



**uff** Universidade  
Federal  
Fluminense  
Campus Volta Redonda

Semana acadêmica  
18-19/out/2016

# Minicurso:

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# Astroquímica e Astrobiologia

Prof. Dr. Sergio Pilling

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[www1.univap.br/spilling](http://www1.univap.br/spilling)





UNIVERSIDADE DO VALE DO PARAÍBA  
São José dos Campos - SP

- 39 cursos de Graduação
- 3 Doutorados  
(Física e Astronomia – nota 4 CAPES)
- 6 Mestrados
- 23 Especialização Lato-Sensu

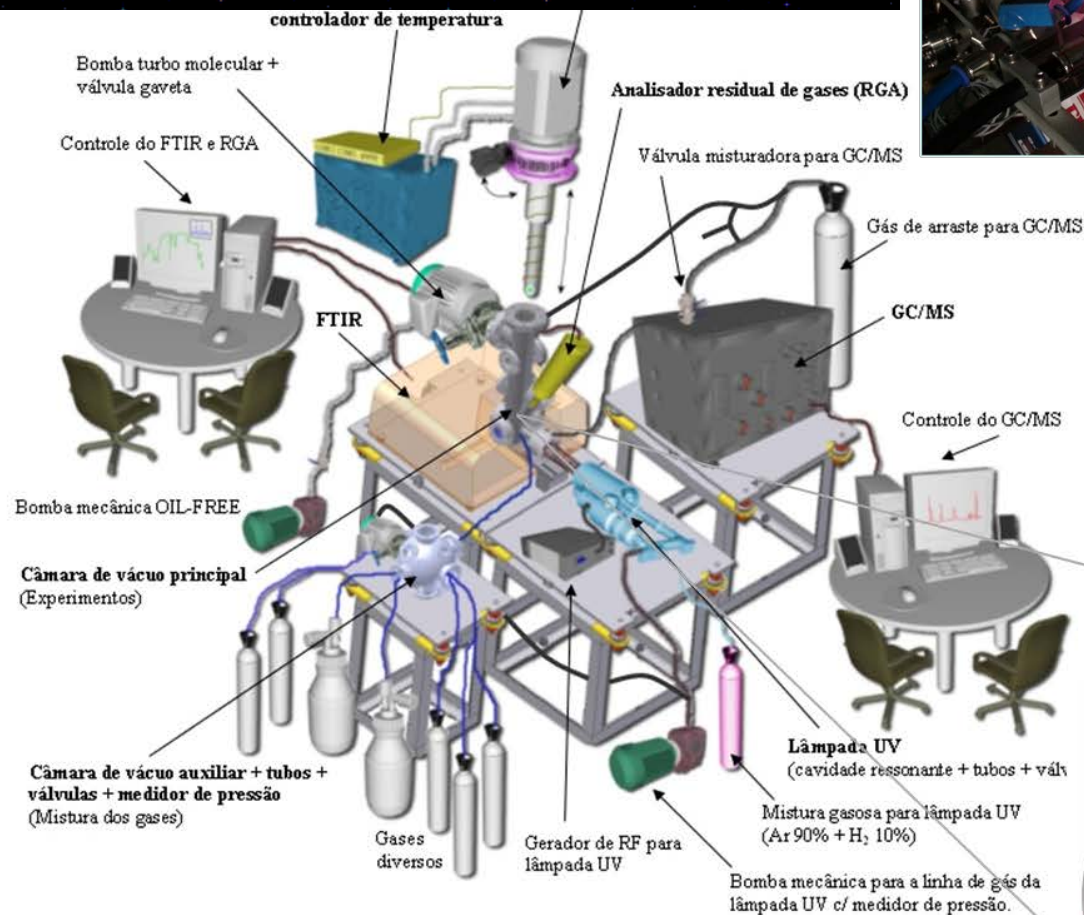


## Instituto de pesquisa (IP&D)

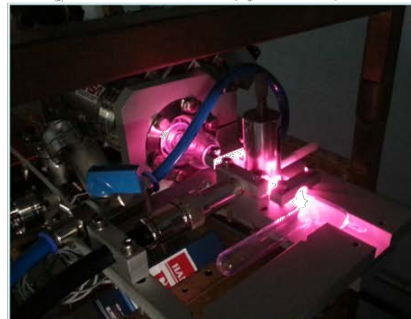




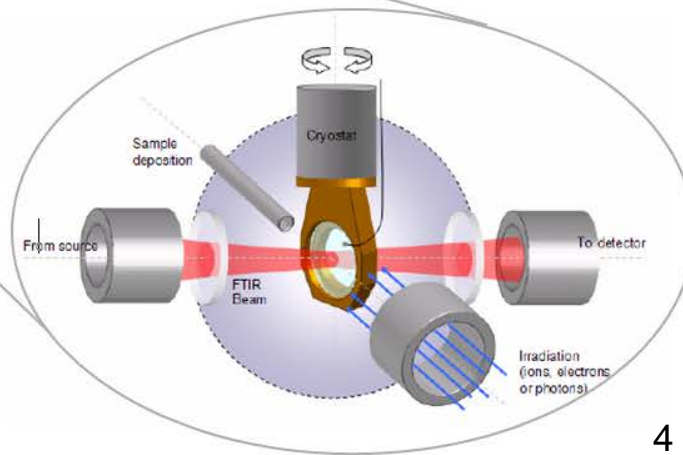
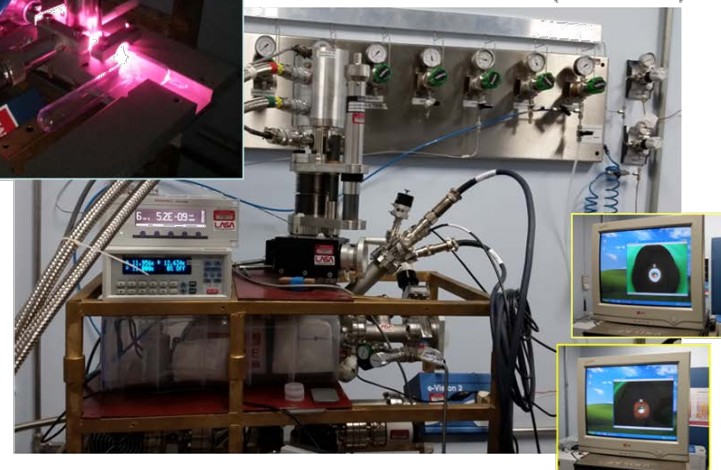
~1 milhão reais  
(FAPESP, CNPQ, FINEP, FVE/UNIVAP)

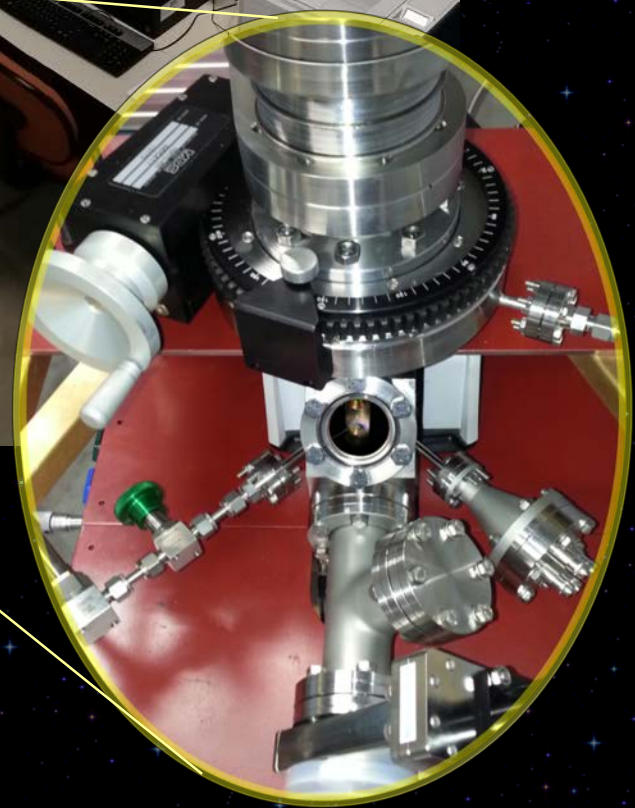
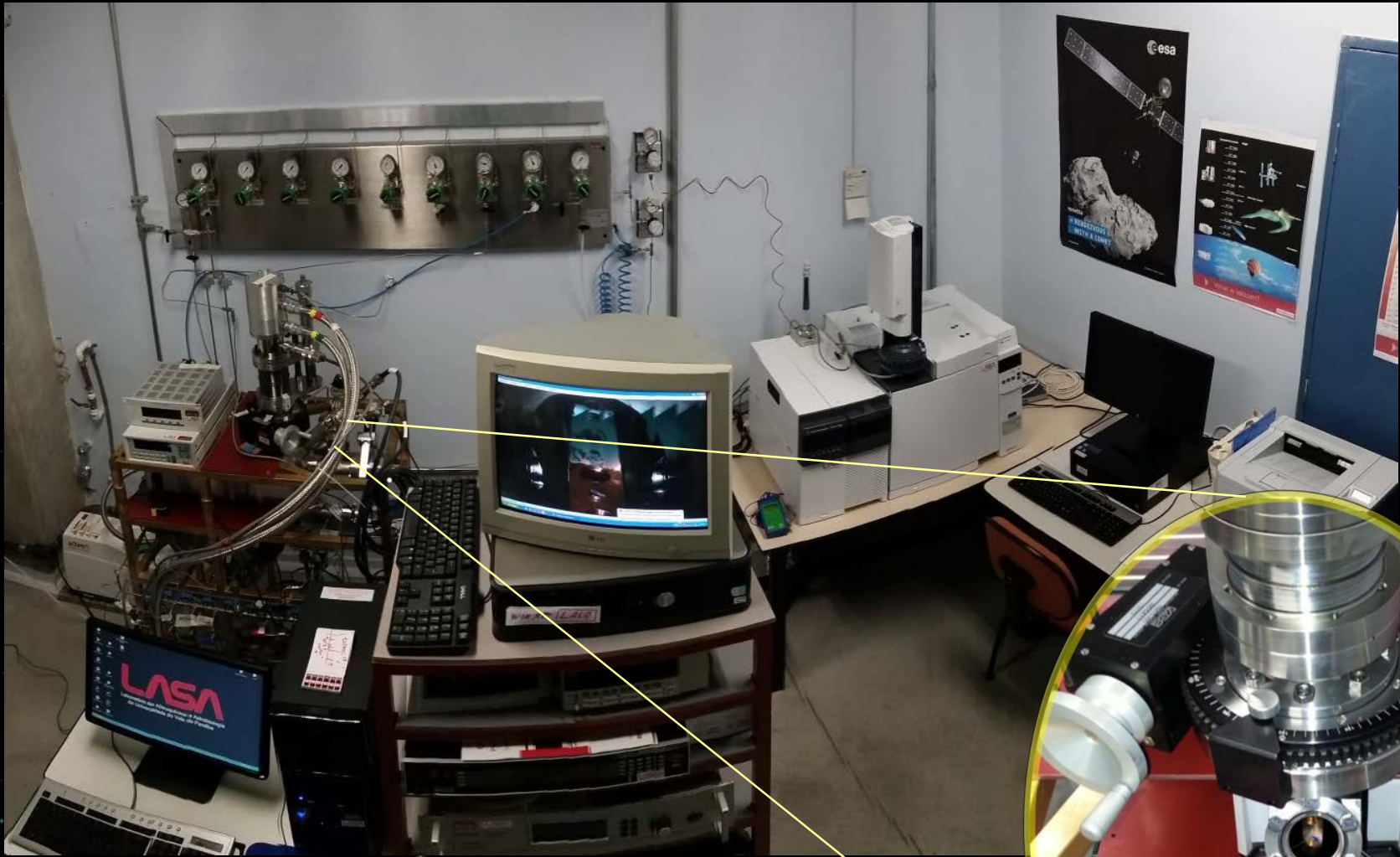


Lâmpada de UV 10.2 eV (Lyman alfa)



Canhão de Elétrons (100eV-5000eV)





LAB ~90m<sup>2</sup>

# GAA – Grupo de Astroquímica e Astrobiologia da Univap (out/2016)

1 posdoc

3 doutorandos

3 mestrandos

3 IC/TCC



## Aula 1:

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# Introdução a Astroquímica e a evolução química do Universo

Nucleossínteses, evolução estelar, meio interestelar, Formação de moléculas nos Céus, Observações (IR e Rádio) e experimentos.

## Aula 2:

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# Introdução a Astrobiologia e vida no contexto cósmico

Exoplanetas, habitabilidade, panspermia, extremófilos.  
Experimentos de astrobio.



## Aula 1:

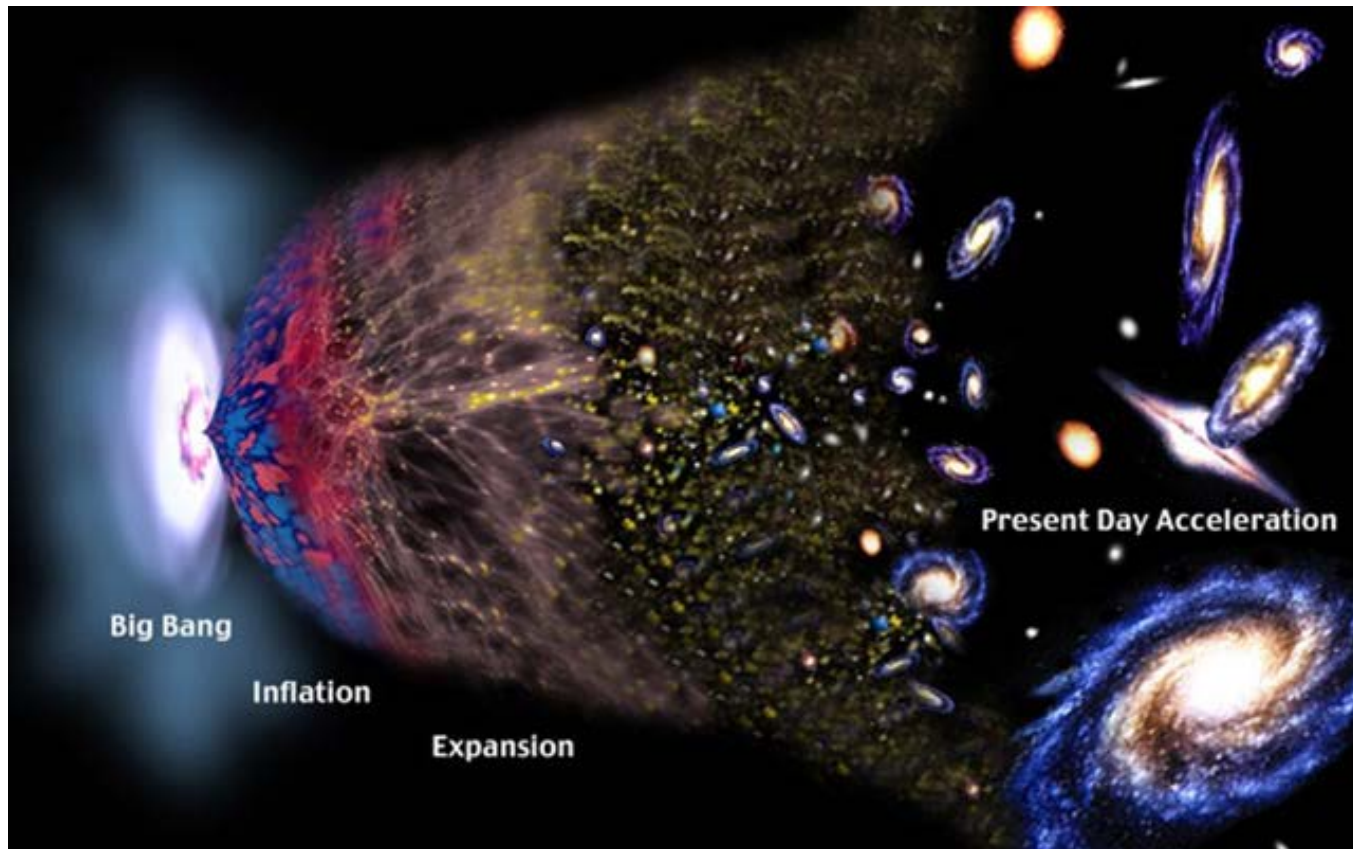
# Introdução a Astroquímica e evolução química do Universo

Nucleossínteses, evolução estelar, meio interestelar, Formação de moléculas nos Céus, Observações (IR e Rádio) e experimentos.



# A) Formação dos primeiros átomos e aumento da complexidade elementar no Universo

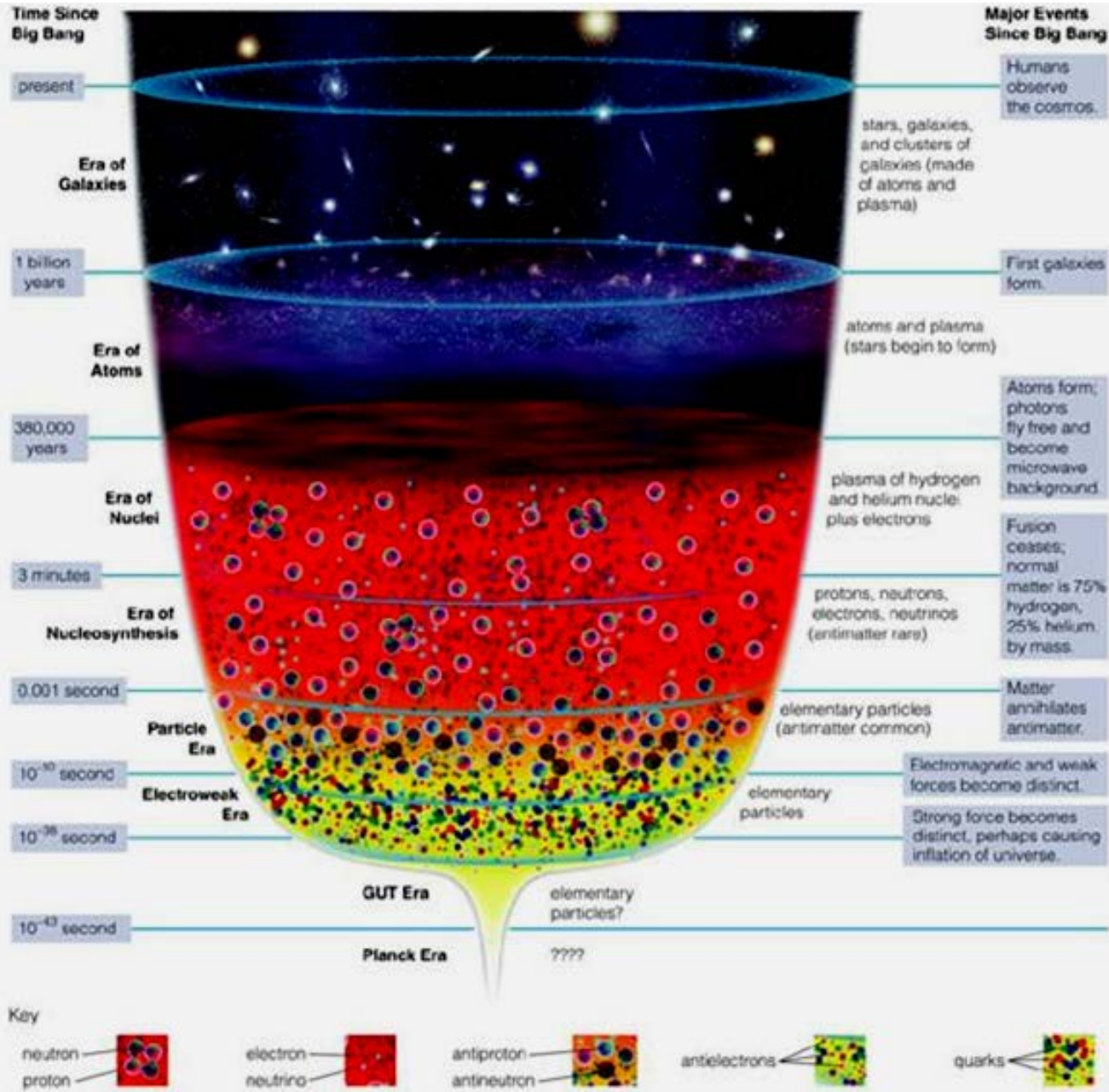
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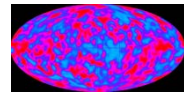


10  
BigBang

# A1) A teoria do BigBang



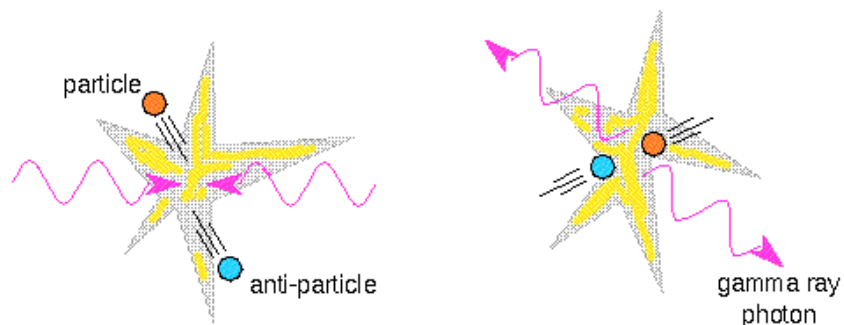
- ← Hoje
- ← Surgimento da vida
- ← 1<sup>as</sup> moléculas orgânicas
- ← 1<sup>as</sup> moléculas
- ← ...
- ← 2<sup>a</sup> geração de estrelas
- ← 1<sup>a</sup> geração de estrelas
- ← 1<sup>os</sup> Átomos
- ← (H, He, Li, Be)
- ← RCF ~ 2.7 K
- ← 1<sup>os</sup> Núcleos
- ← 1<sup>os</sup> prótons e nêutrons
- ← Partículas elementares
- ← Big bang



# A2) Universo primitivo (até ~ 1 seg )

## Formação das partículas elementares e hadrons

Energia radiante (raios gama) é convertida em matéria e anti-matéria.  
 (Eq Einstein,  $E = m.c^2$ )

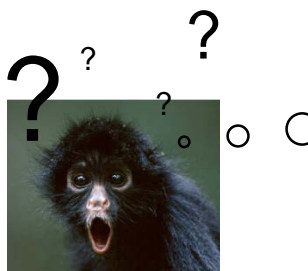
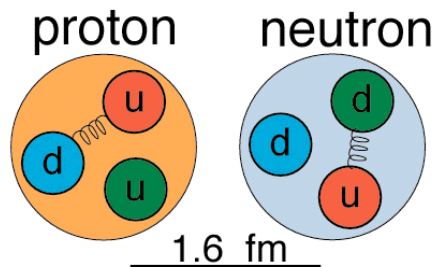


## Partículas elementares ~10<sup>-32</sup> até 10<sup>-6</sup> segundos

	LÉPTONS		QUARKS	
1ª Família	Elétron	Neutrino do elétron	Up	Down
2ª Família	Múon	Neutrino do múon	Charm	Strange
3ª Família	Tau	Neutrino do tau	Top	Botton

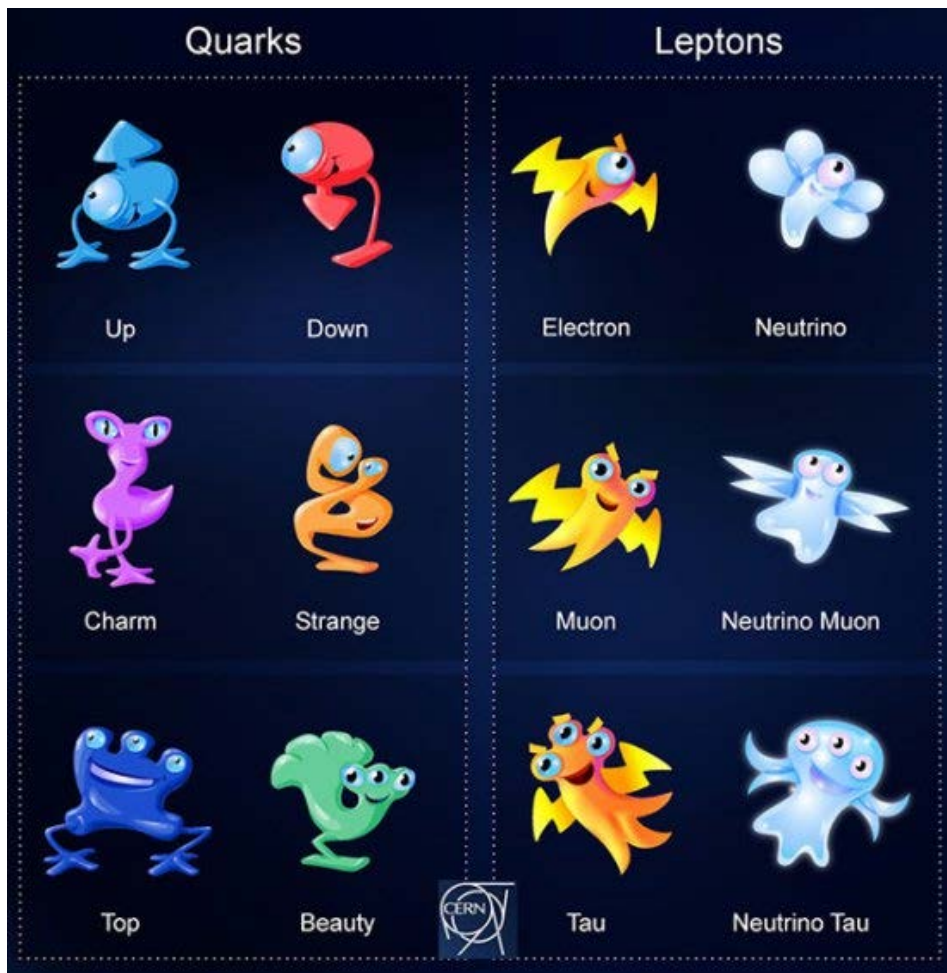
## Formação dos hadrons

10<sup>-5</sup> seg até ~1 seg

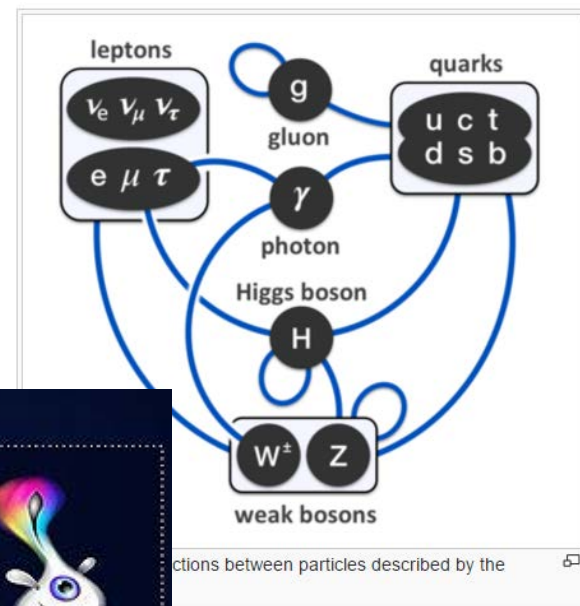


Anti-partículas (1/1bi)?  
 Ex. anti-elétron (pósitron)

# 1ª Grande festa Cósmica (Menos de 1 s após Bigbang)



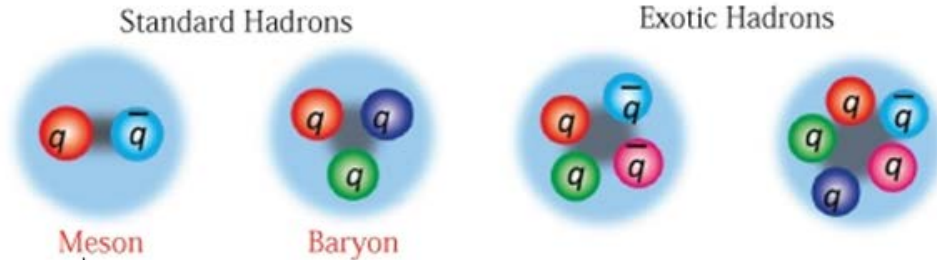
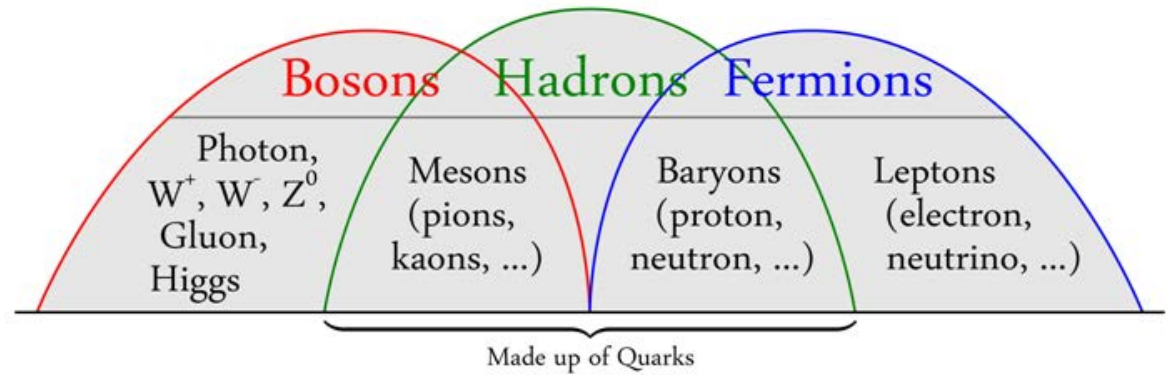
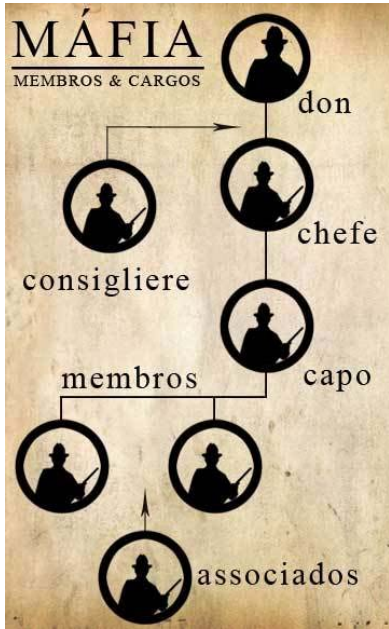
## Panelinhas e Dialetos.



## Local do Evento (Início do Universo)

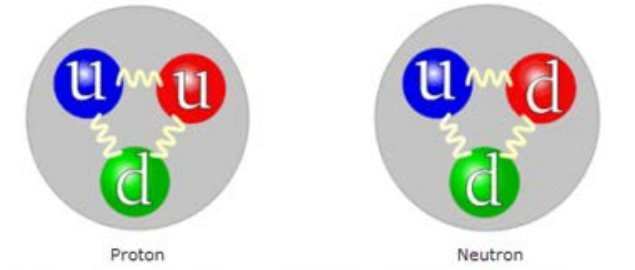


# As primeiras Famílias!



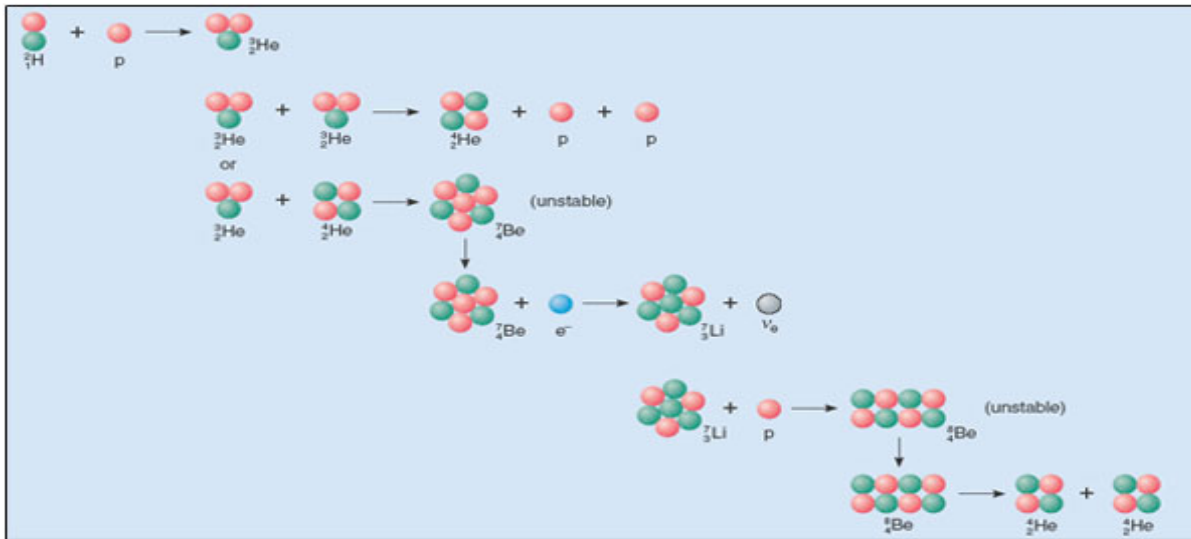
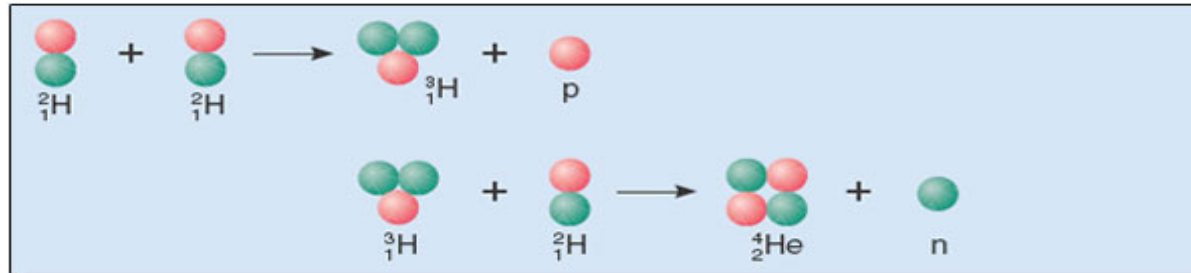
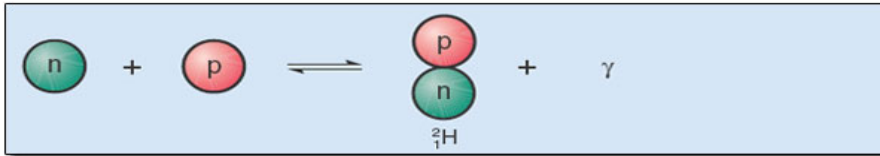
ex.

