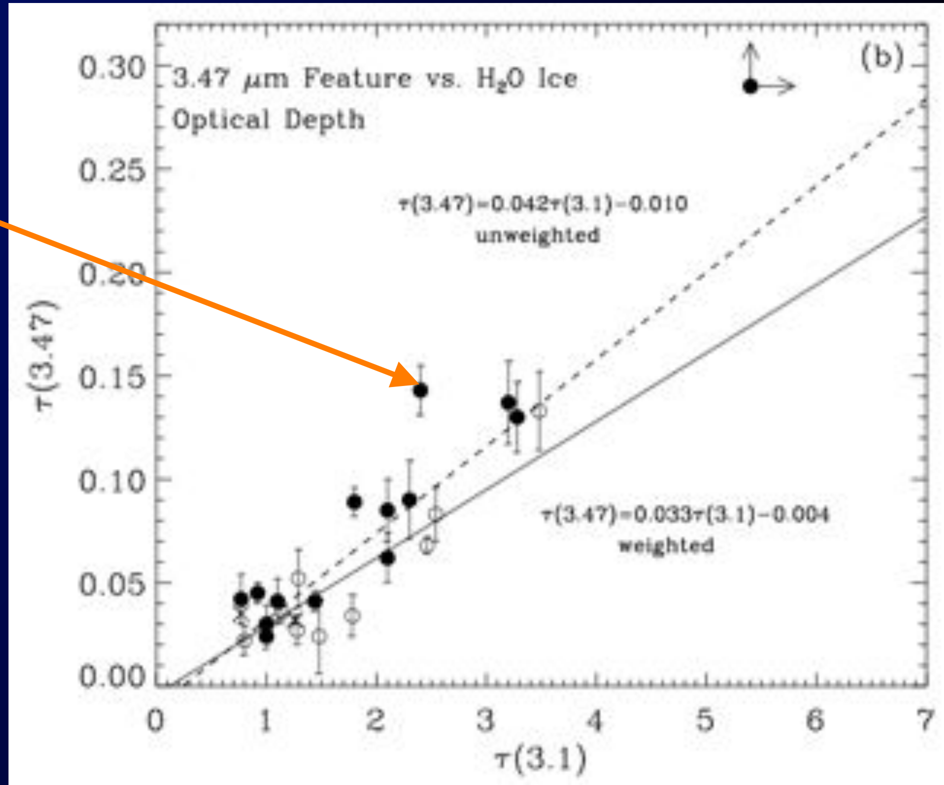
Dartois+2001, 2002



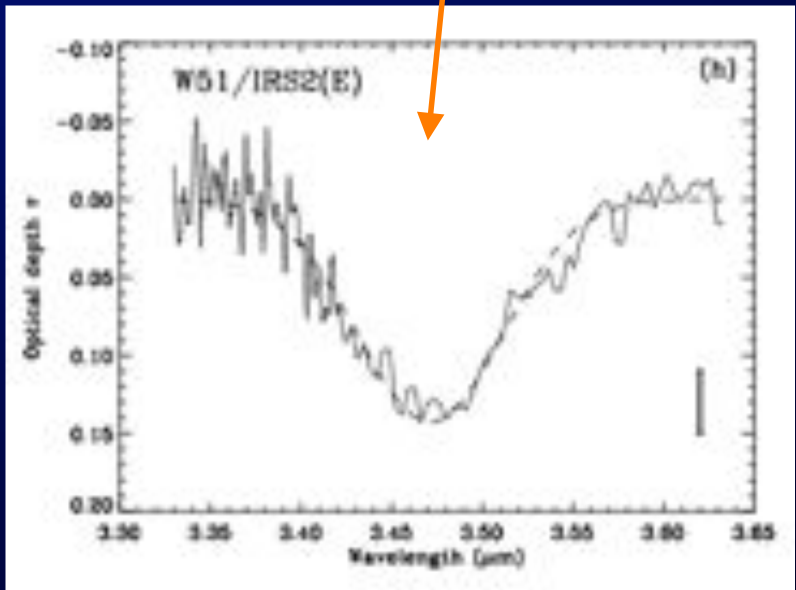
- A new feature ≠ new species
- Interactions must be recorded in the laboratory

NH_3





Brooke & Sellgren 1999

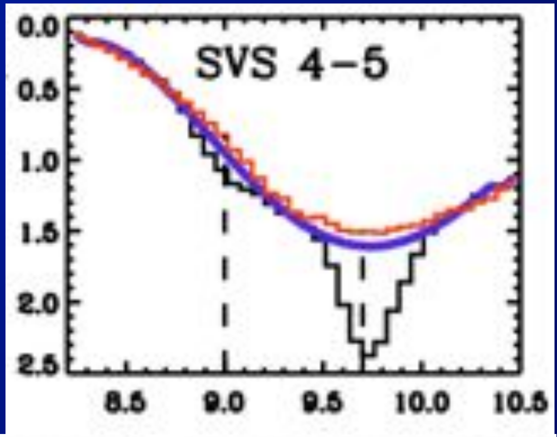


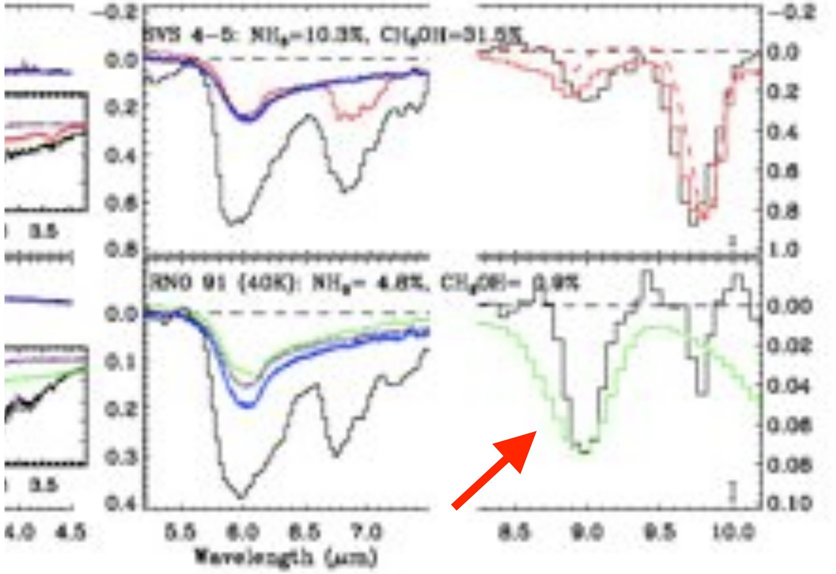
- An interaction giving access to the (ammonia) hydrates limit contribution

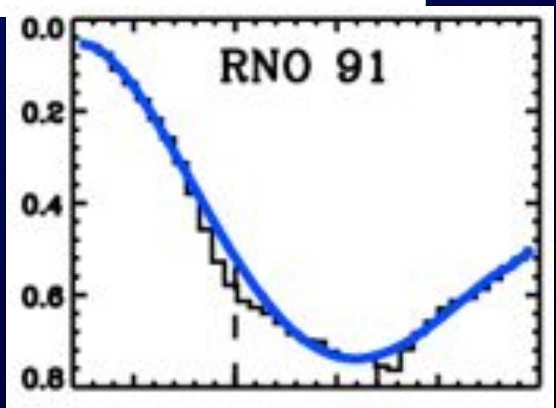
  NH_3 / H_2O ≤ 7%(3.8+-1.8%)

