

Laboratório de Astrofísica

Simulação de ambientes extraterrestres (Cometas, Atmosferas planetárias/lunares, Meio interestelar)



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Interesses científicos:

- Estudar os processos físicos, químicos e físico-químicos envolvendo **átomos e moléculas no espaço**.
 - **Moléculas na fase gasosa e fase condensada (gelos astrofísicos)**
 - Abundâncias, reações químicas, interações com a radiação (fótons + partículas rápidas), seções de choque, taxas de reações, tempos de meia vida.
 - Determinar parâmetros físicos e físico-químicas (temperatura, densidade, velocidades, etc.) de ambientes astrofísicos a partir das observações de átomos e moléculas.
 - Fornecer vínculos para o estudo da evolução química do Universo.
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- **Astroquímica + Geologia espacial:** Rochas e minerais, space weathering
 - **Astroquímica + Astrobiologia:** Moléculas pré-bióticas (açúcares, aminoácidos, bases de DNA), reações catalíticas, Ambientes líquidos, etc.

Moléculas encontradas no cosmos (radio e infravermelho)

Detected cosmic molecules in interstellar and circumstellar environments (adapted from Wootten 2001).

Diatomic	Triatomic	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms	13 atoms
H ₂	C ₃	C-C ₃ H	C ₅	C ₅ H	C ₆ H	CH ₃ C ₃ N	CH ₃ C ₄ H	CH ₃ C ₅ N	HC ₉ N	HC ₁₁ N
AlF	C ₂ H	I-C ₃ H	C ₄ H	I-H ₂ C ₄	CH ₂ CHCN ←	HCOOCH ₃ ←	CH ₃ CH ₂ CN ←	(CH ₃) ₂ CO ←		
AlCl	C ₂ O	C ₃ N	C ₄ Si	C ₂ H ₄	CH ₃ C ₂ H	CH ₃ COOH ←	(CH ₃) ₂ O	NH ₂ CH ₂ COOH ←		
C ₂	C ₂ S	C ₃ O	I-C ₃ H ₂	CH ₃ CN ←	HC ₅ N	C ₇ H	CH ₃ CH ₂ OH			
CH	CH ₂	C ₃ S	c-C ₃ H ₂	CH ₃ NC	HCOCH ₃	CH ₂ OHCHO	HC ₇ N			
CH ⁺	HCN	C ₂ H ₂	CH ₂ CN	CH ₃ OH ←	NH ₂ CH ₃		C ₈ H			
CN	HCO	CH ₂ D ⁺	CH ₄	CH ₃ SH	c-C ₂ H ₄ O					
CO	HCO ⁺	HCCN	HC ₃ N	HC ₃ NH ⁺	CH ₂ CHOH ←					
CO ⁺	HCS ⁺	HCNH ⁺	HC ₂ NC	HC ₂ CHO ←						
CP	HOC ⁺	HNCO	HCOOH ←	NH ₂ CHO						
CSi	H ₂ O	HNCS	H ₂ CHN	C ₅ N						
HCl	H ₂ S	HOCO ⁺	H ₂ C ₂ O							
KCl	HNC	H ₂ CO ←	H ₂ NCN							
NH	HNO	H ₂ CN	HNC ₃							
NO	MgCN	H ₂ CS	SiH ₄							
NS	MgNC	H ₃ O ⁺	H ₂ COH ⁺							
NaCl	N ₂ H ⁺	NH ₃								
OH	N ₂ O	SiC ₃								
PN	NaCN									
SO	OCS									
SO ⁺	SO ₂									
SiN	c-SiC ₂									
SiO	CO ₂									
SiS	NH ₂									
CS	H ₃ ⁺									
HF	SiCN									
SH										

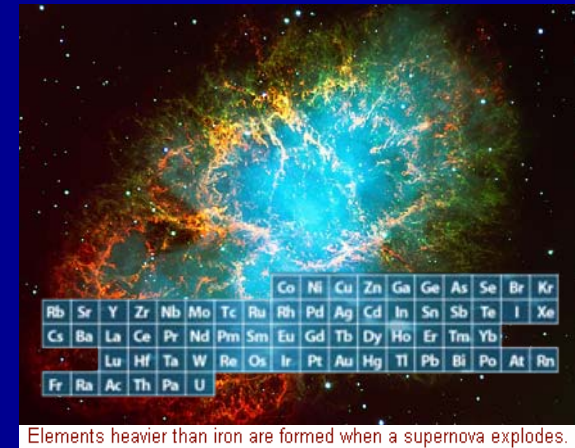
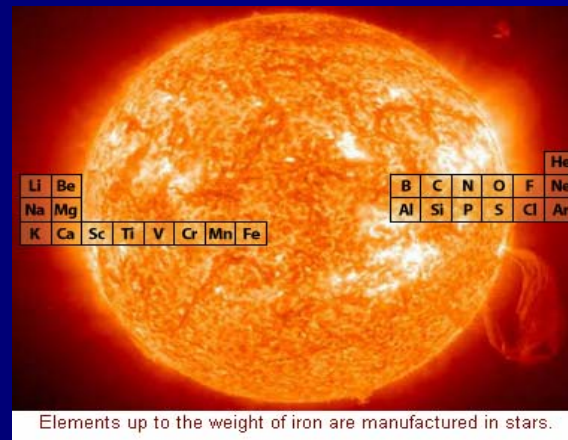
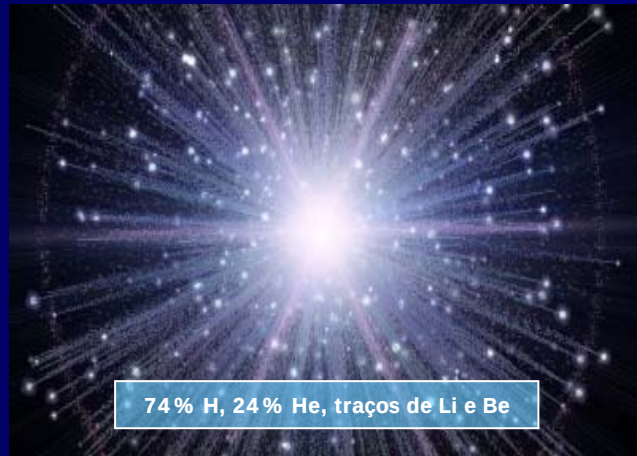
Alcoóis, cetonas, ácidos carboxílicos, aminas, nitrilas, ésteres, ...

Hidrocarbonetos, PAHs,

Nos meteoritos também foram encontrados aminoácidos, bases nitrogenadas e açúcares!

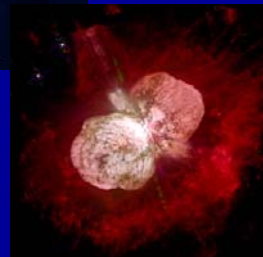
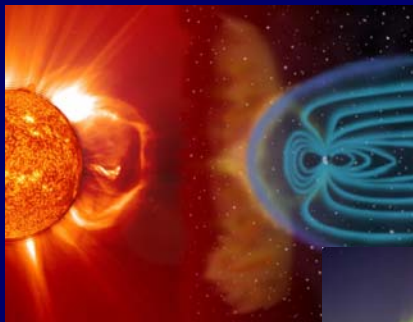
Origem dos átomos:

Nucleossíntese primordial (big bang) + estelar + supernovas.

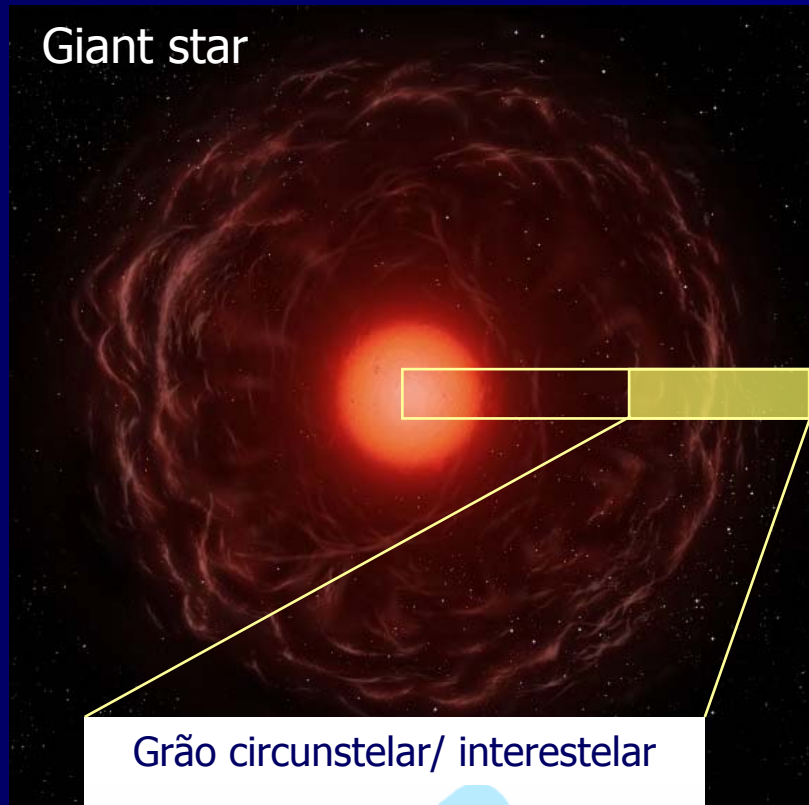


Origem das moléculas:

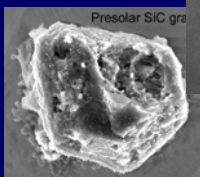
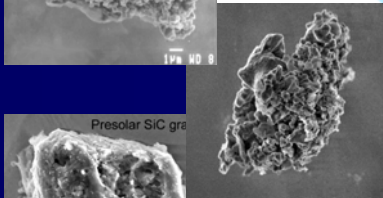
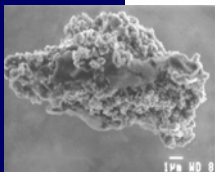
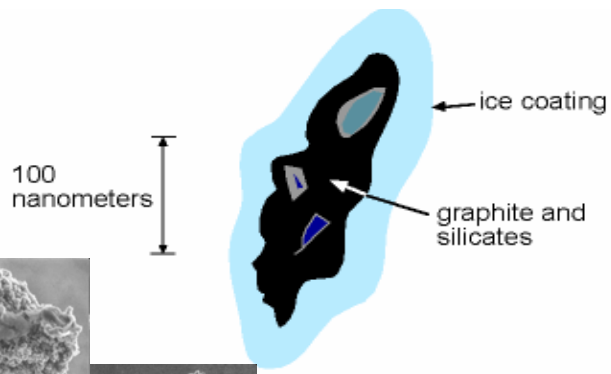
Ventos estelares, reações químicas (gás e superfície), regiões de baixa temperatura.



Giant star



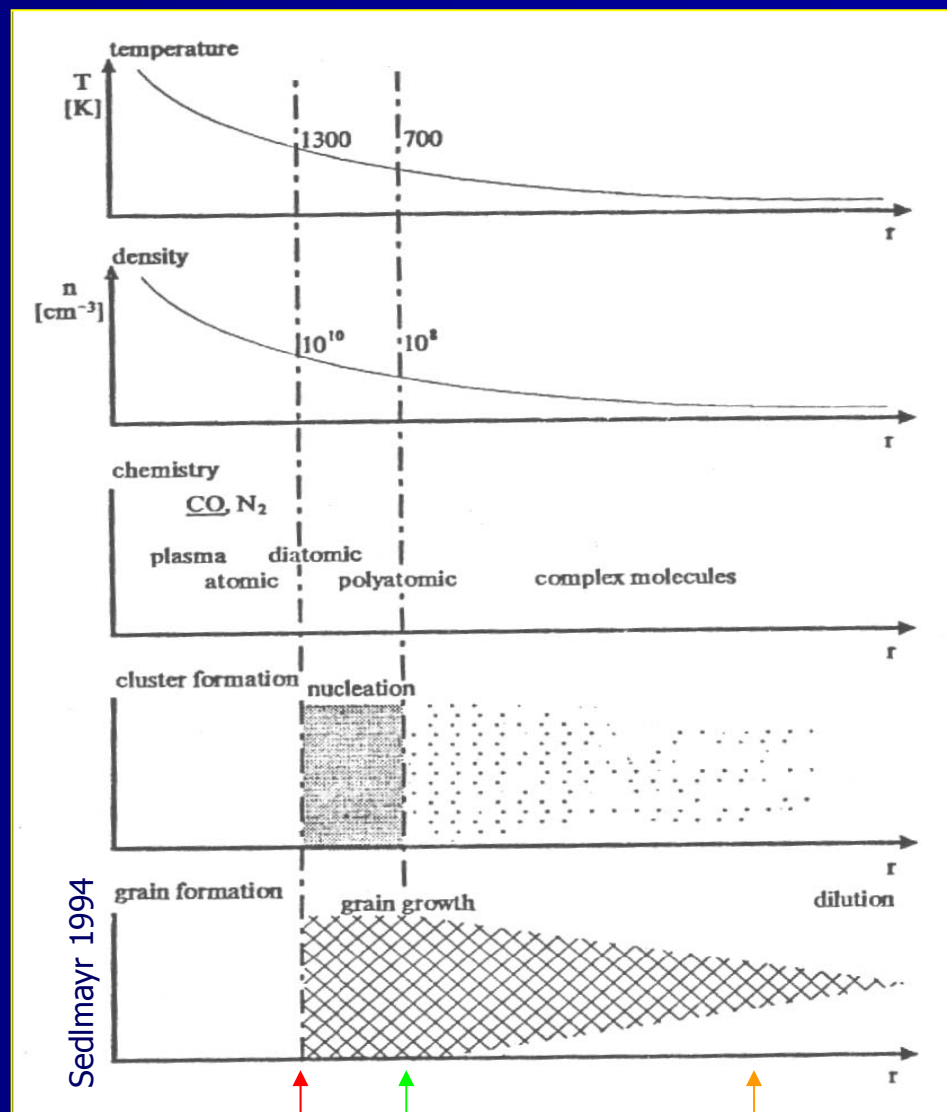
Grão circunestelar/ interestelar



Al_2O_3 (temp $\sim 1700\text{K}$); silicatos (temp $\sim 1400\text{K}$)

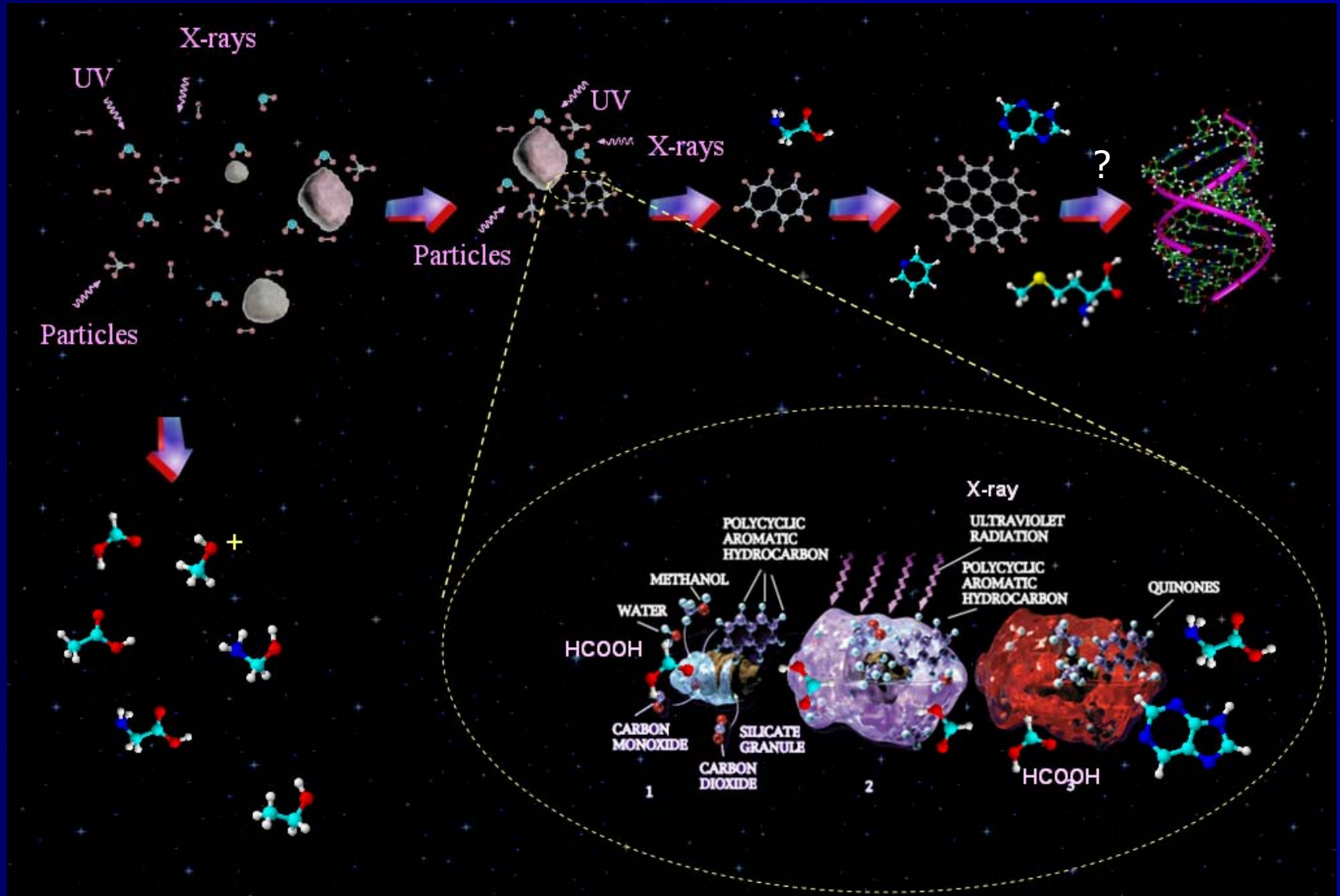
Moléculas carbonáceas (C, PAHs, SiC)

Moléculas voláteis – mantos (H_2O , CH_4 ...)



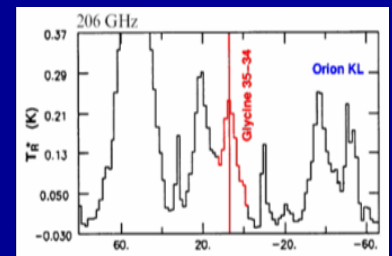
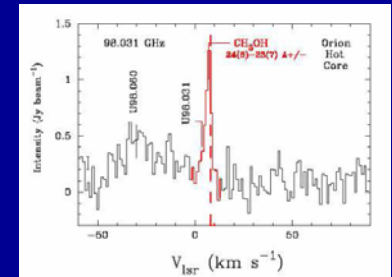
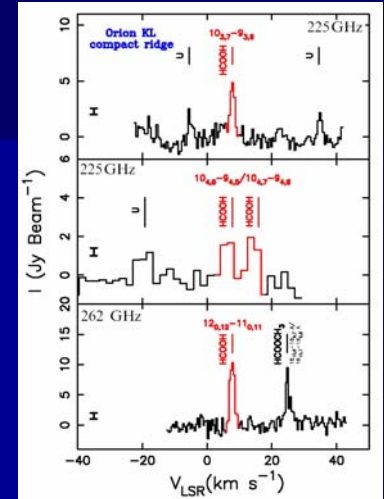
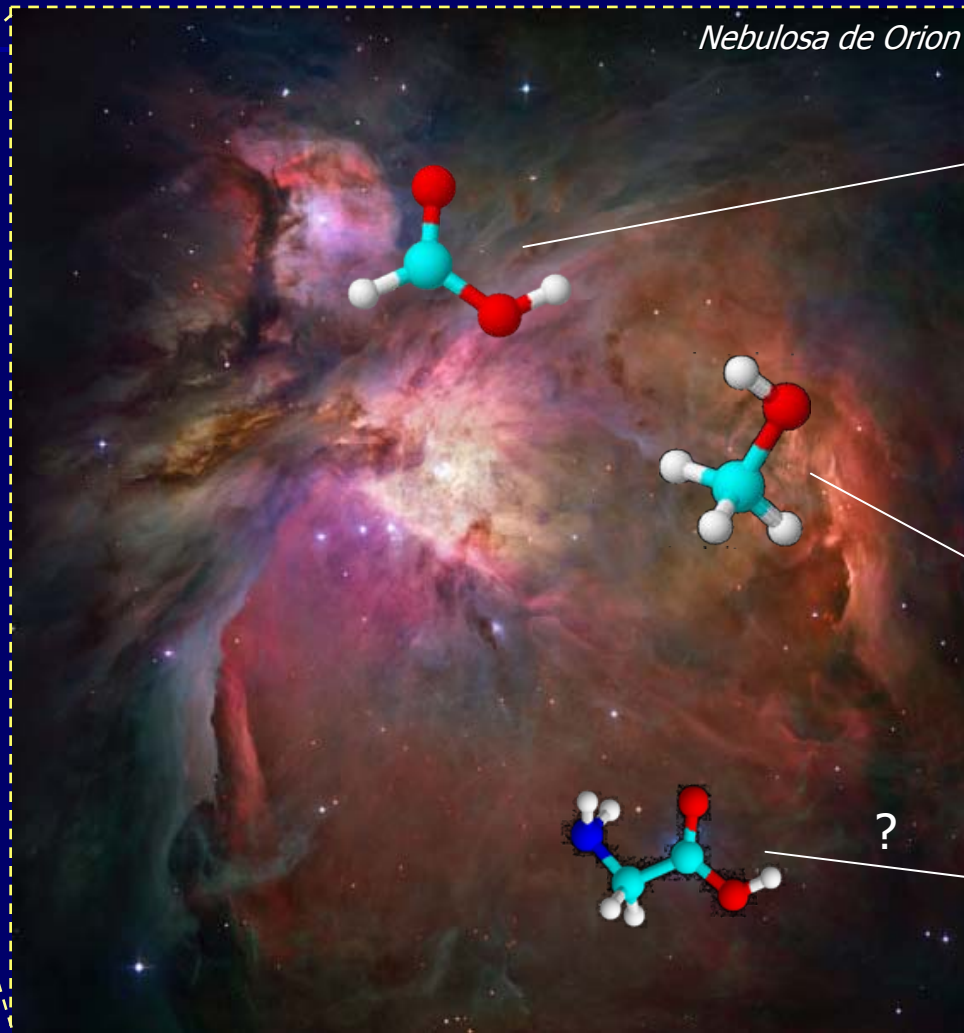
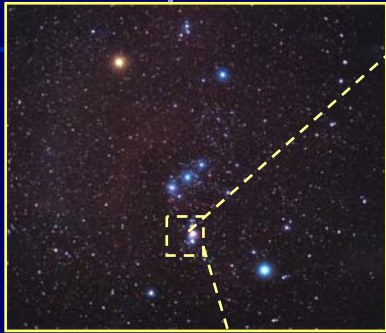
Origem das moléculas maiores:

- Reações na fase gasosa e na superfícies dos grãos (catálise heterogênea)
- Fotólise e radiólise



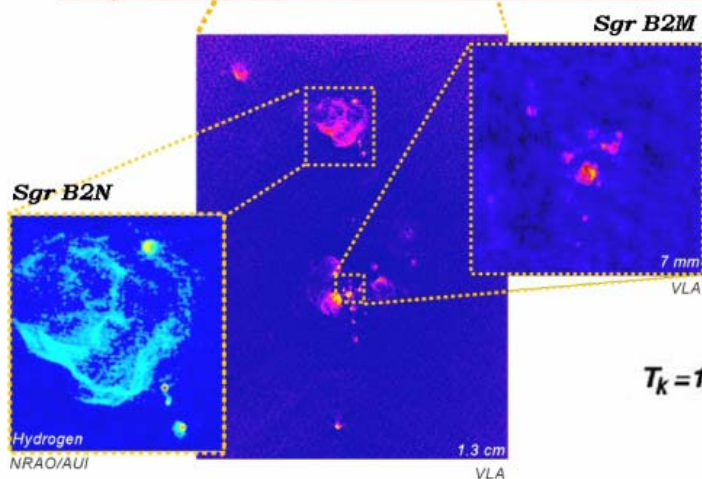
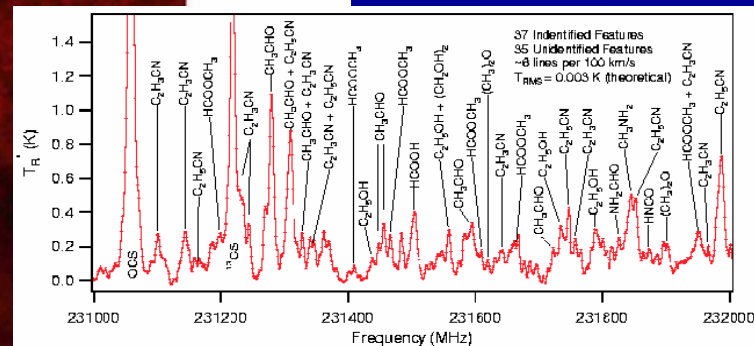
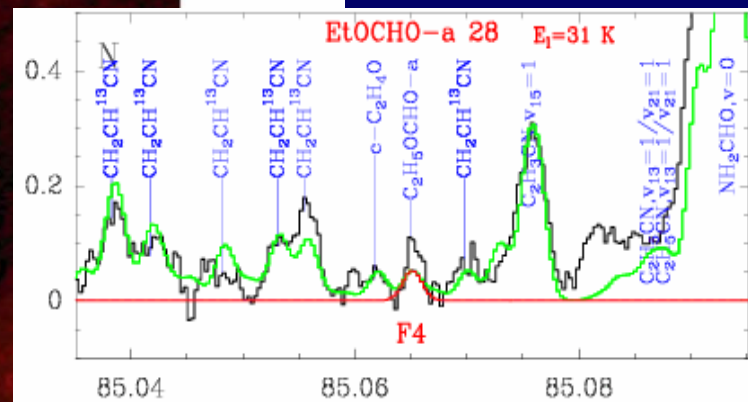
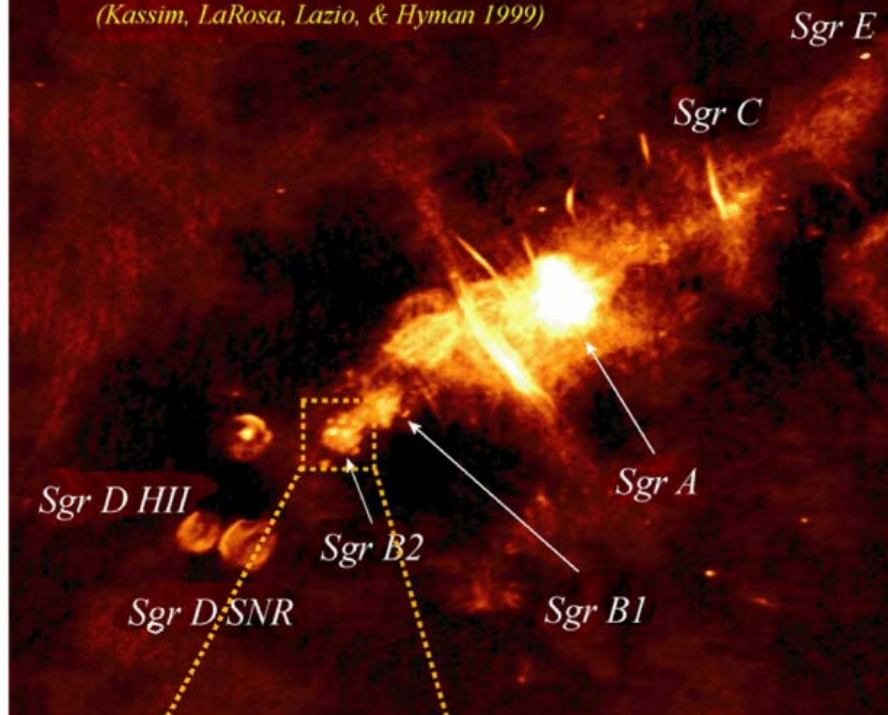
Moléculas na fase gasosa:

Evidências observacionais (Envoltórios de estrelas, MI, nuvens moleculares, atmosferas planetárias, etc.)