Mesons $q\bar{q}$					
Mesons are bosonic hadrons.					
There are about 140 types of mesons.					
Symbol	Name	Quark content	Electric charge	Mass $\text{GeV}/c^2$	Spin
$\pi^+$	pion	$u\bar{d}$	+1	0.140	0
$K^-$	kaon	$s\bar{u}$	-1	0.494	0
$\rho^+$	rho	$u\bar{d}$	+1	0.770	1
$B^0$	B-zero	$d\bar{b}$	0	5.279	0
$\eta_c$	eta-c	$c\bar{c}$	0	2.980	0

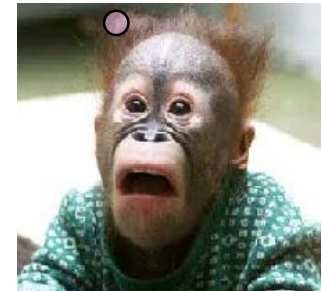


Quark composition of a proton and a neutron (diagrams from Wikipedia)

# A3) Nucleossíntese primordial (~10 seg até ~ 5 min )



Nessa época o Universo era parecido com o núcleo do Sol. Uma sopa de partículas ionizadas (PLASMA)



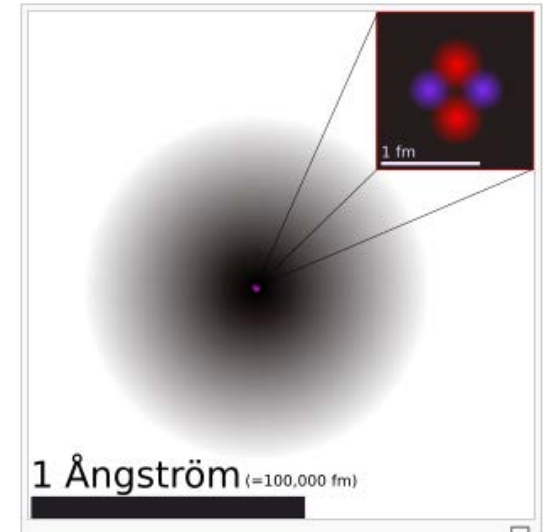
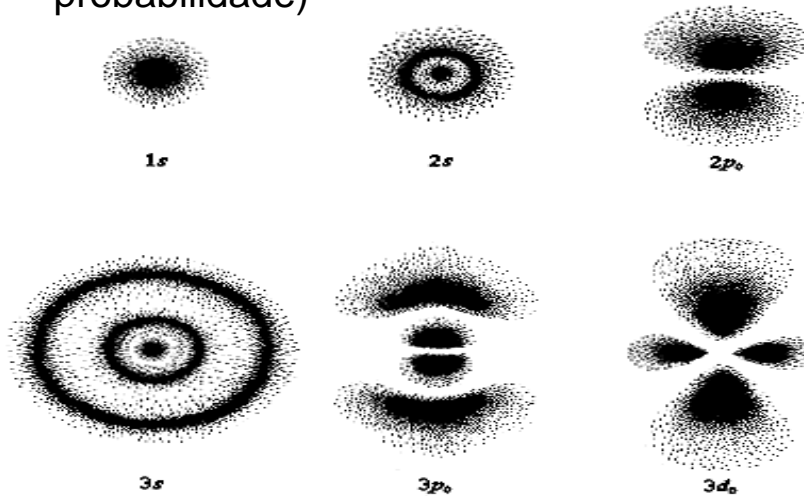
No fim da era da nucleossíntese a composição da matéria bariônica do universo era de **74% prótons**, **24% núcleos de hélio** e traços de núcleos de outros elementos leves como Lítio, Deutério e Berílio.

# A4) Atomossíntese primordial ( de 5 min até ~ 380 000 anos)

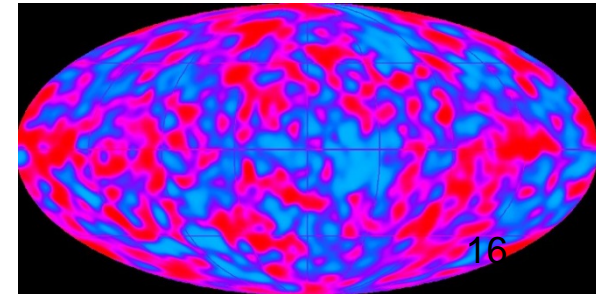
Ao longo dos primeiros 380 mil anos a temperatura do universo decresceu bastante chegando ate cerca de 3000 K, permitindo que os núcleos formados (prótons e nêutrons) combinassem com os elétrons errantes resultando em átomos neutros (recombinação).

Visão quântica (orbitais = distribuição de probabilidade)

Visão clássica (órbitas)



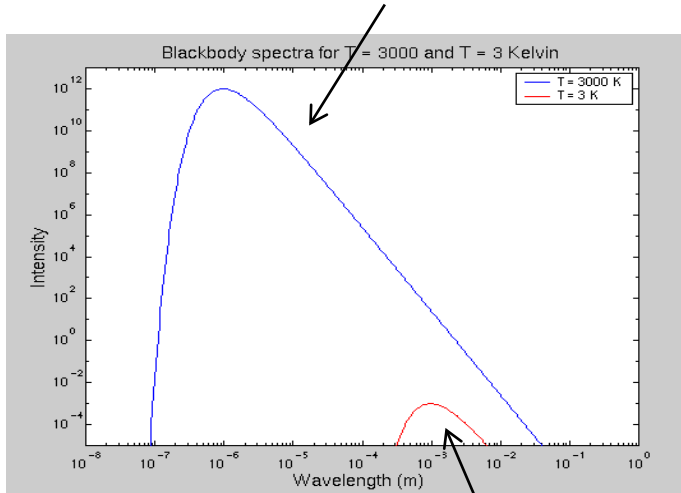
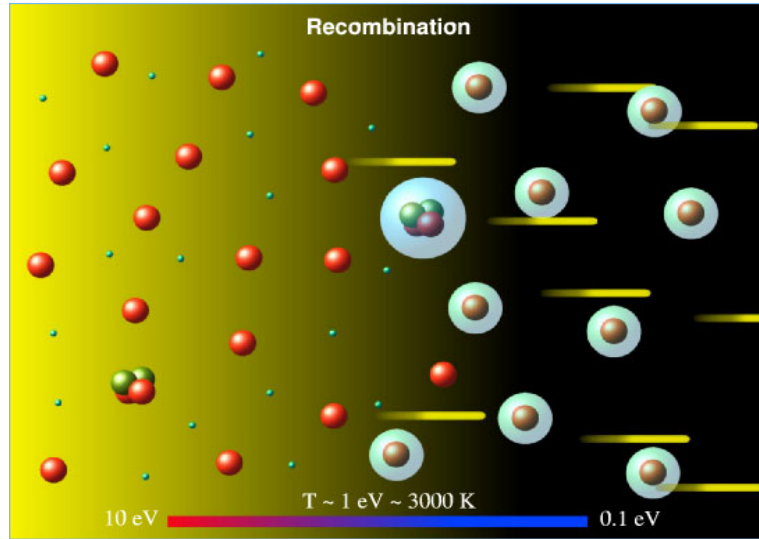
Nessa época o universo deixou de ser opaco a radiação como (o interior solar; espalhamento da luz pelos elétrons livres) e começou a ser transparente. Podendo ser observado nos dias de hoje como a radiação cósmica de fundo (2.7K)



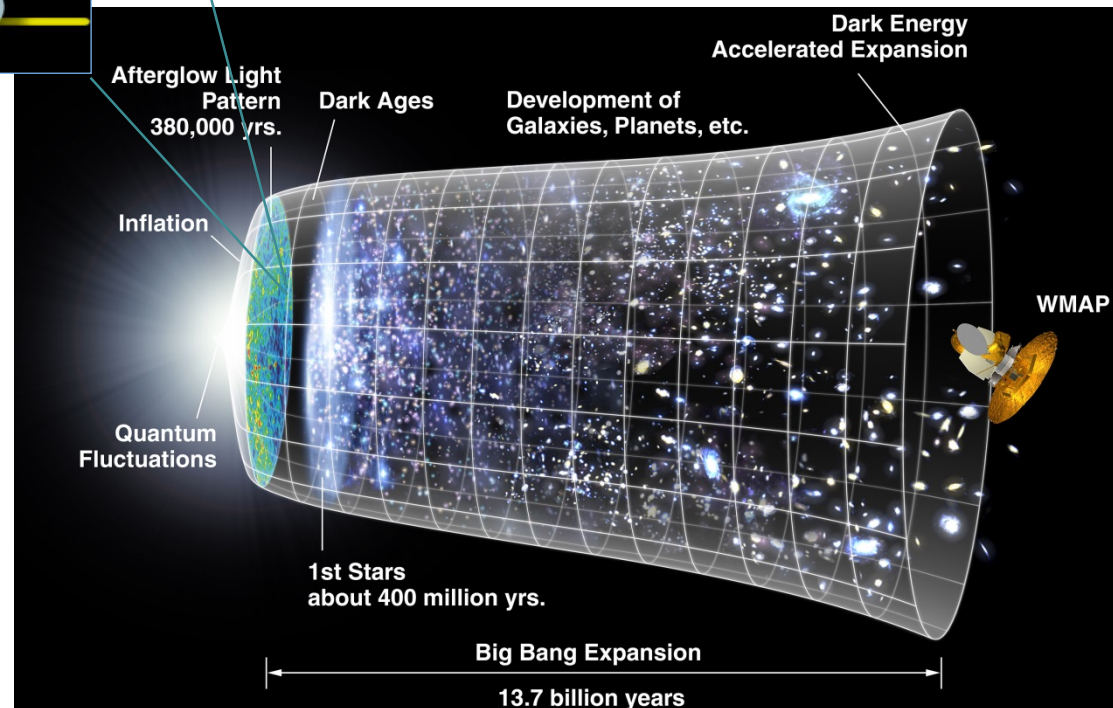


# Mais sobre a radiação cósmica de fundo (RCF).

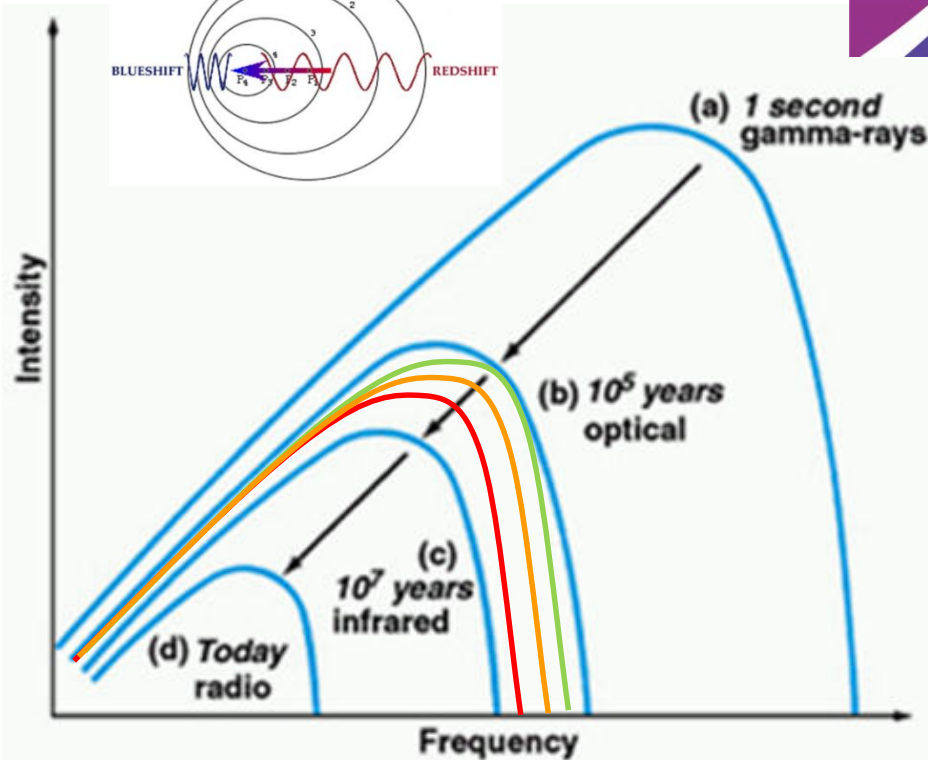
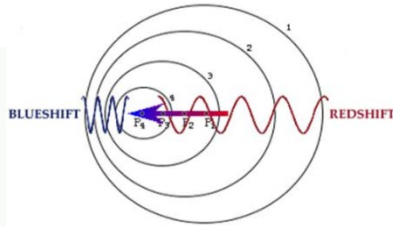
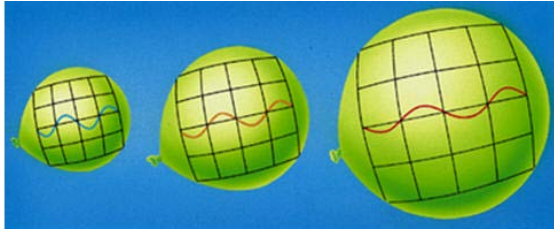
- Recombinação (3000K); **Expansão do Universo + Efeito Doppler ( 2.7 K - Ondas de rádio (mm))**; RCF (Flutuações; galáxias iniciais, Topologia do Universo).



Devido a expansão do universo (efeito Doppler)Hoje

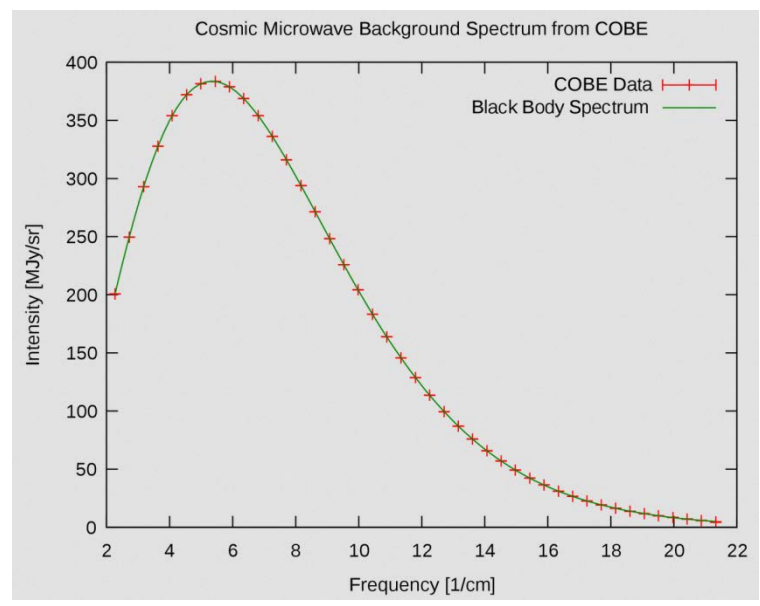
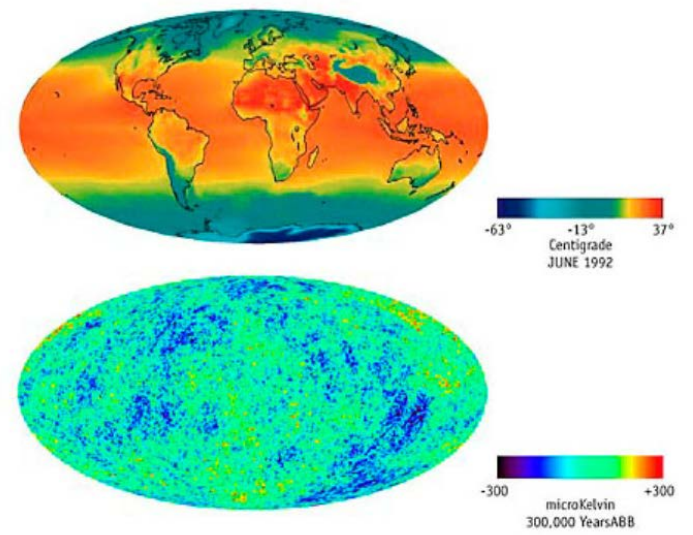
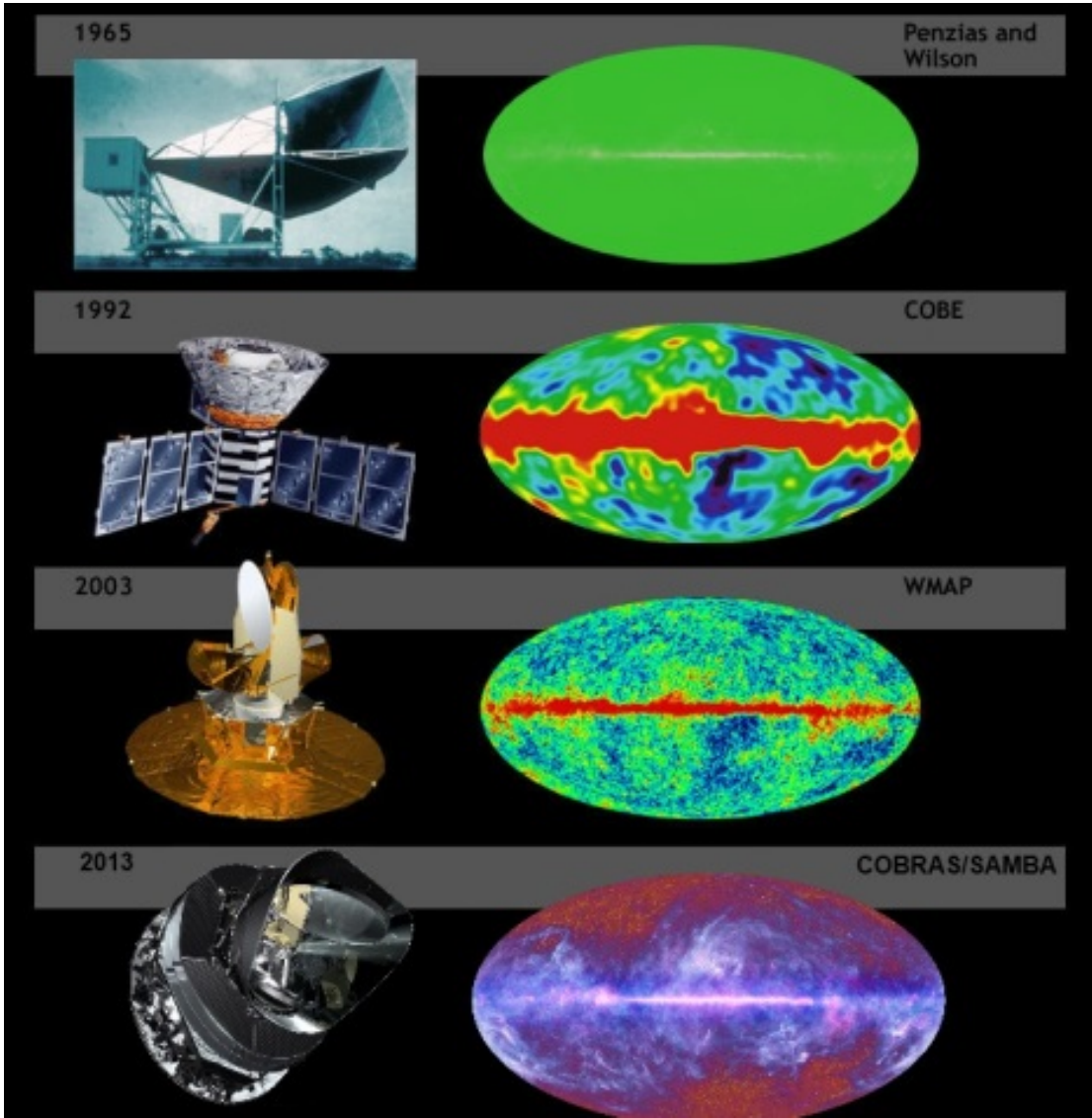


O universo foi “mudando de cor” a medida que evoluiu (expandiu).



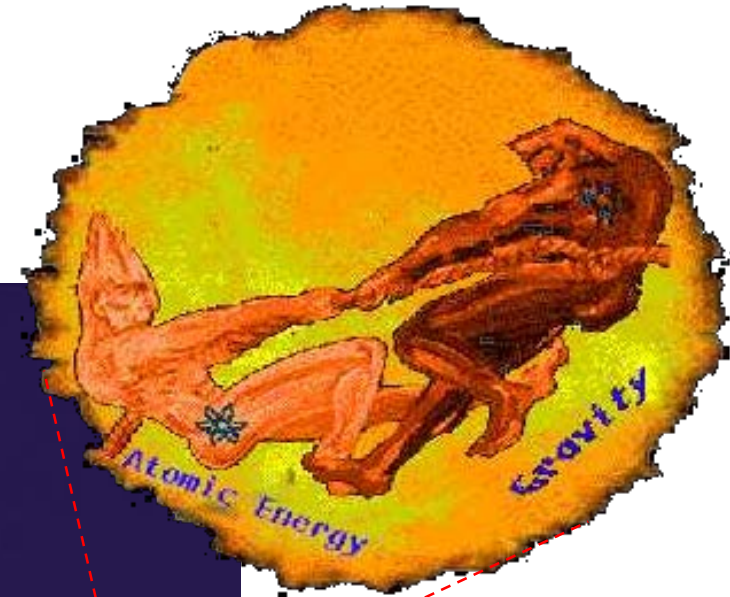
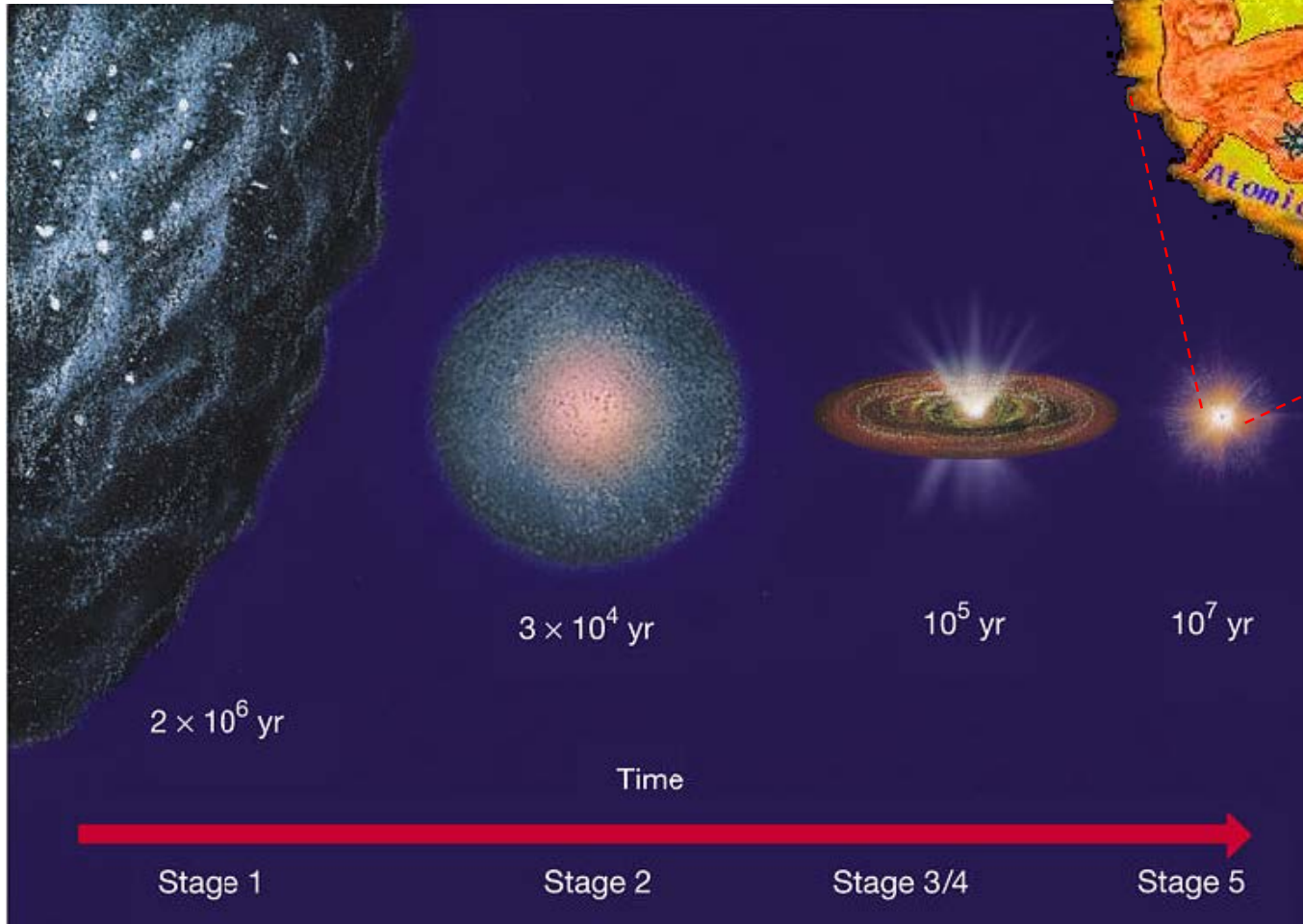
Temperature	peak wavelength
3 K	1mm (radio waves)
300 K (room temperature)	10 microns (infrared)
6000K (surface of sun)	0.5 micron (visible light)
3,000,000 K	1 nanometer (x-rays, gamma-rays)

# Mais sobre a radiação cósmica de fundo.

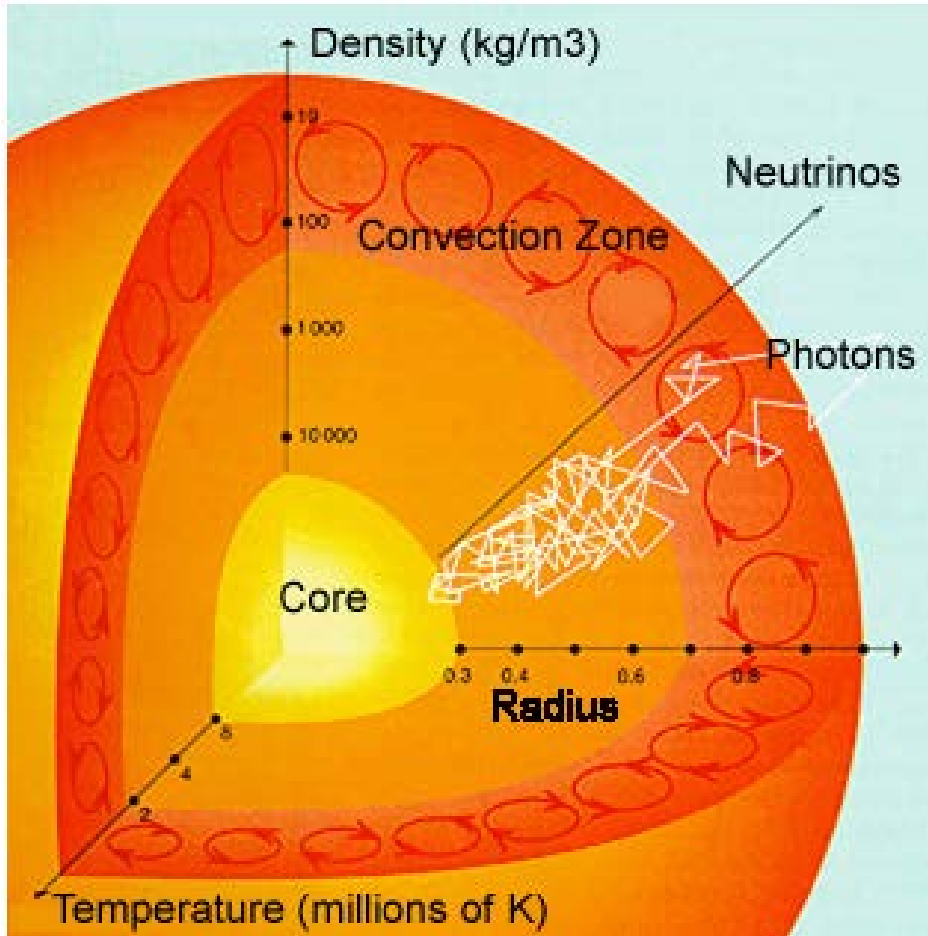


# A5) 1<sup>as</sup> estrelas e nucleossíntese estelar (~ 1bi ano)

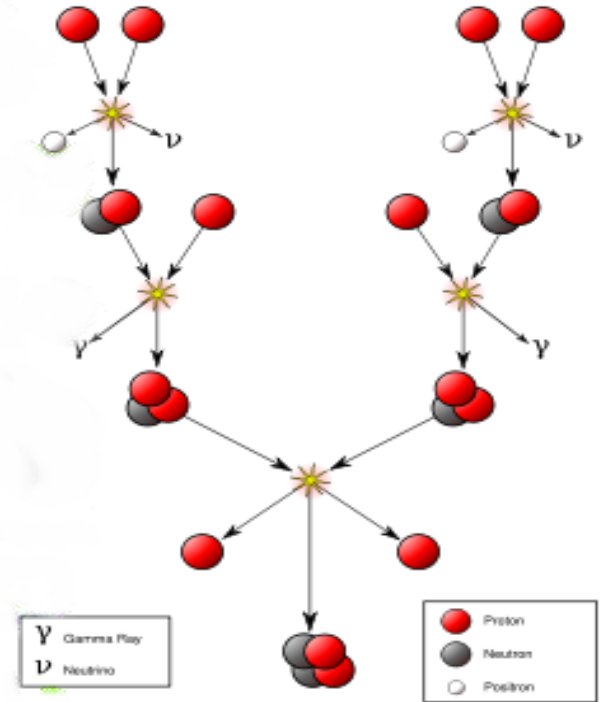
Nuvem de átomos de H, He



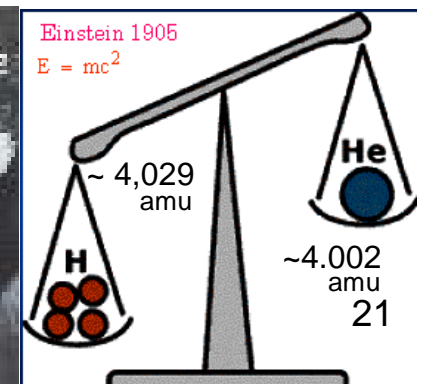
- Estrelas do tipo solar



Queima do hidrogênio (cadeia p-p)

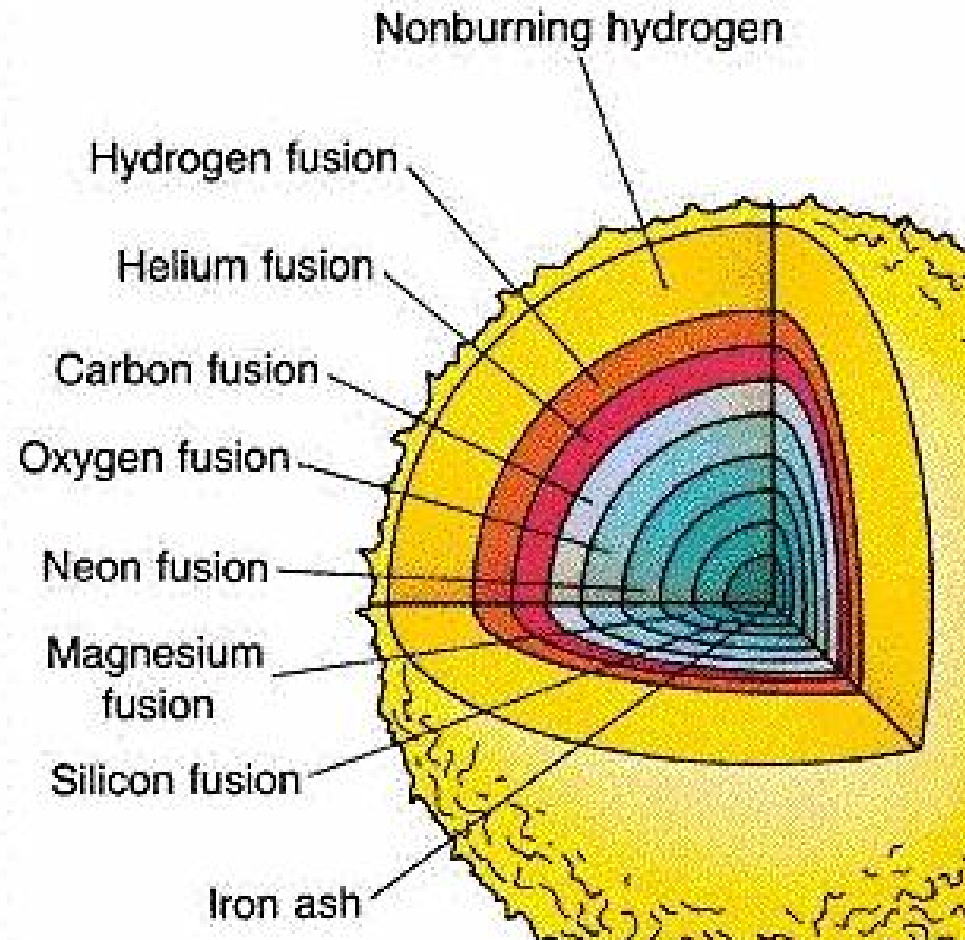
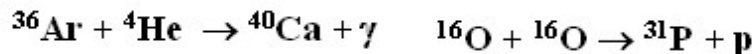
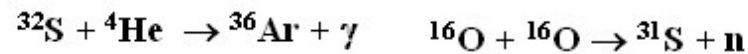
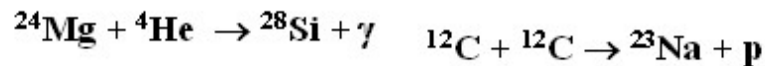
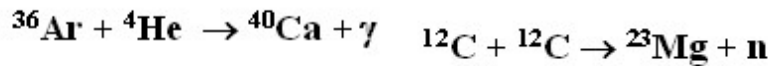
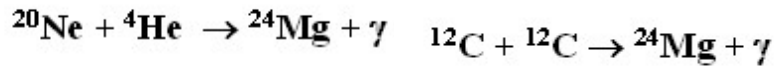
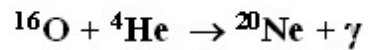
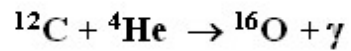


Einstein 1905  
 $E = mc^2$

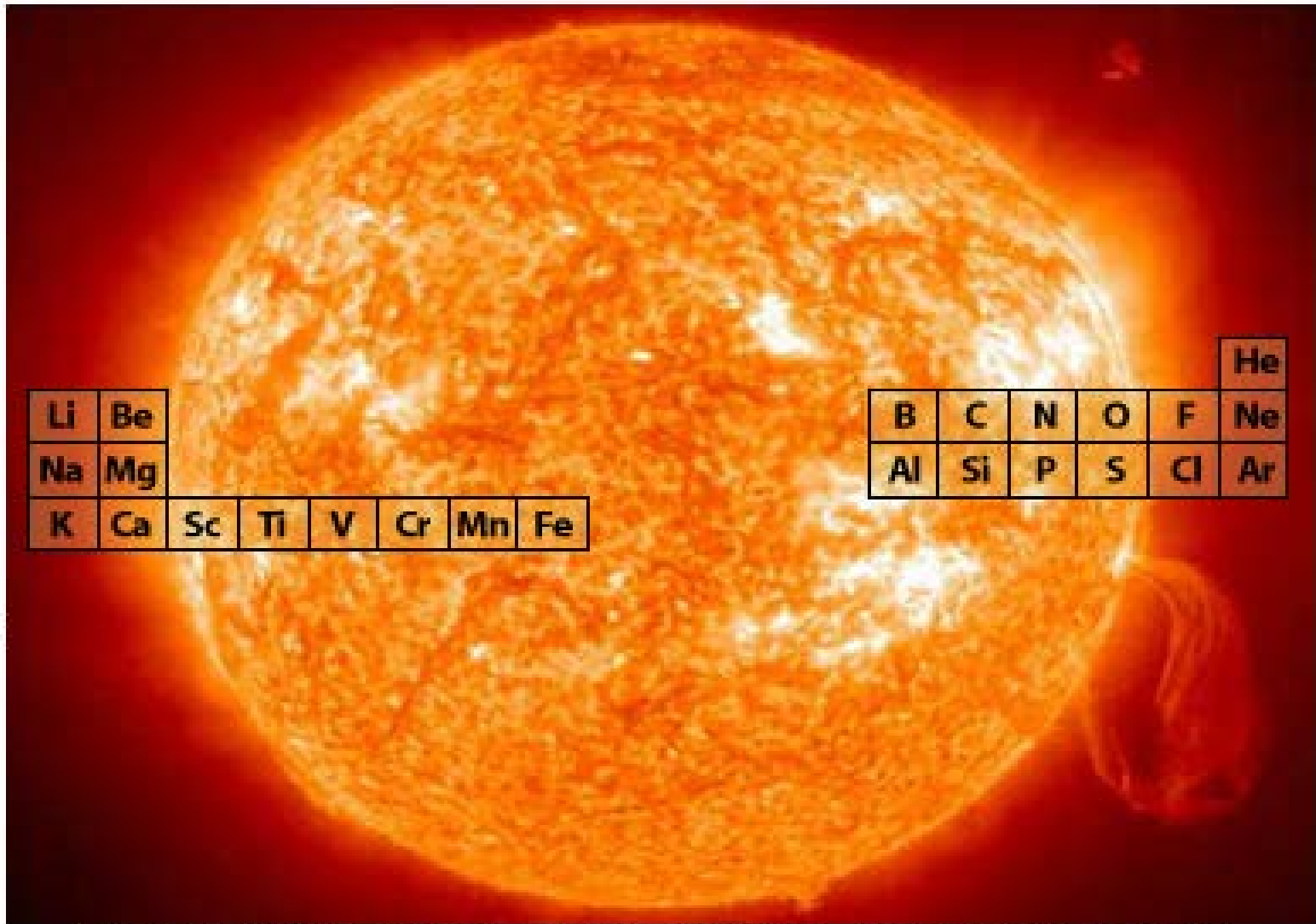


- Estrelas do grade massa

### Exemplo de reações



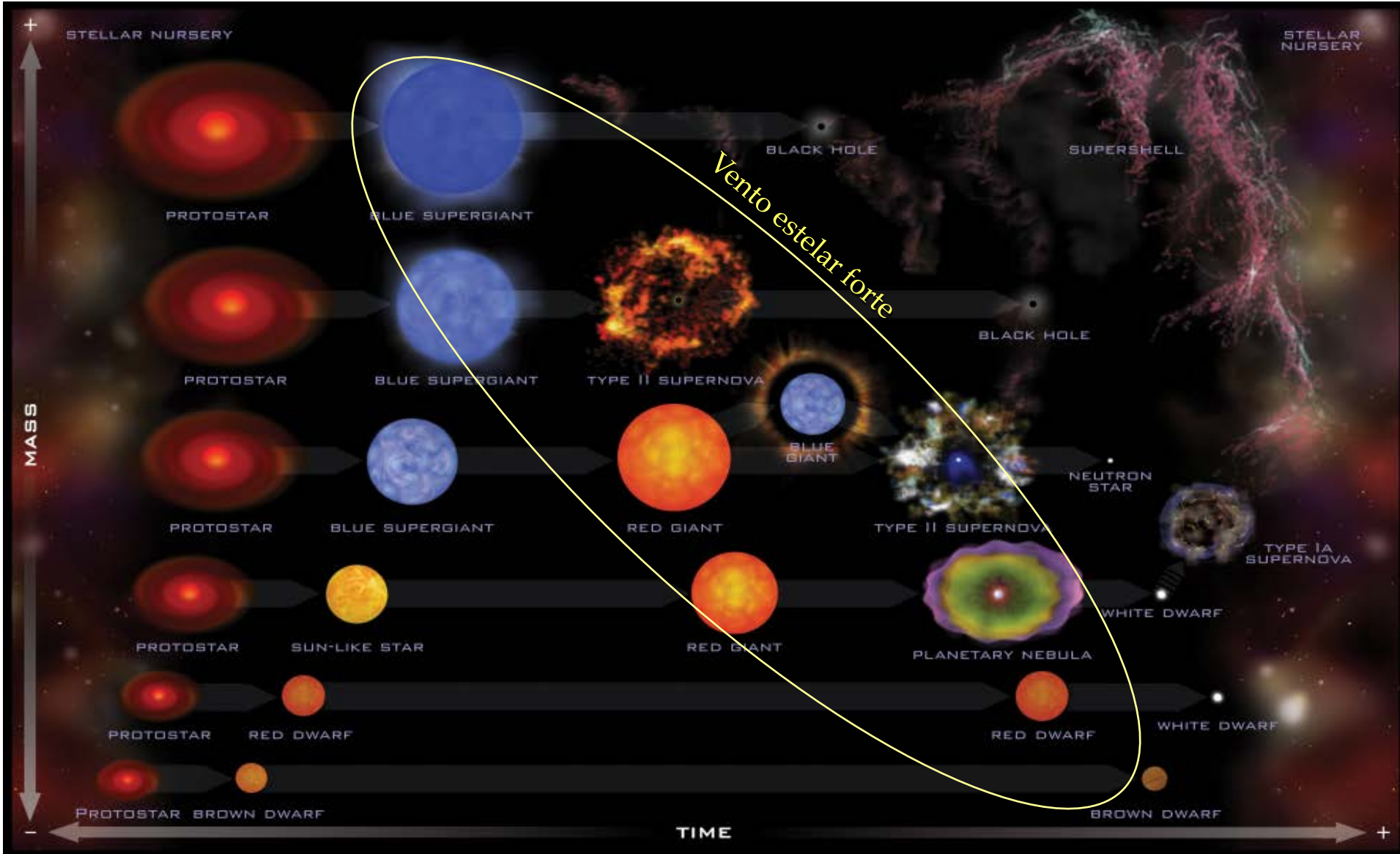
# 1<sup>as</sup> estrelas e nucleossíntese estelar (~ 1bi ano)



Elements up to the weight of iron are manufactured in stars.