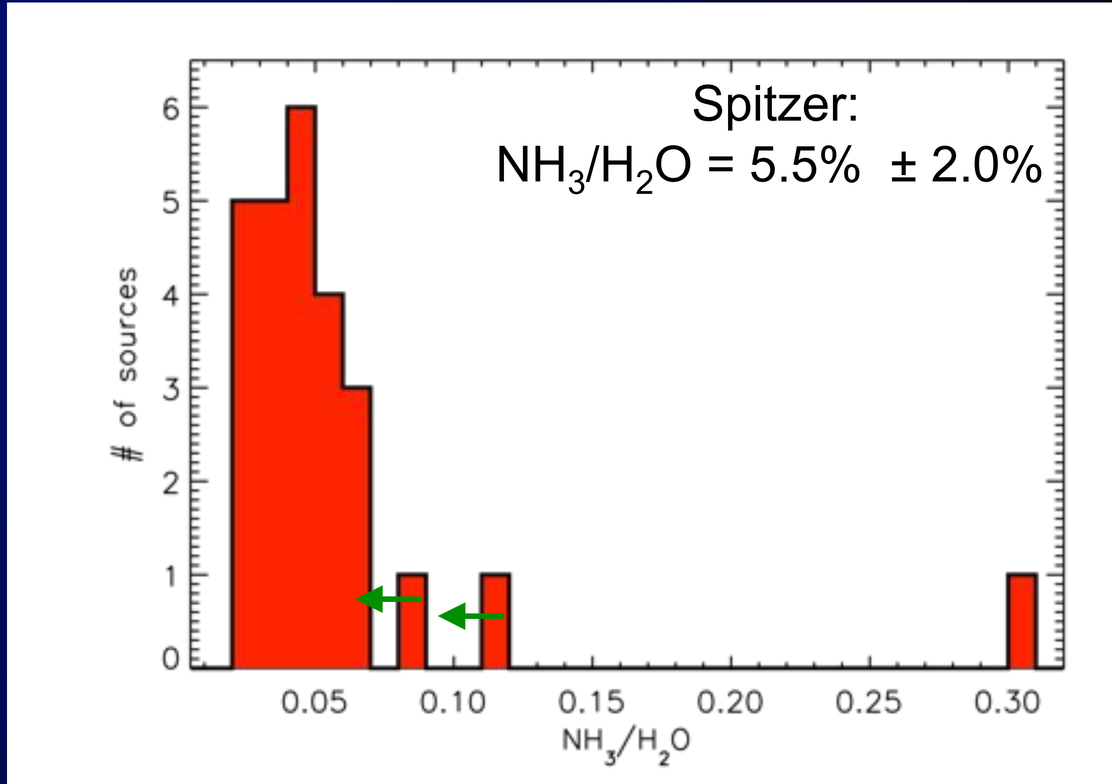
Dartois+2001

Direct observations of the umbrella mode

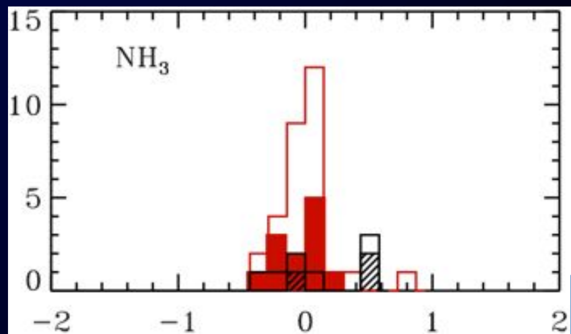






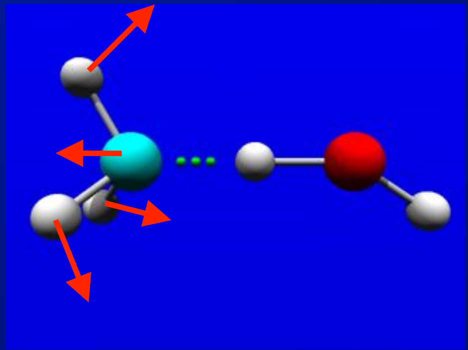


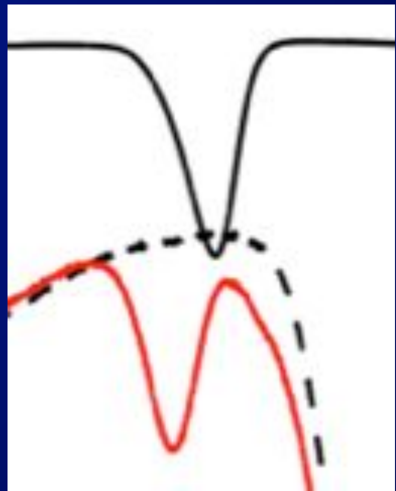
Adapted from Bottinelli+2010

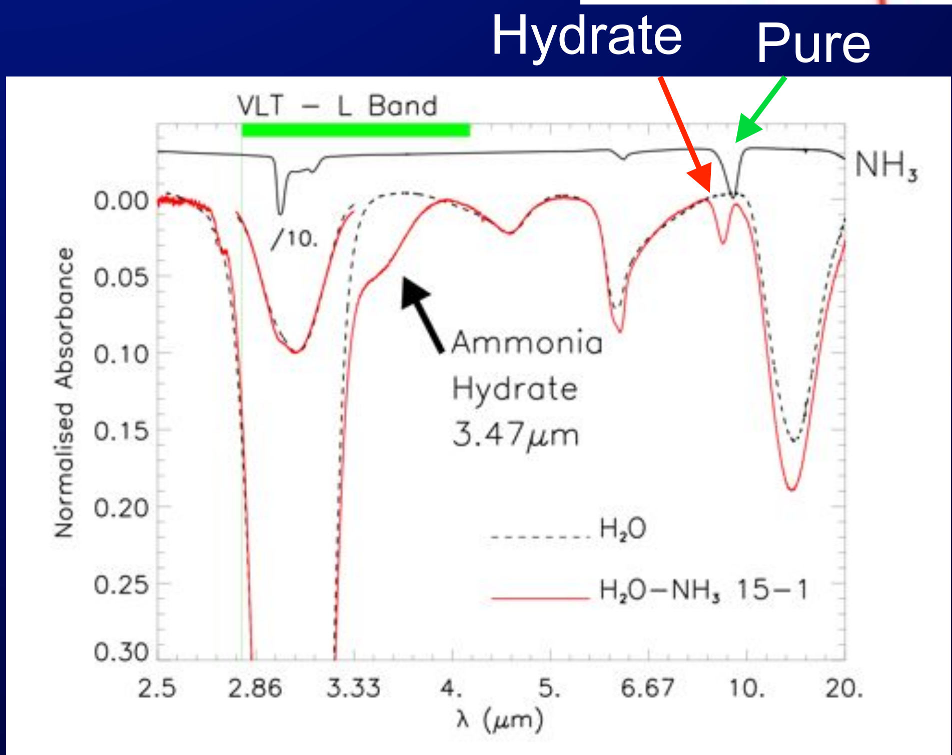


