INTERSTELLAR ICES

E. Dartois, ISMO, Orsay, France
emmanuel.dartois@u-psud.fr

M. Chabot
T. Id Barkach

A.N. Agnihotri
P. Boduch
A. Domaracka
H. Rothard

B. Augé
A. Bacmann

G. M. Muñoz Caro

Workshop PCMI/GDR EMIE, 3-4th October 2019, CNES - Paris

Glaciar Perito Moreno, El Calafate, Argentina

Outline

Astrophysical « icy » environments

Observations of F.S., MYSOs and LYSOs envelopes ices

Detecting ices in disks

Inventory of YSOs envelopes ices

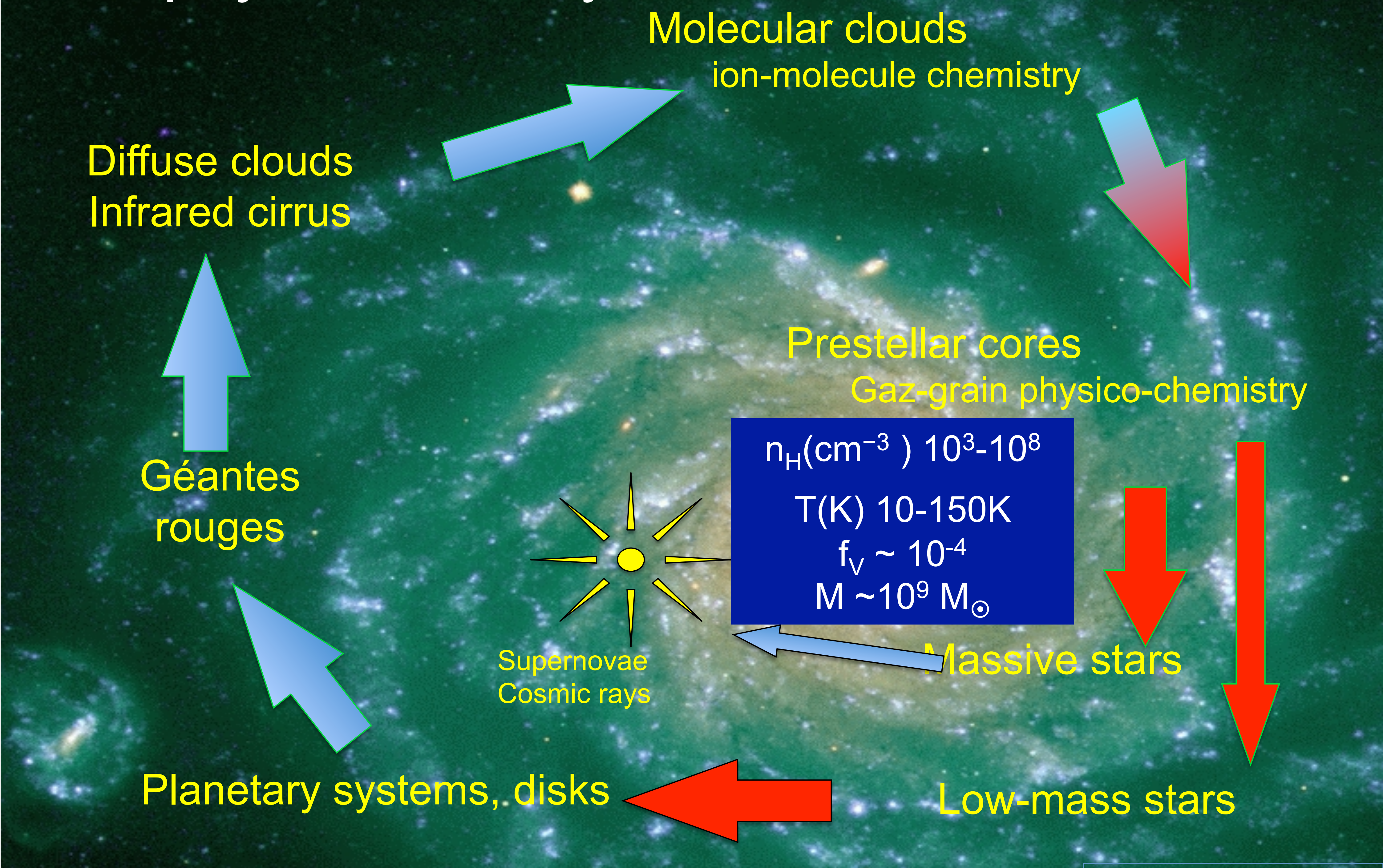
Infos in profiles: structure, composition, heating effects

Energetic processes

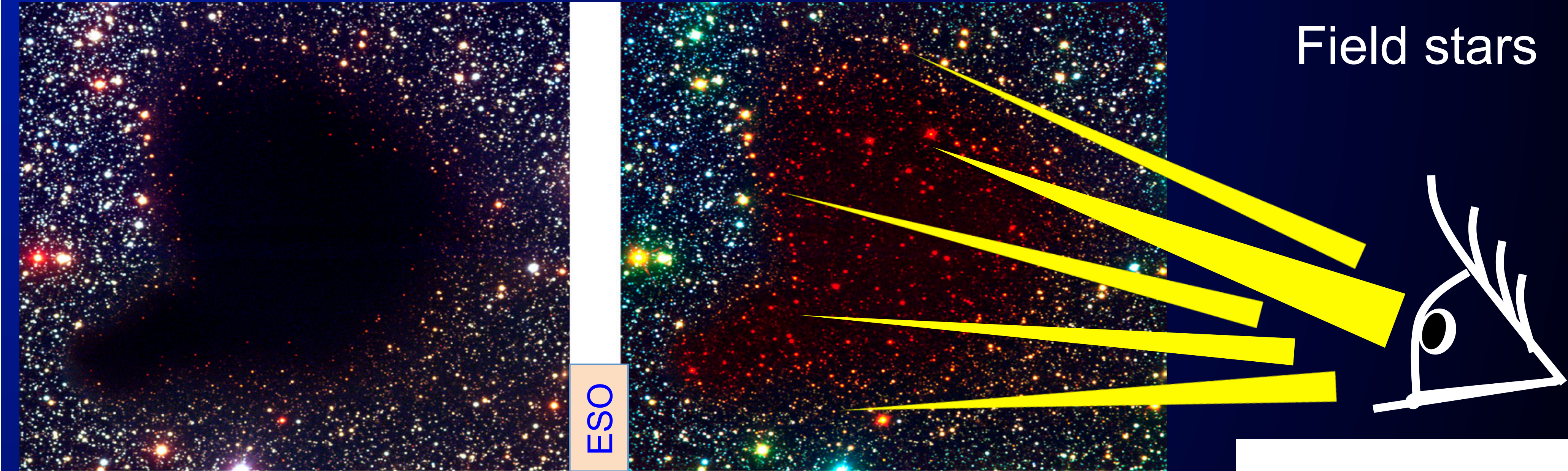
VUV desorption & CR electronic sputtering

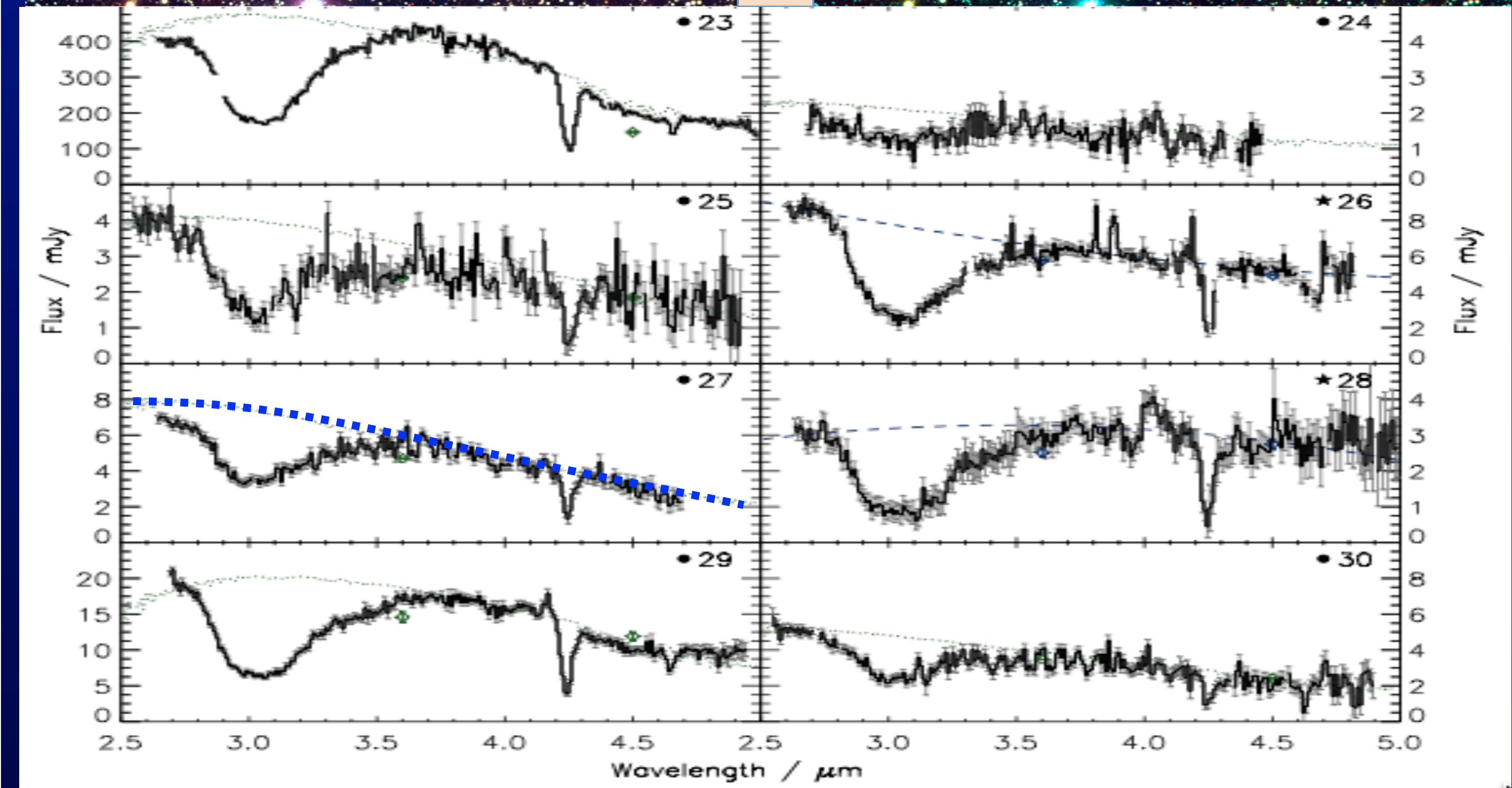
Summary

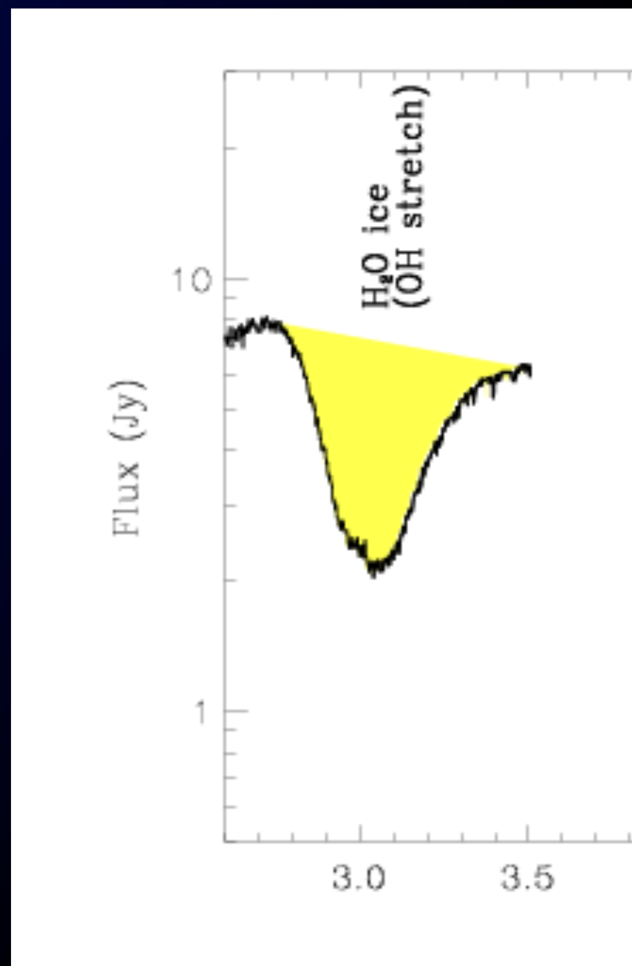
Astrophysical « lifecycle »



Field stars

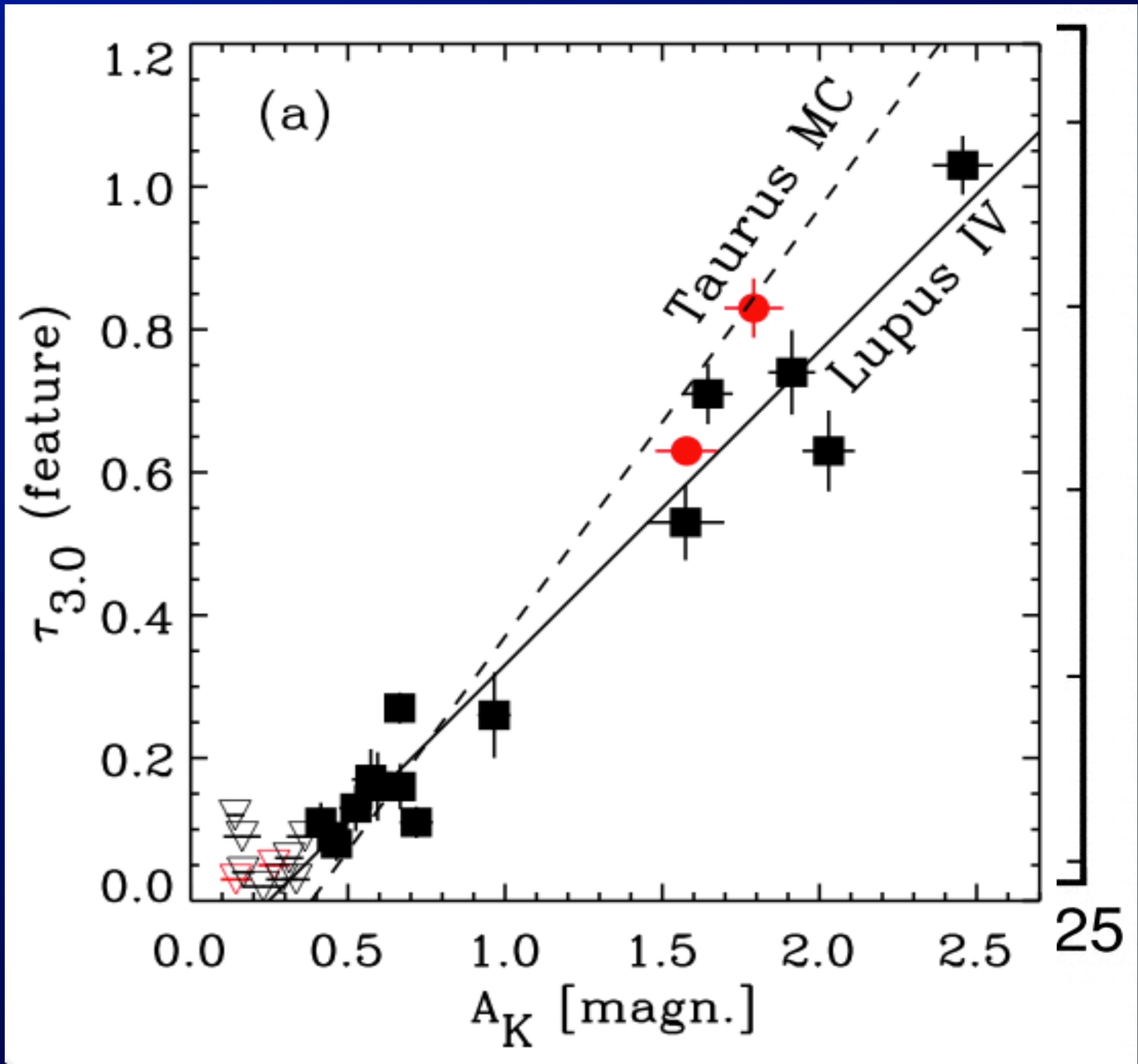






e.g. Noble et al. 2013; Knez et al. 2005, Bergin et al. 2005

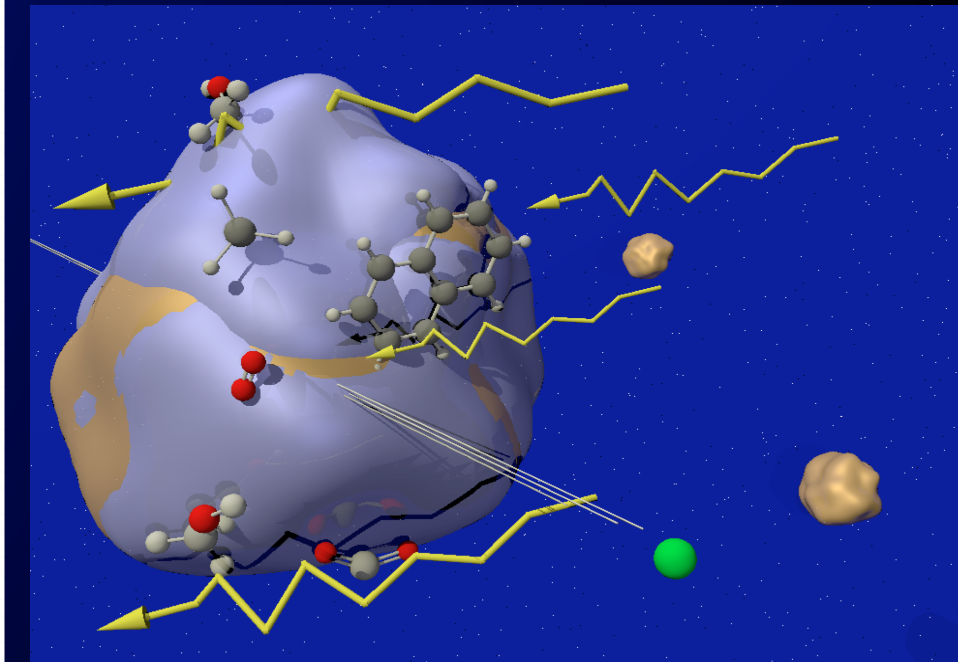
Ices onset and distribution



~ optical depth @ 2.2μm

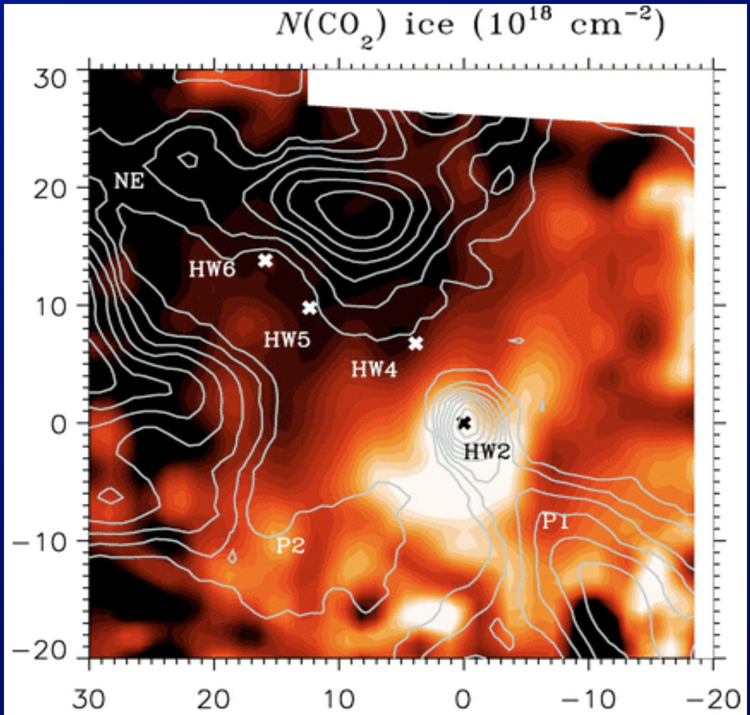
e.g. Boogert et al. 2013; Murakawa et al. 2000; Whittet et al 1998

- $\tau(H_2O) = \alpha(A_V - A_{V\ Seuil})$
- Abundance H_2O : 10^{-5} - 10^{-4} N_H



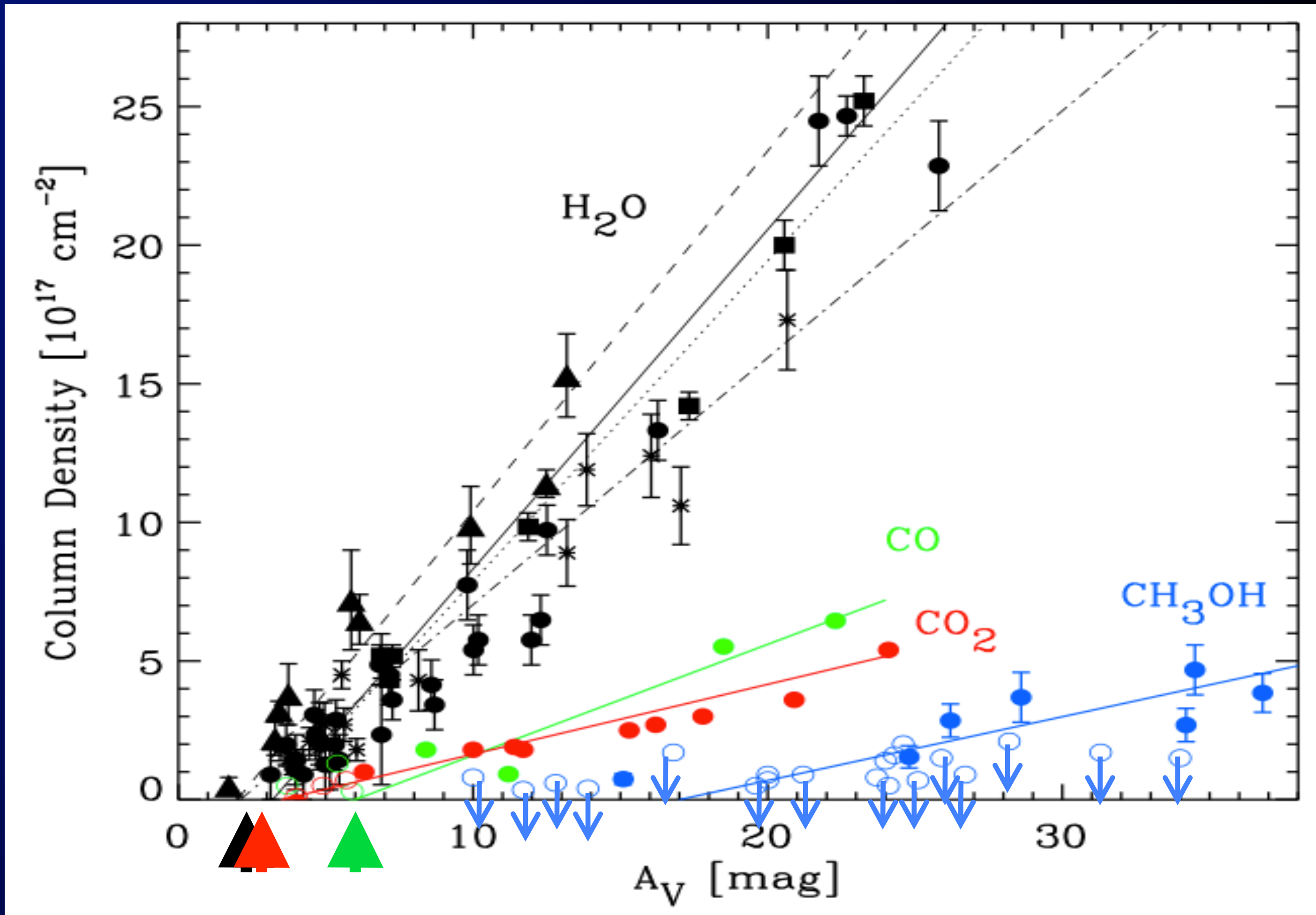
- Typical ice mantle thickness: ~ 100Å

Obs. telescopes & satellites



Sonnentrucker et al. 2008, ApJ 672, 361

Quiescent lines of sights



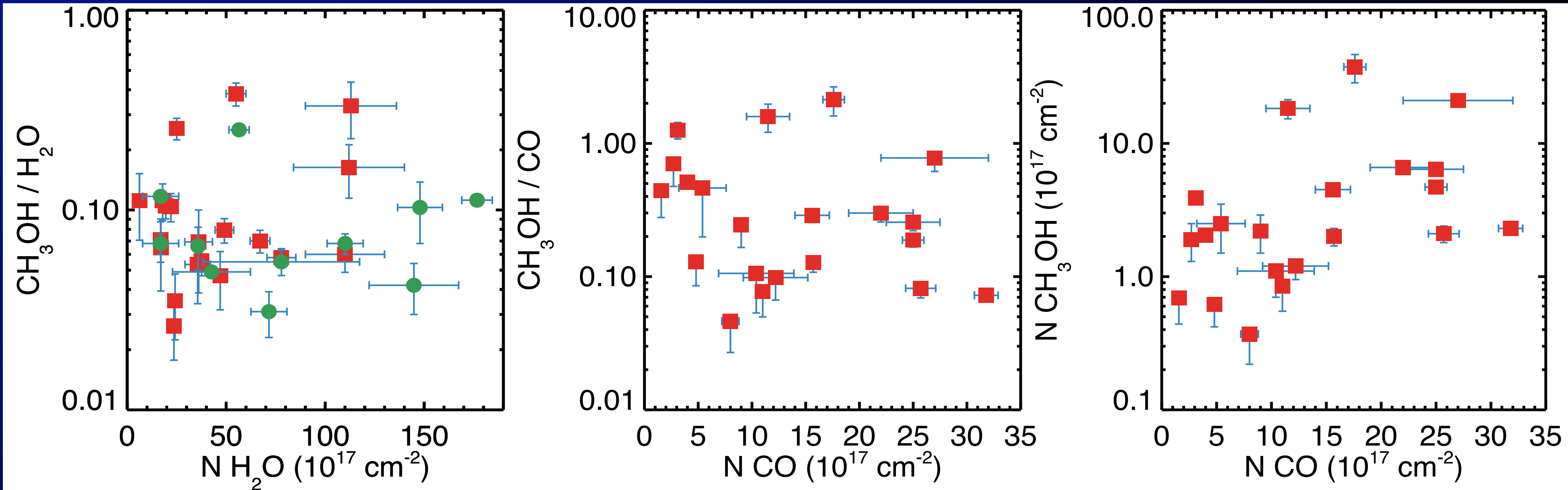
- H_2O and CO_2 seem to share the same Av threshold

e.g. Pontoppidan et al. 2008, Bergin et al. 2005, ApJ 627, L33

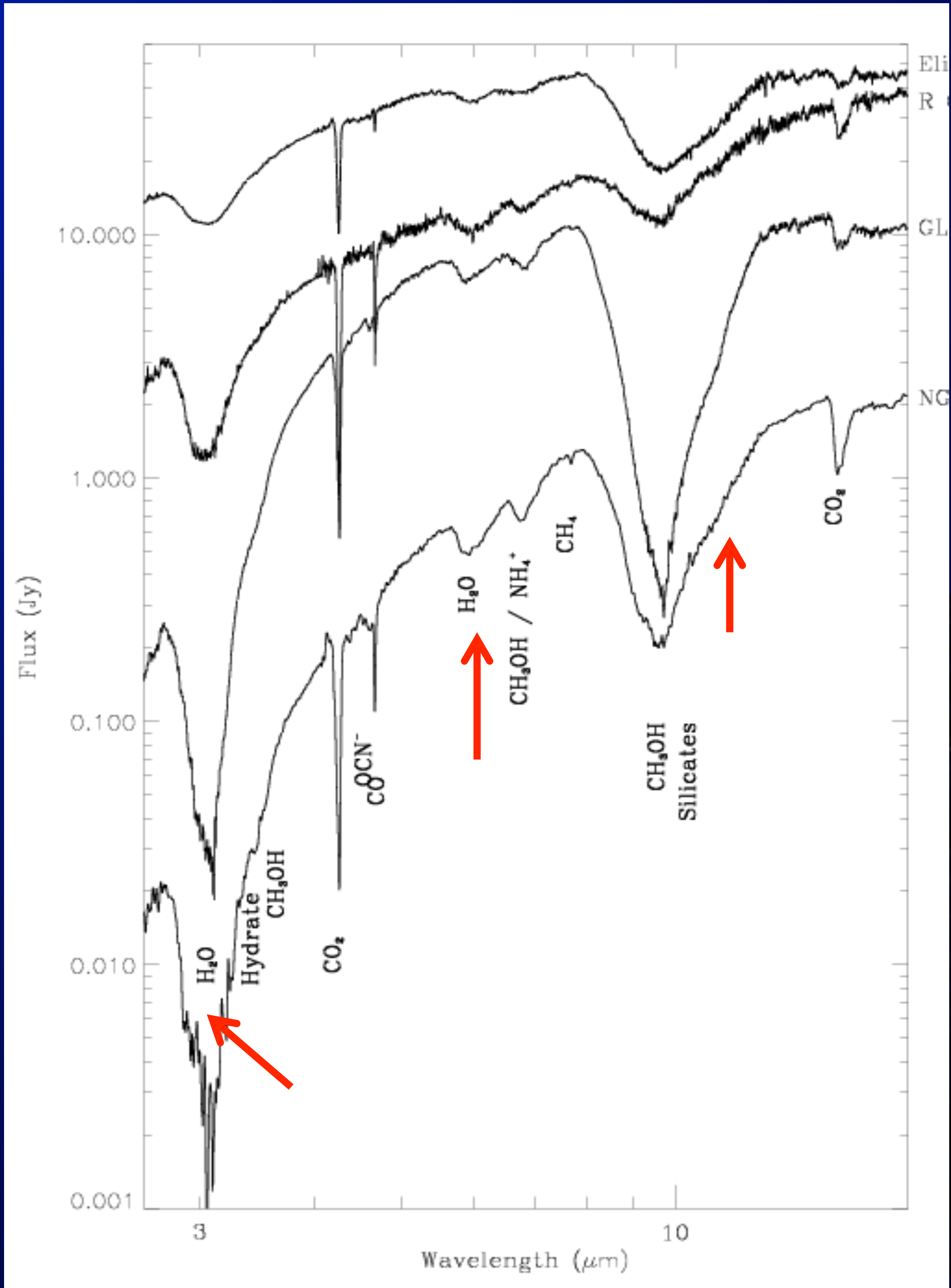
- CO variable and appears later
- CH_3OH highly variable

e.g. Whittet et al. 2011; Boogert et al. 2008, 2015

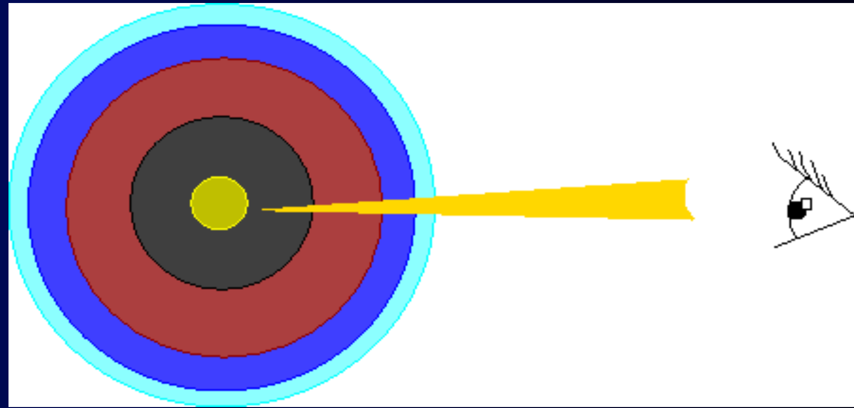
CH_3OH variability



Dartois+ 2019, Whittet+ 2011, Bottinelli+ 2010



ISO database extract



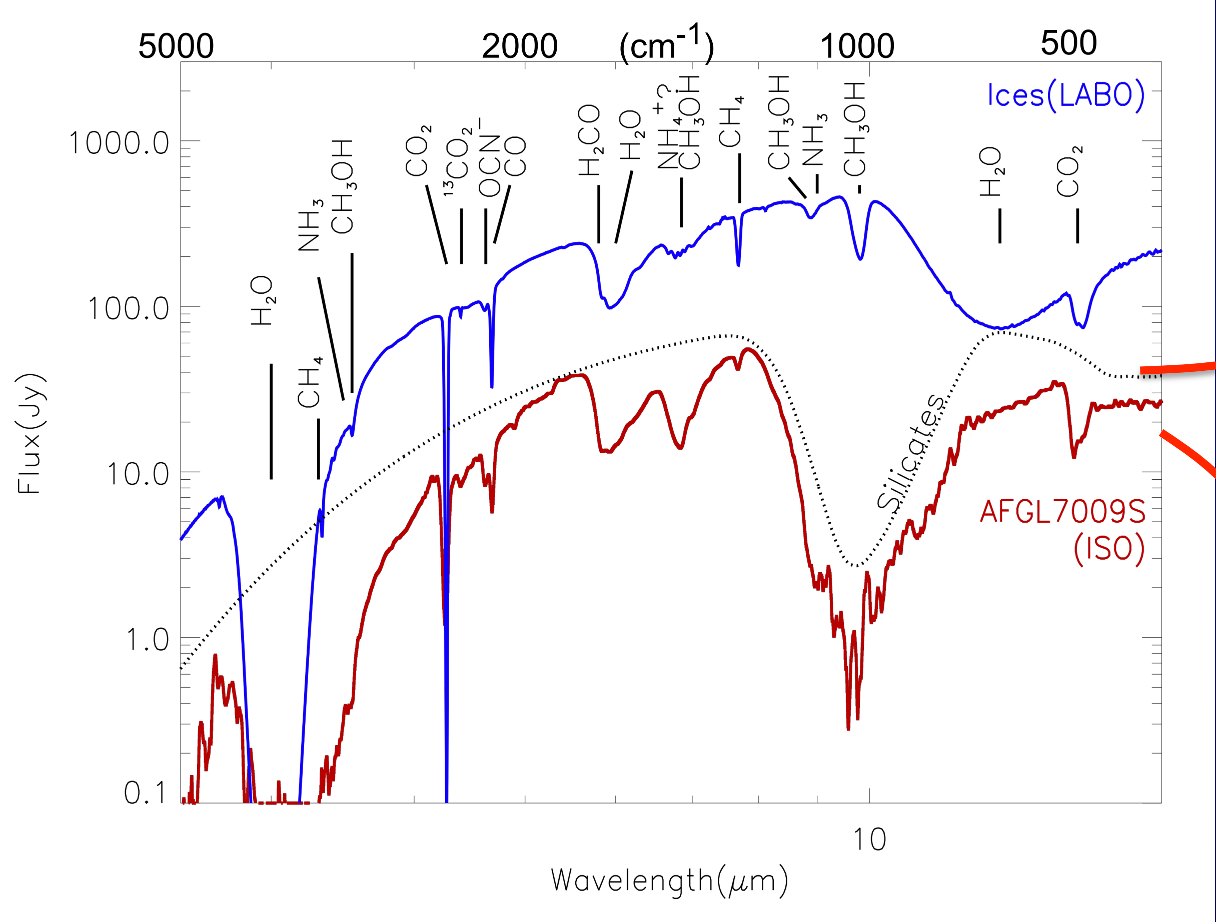
Protostars / Protoplanetary disks

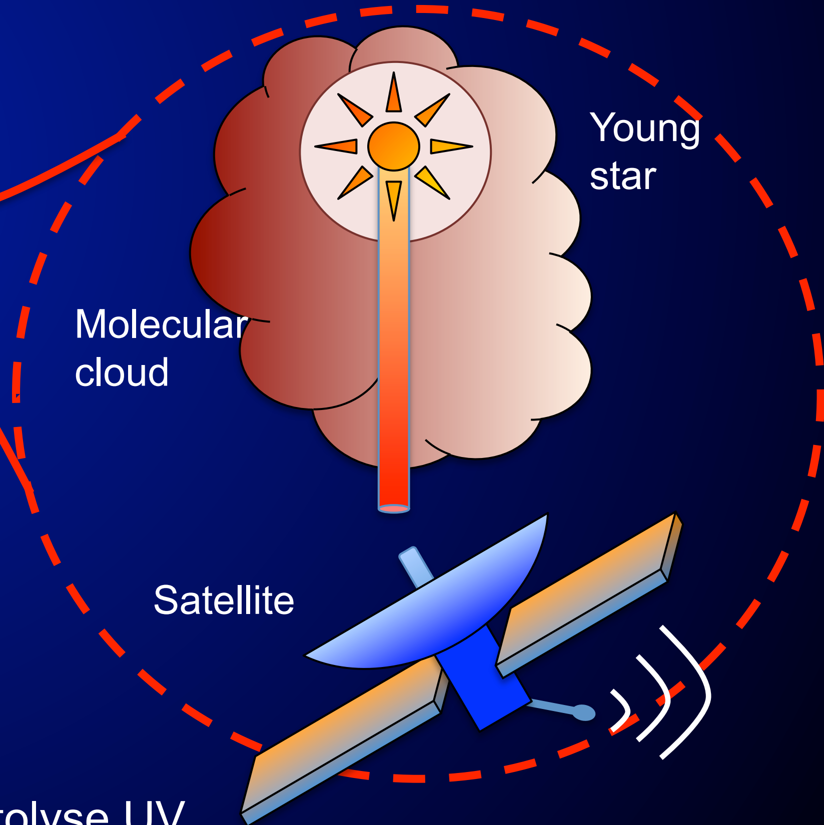
HST / Tau 042021 © C. Gould

Massive YSOs

ISO (1995)