# A6) Um pouquinho sobre Evolução estelar

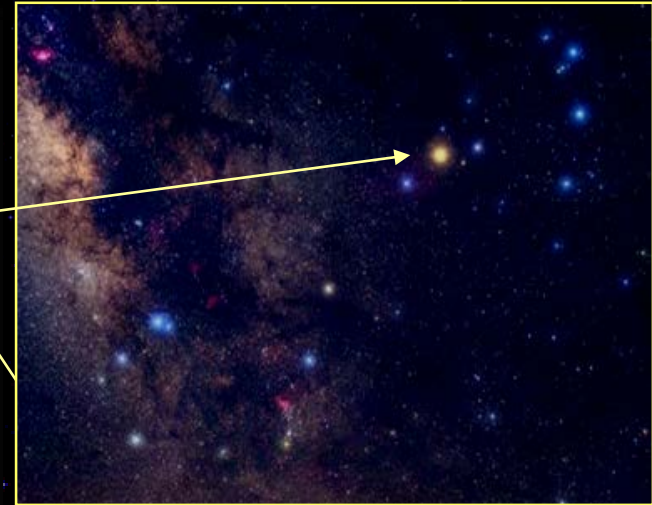
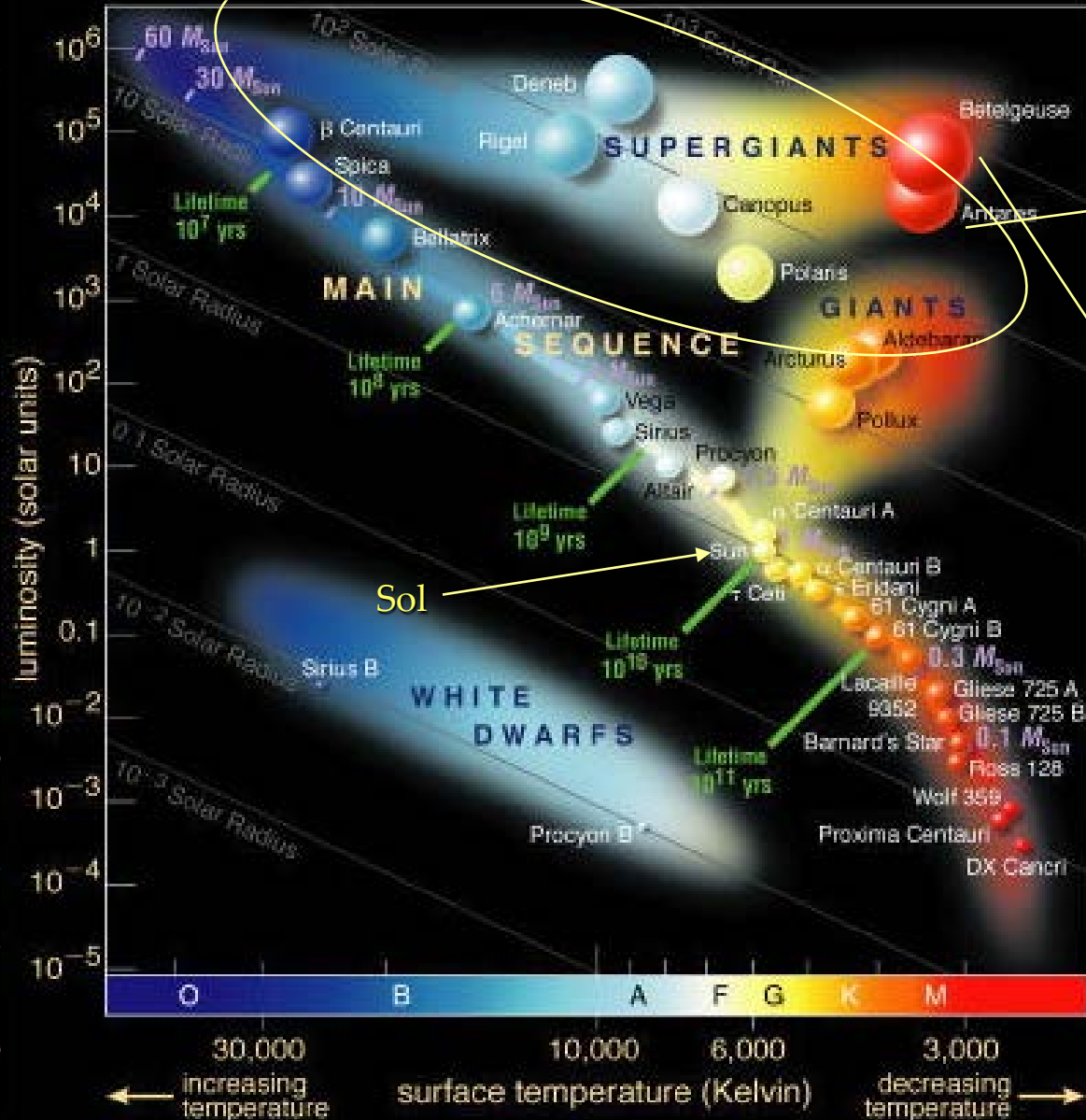
## Biografia estelar





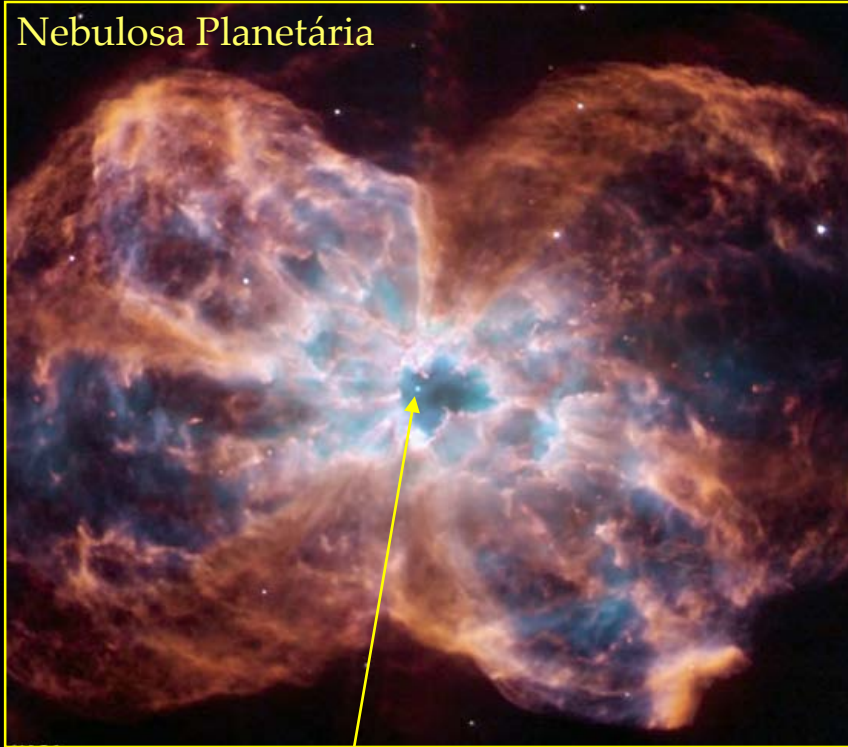
# O Diagrama HR (Hertzprung-Russel)

Vento estelar forte

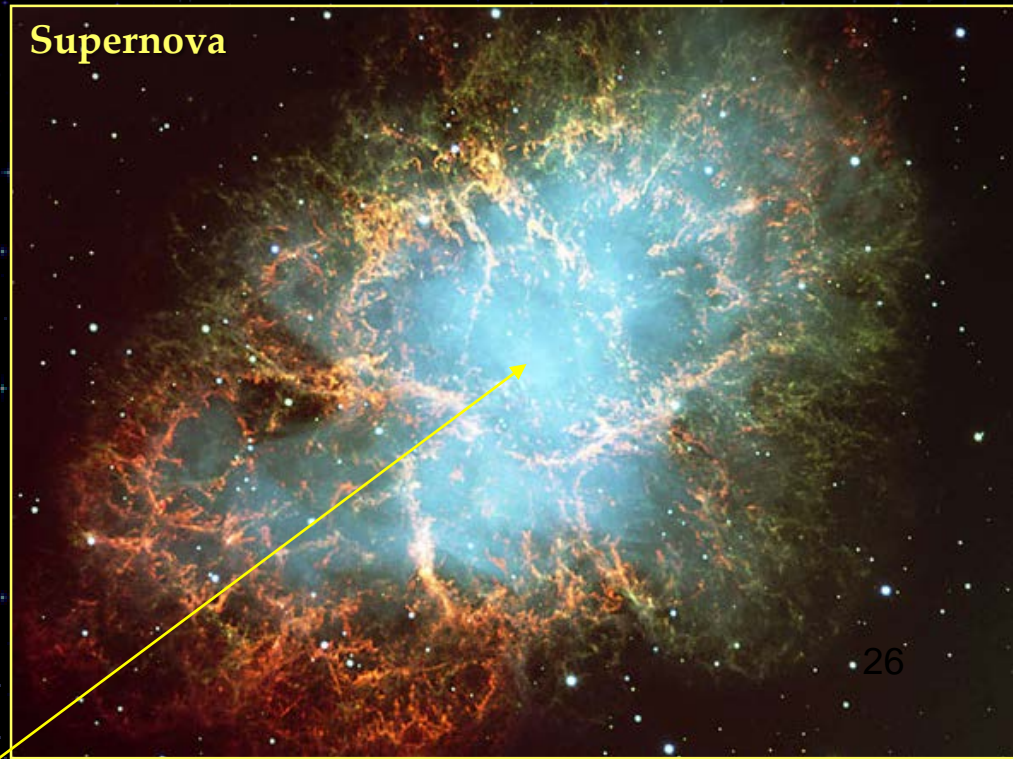


# Estágios finais e Ventos

Estágios finais de estrelas do tipo solar



Estágio finais de estrelas do grande massa



Comparação de tamanhos!!

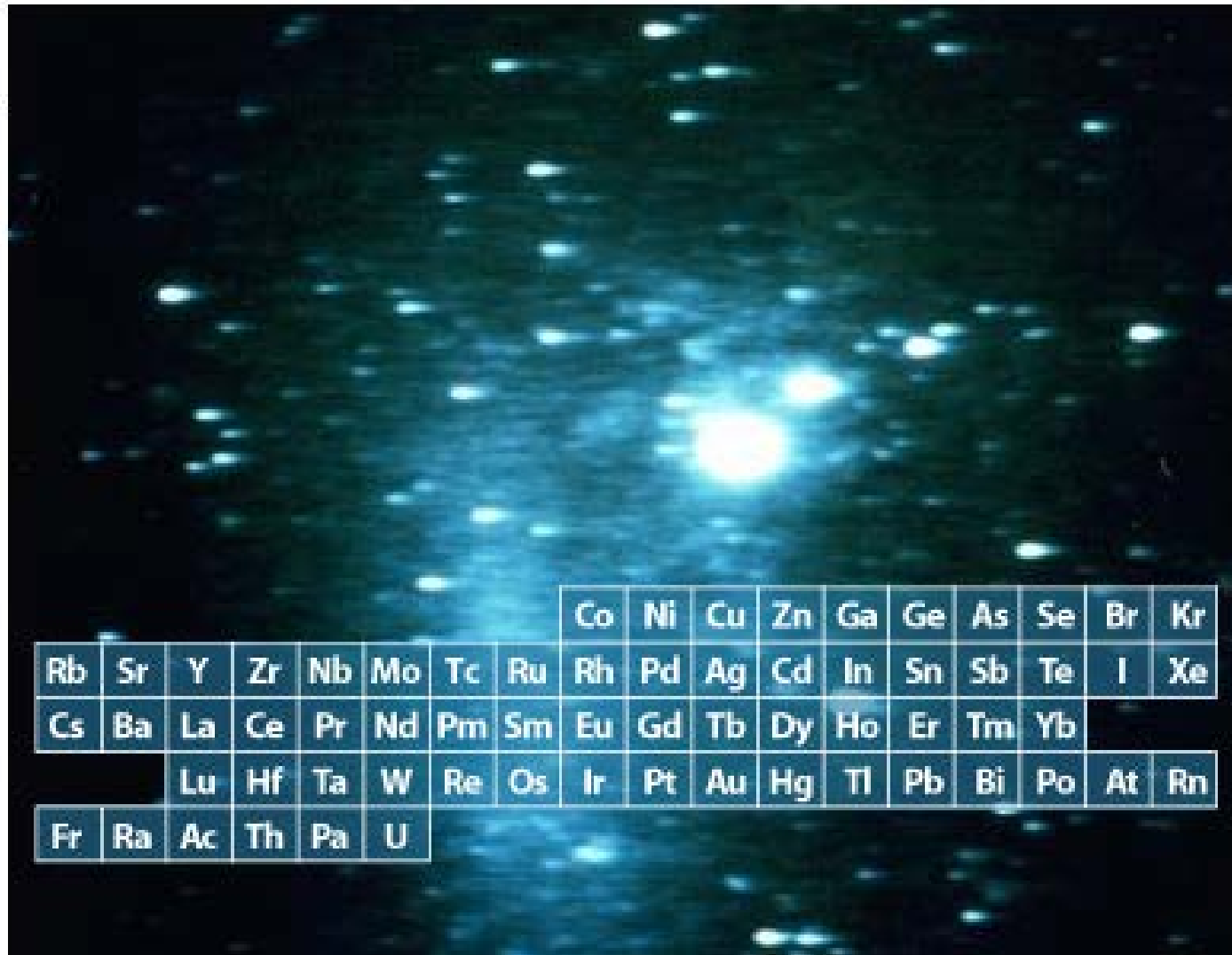


anã branca

Estrelas de nêutrons,  
buraco negro

Ventos estelares: Enriquecem o Meio interestelar átomos novos!!

# 1<sup>as</sup> estrelas e nucleossíntese estelar (~ 1bi ano)



Elements heavier than iron are formed when a supernova explodes.

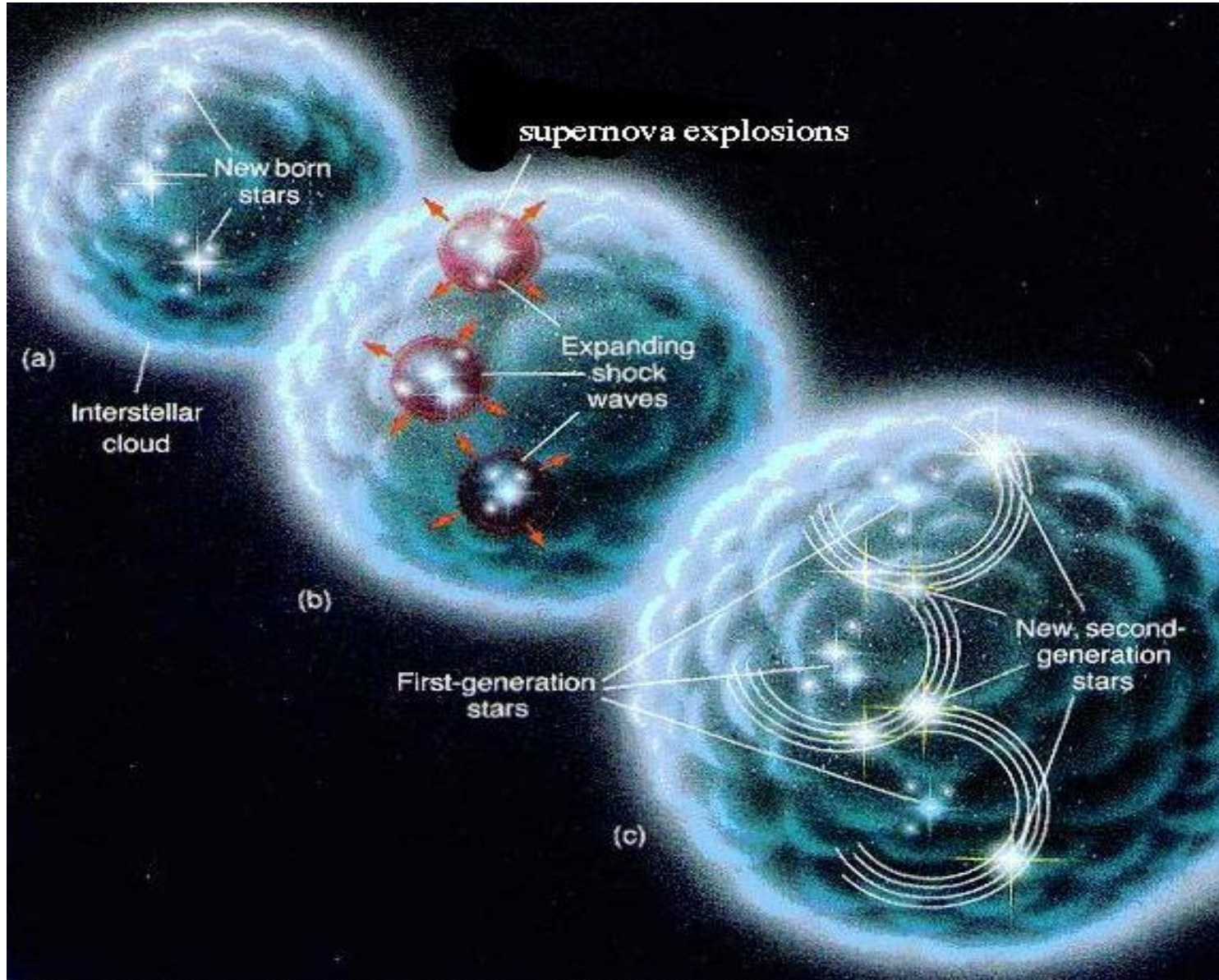
## Tabela Periódica com os átomos e sua origem

H												He						
Li	Be											B	C	N	O	F	Ne	
Na	Mg											Al	Si	P	S	Cl	Ar	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
Cs	Ba			Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra																	
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

- Big Bang
- Supernovae
- Large Stars
- Small Stars
- Cosmic Rays

Estrelas -> supernovas -> estrelas -> .....

Tempo →  
Enriquecimento químico

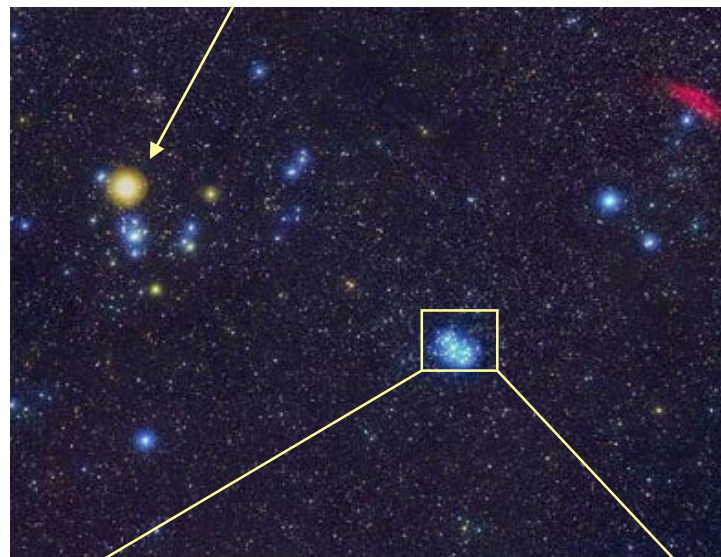


Com as estrelas, apareceram os aglomerados de estrelas ....



*M22, um aglomerado globular*

*Aldebaran (gigante vermelha)*



*aglomerado aberto Pleiades*

# .... as galáxias e aglomerados de galáxias



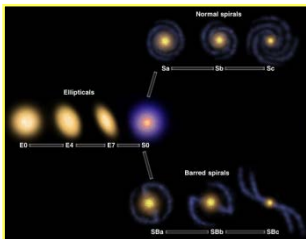
*Andromeda (nossa vizinha)*



*Colisões de galáxias*

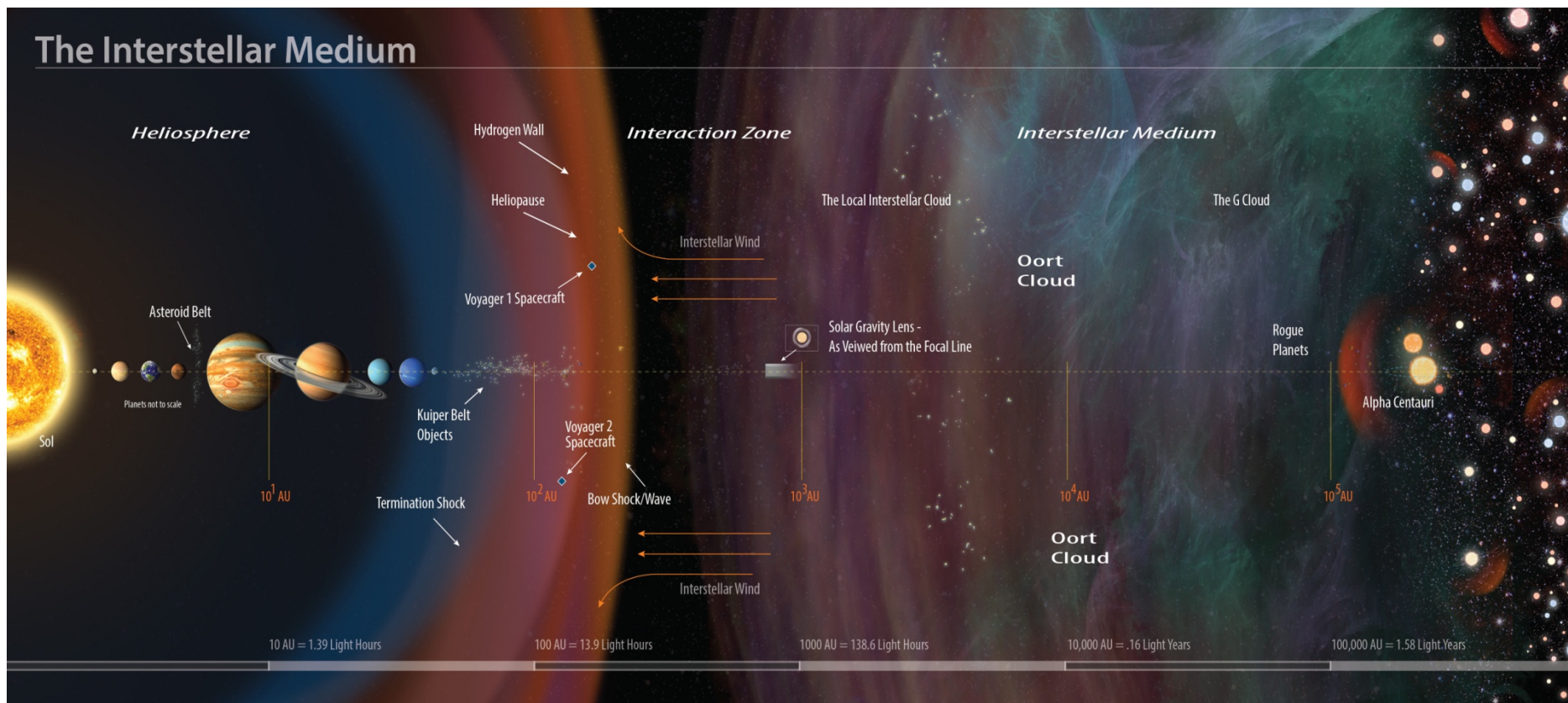


*Galaxy Cluster Abell 2218  
(Gravitational Lensing)*



# B) O meio interestelar

O espaço entre as estrelas esta cheio de coisas (radiação, partículas, campo magnéticos, poeira cósmica , moléculas, etc...)



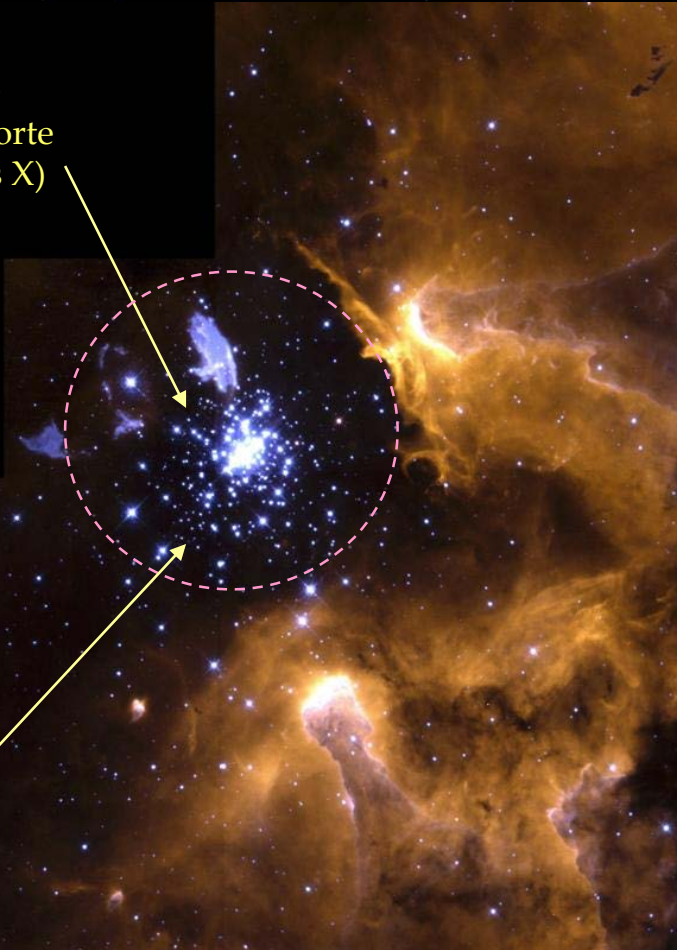


# O meio interestelar (o espaço entre as estrelas)

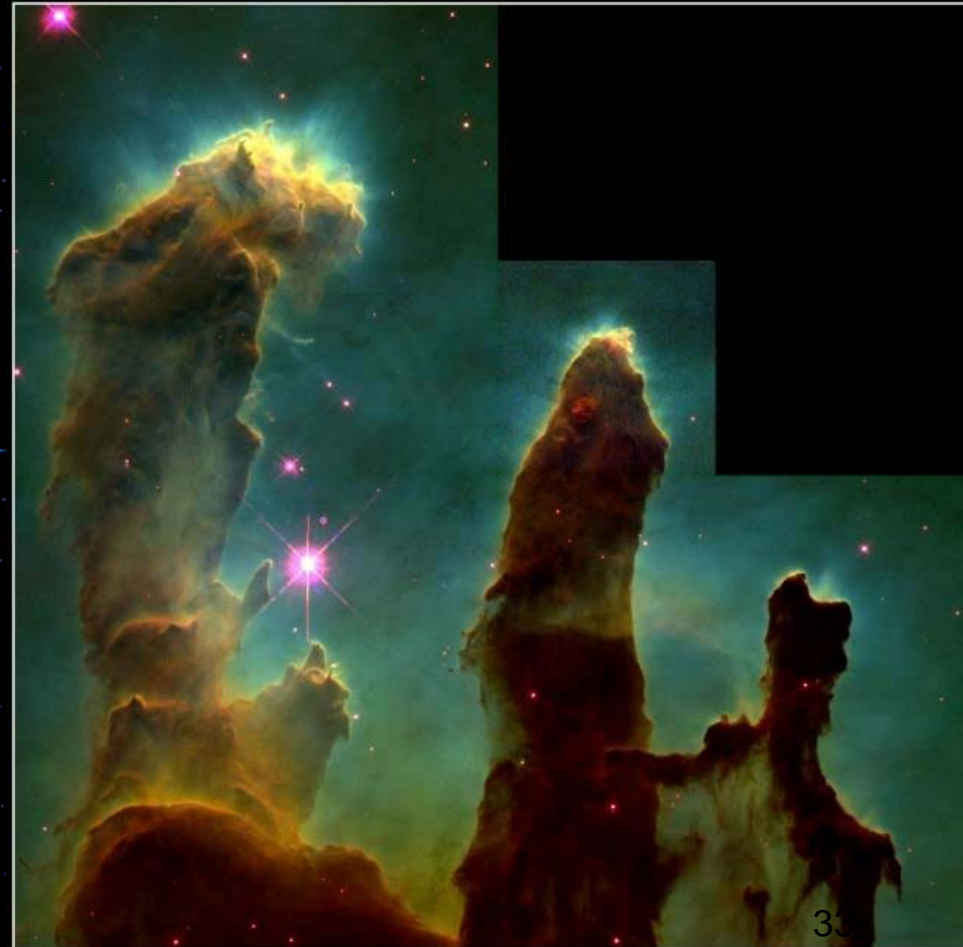
- Evolução estelar → ventos → Enriquecimento do meio interestelar (elemento e moléculas)
- Formação de novas estrelas (+ ricas em metais)

Campo de  
radiação forte  
(UV, Raios X)

Gás ionizado  
HII ( $\sim 10^4$  K)



NGC 3603



Gaseous Pillars · M16

HST · WFPC2

# Propriedades do meio interestelar

- Composição: Átomos, Moléculas, Agregados moleculares, grãos de poeira (agregados de moléculas refratárias. Carbono, Silicatos) e radiação (fotons, eletrons, íons e raios cósmicos)



- Regiões do MI: Nebulosas, Nuvens difusas (quente e rarefeitas  $N < 1$ ); Regiões ionizadas (HII,  $T \sim 10^4 K$ ); Nuvens densas ( $N \sim 10^5$ ), Nuvens Moleculares ( $T \sim 10 K$ ); Glóbulos de bock; Discos proto-planetários, Envoltórios circumstelares, Nebulosas planetárias e outros.

Thackeray's Globules in IC 2944



Hubble  
Heritage

Reflection Nebula in the Pleiades • IC 349



Hubble  
Heritage

# O gás interestelar

Cerca de 99% da matéria interestelar é composta de gás. A poeira constitui cerca de 1%.

Destes 99% temos que cerca de 90% é formado por H ou H<sub>2</sub>, cerca de 9% é He e apenas 1% é formado por elementos mais pesados do que o hélio.