The Galactic Center

*Wide-Field VLA Radio ($\lambda = 90$ cm) Image
(Kassim, LaRosa, Lazio, & Hyman 1999)*



extended envelope:

$$n(H_2) < 10^4 \text{ cm}^{-3}$$

 $R=20 \text{ pc}$

UC HII regions, masers

hot cores:

$$n(H_2) = 10^7 \text{ cm}^{-3}$$

$$T_k = 150-300 \text{ K}$$

hot ring:

$$T_k = 100-120\text{ K}$$

moderate

density cloud:

$$n(H_2) = 10^5 \text{ cm}^{-3}$$

$$T_K = 40-80 \text{ K}$$

Horse head nebula



$$N \sim 10^4 \text{ cm}^{-3}$$

$$T \sim 10\text{-}50\text{K!}$$

Black cloud Nebulosa (B68)



Cruzeiro do Sul e a nebulosa do saco de carvão



Moléculas na fase condensada (gelos astrofísicos):
Evidências observacionais (M1, Nuvens moleculares,
cometas, etc.)



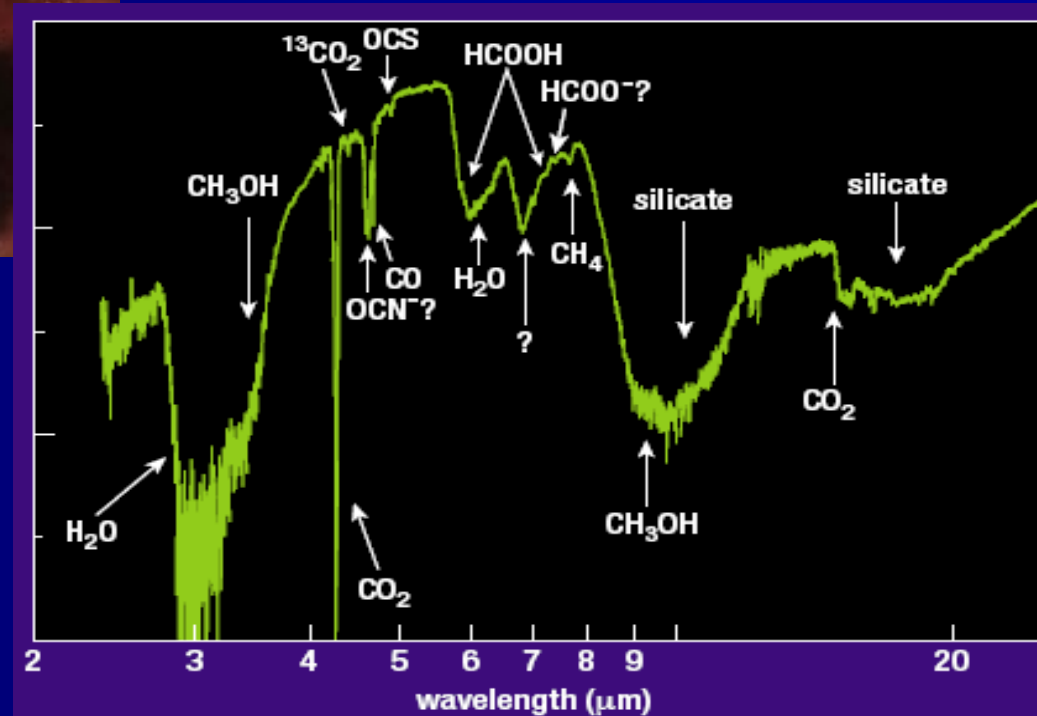
Gelos astrofísicos

Objetos estelares jovens (YSOs) e discos proto planetários



$N \sim 10^4 - 10^8 \text{ cm}^{-3}$

$T \sim 10 - 50 \text{ K}$

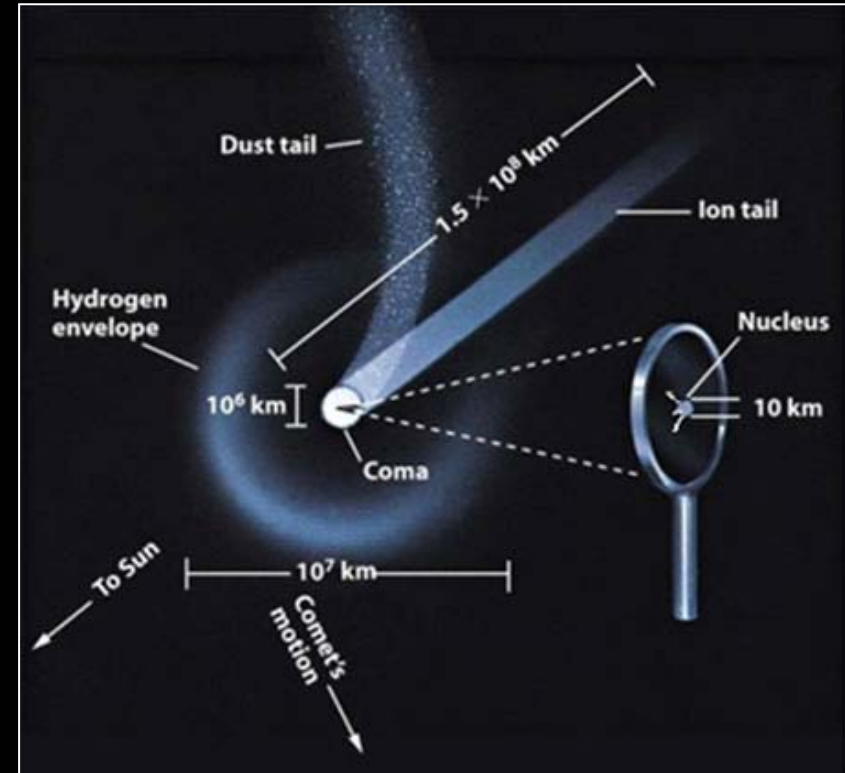
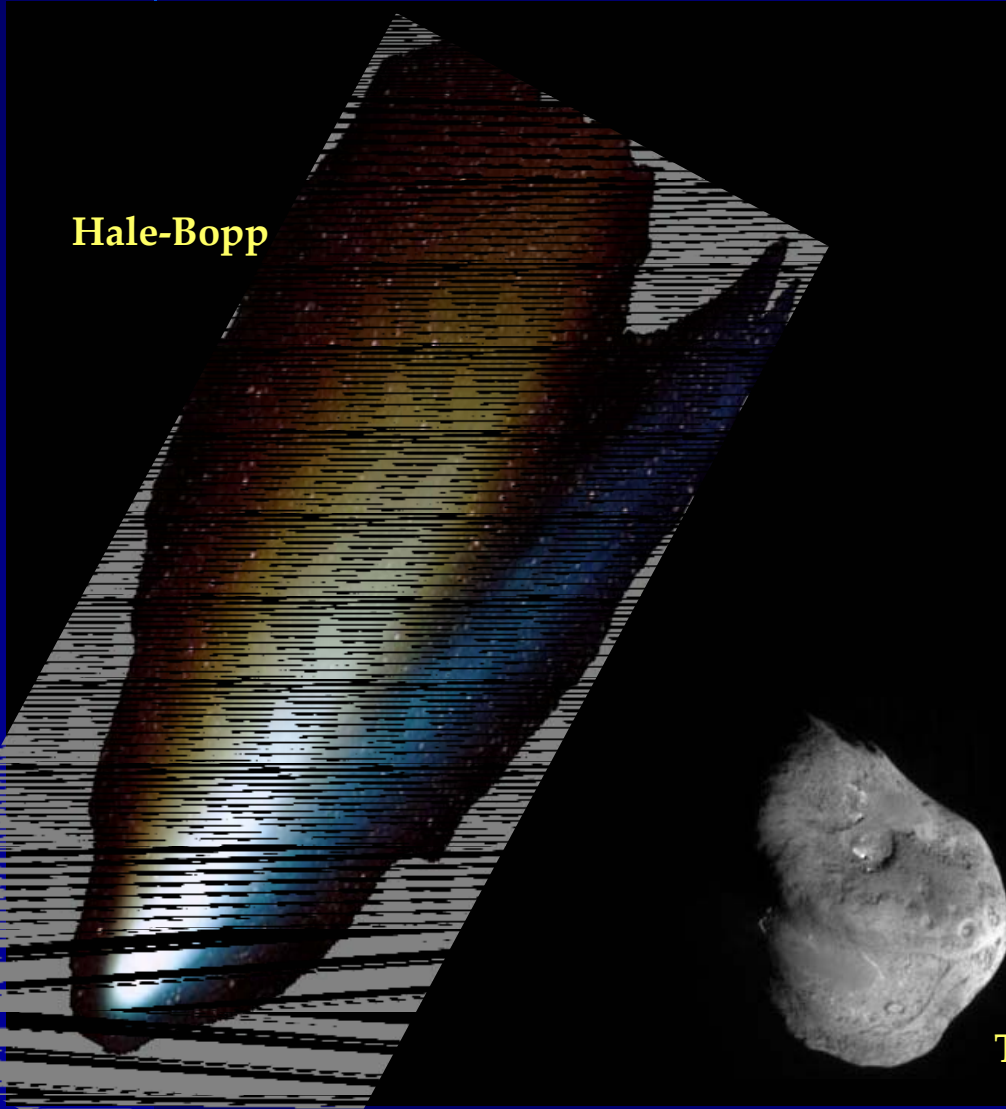


W33a, Protstar (Gibb et al 2000)

Gelos astrofísicos

Cometas ($\sim 80\%$ água. CO , CO_2 , CH_4 ,)

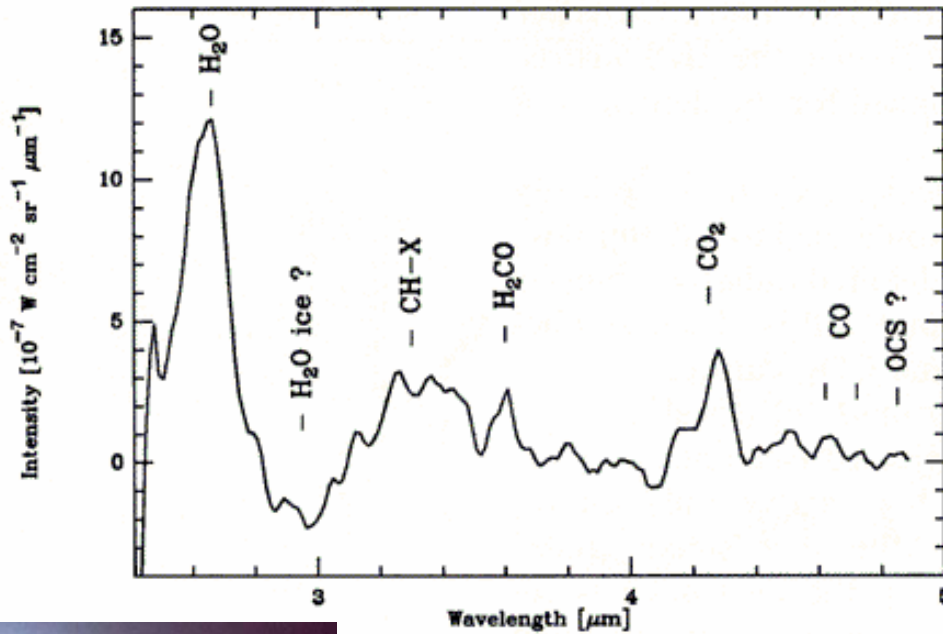
Hale-Bopp



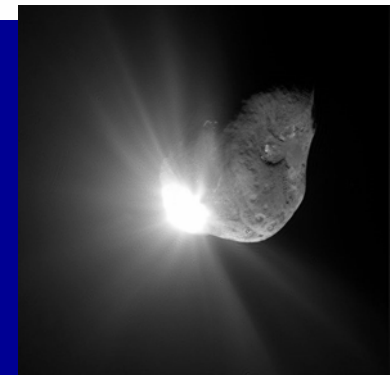
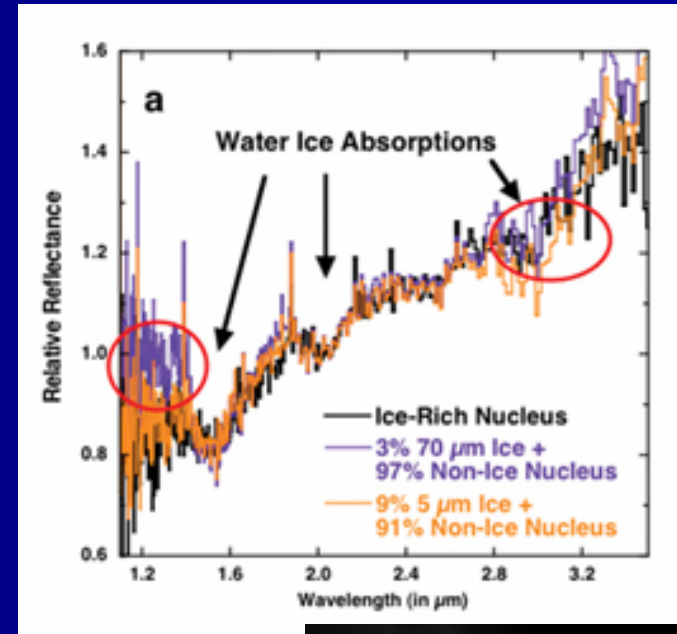
Tempel 1

Gelos astrofísicos

Comet Halley (Combes et al 1988)



Tempel 1 (NASA)



Deep impact Mission

Gelos astrofísicos

• Luas e Planetas.

Artist impressions of Enceladus

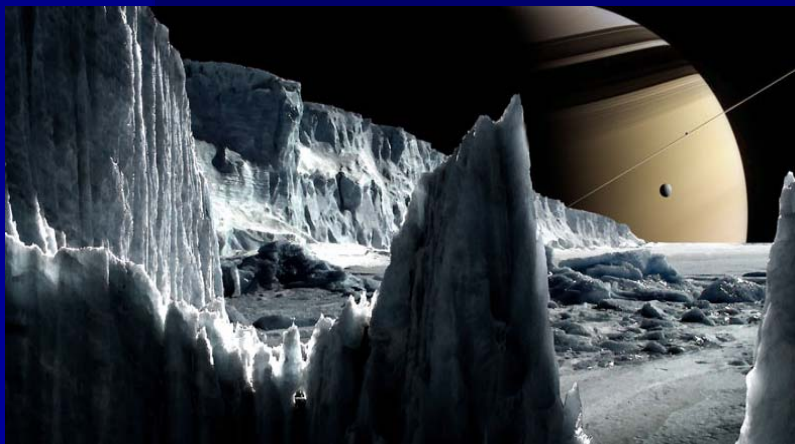
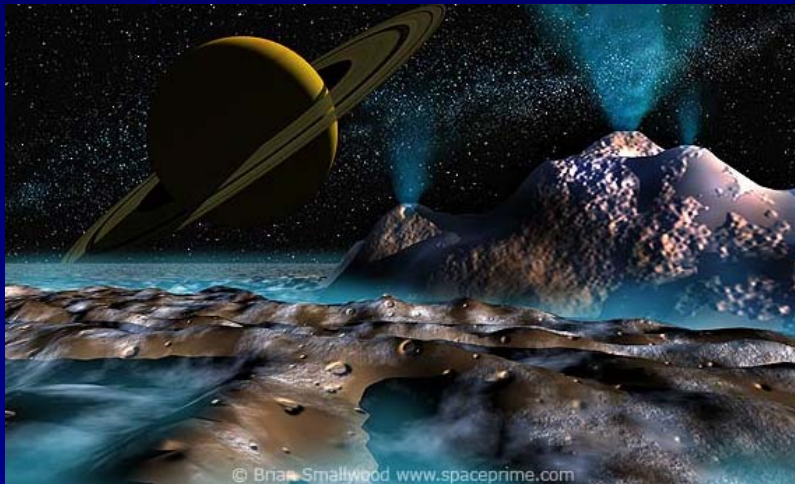


Table 1. Ices in the Solar System.

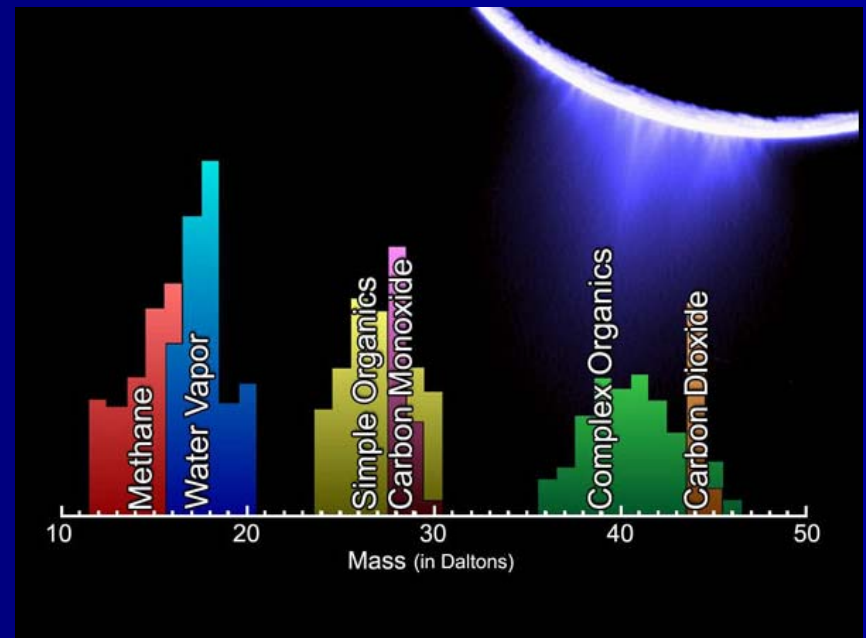
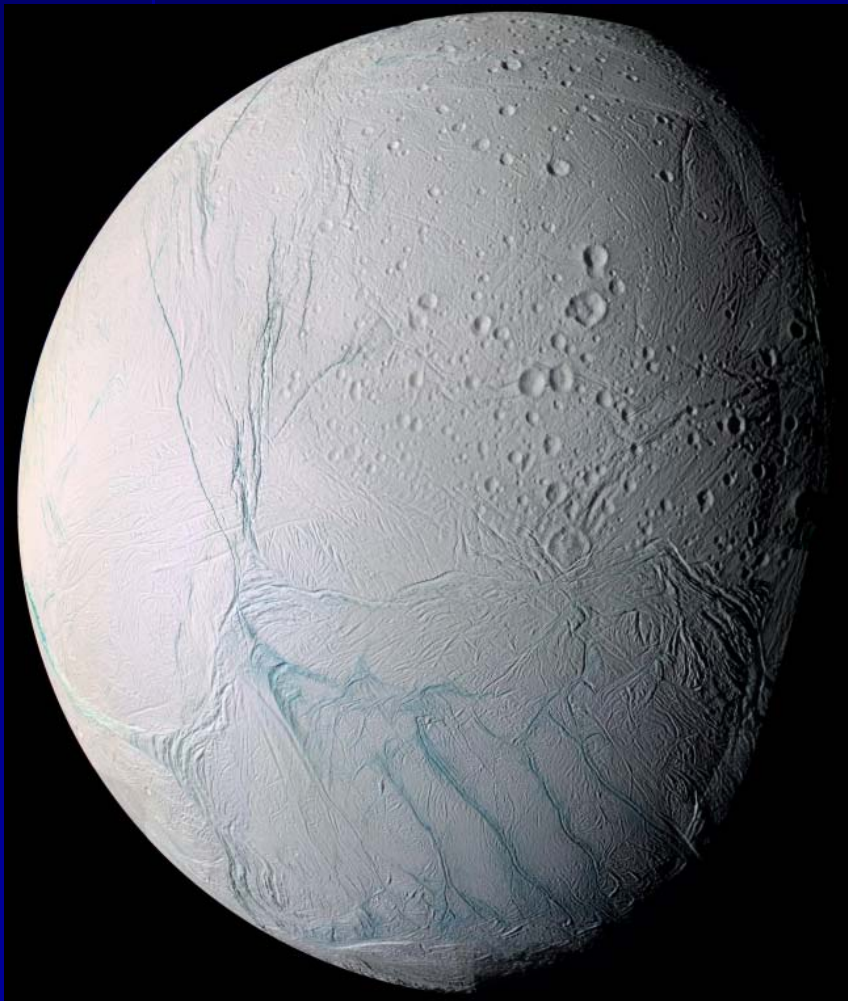
Planet Satellite (Ref.)	Observed Species
Jupiter	
Io	SO ₂ , H ₂ S, H ₂ O
Europa	H ₂ O, SO ₂ , CO ₂ , H ₂ O ₂
Ganymede	H ₂ O, O ₂ , O ₃ , CO ₂
Callisto	H ₂ O, SO ₂ , CO ₂
(Calvin et al. 1995; Nash and Betts 1995)	
Saturn	
Mimas	H ₂ O
Enceladus	H ₂ O
Tetis	H ₂ O
Dione	H ₂ O, O ₃
Rhea	H ₂ O, O ₃
Hyperion	H ₂ O
Iapetus	H ₂ O
(Morrison et al. 1984; Cruikshank et al. 1984; Thomas et al. 1986)	
Uran	
Miranda	H ₂ O
Ariel	H ₂ O
Umbriel	H ₂ O
Titania	H ₂ O
Oberon	H ₂ O
(Cruikshank et al. 1995)	
Neptune	
Triton	N ₂ , CH ₄ , CO, CO ₂ , H ₂ O
(Brown et al. 1995)	
Pluto*	N ₂ , CH ₄ , CO, H ₂ O
Charon	H ₂ O
(Cruikshank et al. 1995)	