Oberg+2010

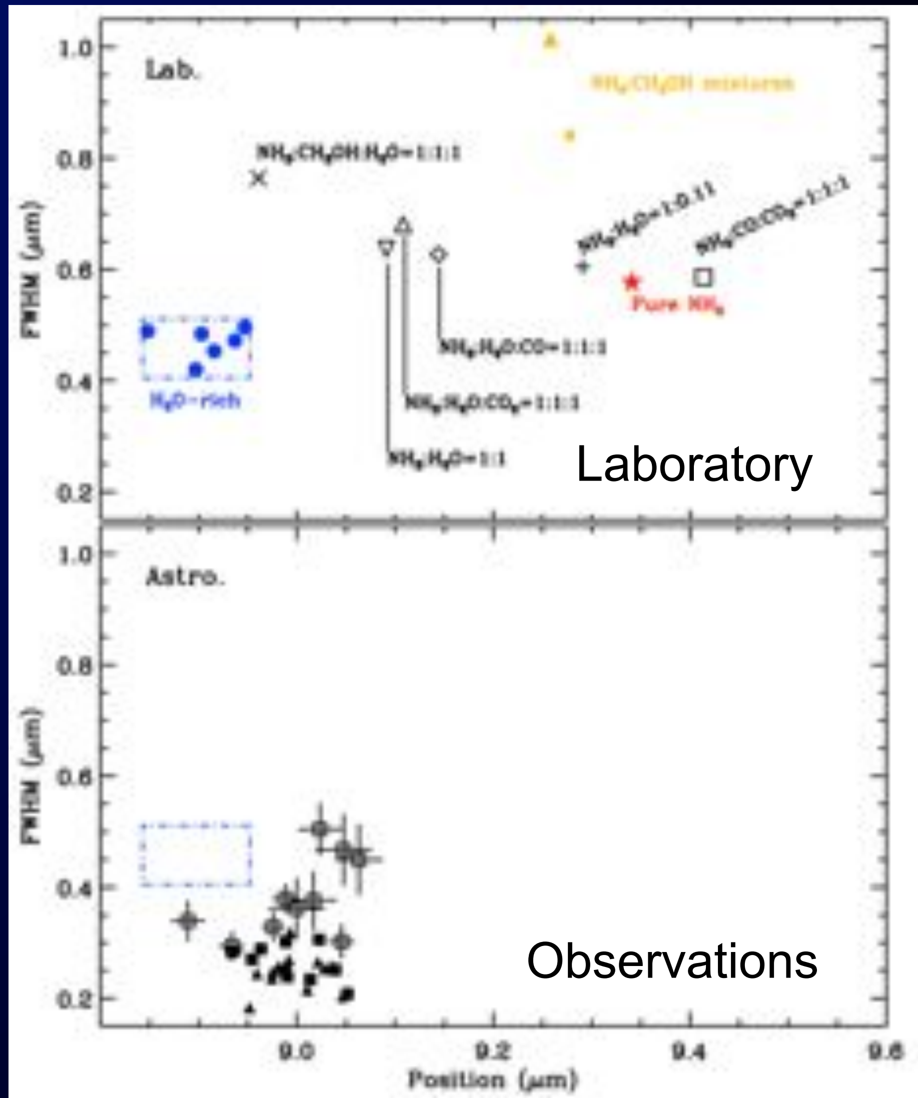
Umbrella mode in a polar environment





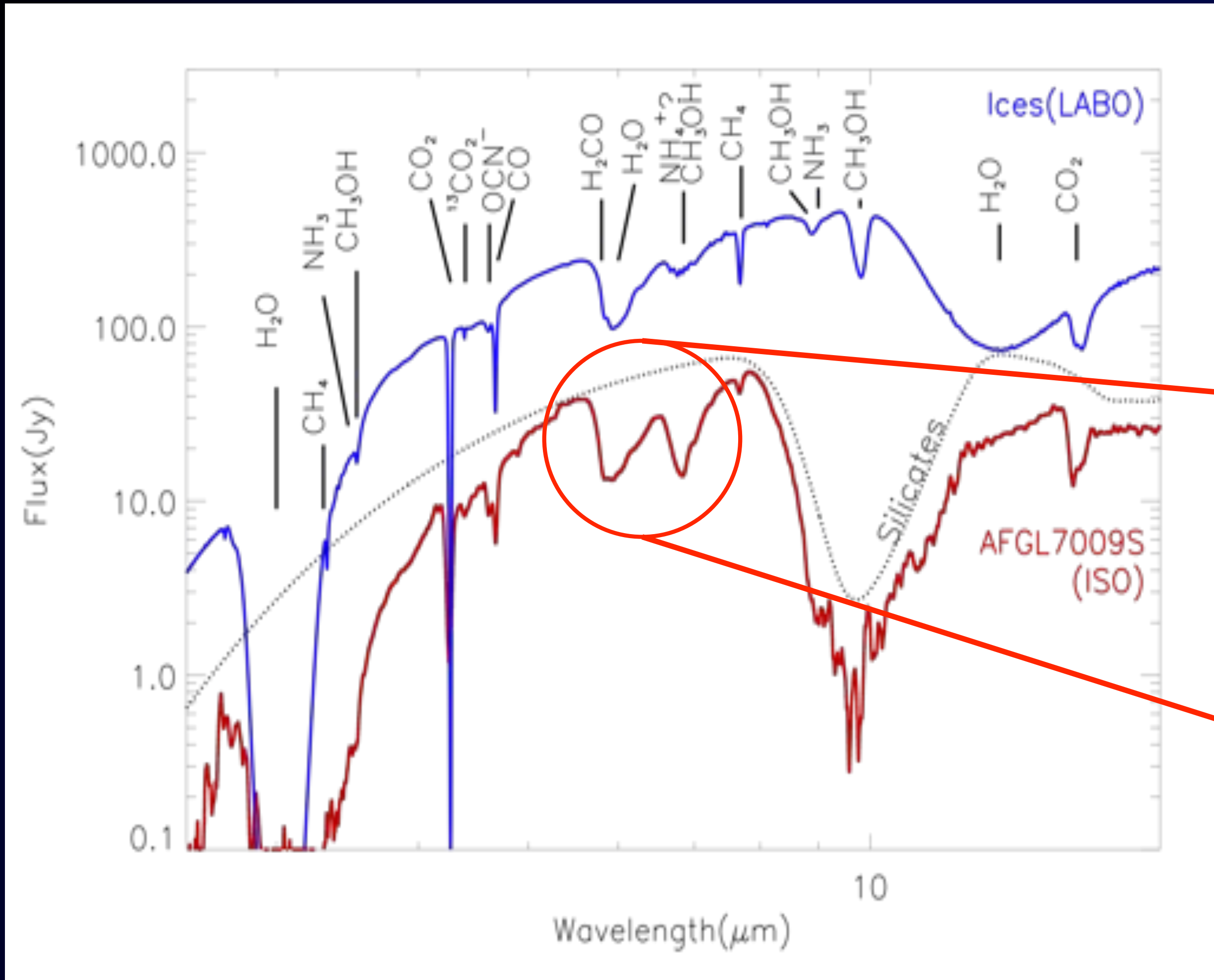


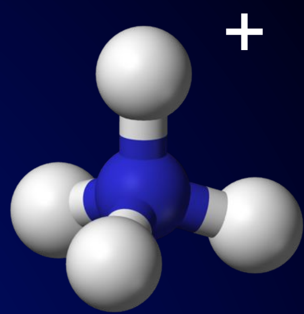
Dartois+2001, 2002

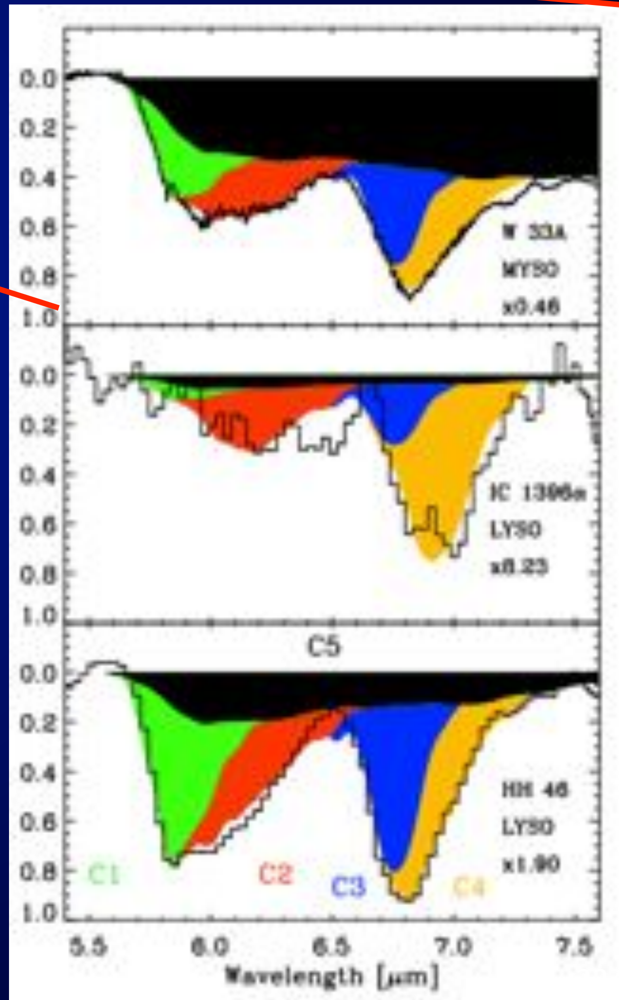


Bottinelli+2010

Related hydride ?