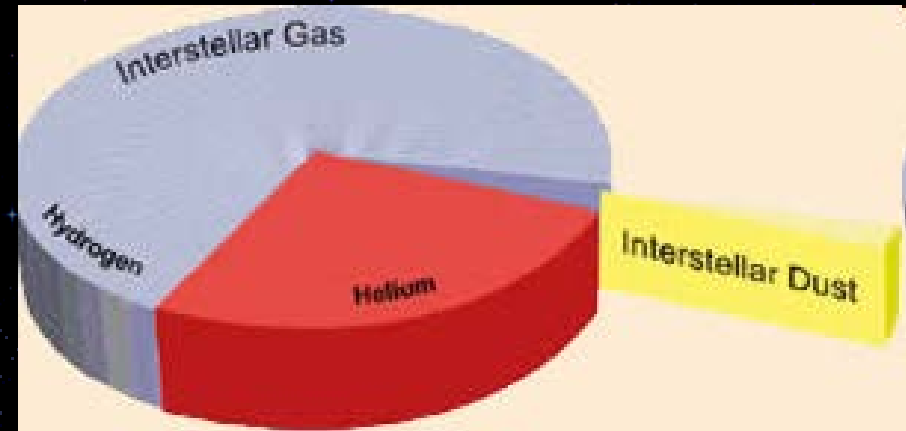


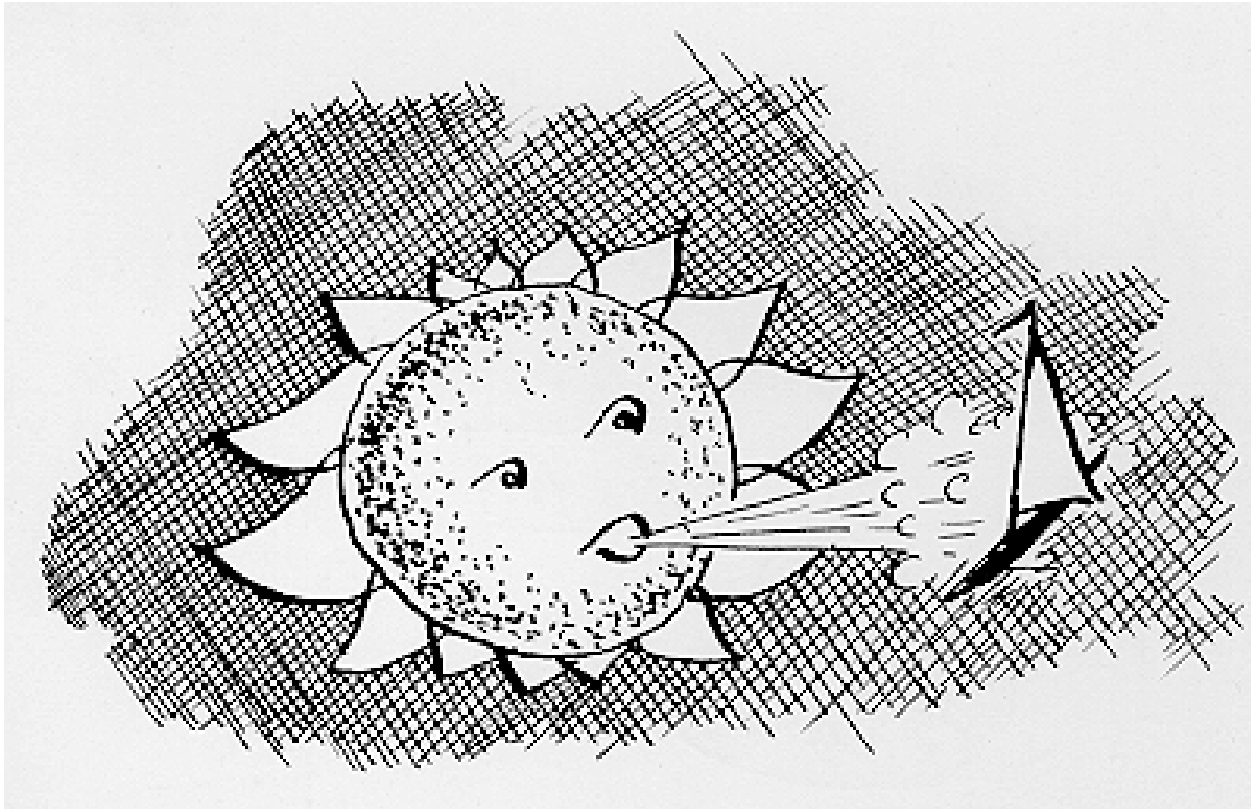
Table 1: Components of the interstellar medium

Component	Fractional Volume	Scale Height (pc)	Temperature (K)	Density (atoms/cm <sup>3</sup> )	State of hydrogen	Primary observational techniques
Molecular clouds	< 1%	70	10—20	10 <sup>2</sup> —10 <sup>6</sup>	molecular	Radio and infrared molecular emission and absorption lines
Cold Neutral Medium (CNM)	1—5%	100—300	50—100	20—50	neutral atomic	H I 21 cm line absorption
Warm Neutral Medium (WNM)	10—20%	300—400	6000—10000	0.2—0.5	neutral atomic	H I 21 cm line emission
Warm Ionized Medium (WIM)	20—50%	1000	8000	0.2—0.5	ionized	H $\alpha$ emission and pulsar dispersion
H II regions	< 1%	70	8000	10 <sup>2</sup> —10 <sup>4</sup>	ionized	H $\alpha$ emission and pulsar dispersion
Coronal gas Hot Ionized Medium (HIM)	30—70%	1000—3000	10 <sup>6</sup> —10 <sup>7</sup>	10 <sup>-4</sup> —10 <sup>-2</sup>	ionized (metals also highly ionized)	X-ray emission; absorption lines of highly ionized metals, primarily in the ultraviolet

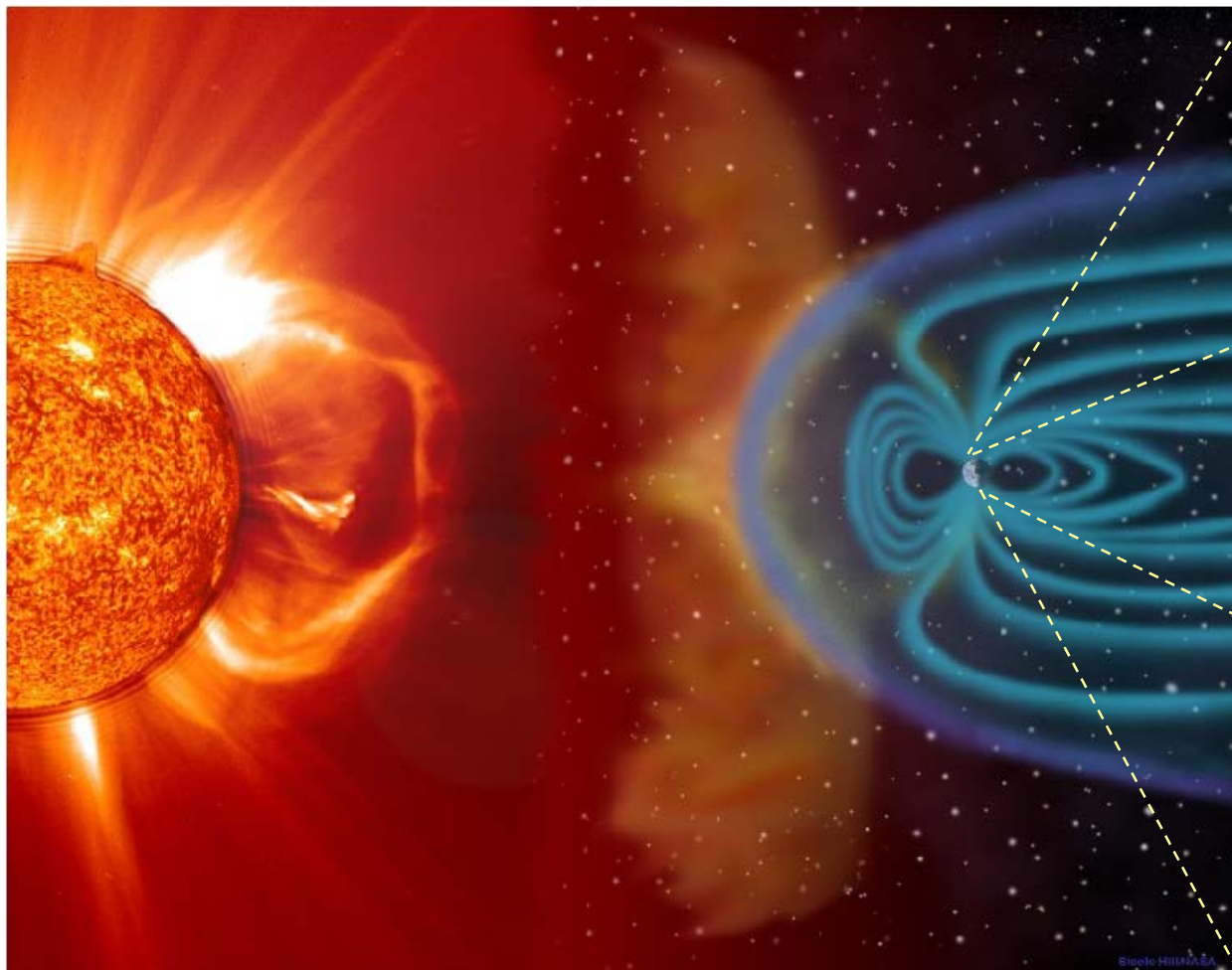
## C) O vento estelar e formação das moléculas

---

O vento estelar tem é essencial para a formação de moléculas circunstelares e interretelares e aumento da complexidade química do meio ionterestelar.



- Vento solar (auroras, tempestades solares,...)
- Vento estelar → formação envoltório circumstelar. Concluinte do meio interplanetário.



# Evolução temporal, aumento da fase de ventos



**Nebulosa Planetária**

*Nebulosa da Ampulheta (MyCn 18)*

Envoltório de Estrela gigante vermelha  $M < 8 M_{\text{sol}}$  (ilustração)

sol



Vento estelar → material circunestelar (estrutura em forma de disco, esférica, bipolar, jatos polares) → meio interestelar

# Mais ventos de nebulosa Planetárias



*Abel 39*



*NGC 6751*



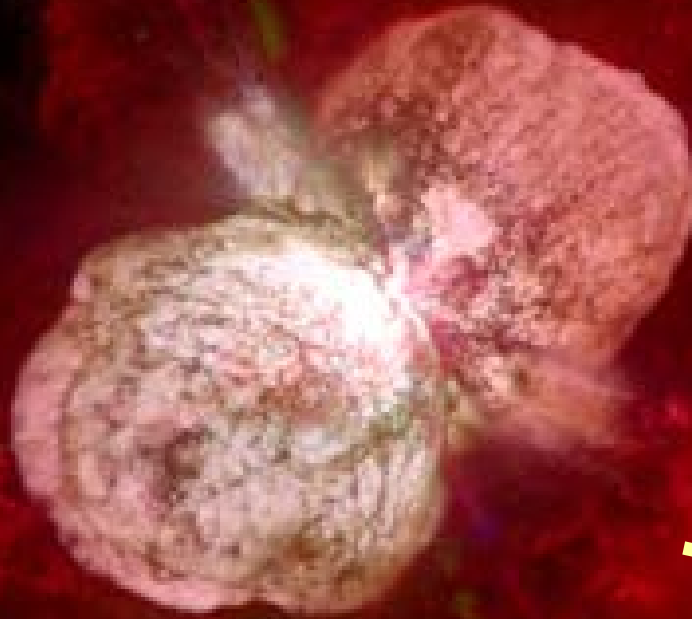
*NGC 6826*



*Twin Jet Nebula M2-9*



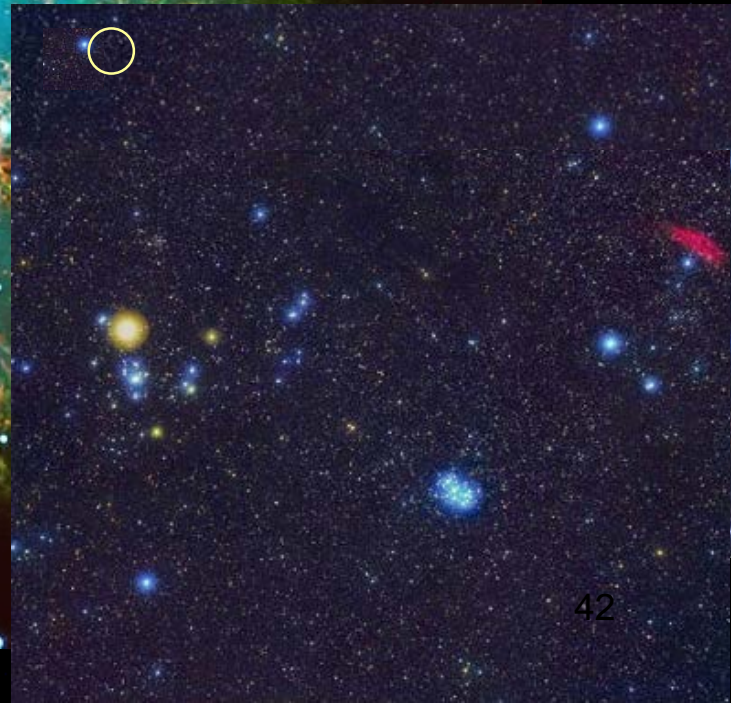
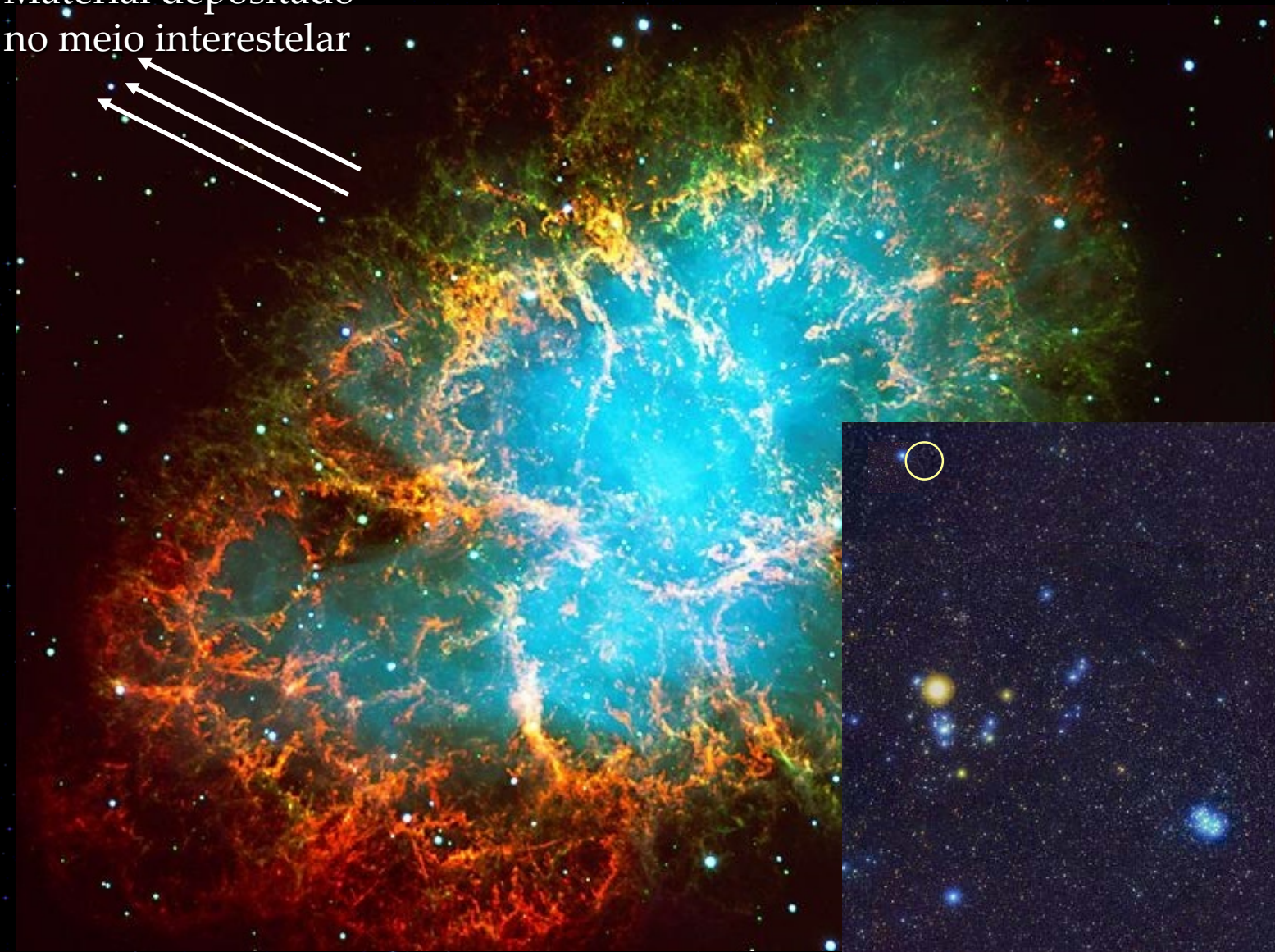
Vento de estrela supermassiva  $M \sim 120 M_{\text{sol}}$   
Eta Carinae



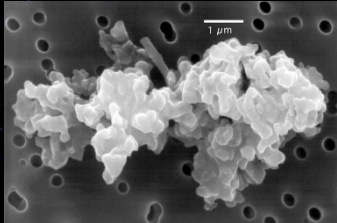
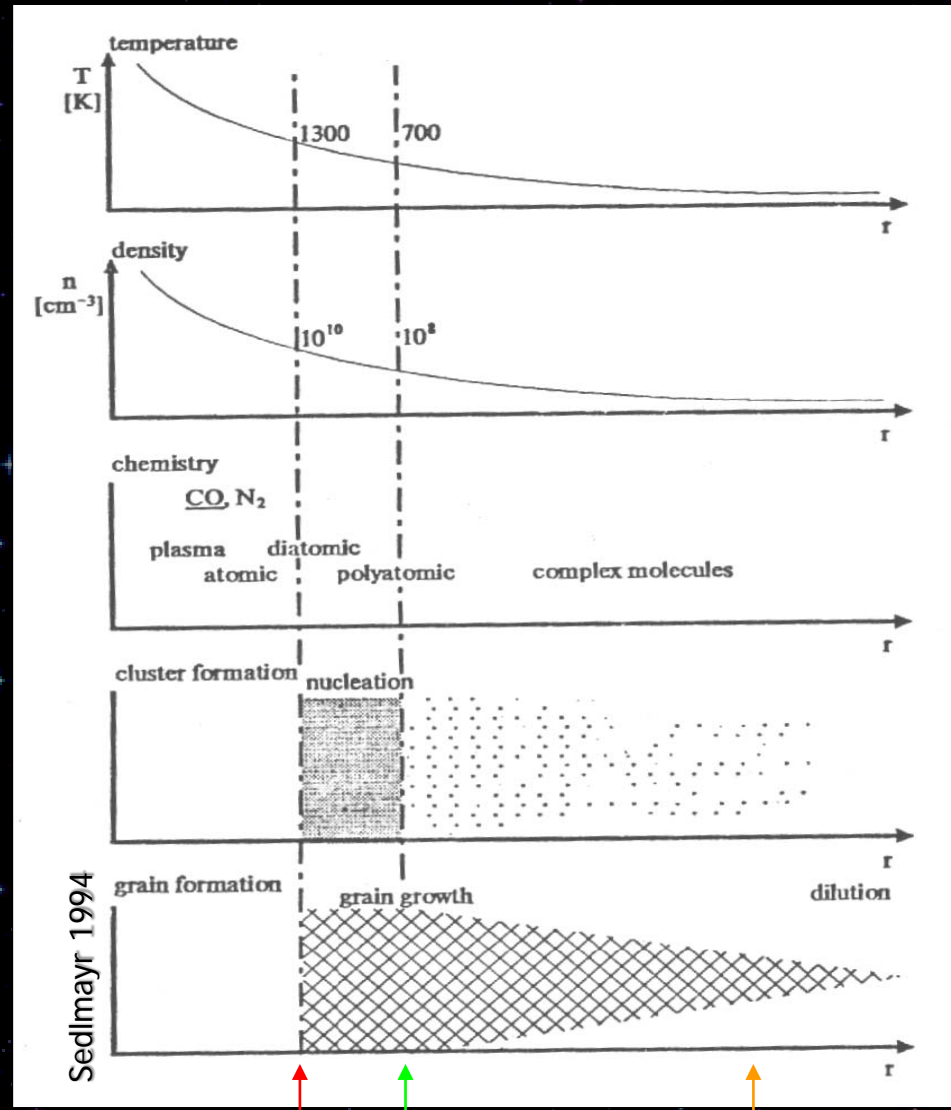
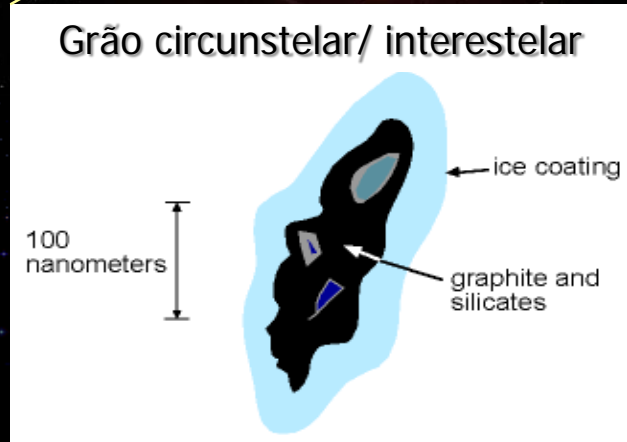
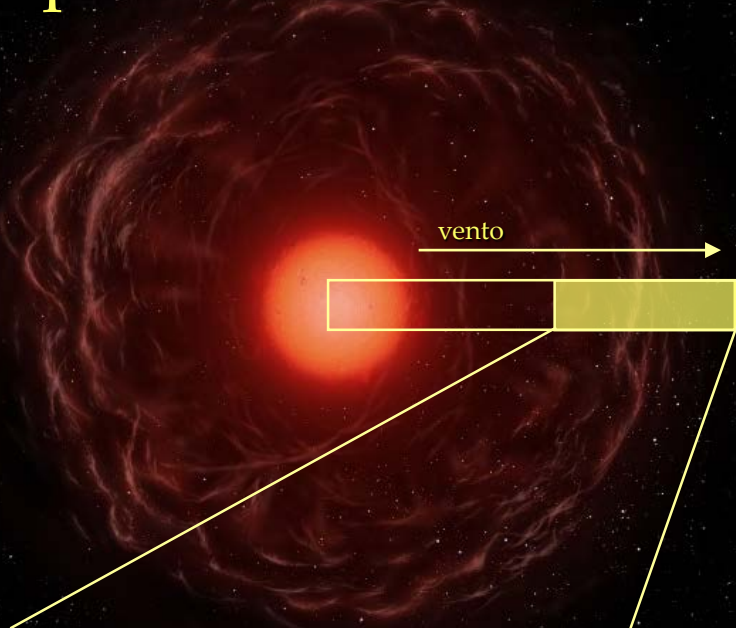
Material depositado  
no meio interestelar

# Ventos de uma remanescentes de supernova nebulosa do caranguejo

Material depositado  
no meio interestelar



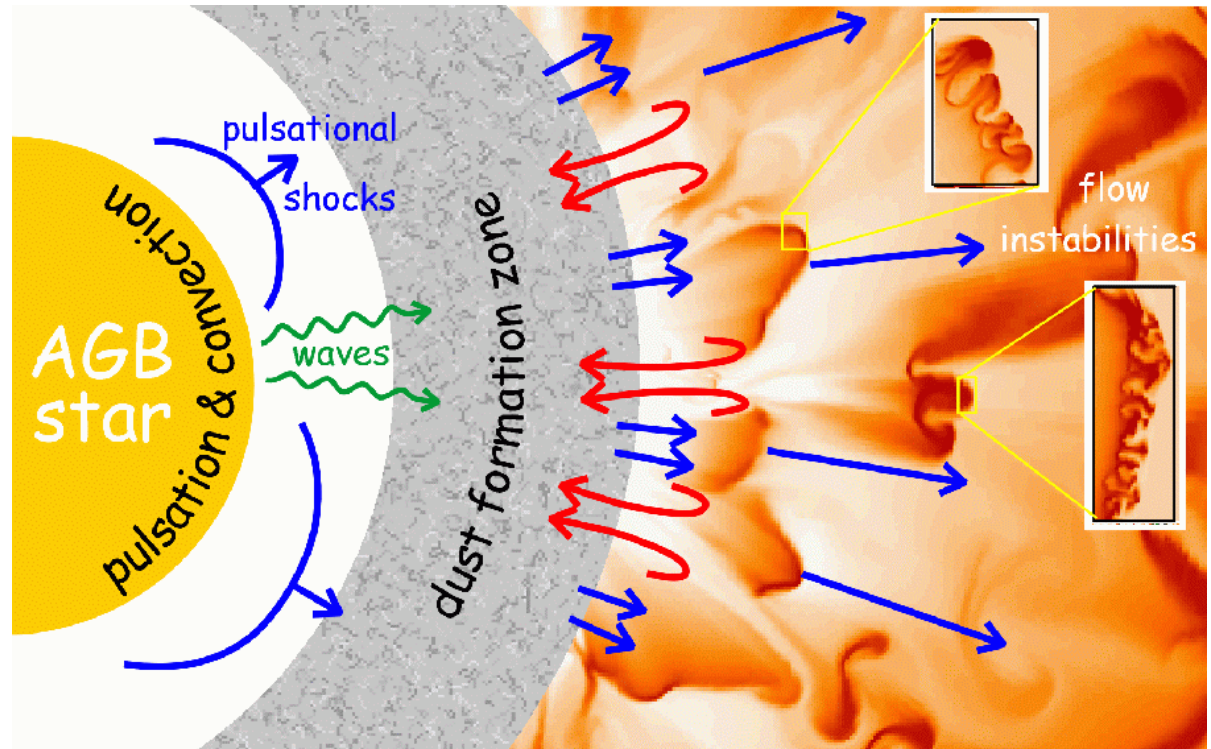
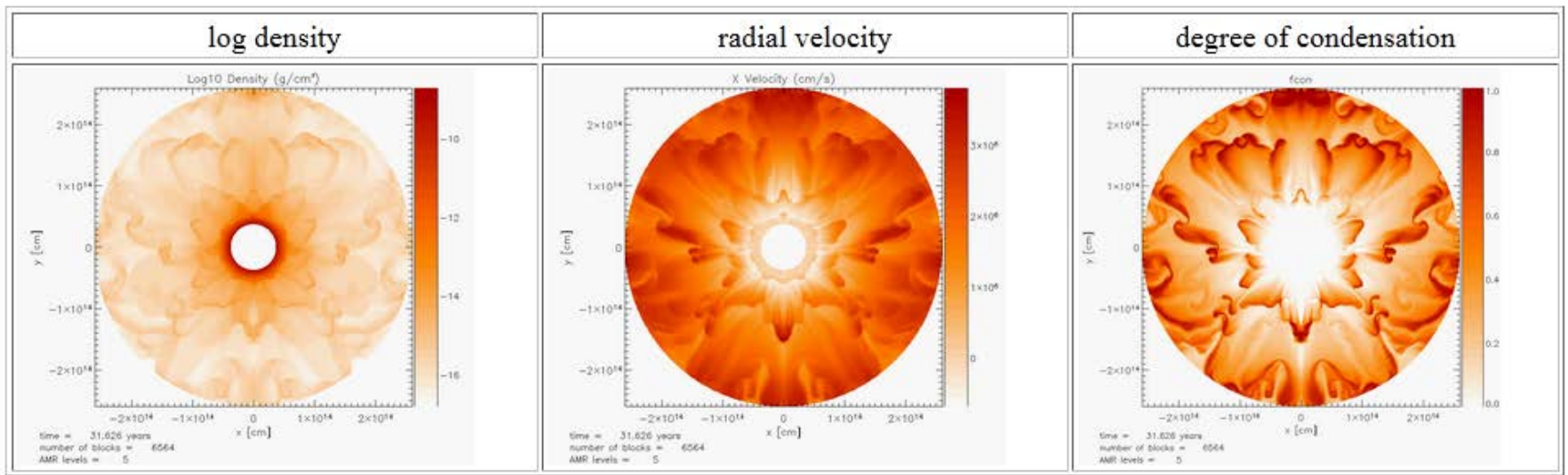
# A poeira interestelar



Al<sub>2</sub>O<sub>4</sub> (temp ~ 1700K); silicatos (temp ~ 1400K)

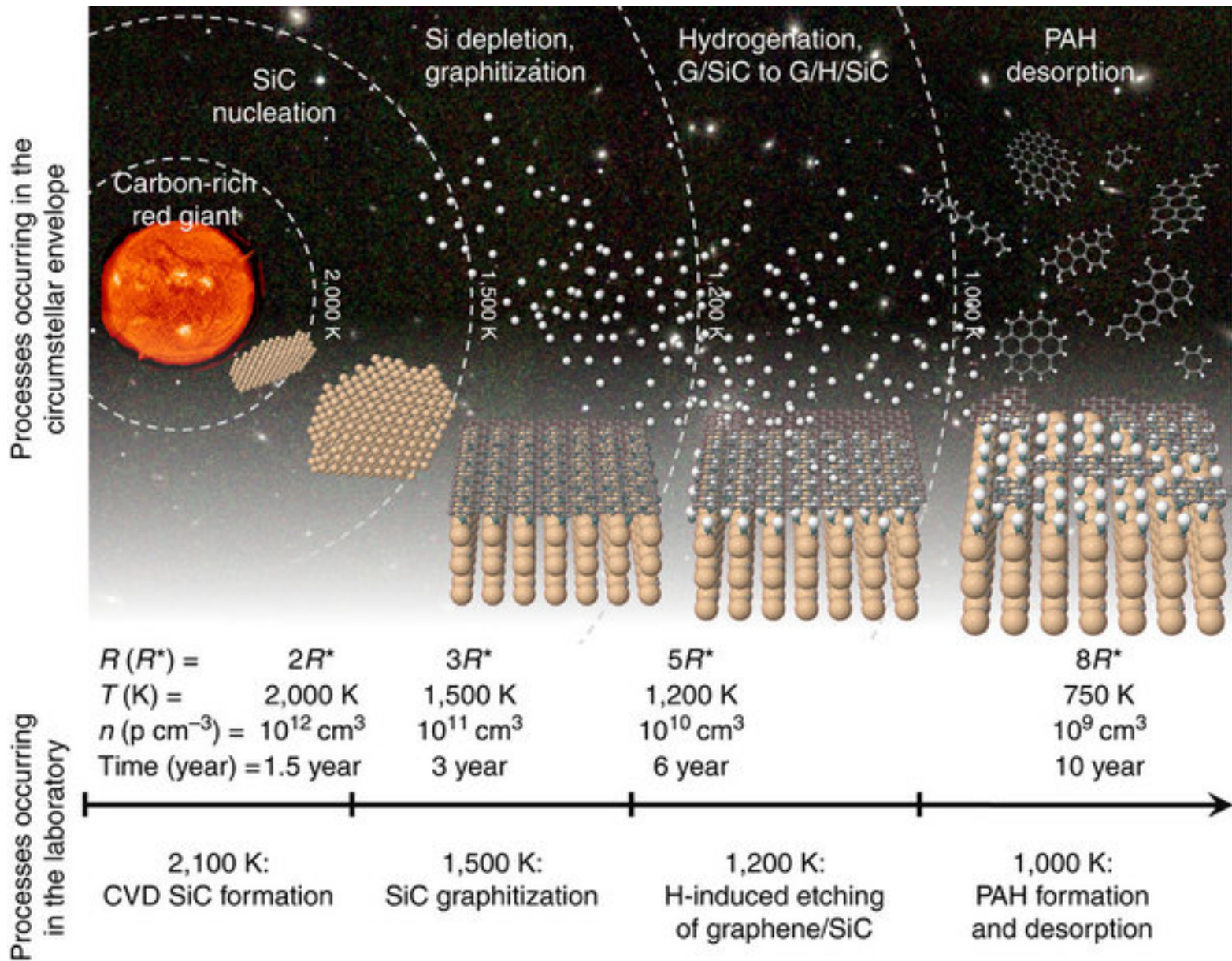
Moléculas carbonaceas (C, PAHs, SiC)

Moléculas voláteis – mantos (H<sub>2</sub>O, CH<sub>4</sub>...)



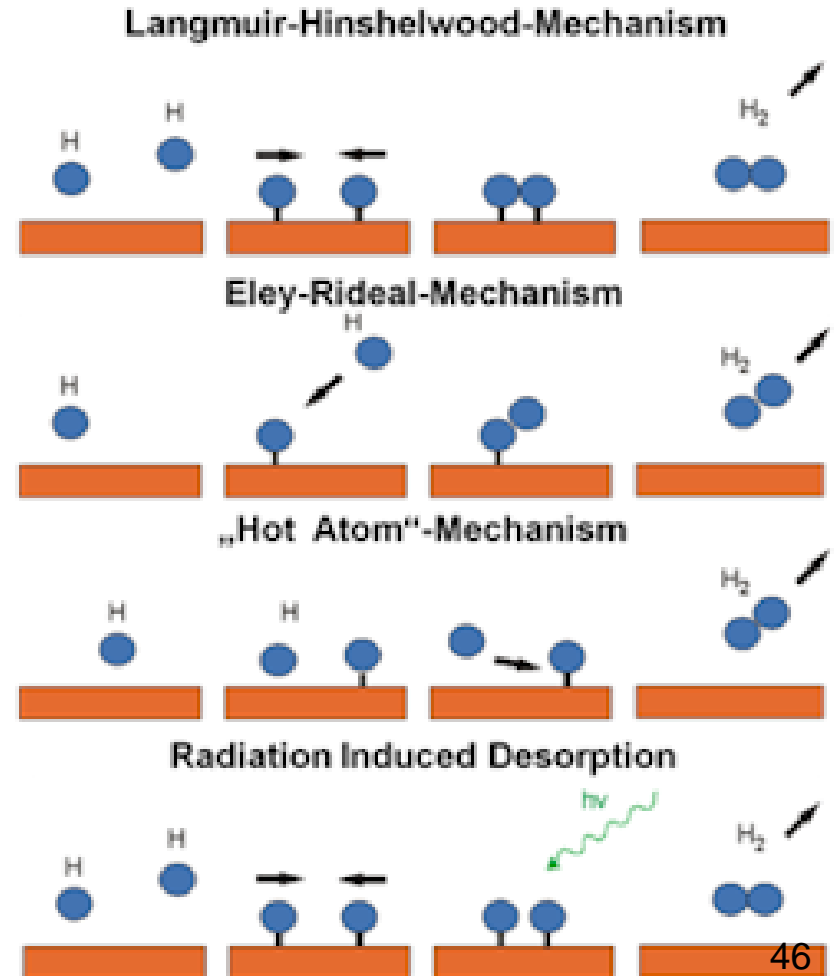
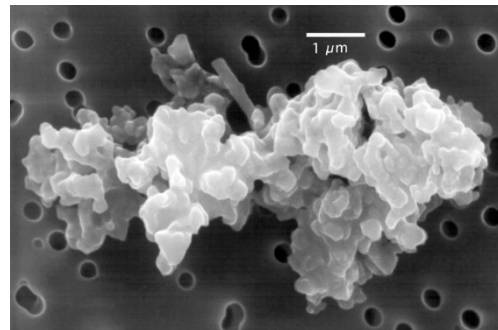
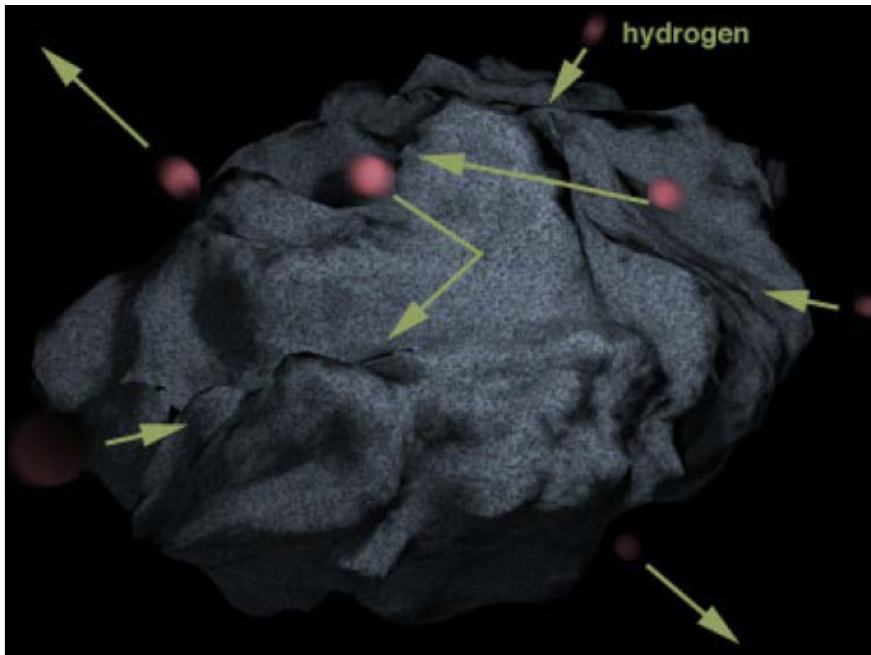
Ver videos:



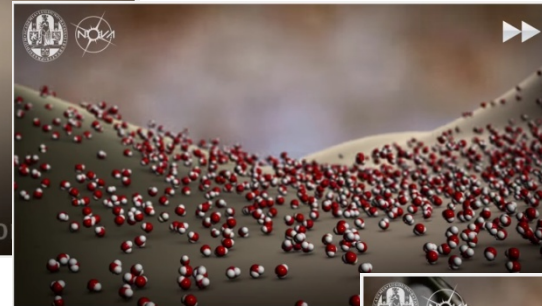
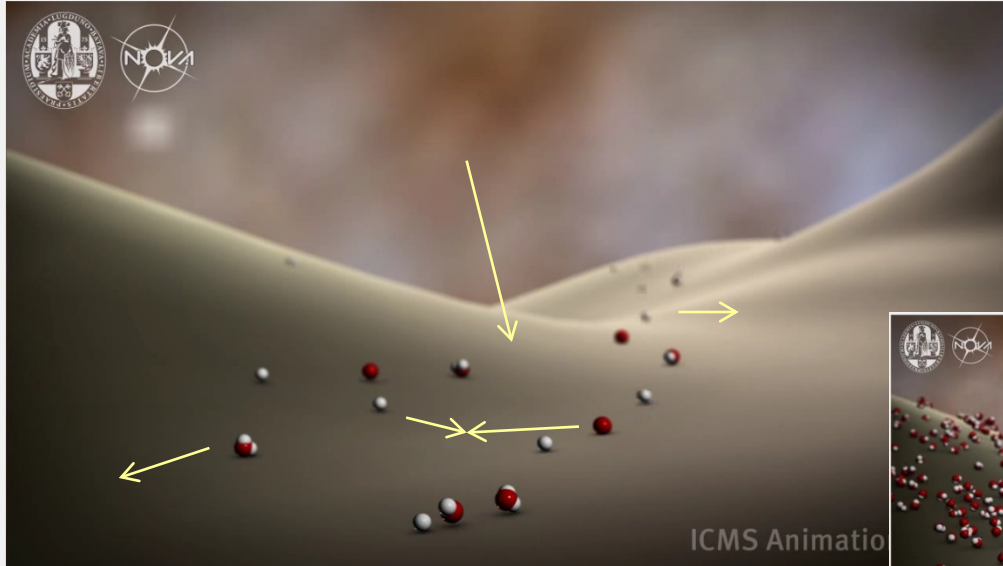


# Grãos interestelares e a formação do $H_2$

- Probabilidade de reação na fase gasosa baixa.
- Grãos ( $T \sim 10K$ ) agem como catalisadores.