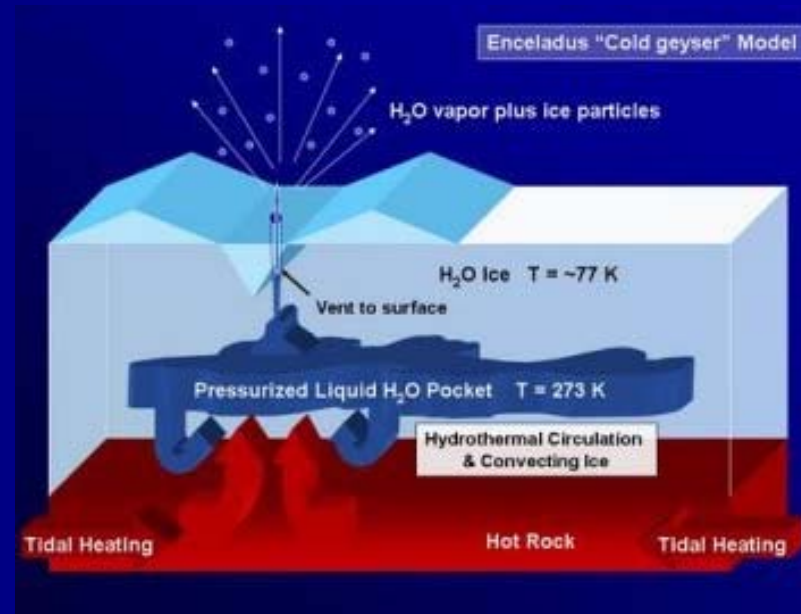
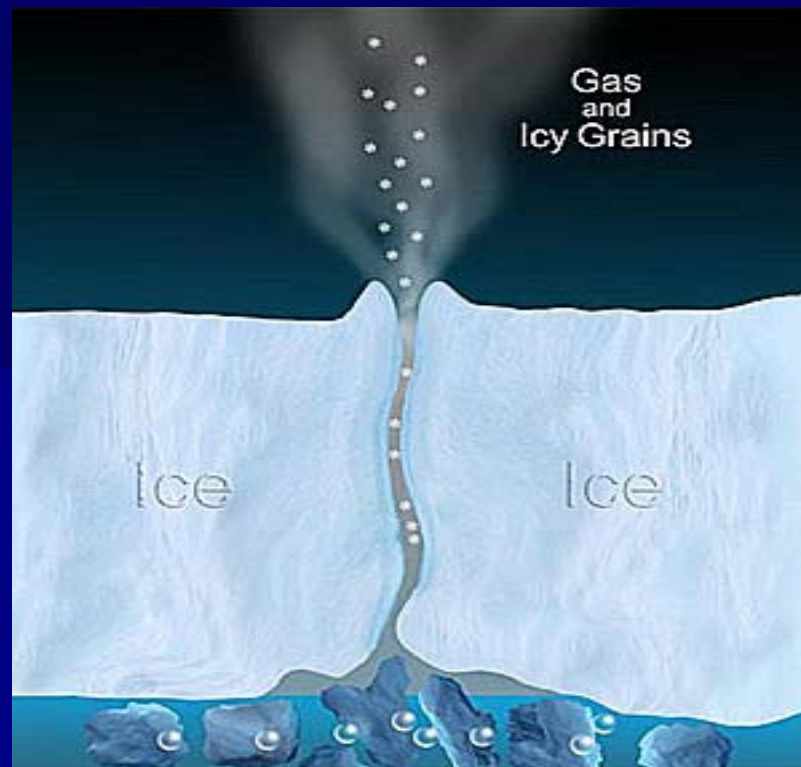
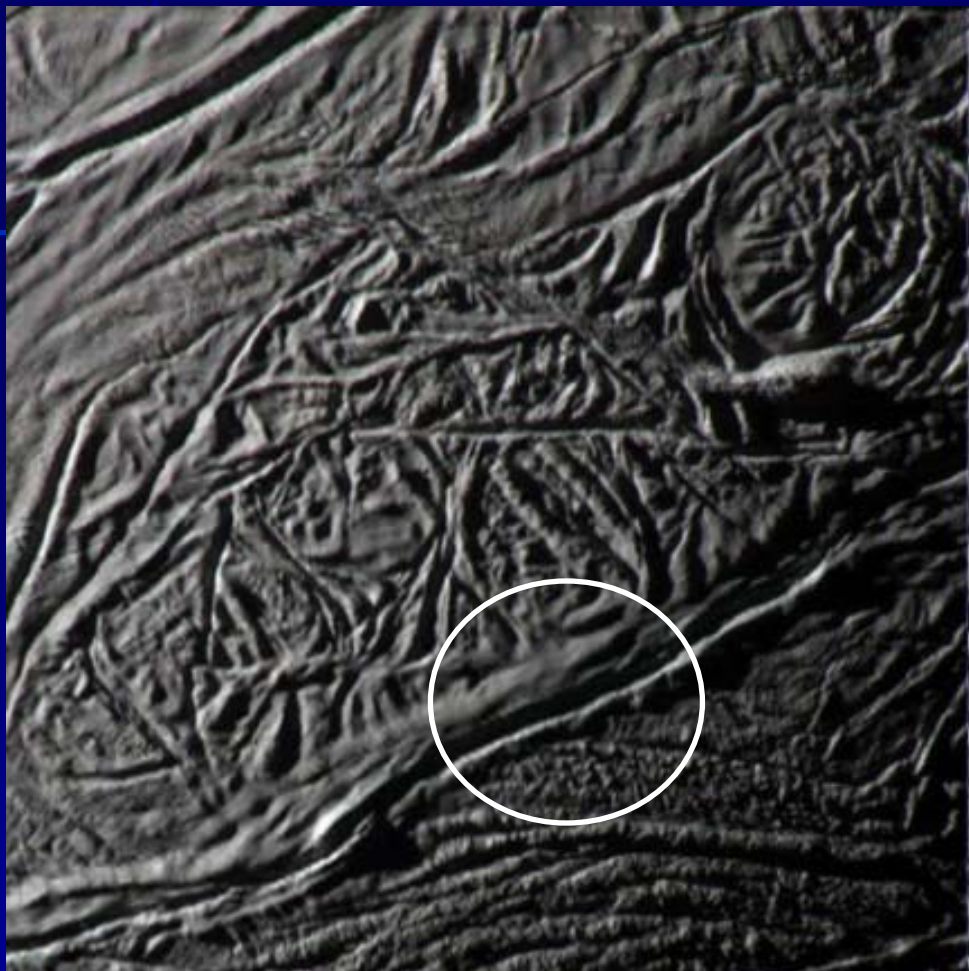
* After IAU resolution, in 2006, Pluto is a *dwarf planet* and is recognized as the prototype of trans-Neptunian objects.

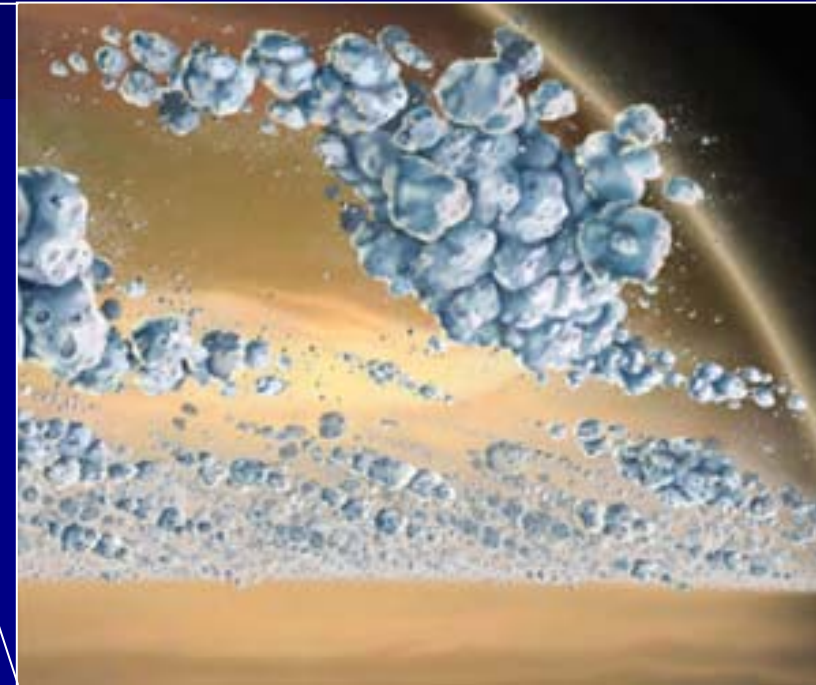
Gelos astrofísicos

Luas e Planetas.

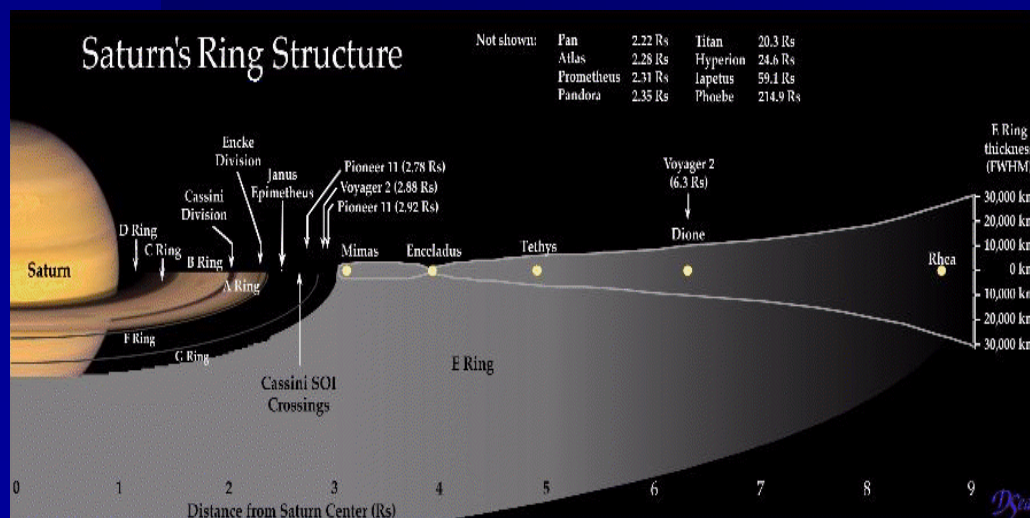
Ex. Enceladus (lua de Saturno).







Gelo de água ~ 99% + silicatos
1 cm - 10 mt.
Enceladus?

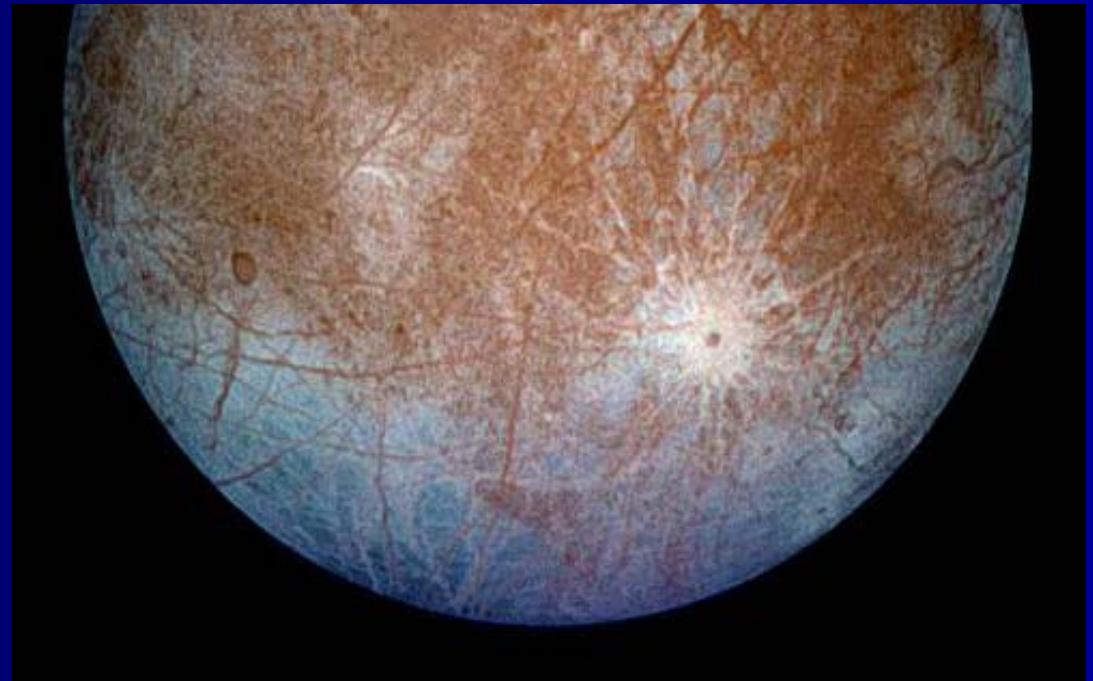
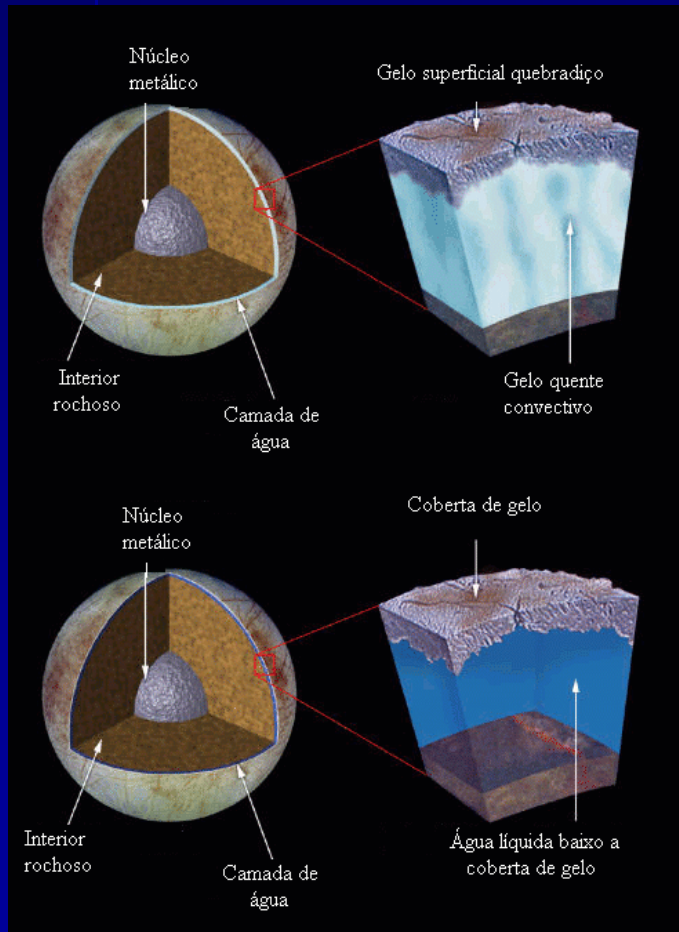


Ex. Anéis de Saturno

Gelos astrofísicos

Luas e Planetas.

Ex. Europa (lua de Jupiter).

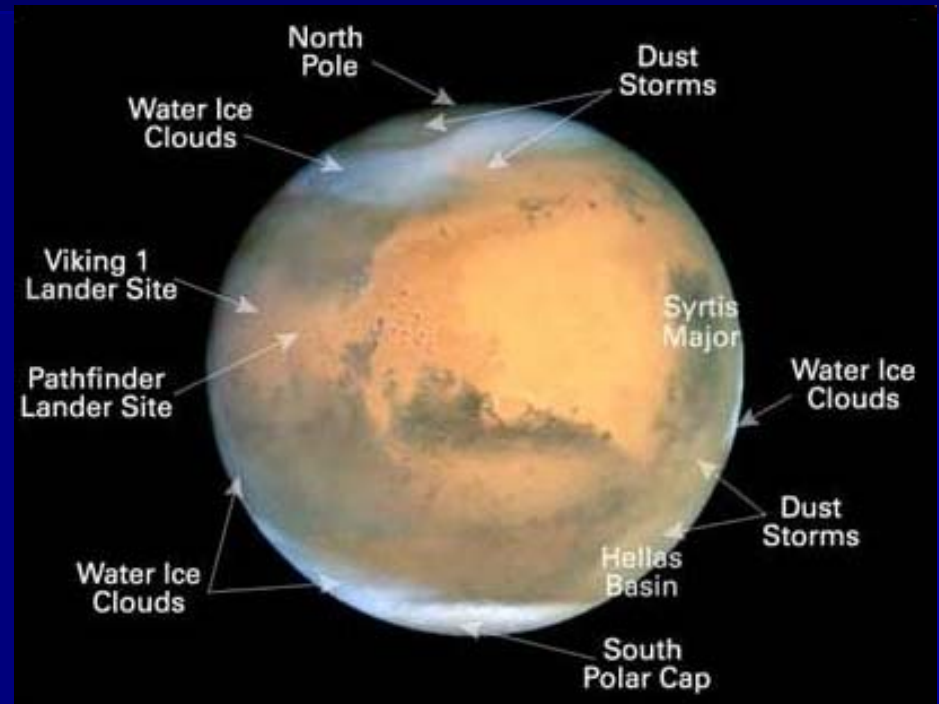


Modelos propostos

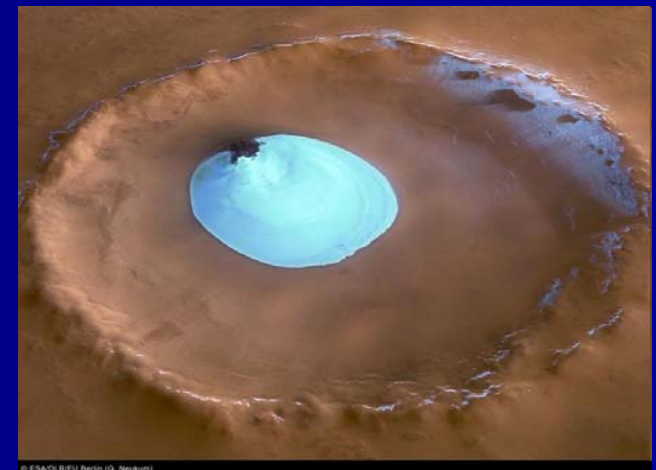
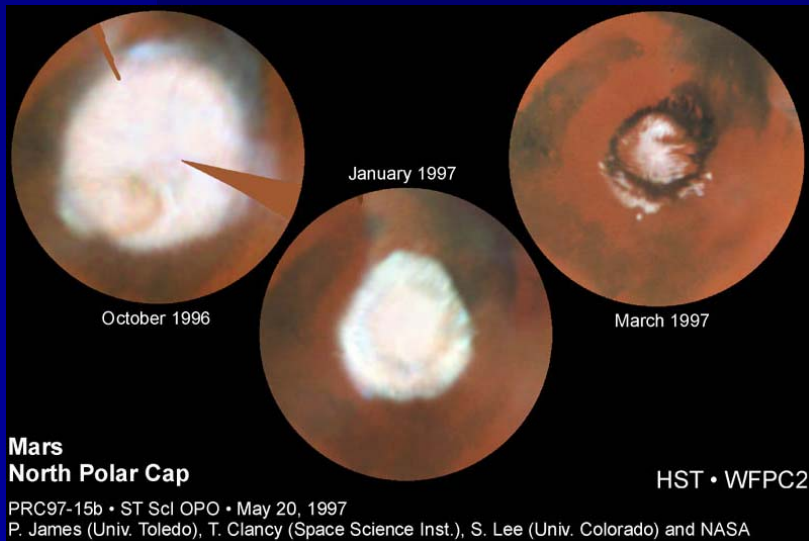
Gelos astrofísicos

- Luas e Planetas

Ex. Marte ($T \sim -46^{\circ}\text{C}$)



Efeito sazonal

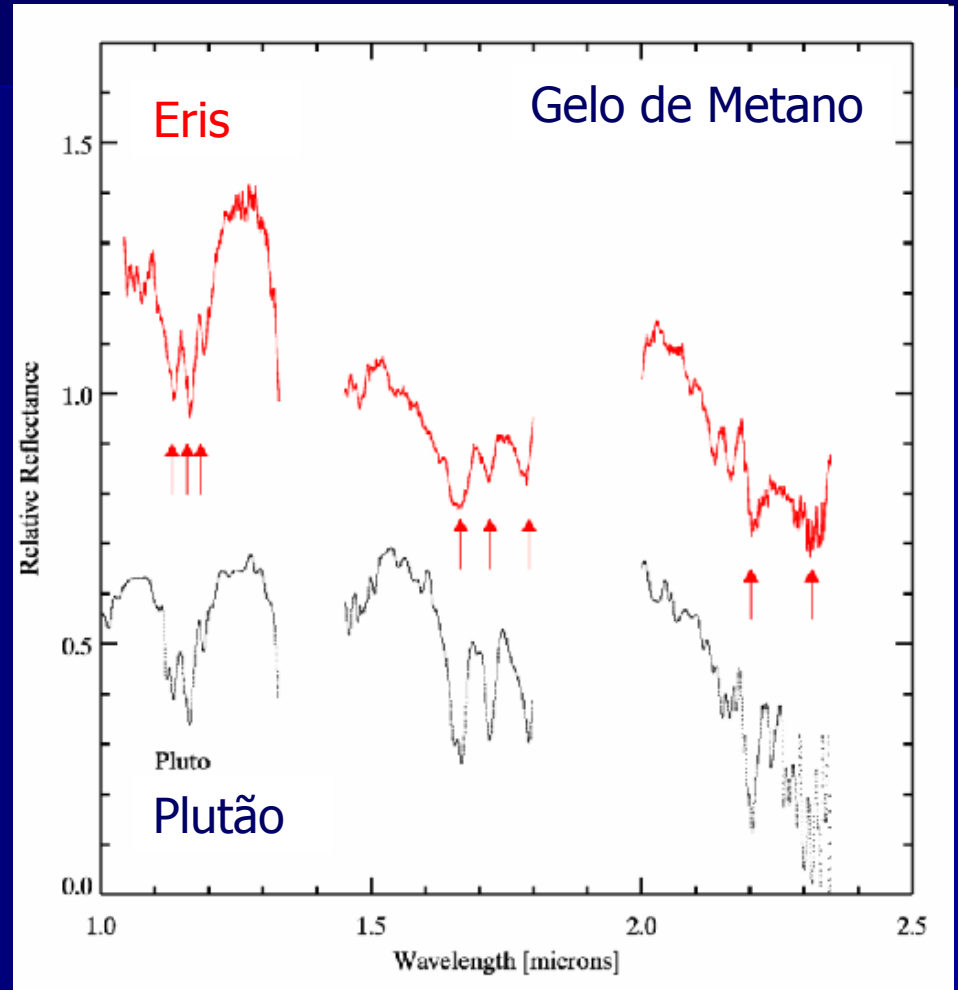


gelo de CO_2 na cratera Vastitas Borealis.