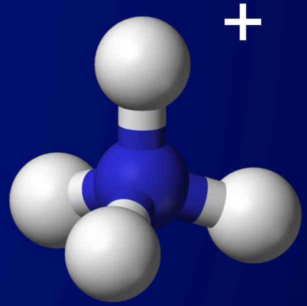


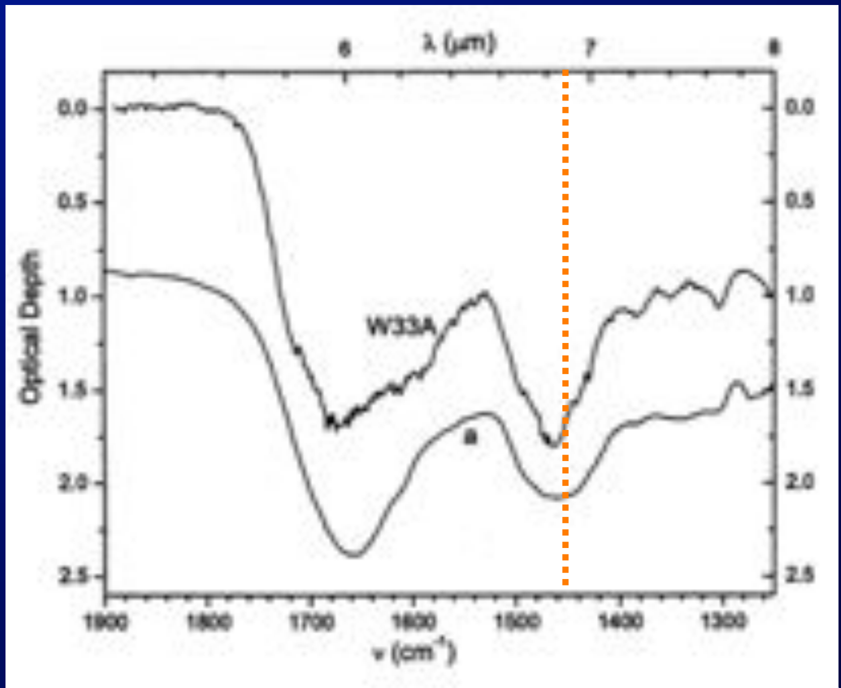
« An interstellar band at 6.8 μm may be absorption by ammonium ions in clay minerals »

Knacke+1982

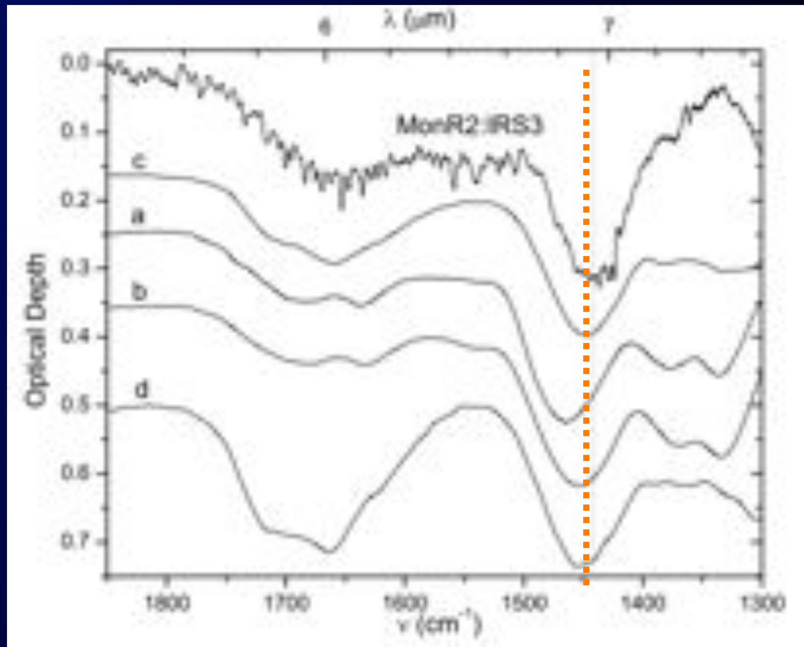
Boogert+2015

Related hydride ?





Schutte+2003

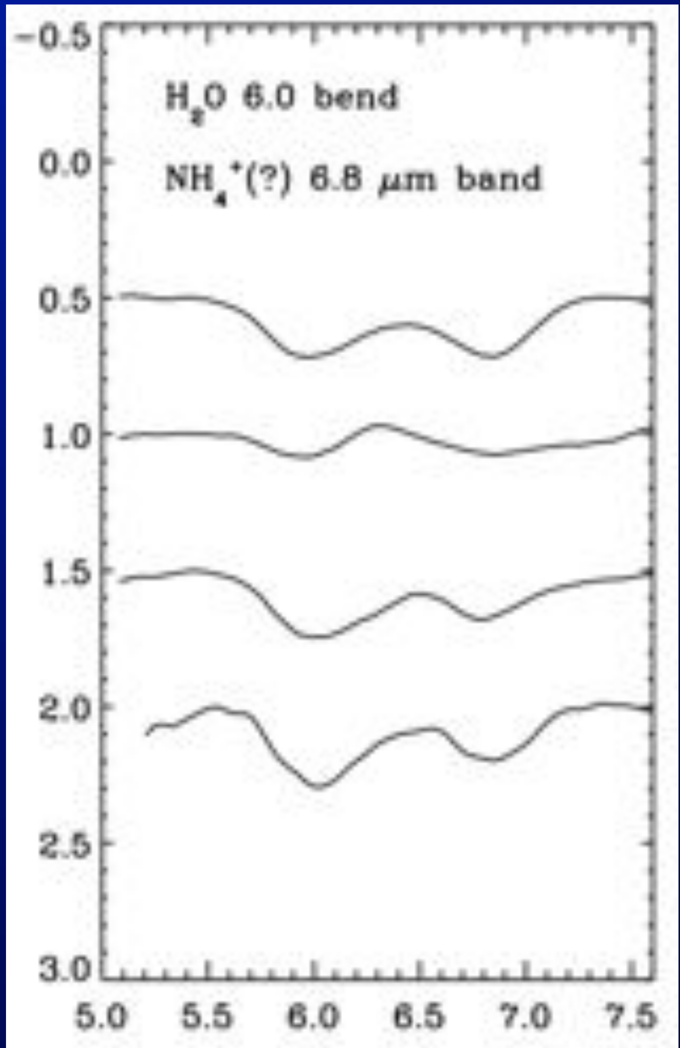


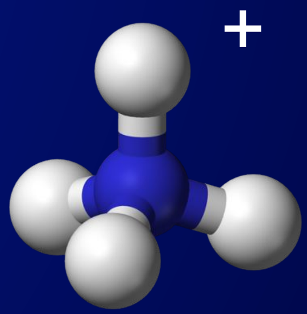
Photolysis of
$H_2O/CO_2/NH_3/O_2$
10/1.2/0.9/0.9
180K

NH_4^+ most likely contributing carrier

Many exp. work

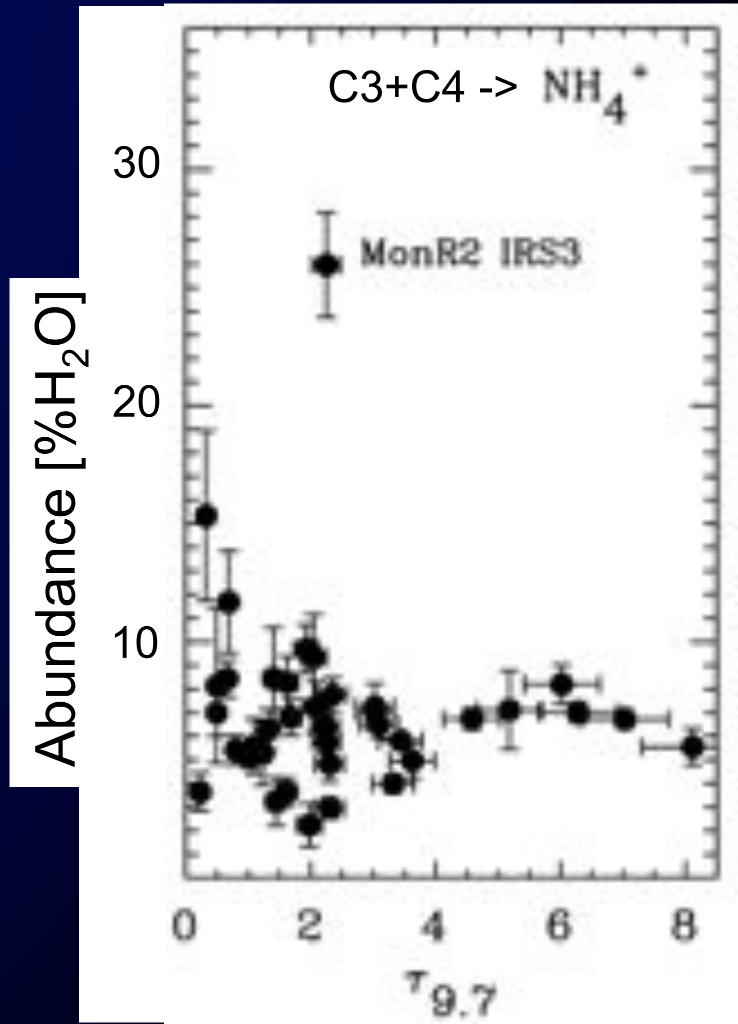
e.g. Demyk+1998, Novozamsky+2001, Raunier+2004, Guennoun+2006, Moon+2010, Galvez+2010