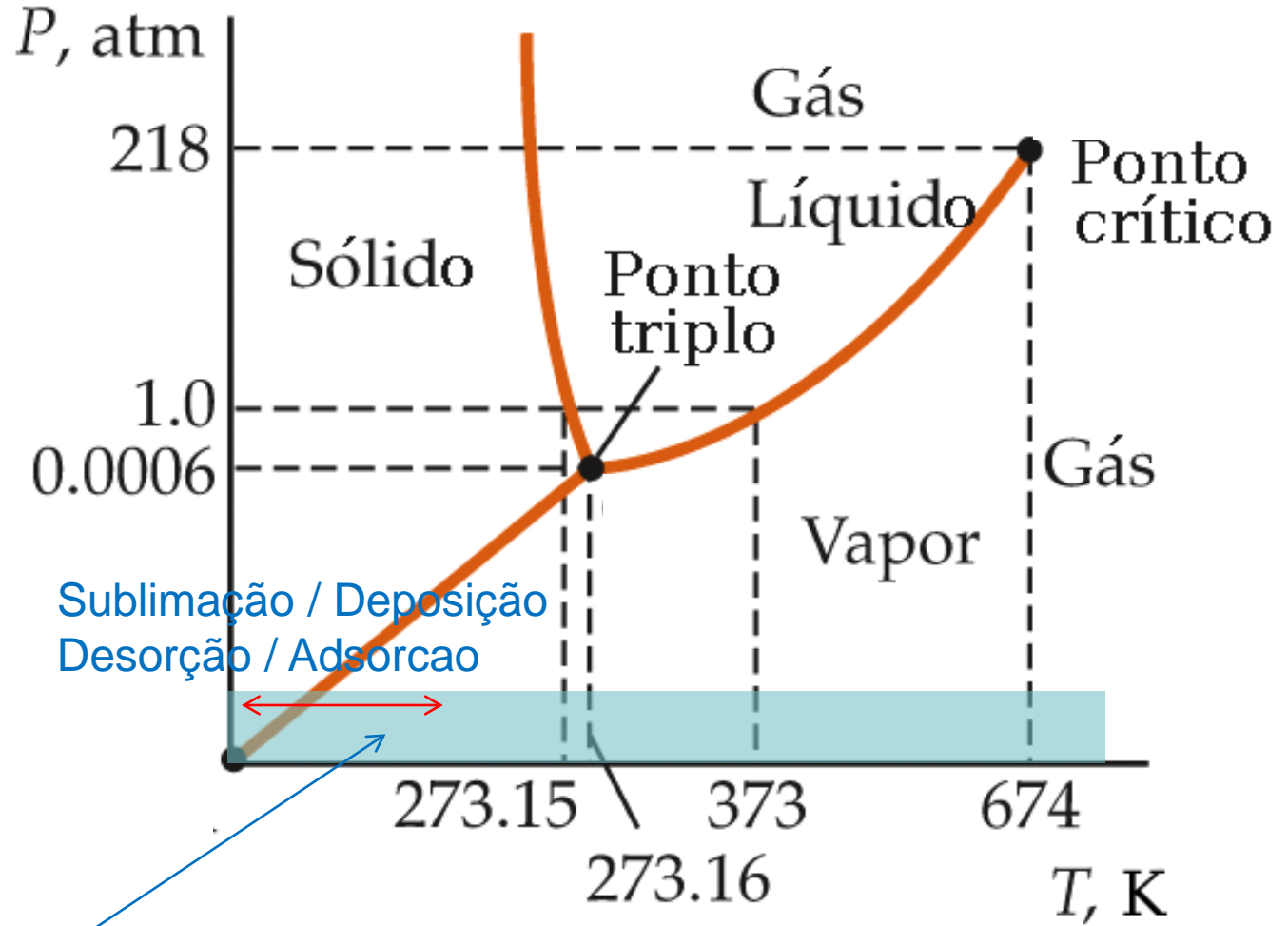
# Formação de gelos de água no espaço



Ver vídeo:



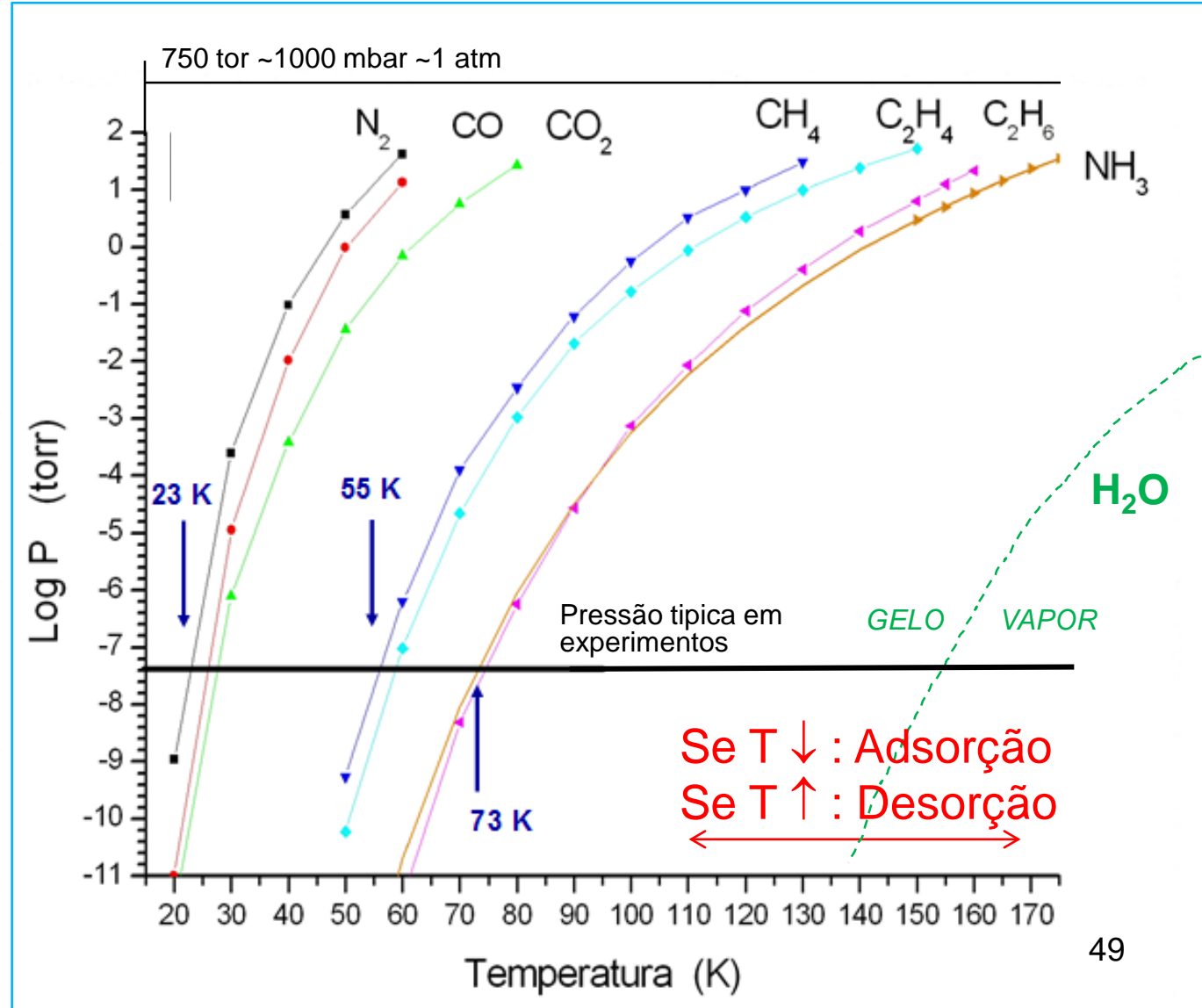
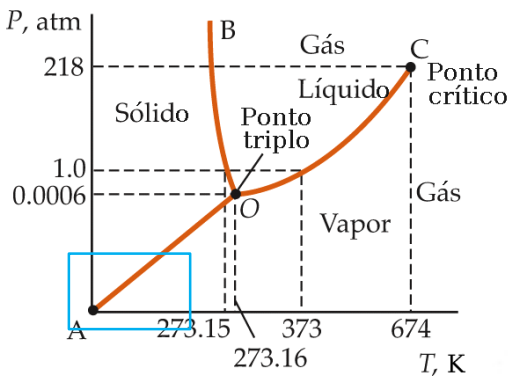
# Diagrama de Fase e Pressão de Vapor



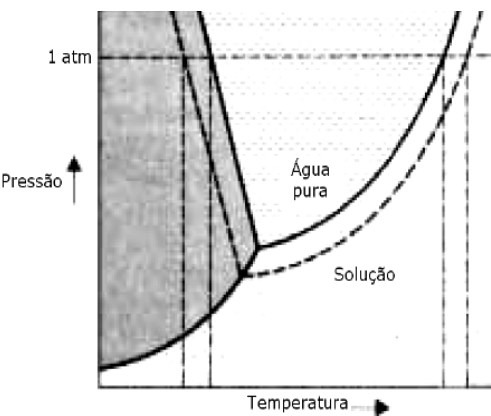
No espaço!!!



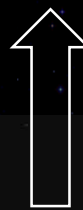
# Diagrama de Fase e Pressão de Vapor



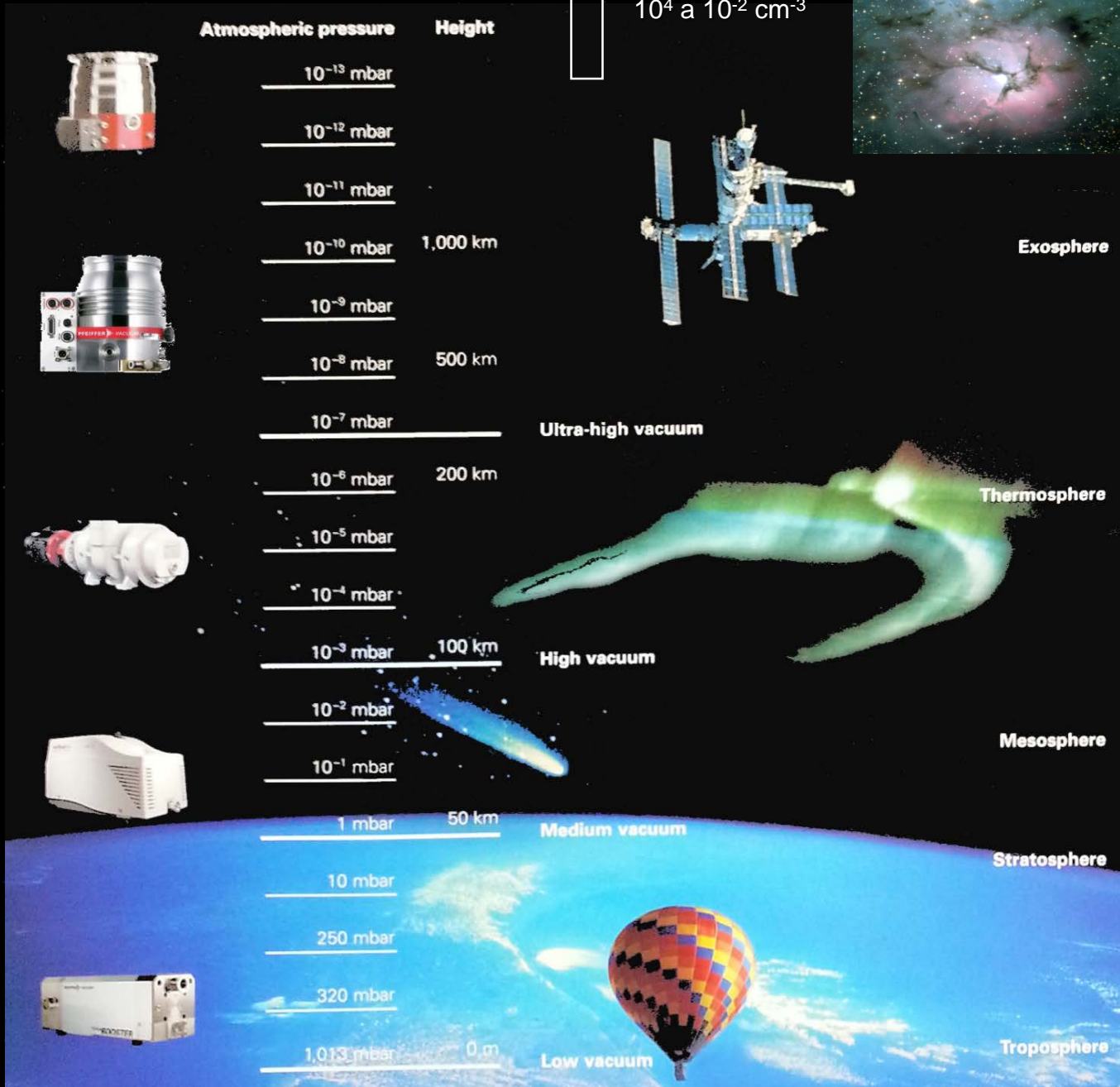
Obs: Soluções



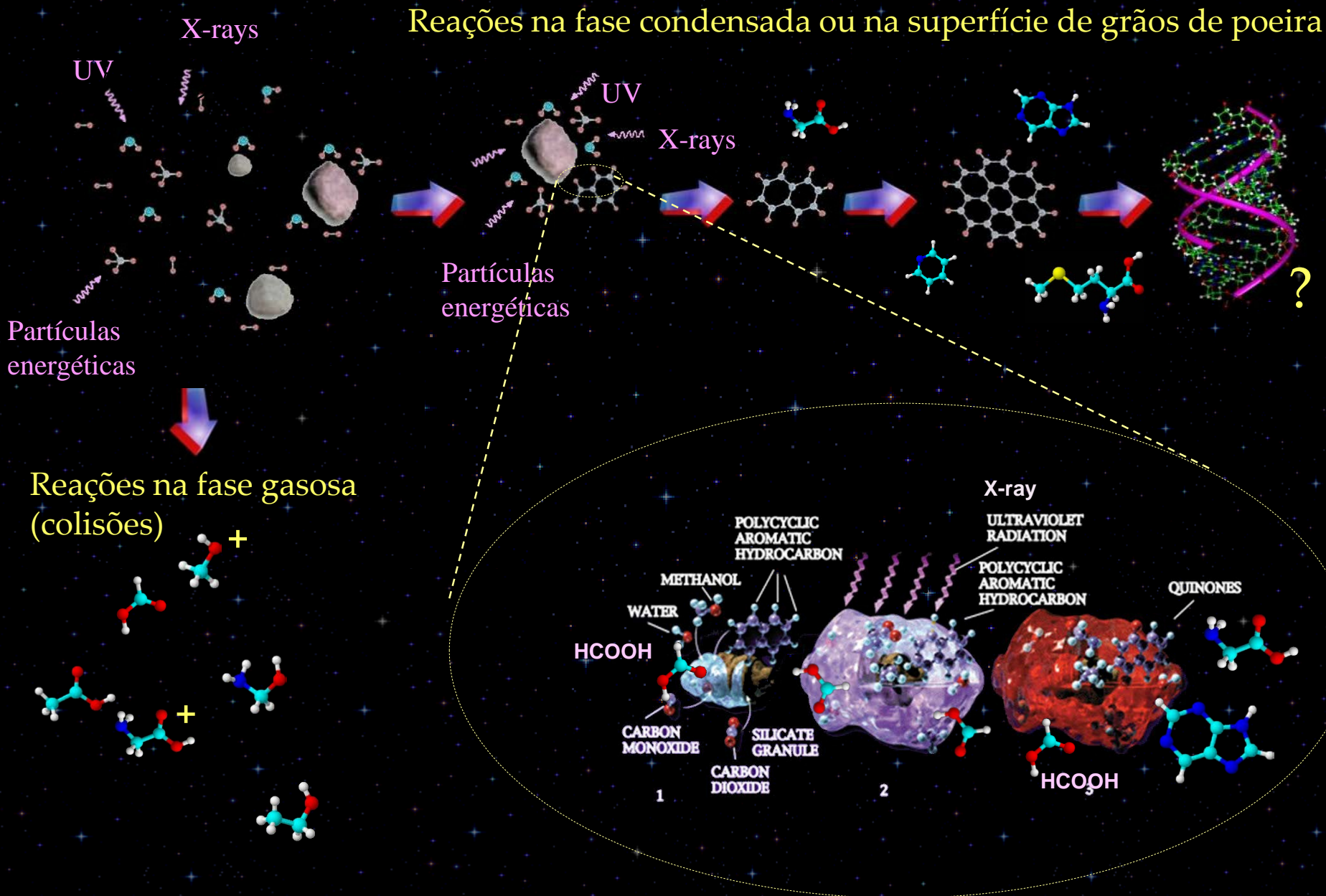
# Faixas de Pressão



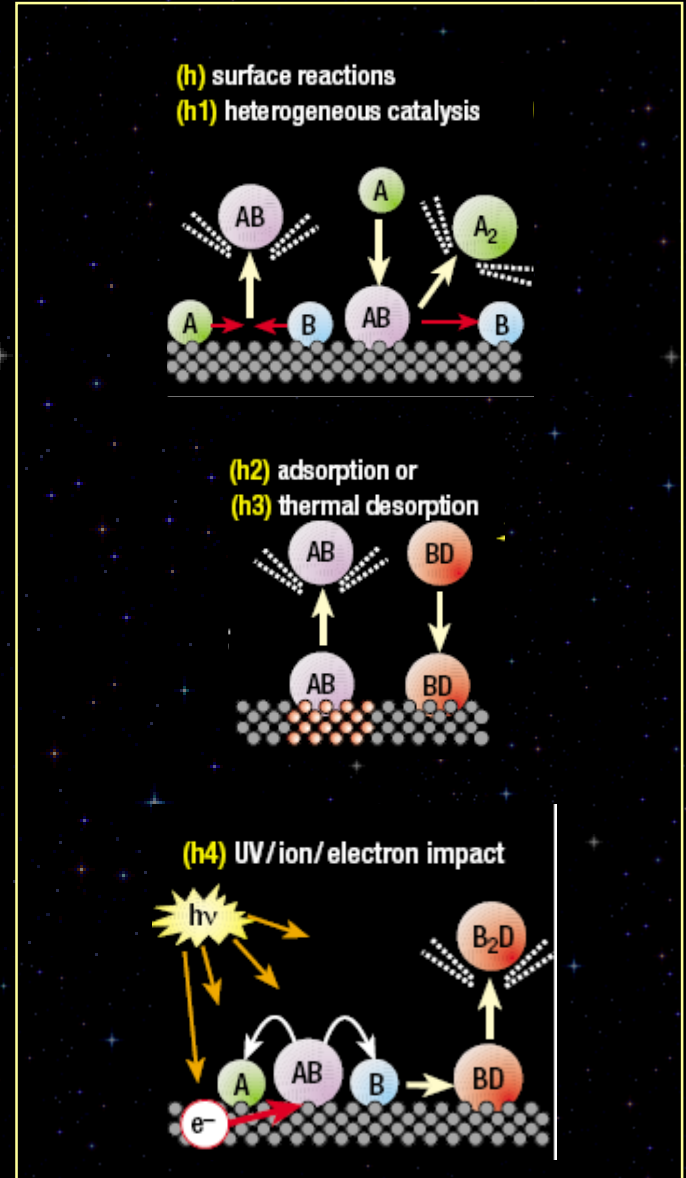
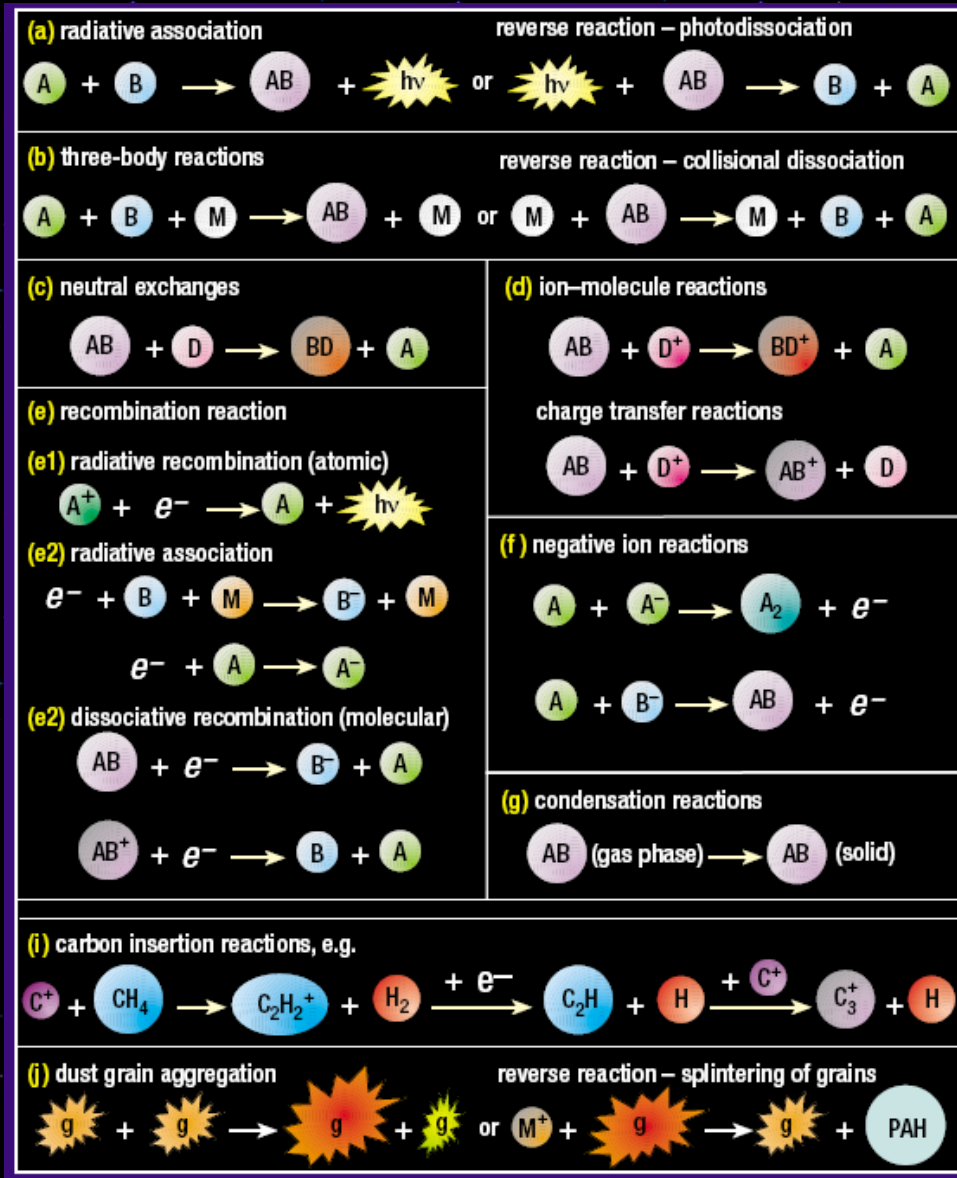
Meio interestelar  
 $10^{-12}$  a  $10^{-18}$  mbar  
 $10^4$  a  $10^{-2}$  cm<sup>-3</sup>



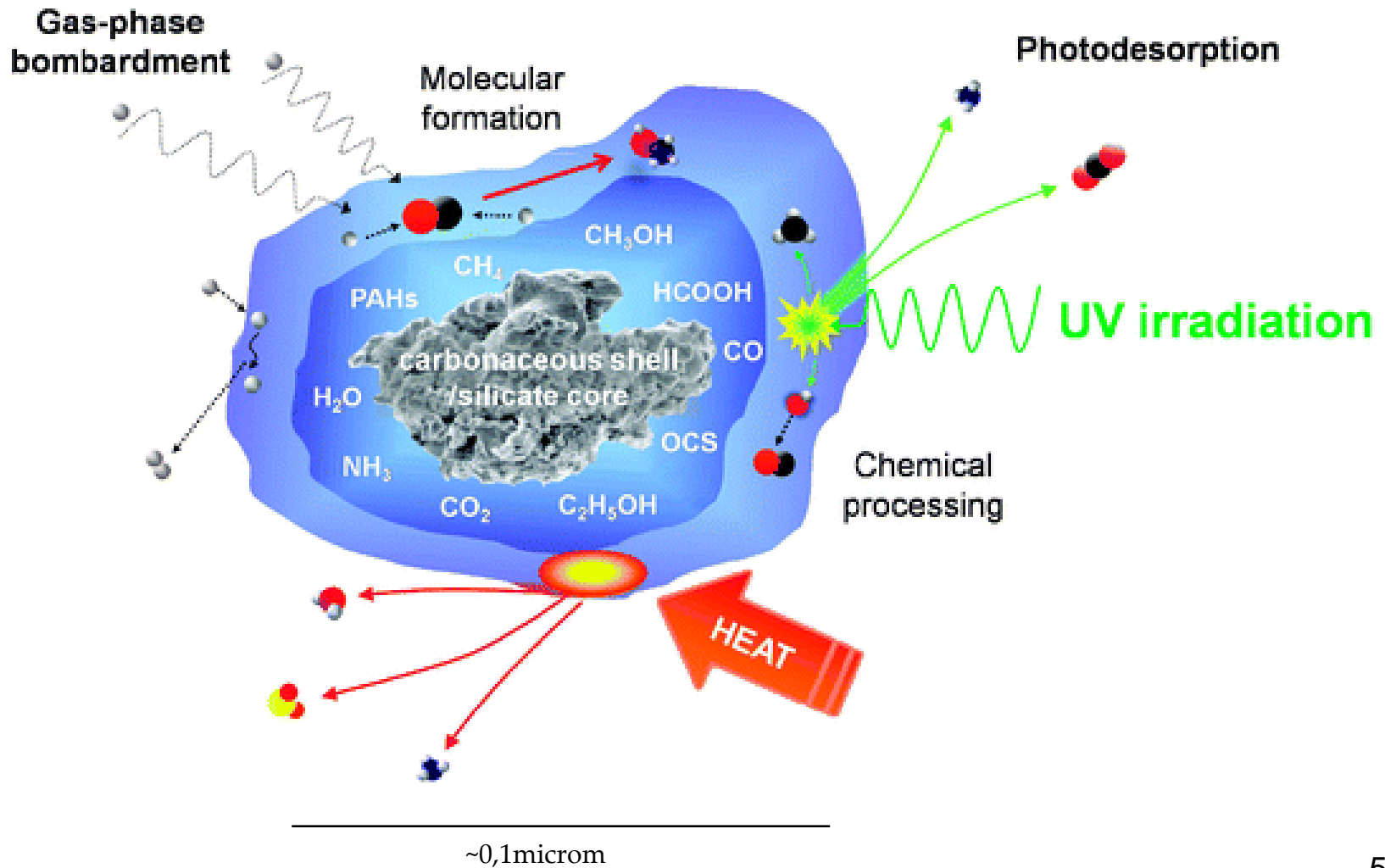
# Formação de outras moléculas no espaço



# Algumas reações típicas na fase gasosa e fase condensada.



# Grão interestelar típico (coberto por um manto de gelo)

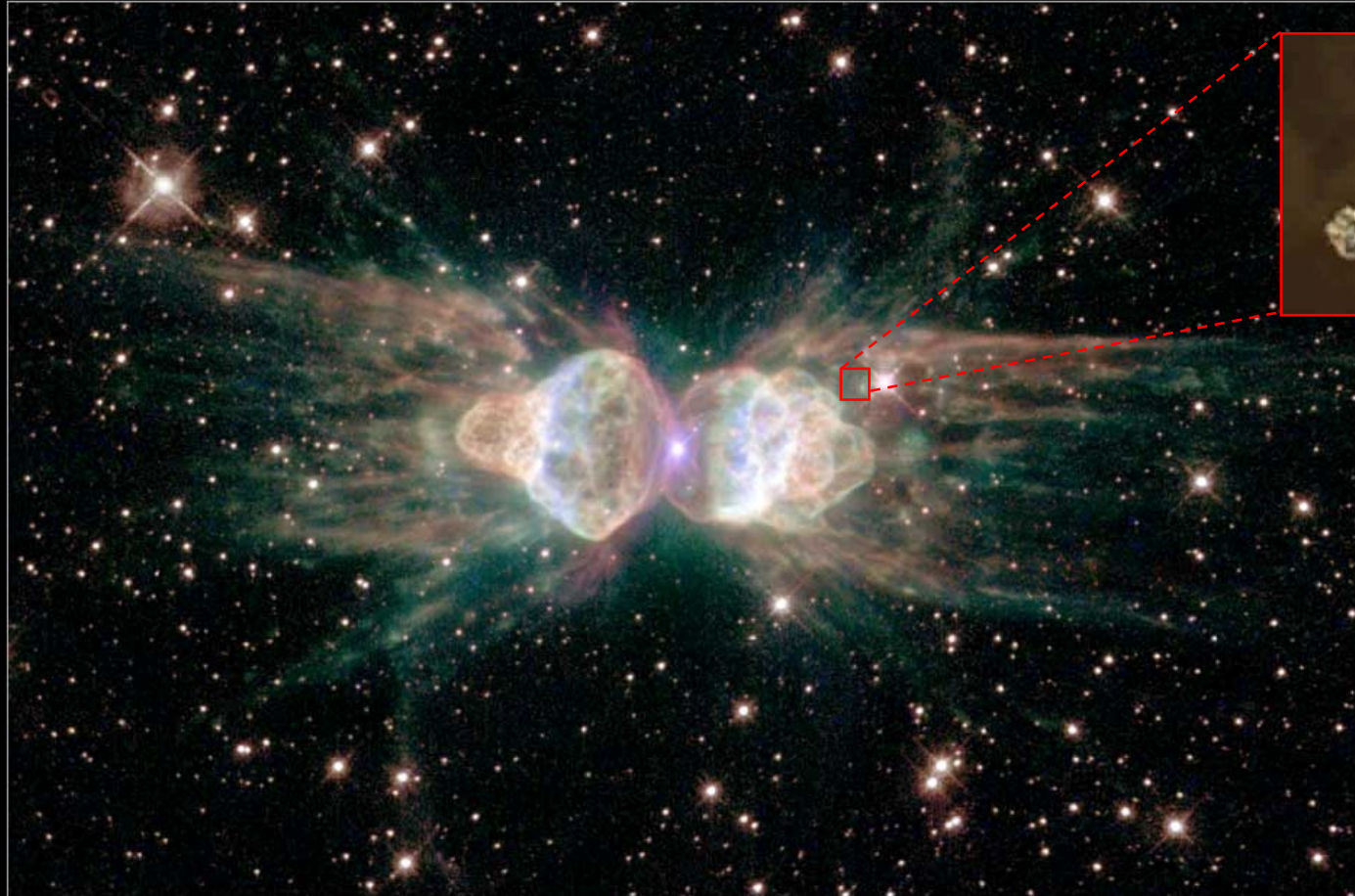


# Mais sobre gelos astrofísicos

- Grãos de poeira fria: núcleos de silicatos/carbono + cobertura de moléculas voláteis condensadas ( $\text{H}_2\text{O}$ ,  $\text{CO}$ ,  $\text{N}_2$ ,  $\text{NH}_3$ , etc...)



# Planetary Nebula Mz3



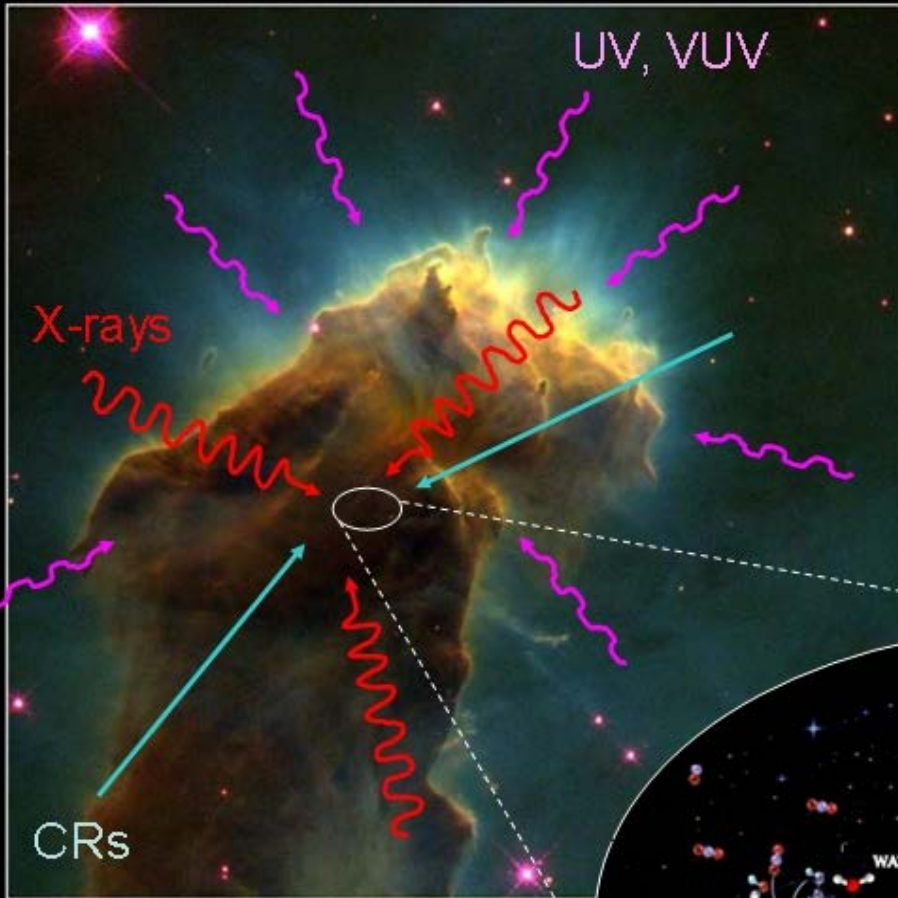
Hubble  
Heritage

NASA, ESA, and The Hubble Heritage Team (STScI/AURA) • Hubble Space Telescope WFPC2 • STScI-PRC01-05

# Processamento pela Radiação:

Fótons,  
eletrons,  
íons.