Gelos astrofísicos

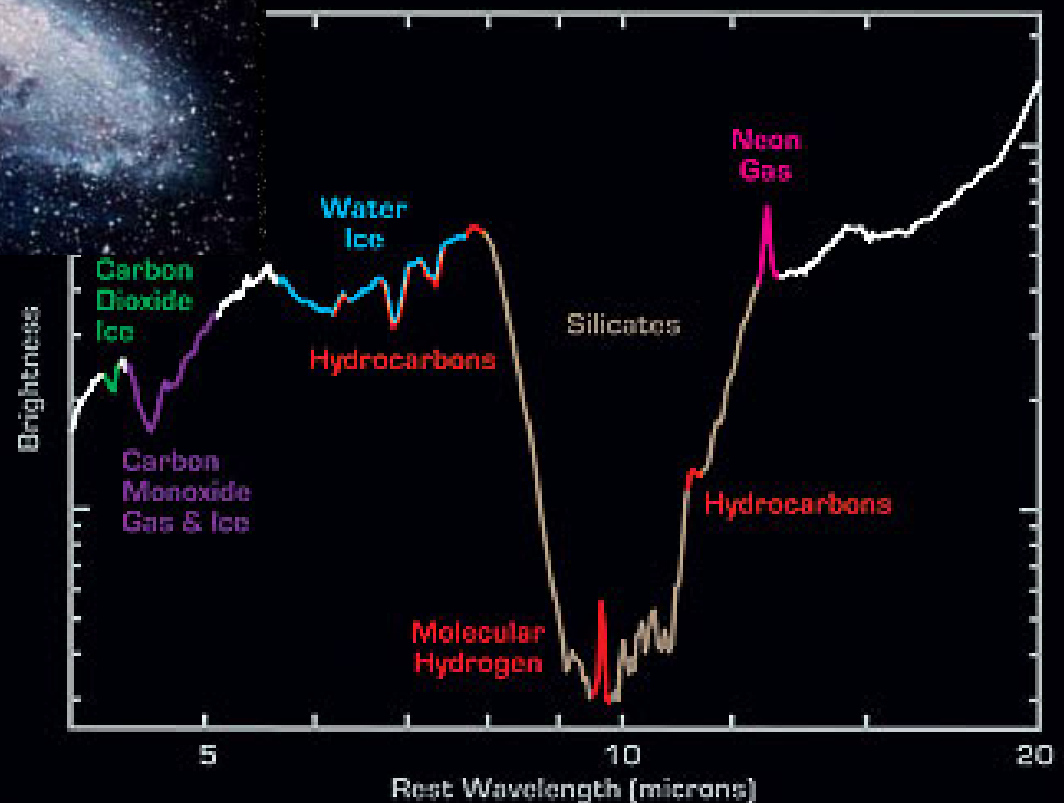
Planetas anões

Ex. Plutão e Eris



Gelos astrofísicos

- Outras galáxias



Galaxy IRAS F00183-7111

NASA / JPL-Caltech / L. Armus (SSC/Caltech)

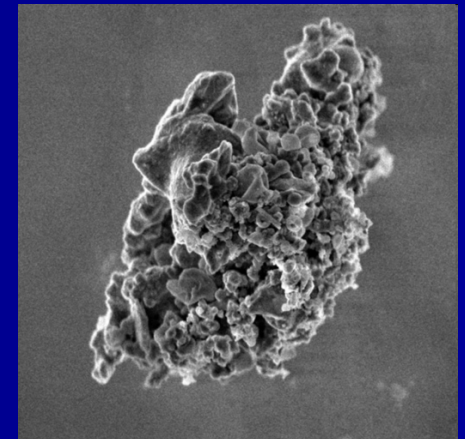
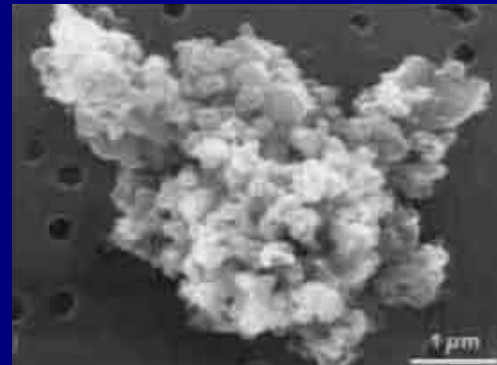
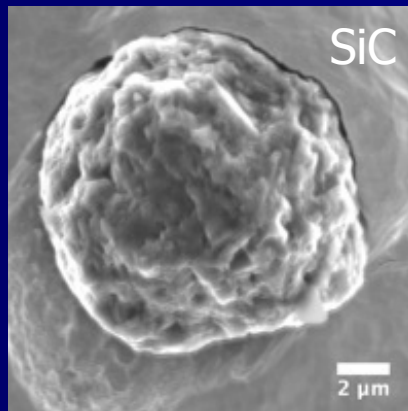
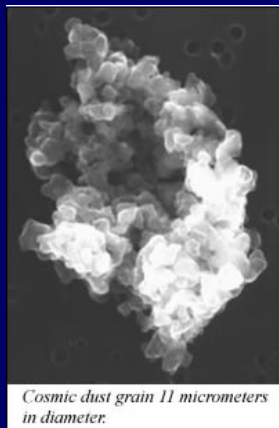
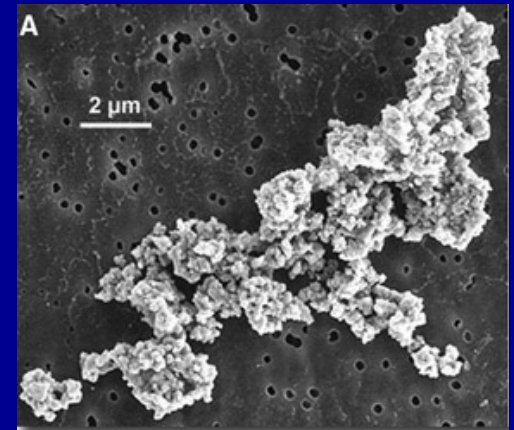
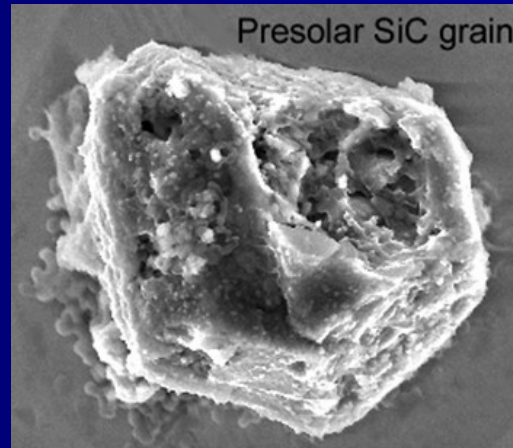
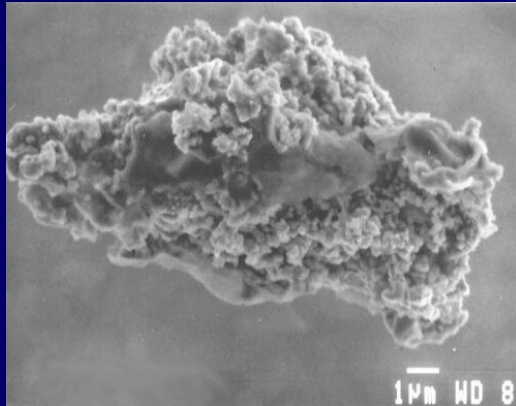
Spitzer Space Telescope • IRS

Inset: visible (SSC)

ssc2003-06h

Processos de crescimento, alteração e destruição dos gelos astrofísicos e experimentos de laboratório

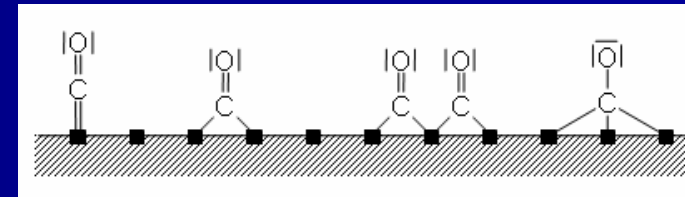
Ex. Grãos interplanetários



1) Processos de crescimento: adsorção

■ Quimissorção (Chemisorption)

- Ligações químicas entre superfície-adsorbato ($\sim \text{eV}$)
- Sítios específicos de absorção.
- Envolve energia de ativação.
- 1ª monocamada,

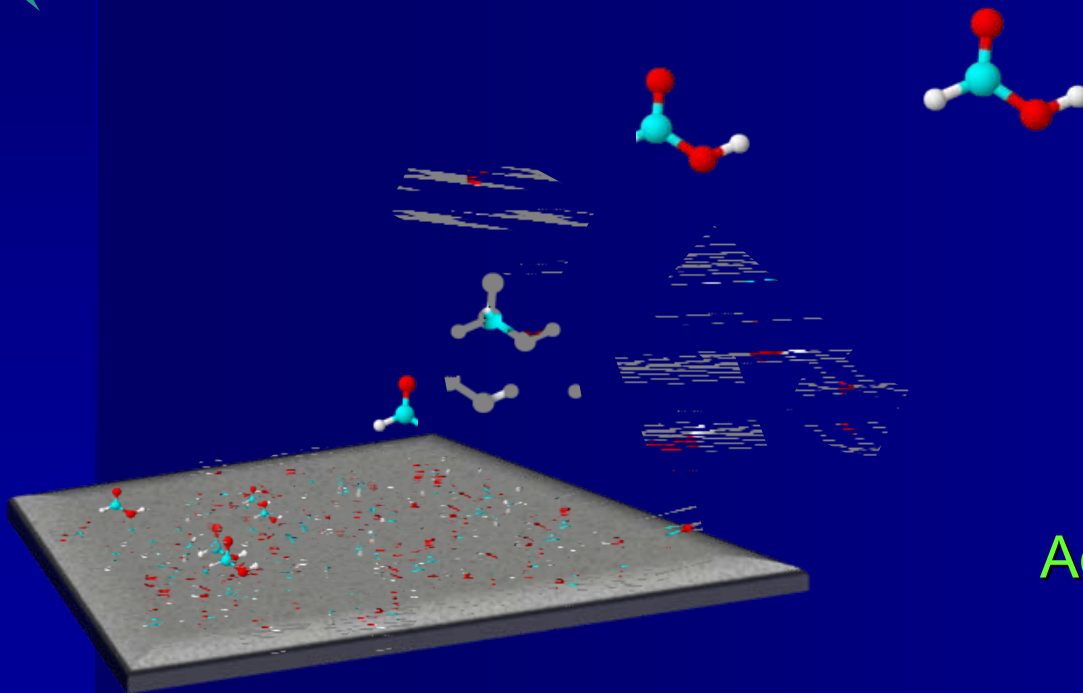


■ Fisissorção (Physisorption)

- Forças intermoleculares (Ligações fracas): Pontes de hidrogênio, dipolo, dipolo induzido, van der Waals, ... ($\sim \text{meV}$)
- Não envolve sítios específicos: Toda a superfície!
- Não envolve energia de ativação.
- Moléculas podem caminhar bastante na superfície (difusão alta)
- Multicamadas; Preenchimento de microporos.
- Em equilíbrio: o n de moléculas que “colam” na superfície é igual ao numero de moléculas que “descolam” superfície.

2) Processos de Alteração e Destruição:

- FOTÓLISE: Fótons (UV, Raios X)
- RADIÓLISE: Partículas (e^- , íons, CRs); Vento solar.
- AQUECIMENTO: Colisão entre os grãos



Reações químicas
Desorção
Aquecimento e Evaporação
Sputtering (erosão)
Compactação

3) Experimentos de Laboratório

- Diferentes domínios de energia (alta, intermediária, media e baixa) envolvendo fótons, elétrons, íons e átomos neutros.
 - Estudos de superfície ou volume
-

3.1) Energias Altas (ex. > 1 keV) → Sputtering, dissociação

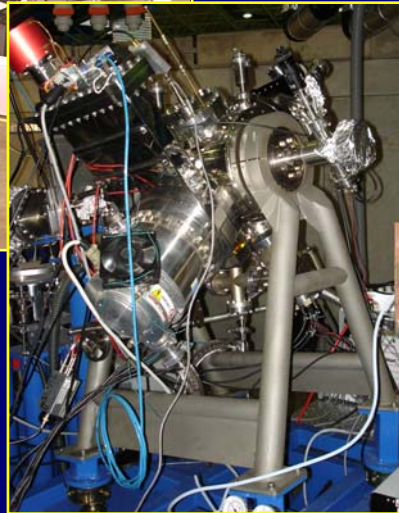
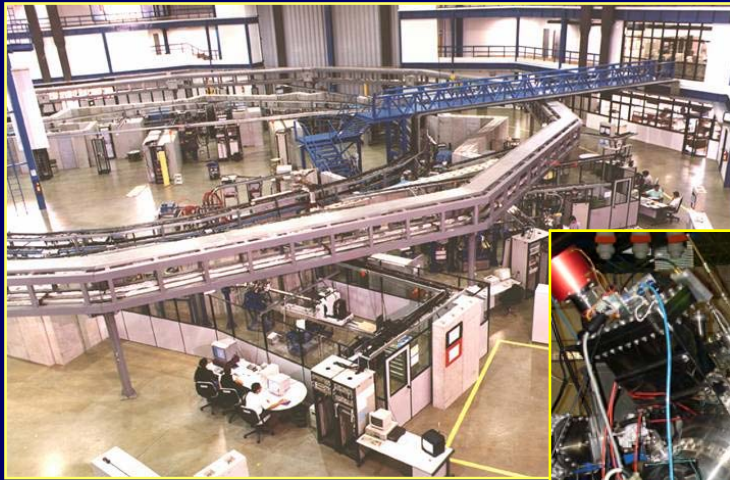
Fótons (X-ray): ionização e dissociação molecular, reações químicas (radicais, espécies iônicas), Sputtering (para energias altas), Seções de choque de absorção (camada interna).

Íons rápidos: compactação, clusters, Grande Sputtering, reações, seções de choque diss.

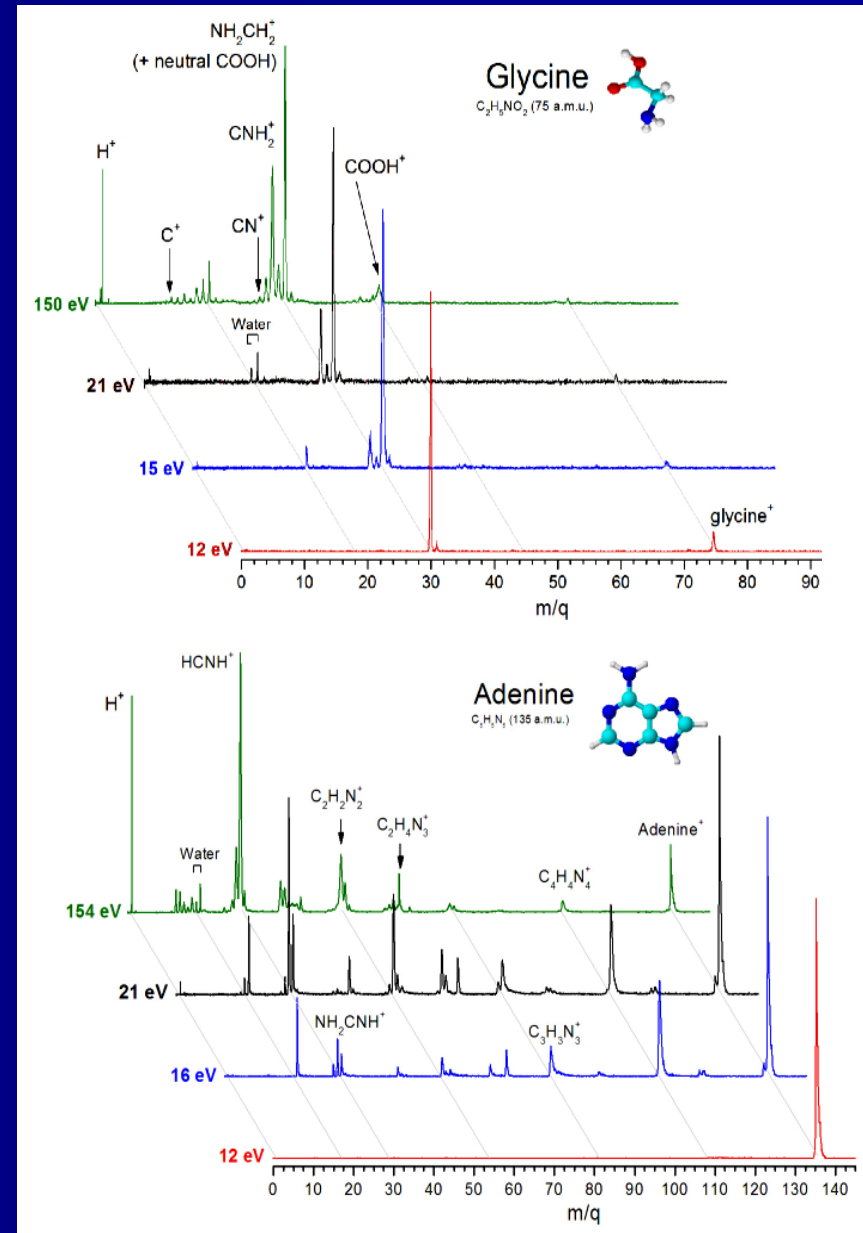
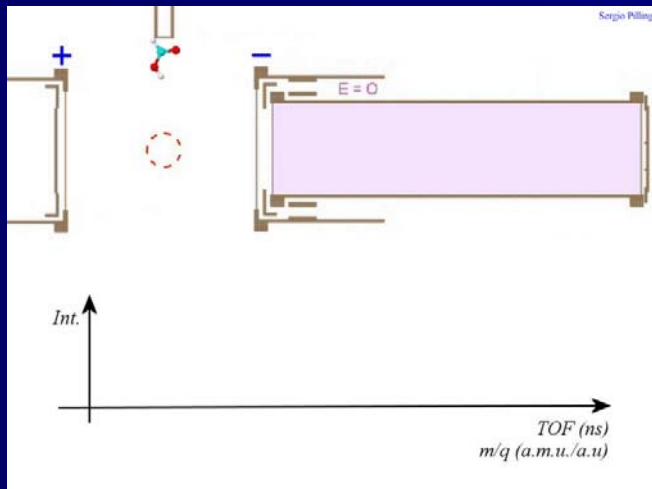
OBS: A penetrabilidade os íons é maior do q a dos fótons e elétrons. Stopping power: Energia depositada.

Técnicas investigativas: PDMS, PSID, TOF-MS, FTIR, QMS.

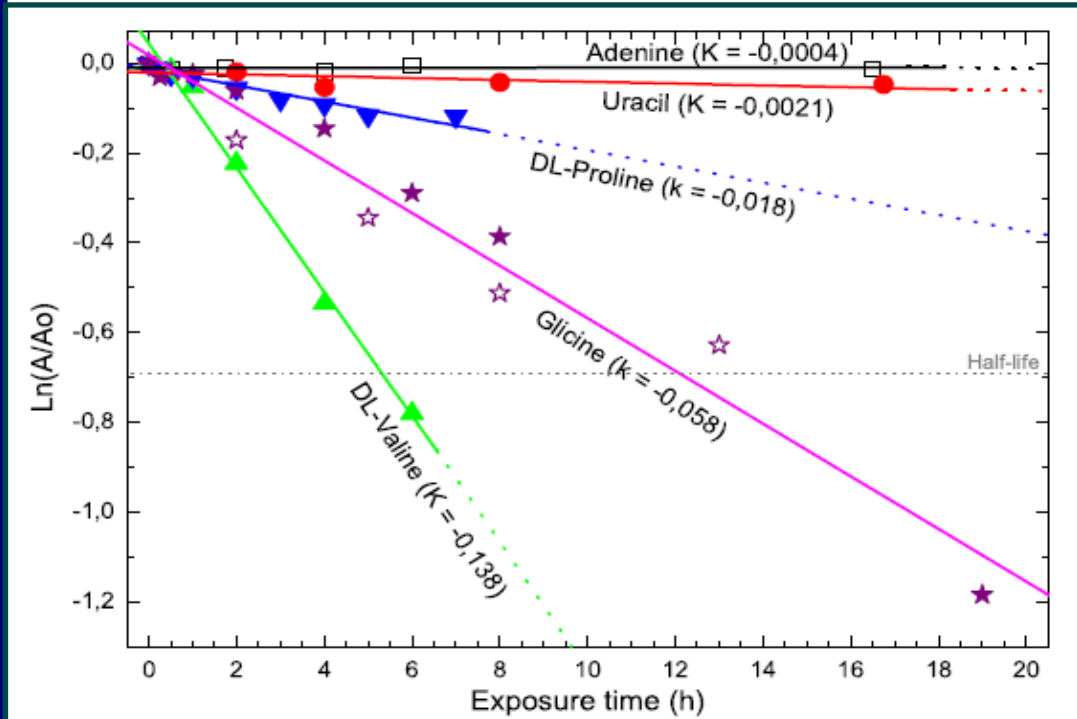
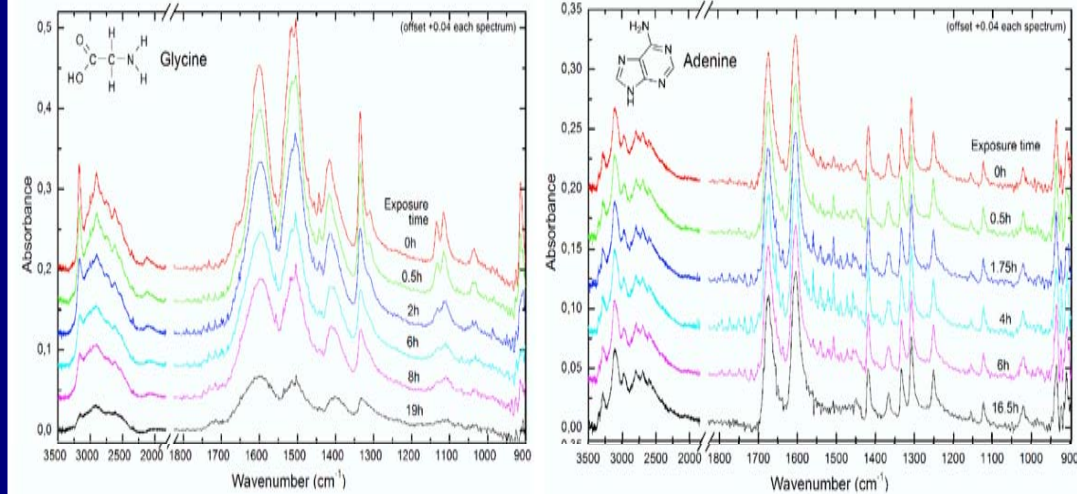
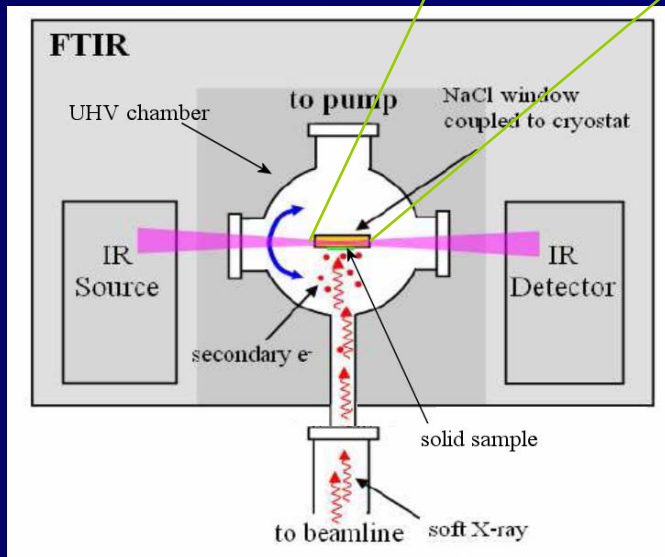
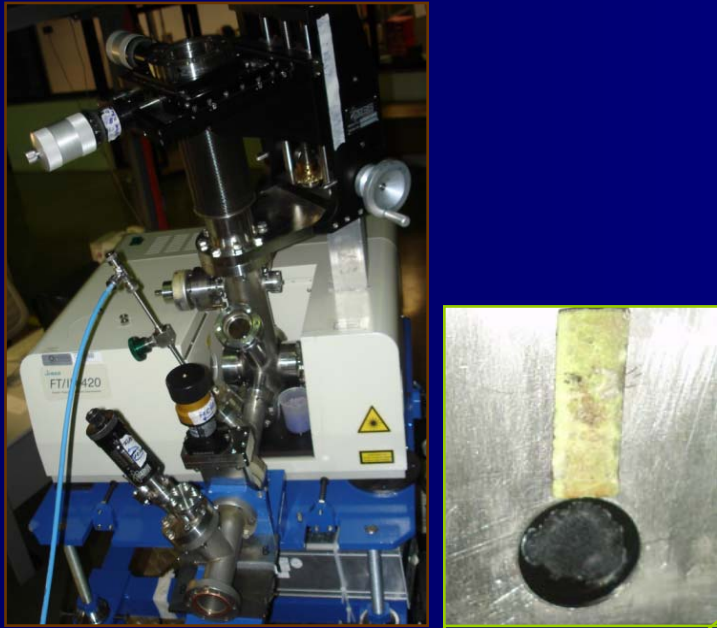
Ex. Experimentos de interação com fótons energéticos (fase gasosa)



- LNLS (raios X moles)
- TOF-MS
- Br. ratio e Seções de choque.