Ophiuchus-F core
No variation within the same cloud

Pontoppidan+2006



Boogert+2008

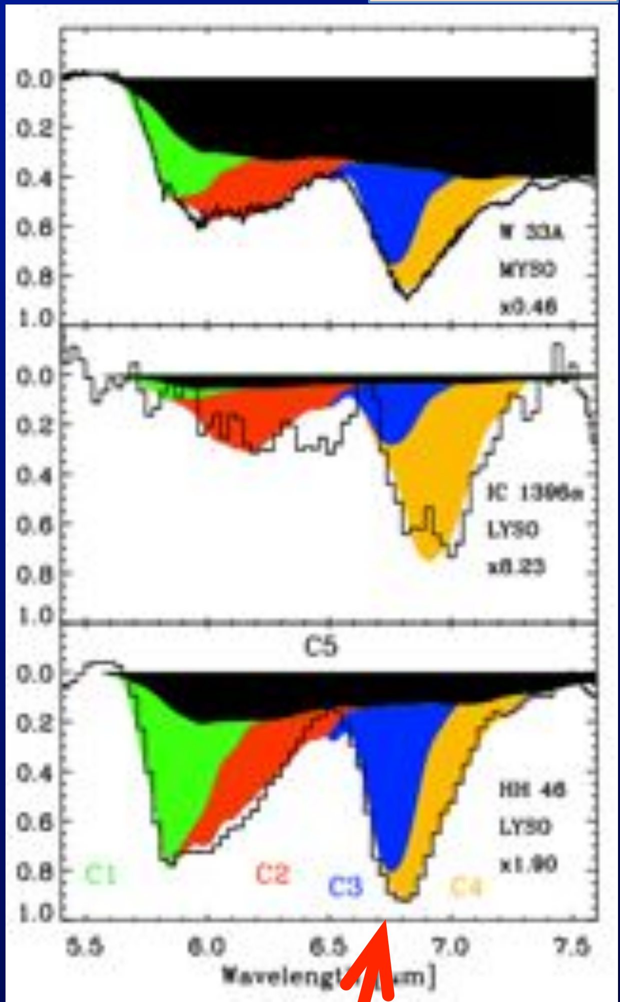
Astrophysical profile still discussed

NH_4^+ would represent about 7-11% of H_2O

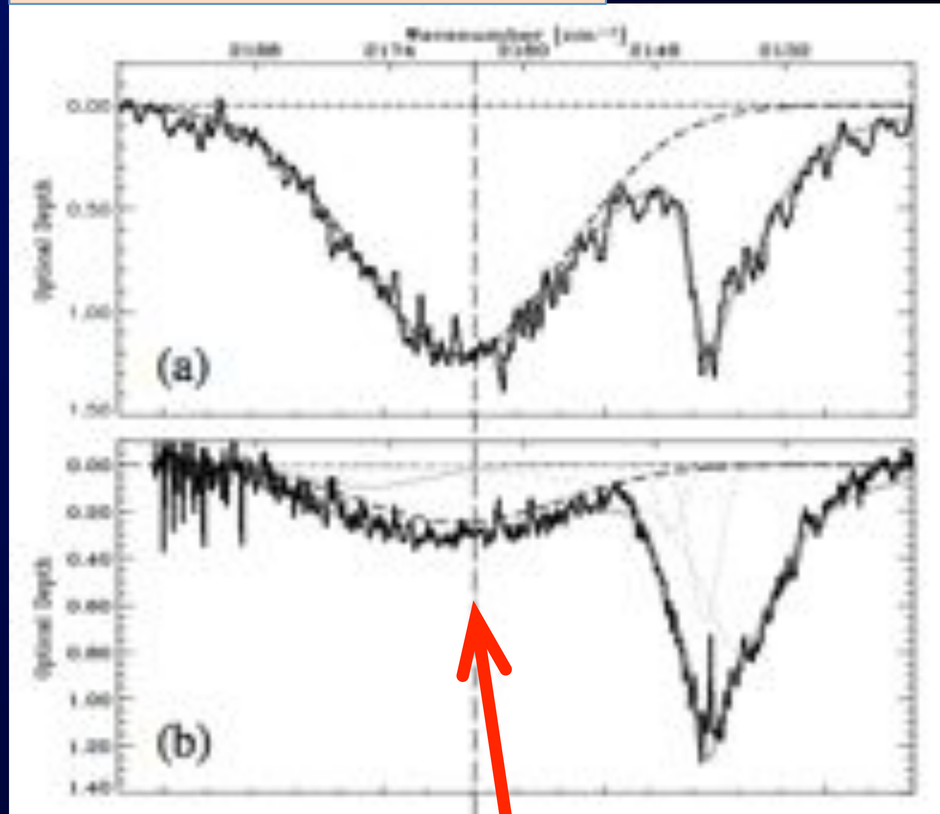
NH_2 observed in the lab ice, not in the astro. obs. (solid)

Counterion ?

Boogert+2015



Van Broekhuizen+2005 & ref therein

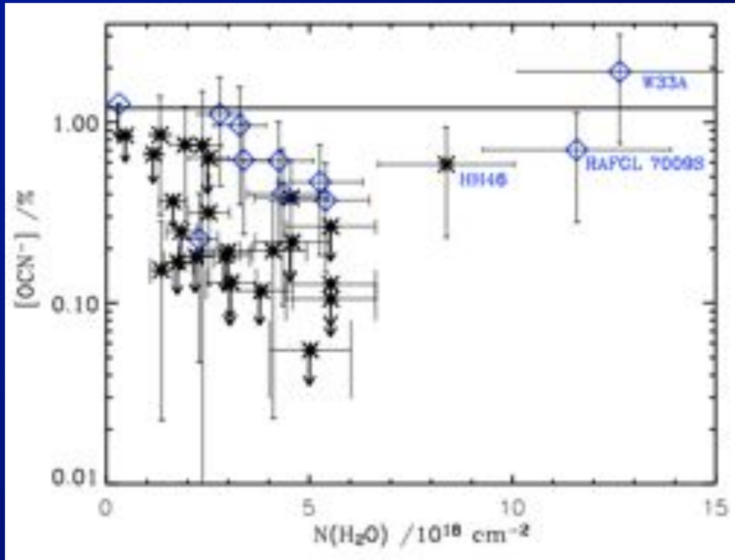


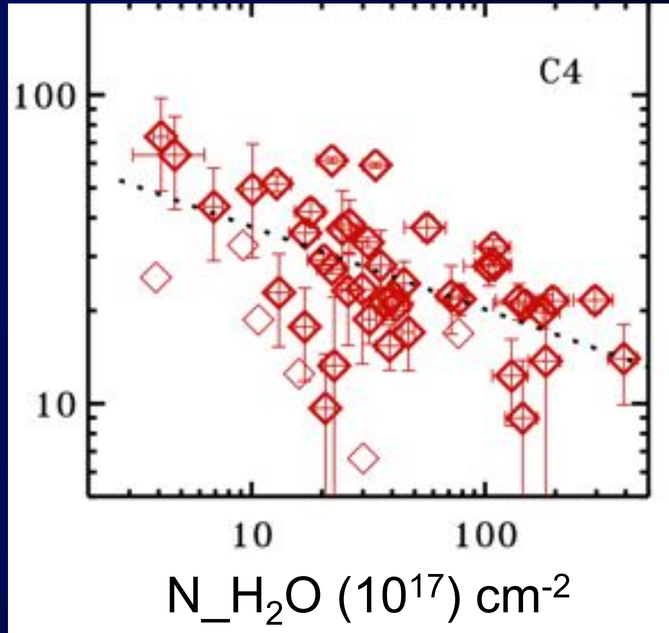
NH_4^+

OCN^-

OCN^- (2165 cm^{-1})