ISO SWS
(Complete coverage 2.5 – 45 μm, bright & massive sources)



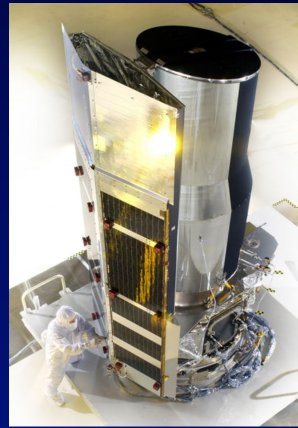


Gerin+2015; Dartois 1998

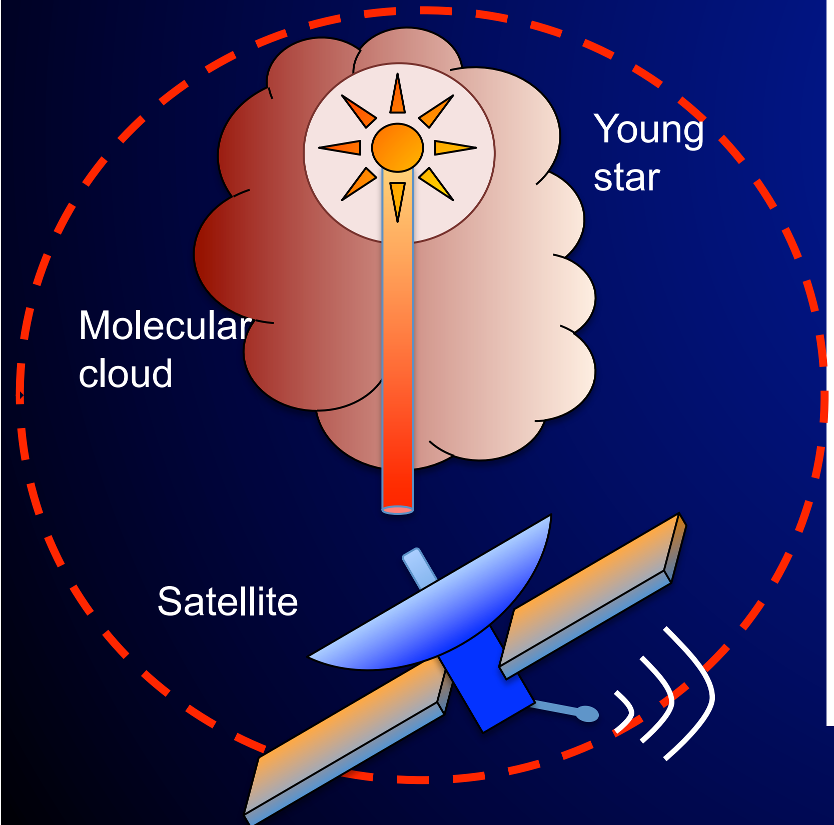
Film $H_2O/CO/CH_4/NH_3$ @ 10 K + photolyse UV

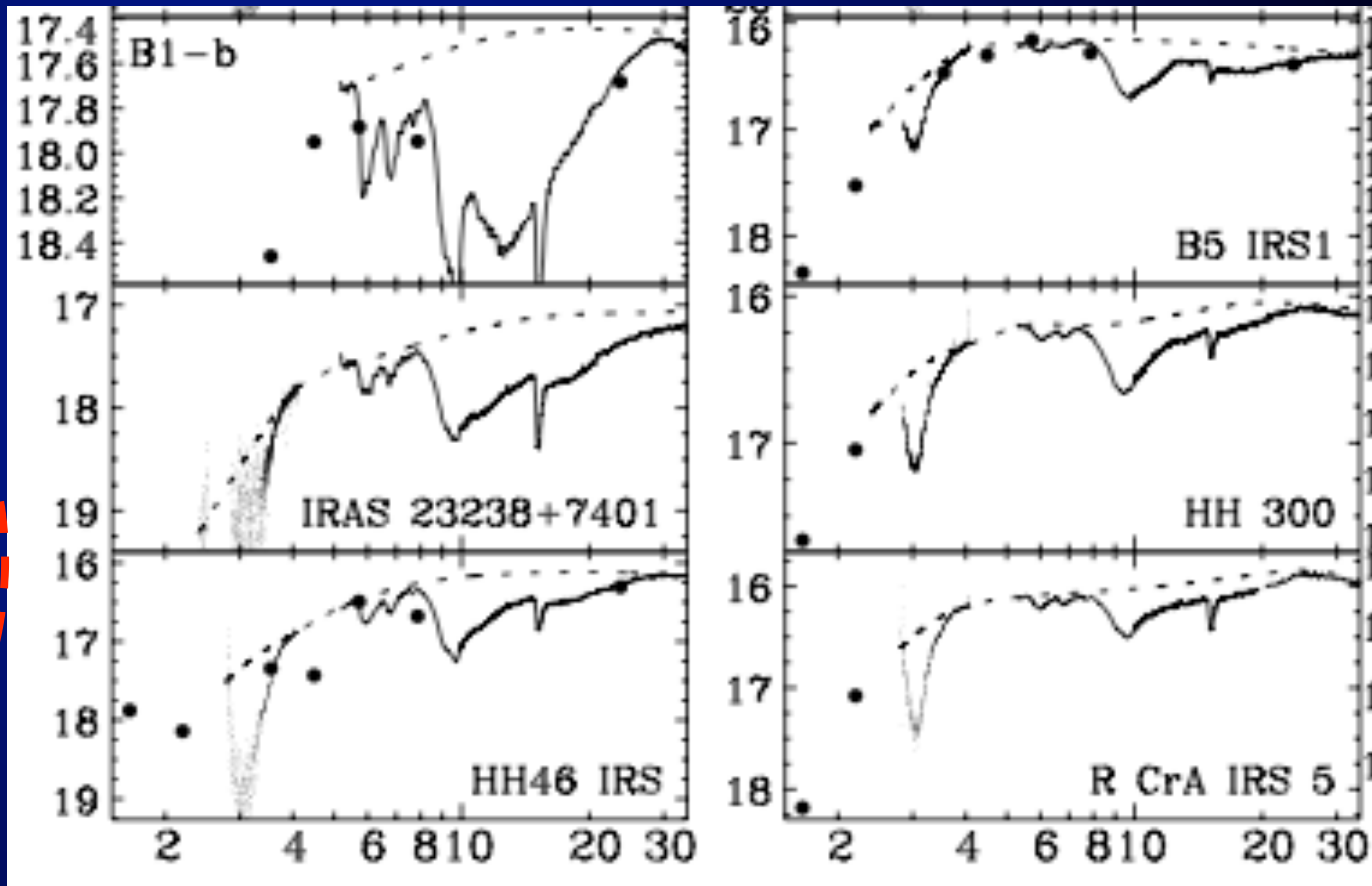
Low mass YSOs

Spitzer IRS
(5 – 40 μm, extension to LYSOs, low spectral res @ low lambda)



Spitzer (2003)





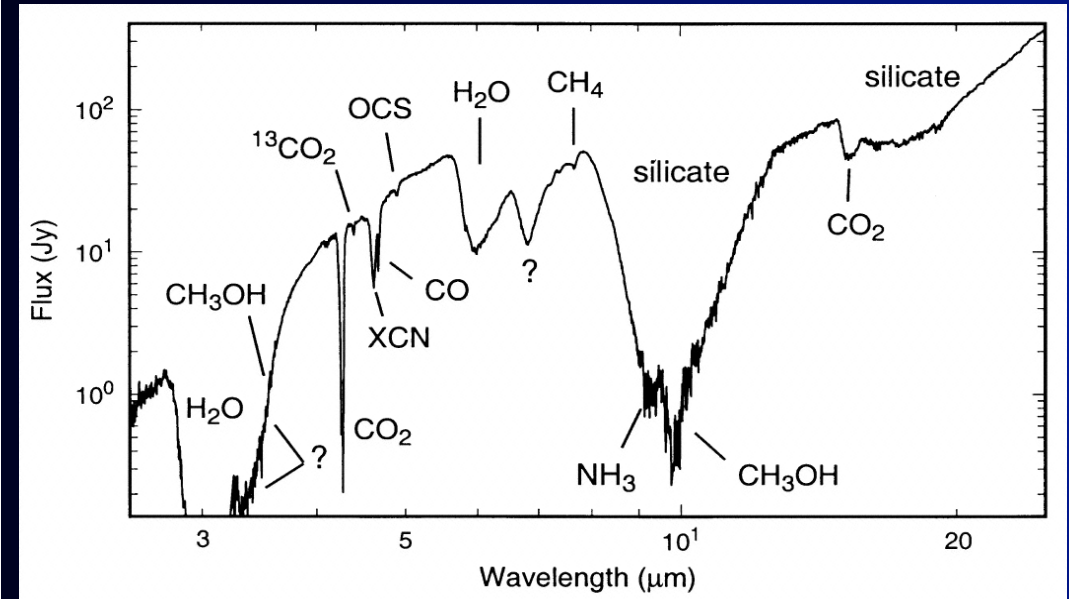
Boogert+2008

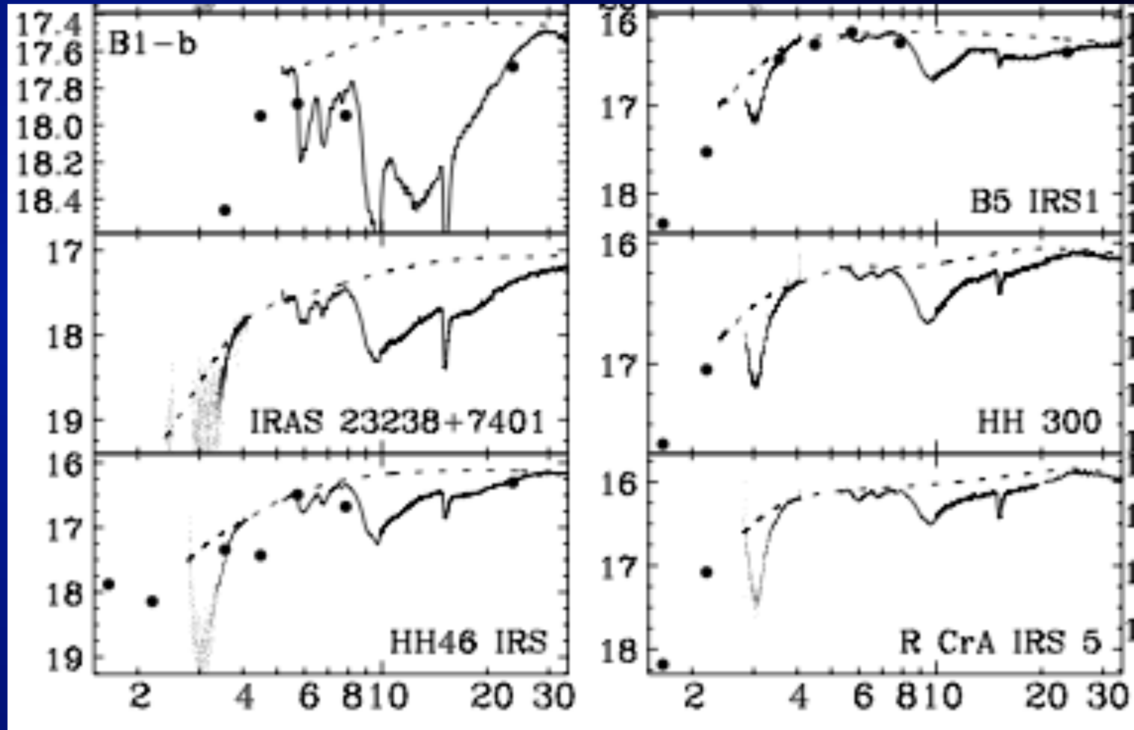
MYSOs & LYSOs

Traditionally separation between MYSOs and LYSOs

MYSOs (ISO)

LYSOs (Spitzer)





Gibb+2000

W33a ~10^5 L_{Sun}

Boogert+2008

Similar main ices within a factor of two

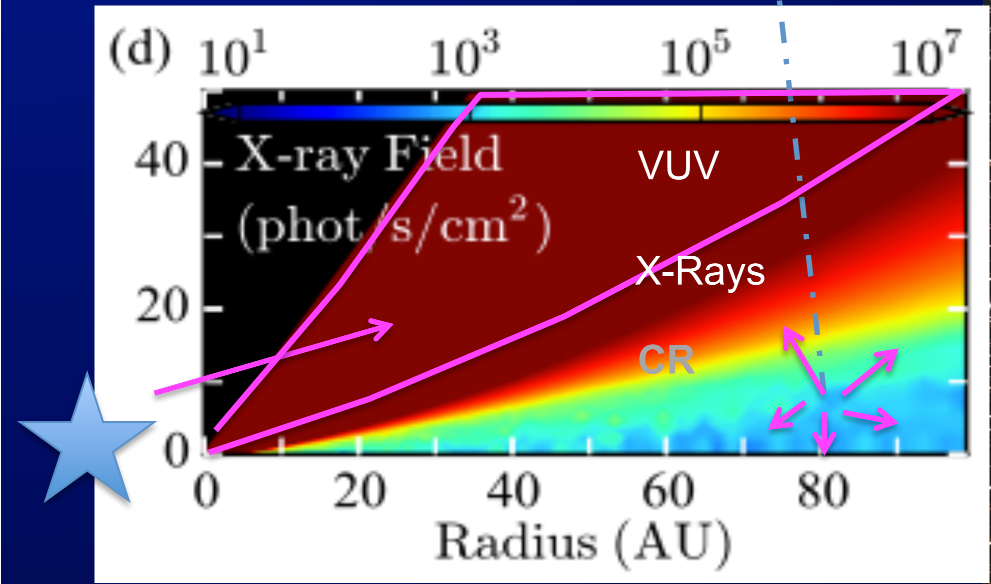
Energy sources of evolution

<u>Photon sources</u>

VUV photolysis:

- ambient
- stellar
- CR induced

X-Rays



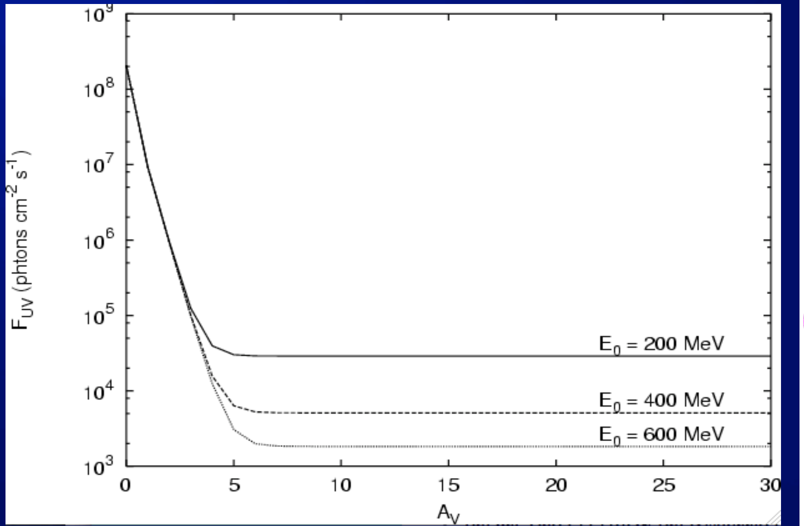
Anderson+2017

<u>Particles sources</u>

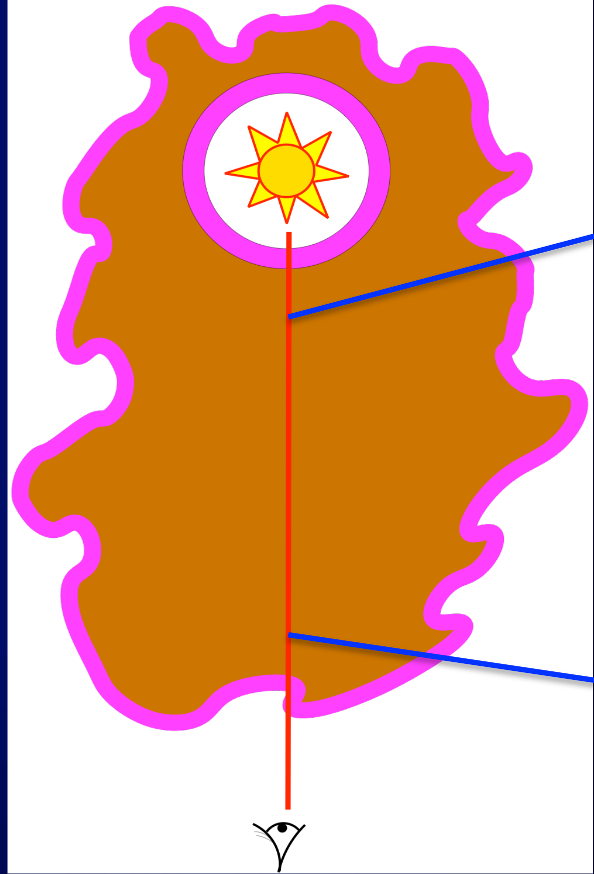
electrons

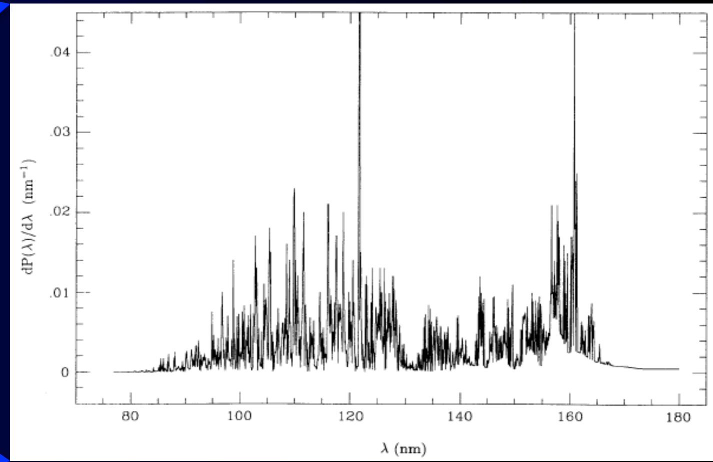
Cosmic rays

Diffuse Interface Dense



Shen & Greenberg 2004





Gredel+1989

Radiative environments in MYSOs & LYSOs:
The cosmic rays induced UV photons make photochemistry and radiolysis
~~stellar light, ISRF~~
…not heavily ~~affected~~ by the SpT

But differences in evolution timescale for e.g. surface reaction (& densities ?)

Statistically MYSOS more affected by rapid central star evolution

Mixing ice phases along the l.o.s.

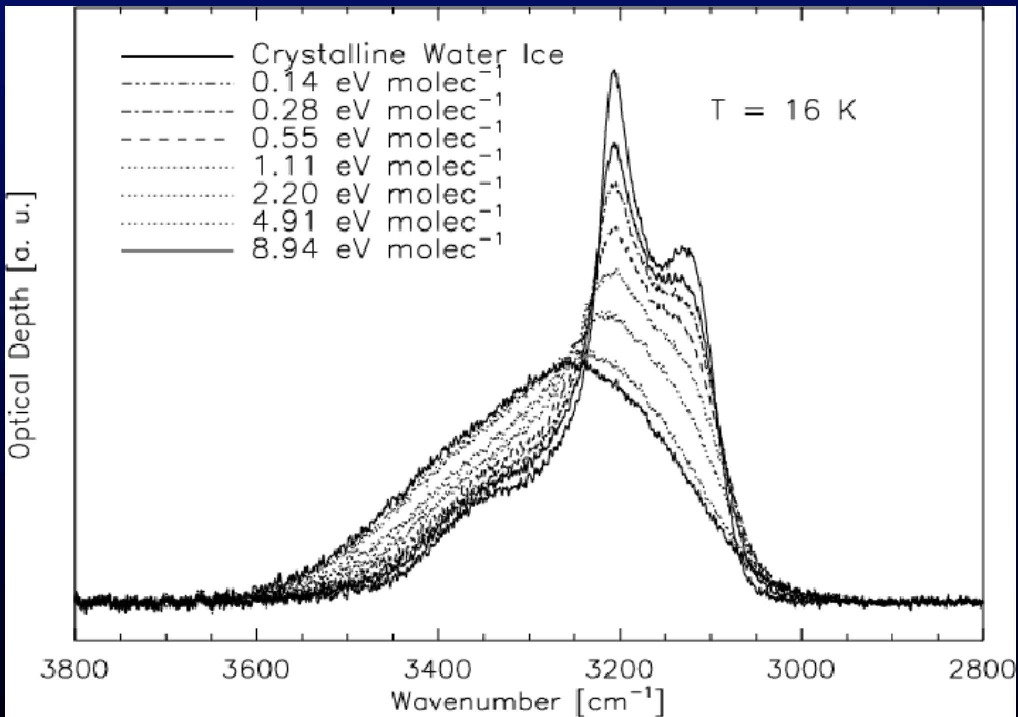
Ice/gas interface process (e.g. desorption)

Evolution

Φ

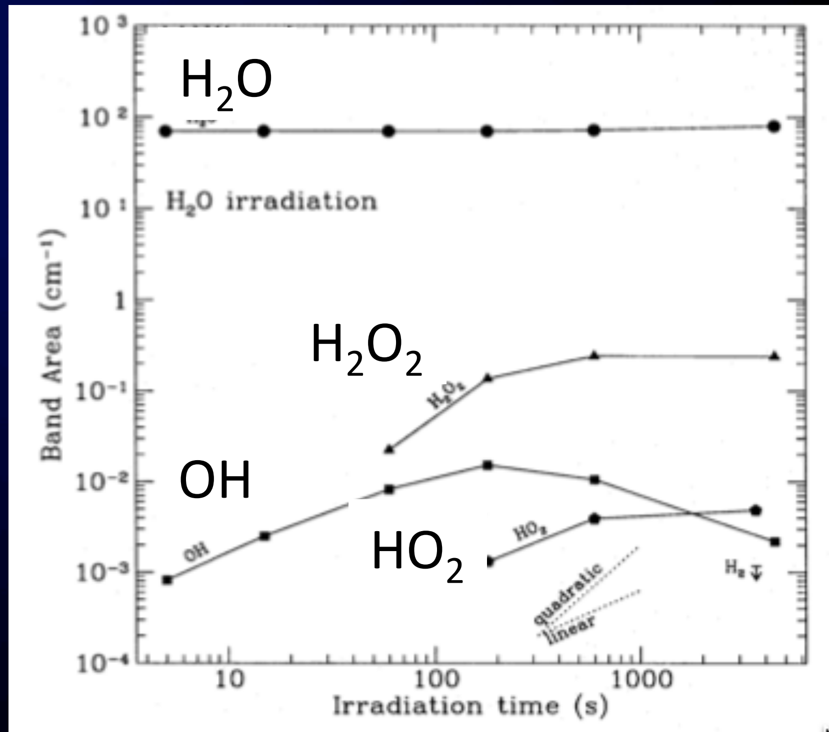
χ

Amorphisation/compaction



Leto 2003

Photochimie UV de glace pure

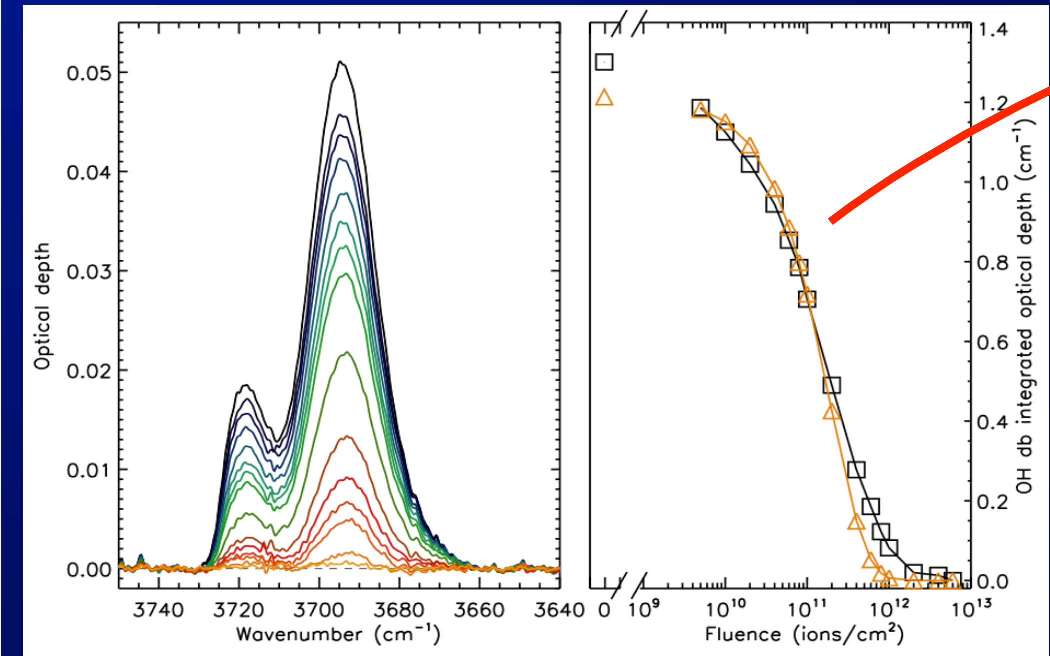


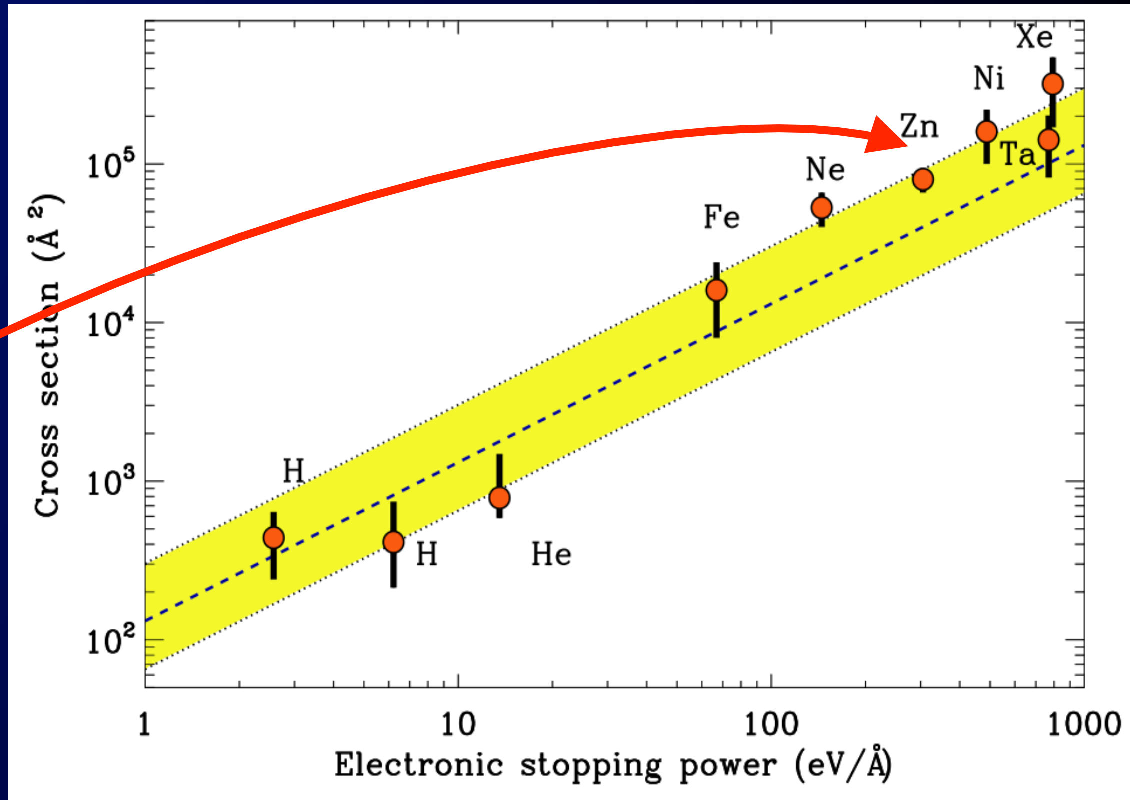
Photolyse UV interstellaire de la glace

Gerakines 1996

Accelerator experiments on ice structure evolution

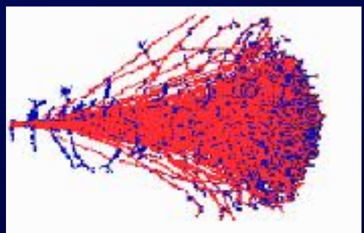
OH-dB evolution





Dartois et al. 2015; 2013; Palumbo et al. 2006; Moore & Hudson 2000; Famá et al. 2010; Raut et al. 2007; 2008; Mastrapa & Brown 2006; Baragiola et al. 2005; Guillot & Guissani 2004; Leto & Baratta 2003; Strazzulla et al. 1992; Moore & Hudson 1992; Baratta et al. 1991

Se(Z,E)



Ziegler et al. 2010

$\sigma(Z,E) = f(Se(Z,E))$

Inventories of ices

Identified vs likely species

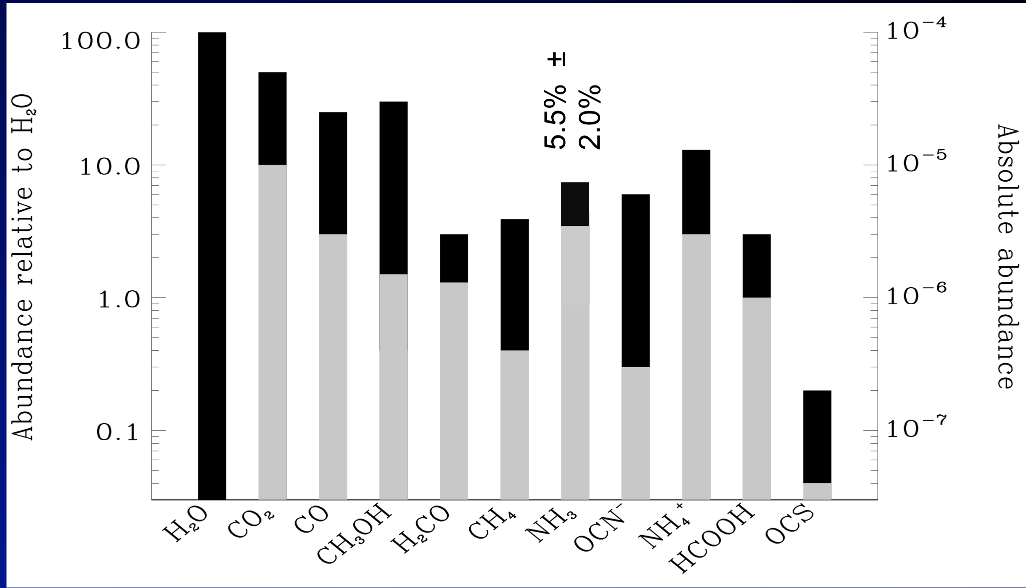
identified

	MYSOs	LYSOs
H_2O^e	100	100
CO^e	7_4^{15} (7)	21_{12}^{35} (18)
	3-26	(<3)-85
$CO_2{}^e$	19_{12}^{25}	28_{23}^{37}
	11-27	12-64
CH_3OH	9_5^{23} (5)	6_5^{12} (5)
	(< 3)-31	(< 1)-25
NH_3		6_4^8 (4)
	$\sim 7^f$	3-10
CH_4		4.5_3^6 (3)
	1-3	1-11

likely

	MYSOs	LYSOs
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
OCS	0.03-0.16	≤1.6

Boogert+ 2015



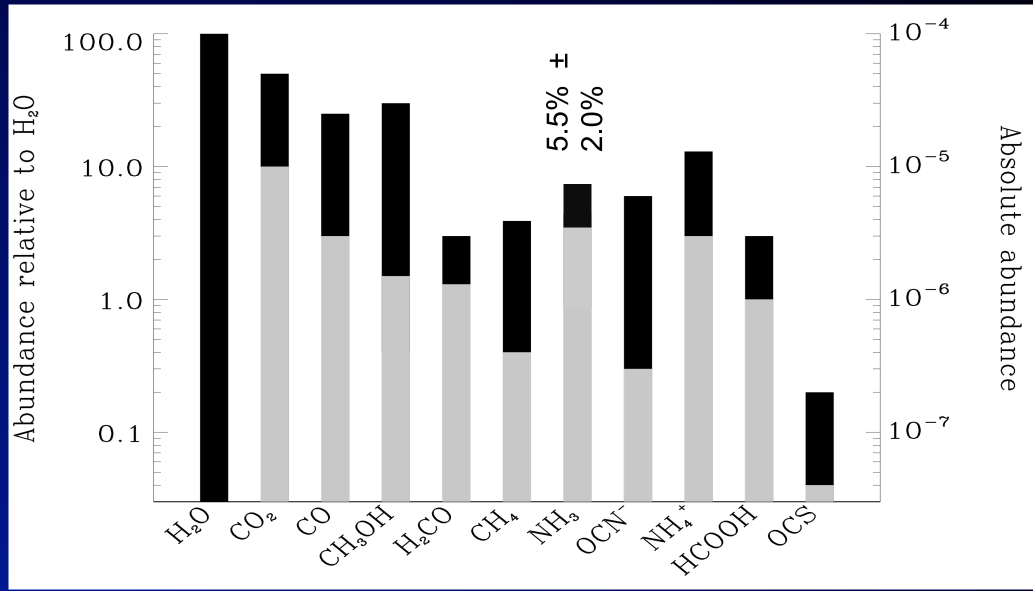
Dartois 2005, SSRv

Inventories of ices

Identified vs likely species

		MYSOs	LYSOs
identified	H_2O^e	100	100
	CO^e	7^{15}_{4} (7) 3-26	21^{35}_{12} (18) (<3)-85
	$CO_2{}^e$	19^{25}_{12} 11-27	28^{37}_{23} 12-64
	CH_3OH	9^{23}_{5} (5) (< 3)-31	6^{12}_{5} (5) (< 1)-25
	NH_3	$\sim 7^f$	6^{8}_{4} (4) 3-10
	CH_4	1-3	4.5^{6}_{3} (3) 1-11
likely	H_2CO	~2-7	~6
	OCN^-	$0.6^{0.7}_{0.3}$ 0.1-1.9	$0.6^{0.8}_{0.4}$ (0.4) (< 0.1)-1.1
	OCS	0.03-0.16	≤1.6

Boogert+ 2015



Dartois 2005, SSRv

LYSO/MYSO ~3

≠ profiles

Envelopes T sup, processed

Higly variable,
no consensus on formation pathway

Seems contemporaneous to H_2O

To be further constrained

Wich process ?