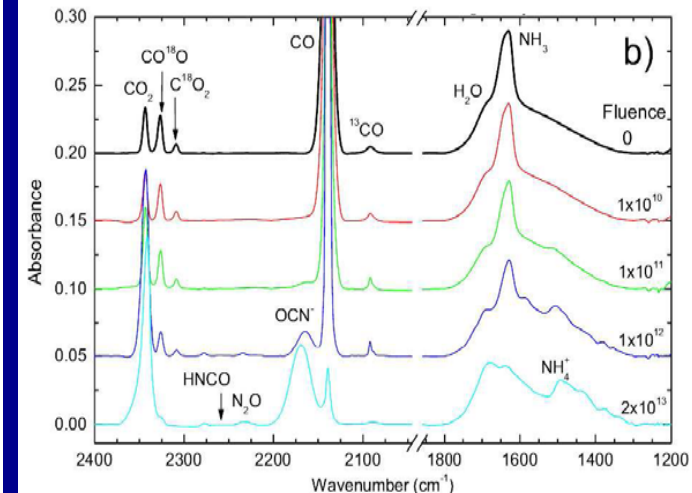
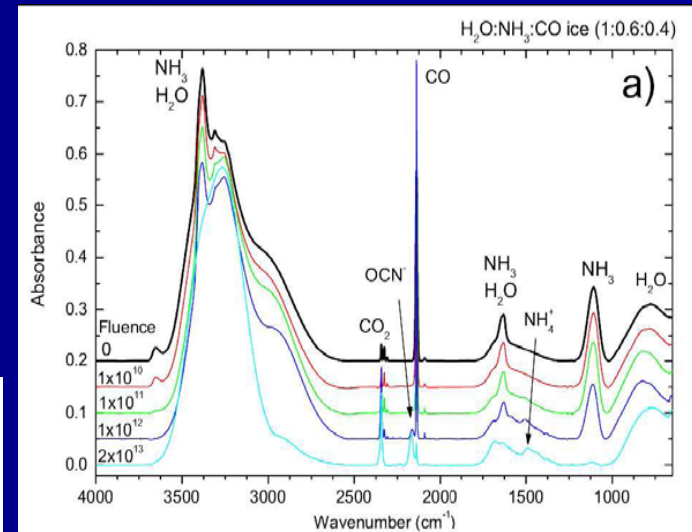
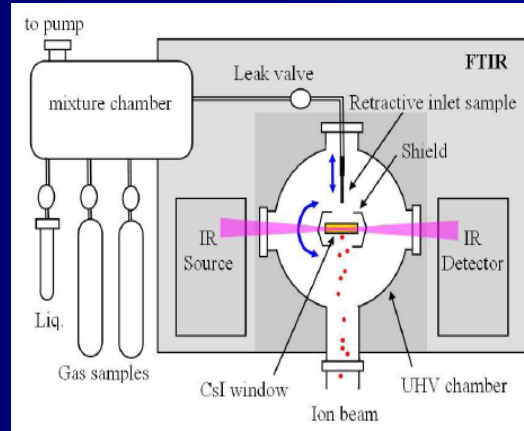
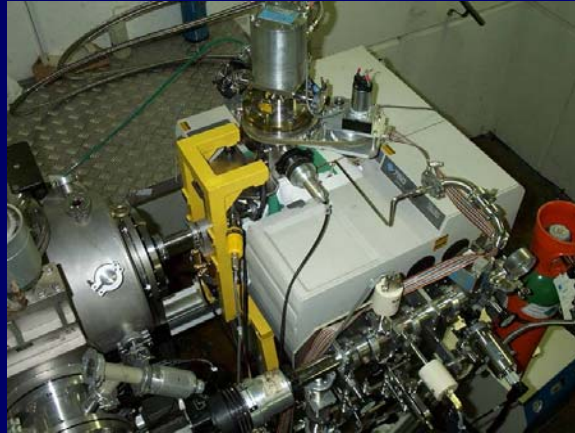
Ex. Experimentos de interação com fótons energéticos (fase condensada)



Ex. Experimentos de interação com ions energéticos (fase condensada)

- Simulação do efeitos de raios cósmicos em gelos astrofísicos.

S. Pilling, et al. 2009 A&A, Submt



Typical dense cloud grain

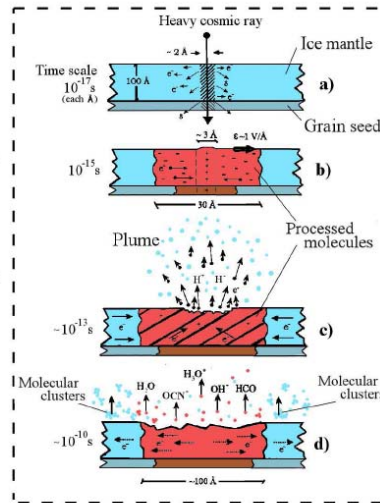
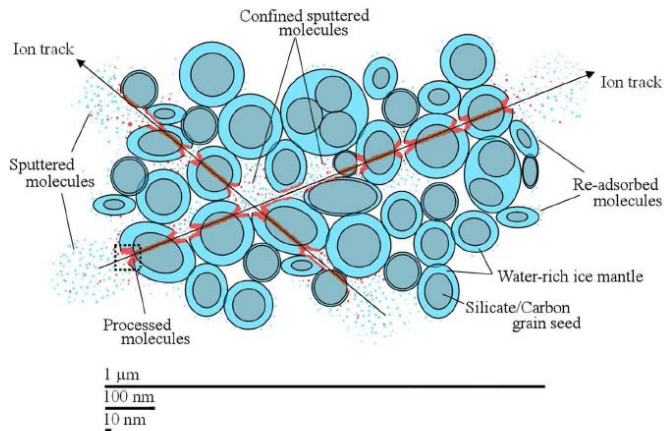


Fig. 7. Schematic view showing the interaction between heavy ion cosmic ray with a typical interstellar grain inside dense clouds. The ion track along the coagulate sub-micron size grains, the grain mantles, the processed and the sputtered molecules are indicated. Figure insets were adapted from Andrade et al. (2008) and indicate the physical-chemical changes on the grain mantle due to the impact with heavy ion. See details in text.

Sputtering e seção de choque de dissociação

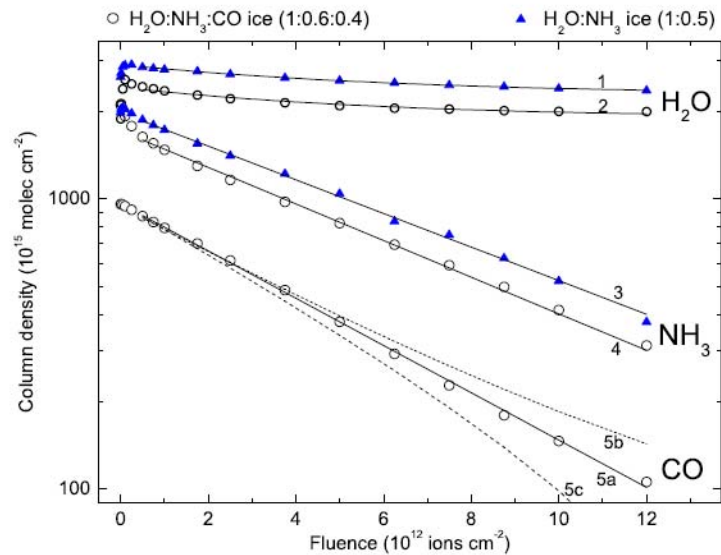


Fig. 3. Variation of the column density of water, ammonia and CO as a function of fluence. The solid lines are the fittings using Eq. 6 and Eq. 7. Triangles and circles correspond to different ice samples. The model parameters are listed in Table 3. See details in text.

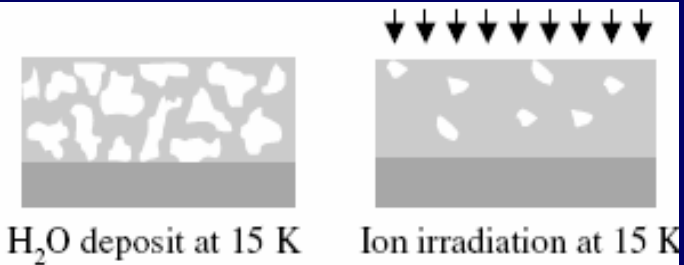
$$N_i = N_{0i} \exp(-\sigma_{d,i}F) \quad \text{for } i \neq 1 \text{ species}$$

and

$$N_1 = (N_{01} - N_{\infty,1}) \exp(-\sigma_{d,1}F) + N_{\infty,1}$$

where $N_{\infty,1} = (L_1 - Y_1)/\sigma_{d,1}$ is the asymptotic value of column density at higher fluences due to the presence of layering. N_i and N_{0i} are the column density of species i at a given fluence and at the beginning of experiment, respectively.

Compactação



H₂O deposit at 15 K

Ion irradiation at 15 K

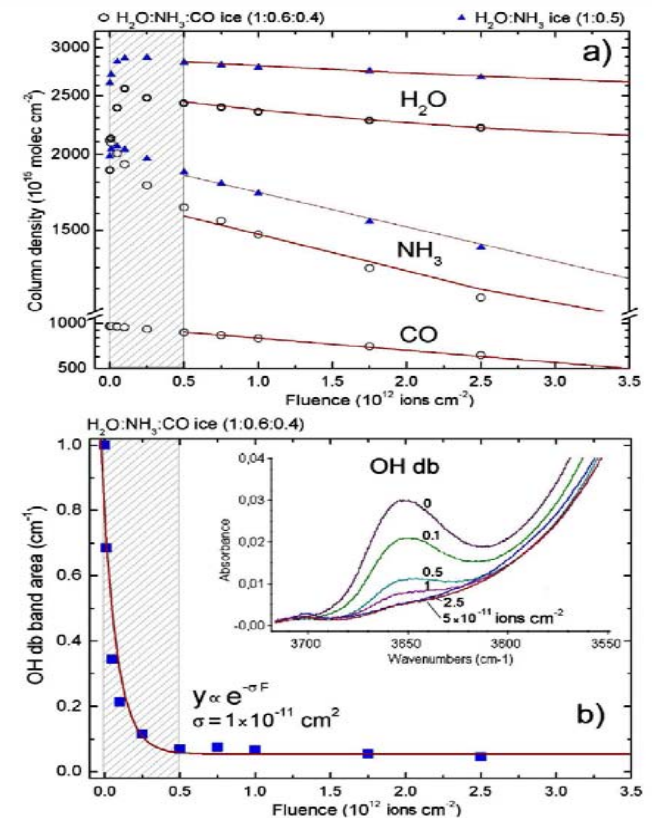


Fig. 4. a) Expanded view of Fig. 3 at the beginning of irradiation. Note the drastic changes in column density of water and ammonia up to fluence of 5×10^{11} ions cm^{-2} . The hatched strip indicates the regions where the compaction is occurring. b) OH dangling bond feature area (cm^{-1}) in the H₂O:NH₃:CO ice (1:0.6:0.4) as a function of fluence. Figure inset is the OH db feature from non irradiated ice and at fluences 0.1, 0.5, 1, 2.5 and 5×10^{11} ions cm^{-2} .

Formação de espécies novas (OCN⁻; Glicina?)

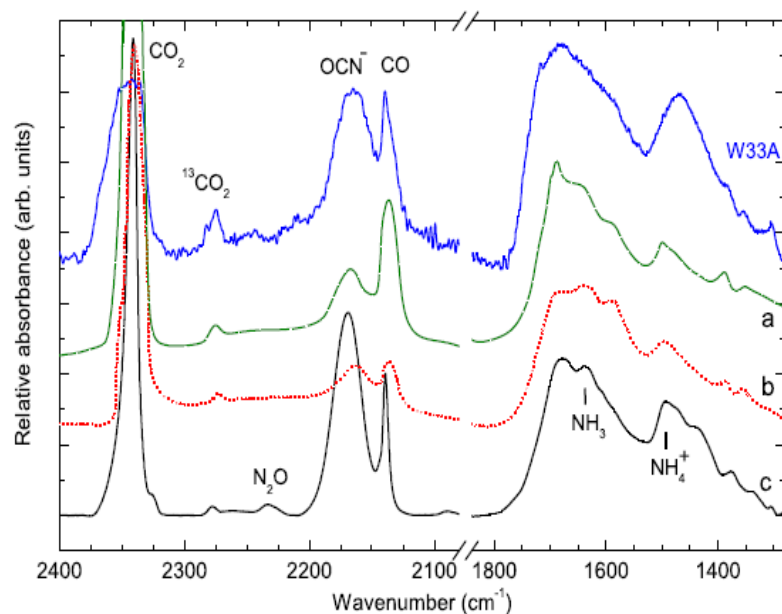
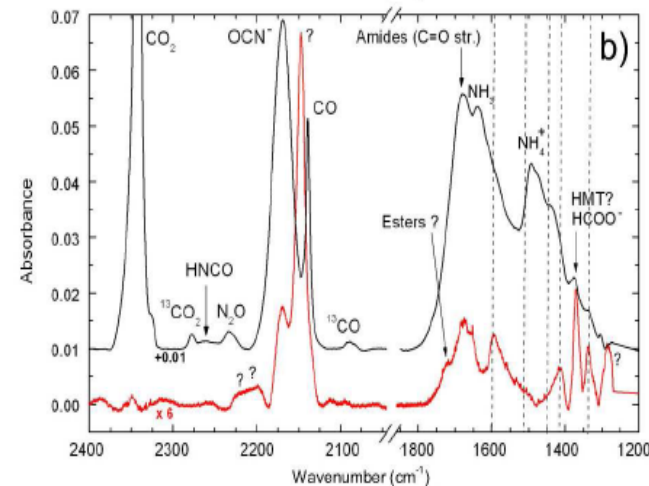


Fig. 5. Comparison between IR spectra of interstellar and laboratory ices. The upper trace is the infrared spectra of protostellar source W33A obtained by Infrared Space Observatory (ISO). Lower traces indicates lab spectra of H₂O:NH₃:CO ices at 13-15 K after processing by ionizing radiation. a) H₂O:NH₃:CO (1:0.2:0.2) ice processed by UV photons (Hudson & Moore 2000); b) H₂O:NH₃:CO (1:0.2:0.2) ice bombarded by 0.8 MeV protons (Hudson & Moore 2000); c) H₂O:NH₃:CO ice (1:0.6:0.4) irradiated by 46 MeV Ni ions simulating heavy and energetic cosmic rays (this work).



b) Comparison between the organic residue at 13 K and 300 K. Vertical dashed lines indicate the frequencies of some vibration modes of zwitterionic glycine (NH₃⁺CH₂COO⁻).

Table 4. Infrared absorption features produced by the radiolysis of the H₂O:NH₃:CO ice (1:0.6:0.4) by heavy, charged and energetic ions and the assignment of the observed bands at 13 K and 300 K.

Frequency (cm ⁻¹)	Wavelength (μm)	Temp. (K)	Molecule	Vibration mode (cm ⁻¹)	Notes
~2280	4.38	13	HNCO	(~2265)	[1,3,7]
2233	4.48	13	N ₂ O	N-N str.(2235)	[1,2]
2218 ^d	4.51	300	aryl nitriles	Ar-C≡N (2210)	[8]
2200	4.54	300	conjug. nitriles	(~2180)	[8]
2168	4.61	13, 300	OCN ⁻	(~2165)	[1,3,4,7]
2147 ^d	4.66	300	aliph. isocyanide	R-N≡C (2150)	[8]
~2112	4.73	300	NCO ₂	ν ₁ (2115)	[2]
1725 ^d	5.80	300	ester ^a	C=O str. (~1742)	[5]
1683	5.94	300	amides ^b	C=O str. (~1680)	[5]
1652 ^d	6.05	300	N ₃ ; asym-N ₂ O ₃	(1652)	[2]
1637	6.11	13	?		
1593 ^d	6.28	300	NH ₃ ⁺ CH ₂ COO ⁻	COO ν _{as} (1596)	[6]
1558	6.42	300	?		
1533	6.52	300	?		
1506 ^d	6.64	300	NH ₃ ⁺ CH ₂ COO ⁻	NH ₃ δ _s (1505)	[6]
~1490	6.71	13	NH ₃ ⁺	ν ₄ (~1485)	[1,3,7]
1474	6.78	13	NO ₂ ?	(1471)	[2]
1440 ^d	6.94	13	NH ₃ ⁺ CH ₂ COO ⁻	NH ₃ δ (1444)	[6]
1415 ^d	7.07	300	NH ₃ ⁺ CH ₂ COO ⁻	COO ν _s (1415)	[6]
~1370 ^d	7.30	13, 300	HMT ^c	CH seis (1375)	[5]
			HCOO ⁻	CH seis	[5]
1338 ^d	7.47	13, 300	NH ₃ ⁺ CH ₂ COO ⁻	CH ₂ ω (1342)	[6]
			NH ₃ CH ₂ COO ⁻	ν ₉ (1342)	[6]
1305	7.66	13	N ₂ O ₃ ; N ₂ O ₄ ; N ₂ O ₅	ν ₁ ; ν ₃ ; ν ₂ (1303)	[2]
1283 ^d	7.80	300	N ₂ O	N-O str. (1288)	[2]

^a amides, H₂NC(=O)-R; ^b esters, R-C(=O)-O-R; ^c HMT - hexamethylenetetramine, (CH₂)₆N₄; ^d tentative assignment. [1] Proton bombardment of several ices (Hudson et al. 2001); [2] Electron bombardment of N₂:CO₂ (Jamieson et al. 2005); [3] Hudson & Moore 2000; [4] van Broekhuizen et al. 2005; [5] UV photolysis of H₂O:NH₃:CH₃OH:CO:CO₂ ice (Munoz Caro and Shutte 2003); [6] Electron bombardment of CH₃NH₂:CO₂ ice (Holtom et al. 2005); [7] UV photolysis of ammonia-rich ices (Demyk et al. 1998); [8] UV photolysis of N₂:CH₄ ices at various pressures (Imanaka et al. 2004).

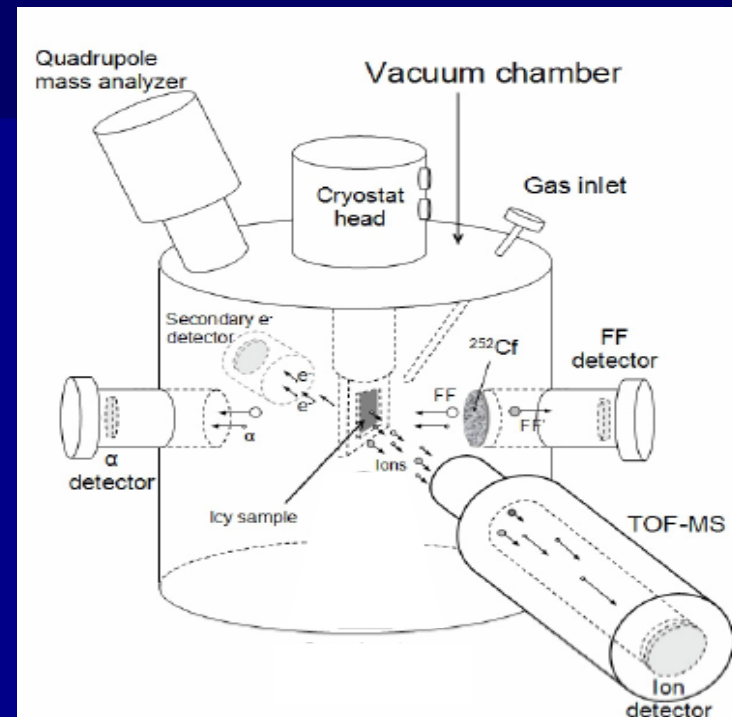
Ex. Investigações da superfície pelo impacto de íons rápidos

PDMS – Cf: Plasma Desorption Mass spectrometry by ^{252}Cf fission frag.

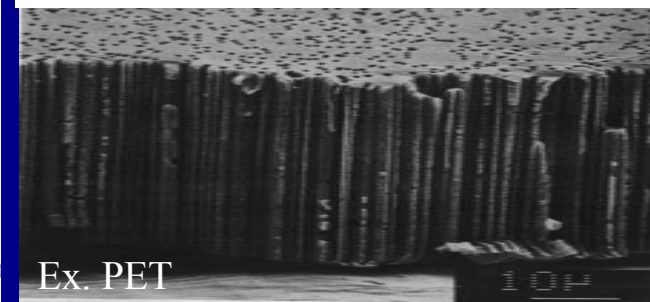
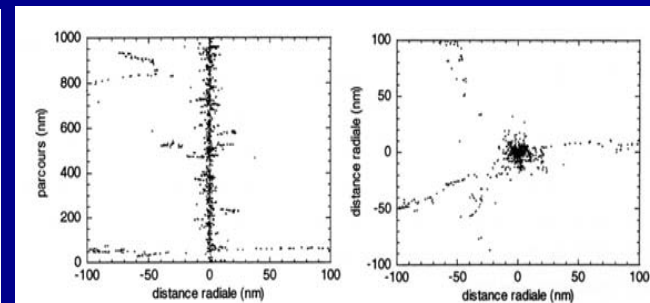
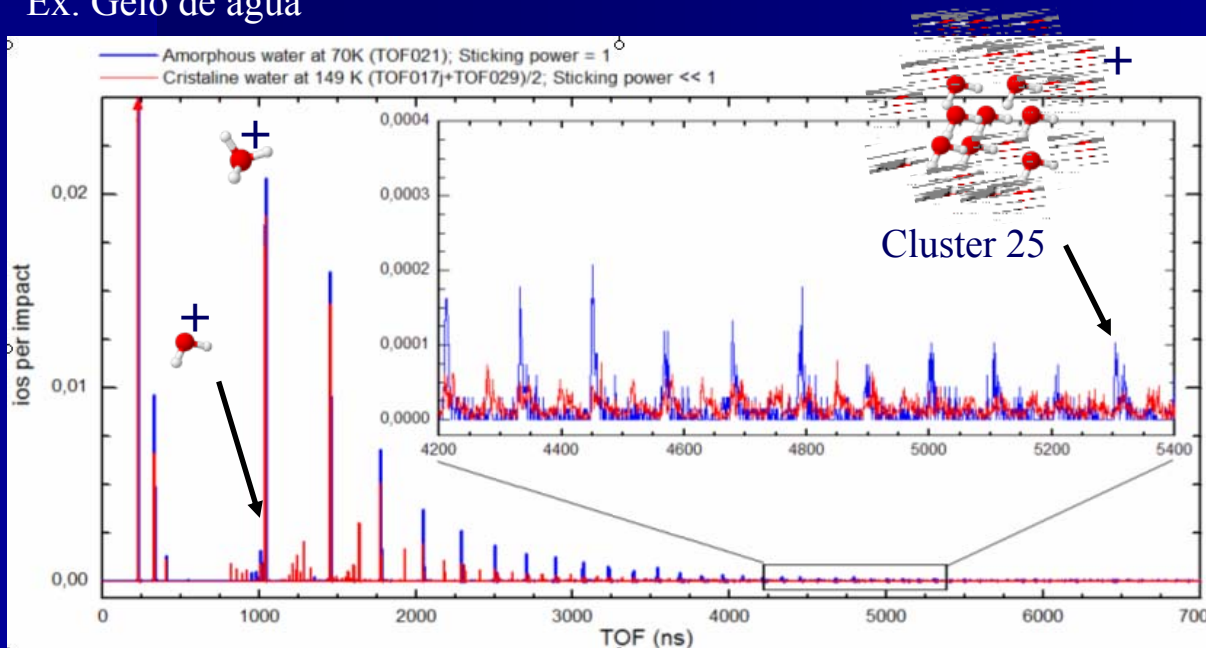
- $E \sim 65\text{MeV}$; (Regime eletrônico)
- Baixo fluxo $\sim 1000\text{ cm}^{-2}\text{ s}^{-1}$.