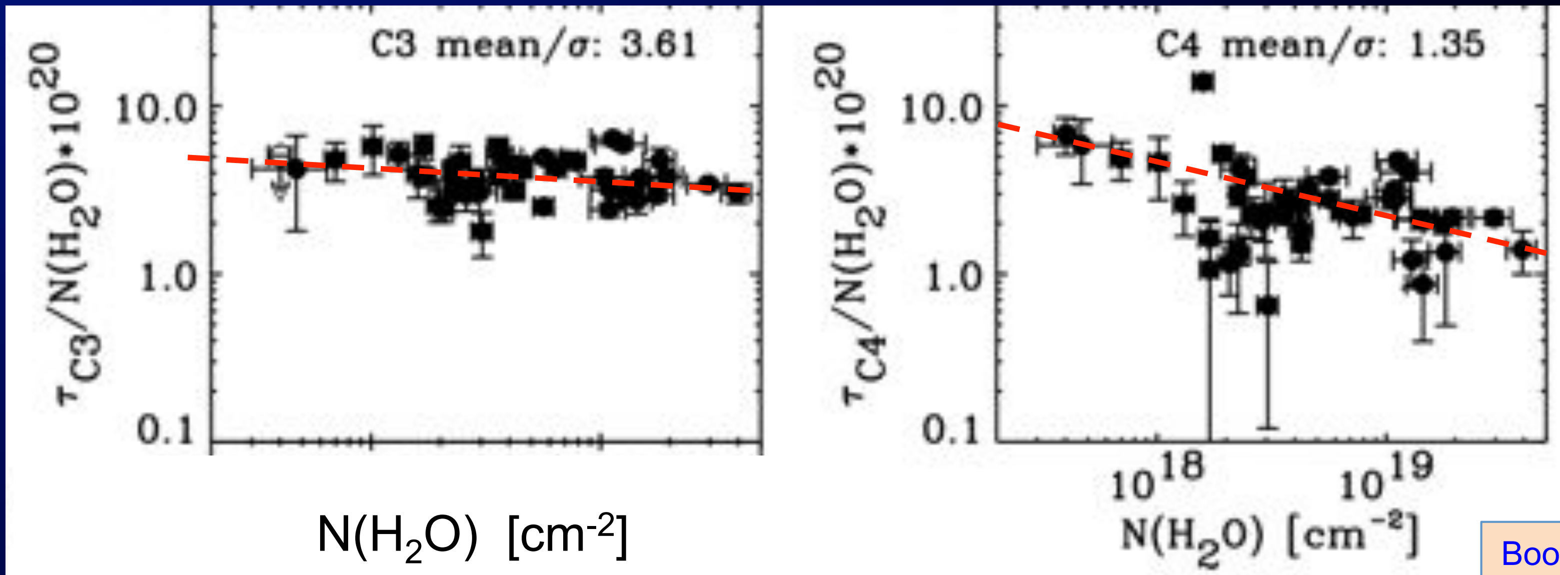
Van Broekhuizen+2005





Oberg+2011

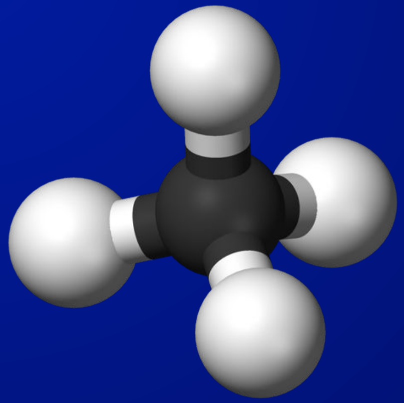
NH_4^+ (1485 & 1440 cm^{-1})