Photolysis
Radiolysis
Surface/thermal

Possible, « Speculative » list

	MYSOs	LYSOs	
$HCOOH^{i}$	4_{3}^{5} (3)		
	(< 0.5)-6	(< 0.5)-4	
$C_2H_5OH^{i}$	$\sim X_{H_2O}$(HCOOH)		?
$HCOO^{-j}$	$0.5_{0.5}^{0.7}$ (0.5)		which process ?
	0.3-1.0	~0.4	
$C_2H_4O^{j}$	$X_{H_2O}(HCOO^{-})\times 11$		
NH_4^+	11_{9}^{13}	11_{7}^{15}	which process ?
	9-34	4-25	
SO_2	(< 0.9)-1.4	~0.2	

Boogert+ 2015

Upper limits (~MYSOs)

Possible, « Speculative » list

	MYSOs	LYSOs
$HCOOH^{i}$	4^{5}_{3} (3)	
	(< 0.5)-6	(< 0.5)-4
$C_2H_5OH^{i}$	$\sim X_{H_2O}(HCOOH)$	
$HCOO^{-j}$	$0.5^{0.7}_{0.5}$ (0.5)	
	0.3-1.0	~0.4
$C_2H_4O^{j}$	$X_{H_2O}(HCOO^-)\times 11$	
NH_4^+	11^{13}_{9}	11^{15}_{7}
	9-34	4-25
SO_2	(< 0.9)-1.4	~0.2

C_2H_5OH: ?

$HCOO^-$: which process ?

NH_4^+: which process ?

Boogert+ 2015

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

N_2, O_2: ?

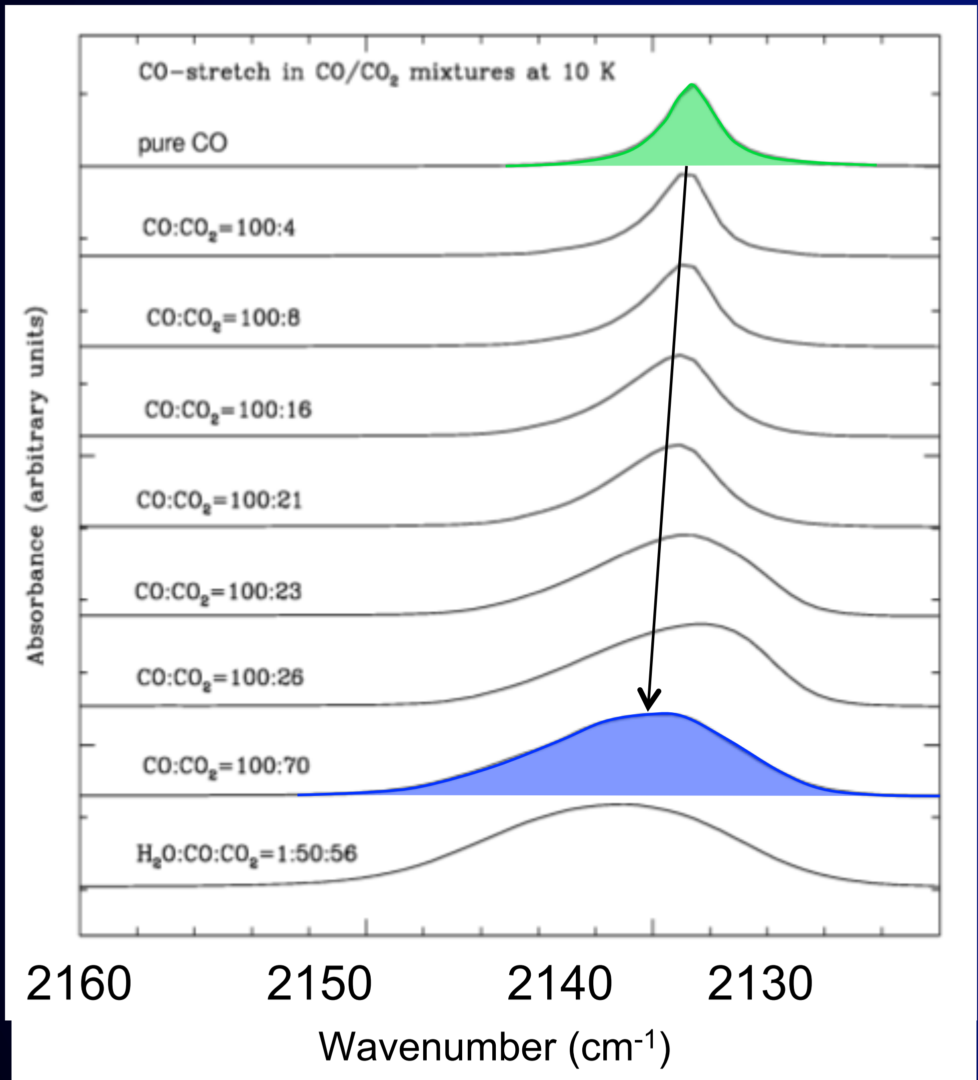
H_2S: Higher in comets

HNCO: Relation to OCN- ?

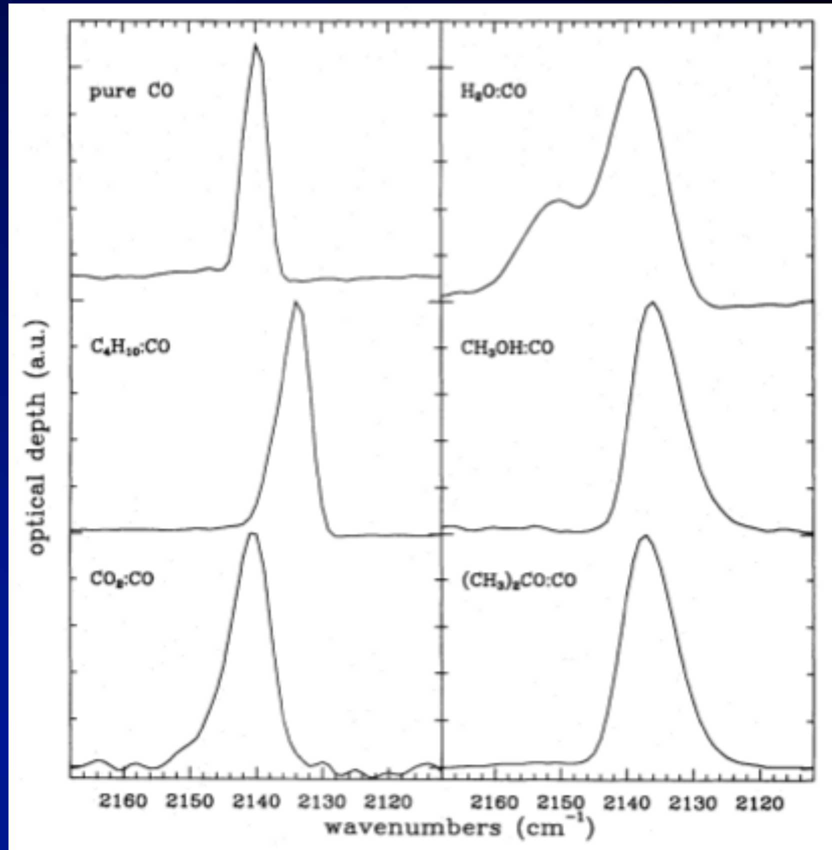
…. HCO^+, HCN, N_2O

Information in band profiles

polar versus apolar ices



Ehrenfreund+1996



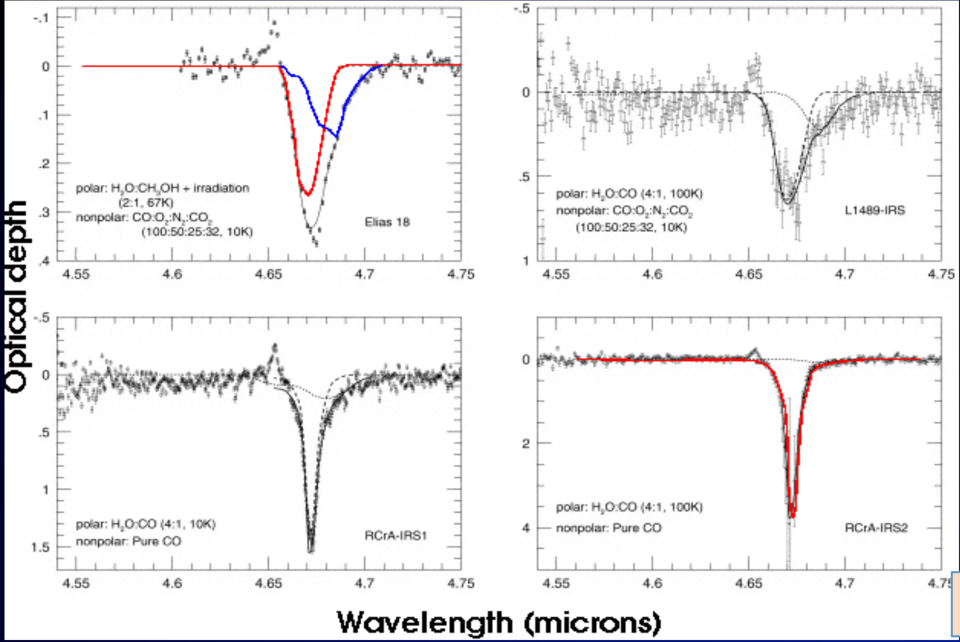
Palumbo+1993

Band widths and positions depend on the interactions in the solid

Initially traced by the CO ice observable from the ground.

Tielens+1991

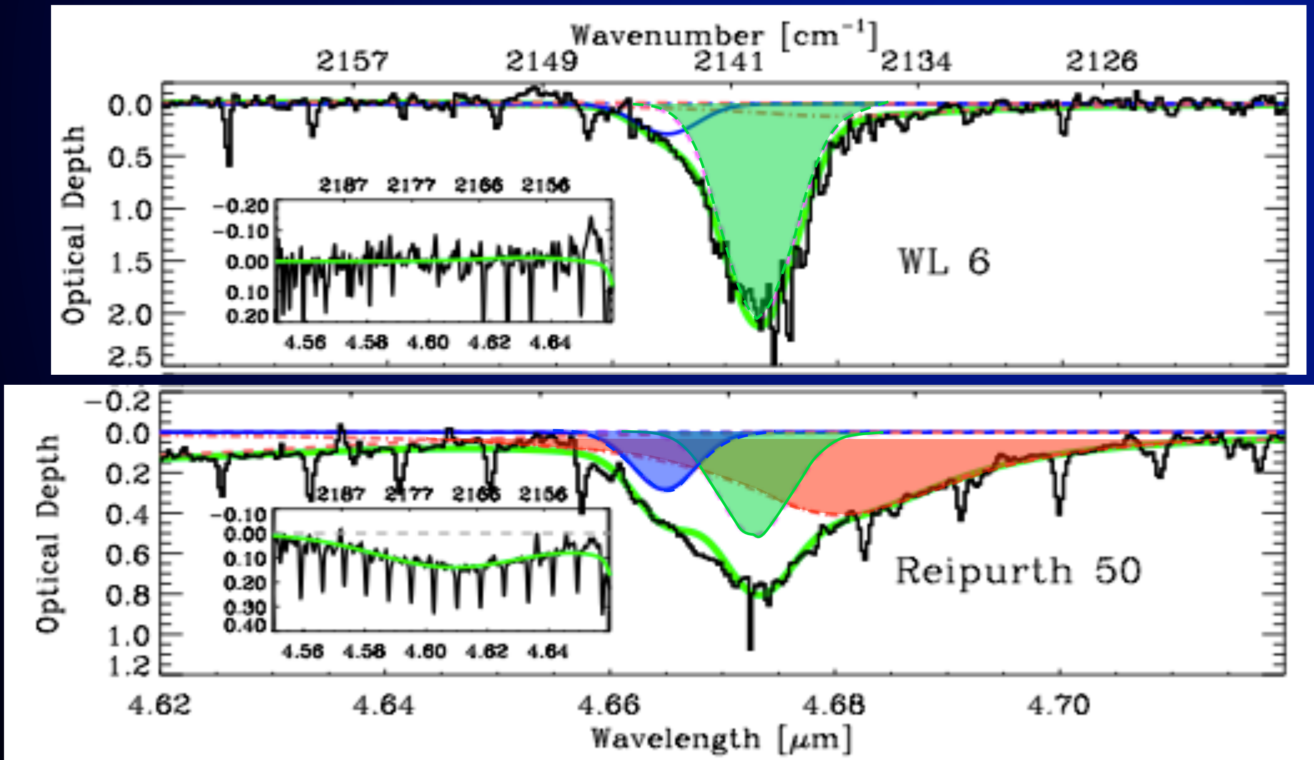
The ice phases linear hypothesis

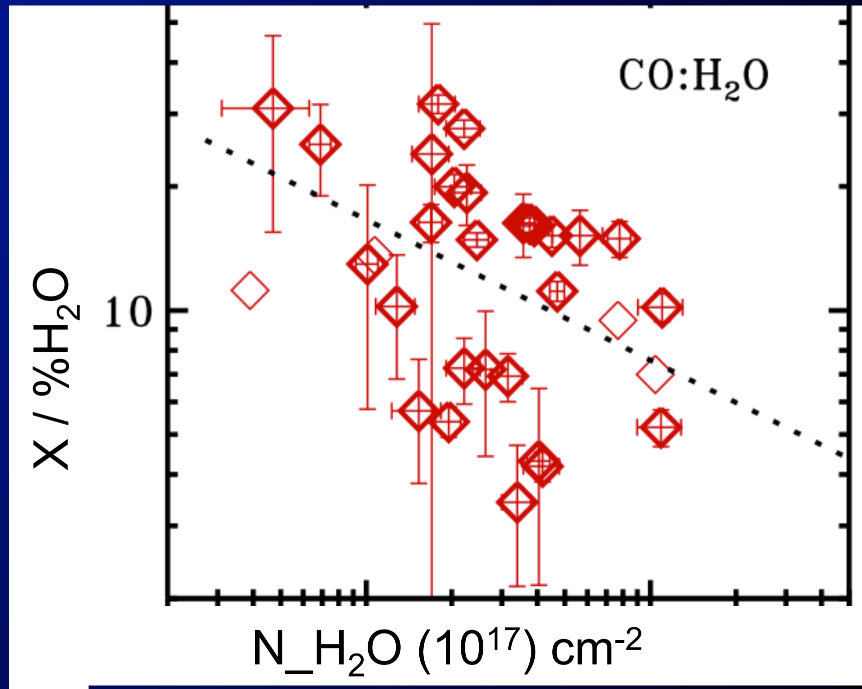


Chiar+1998

<u>Pros</u>: observations deconvolved on the basis of lab spectra combinations

<u>Cons</u>: Strong underlying hypothesis (naïve?) of no phases interactions



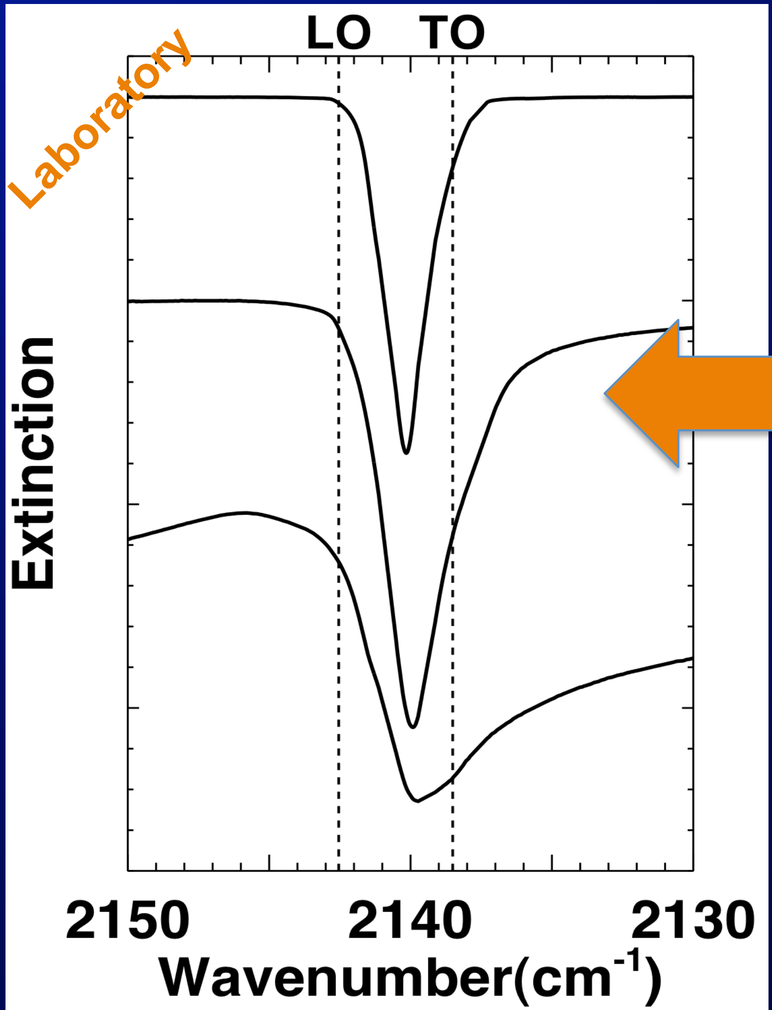


Pontoppidan+2003

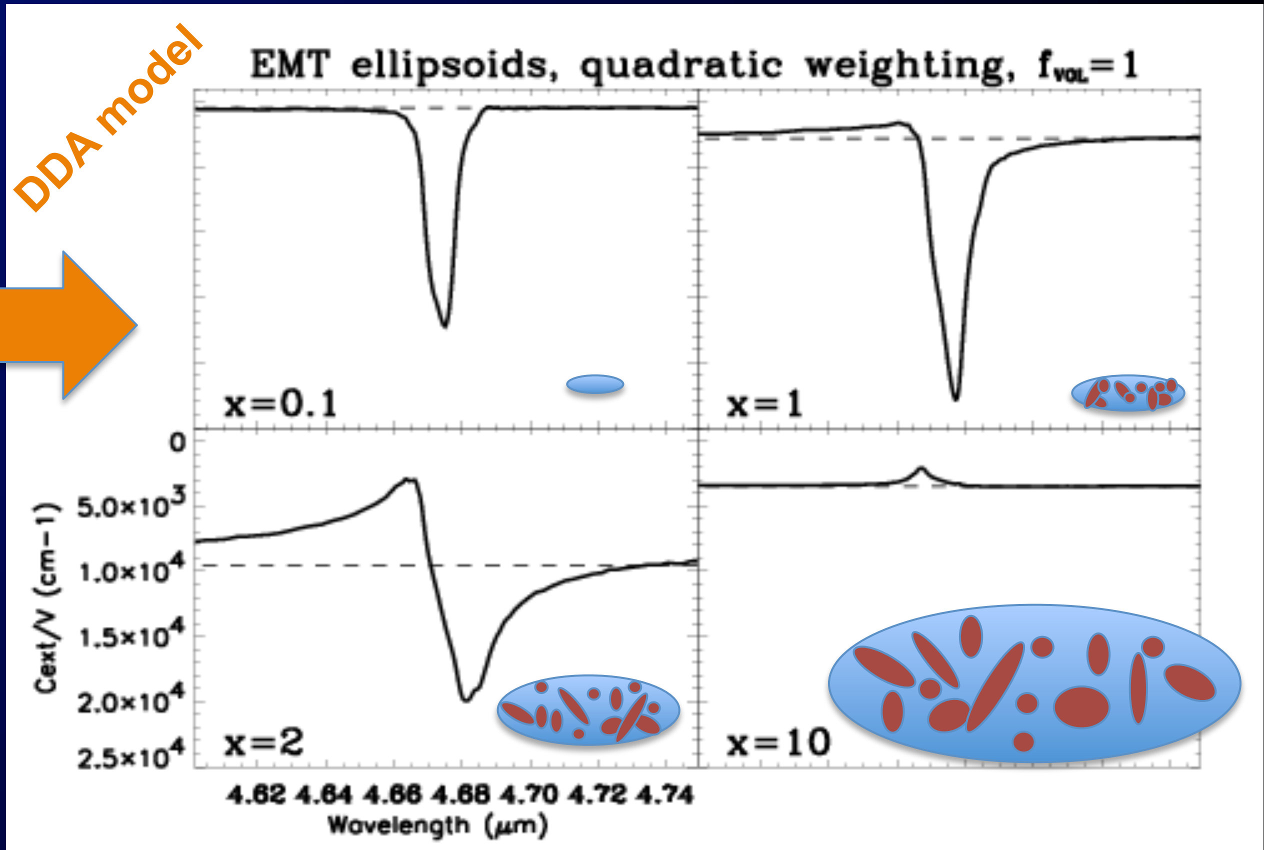
Oberg+2011

Band profiles – grain growth influence

Measured in the lab with
A collisional cell



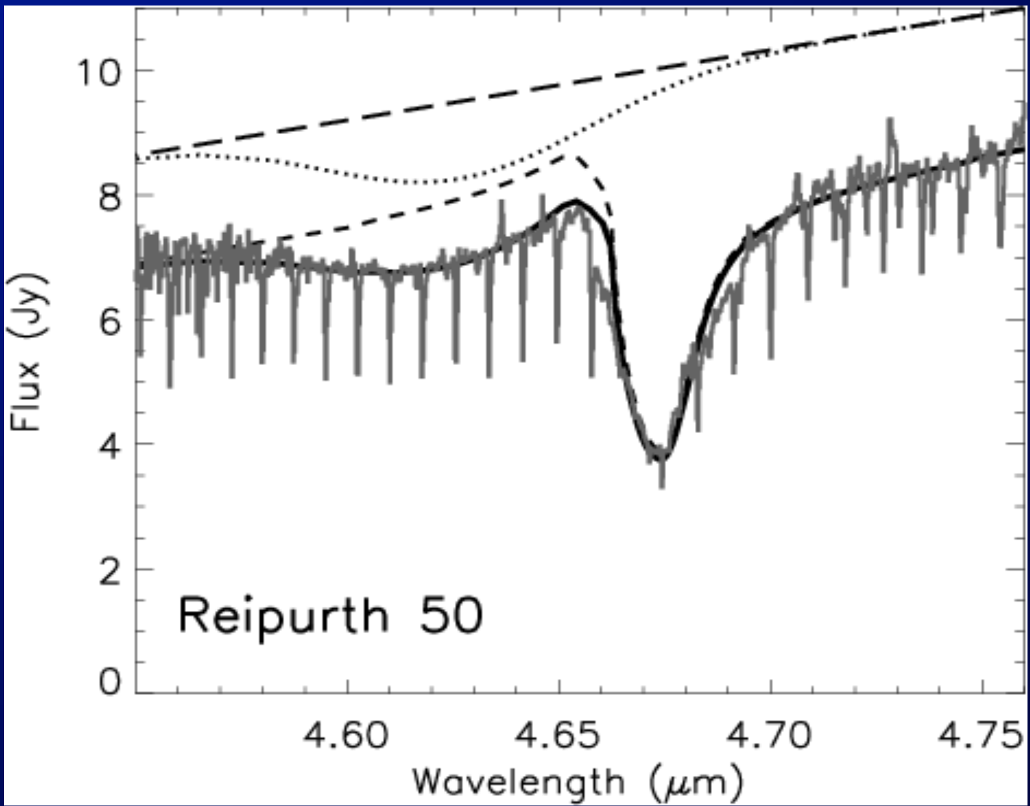
Dartois & Bauerecker 2008



Modification of the profile for pure CO

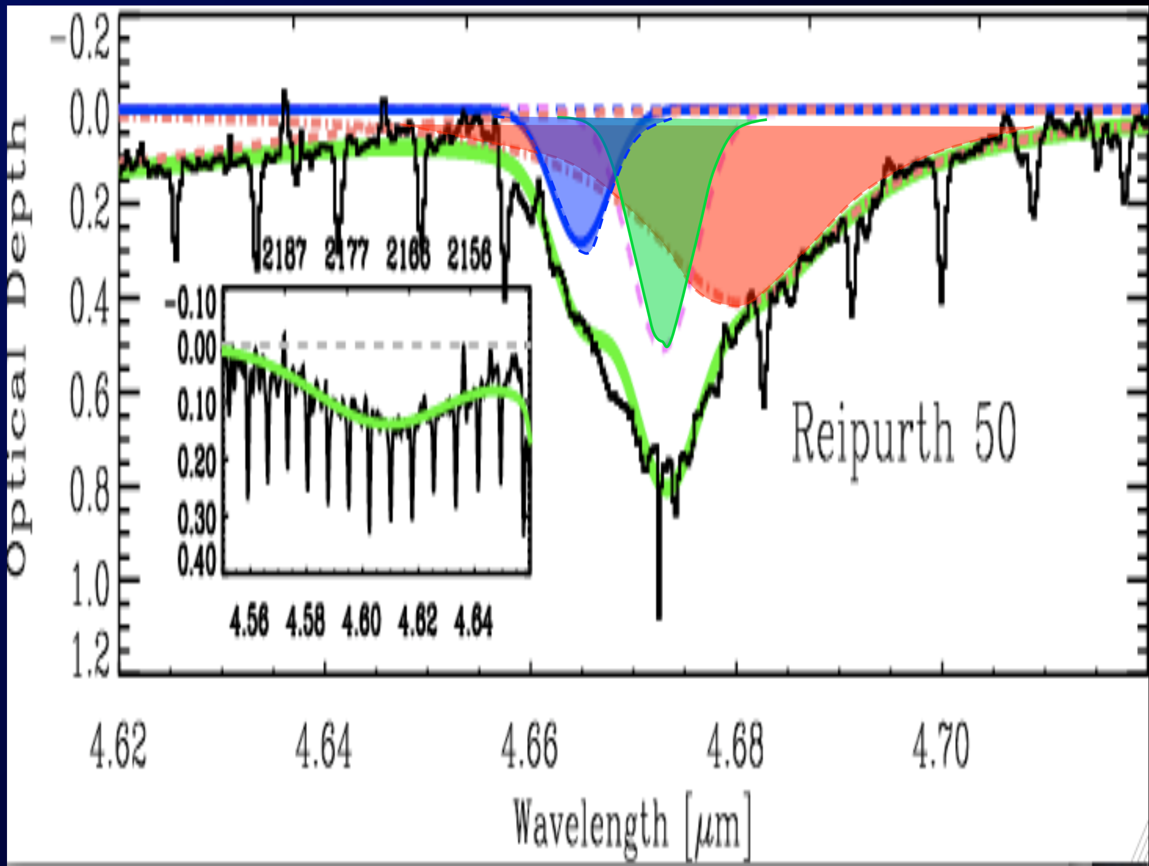
Band profiles –shape and size influence

Growth
CO pure mixed with silicates



Dartois+2006

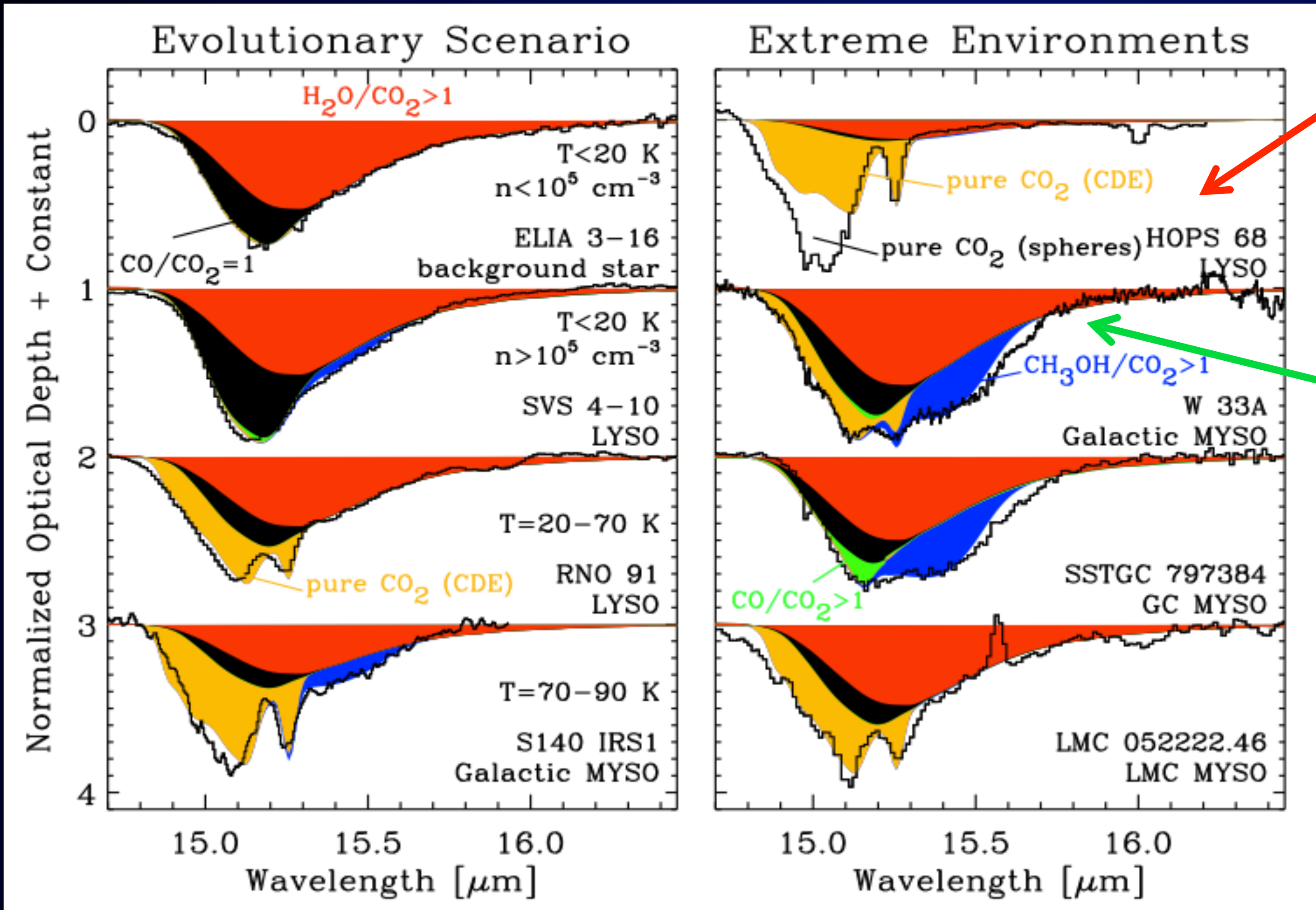
« Polar / Apolar »
Deconvolution with 3 components