UVH + TOF-MS

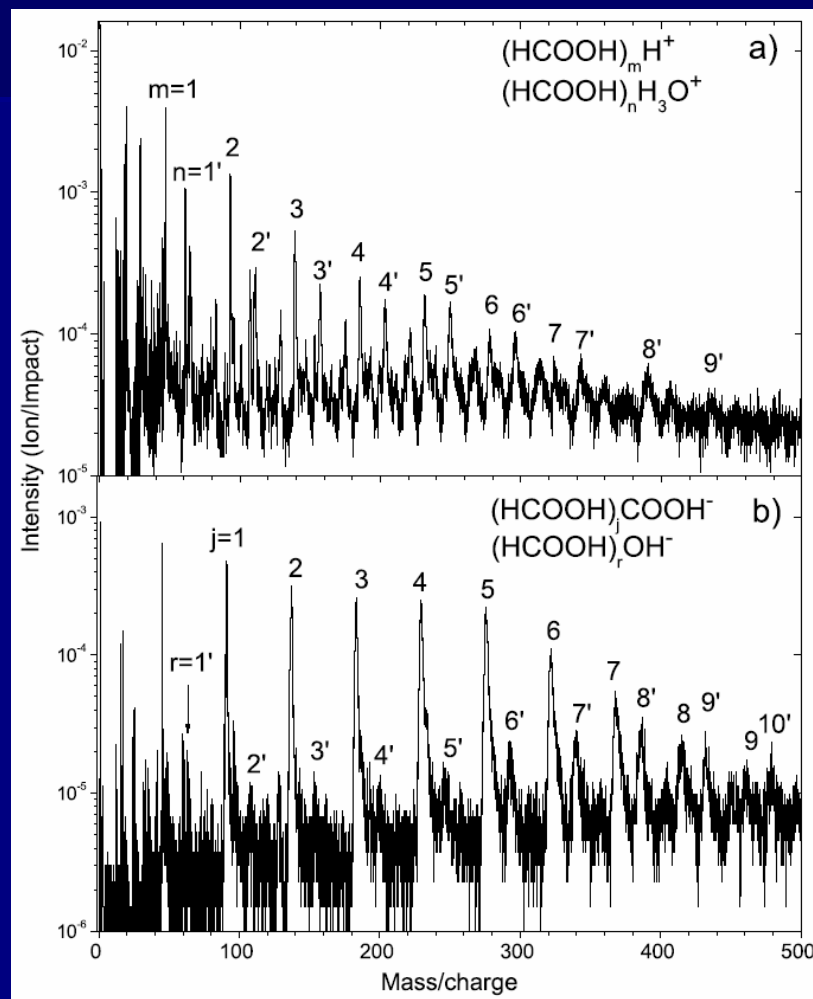
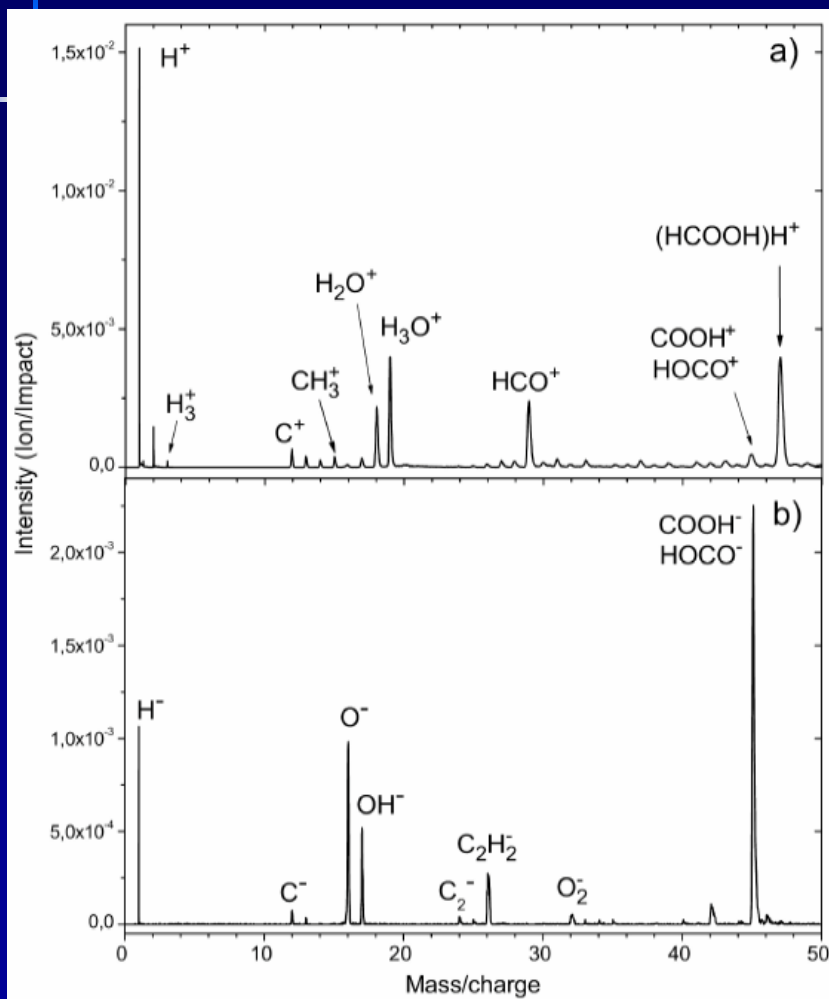
- Track: Atomização e molecularização
- Dissociação molecular (via secondary e^-).
- Novas espécies (via secondary e^-).
- **Clusters; íons positivos e negativos.**



Ex. Gelo de água



Ex. Gelo de ácido Fórmico (HCOOH) à 55K



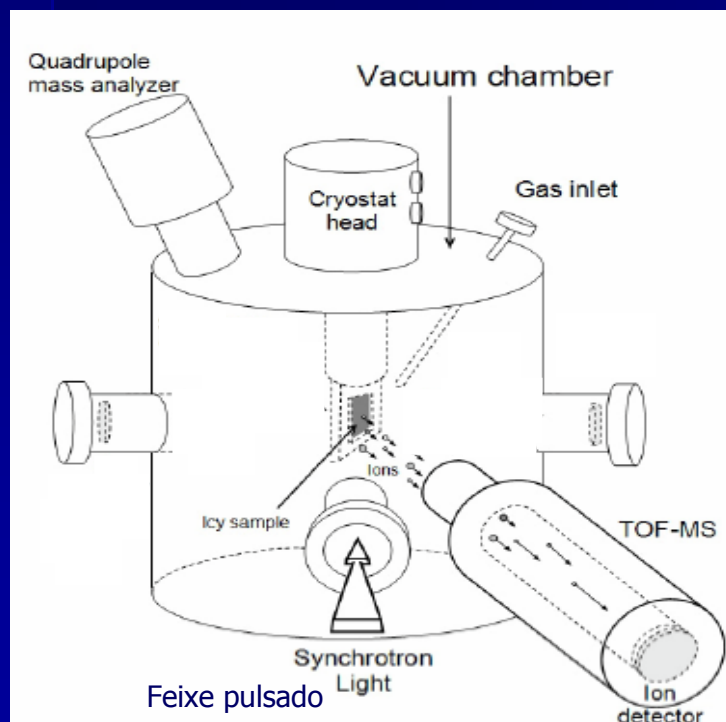
Ex. Investigações da superfície pelo impacto de fótons energéticos

PSID – Photon Stimulation Ion Desorption

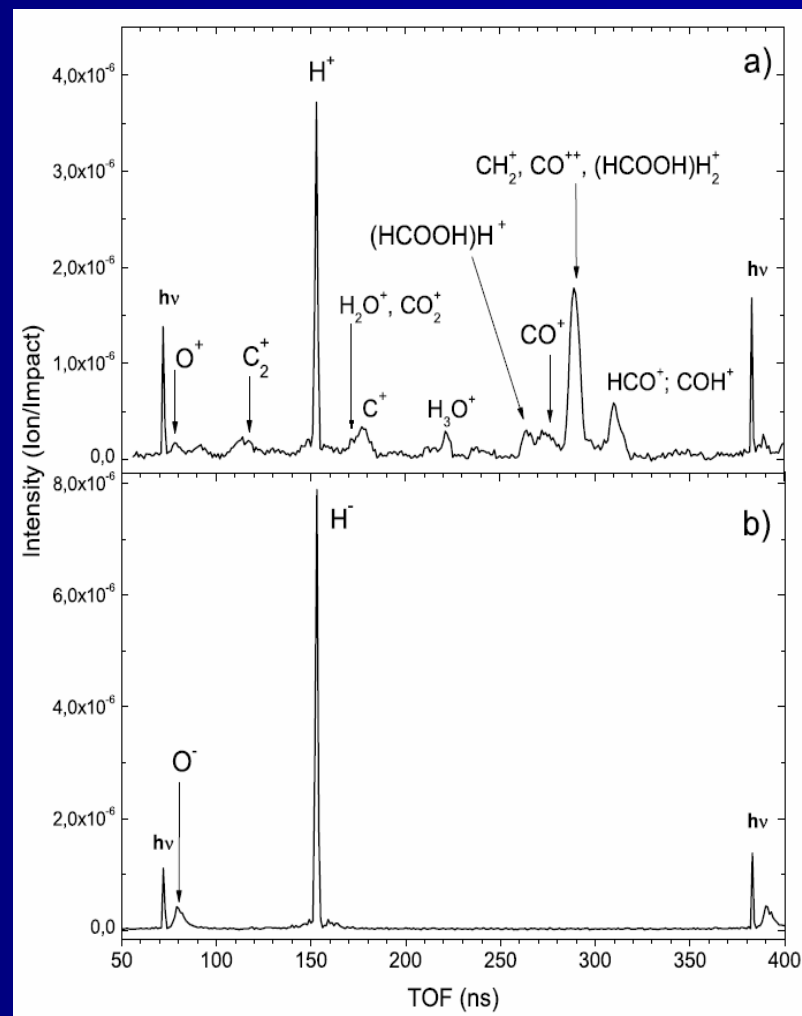
- Raios X; Feixe Pulsado (LNLS)

UVH + TOF-MS

- Dissociação molecular.
- Desorção estimulada.
- Íons positivos e negativos.
- NÃO produz Clusters



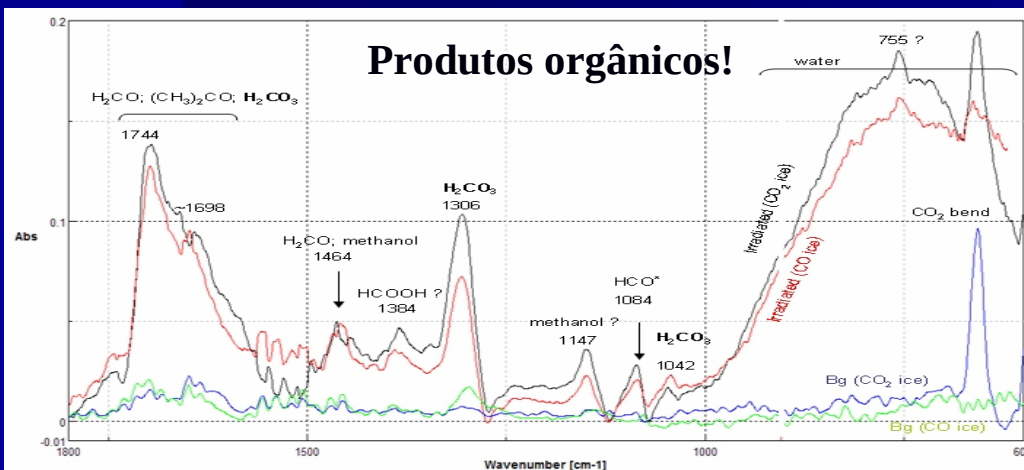
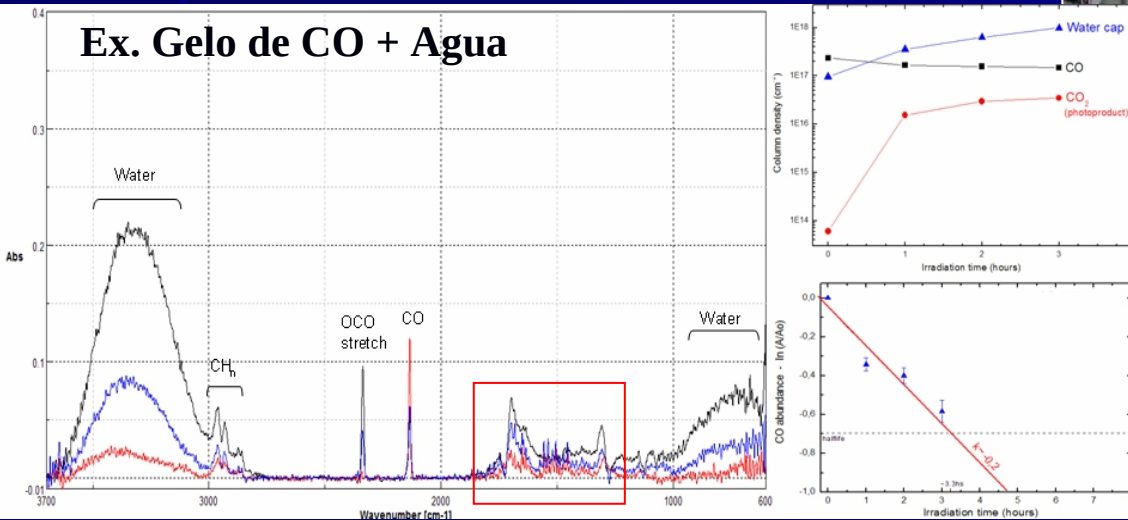
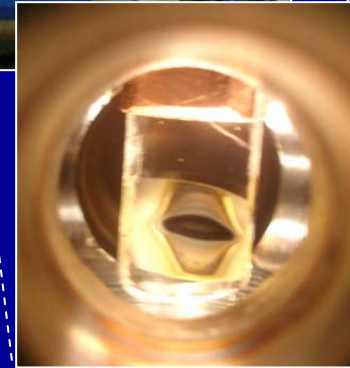
Ex. Gelo de ácido Fórmico (HCOOH) à 55K



Andrade et al. 2008

Ex. Fotoquímica de gelos de CO e CO₂ dentro de nuvens moleculares simuladas

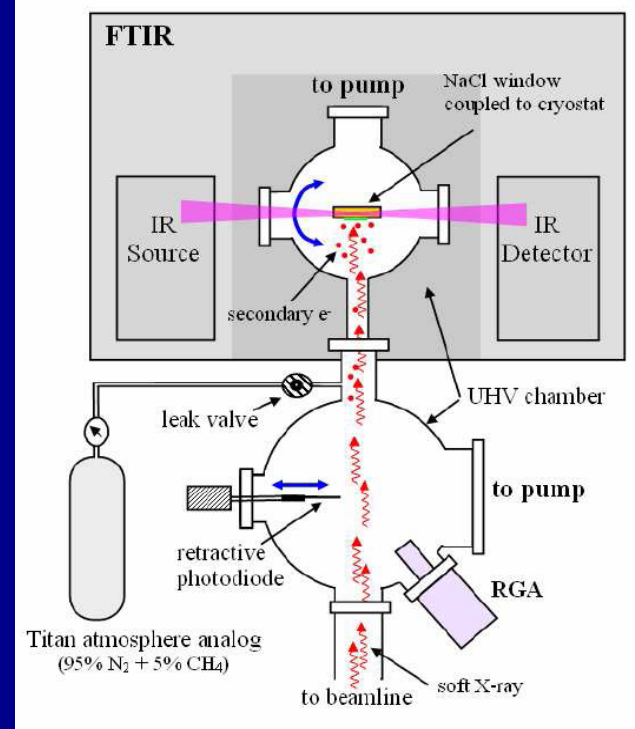
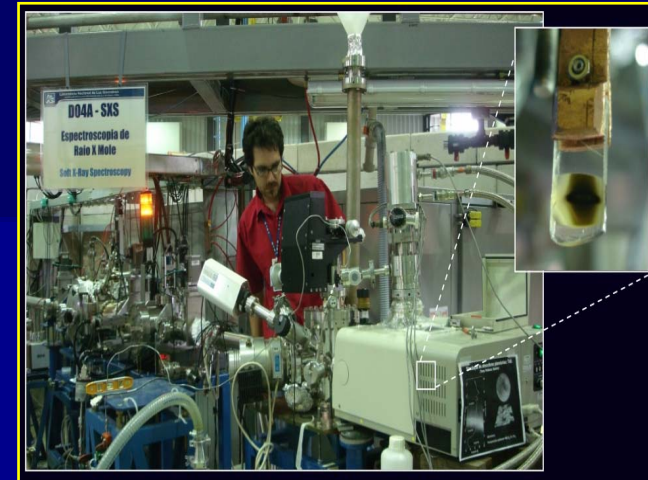
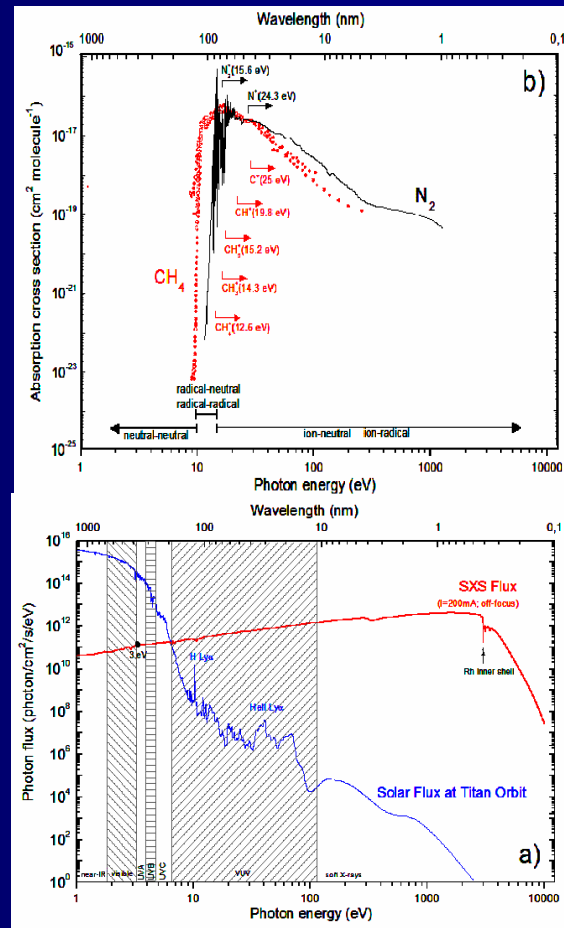
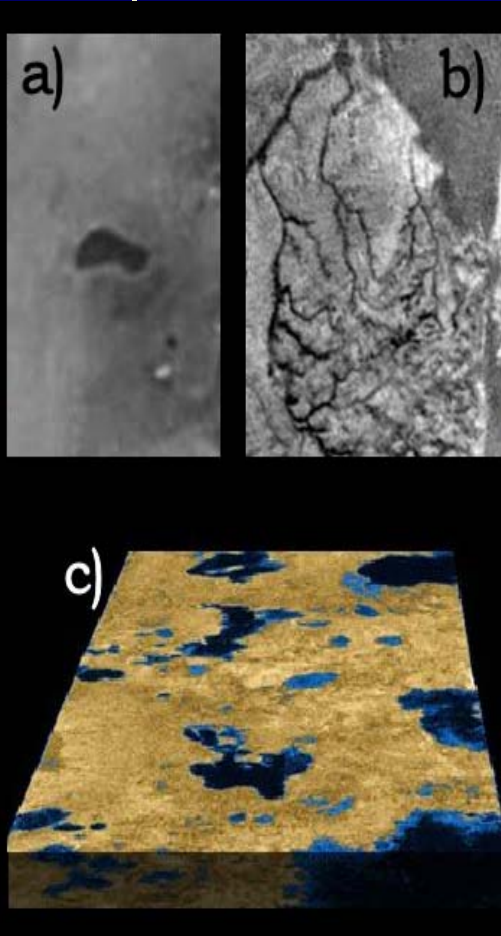
- Cryo-IR_β (NaCl; 12 K; 10⁻⁷ mbar)
- SXS (white beam; 0.5-3 keV)
- k , σ , $\tau_{1/2}$

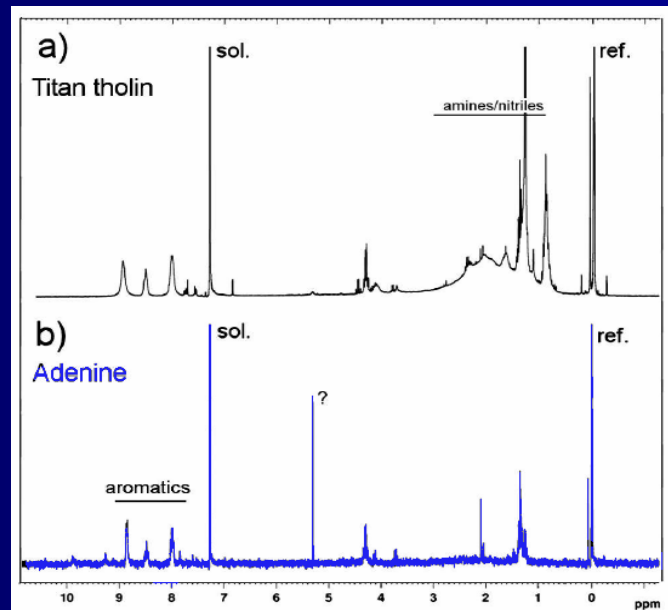
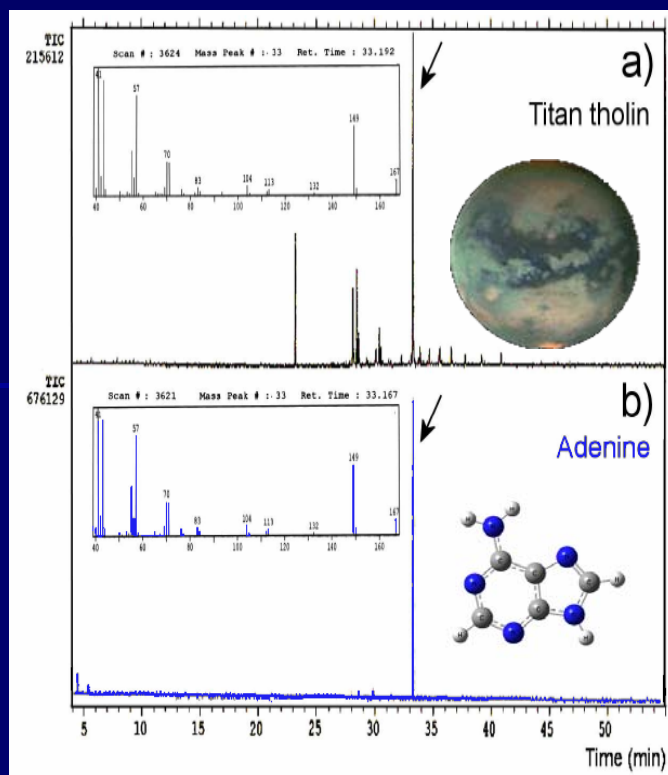
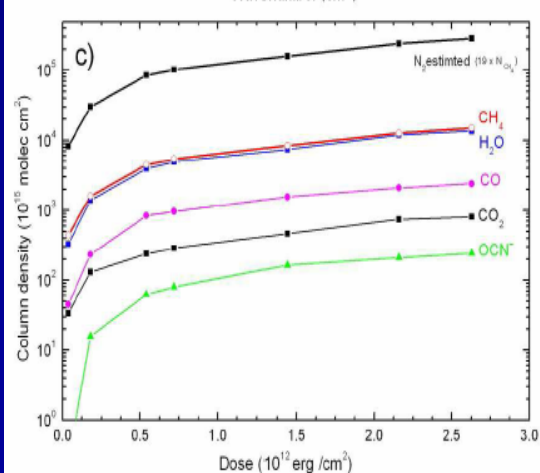
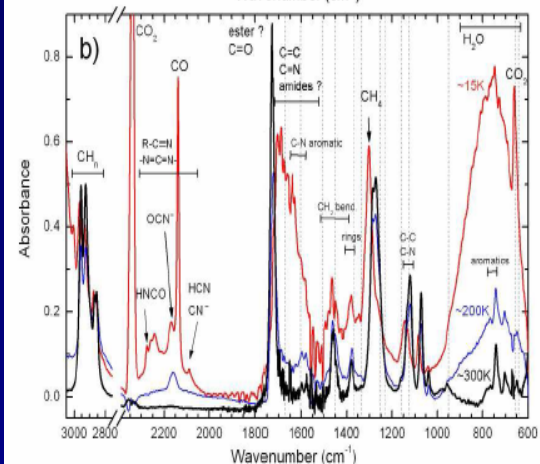
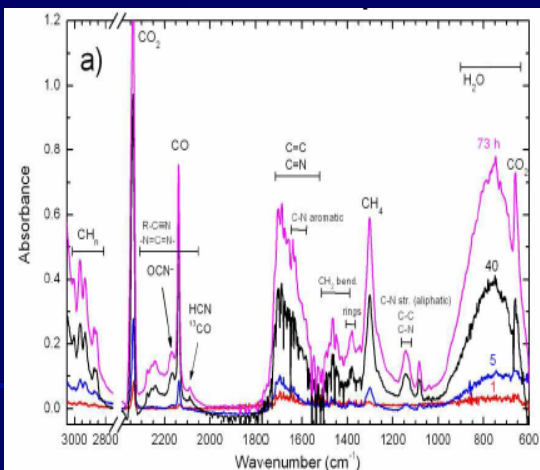


	Photon flux at soft X-ray range	Half life of CO	Half life of CO ₂
Experimental	2x10 ⁴ erg/cm ² s	3.4 hs	6.7 hs
Typical XDR	10 erg/cm ² s	~ 4 x 10 ³ hs	~ 7 x 10 ³ hs
Dense Cloud (AFLGL 2591)	10 ⁻² erg/cm ² s	~ 5 x 10 ³ years	~ 10 ⁴ years

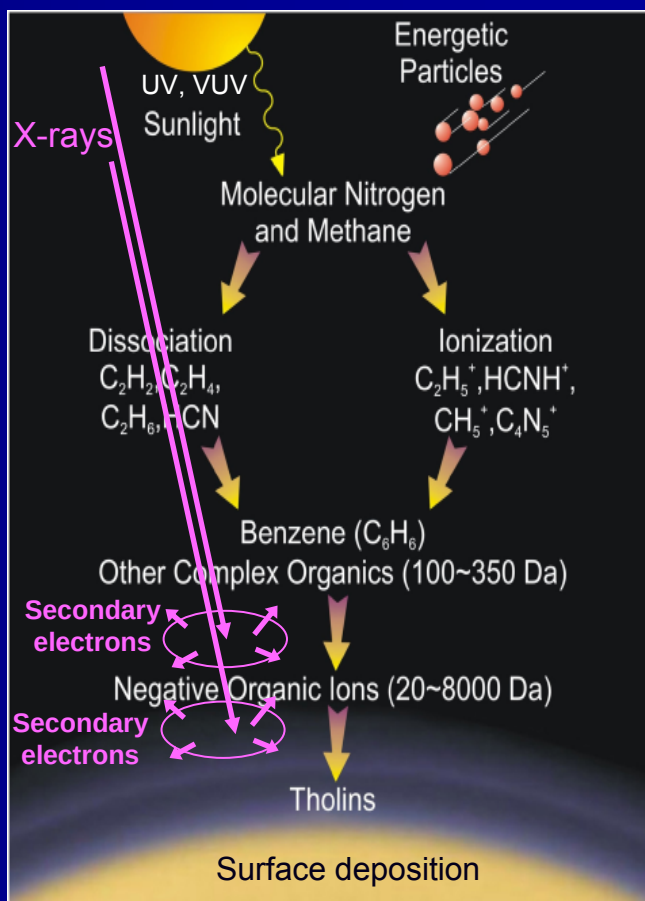
Ex. Fotoprodução de biomoléculas na atmosfera de Titã por raios X

- Cryo-IR_p (NaCl; 12 K; 10⁻⁸ mbar)
- N₂ 95% + CH₄ 5% (+ traços H₂O): 10⁻⁶ mbar
- SXS (white beam; 0.5-3keV; ~10¹² fótons/cm s)
- *In-situ* FTIR, *in-situ* Q-MS, GC-TOFMS, RMN: **ADENINA**





- 73 hs de irradiação com luz sincrotron!
- ~ 7 milhões de anos de raios X solares em Titã
- Adenina: formação promovida por elétrons secundários produzido a partir da dissociação de moléculas por fótons de raios X.