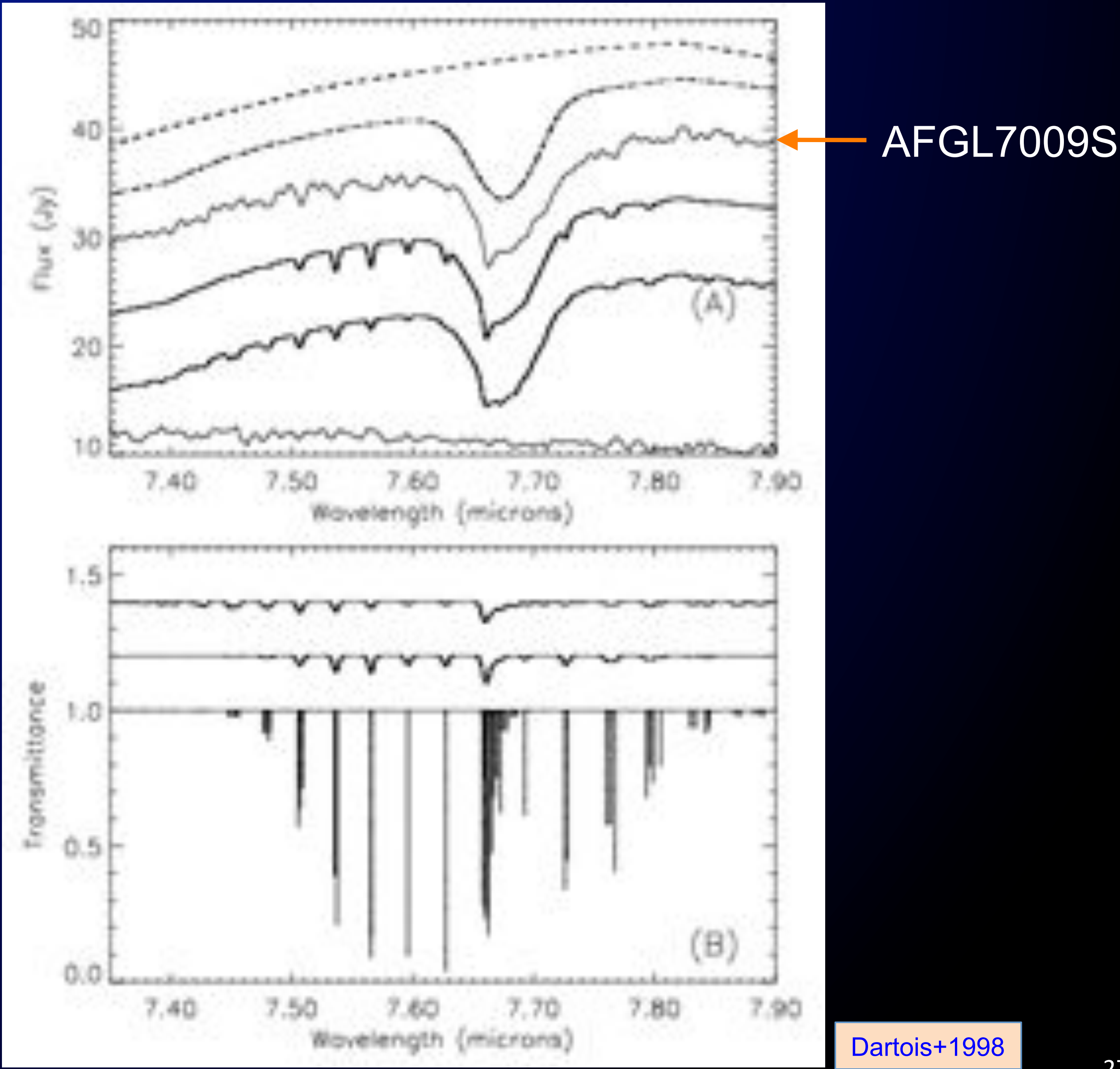


Boogert+2008

Charge equilibrium summing solid ions contributions not respected

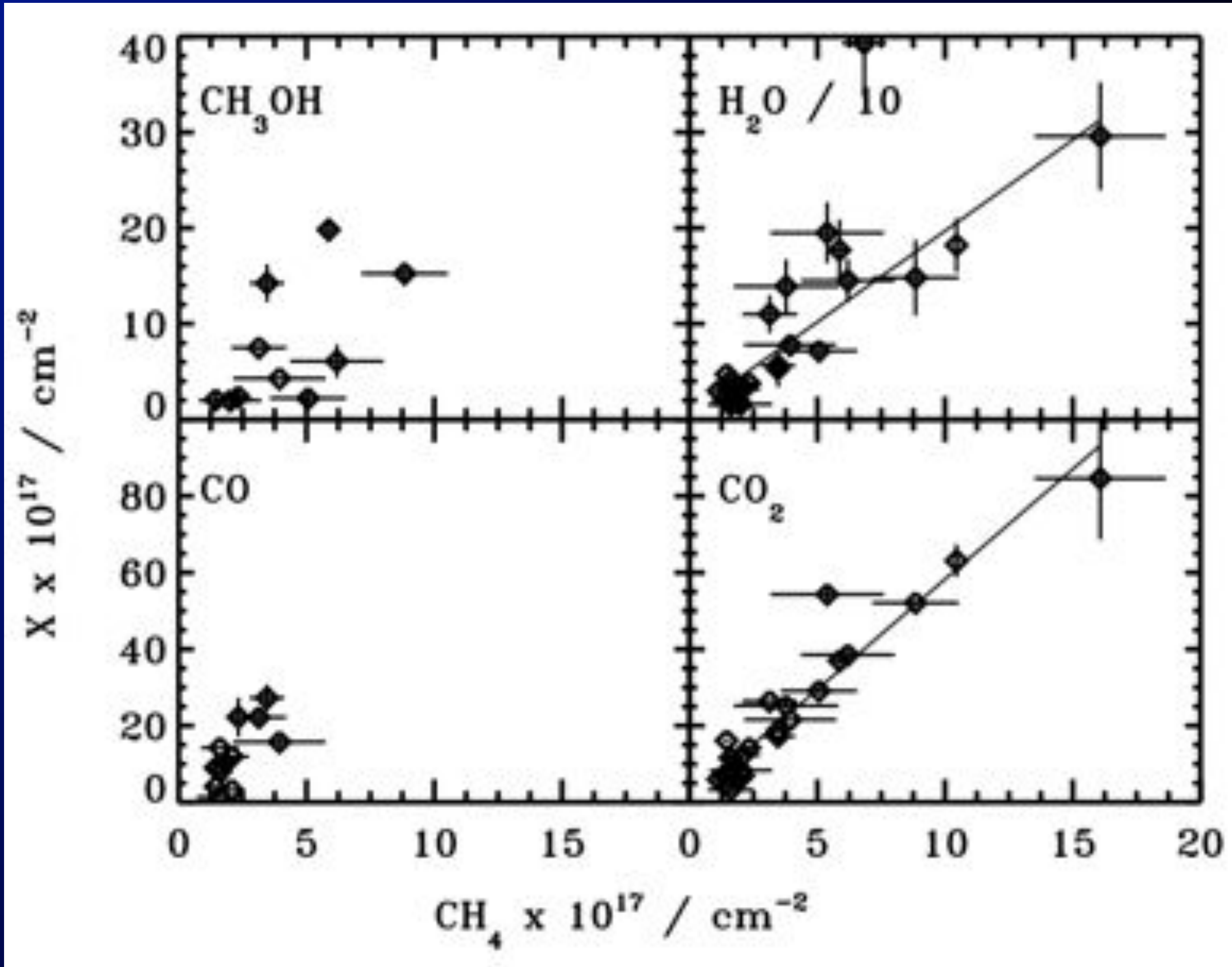
Ions with great importance to pin point underlying processes