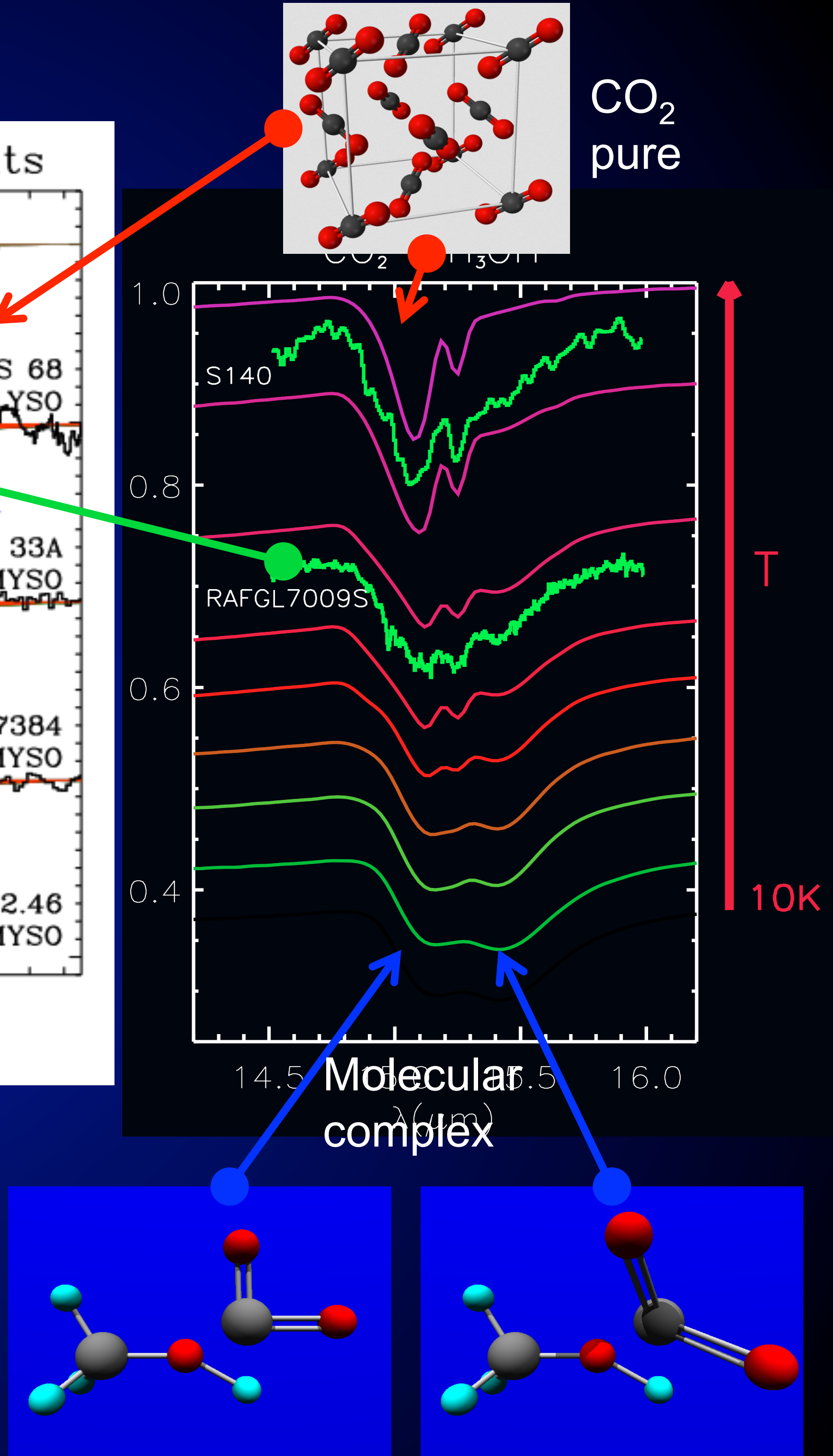


Pontoppidan+2003

Shape and size influence profile (generally overlooked) in addition to chemical composition

Bands profiles



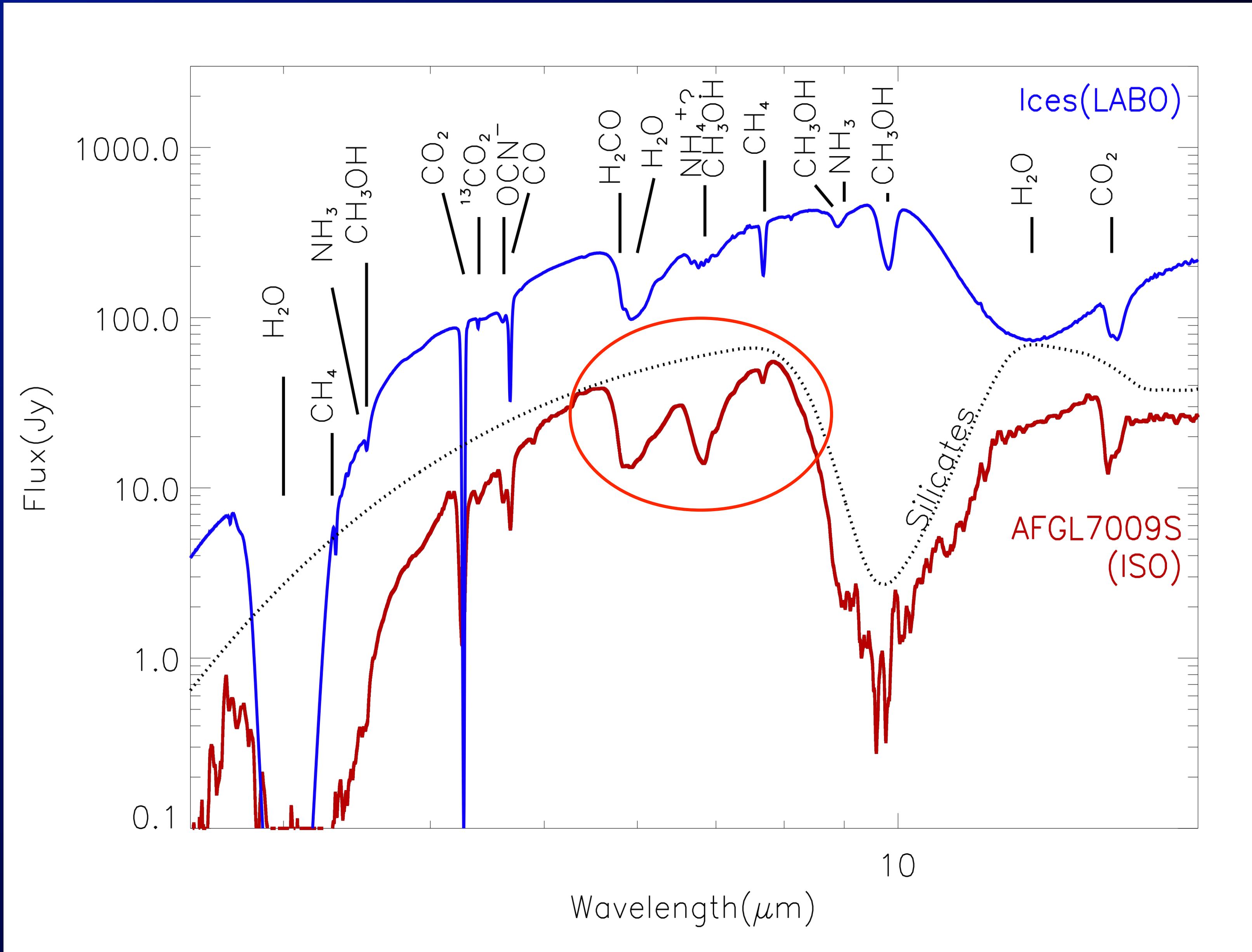


Boogert+2015, Gerakines+1999, Bergin+2005, Pontoppidan+2008, An+2011, Seale+2011, Poteet+2013, Klotz+2004, Dartois+1999

Info on envelopes T, composition, mix along l.o.s., shape and grain size…

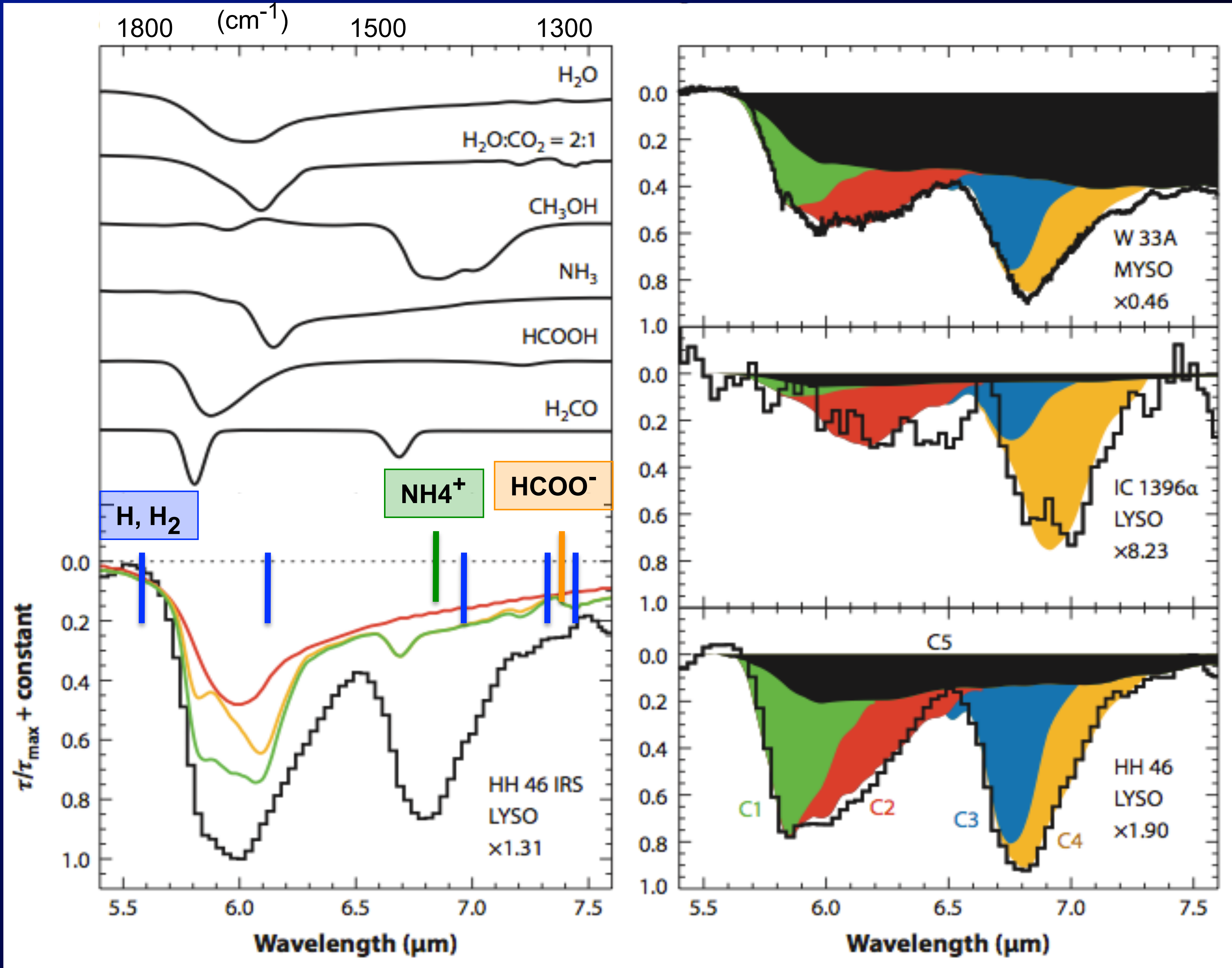
The fingerprint region for COMs identification ?

film$H_2O/CO/CH_4/NH_3$ @ 10 K + UV photolysis



Gerin+2015; Dartois 1998

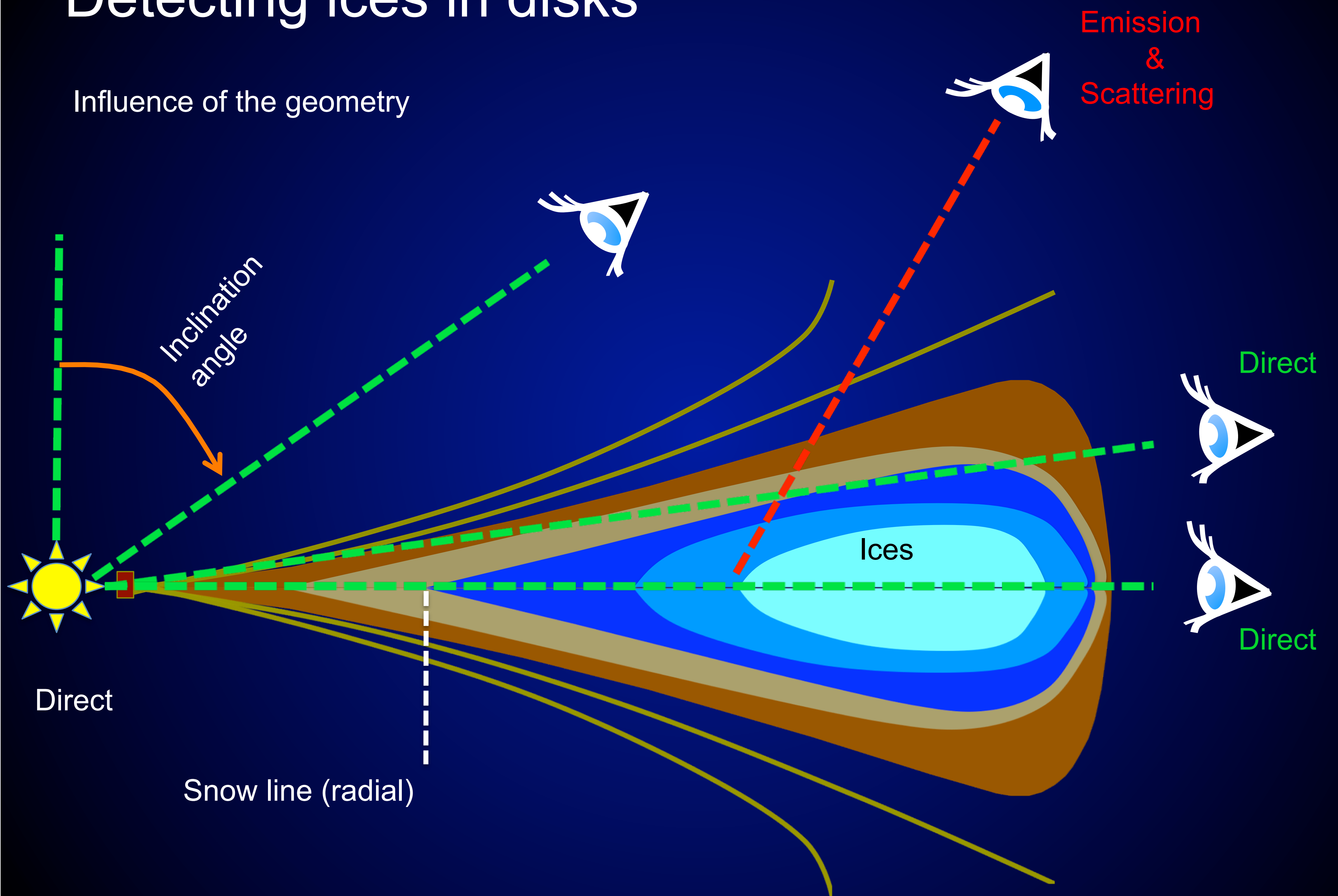
« Fingerprints » range : need JWST spectral res



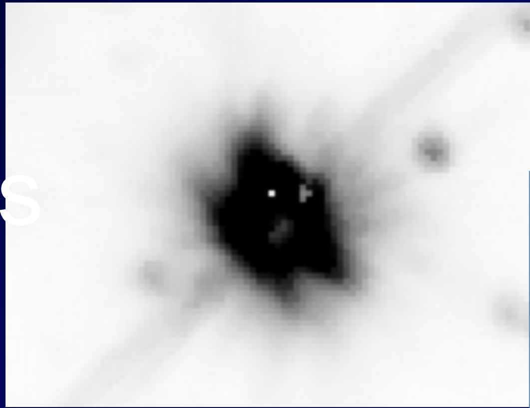
Boogert+ 2015

Detecting ices in disks

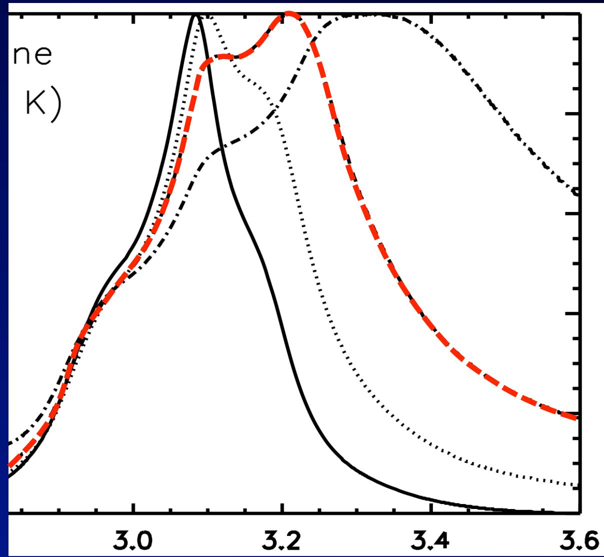
Influence of the geometry



Detecting ices in disks

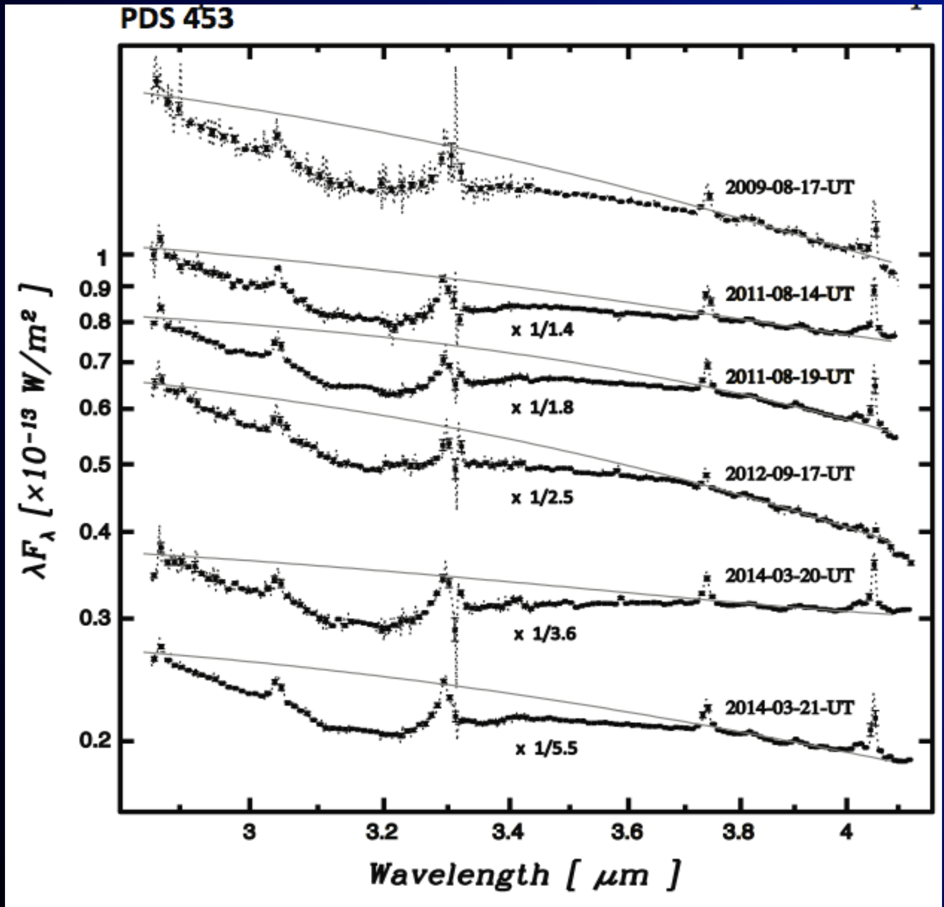


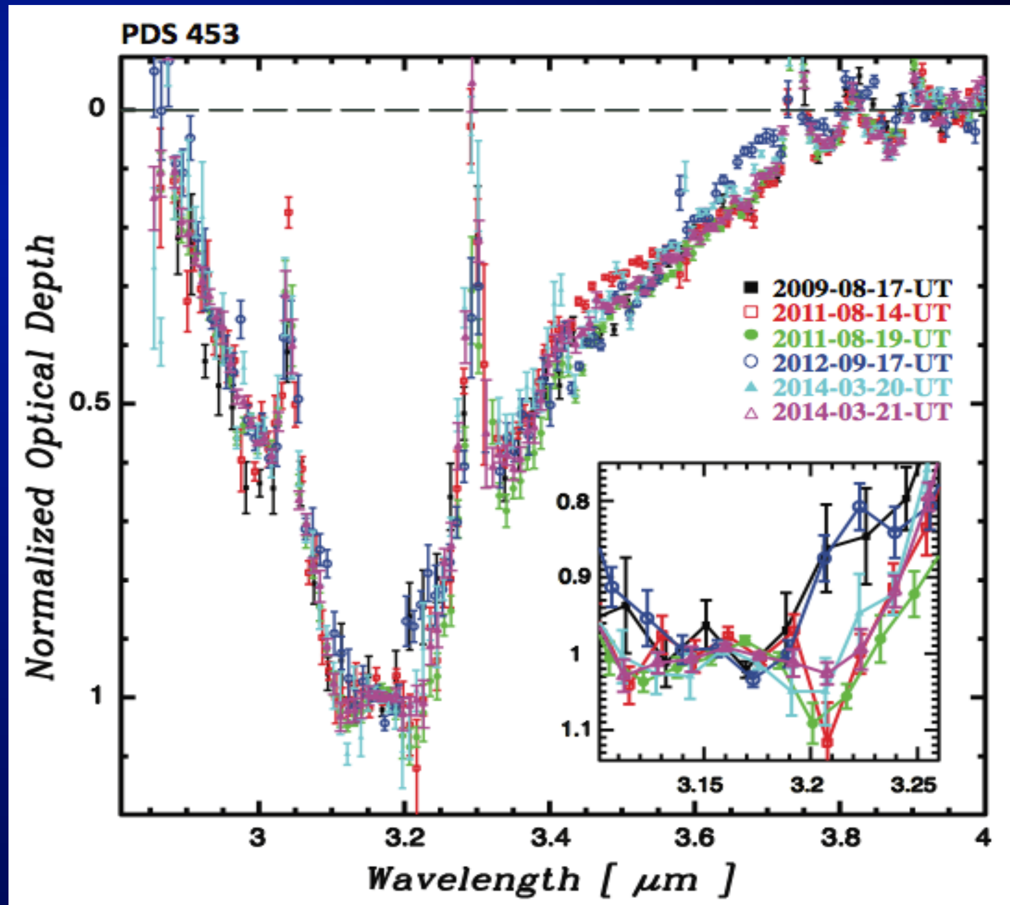
PDS453 / HST



Schegerer & Wolf 2010

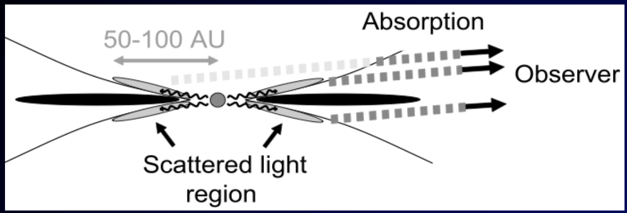
F2V; Herbig Ae d~140pc Incl. ~79deg





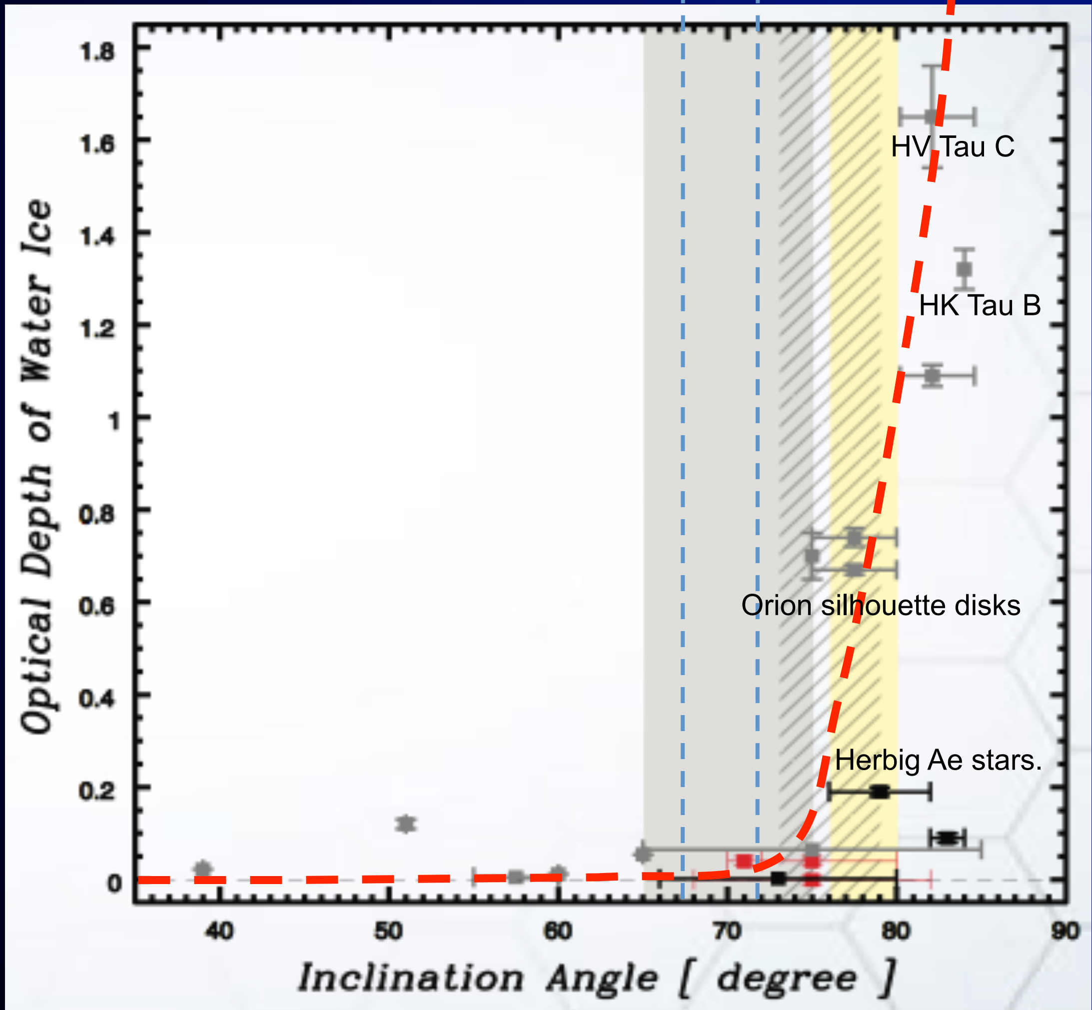
Terada & Tokunaga 2017

Inclination & flaring determines what is probed

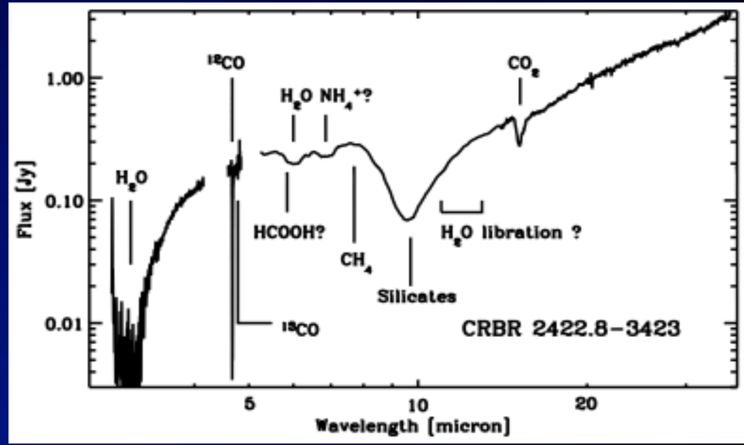


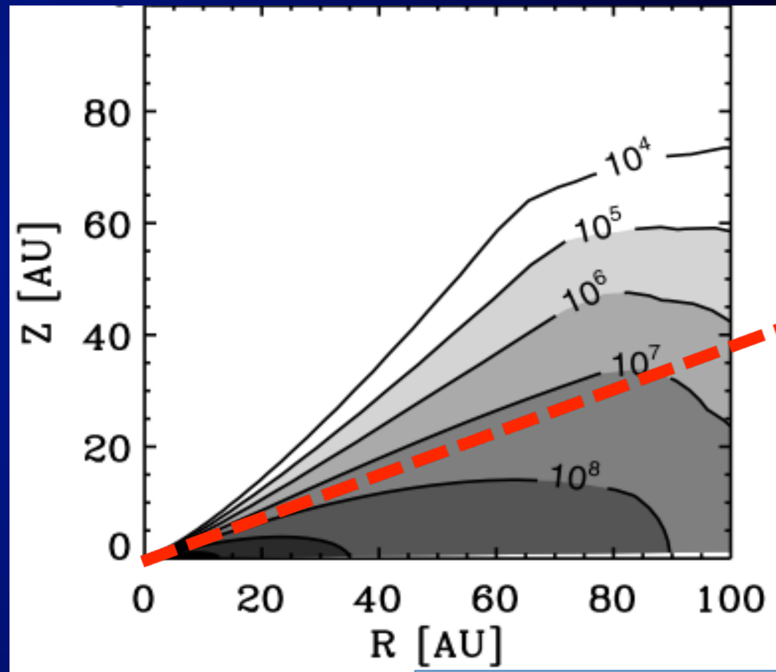
Terada+2007

CRBR 2422.8- 3423
0.8 Msun



Terada & Tokunaga 2016

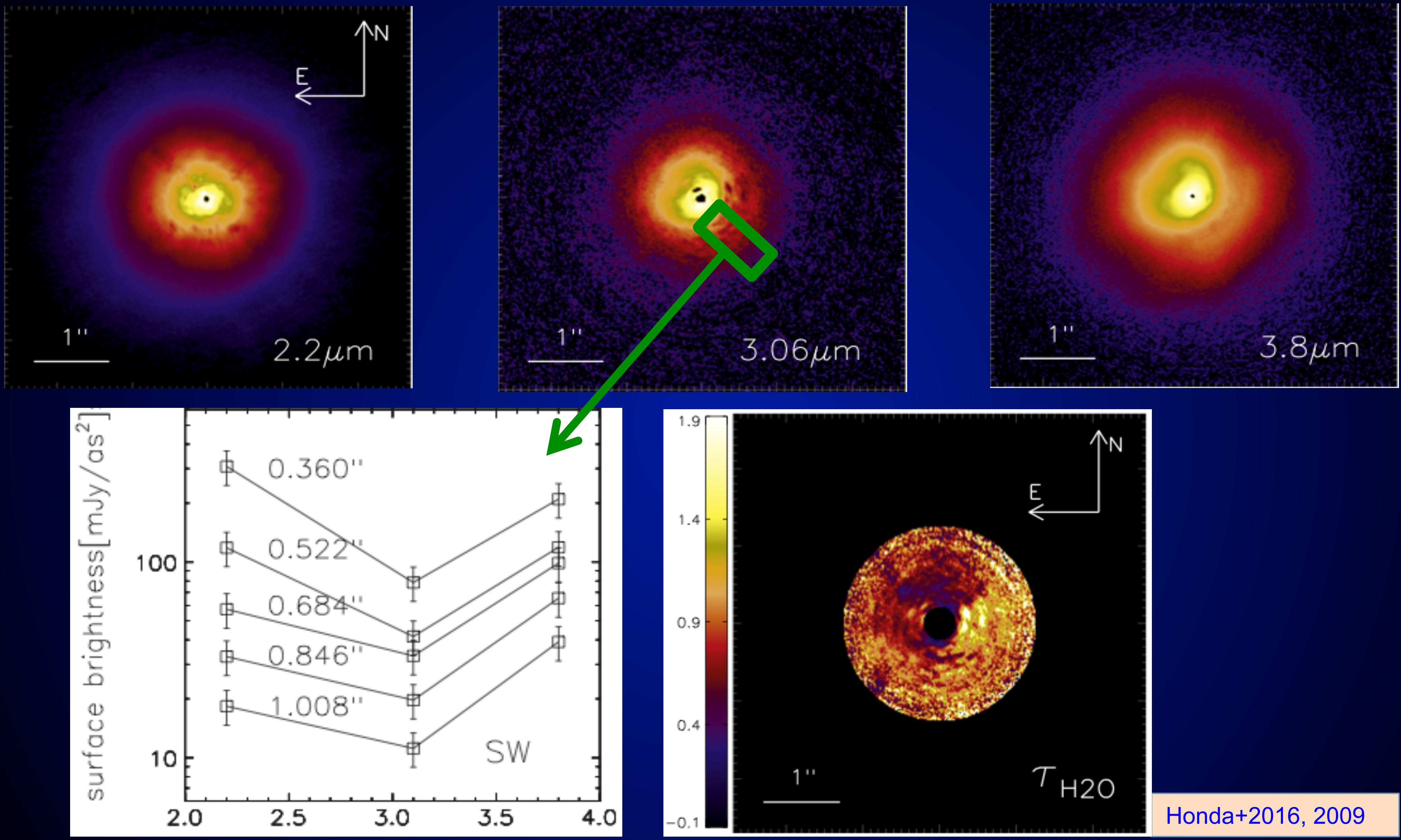




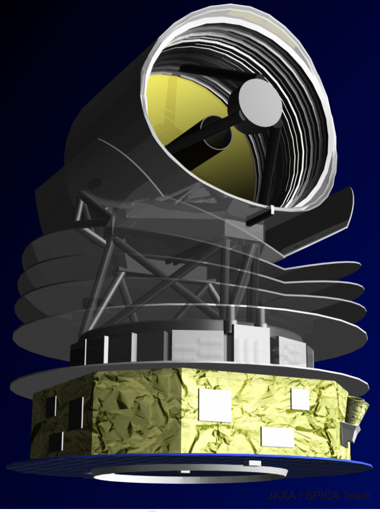
Pontoppidan+2005

« Because of the high optical depths of typical disk midplanes, ice absorption bands will often probe warmer ice located in the upper layers of nearly edge-on disks. »