Ex. Amorfização da estrutura cristalina (alta energia e energia intermediária)

UV

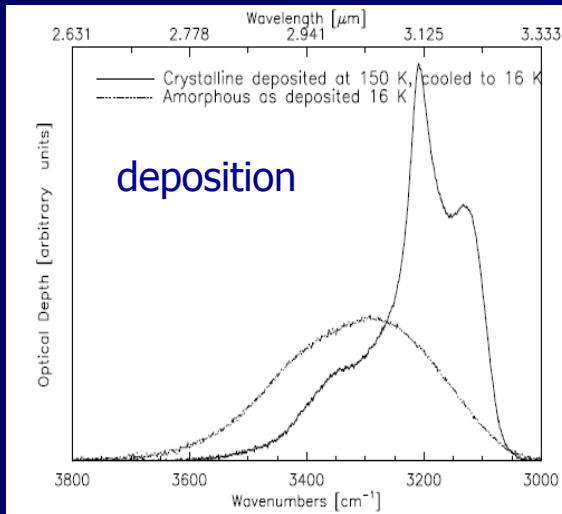


Fig.1. The 3-micron OH band in the case of crystalline and amorphous water ice.

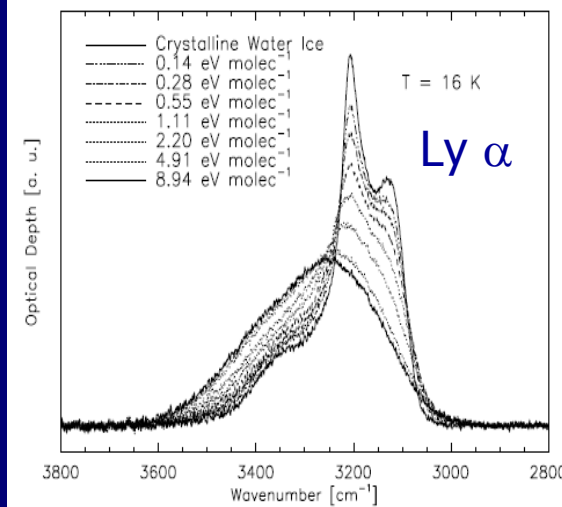
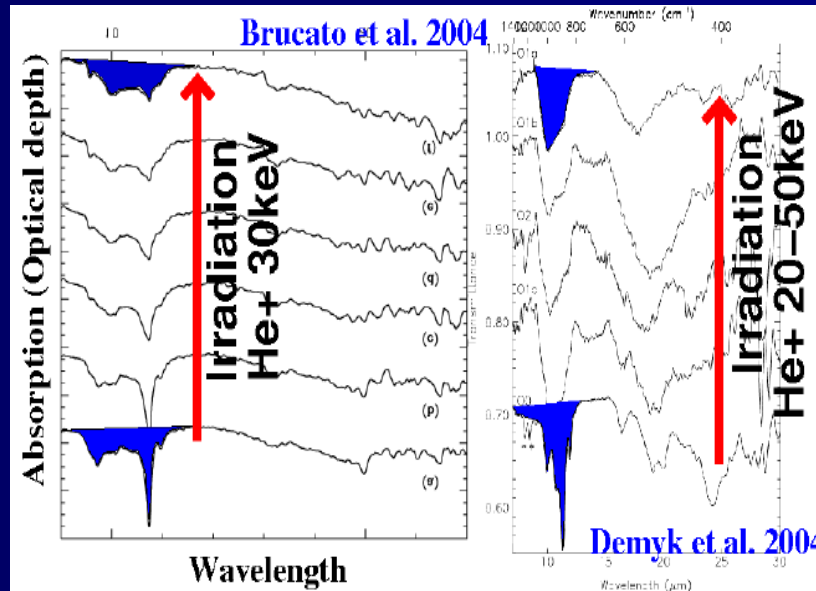


Fig.3. Evolution of the crystalline water ice band under UV photolysis.

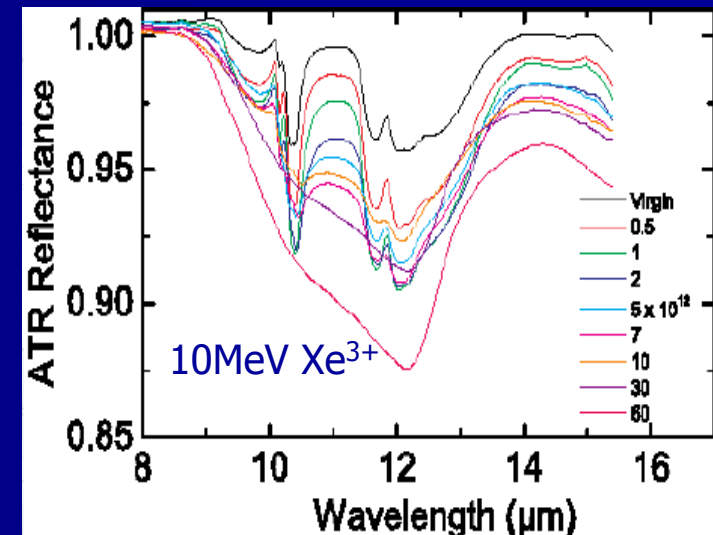
Leto 2003 A&A



Brucato et al. 2004

Demyk et al. 2004

CRs



Bringa et al 2007 A&A

3.2) Energias intermediárias (ex. $\sim 1-10$ eV) $\rightarrow$ Ionização, Dissociação, Rearranjos moleculares, Reações químicas.

Fótons (UV) e elétrons: ionização e dissociação molecular, reações químicas (radicais, espécies iônicas), Sputtering (para energias altas) Seções de choque de absorção (valência), dissociação iônica, dissociação neutra, dissociação por captura eletrônica.

Íons lentos: Implantação, aquecimento, reações.

Técnicas investigativas: Low energy ion/eletrom beam, TOF, FTIR, QMS.

Ex. Produção de aminoácidos a partir do processamento de gelos astrofísicos simulados

- Misturas: $\text{H}_2\text{O} + \text{NH}_3 + \text{CH}_4$ ou $\text{H}_2\text{O} + \text{CH}_3\text{OH} + \text{N}_2$
- UHV, Fonte de ionização (fótons, e^- , íons)
- Monitoramento *in-situ*: **FTIR**
- Análise *ex-situ*: **Cromatografia Líquida (HPLC) e gasosa (GC-MS)**

Mon. Not. R. Astron. Soc. 384, 695–710 (2008)

doi:10.1111/j.1365-2966.2007.12687.x

Amino acids produced from the ultraviolet/extreme-ultraviolet irradiation of naphthalene in a $\text{H}_2\text{O} + \text{NH}_3$ ice mixture

Y.-J. Chen,¹ M. Nuevo,^{1*} T.-S. Yih,¹ W.-H. Ip,² H.-S. Fung,³ C.-Y. Cheng,⁴ H.-R. Tsai⁴ and C.-Y. R. Wu⁵

THE ASTROPHYSICAL JOURNAL, 660:911–918, 2007 May 1

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MECHANISMS OF AMINO ACID FORMATION IN INTERSTELLAR ICE ANALOGS

JAMIE E. ELSILA,^{1,2} JASON P. DWORKIN,³ MAX P. BERNSTEIN,¹ MILDRED P. MARTIN,^{3,4} AND SCOTT A. SANDFORD¹



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Advances in Space Research 36 (2005) 190–194

ADVANCES IN
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Abiogenic photochemical synthesis on surface of meteorites and other small space bodies

Michael B. Simakov*, Eugenia A. Kuzicheva

A&A 457, 741–751 (2006)
DOI: 10.1051/0004-6361:20042018
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Astronomy
&
Astrophysics

The effects of circularly polarized light
on amino acid enantiomers produced
by the UV irradiation of interstellar ice analogs

M. Nuevo^{1,2}, U. J. Meierhenrich^{3,4}, G. M. Muñoz Caro^{1,5}, E. Dartois¹, L. d'Hendecourt¹,
D. Deboffle², G. Auger⁶, D. Blanc⁶, J.-H. Bredehoft⁷, and L. Nahon^{8,9}

NATURE | VOL 416 | 28 MARCH 2002

letters to nature

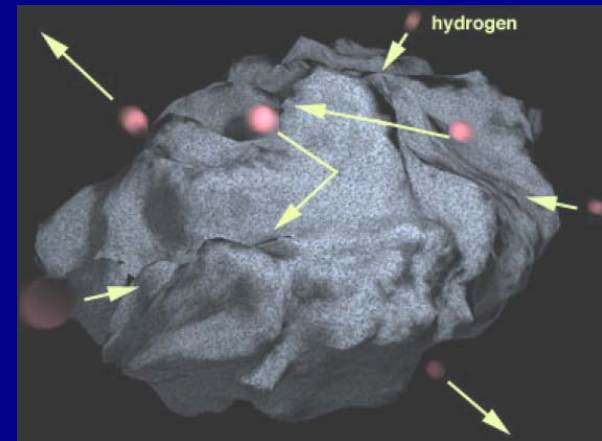
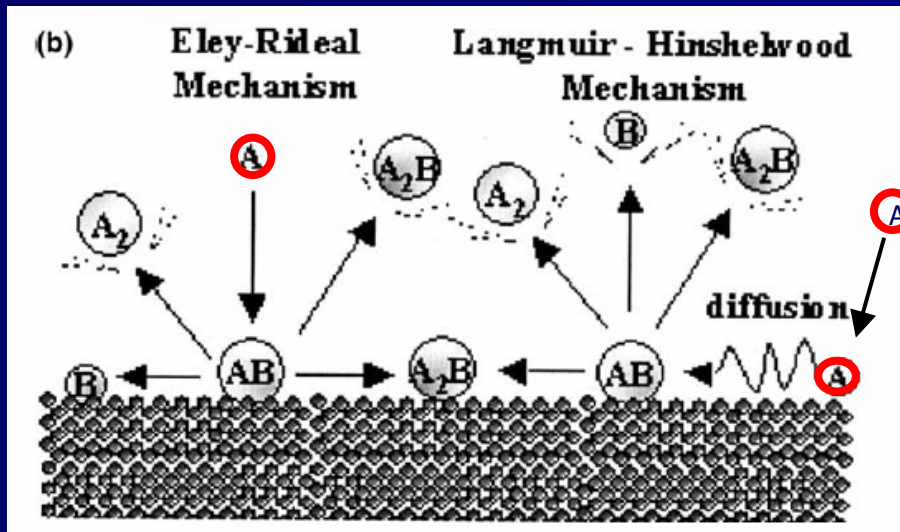
**Racemic amino acids from the
ultraviolet photolysis of
interstellar ice analogues**

Max P. Bernstein^{*,†}, Jason P. Dworkin^{*,†}, Scott A. Sandford[†],
George W. Cooper[†] & Louis J. Allamandola[†]

3.3) Energias baixas (ex. $\sim 0.1-1$ eV) $\rightarrow$ Reações seguidas por evaporação

- Sticking $\rightarrow$ diffusion $\rightarrow$ reaction $\rightarrow$ evaporation
 - Eley-Rideal/hot-atom reaction
 - Langmuir-Hinshelwood reaction
 - Experimentos de Formação do H_2 ,
 - Formação de H_2O a partir de $O_2 + H_2$, etc.
- Técnicas investigativas: TPD, FTIR, QMS.
- **Dissociation by electron association**

Exemplos.



Ex. Formação do H_2
(catalise heterogênea)

3.4) Energias muito baixas (ex < 0,01 eV) → Aquecimento - evaporação

- Fótons de IR, Visível, colisões entre grãos.
- Técnicas investigativas: TPD, FTIR, QMS.

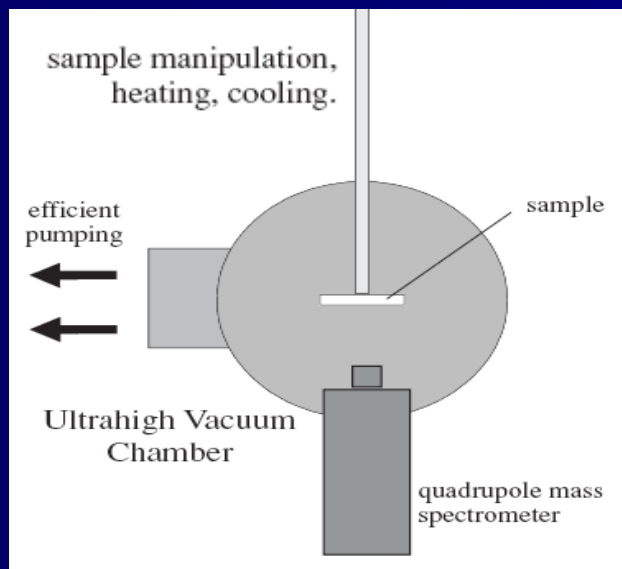
Ex. Experimentos para o estudo da evaporação de gases em gelos astrofísicos (TPD)

TPD – Thermal Programed Desorption

UHV + Aquecimento controlado + QMS

UHV (10^{-9} mbar → ~ 1 monolayer per hour $\sim 10^{12}$ mols/cm² s); Bombeamento eficiente para prevenir acumulação de gás na câmara; Rampa de aquecimento constante (ex. $\beta=1$ K/s); estudar o aprisionamento de gases; “Anelamento” de gelos astrofísicos.

Esquema experimental típico



Polanyi-Wigner equation

Taxa de desorção, $R(T)$

Fator pré-exponencial

$$R(T) = -\frac{dN_s}{dT} = \frac{A}{\beta} N_s^m \exp^{-E_d / k_B T}$$

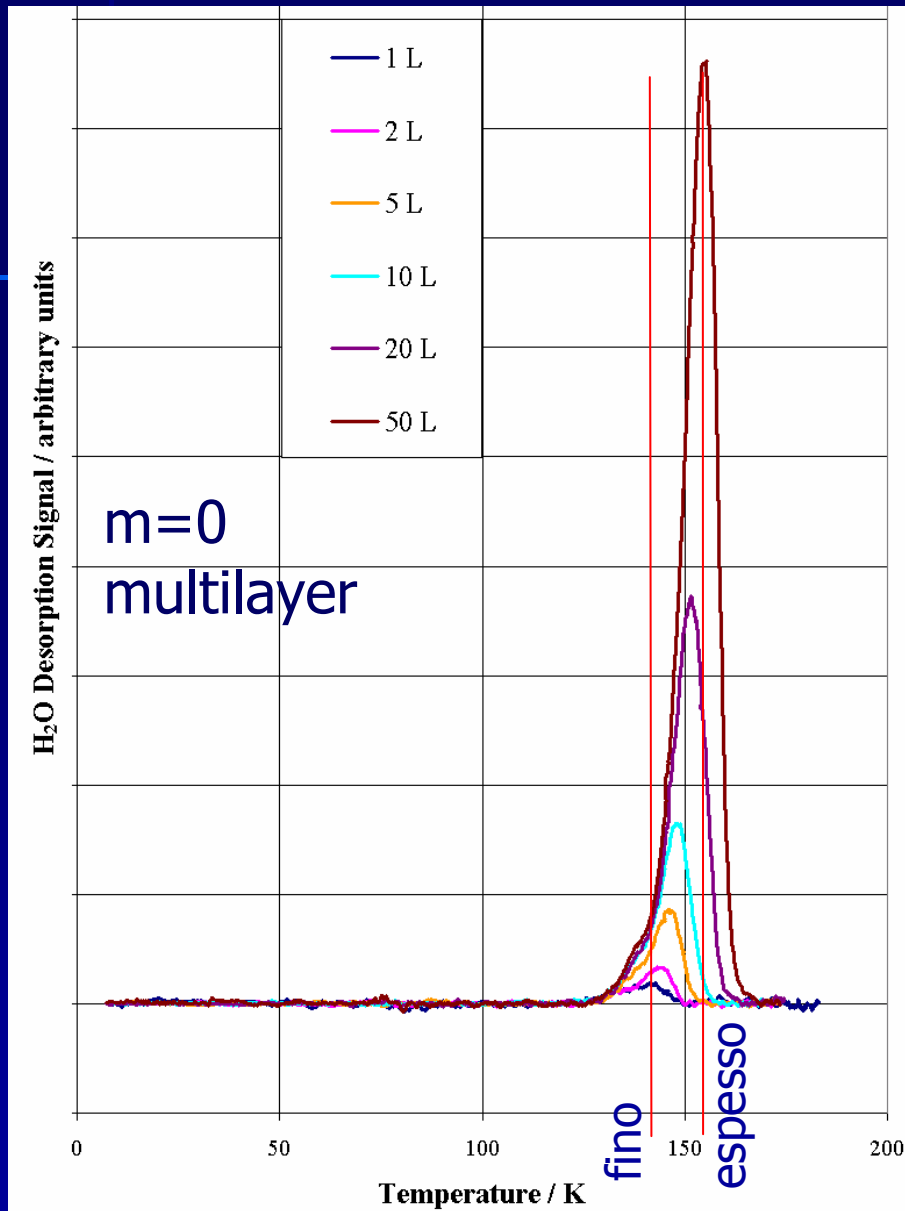
Rampa de aquecimento

$m=0 \rightarrow$ multilayer ices (bulk of solid ices)

$m=1 \rightarrow$ monolayer (molecule-surface region)

$$E_d \approx \Delta_{sub} H$$

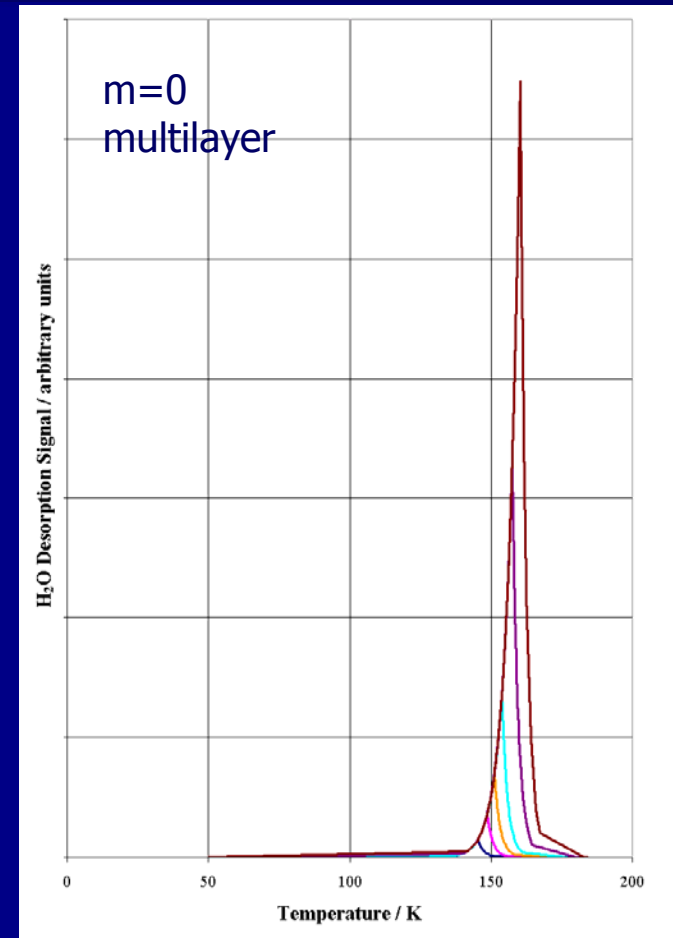
TPD da Agua Pura (sobre Au)



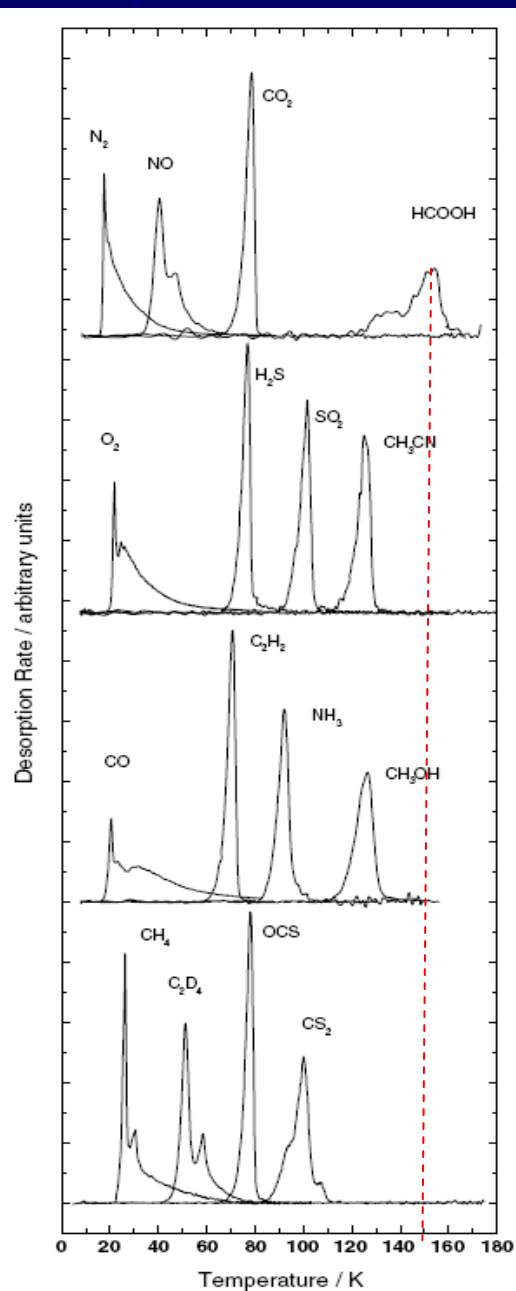
$$-\frac{dn_{H_2O(bulk)}}{dt} = 10^{30 \pm 2} e^{-48,000 \pm 500 / RT} \text{ molec cm}^{-2} \text{ s}^{-1}$$