Dartois+1998

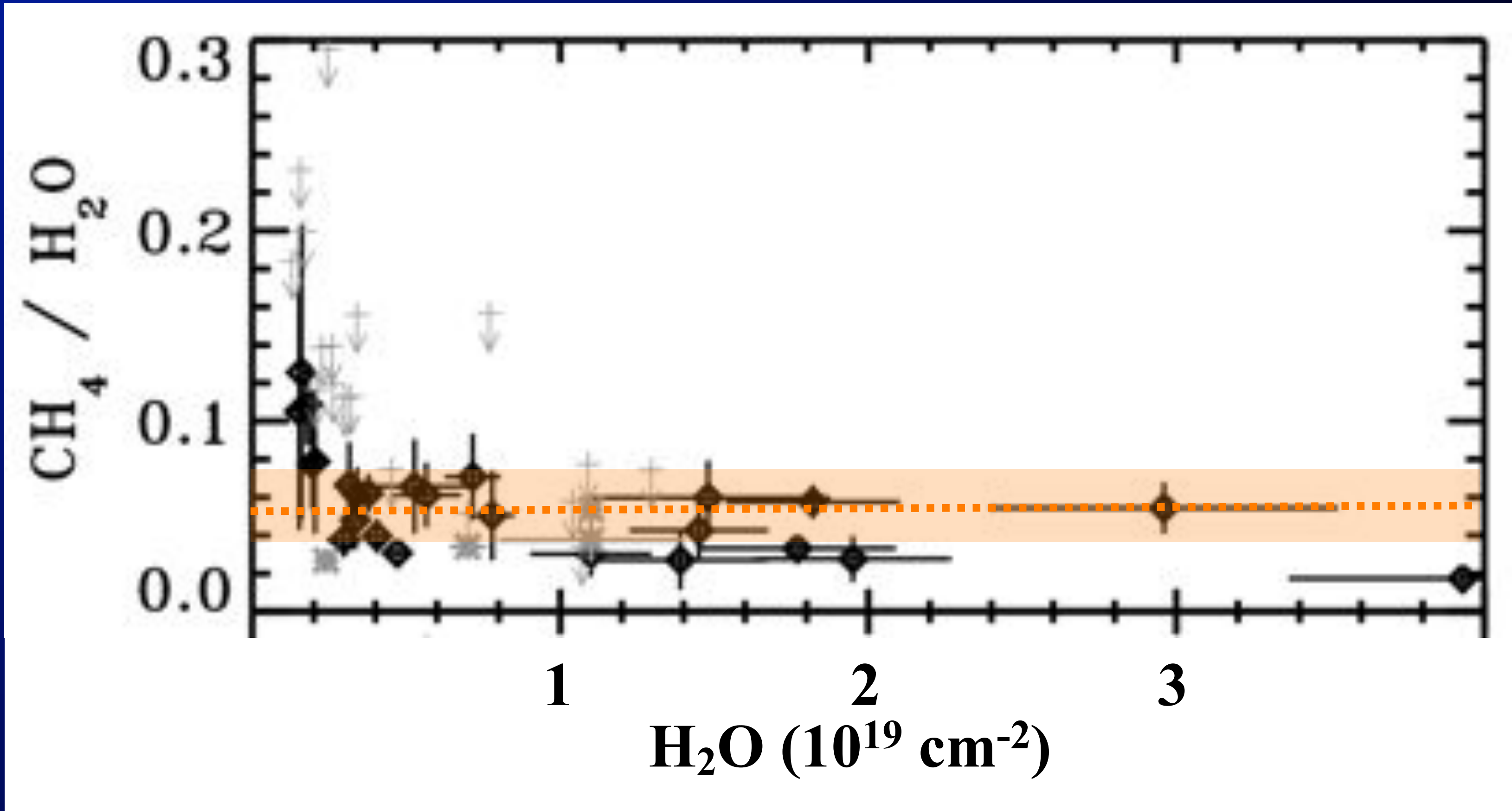
CH_4



Oberg et al. 2008

Correlate strongly with H_2O and CO_2, no other ice

CH_4



4.7%

Oberg et al. 2008

Similar abundances variations in low- and high-mass YSOs

Abundance

Species	$X_{H_2O}^{a}$ [%]				X_{H}^{b} [10^{-6}]		
	MYSOs	LYSOs	BG Stars[c]	Comets	MYSOs	LYSOs	BG Stars[c]
Securely identified species[d]:							
H_2O^e	100	100	100	100	31^{+16}_{-12}	38^{+31}_{-22} (42)	40^{+18}_{-21} (39)
					12-57	14-99	(< 9)-62
CO^f	7^{+15}_{-4} (7)	21^{+35}_{-13} (18)	25^{+43}_{-20}		$2.6^{+8.8}_{-0.2}$ (1.9)	$9.6^{+17}_{-4.8}$ (8.1)	12^{+20}_{-9}
	3-26	(<3)-85	9-67	0.4-30	(< 0.4)-12.8	(< 1.2)-26	3-21
CO_2^g	19^{+25}_{-12}	28^{+37}_{-23}	26^{+39}_{-18}	15^{+24}_{-10}	$3.7^{+13}_{-2.3}$	$11.8^{+25}_{-5.5}$	$13.2^{+18}_{-4.2}$
	11-27	12-64	14-43	4-30	1.8-15.6	2.4-38	5.2-26
CH_3OH	9^{+23}_{-5} (5)	6^{+12}_{-2} (5)	8^{+10}_{-6} (6)		$3.7^{+11}_{-1.9}$ (1.7)	$3.3^{+7.2}_{-2.1}$ (2.3)	$5.2^{+6.4}_{-3.2}$ (2.4)
	(< 3)-31	(< 1)-25	(<1)-12	0.2-7	(< 0.4)-16.6	(< 0.2)-15	(< 0.6)-6.6
NH_3		6^{+8}_{-4} (4)				$3.6^{+5.4}_{-2.3}$ (2.6)	
	$\sim 7^f$	3-10	< 7	0.2-1.4	$\sim 4^f$	(< 0.4)-6.4	< 4
CH_4		4.5^{+6}_{-3} (3)				$2.3^{+7}_{-1.5}$ (1.4)	
	1-3	1-11	< 3	0.4-1.6	0.4-1.8	(< 0.2)-5.6	<1.2

Boogert et al. 2015

$A_V/N_H \sim 10^{-21} cm^2$ then for A_v eq 5

$N_{H2O} \sim 10^{17} cm^{-2}$

~200 times NH_3 in

Roueff et al. 2005

Upper limits

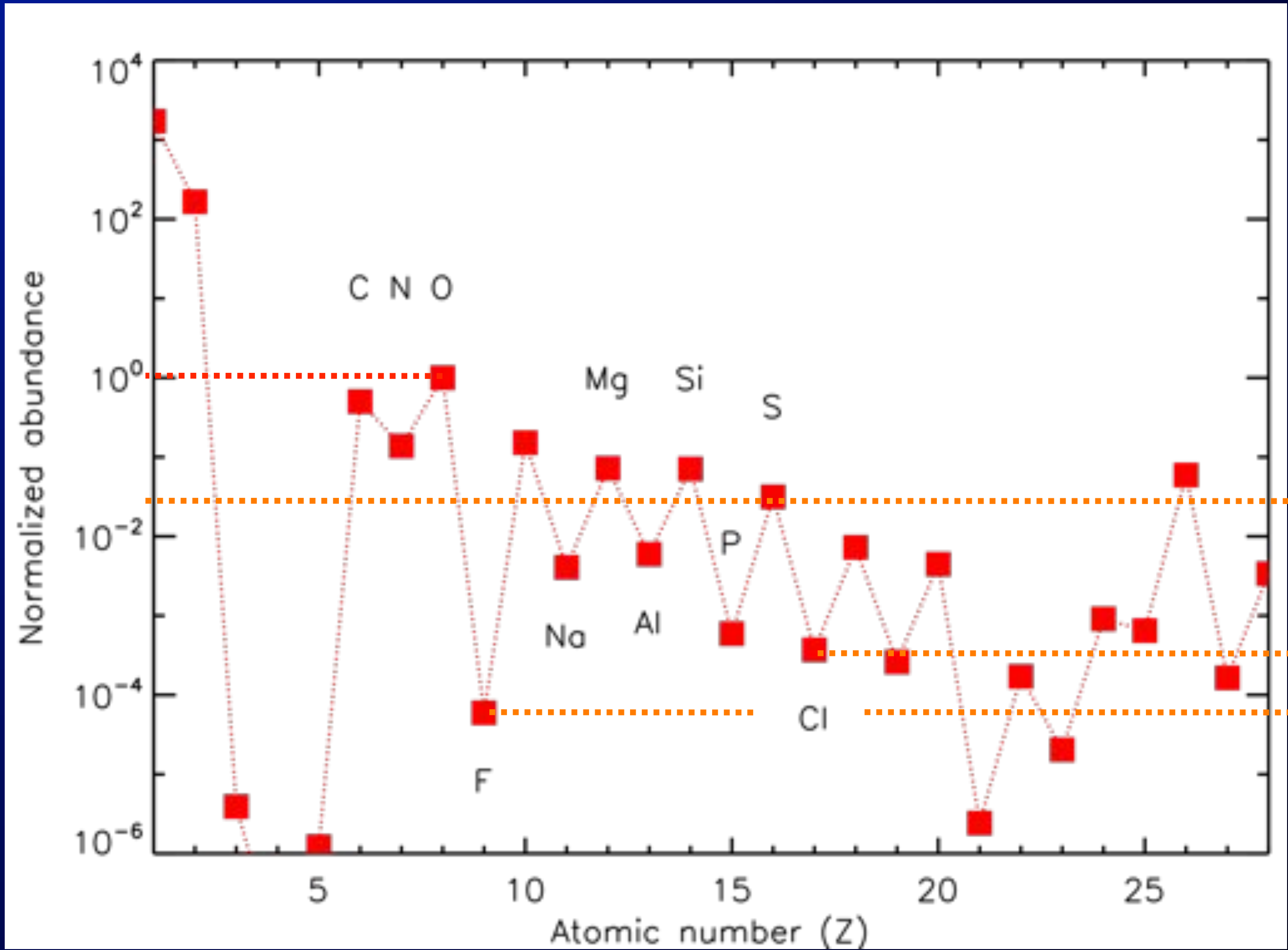
Species	X_{H_2O} %	X_H 10^{-6}	Environment[a] (reference)[b]
N_2	$< 0.2 - 60$	$< 0.1 - 28$	Taurus cloud (1, 2, 3)
O_2	< 39	< 60	LYSO R CrA IRS2 (4)
	< 15	< 30	MYSO NGC 7538 IRS9 (4)
H_2	< 68	< 14	LYSO WL 5 (5)
H_2S	$< 0.3 - 1$	$< 0.04 - 0.12$	MYSOs (6)
	$< 1 - 3$	$< 0.6 - 1.6$	Taurus cloud (6)
H_2O_2	$< 2 - 17$	$< 0.6 - 8$	YSOs, Taurus cloud (7)
C_2H_2	$< 1 - 10$	$< 0.4 - 4$	MYSOs (8)
C_2H_6	< 0.3	< 0.14	MYSO NGC 7539 IRS9 (8)
C_5H_{12}	< 15	< 10	MYSO W 33A (12)
C_3O_2	< 5	< 2	YSOs (9)
N_2H_4, $N_2H_5^+$	< 10	< 4	MYSOs (8)
HNCO	$< 0.3 - 0.7$	$< 0.10 - 0.24$	MYSOs (11)
$HCONH_2$	< 1.5	< 1	MYSO W 33A (12)
NH_2CH_2OH	$< 3 - 6$	$< 2 - 4$	MYSO W 33A (13)
NH_2CH_2COOH[d]	< 0.3	< 0.1	MYSO W 33A (10)

Boogert et al. 2015

Corollary: every detected ice is a major species

Cosmic abundance and ices detectivity

Upper limits (H_2S, HF, HCl)



S/O 3.0%

Cl/O $<<10^{-3}$

F/O $<<10^{-4}$

Lodders 2003

Thank you
for your attention