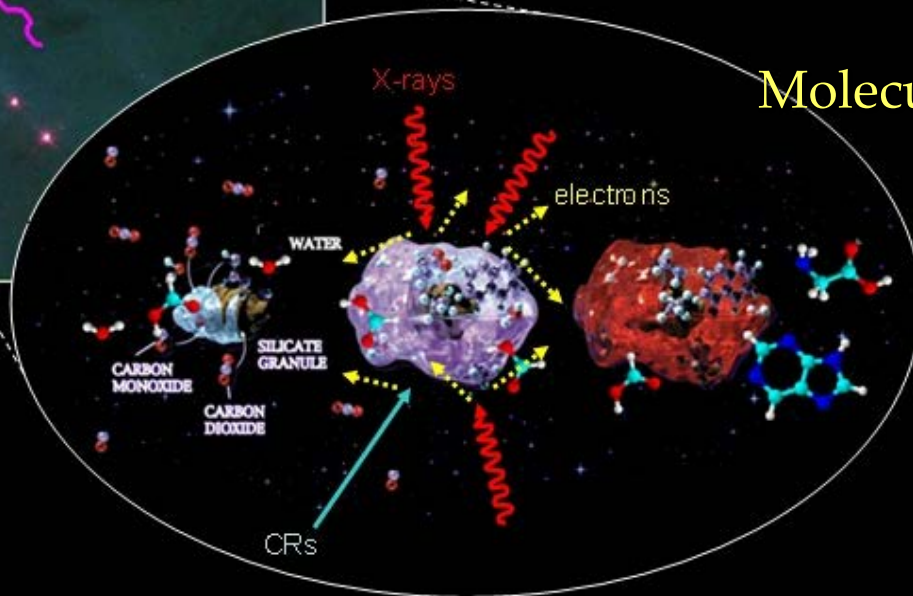
Sol,  
Galáxia,  
Magnetosfera.



Star-Birth Clouds · M16

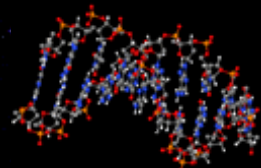
PRC95-44b · ST ScI OPO · November 2, 1995  
J. Hester and P. Scowen (AZ State Univ.), NASA

HST · WFPC2



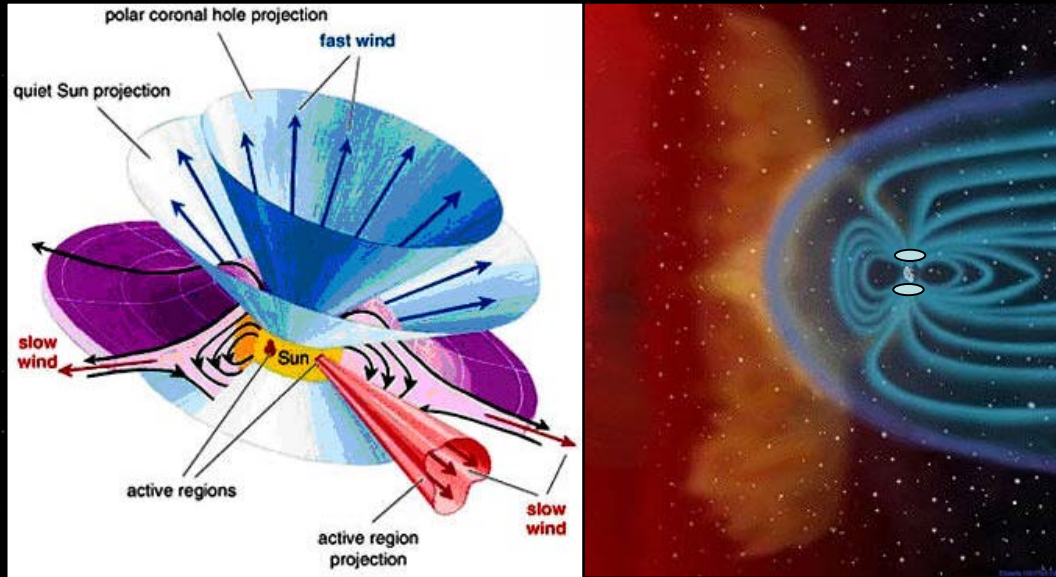
Moléculas complexas!  
- Aminoácidos.

Peptídeos,  
RNA, DNA?





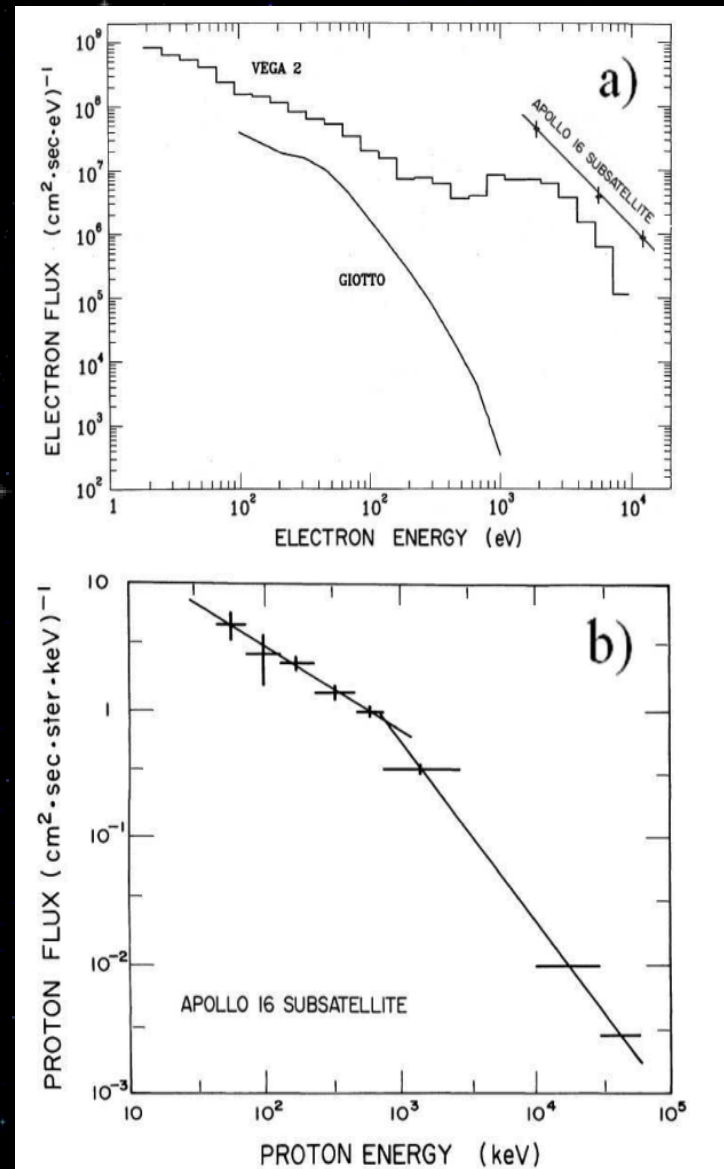
# Vento solar (íons baixa energia)



**Table 1.** Averaged properties of solar wind at 1 au (adapted from Kroll & Trivelpiece 1973, Toptygin 1985 and Zirin 1988).

Properties	Quiet times	Disturbed times
Density <sup>a</sup>	$\sim 10 \text{ ions cm}^{-3}$	$20\text{--}40 \text{ ions cm}^{-3}$
Bulk speed	$\sim 450 \text{ km s}^{-1}$ ( $100\text{--}600 \text{ km s}^{-1}$ )	$\sim 750 \text{ km s}^{-1}$ ( $700\text{--}900 \text{ km s}^{-1}$ )
Ion temperature	$\sim 8 \times 10^4 \text{ K}$	$\sim 3 \times 10^5 \text{ K}$
Proton energy	$\sim 0.6 \text{ keV}$	$\sim 3 \text{ keV}$ ( $1\text{--}10^4 \text{ keV}$ )
Electron energy	$\sim 0.3 \text{ eV}$ ( $0.1\text{--}10^4 \text{ eV}$ )	$\sim 1.5 \text{ eV}$ ( $0.1\text{--}10^4 \text{ eV}$ )
Magnetic field	$3\text{--}8 \times 10^{-5} \text{ G}$	$10\text{--}30 \times 10^{-5} \text{ G}$
Energy flux	$\sim 0.5 \text{ erg cm}^{-2}$	$\sim 15 \text{ erg cm}^{-2}$

<sup>a</sup>95 per cent  $\text{H}^+$ , 4 per cent  $\text{He}^{++}$  and traces of C, N, O, Ne, Mg, Si and Fe ions.



**Figure 1.** (a) Electron fluxes in comet Halley measured by the Vega 2 (Gringauz et al. 1986), Giotto (D'Uston et al. 1989) and at lunar orbit measured by APOLLO 16 subsatellite (adapted from Lin et al. 1974). (b) The proton energy spectrum due to solar wind at lunar orbit measured by APOLLO 16 subsatellite (Lin et al. 1974).

# Raios cósmicos e partículas energéticas do vento solar

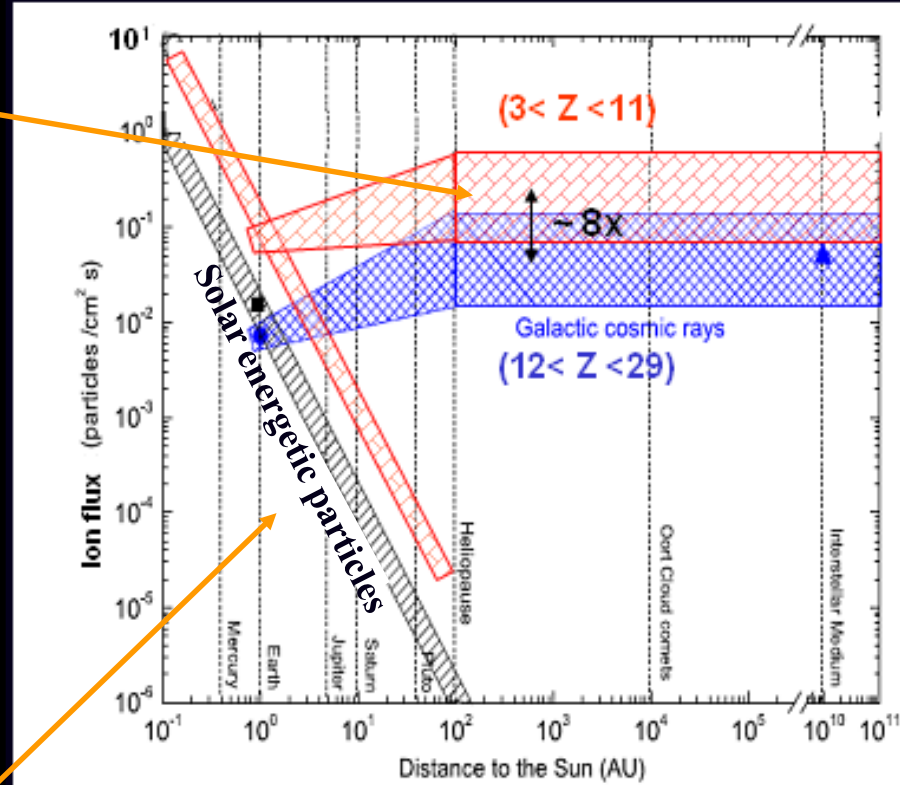
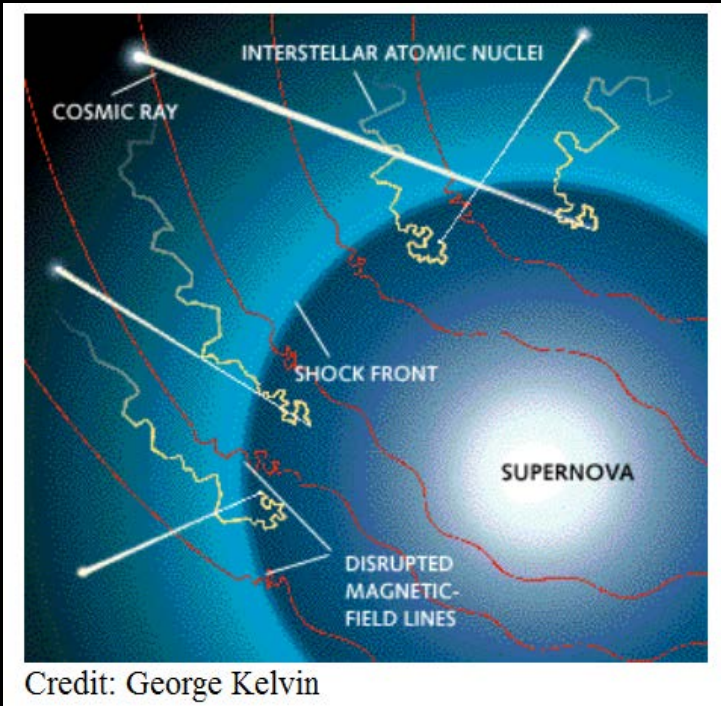
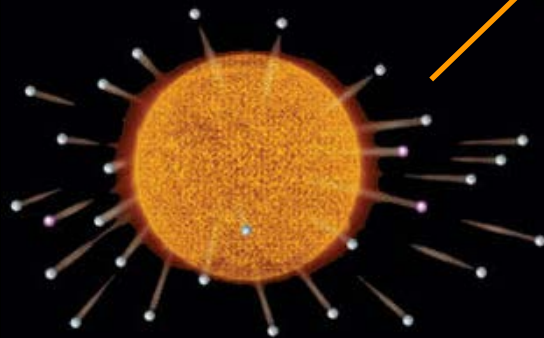
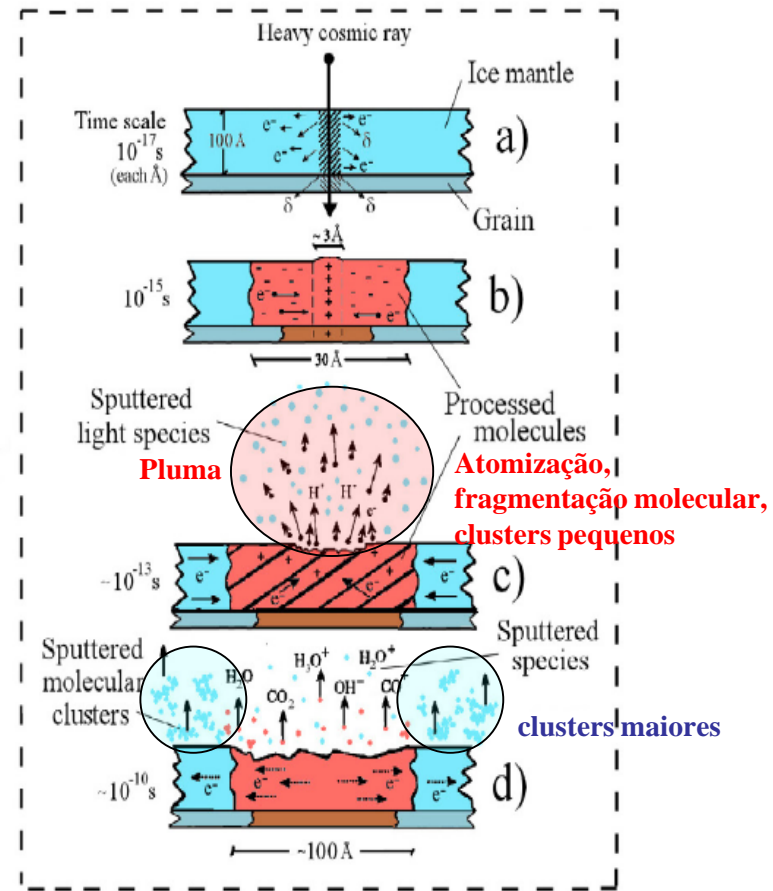
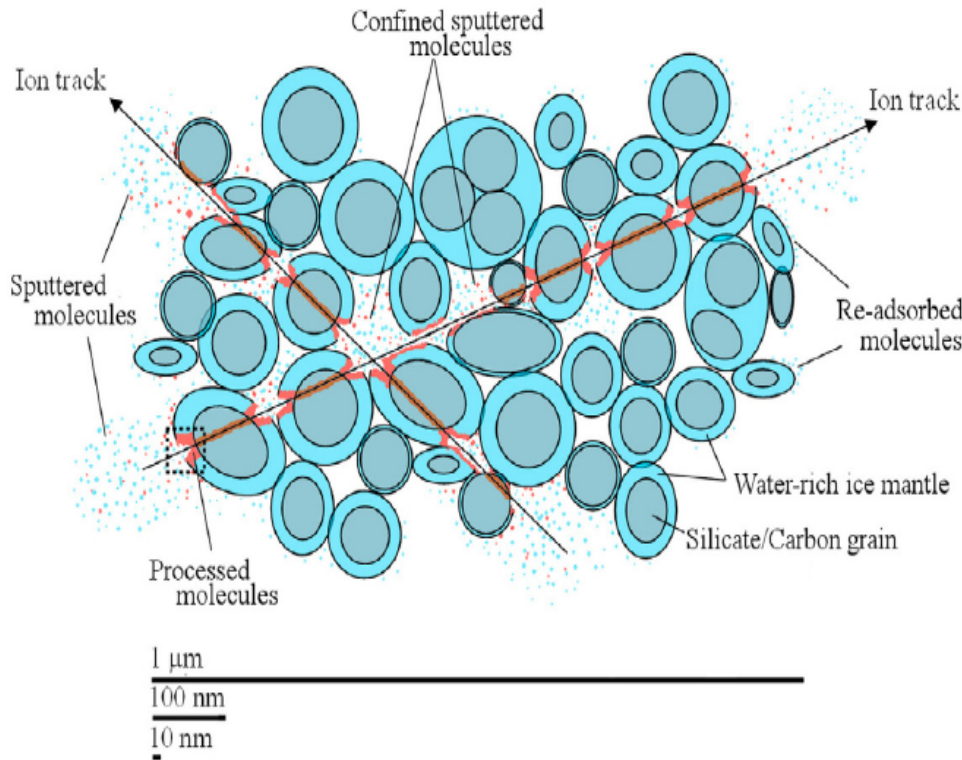


Fig. Estimated value of the integrated ion flux ( $3 < Z < 11$ ) and ( $12 \lesssim Z \lesssim 29$ ) with energy between 0.1-10 MeV/u inside solar system and at interstellar medium as a function of distance to the Sun. Both Galactic cosmic rays and solar wind particles are displayed. Square: integrated flux of solar wind ions. Circle and triangle: integrated flux of cosmic rays.



# Typical dense cloud grain

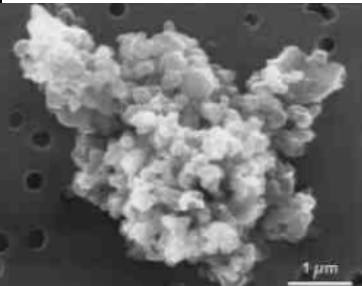


**Fig. 7.** Schematic view showing the interaction between a heavy-ion cosmic ray and a typical interstellar grain inside dense clouds. The ion track along the coagulate sub-micron size grains, the grain mantles, the processed and the sputtered molecules are indicated. Figure insets were adapted from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

Pilling et al. 2010, A&A

Radiólise  $\rightarrow$  Elétrons secundários  $\rightarrow$  Energia extra no sistema.

Atomização, moléculas novas, sputtering, clusters



Dust grain or IDP, interstellar dust particle  
Credit: UWSTL, NASA Hubble

# D) Como essas moléculas são detectadas?

## Telescópios Infravermelhos (bandas vibracionais)



GEMINI Sul (8.1m)



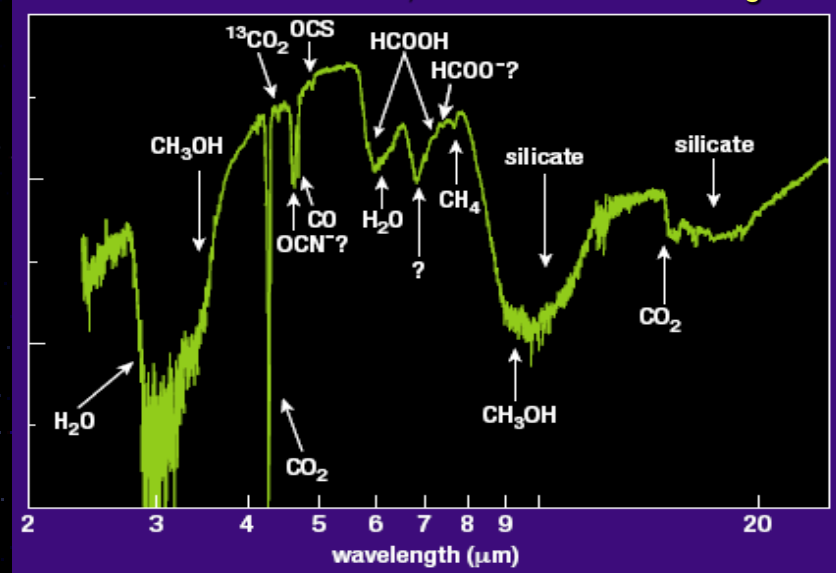
SPITZER

ISO

SOAR (4.2m)



W33a, Proto estrela – Gelo orgânico!



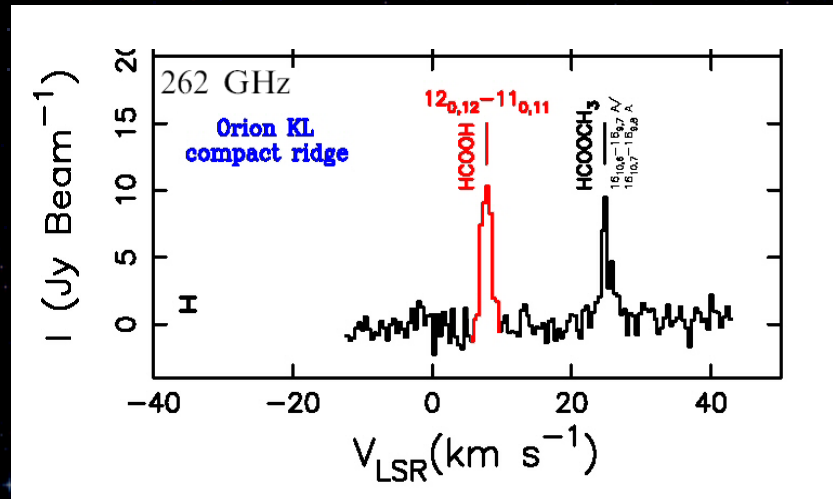
## Radiotelescópios (linhas rotacionais e ro-vibracionais)



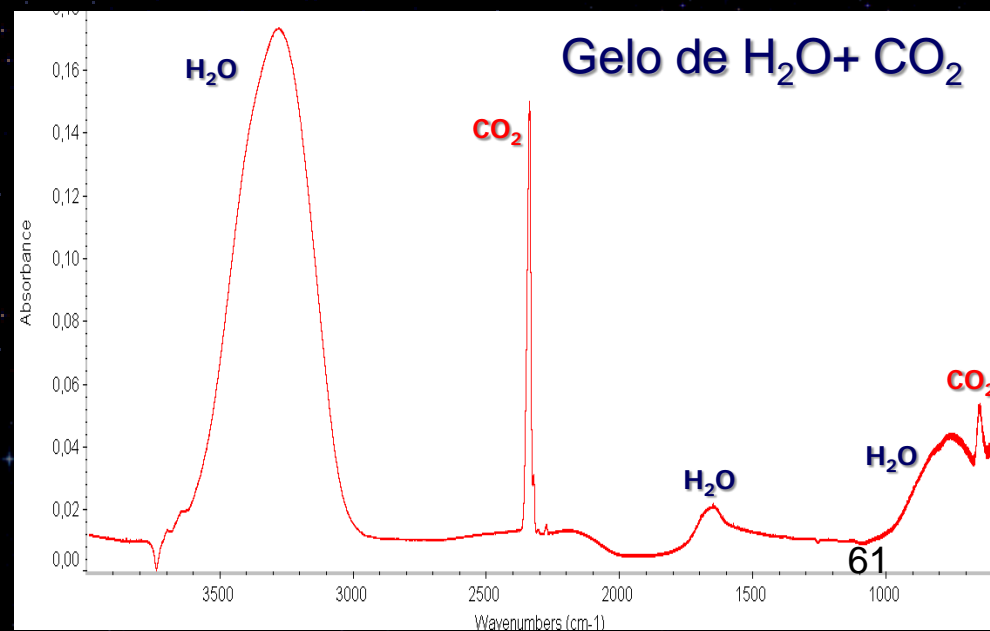
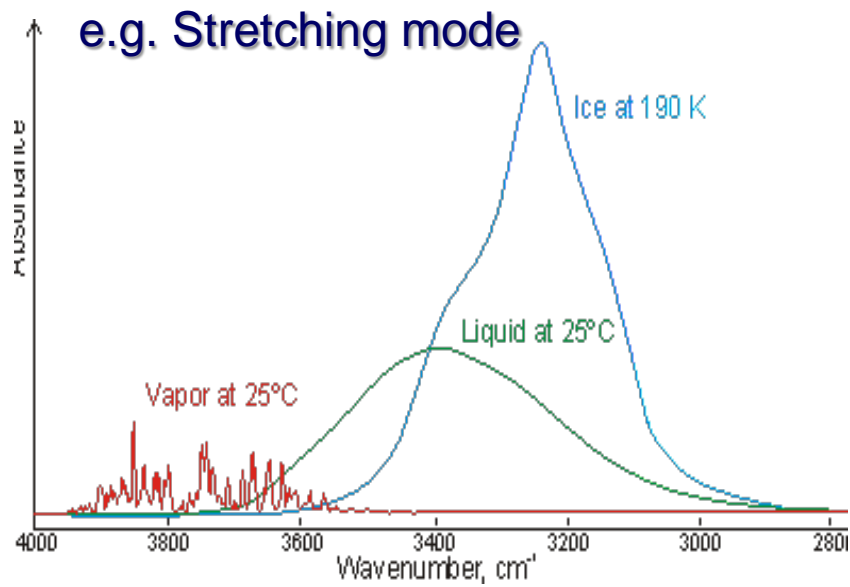
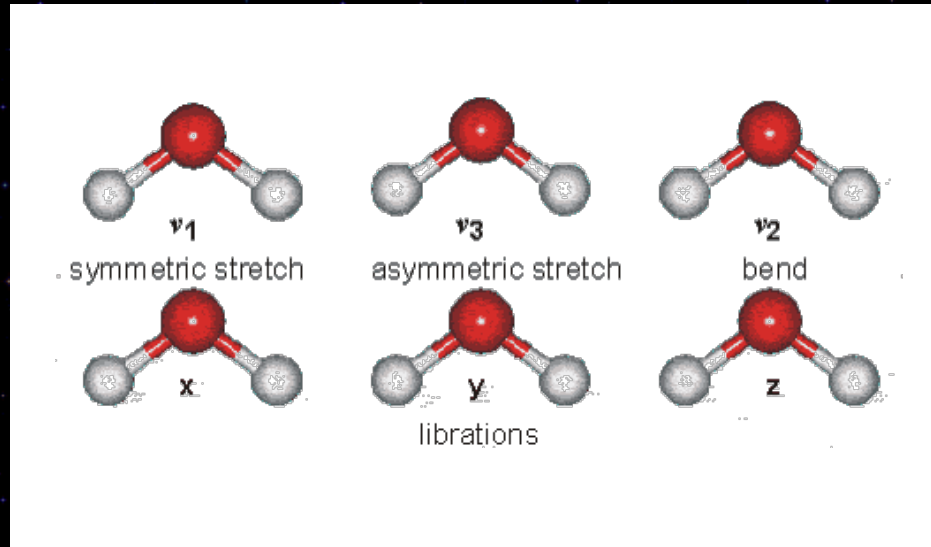
VLA



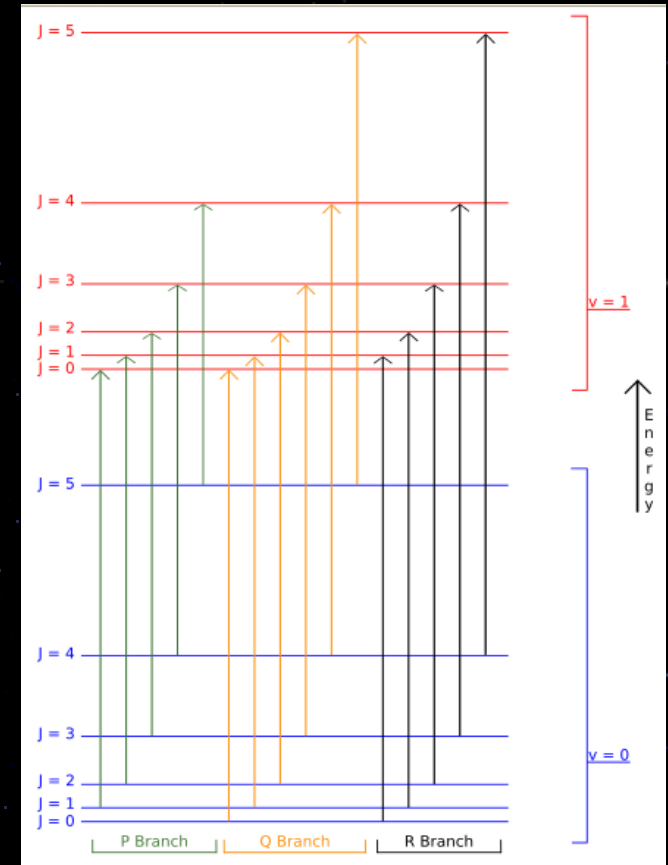
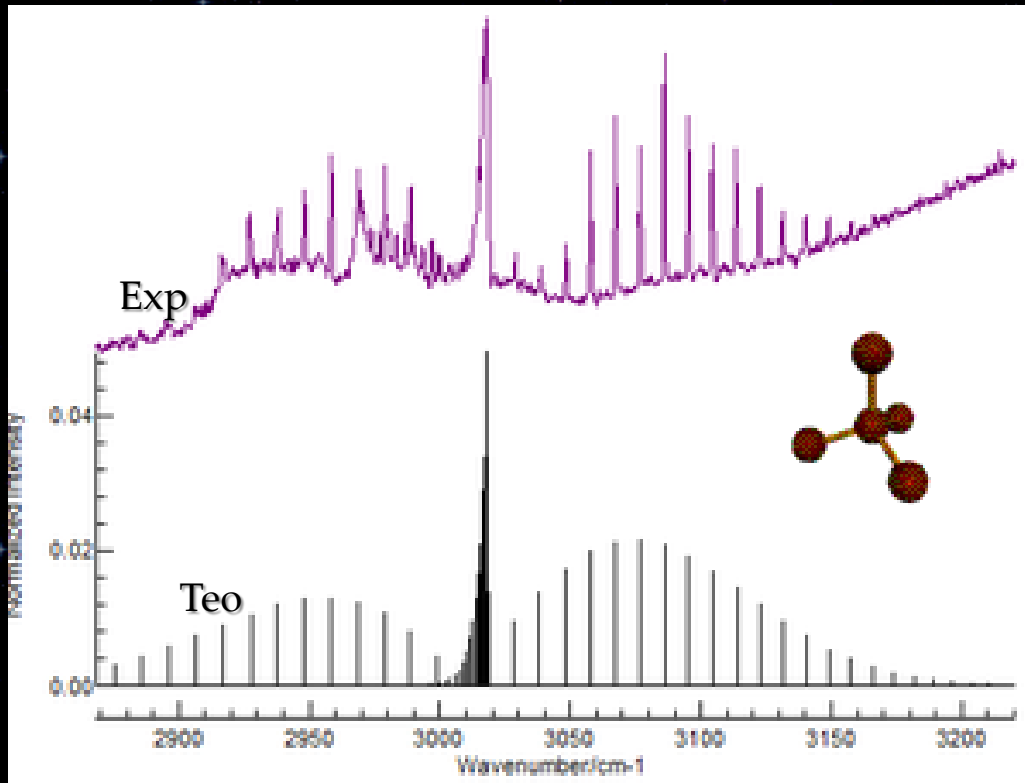
Itapetinga, SP



# Espectroscopia Molecular no IR – Bandas vibracionais (GELO)

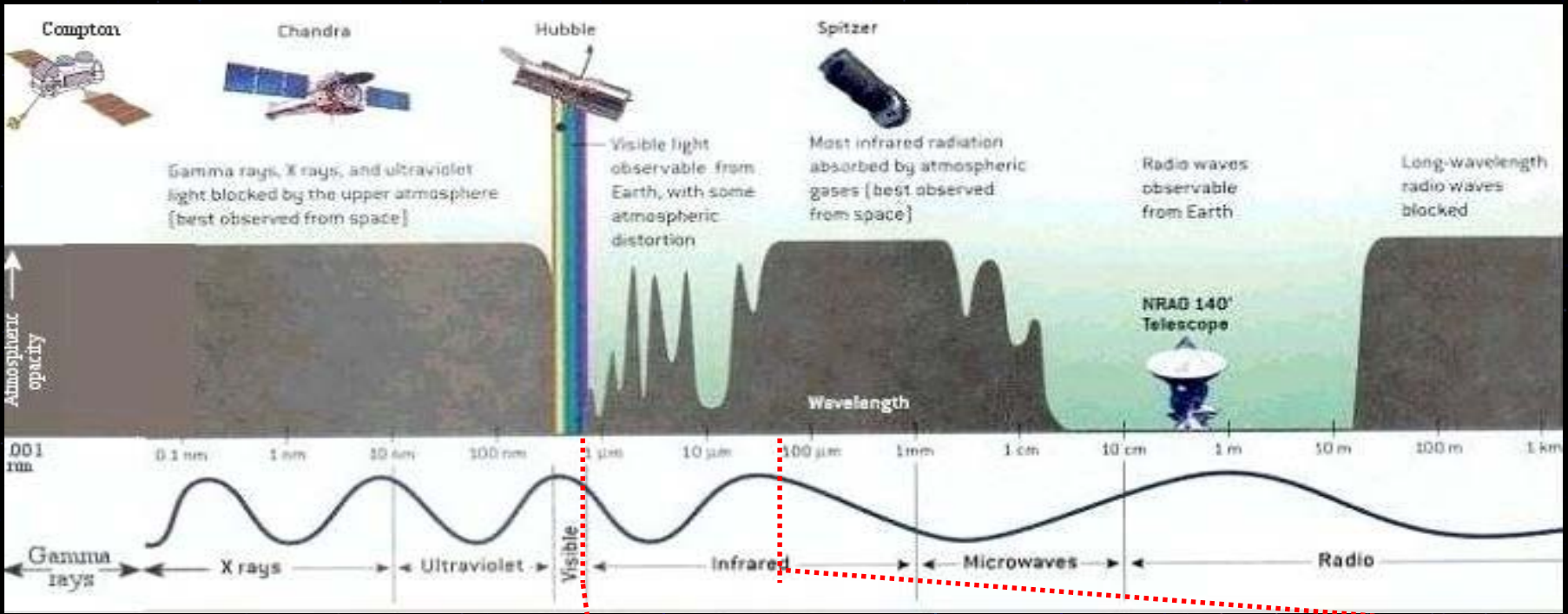


# Espectroscopia Molecular no microondas/rádio – Bandas rotacionais-vibracionais e bandas rotacionais (FASE GASOSA)

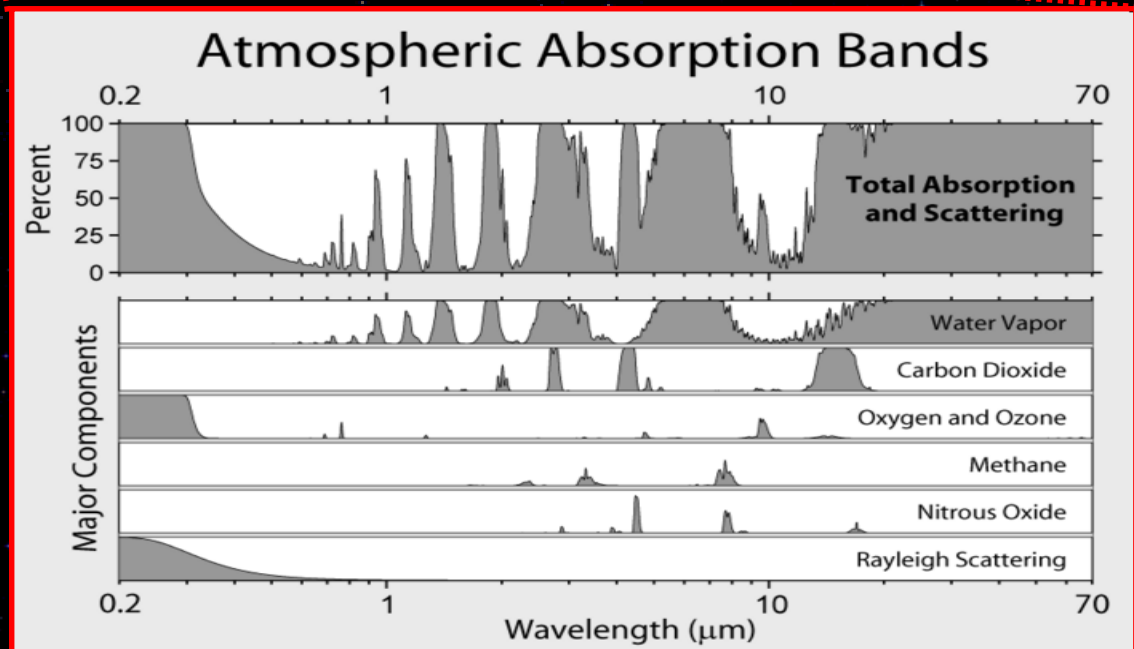


<http://web.mit.edu/5.33/www/lec/spec5.pdf>

[http://www.ias.ac.in/initiat/sci\\_ed/resources/chemistry/rotational.pdf](http://www.ias.ac.in/initiat/sci_ed/resources/chemistry/rotational.pdf)



# Absorção da radiação pela atmosfera



# Observatórios IR



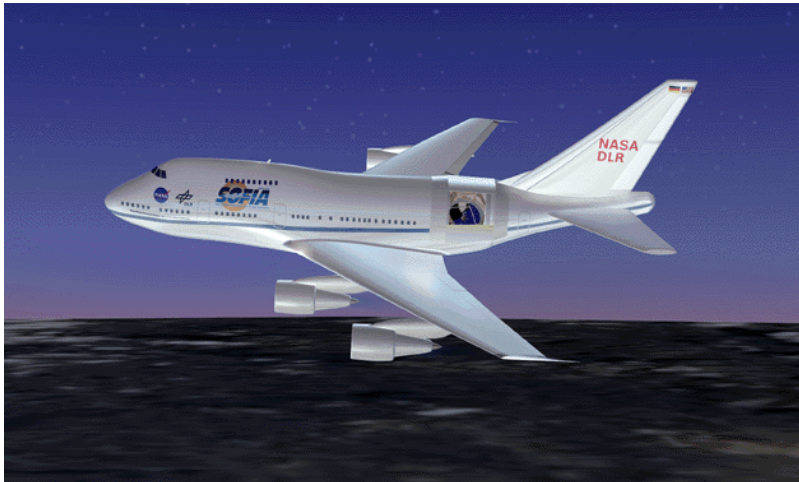
Gemini (Hawai e Chile)



SOAR (Chile)



UKIRT – Hawai



SOFIA (nasa)



VLT (Chile) – Interferometria

Coisa em comum?  
Grandes altitudes.