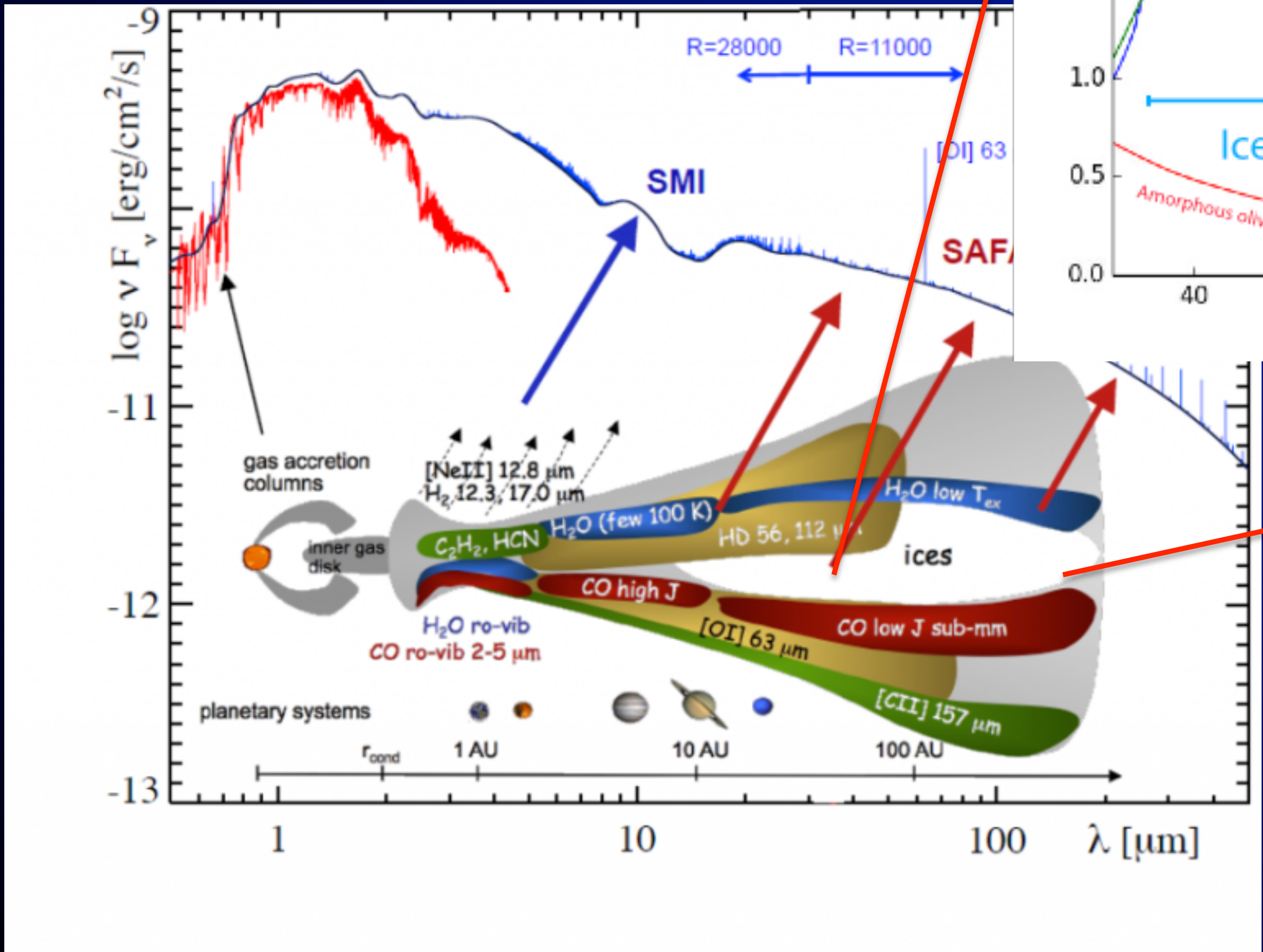
Face on disks will be observed in scattering

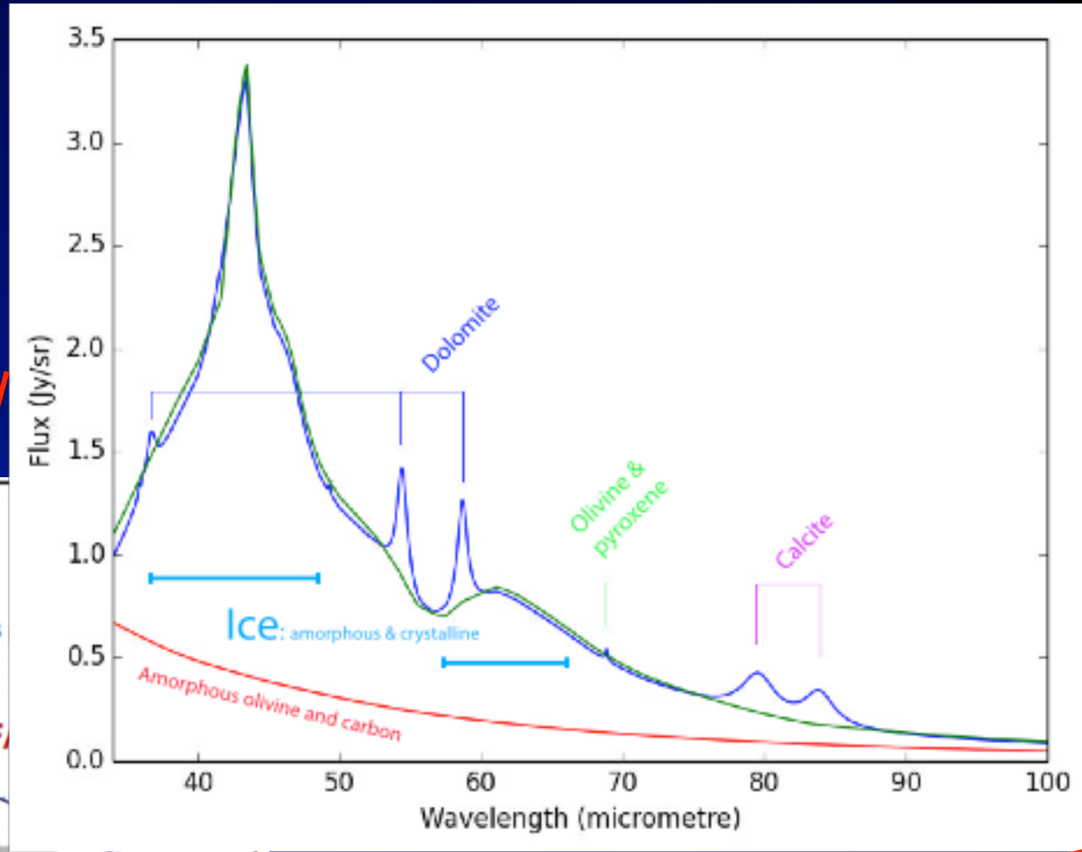


Honda+2016, 2009



https://spica-mission.org/





A full inventory like in YSOs is long term…

Gas/grains ice mantles interactions & energetic processes

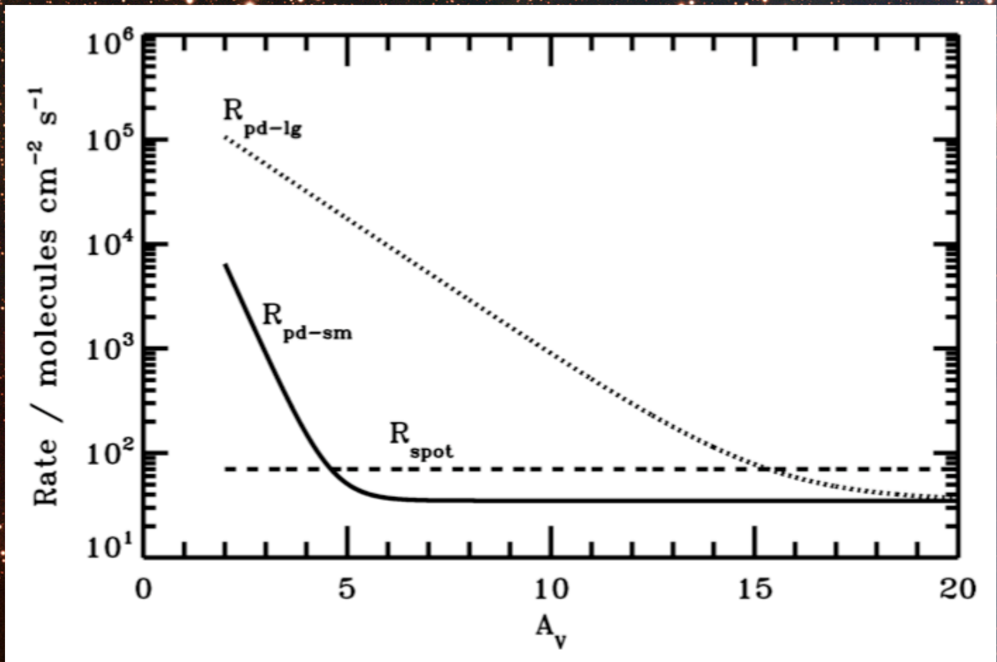
Process	Observationnally ?
Surface reactions	Indirect, composition evol
Cosmic rays Radiolysis	Specific radicals, ions ?
Sputtering (CR desorption)	Indirect, gas chemistry?
VUV Photolysis (*, ambiant, RC induced)	Ions ?
Photodesorption	Indirect, gas chemistry?
Radical Recombinaison	Release ?
Chemical desorption	
Thermal evolution	Band profiles ?

Desorption and Sputtering

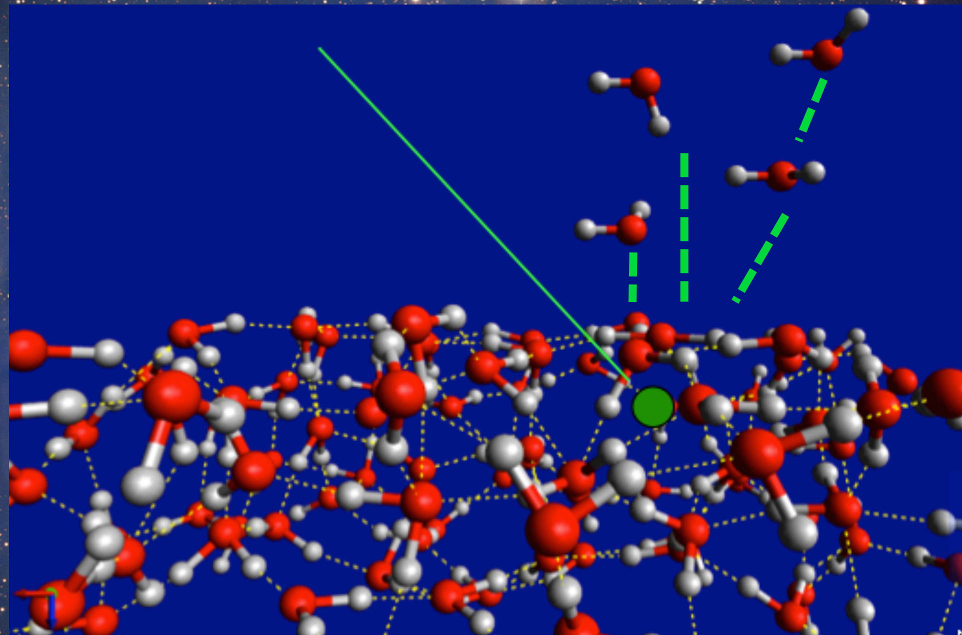
- Gas phase accretion timescale

  ~10^9 years / n_H

  ➡ everything should condense



Oberg+2007



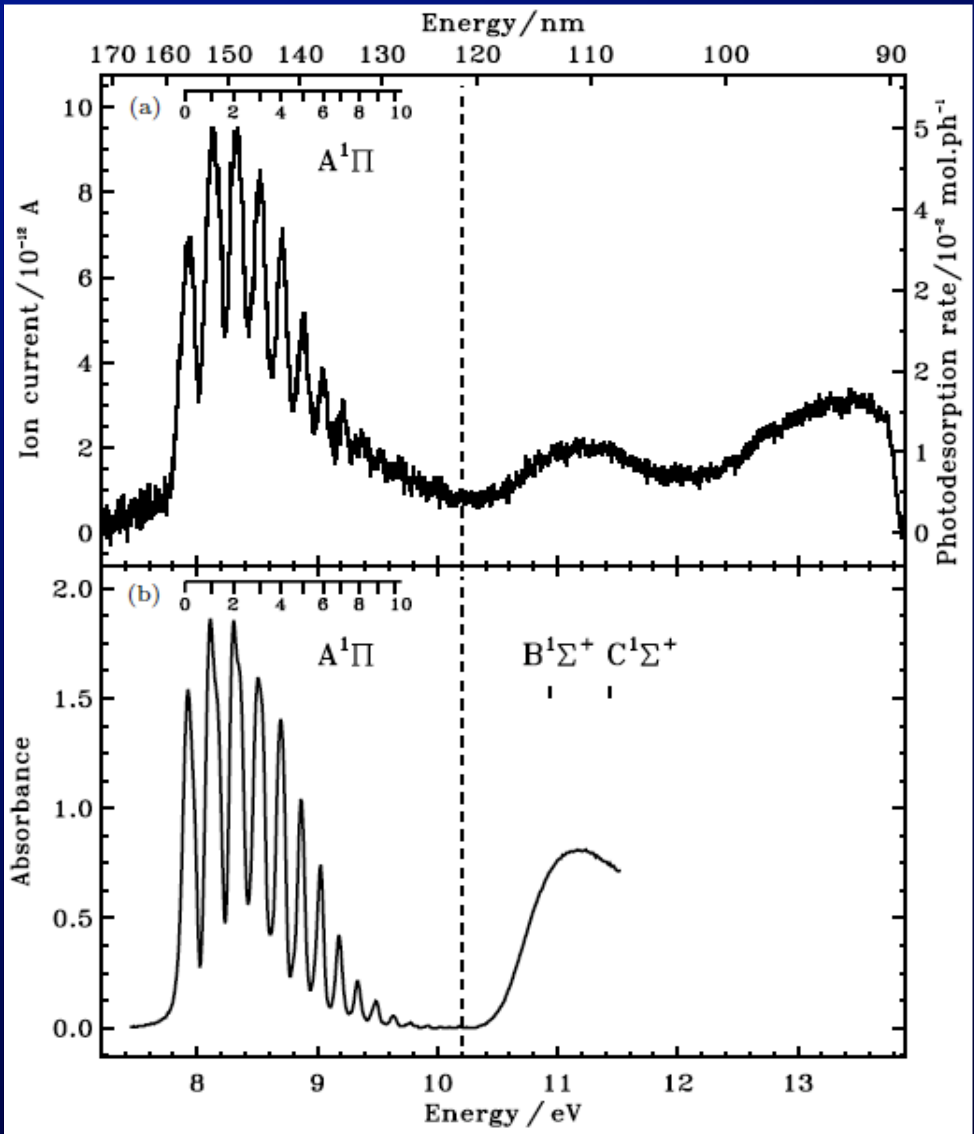
Dartois+2015

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

Lupus 3 dark cloud © ESO/F. Comeron

VUV photons desorption

Wavelength dependent measurements point that photodesorption is induced by electronic transition



Fayolle et al. 2011

CO

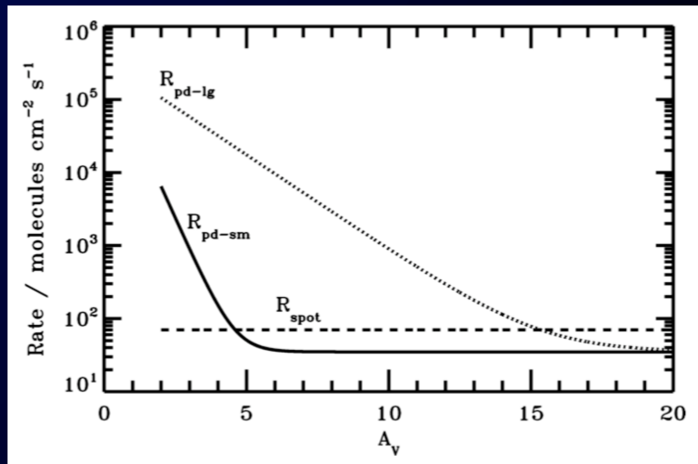
$8{\times}10^{-2}$ to 10^{-3} per hν

Oberg+ 2007, Muñoz Caro+2010,2011, Fayolle+2011, Bertin+2012, Chen+2014

In YSOs envelopes, for 10^4 hν cm^2 s^{-1}

CO rate (10^{-3}) of ~10 molecules cm^2 s^{-1}

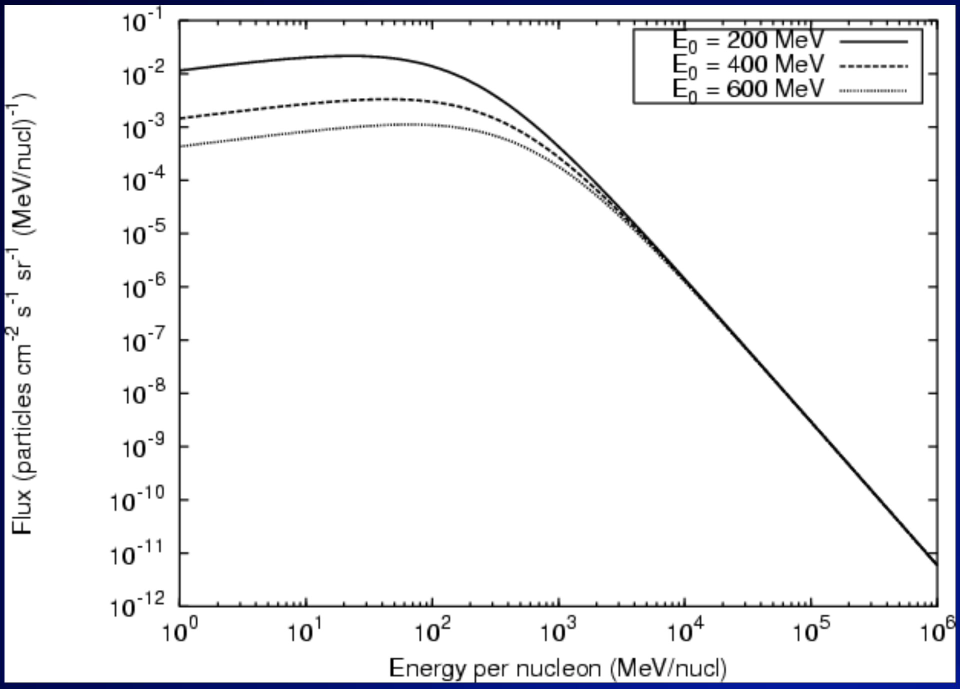
For 10^{-5} rate of ~0.1 molecules cm^2 s^{-1}



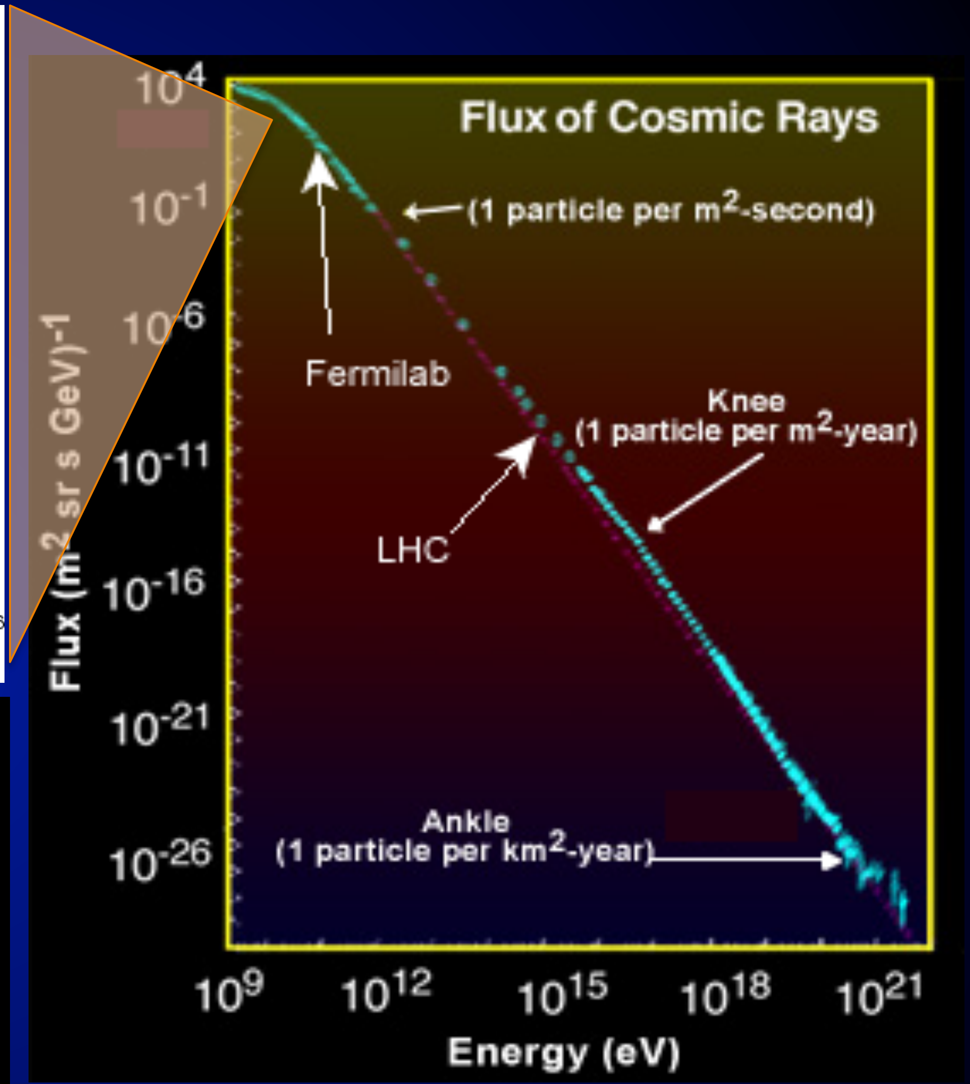
Efficient at the border of clouds, inside provide a few per thousand/percent gas phase injection

Oberg et al. 2007

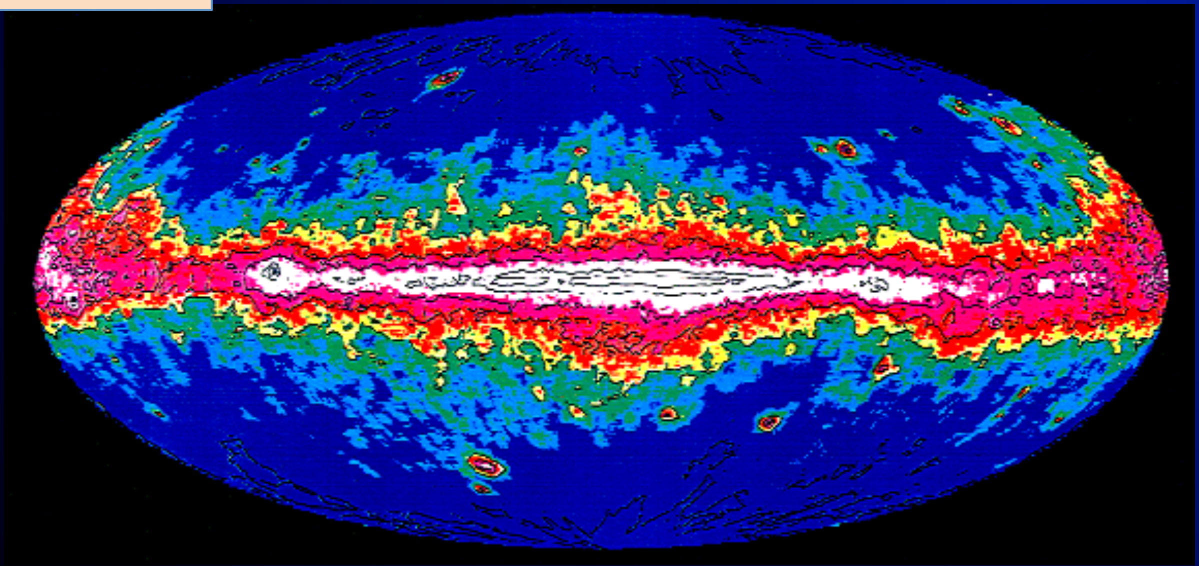
Influence of energetic cosmic rays on ices ?