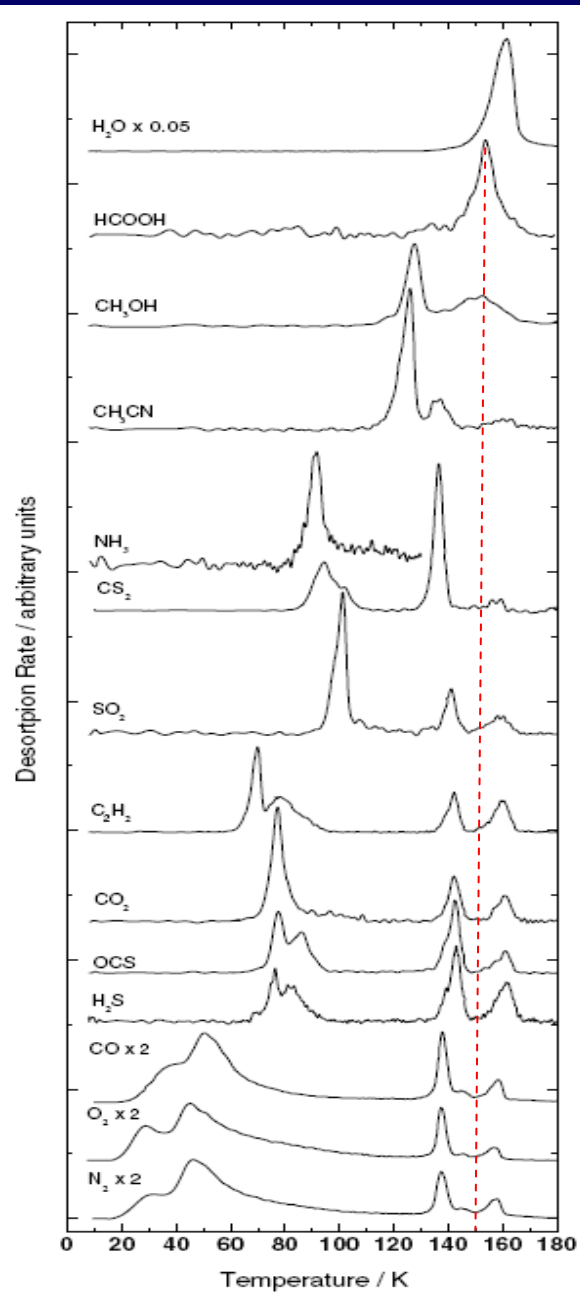
Ajuste



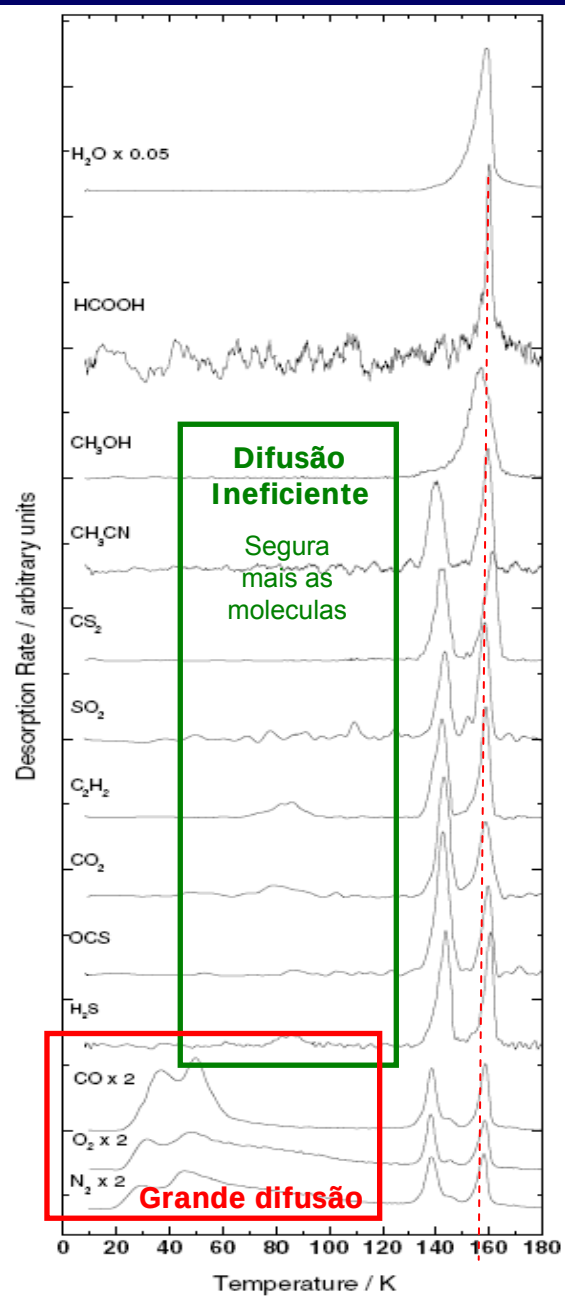
Amostras puras (sobre Au)



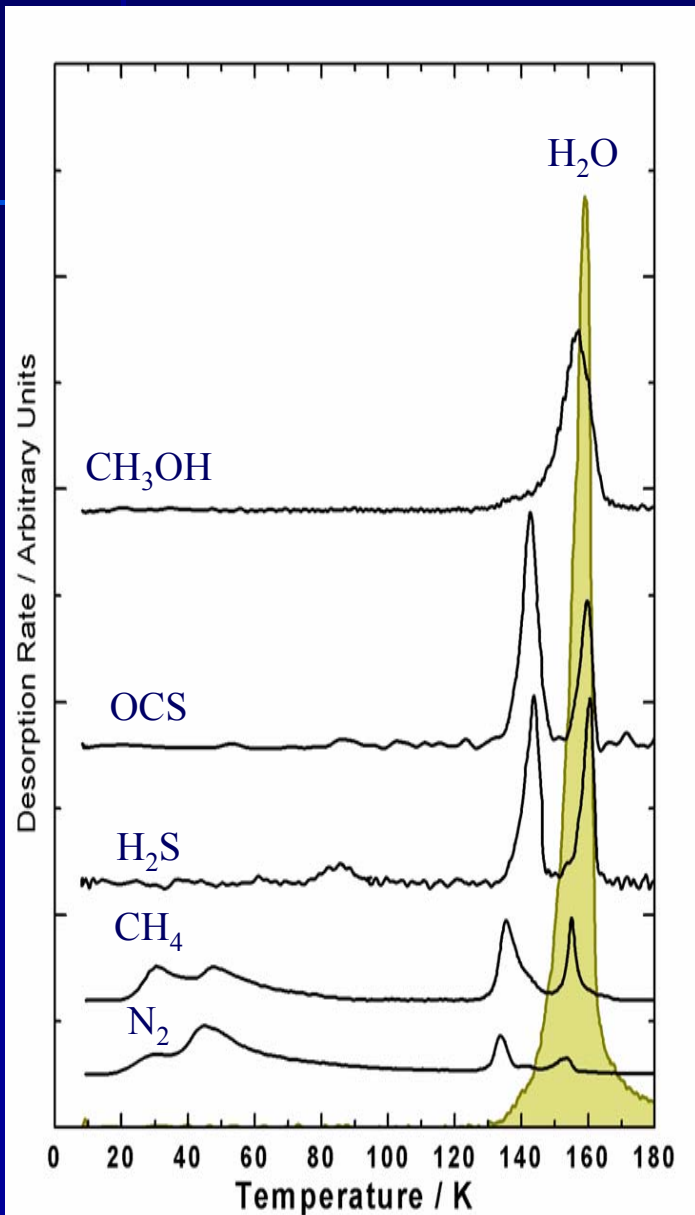
Amostras puras (sobre Gelo Agua)



Amostras misturadas com Água



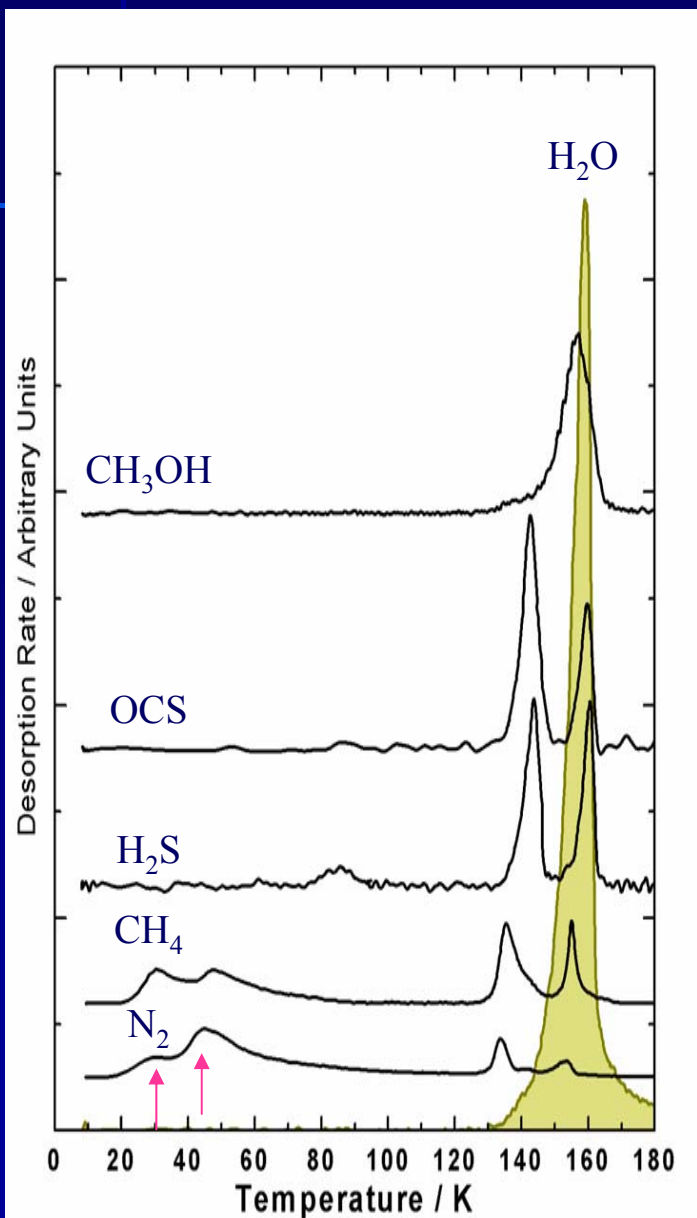
TPD de misturas contendo água (Caso real dos gelos astrofísicos)



TIPO 1 – Moléculas que fazem pontes de hidrogênio (ex. NH_3 , CH_3OH , ...). Desorvem quando o gelo de água desorve.

TIPO 2 - Espécies que tem $T_{\text{sub}} > T_{\text{pore-collapse}}$ (Ex. H_2S , CH_3CN , ...) Apresentam uma habilidade limitada de difusão não sendo aprisionadas (trap) quando sobrepostas pelo gelo de água mas possuem um grande potencial de aprisionamento em situações de misturas gasosas.

TPD de misturas contendo água (Caso real dos gelos astrofísicos)



TIPO 3 – Espécies que tem $T_{\text{sub}} < T_{\text{pore-collapse}}$ (ex. N_2 , O_2 , CH_4 , CO ...). Difundem rapidamente e se comportam como CO exibindo quatro características no espectro TPD quando em misturas. Espécies muito voláteis! Os dois picos da esquerda são da desorção das multicamadas e da monocamada.

MIXTURA (CO sobre gelo de agua)

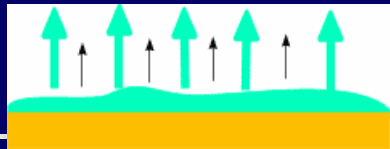
Sublim. of CO into the water porous
m=1 (first order)

Sublim. Solid CO

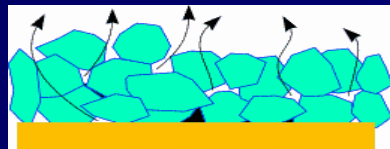
Sublim. some trapped CO

Subl. of water

Temperature



160 K



135 - 140 K



Pore Colapse!
30 - 70 K

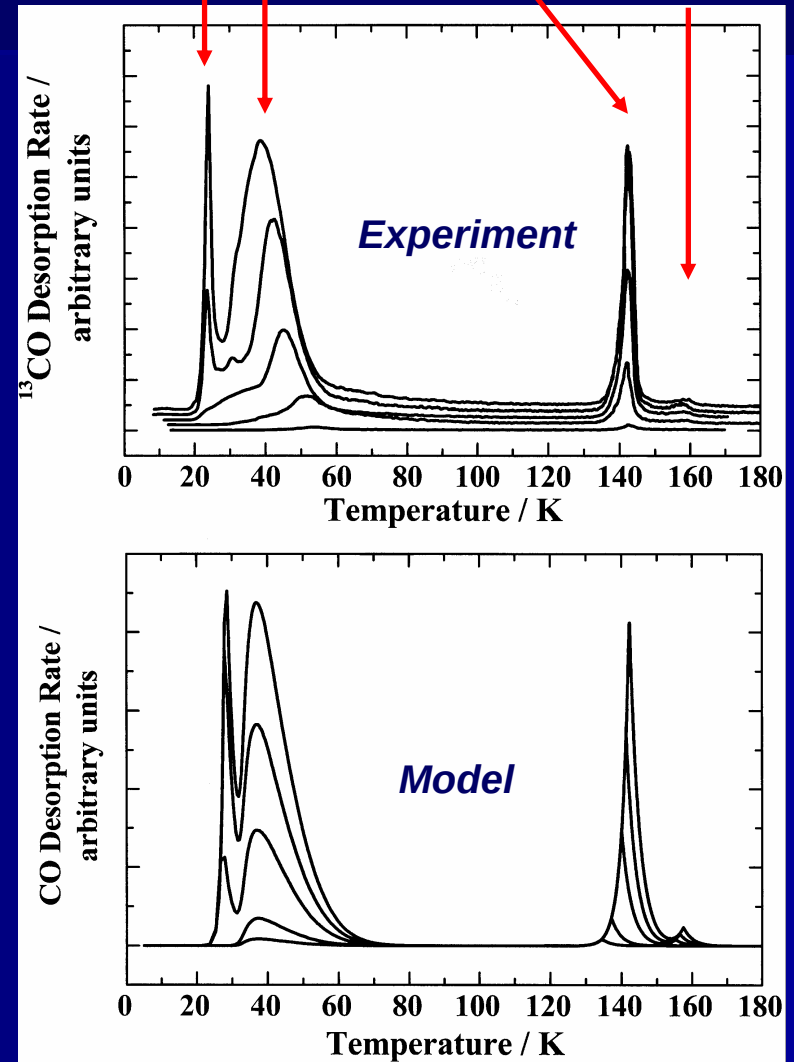


10 - 20 K



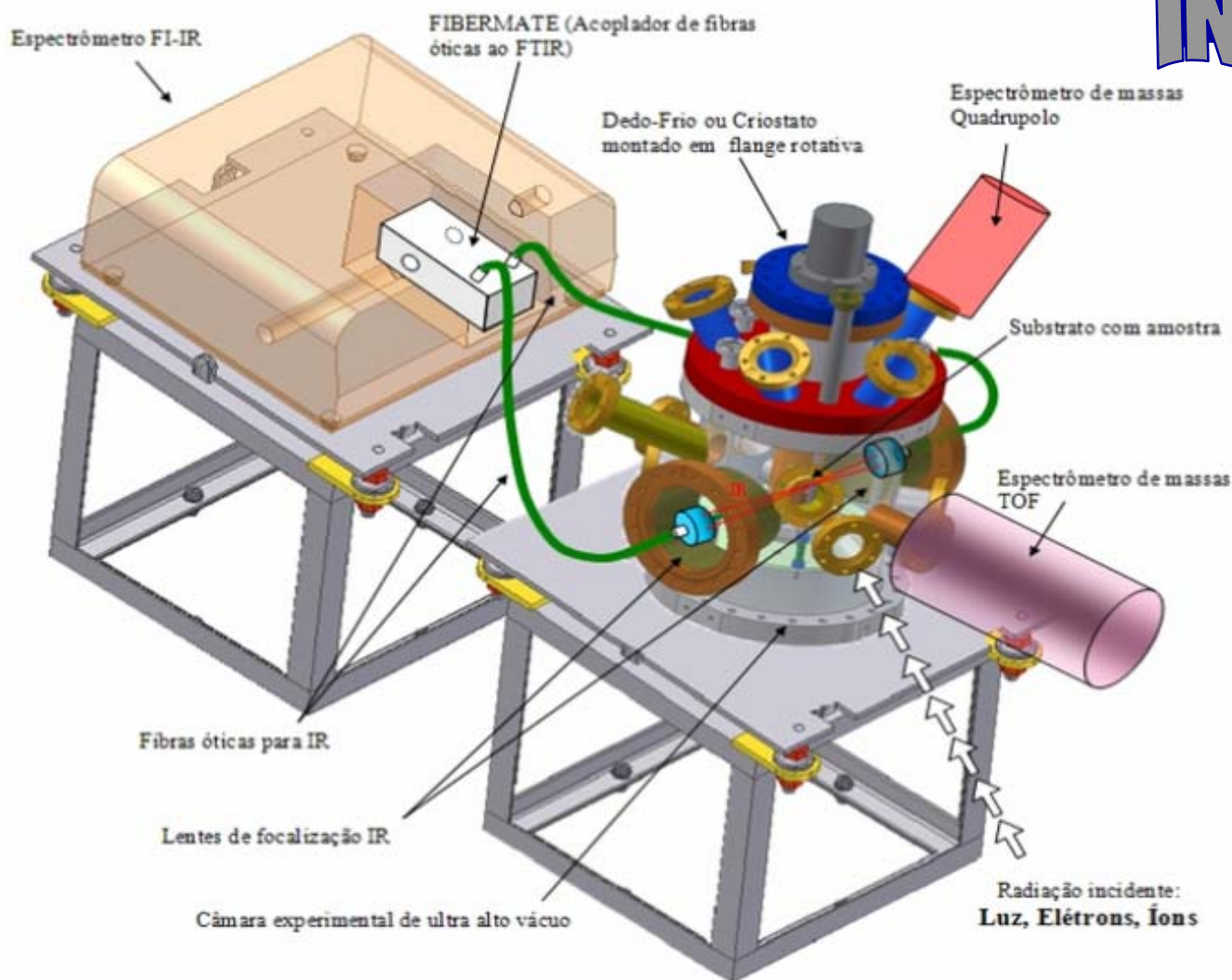
< 10 K

CO
H₂O



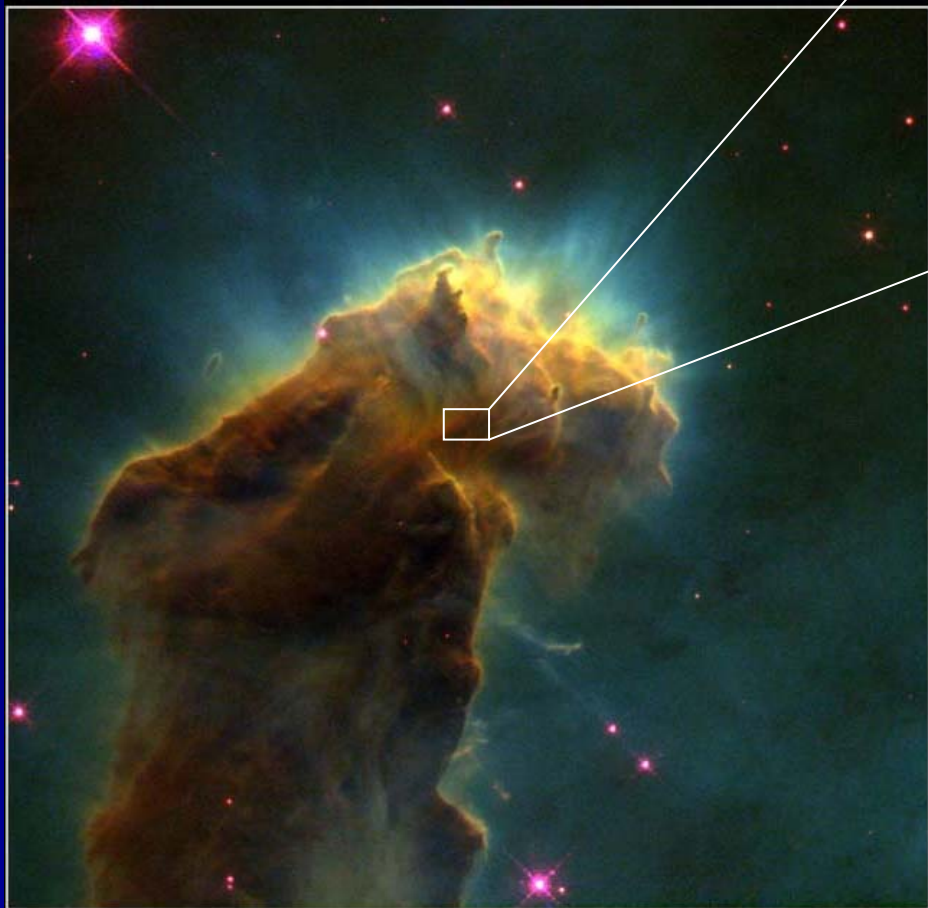
FUTURO: Investigações da superfície e bulk ao mesmo tempo pelo impacto de fótons ou íons energéticos

INÉDITO!



Obrigado pela atenção.

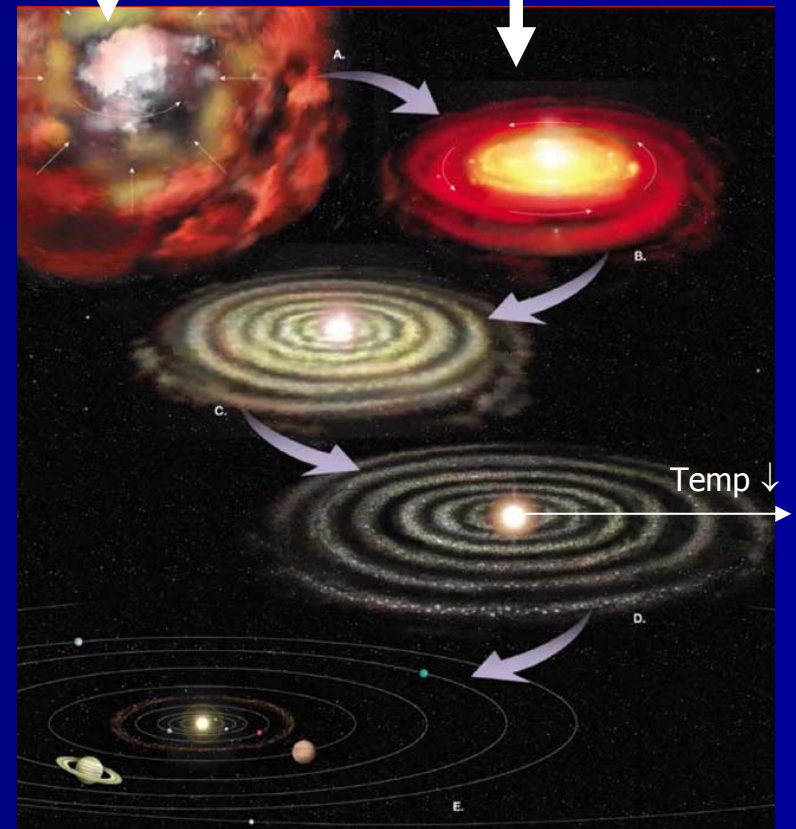
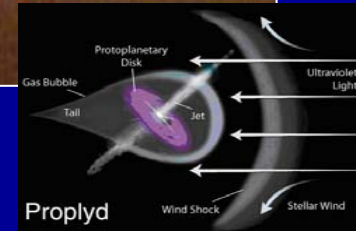
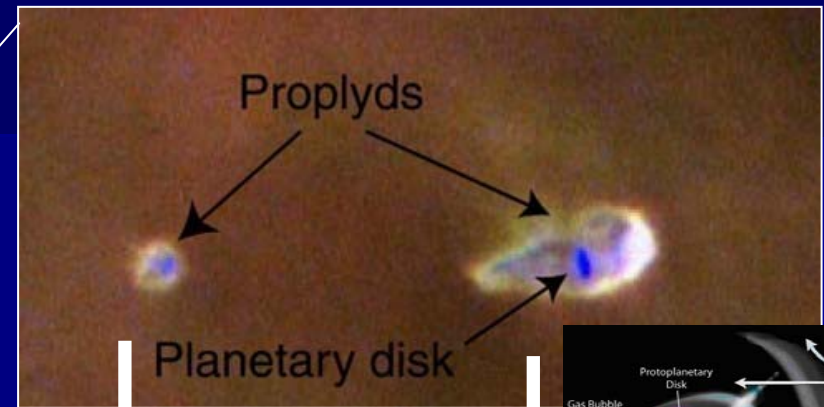
Gelos interestelares vs Gelos interplanetários



Star-Birth Clouds • M16

HST • WFPC2

PRC95-44b • ST ScI OPO • November 2, 1995
J. Hester and P. Scowen (AZ State Univ.), NASA



Gelos interplanetários são os resquícios da nuvem protosolar

Kuiper belt,

- Cometas curto período
- Planetas anões
- Asteróides

Plan. Gigantes



Cinturão de asteróides
- Asteróides

Plan. Rochosos



Nuvem de Oort
- cometas Longo Período