# Telescópios espaciais e Sondas



IRAS (1983)

ISO (1995-1998)

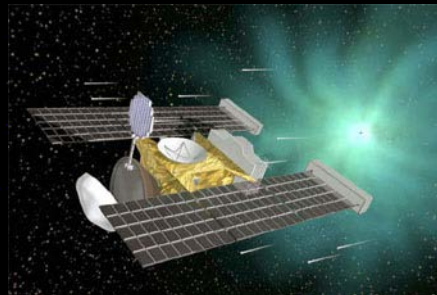


Spitzer (2003-2009)

## Spacecrafts



HST(1999, ...)

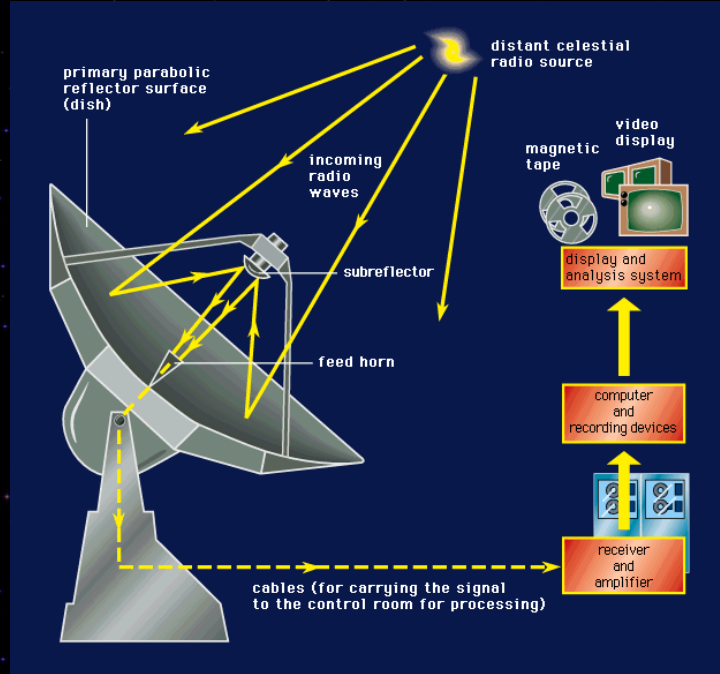


Ex. Stardust, Cassini, Mars Rovers

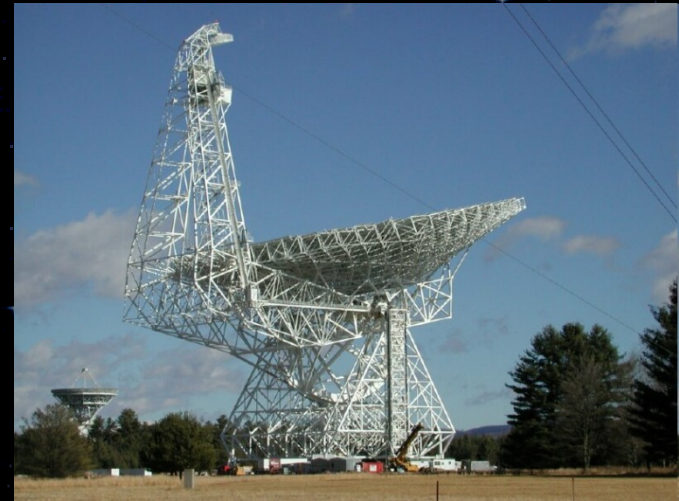
# Observatórios na faixa de microondas e rádio



Single Dishes



305-meter Arecibo

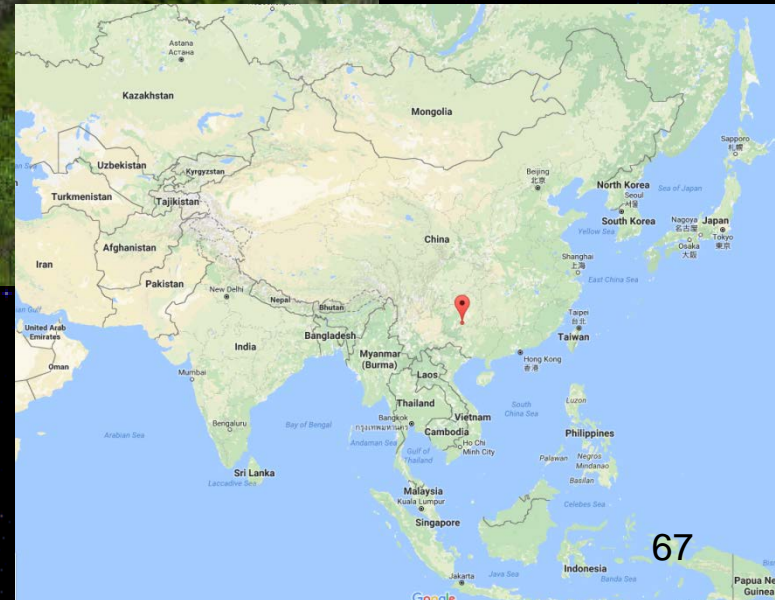


100-Meter Green Bank Radio Telescope

# Radio telescópio FAST, China (Maior do mundo, 500m diâmetro)

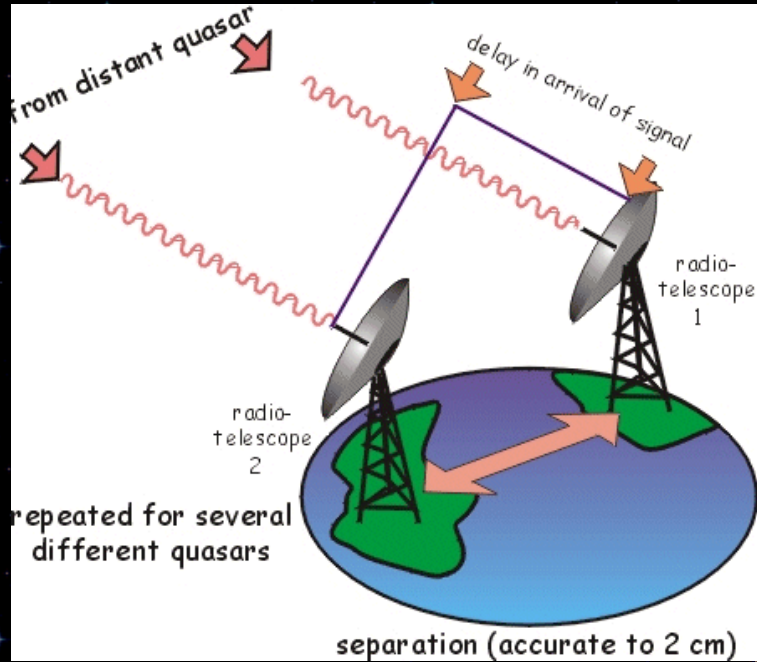


FAST's surface is made of 4450 triangular panels (11 m side)  
Pointing: anywhere within  $\pm 40^\circ$  from the zenith  
Working frequency range: 70 MHz to 3.0 GHz.



# Observatórios na faixa de microondas e rádio

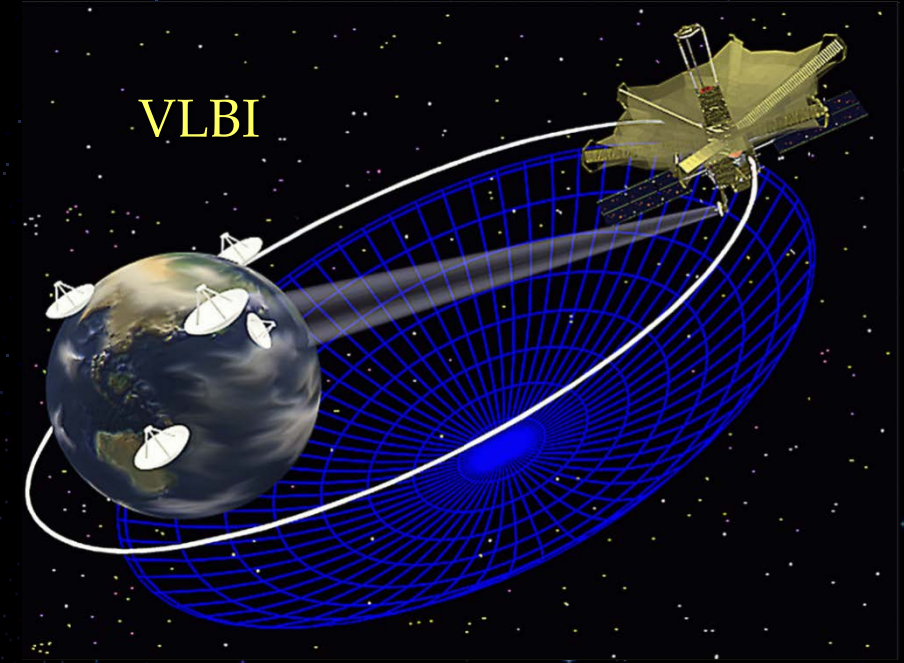
## Multi-dishes Interferometry



VLA

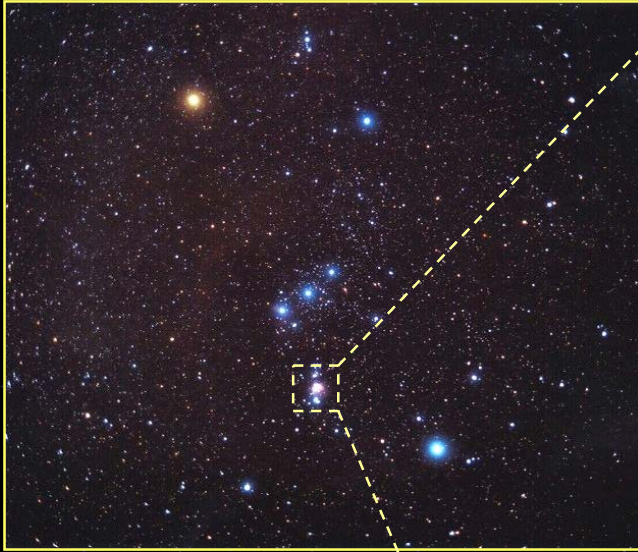


Austrália

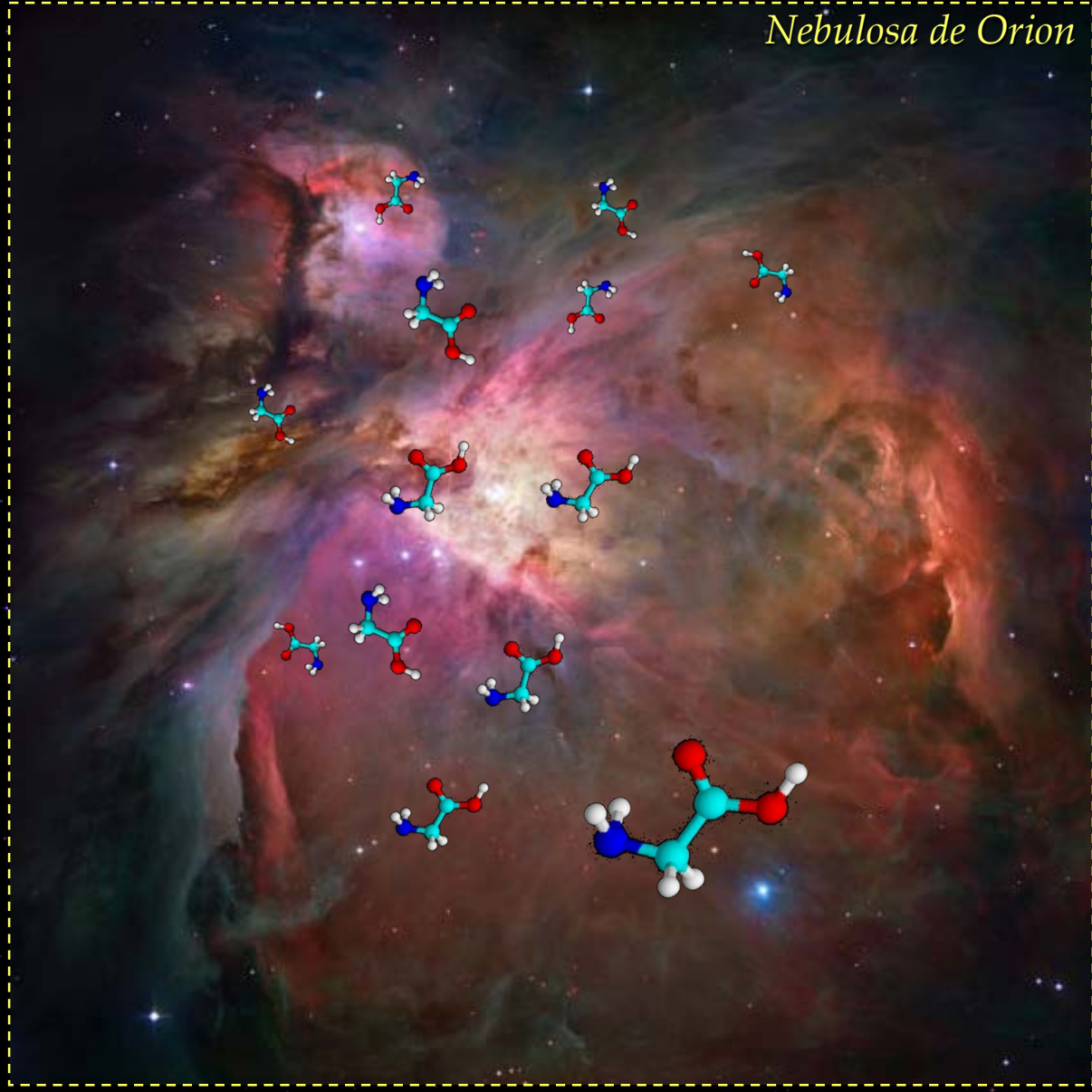
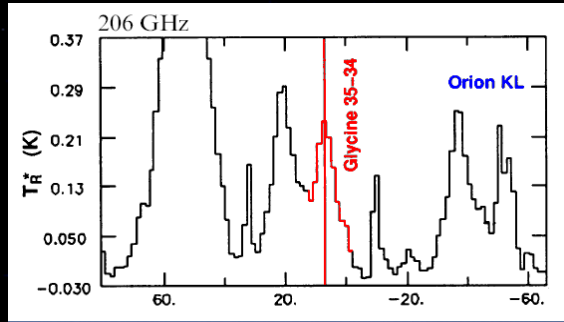


VLBI

# Nuvens moleculares: berçário estelar

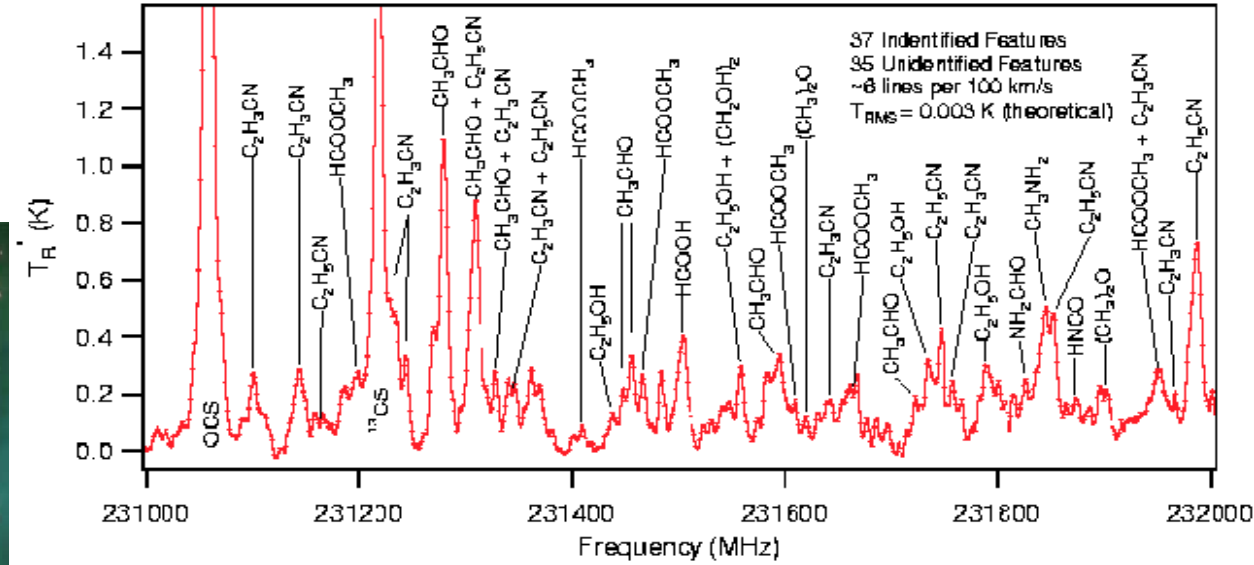


# Nuvens moleculares: berçário estelar



# Aonde mais essas moléculas são encontradas?

Gaseous Pillars – Eagle Nebula



Sgr B2 with ALMA

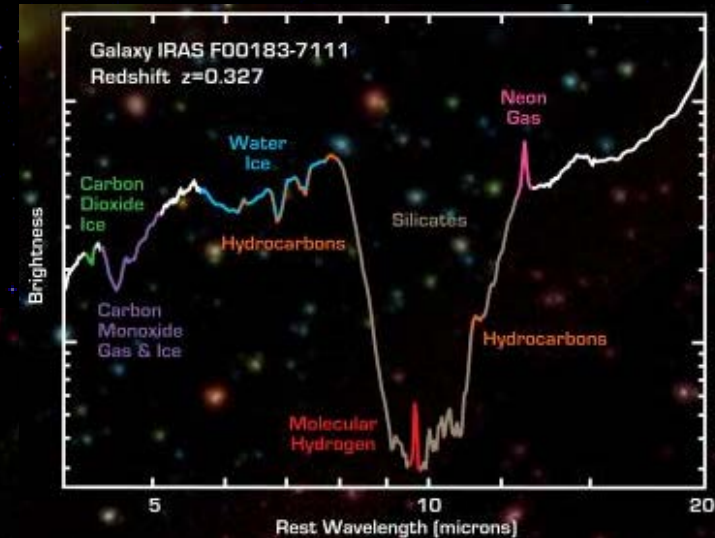
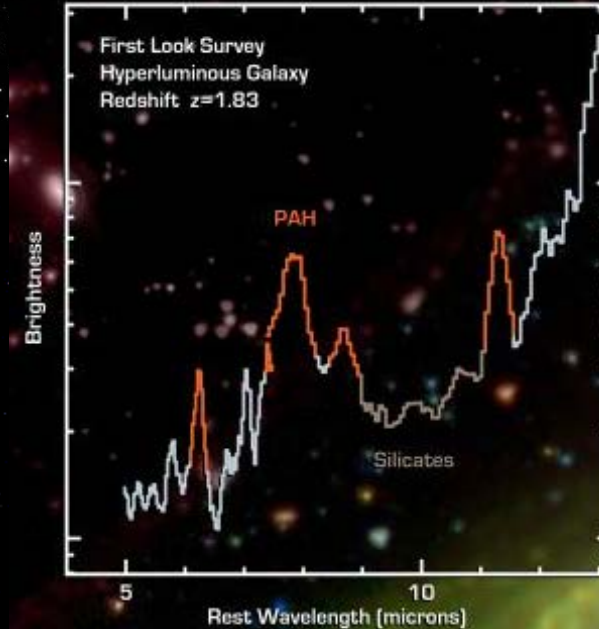


# Moléculas em Galáxias distantes.

1ª moléculas orgânicas (idade do universo ~2 -3 bi anos)



Telescópio espacial  
SPITZER

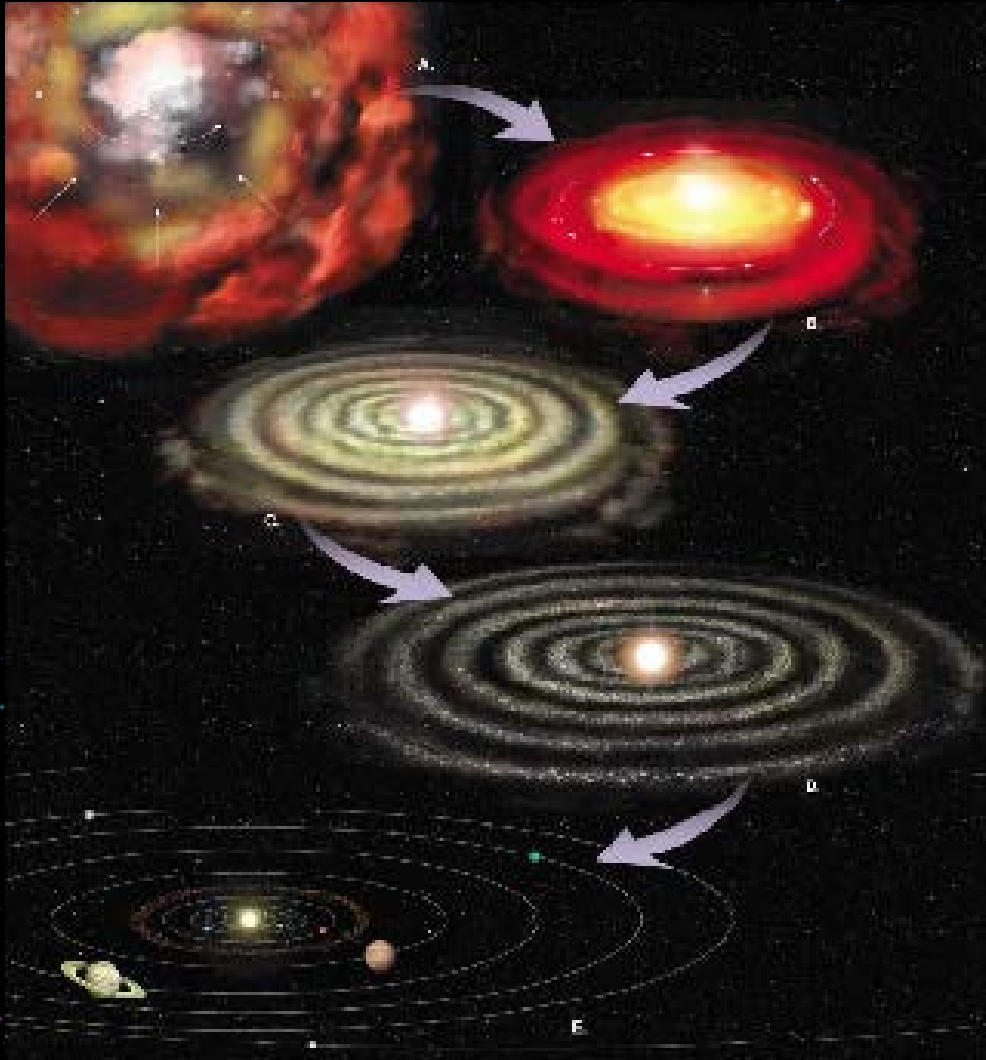


Moléculas orgânicas em galáxias distantes!

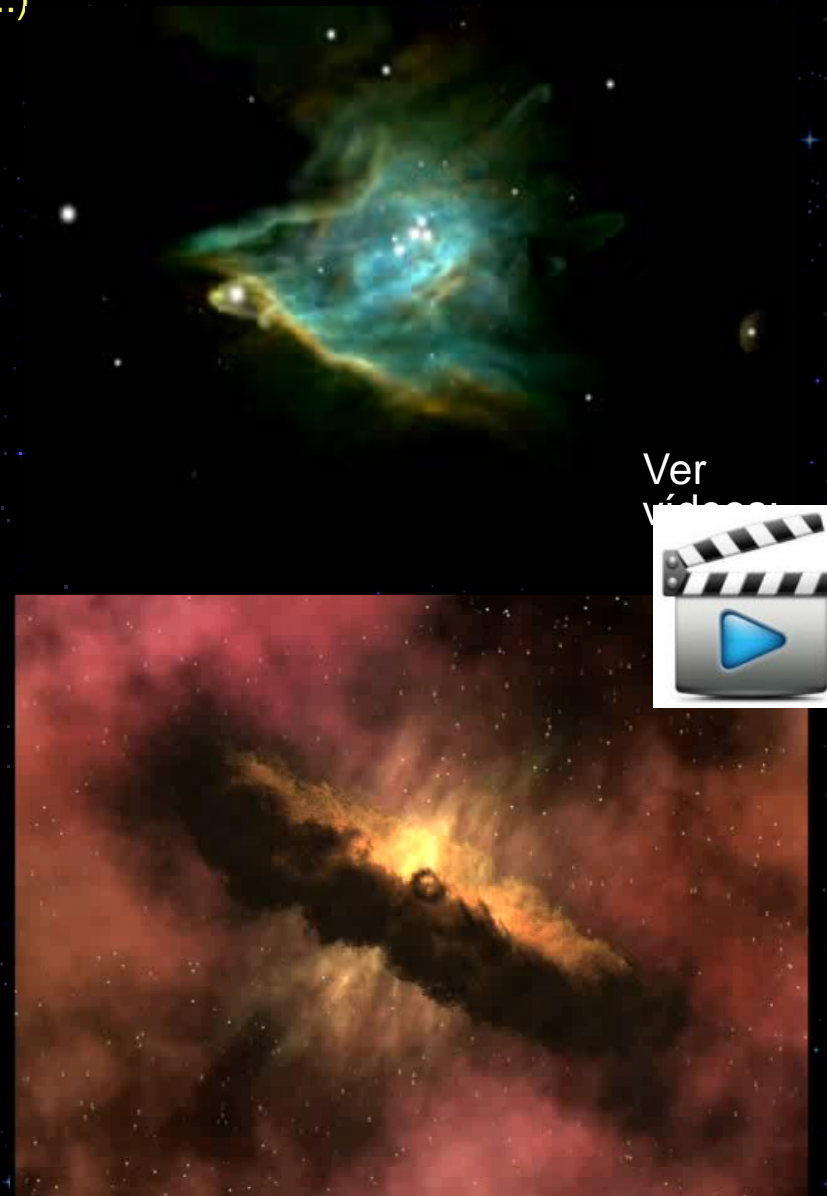


# Moléculas em discos protoestelares (gás e gelos)

Nuvem de átomos (ex. H, He, C, N, O, ...) e moléculas (ex. H<sub>2</sub>, silicatos, água, CO, CO<sub>2</sub>, etanol, acetona, amônia, ....)



Sistemas planetários, cometas, etc.



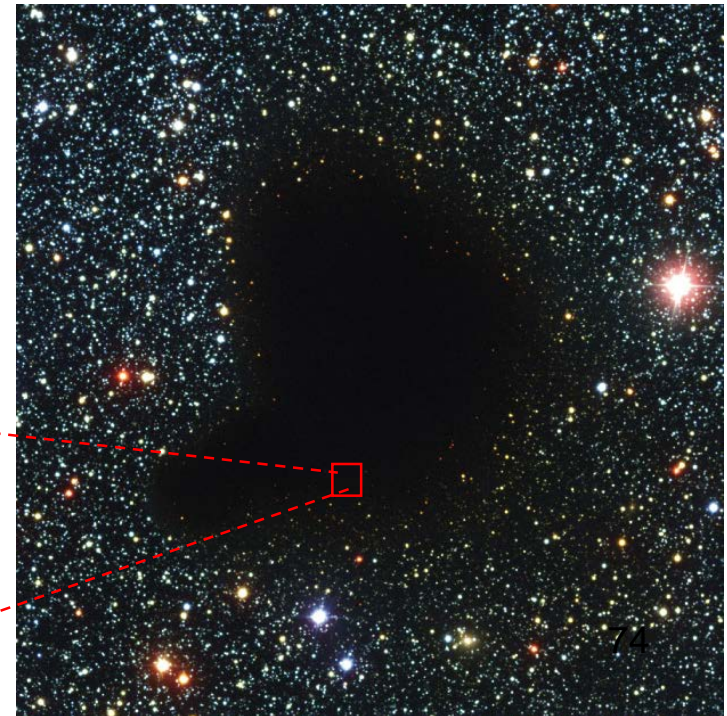
# Moléculas em discos protoestelares e nuvens densas

- Grãos de poeira fria: núcleos de silicatos/carbono + cobertura de moléculas voláteis condensadas (H<sub>2</sub>O, CO, N<sub>2</sub>, NH<sub>3</sub>, etc...)



Objetos estelares jovens (YSOs) e discos proto planetários ( $N \sim 10^4\text{-}10^8 \text{ cm}^{-3}$ ;  $T \sim 10\text{-}50 \text{ K}$ )

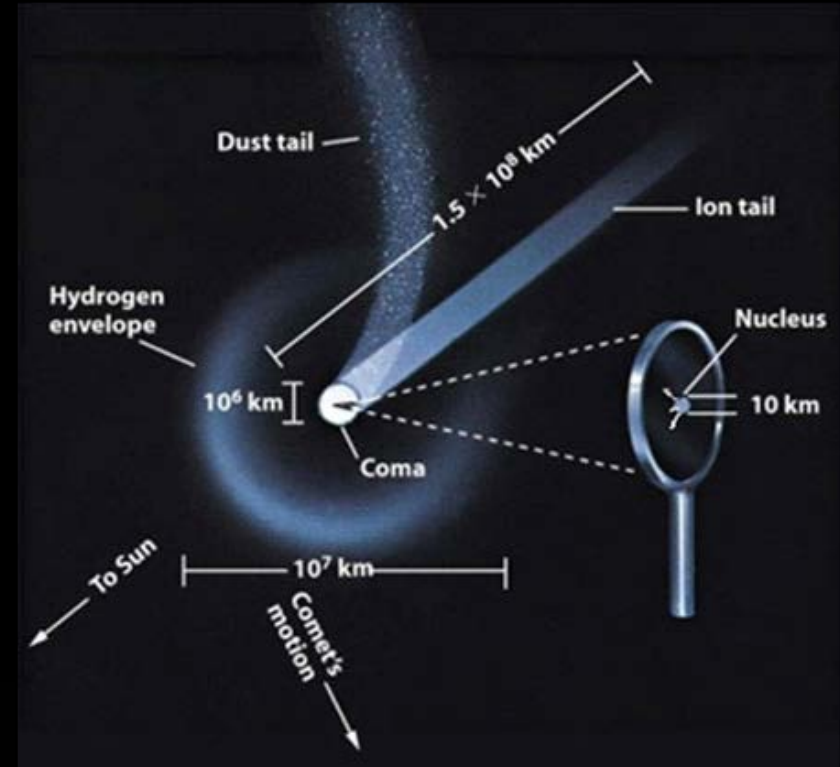
Ver vídeos:



# Moléculas em cometas

Composição básica dos cometas:  
(~80% água. CO, CO<sub>2</sub>, CH<sub>4</sub>, ....)