Webber & Yushak 1983, Shen 2004

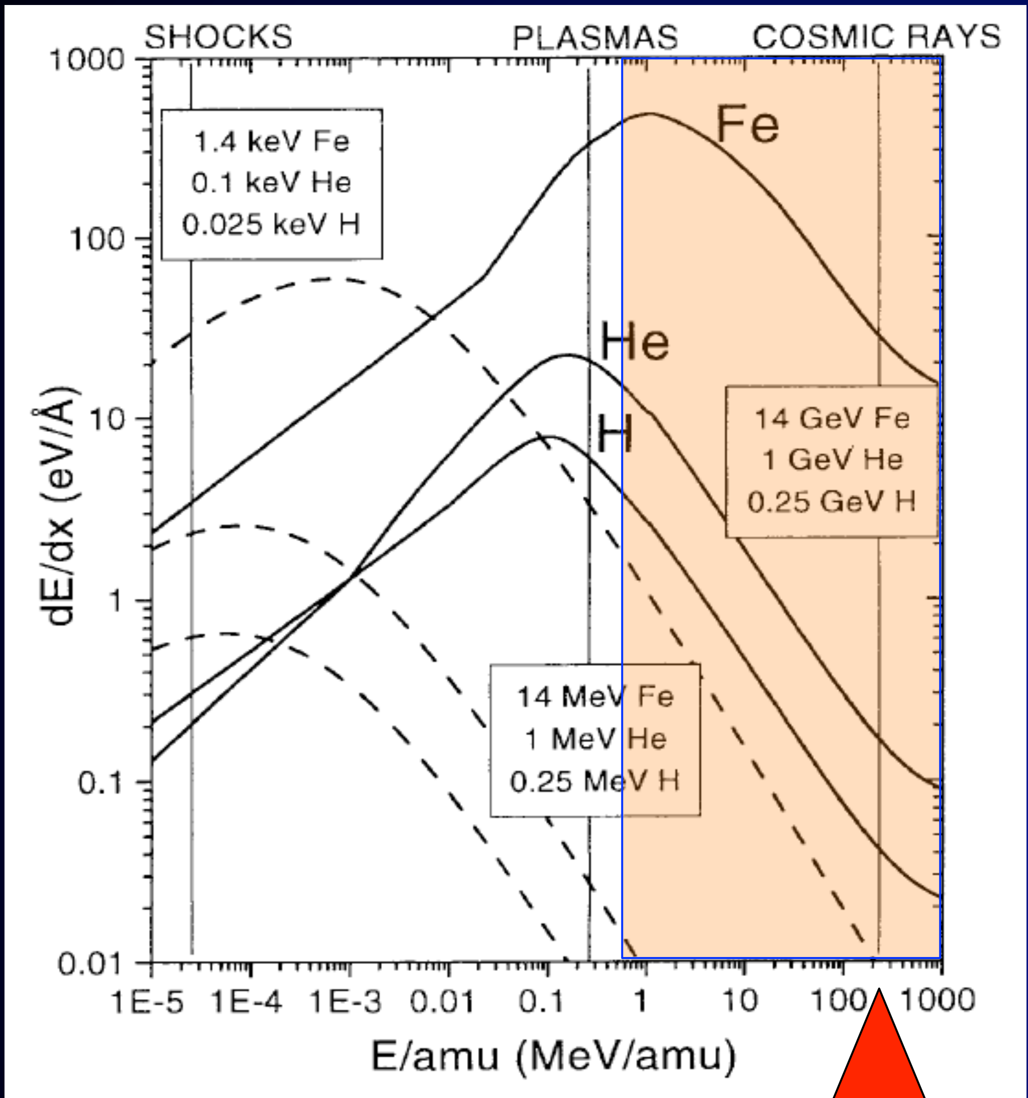


LPSC Grenoble

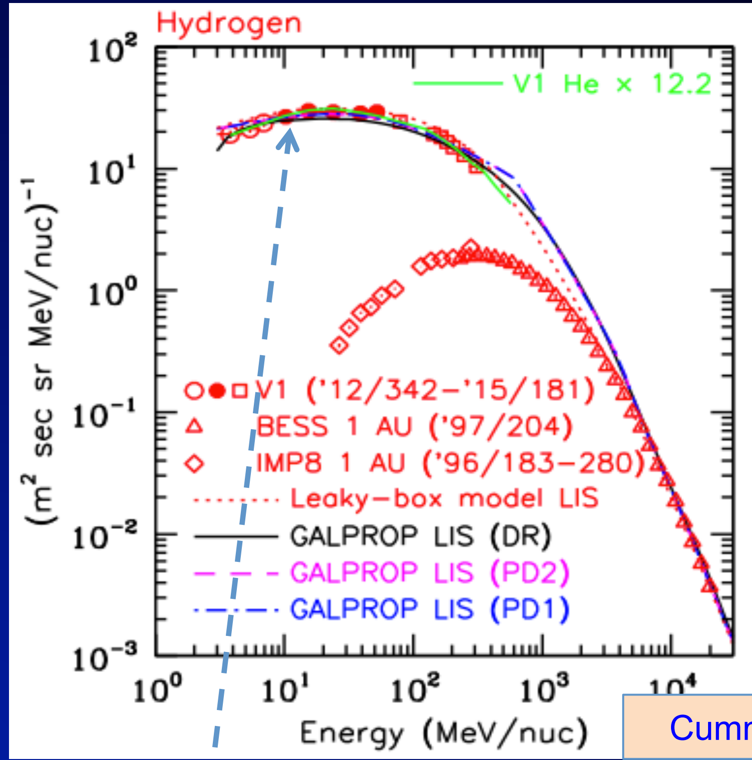


EGRET Gamma ray Galactic map

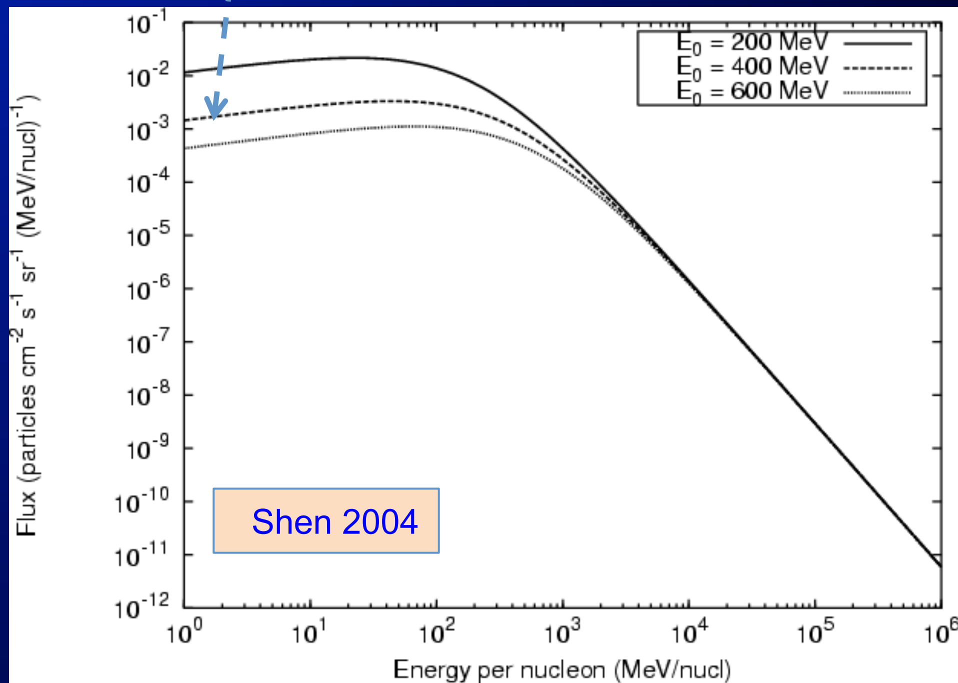
Nrj for dust astrophysics



Bringa 2003



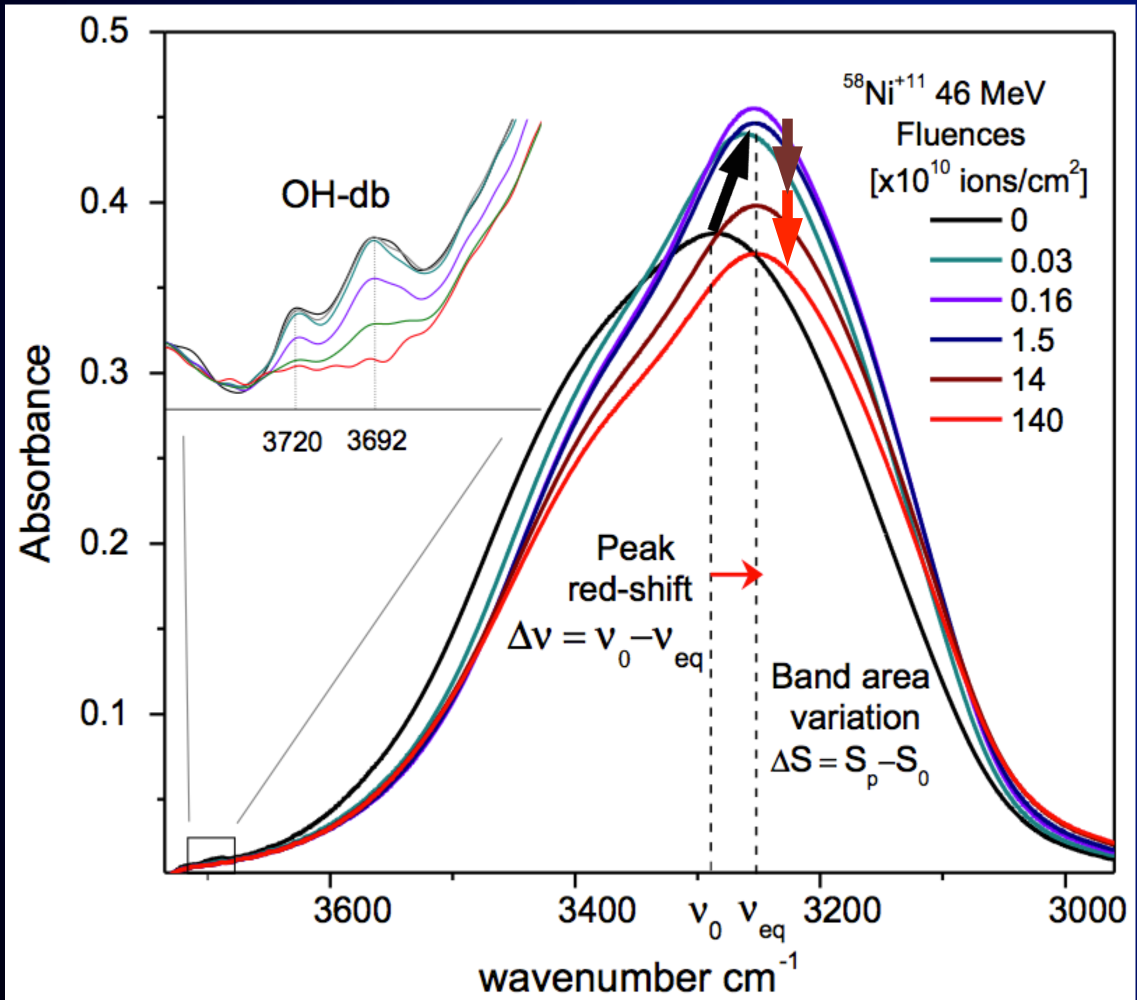
Cummings 2016



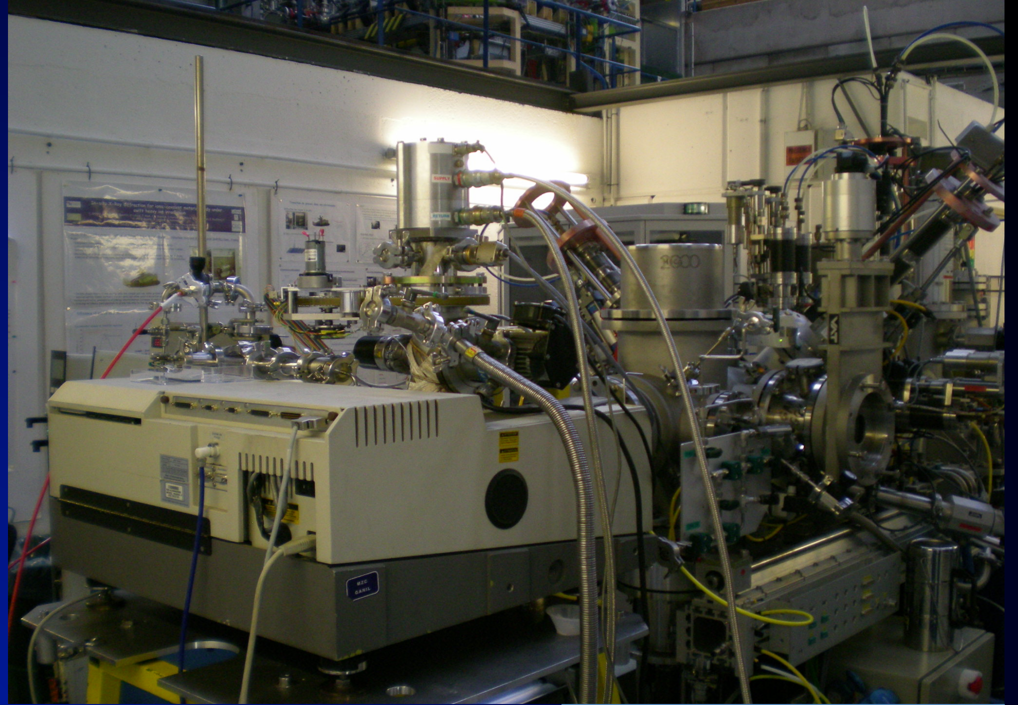
Shen 2004

~ a few 100 MeV/nucl

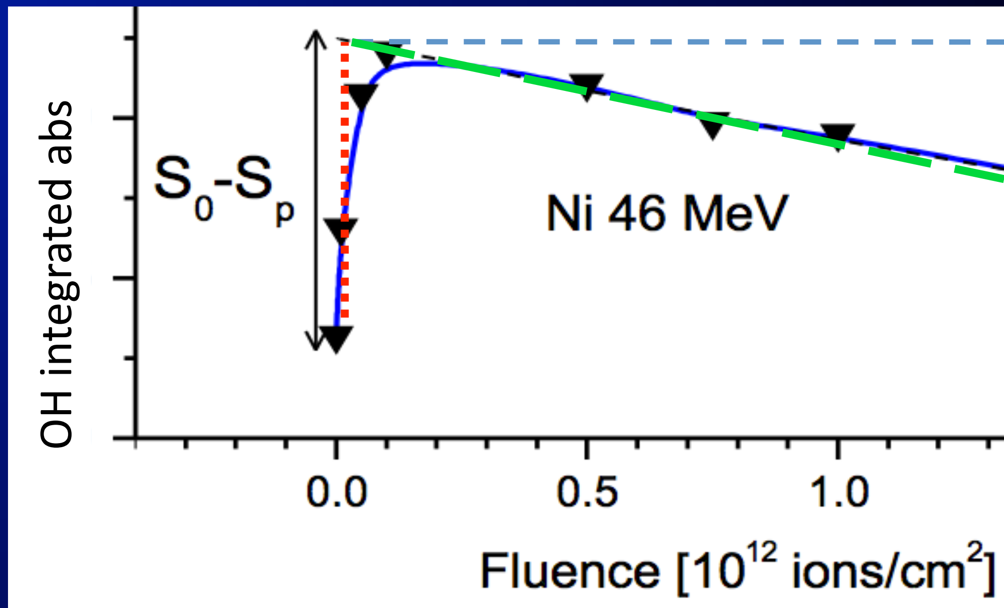
Measuring the CR sputtering yield with IR: the pure H_2O ice case



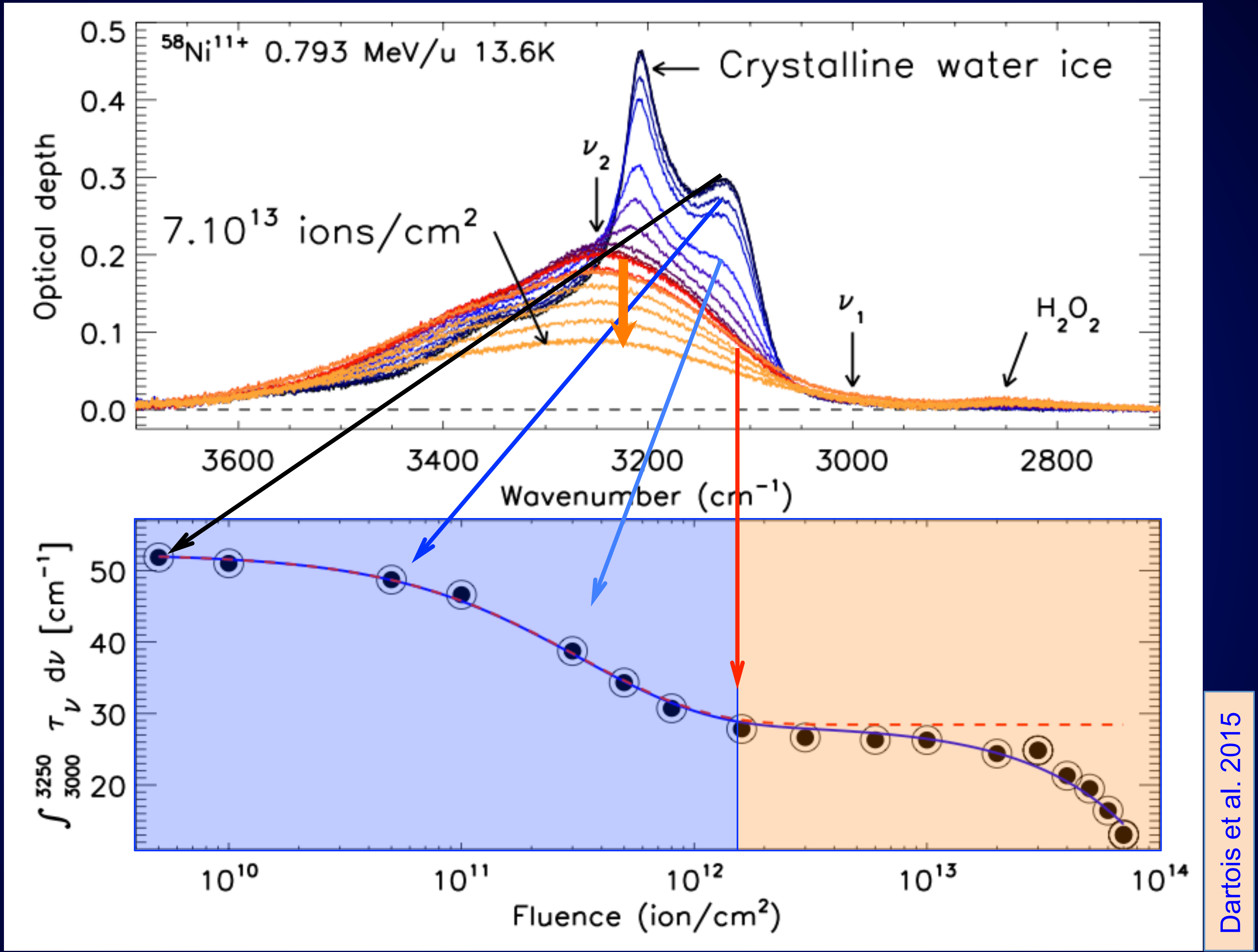
Mejia+2015, Dartois+2015, Rothard+2016

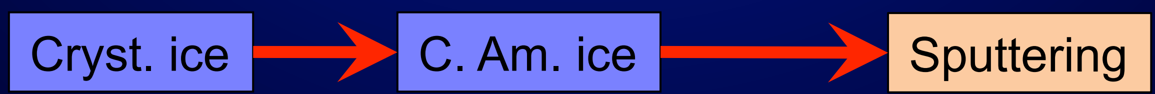


CASIMIR Setup/GANIL

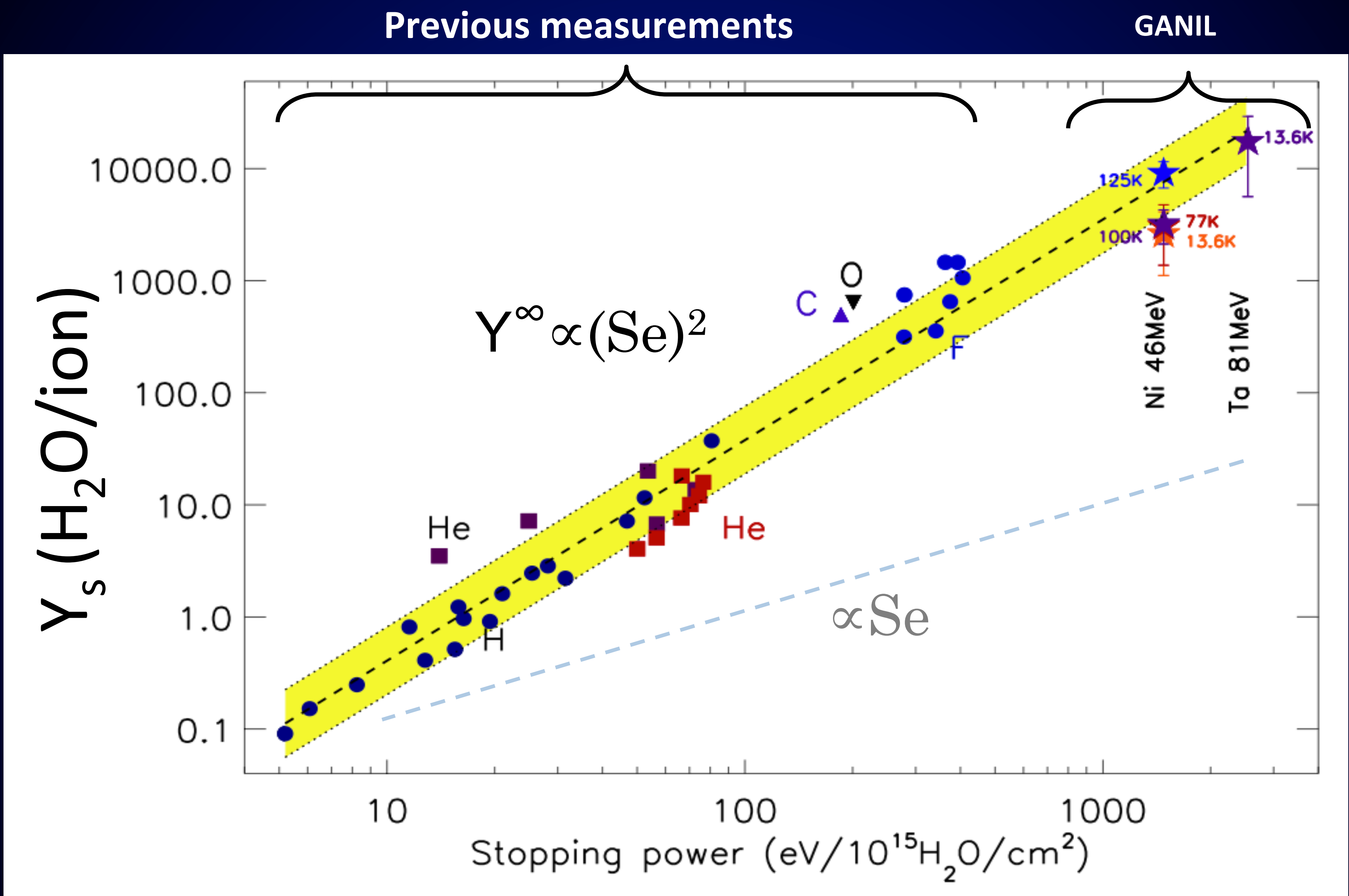


Measuring the sputtering with IR



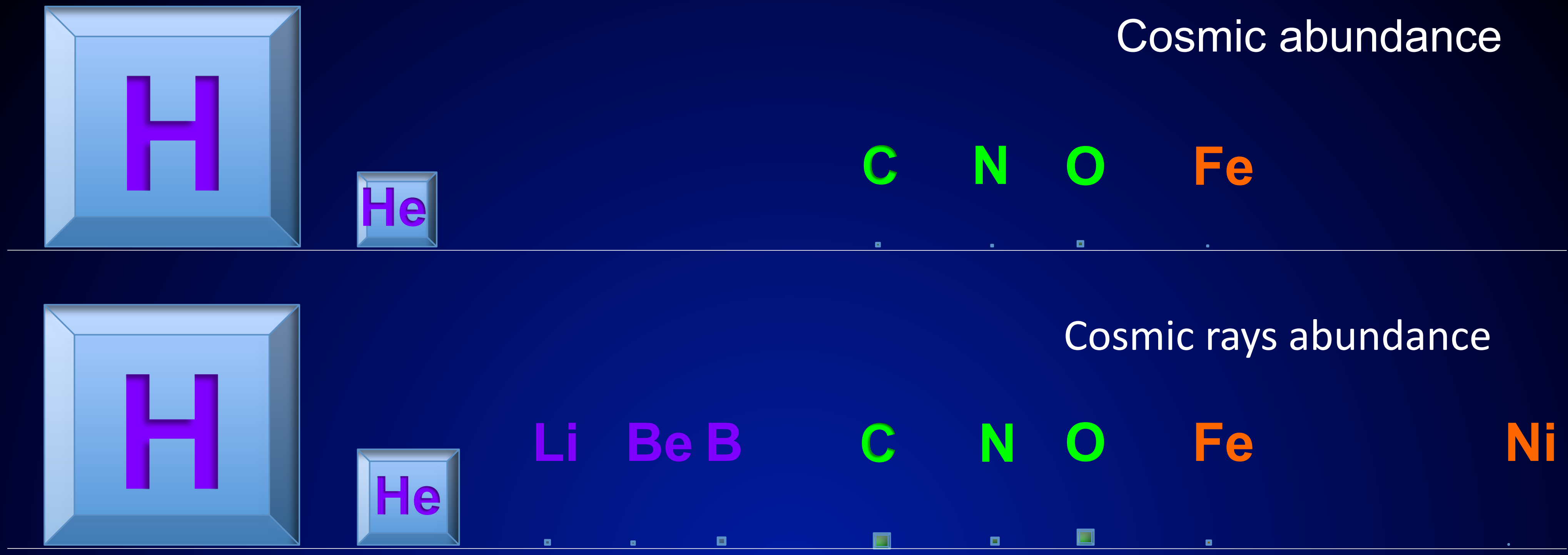


Semi-∞ sputtering yield

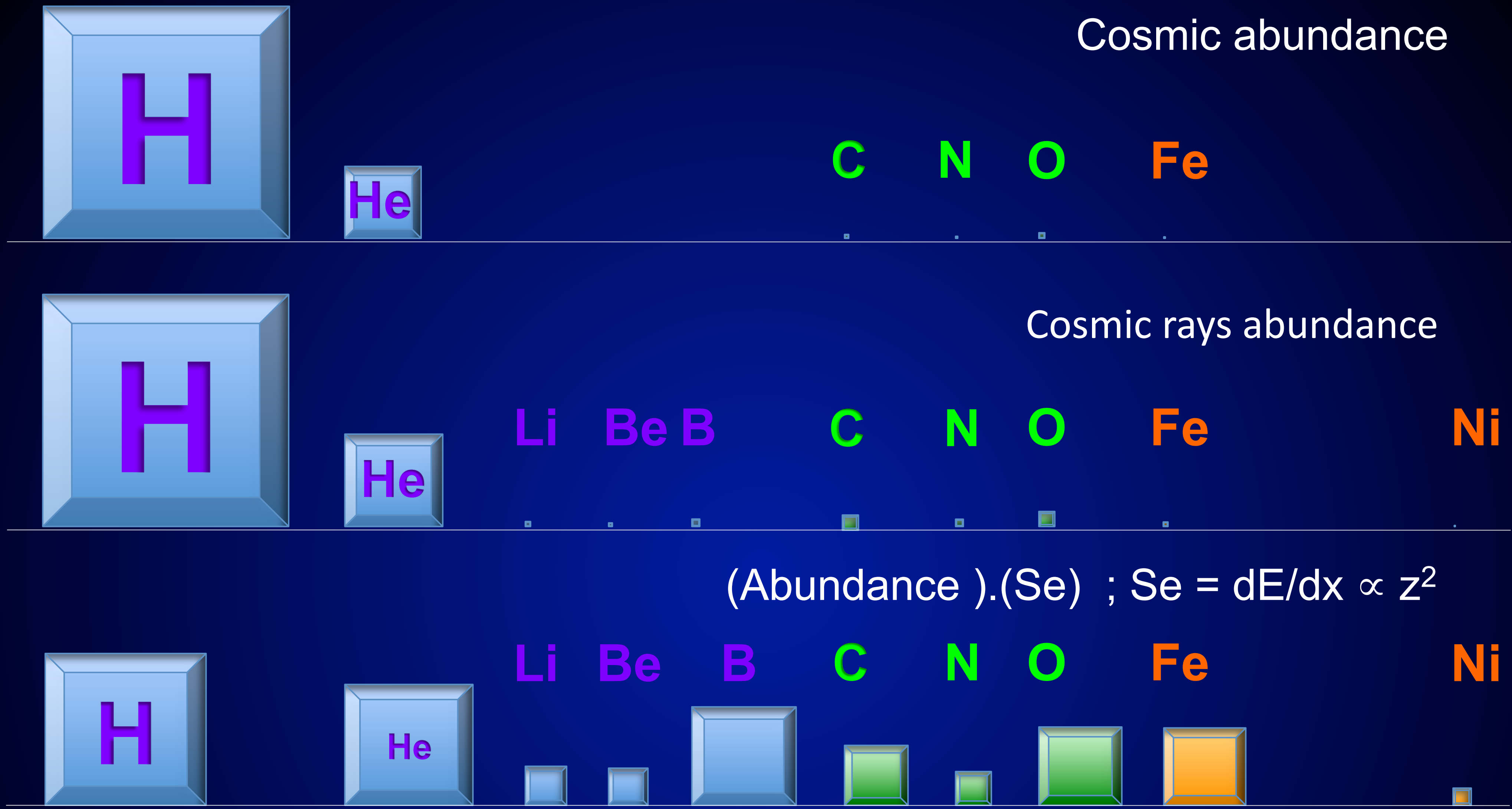


Brown et al. 1984 and ref therein

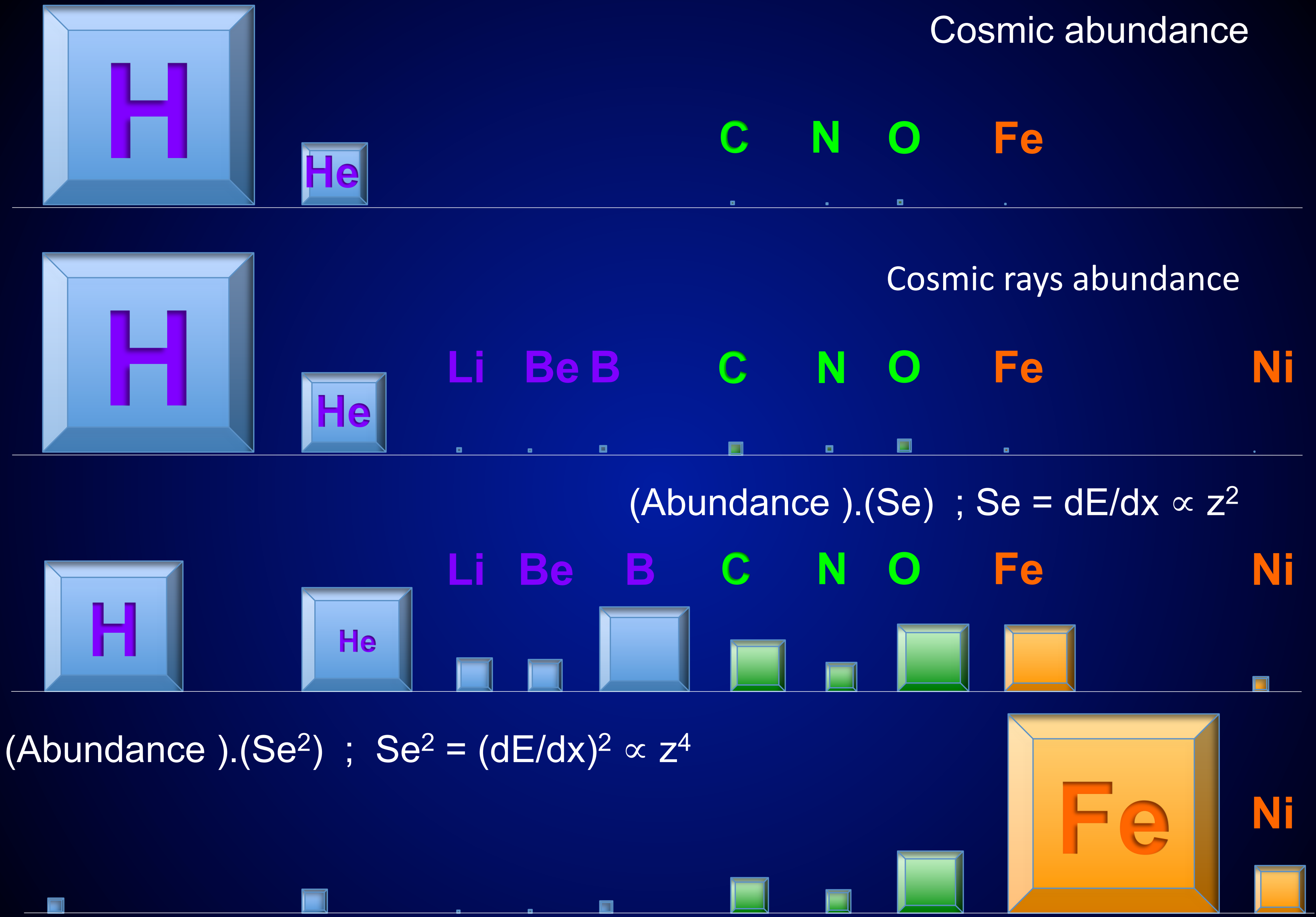
Dartois et al. 2015


Cosmic abundance
H
He
C
N
O
Fe
Cosmic rays abundance
H
He
Li
Be B
C
N
O
Fe
Ni

Chabot 2018

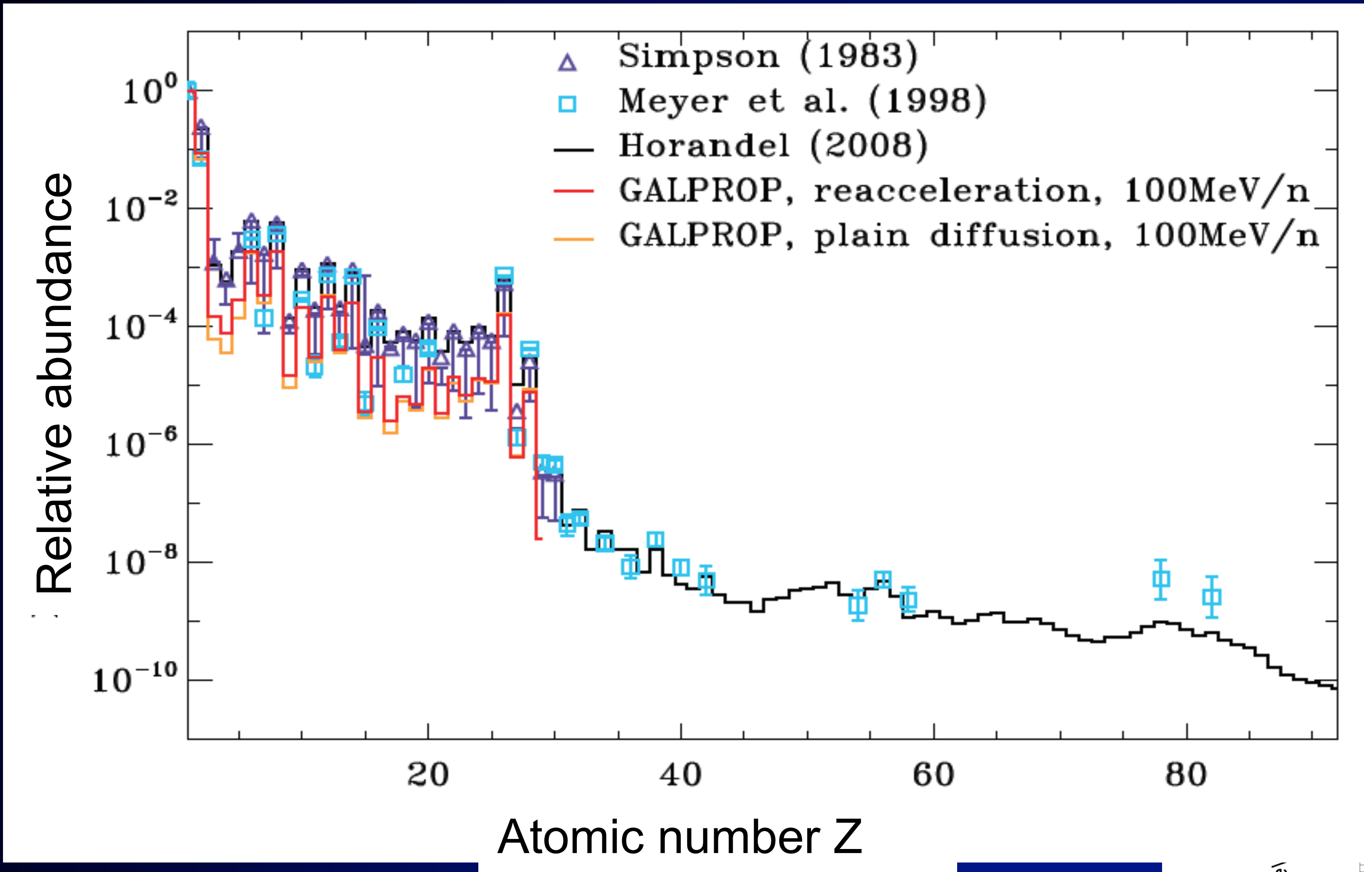

Cosmic abundance
H
He
C
N
O
Fe
Cosmic rays abundance
H
He
Li
Be B
C
N
O
Fe
Ni
(Abundance).(Se) ; Se = dE/dx $\propto z^2$
H
He
Li
Be
B
C
N
O
Fe
Ni

Chabot 2018


Cosmic abundance
H
He
C
N
O
Fe
Cosmic rays abundance
H
He
Li
Be
B
C
N
O
Fe
Ni
(Abundance).(Se) ; Se = dE/dx ∝ z^2
H
He
Li
Be
B
C
N
O
Fe
Ni
(Abundance).(Se^2) ; Se^2 = $(dE/dx)^2$ ∝ z^4
Fe
Ni

Chabot 2018

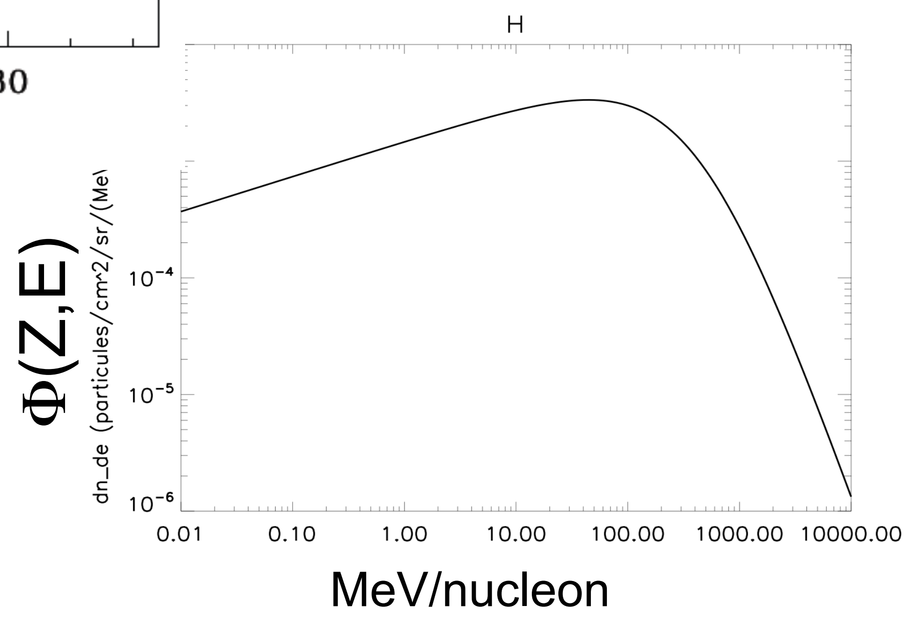
Inserting into astrophysical models

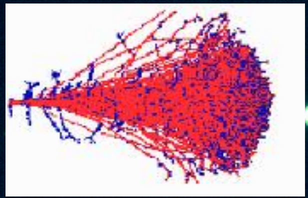


f (Z)

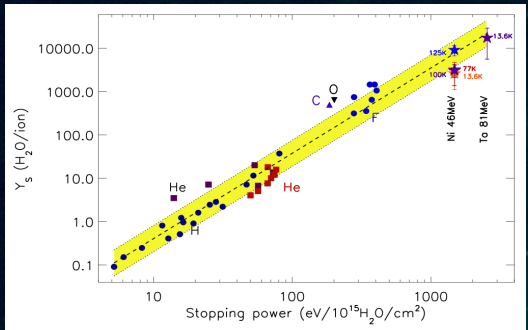
Godard et al. 2011

$\Phi(Z,E)$





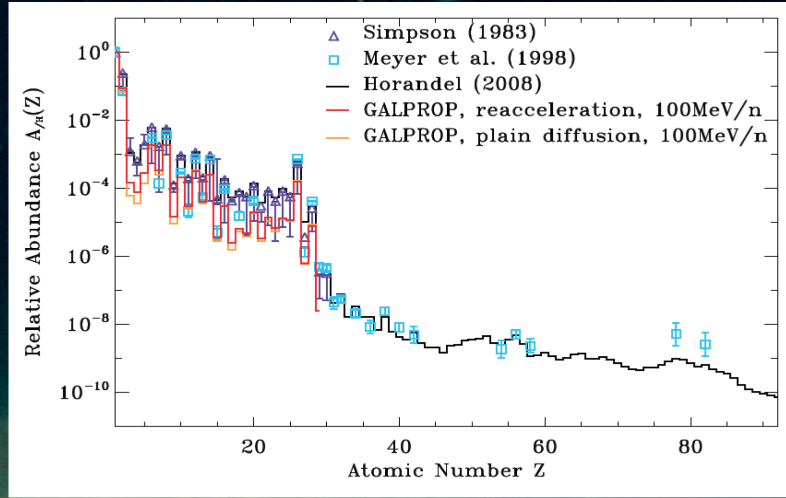
Se(Z,E)



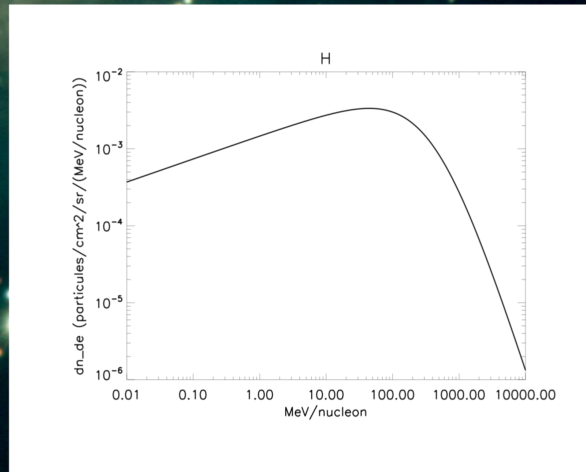
Y^∞(Se)

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

f (Z)



Φ(Z,E)

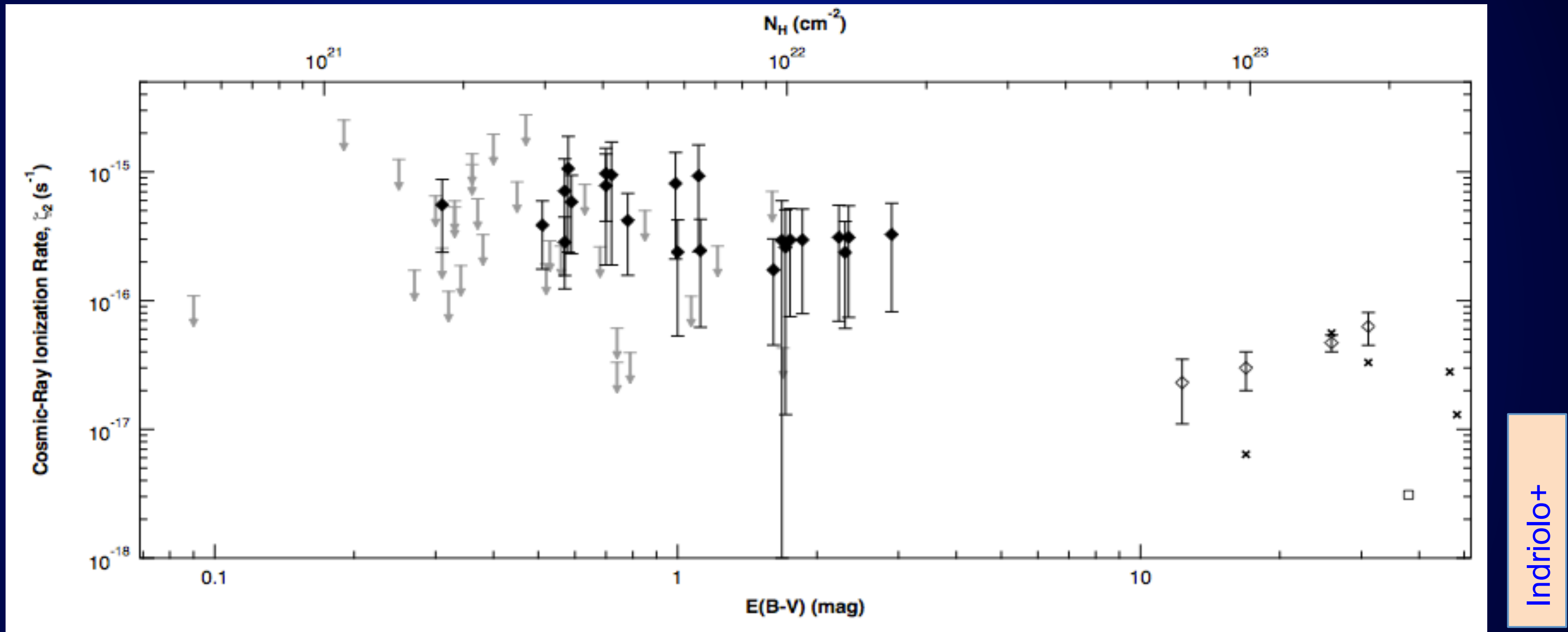


CR desorption rate:

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

H_2O CR sputtering rate

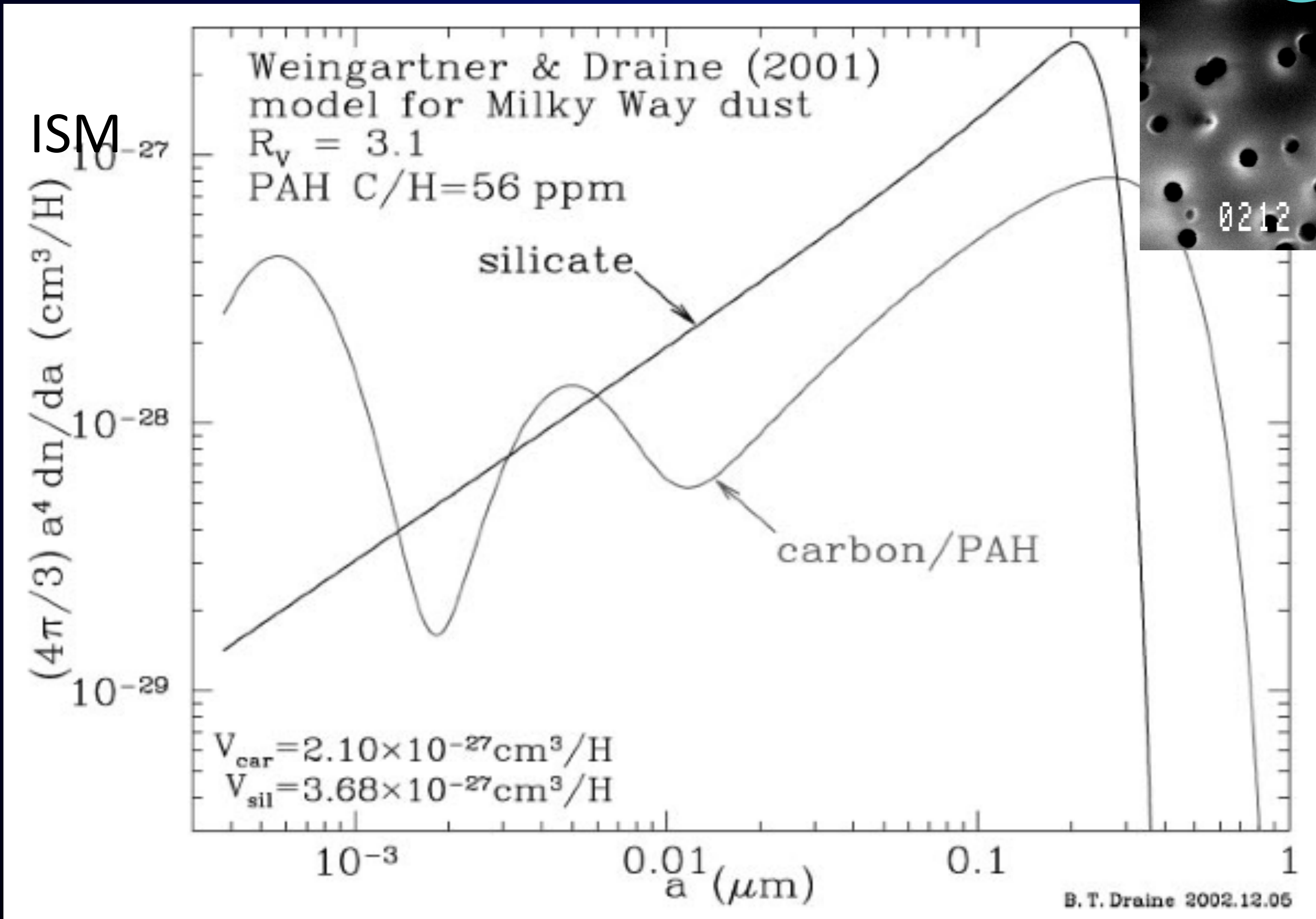
$\eta_{\text{CR sputtering}} \approx 10\ H_2O/cm^2/s$ for $\zeta = 10^{-16} s^{-1}$

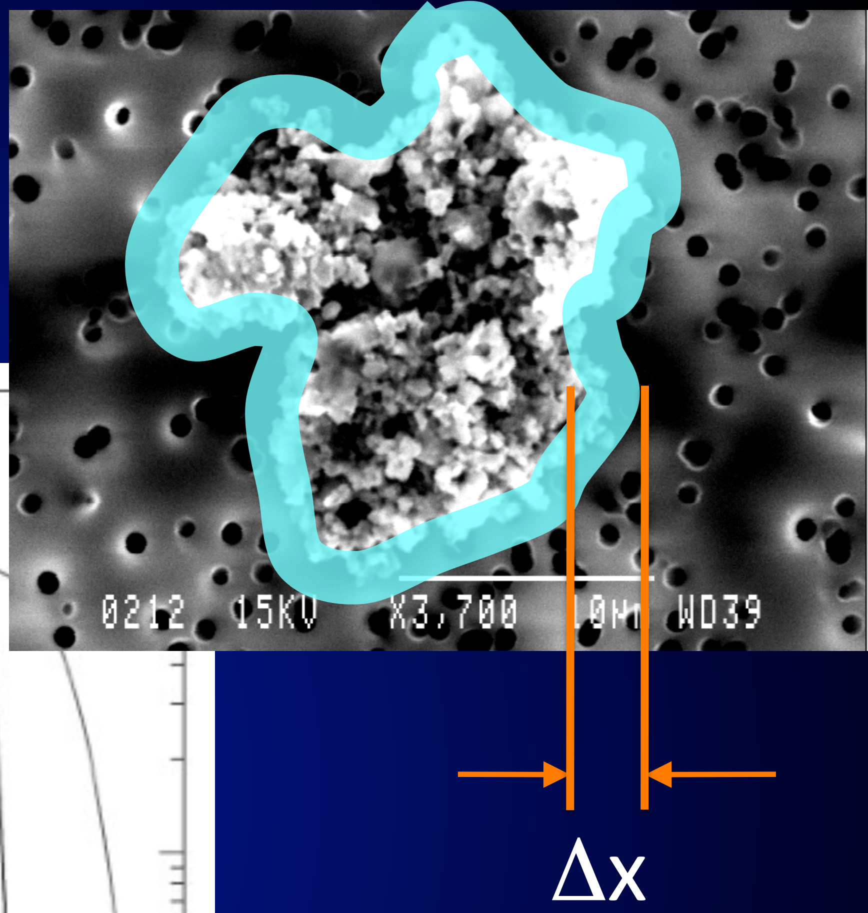


Comparison to energetic secondary photons induced by CRs:

$\eta_{\text{photodesorption}} \approx 10\ H_2O/cm^2/s\ (Y \approx 10^{-3})$

Interstellar
Grain size distribution ?

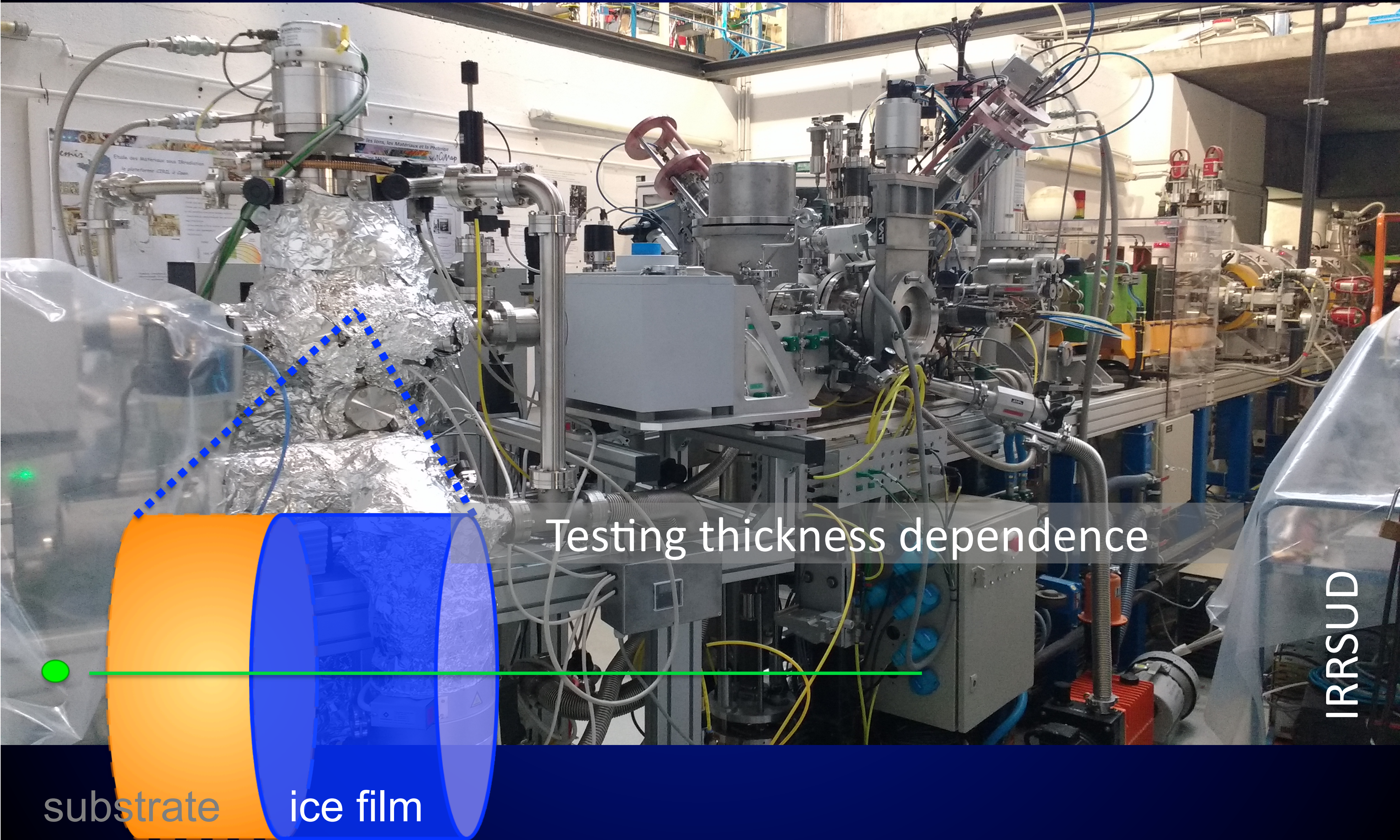




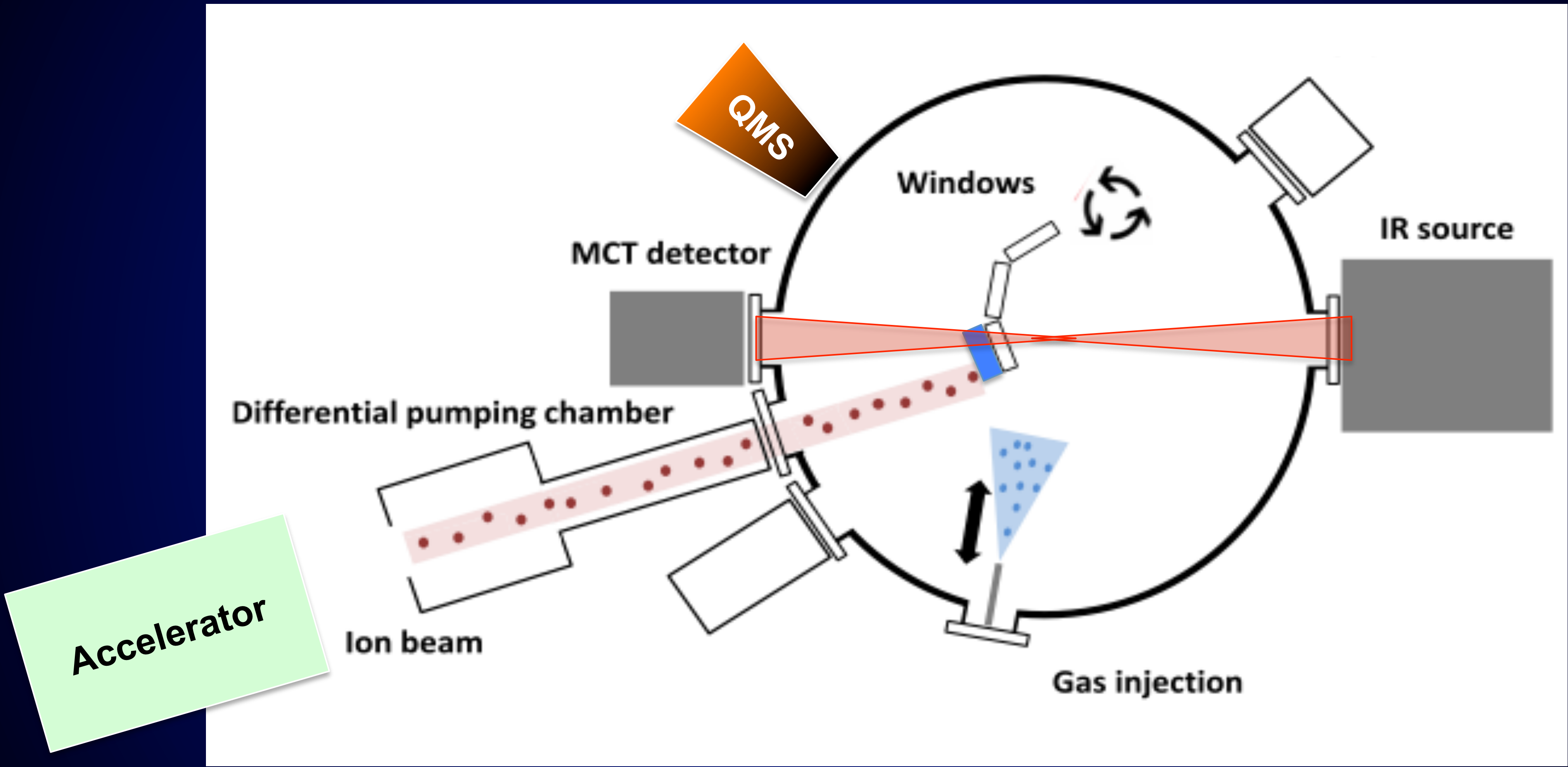
Ice mantle thickness

ANR IGLIAS (CIMAP/IPNO/ISMO) : New setup

Thèse Basile Augé 2017

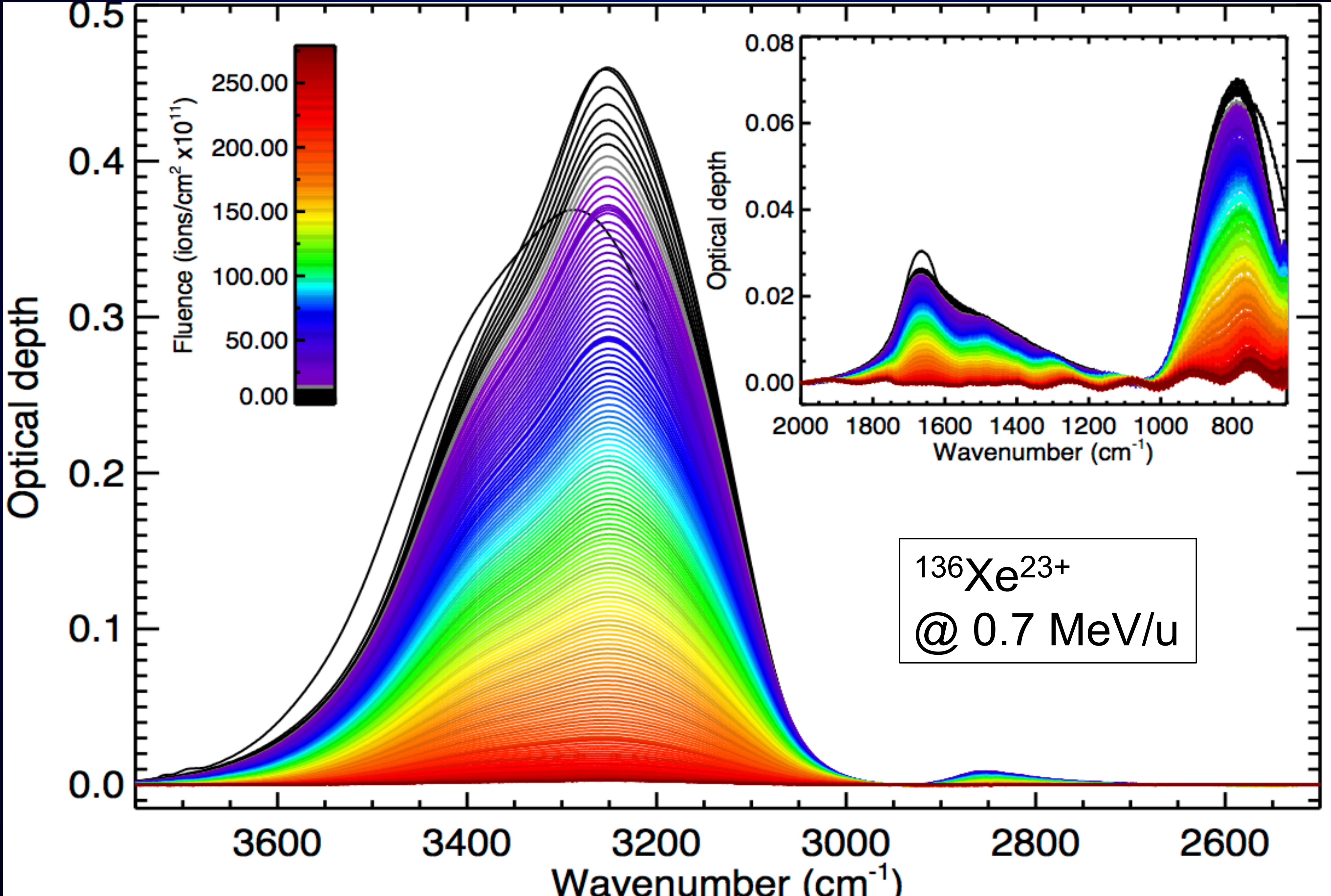


IGLIAS

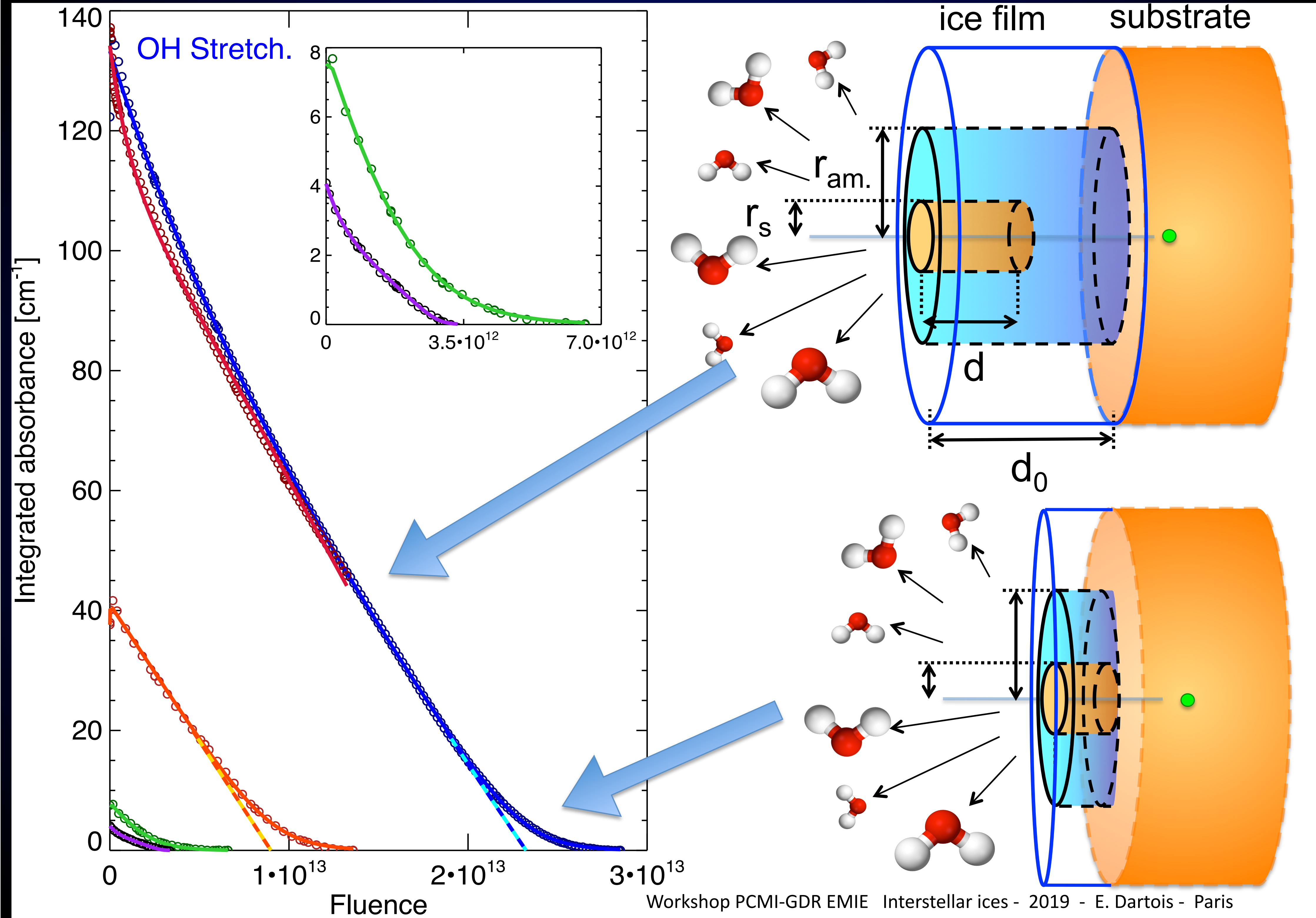


Augé+2018

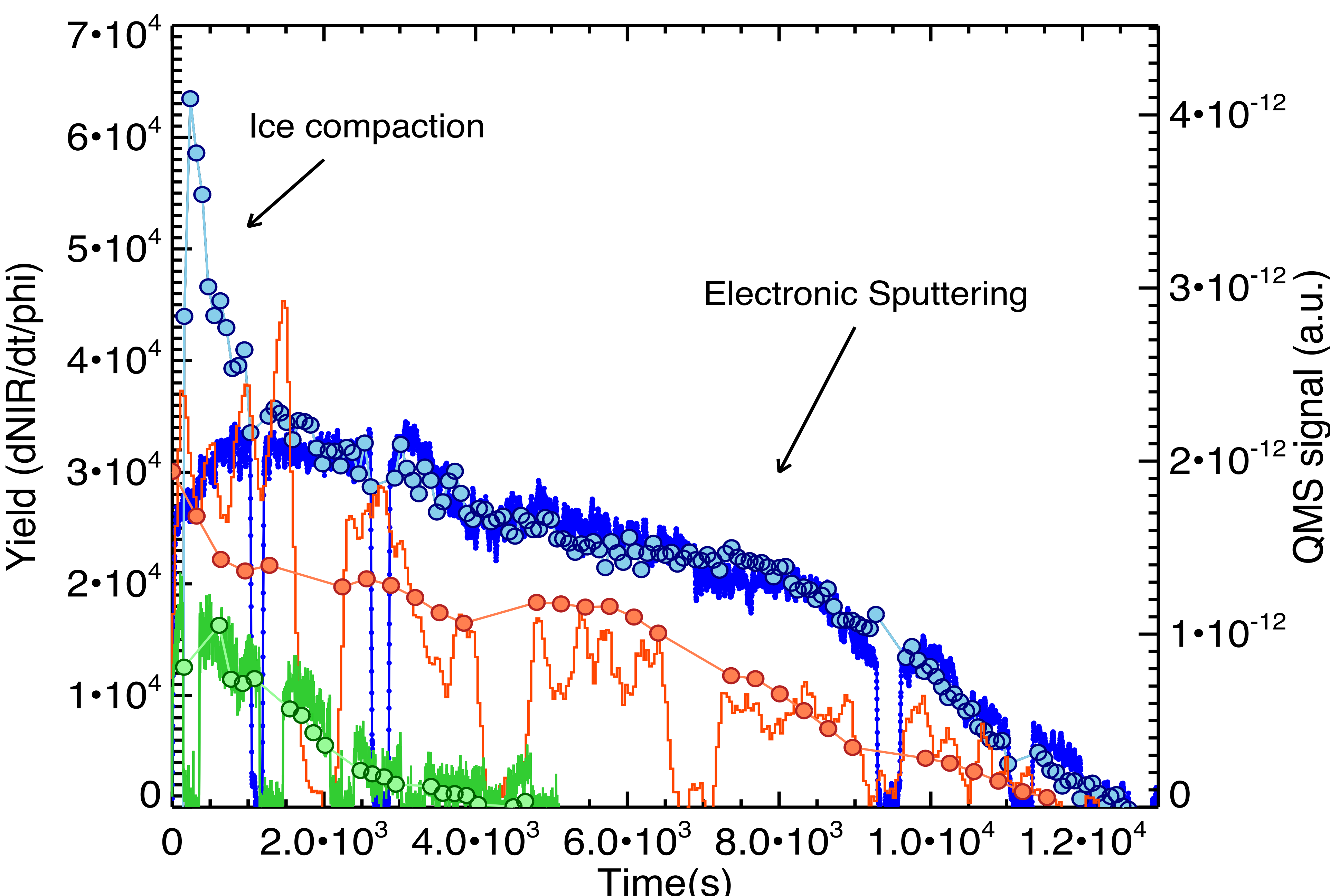
Ice infrared spectra evolution upon SHI irradiation



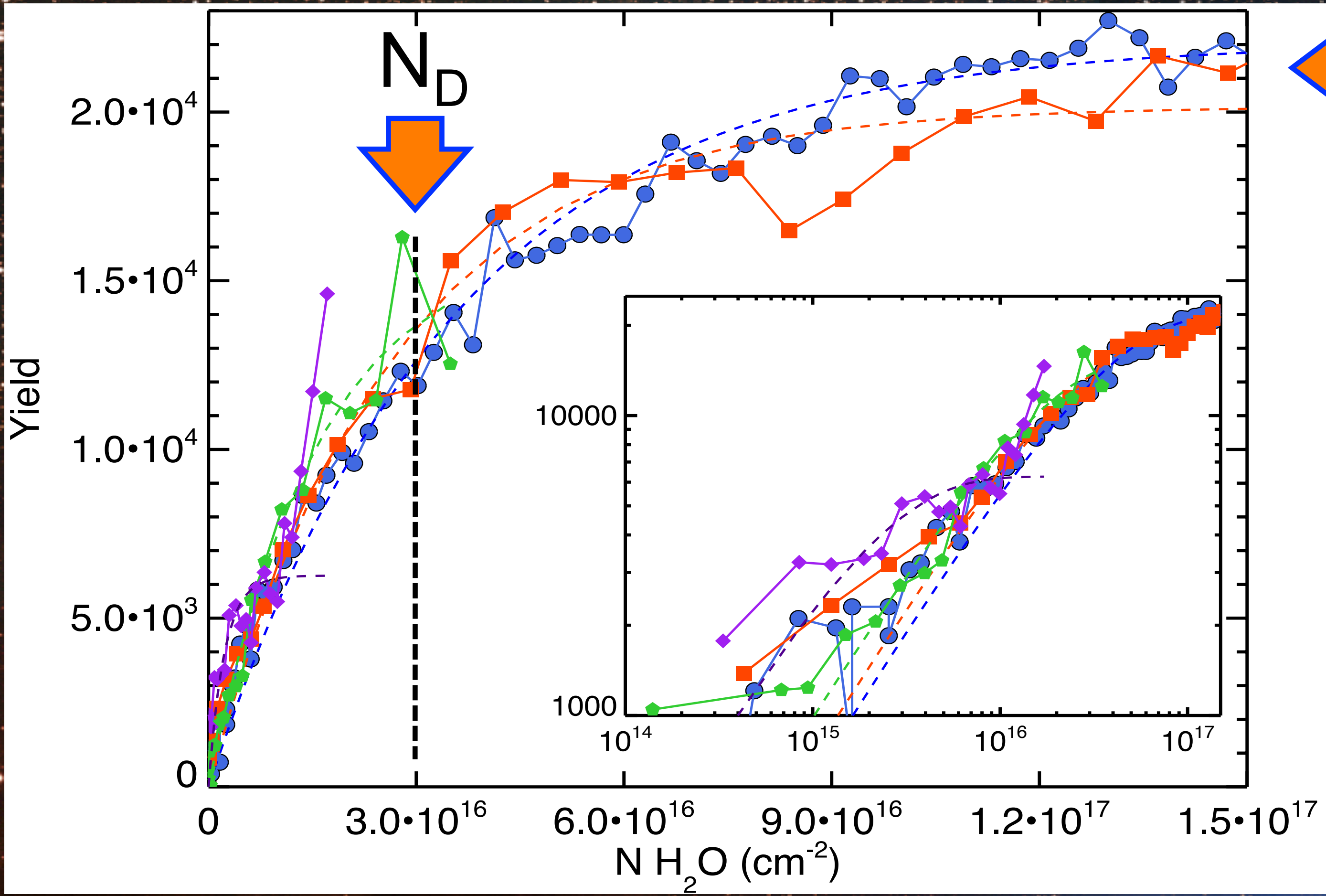
Dartois+2018

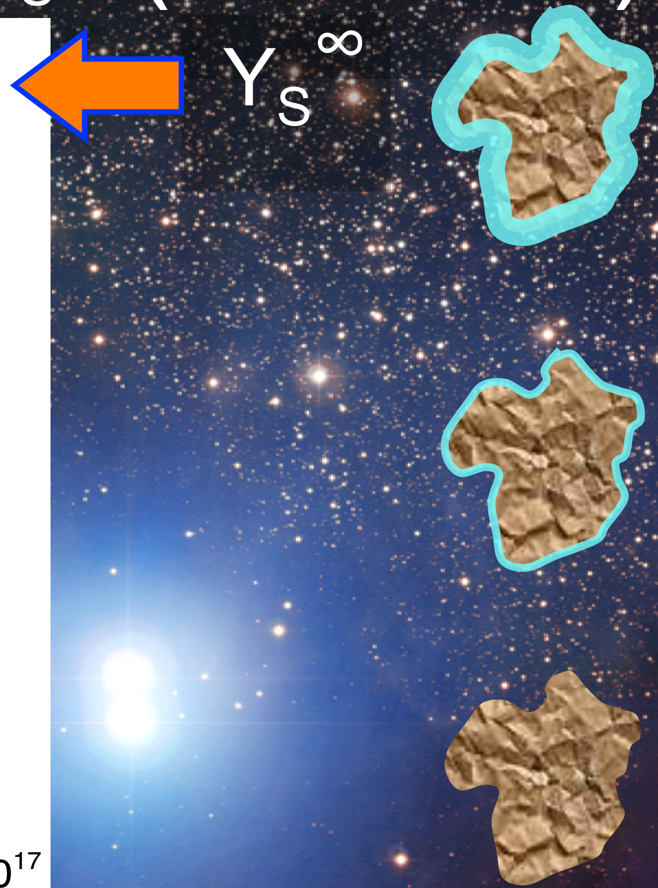

OH Stretch.
Integrated absorbance [cm-1]
Fluence
0
1•10^13
2•10^13
3•10^13
3.5•10^12
7.0•10^12
ice film
substrate
r_am.
r_s
d
d_0

QMS versus Infrared



Yield thickness dependence $\approx -Y_S^{\infty}\left(1-e^{(-N/Nd)}\right)$



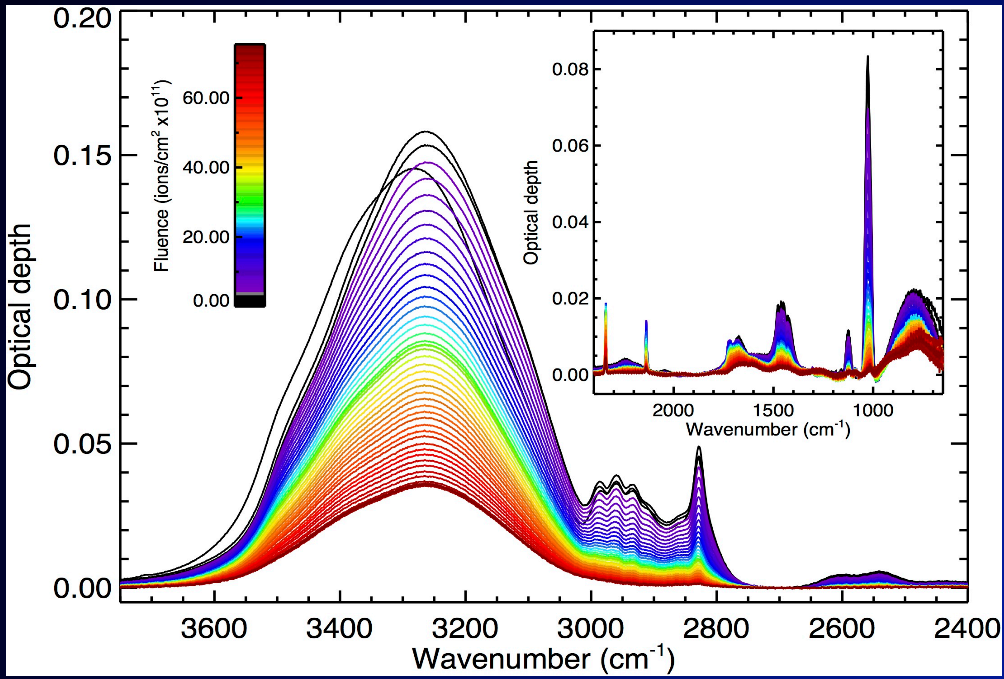


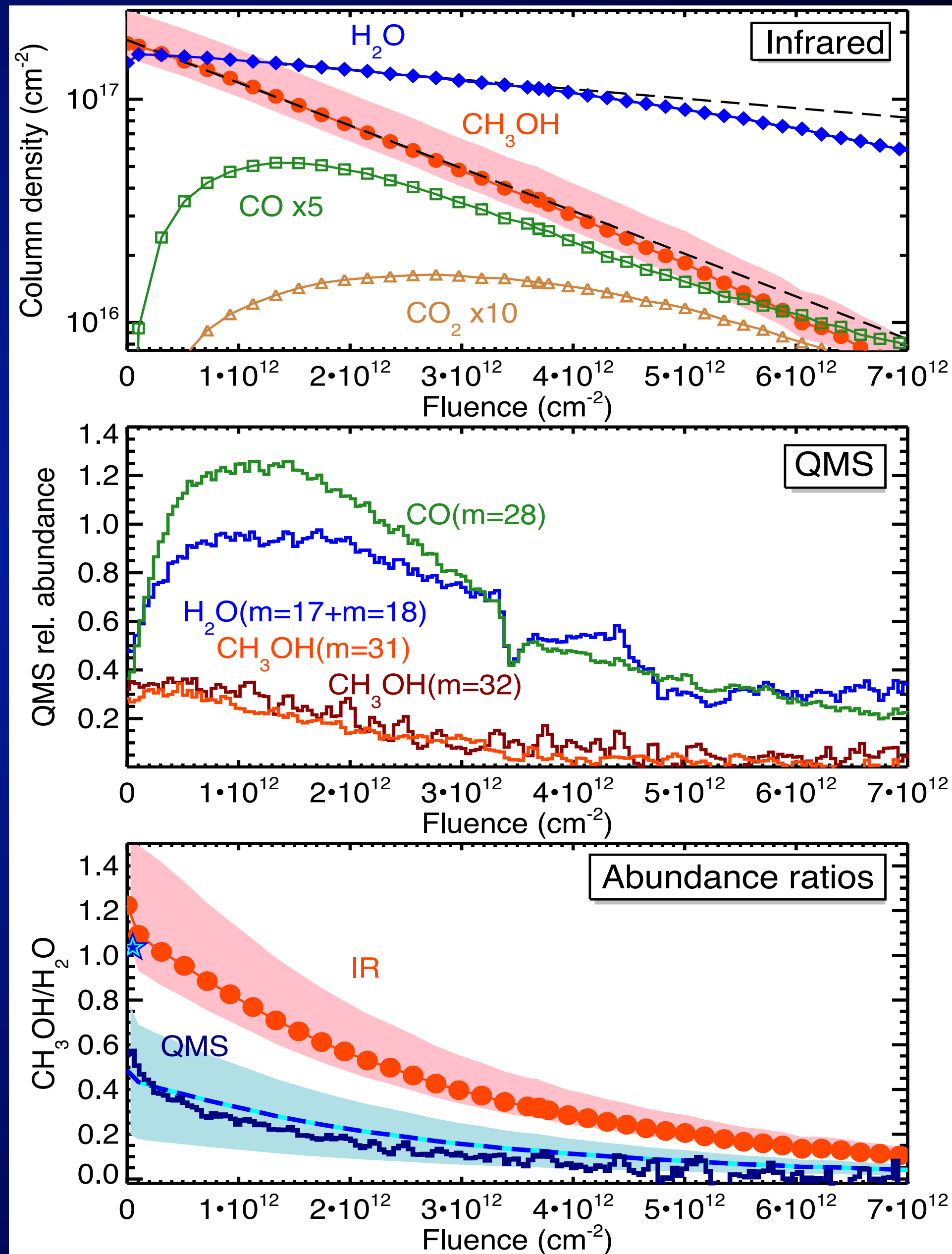
$Y_S^{\infty} \sim 2.10^4\ H_2O/ion$

$Nd \sim 3.10^{16}\ H_2O/cm^2$, i.e. about 30 ml

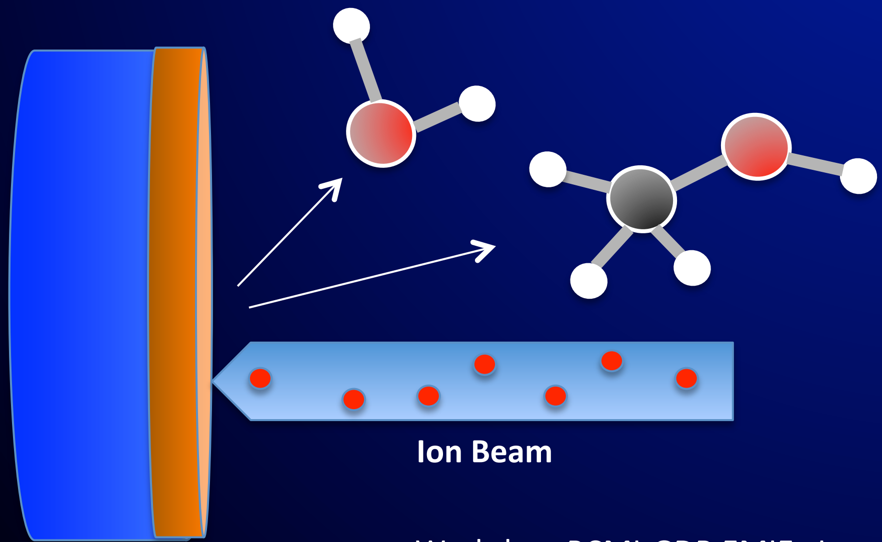
- Provides Anchor point
- Prescription (A.R.) of dependency with Se for astro

C.R. sputtering of complex organic molecules in ice:
the CH_3OH/H_2O case

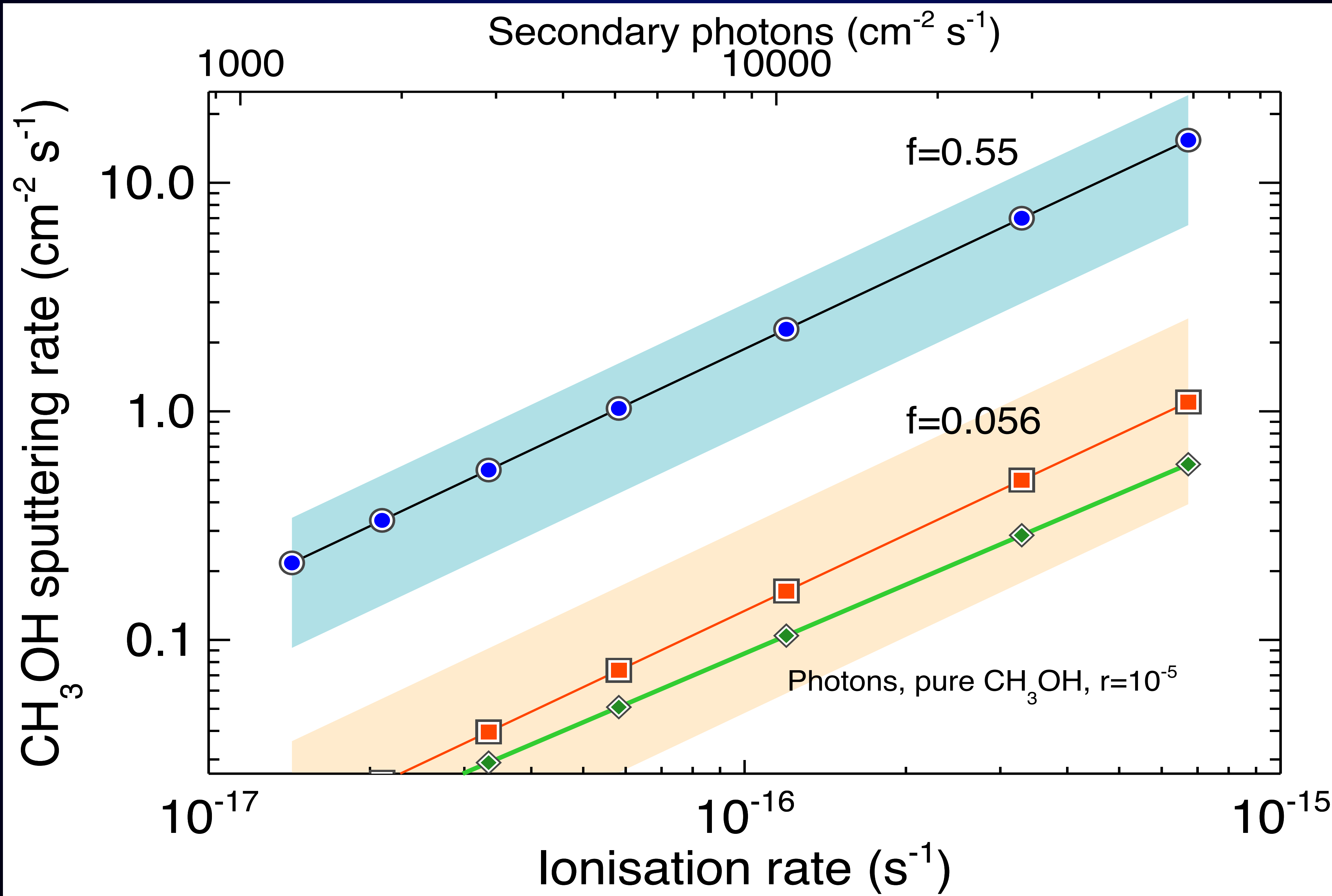




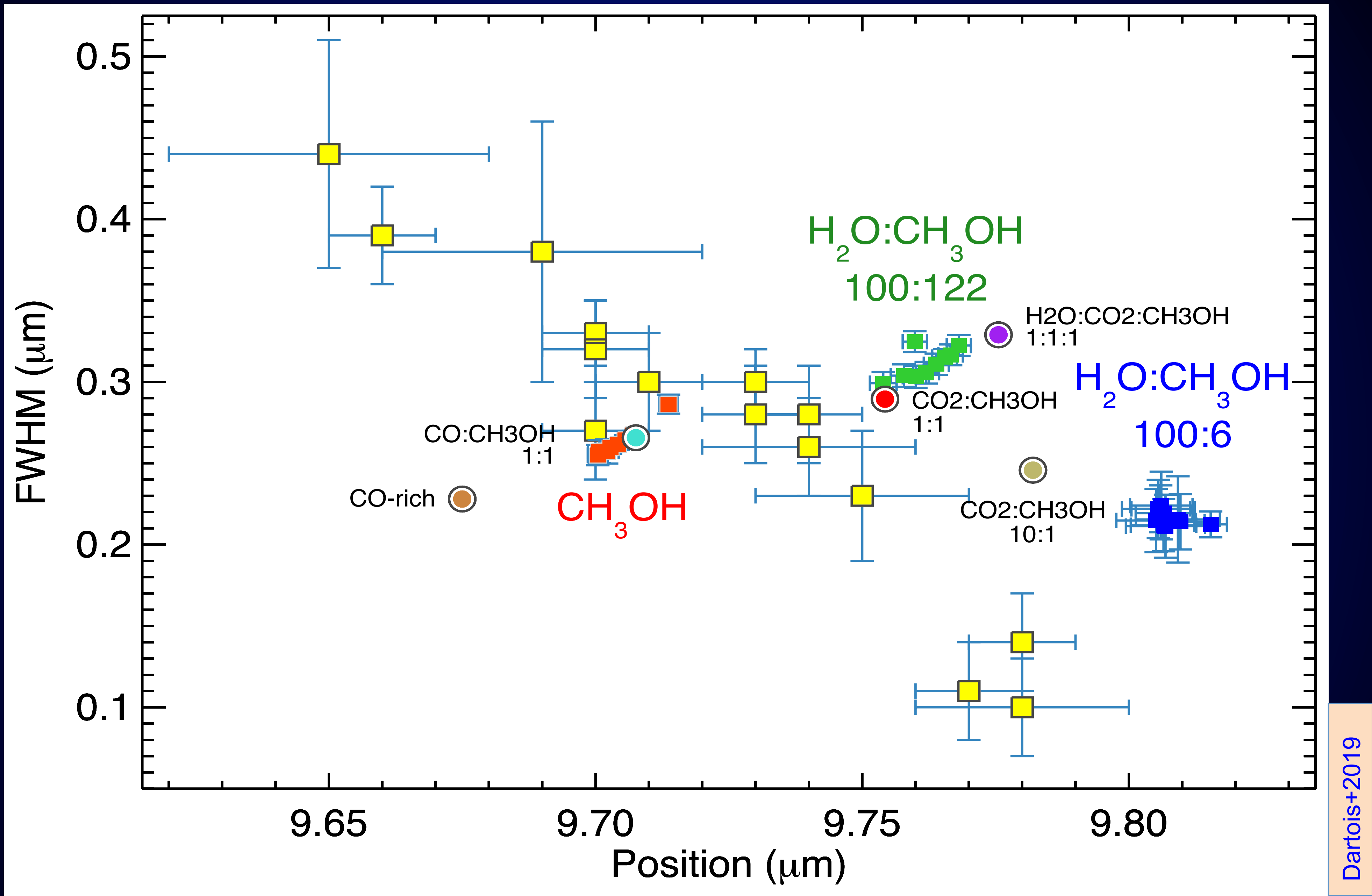
Dartois+2019



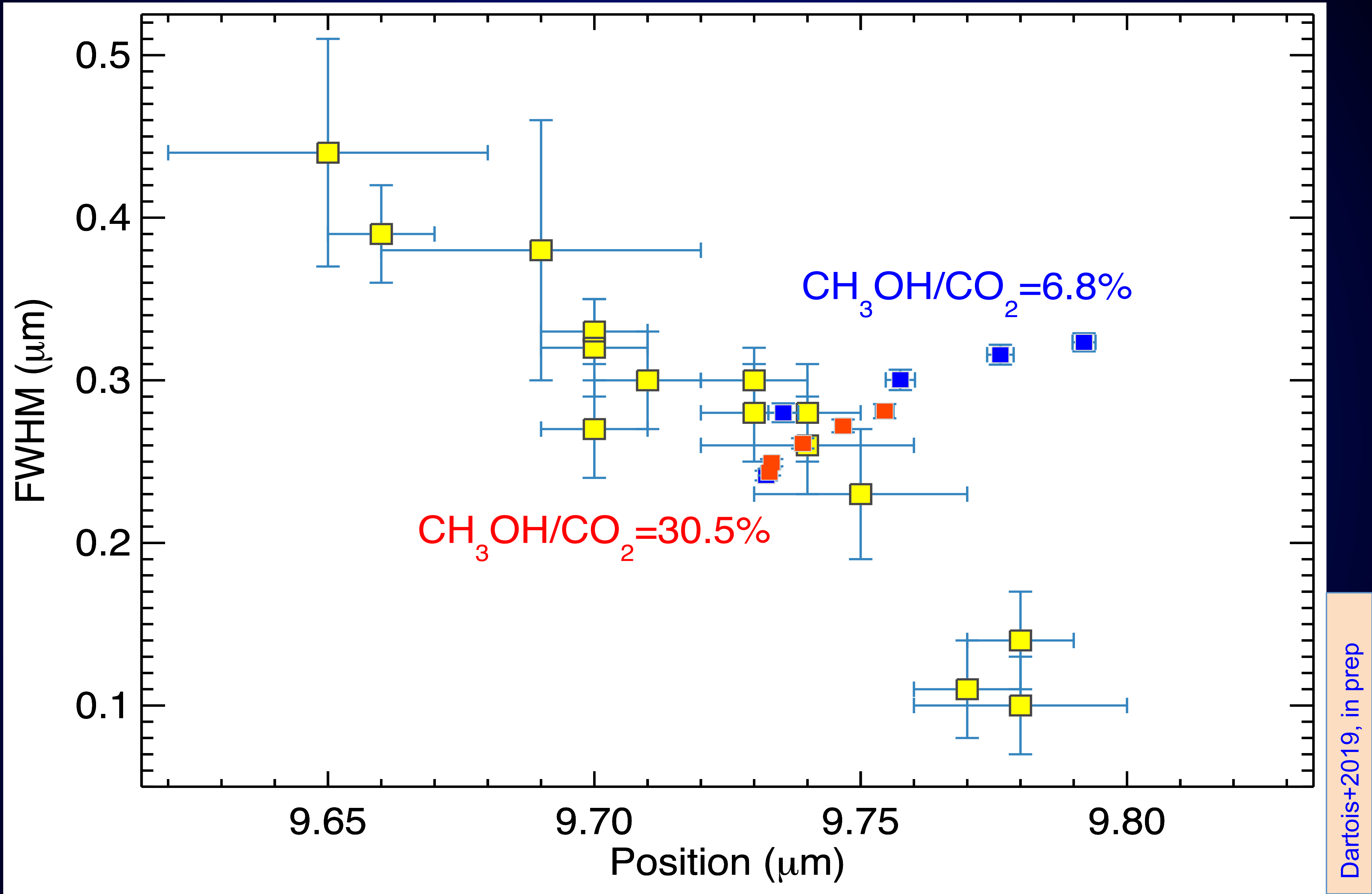
Sputtering rate as a function of the cosmic-ray ionisation rate



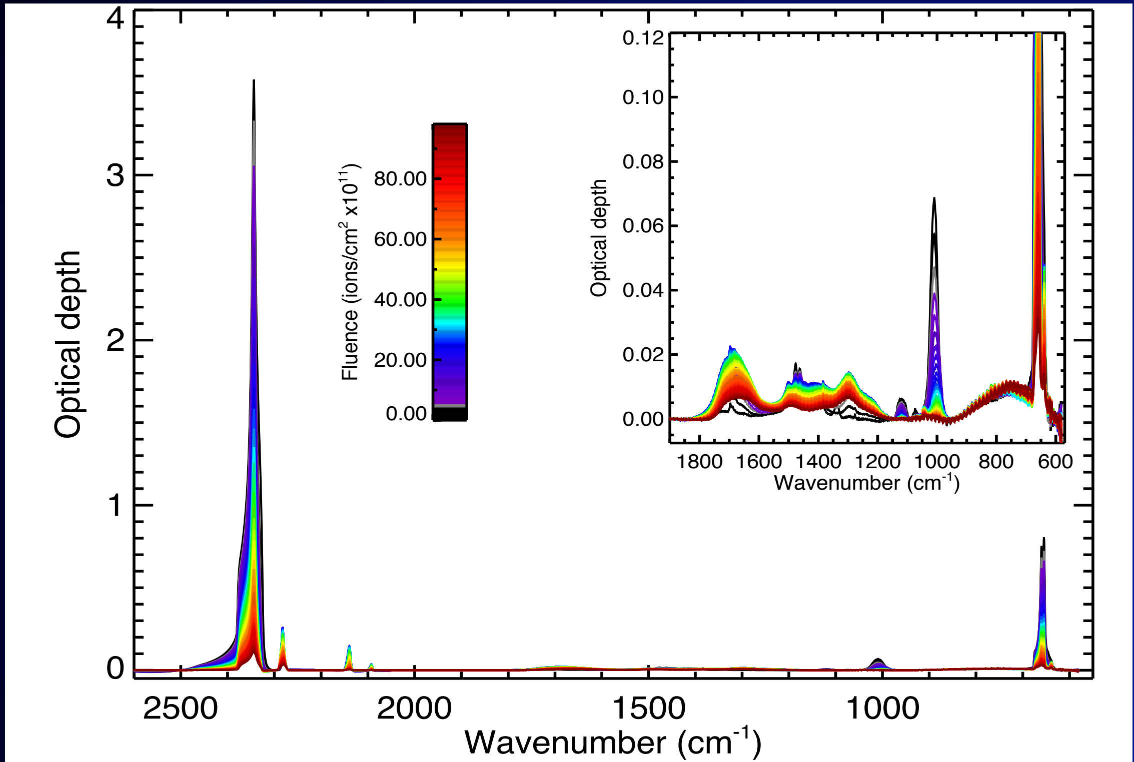
Methanol C-O stretching-mode position–FWHM



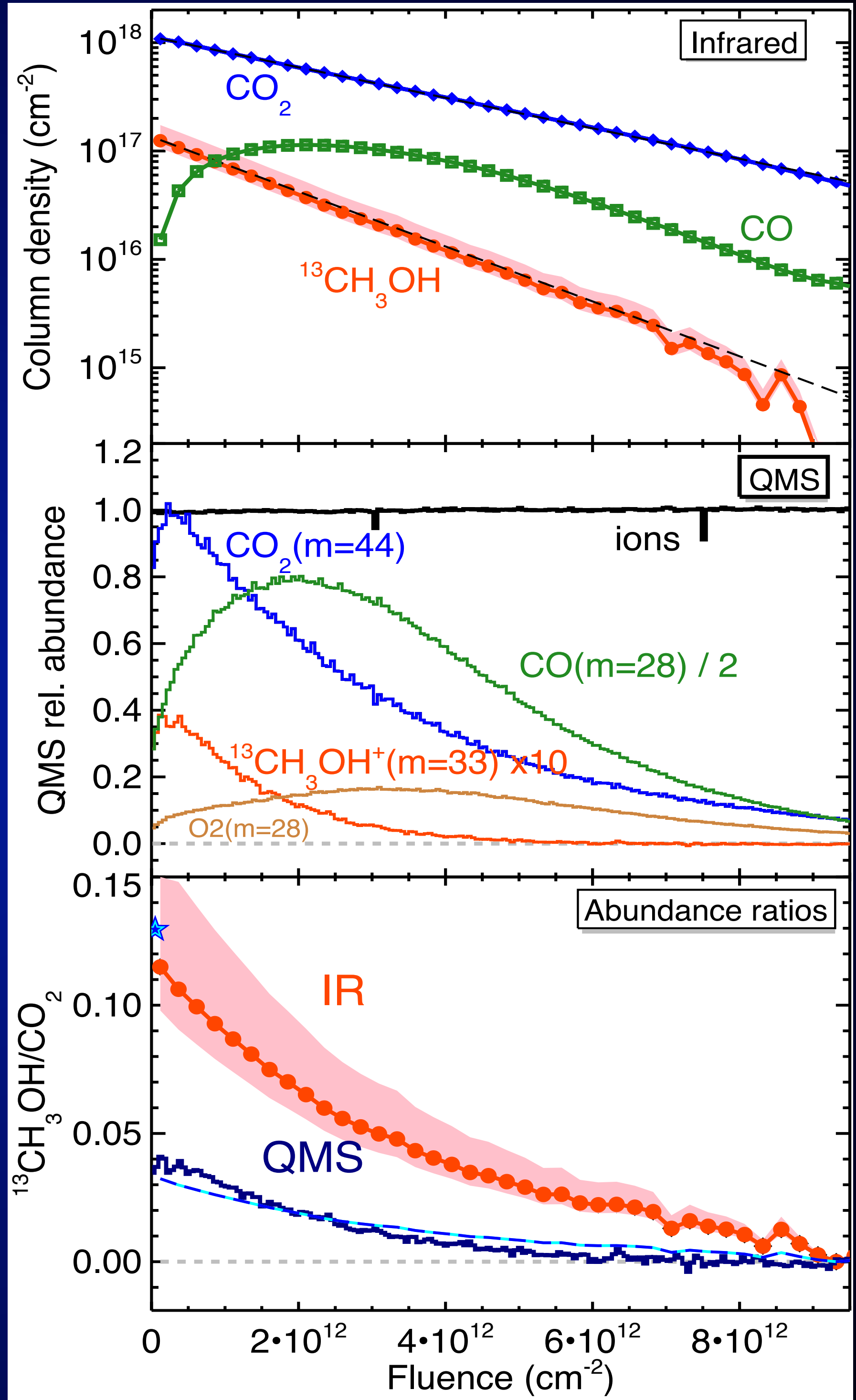
Methanol C-O stretching-mode position–FWHM



C.R. COM sputtering:
CH_3OH/CO_2 mixtures



Dartois+2019, in prep



Sputtering efficiency close to that of the carbon dioxide ice matrix

CO_2 ~8 x higher sputtering than H_2O

~1/3 CH_3OH sputtered intact

The JWST successor of the HST
a 6.5 meter InfraRed telescope in Space

Four Instruments on board:

- NIRIS (0.6-5 μm) (Canada)
- NIRCAM (1-5 μm) (US)
- NIRSPEC (1-5 μm) (ESA)
- **MIRI : (5-28 μm) (Europe – US)**

To be launched by an Ariane rocket in March 2021
to be in operation for 5 to 10 years

Four Scientific Themes:

- First light and the reionisation
- Assembly of galaxies
- Birth of stars and proto-planetary systems
- Planetary systems and the origin of life

JWST : some spatial information & sensitivity expectations

How ice thresholds vary as a function of molecular clouds (small scale structuration) ?

Which fraction of the dispersion in ice correlations is due to sensitivity / intrinsic ?

Secure the identification of complex molecules in interstellar ice mantles (the most complex are probably the best targets to constrain formation processes/ chemical networks)

How ice properties change from molecular clouds to disks

Unique access to large distances from stars (10's to 100's AU)

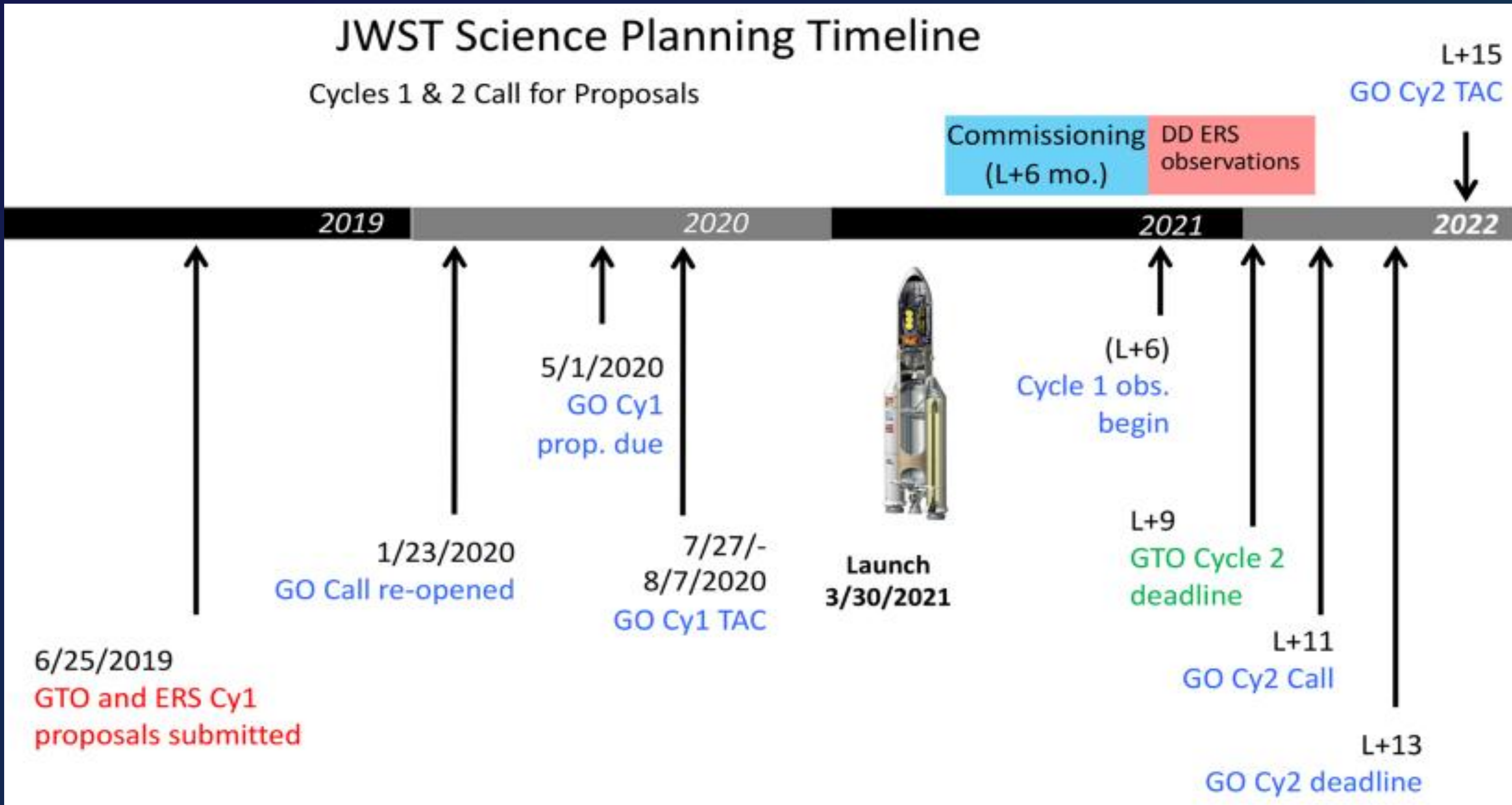
Low mass stars ($< 2\ M_{\odot}$)

Can we explore new regimes in newly accessible regions ?

JWST Science planning timeline

Guaranteed Time Observations (GTO) 450 hours / 3 large progr. exoplanets, disks, extragalactic

GTO target list finalised and APT files submitted by 25th June **2019**



Early Science Release (ERS) (500 hours)
*November **2017***
13 ERS science programs selected

ERS : no proprietary period (data available immediately); GTO and GO: 1 year proprietary period

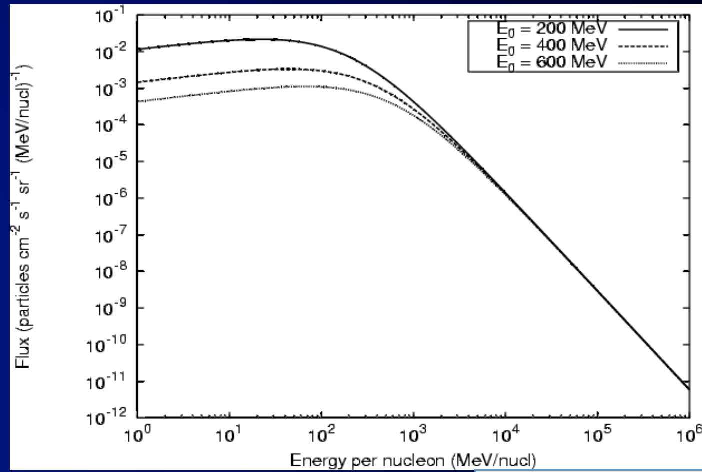
But most of the time « **open time** » attributed following calls for General Observations (GO).
*1st call: Jan 2020; deadline: **May 2020**.*
*2nd call: L+11; deadline: **L+13***

*On sky commissioning in 2021, then **GTO, ERS and GO observations will start end of 2021.***
ESA will organize a train-the-trainer master class workshop in Europe in January 2020

Echelle de temps astrophysique pour la compaction de la glace par le rayonnement cosmique

	GCR		
	$E_0 = 200$	$E_0 = 400$	$E_0 = 600$
$\zeta(s^{-1})^a$	3.34(–16)	5.89(–17)	2.12(–17)
$E_{th} = 0$ eV/Å^b			
Light^c	0.589	0.580	0.576
$Z \geq 3^d$	0.411	0.420	0.424
Fe	0.073	0.078	0.080
$\tau(\mathrm{My})^e$	0.14	0.71	1.82

Dartois et al. 2013



Shen 2004

Durée de vie d'un nuage moléculaire
~ qq 10^7 ans