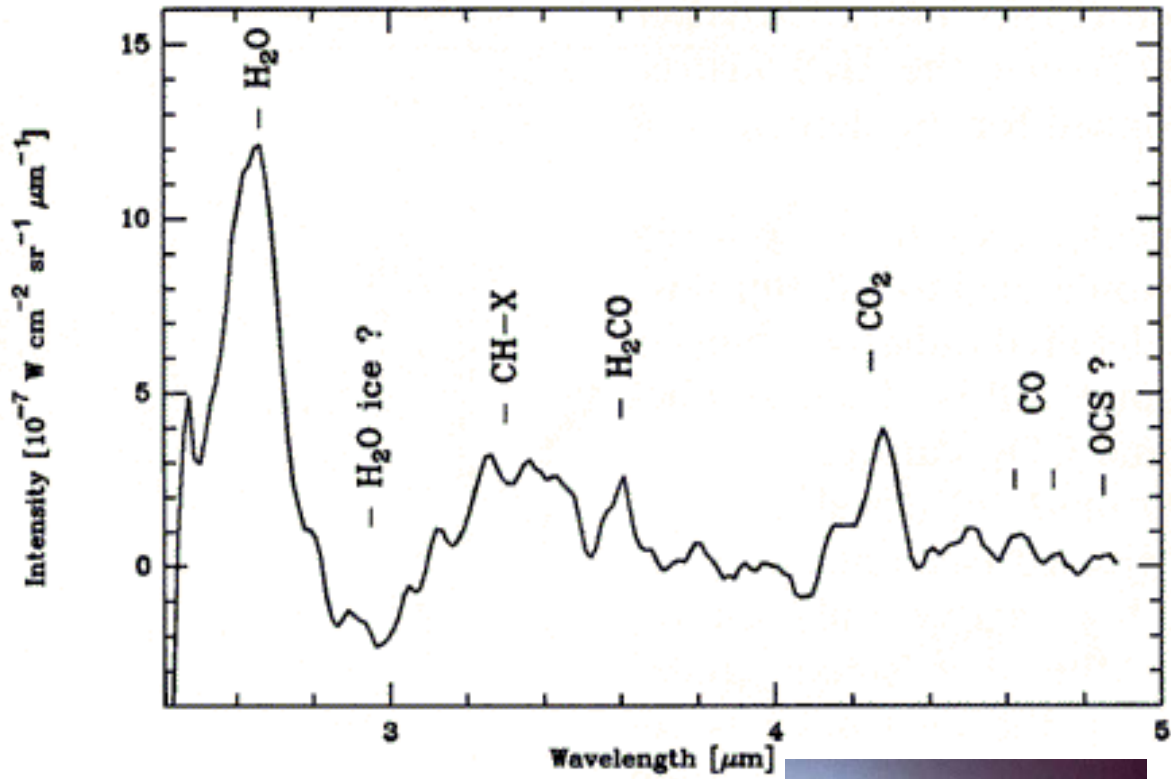
Hale-Bopp



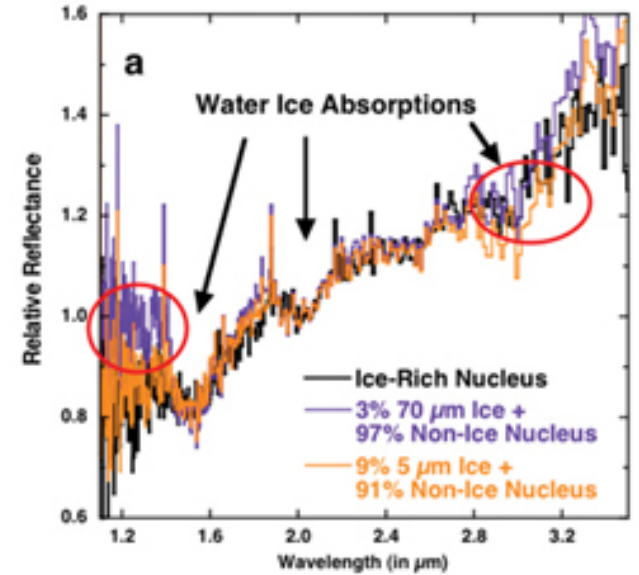
Tempel 1

# Exemplo de Espectroscopia de Cometas no IR

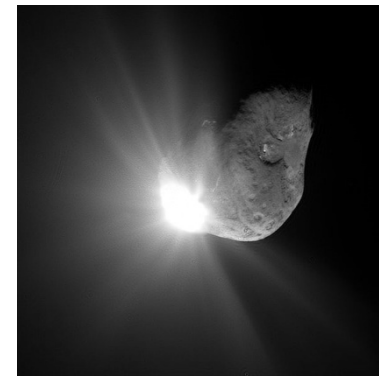
Comet Halley (Combes et al 1988)



Tempel 1 (NASA)  
Deep impact Mission

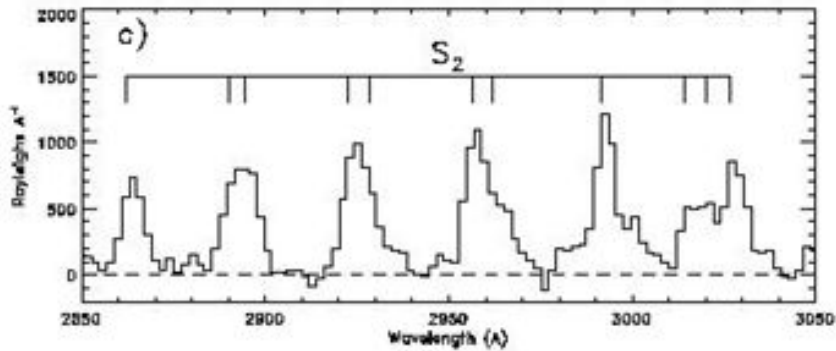
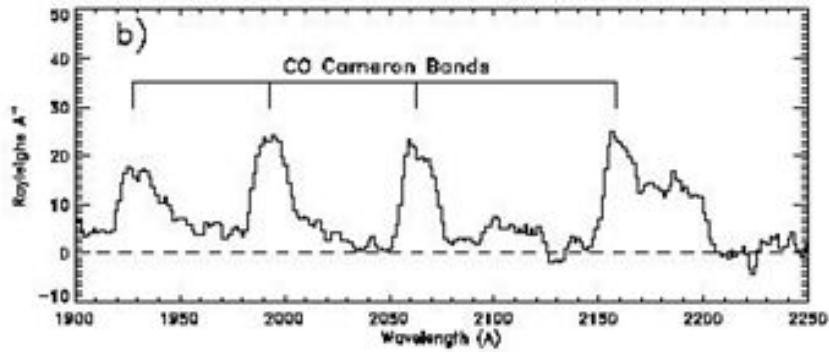
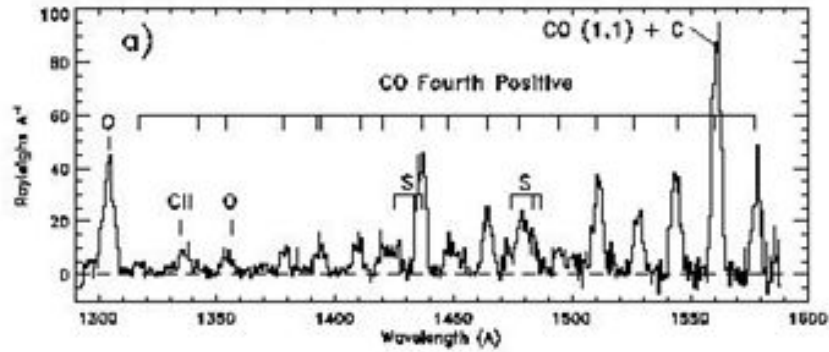


Comet Halley

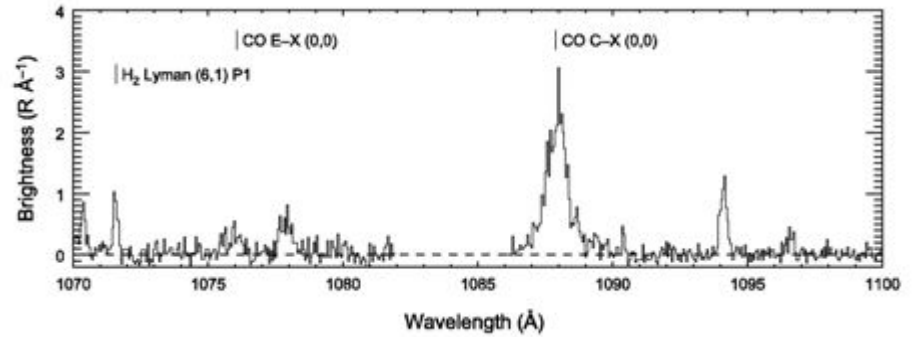


Tempel 1

# Exemplo de Espectroscopia de Cometas no UV



HST Espectro do Hyakutake (C/1996 B2)

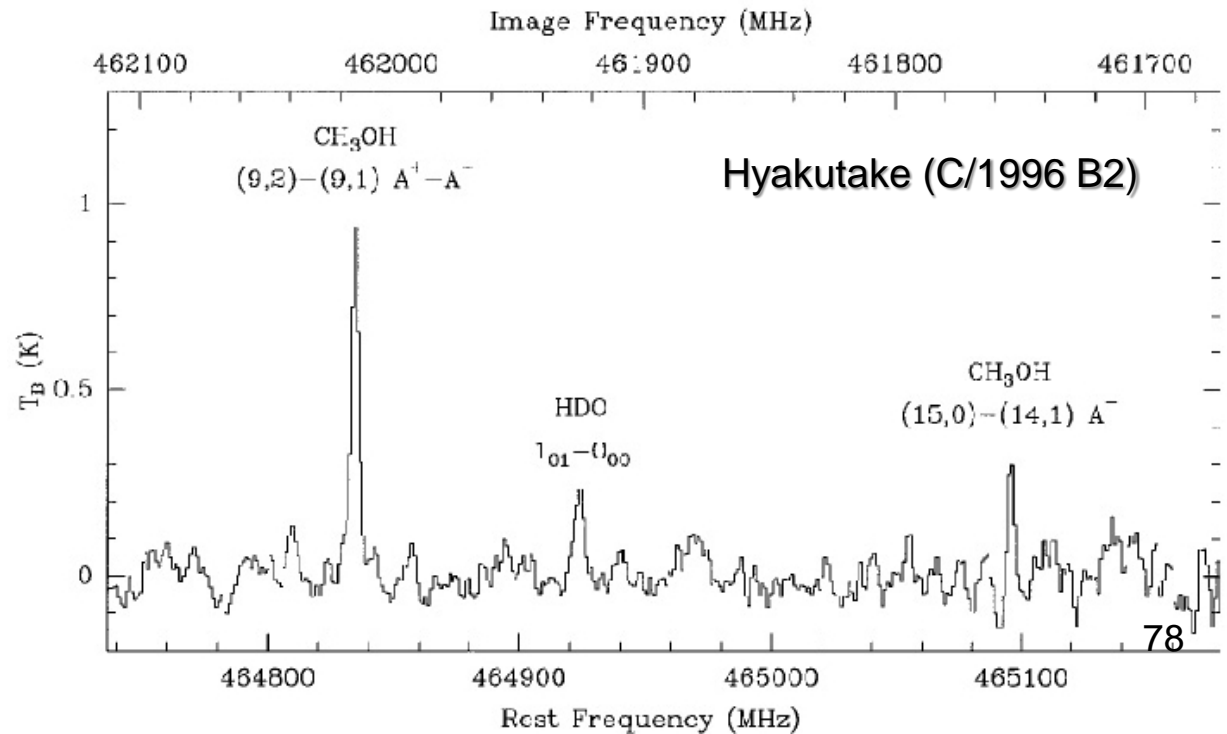
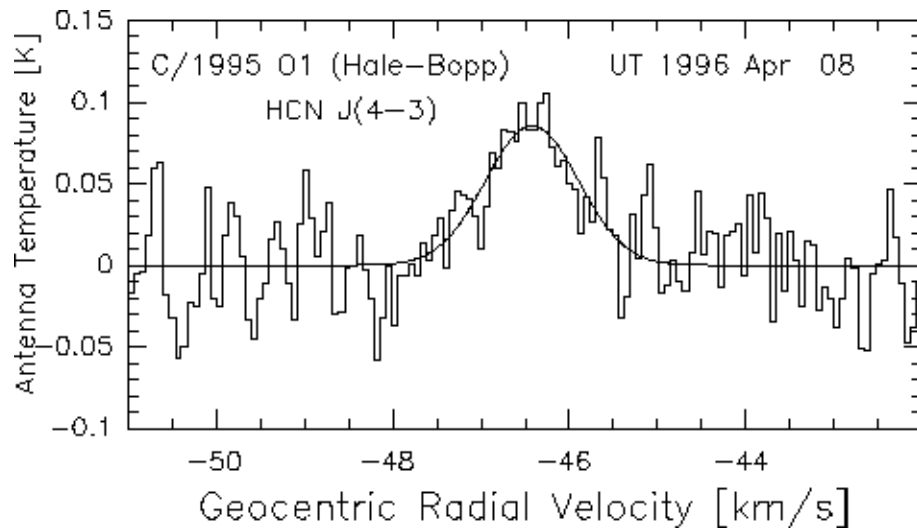


FUSE Espectro do cometa Linear (C/2001 A2)



Hyakutake (C/1996 B2)

# Exemplo de Espectroscopia de Cometas na faixa radio

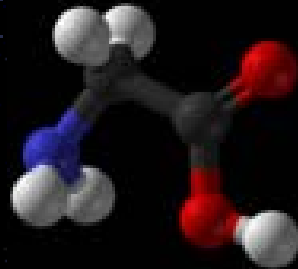
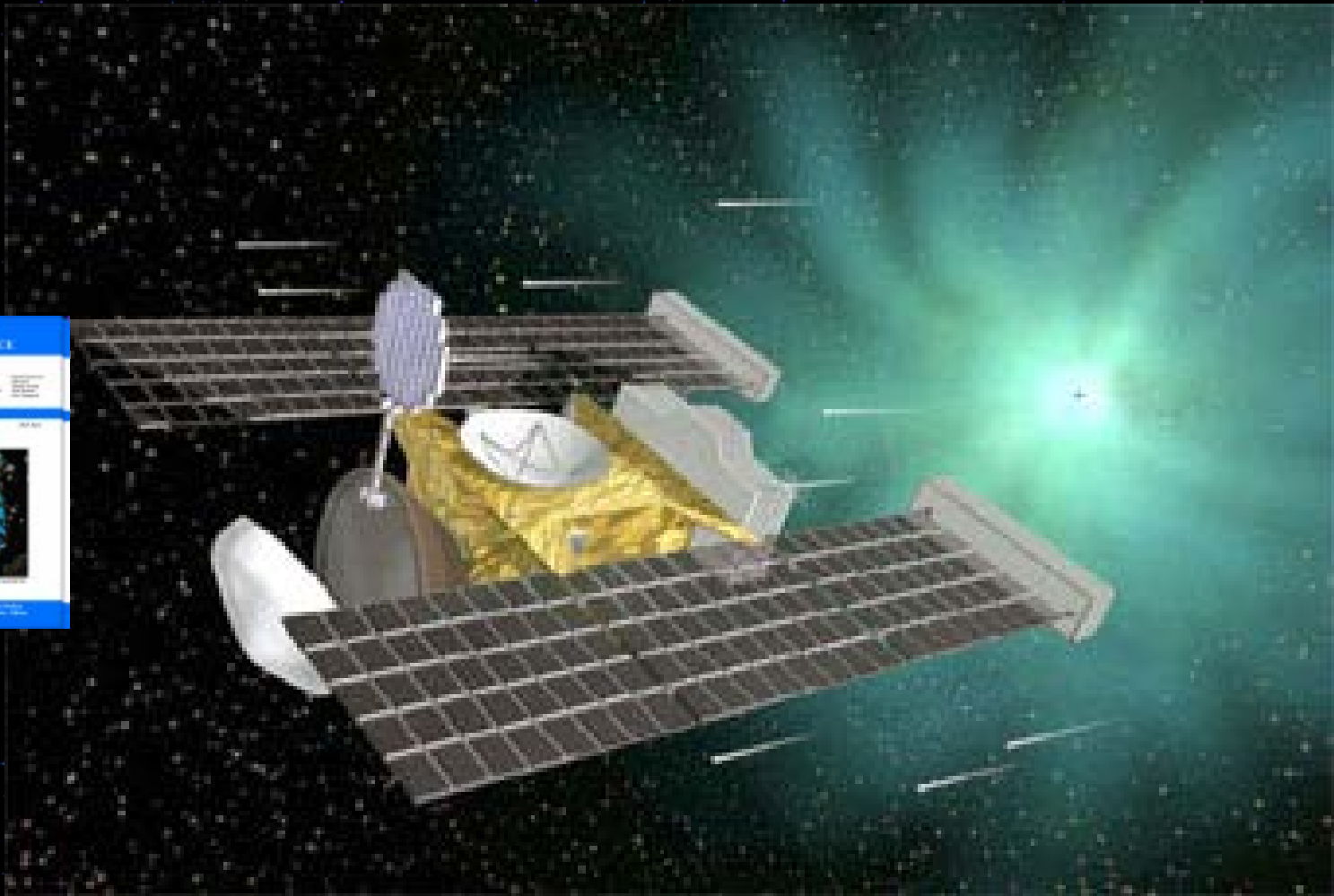


Science

19 December 2008 1113



Stardust



Glicina

# Moléculas em gelos extraterrestres: outras evidências observacionais

## • Luas e Planetas

### Artist impressions of Enceladus

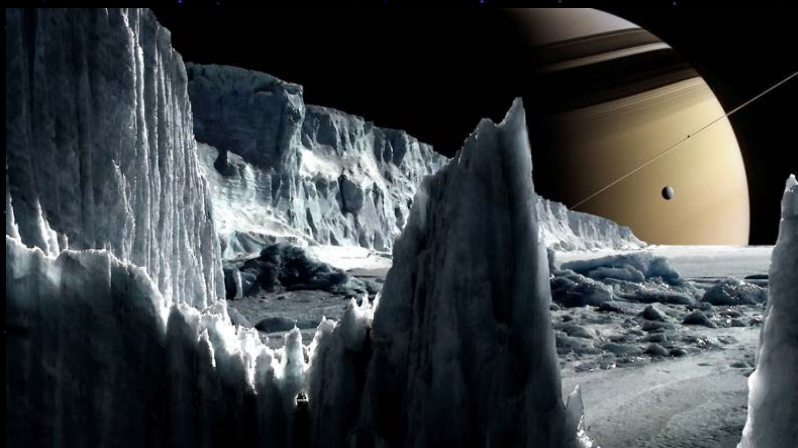
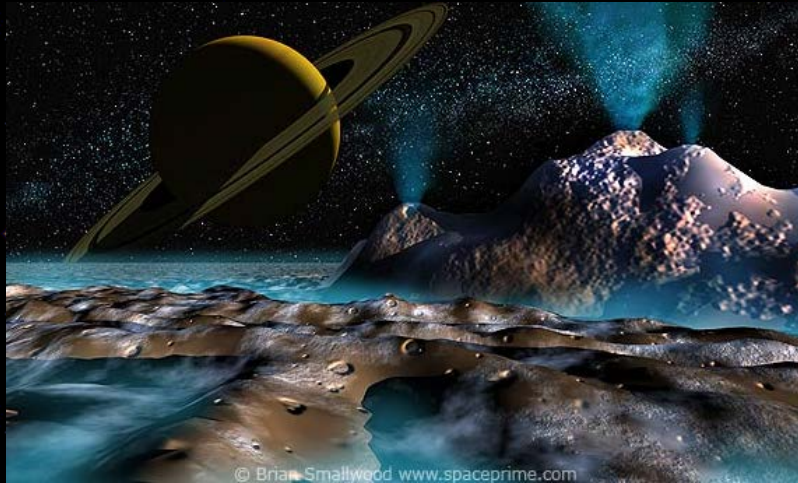


Table 1. Ices in the Solar System.

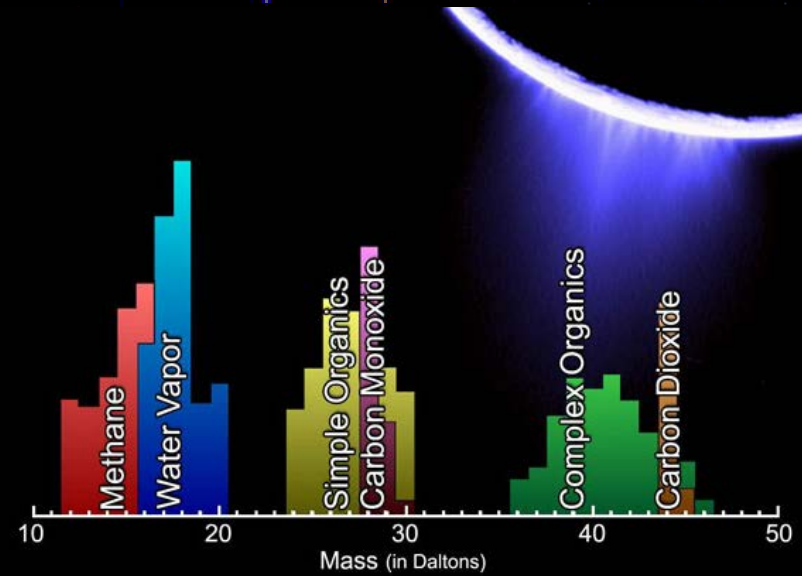
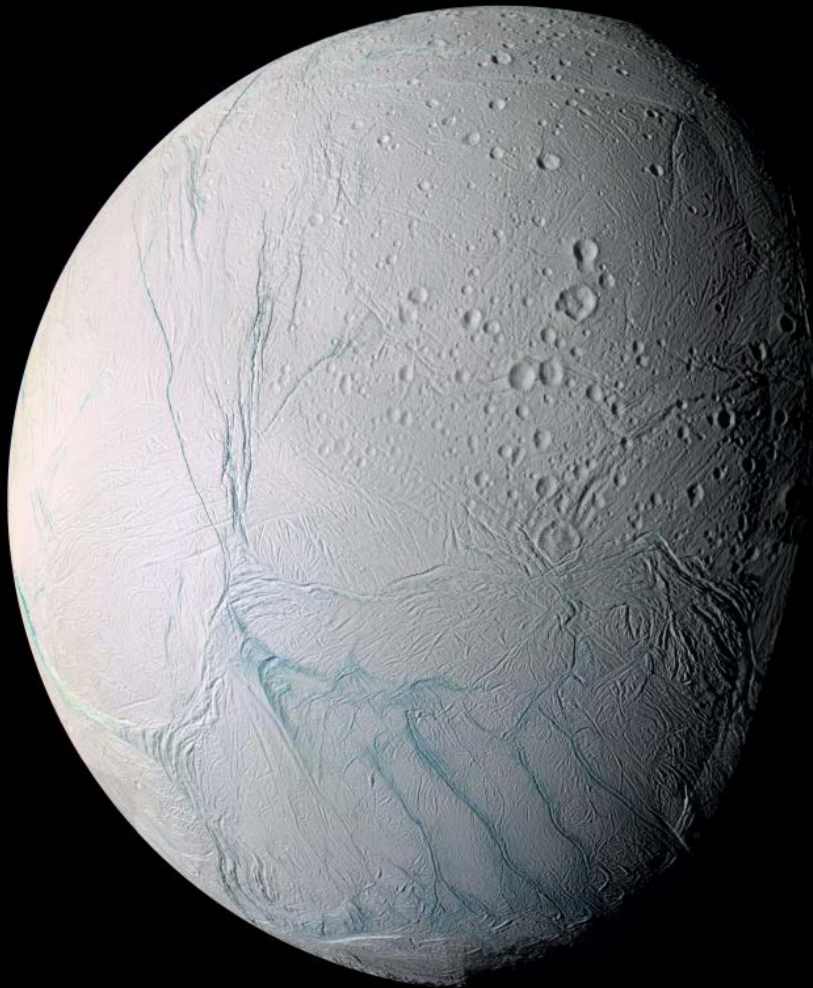
<u>Planet</u> Satellite (Ref.)	Observed Species
<u>Jupiter</u>	
Io	SO <sub>2</sub> , H <sub>2</sub> S, H <sub>2</sub> O
Europa	H <sub>2</sub> O, SO <sub>2</sub> , CO <sub>2</sub> , H <sub>2</sub> O <sub>2</sub>
Ganimede	H <sub>2</sub> O, O <sub>2</sub> , O <sub>3</sub> , CO <sub>2</sub>
Callisto	H <sub>2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



- Luas e Planetas

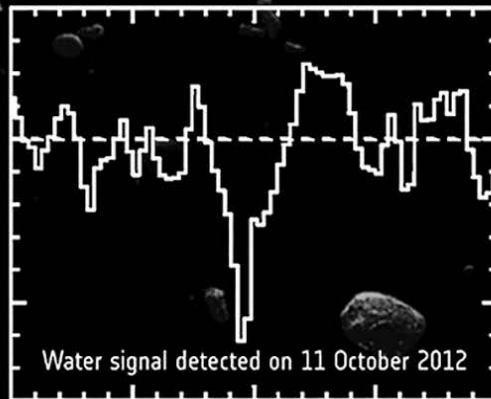
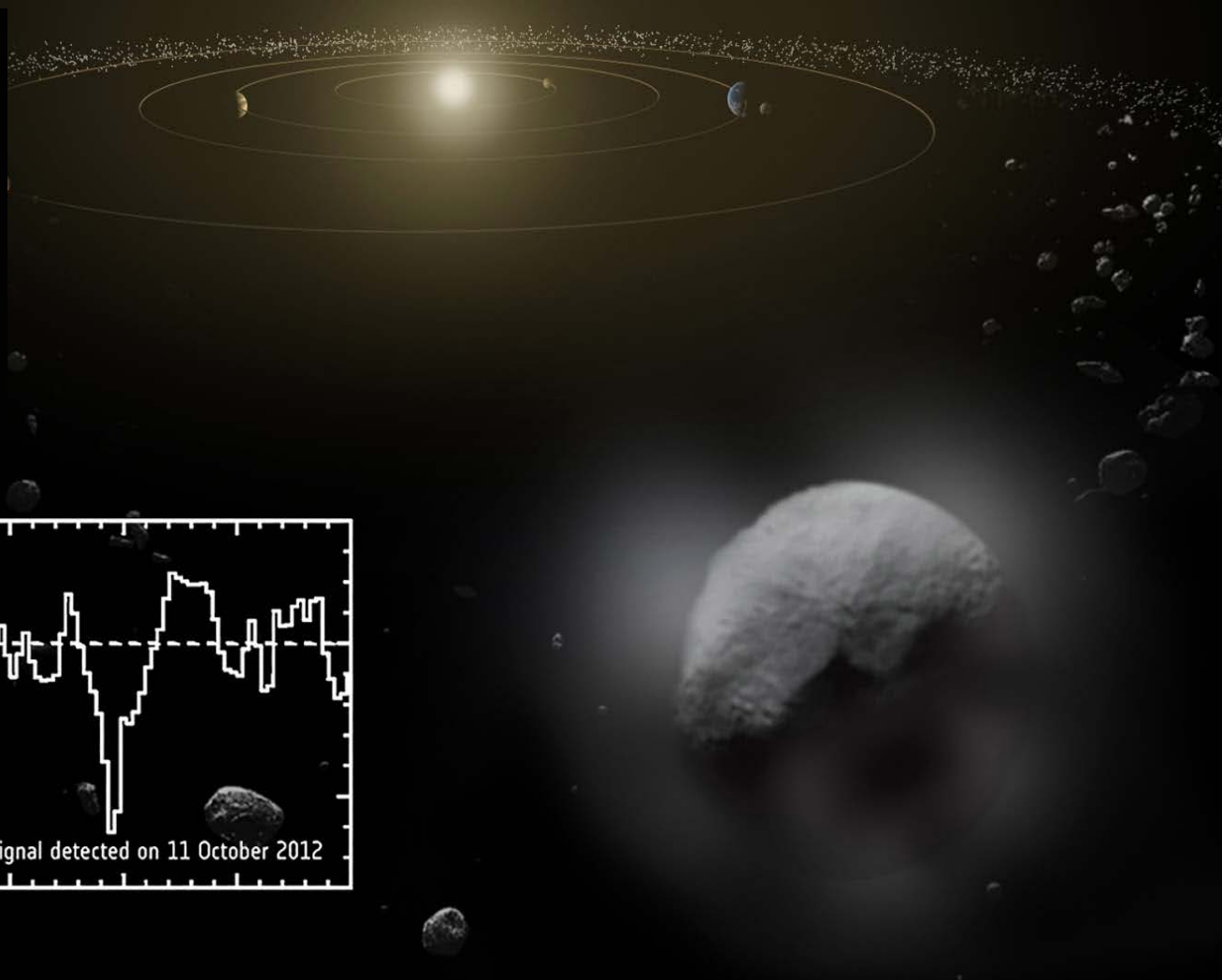
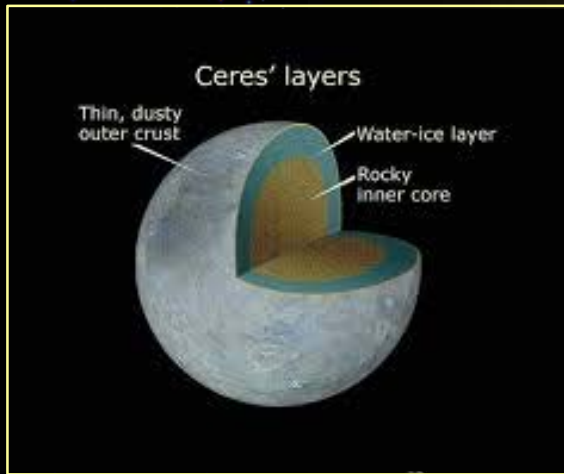
- Enceladus (lua de Saturno).



- Planetas anões

Detecção de água em Ceres (atmosfera tênue de vapor de água)

ESA's Herschel space observatory between 2011 and 2013

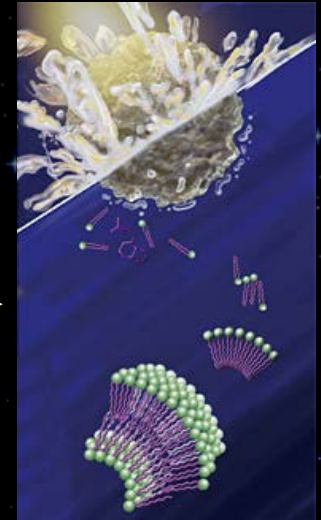


# Aonde mais essas moléculas são encontradas?

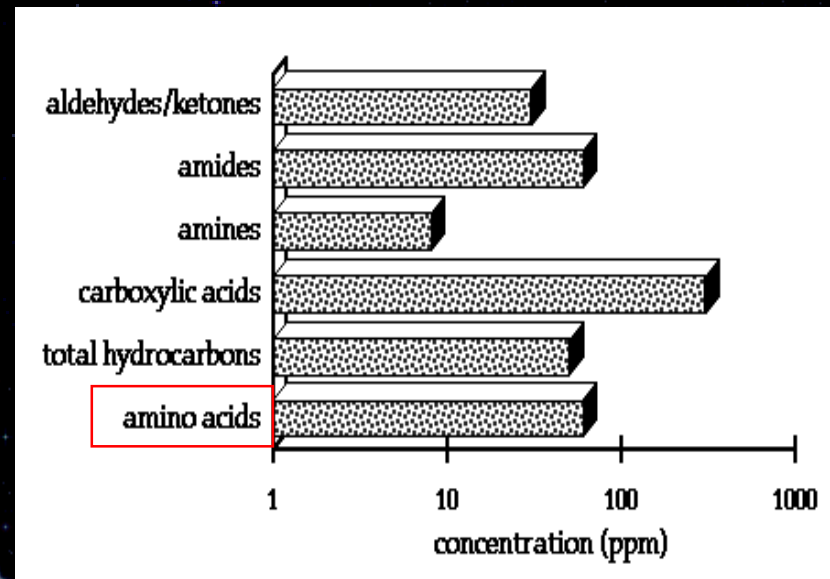


Murchison meteorite

- Aminoácidos
- Bases de DNA.
- Açúcares
- Precursores de Fosfolipídios →



	Sugars	Sugar Alcohols	Sugar Acids	Dicarboxylic Sugar Acids
3C	$\begin{array}{c} \text{CH}_2\text{OH} \\   \\ \text{C}=\text{O} \\   \\ \text{CH}_2\text{OH} \end{array}$ Dihydroxyacetone	$\begin{array}{c} \text{CH}_2\text{OH} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{CH}_2\text{OH} \end{array}$ Glycerol	$\begin{array}{c} \text{CO}_2\text{H} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{CH}_2\text{OH} \end{array}$ Glyceric acid	—
4C	—	$\begin{array}{c} \text{CH}_2\text{OH} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{CH}_2\text{OH} \end{array}$ Erythritol & Threitol	$\begin{array}{c} \text{CO}_2\text{H} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{CH}_2\text{OH} \end{array}$ Erythronic & Threonic acid	$\begin{array}{c} \text{CO}_2\text{H} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{HO}-\text{C}-\text{H} \\   \\ \text{CO}_2\text{H} \end{array}$ Tartaric & Mesotartaric acid
5C	—	$\begin{array}{c} \text{CH}_2\text{OH} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{CH}_2\text{OH} \end{array}$ Ribitol + isomers	$\begin{array}{c} \text{CO}_2\text{H} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{CH}_2\text{OH} \end{array}$ Ribonic acid + isomers	$\begin{array}{c} \text{CO}_2\text{H} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{CO}_2\text{H} \end{array}$ 2,3,4-Trihydroxy Pentanedioic acid



# Moléculas em outros planetas

Ver vídeos:



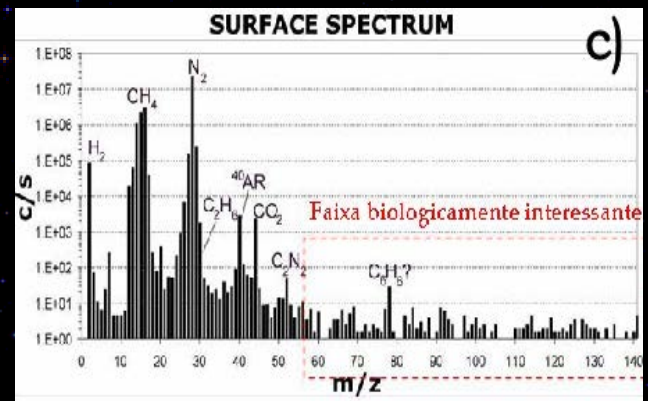
Titã

Metano e gelo de água fazem o papel da água e silicatos na terra.

$T_{\text{sup}} \sim 100\text{K}$ ,  $P_{\text{sup}} \sim 1.5 \text{ atm}$ .



Cassini-Huygens spacecraft, 2004



# Universo Molecular!

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

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

Hidrocarbonetos, PAHs, ....

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

# The Astrochymist

## Resources for Astrochemists & Interested Bystanders

### Astromolecule of the Month



July 2016

#### – Astrochemistry News –

Chiral propylene oxide detected

### NEWS ARCHIVE

#### New Detections

propylene oxide

formamide (iso)

isocyanic acid (iso)

ethyl cyanide (iso)

#### Detections in the Pipeline

#### Astrochemistry Outstanding Doctoral Dissertation Award

sponsored by the ACS Astrochemistry Subdivision  
2016 Winner: Brian Hays

Created and maintained by DE Woon  
Site updated 27 July 2016

### arXiv Preprints

Updated 24 July 2016

### Current Astrochemistry Publications

9 new papers added 24 July 2016

### A Bibliography of Astromolecules

molecules detected (or not) in various astronomical environments

### Astrochemistry Conferences

professional meetings of interest to astrochemists

### Astrochemistry Texts & Books

texts or books about astrochemistry

### Who's Who in Astrochemistry

links to the world-wide community of astrochemists

### Astrochemistry Links

links to other astrochemistry sites

### Astrochemistry FAQ

the basics of astrochemistry

### About This Website...

why this website was created

# A HYPER-BIBLIOGRAPHY OF KNOWN ASTROMOLECULES

**Recently Added Non-Detections:** [HSO](#), [CH3OCN](#), [CH3NCO](#)

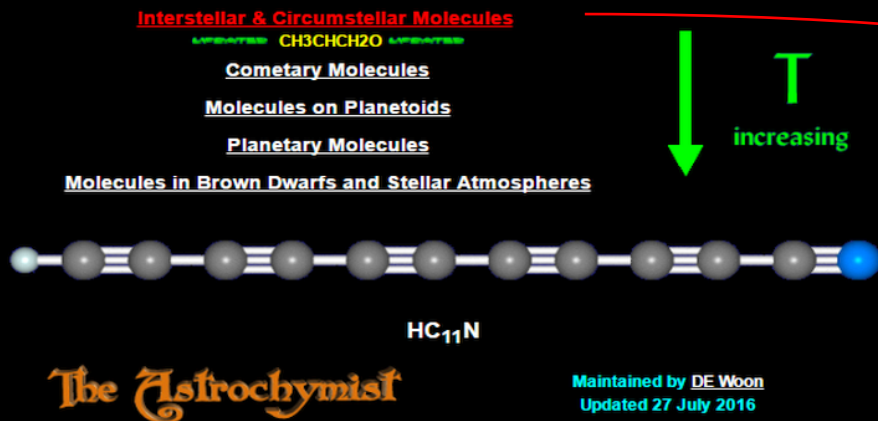
**Recently Added Isotopologues:** [CH2CHO](#), [HNCO](#), [CH3CHCN](#)

Molecules can exist in a wide range of astrophysical environments, from the extremely cold regions between stars to the atmospheres of stars themselves.

To date, nearly 200 molecular species have been tentatively or definitively identified in interstellar or circumstellar clouds, while about 50 have been identified in studies of comets in our solar system. Numerous **isotopologues** of interstellar and circumstellar molecules have also been observed.

Some detections reported on these pages may be controversial, but all are taken from the peer-reviewed astronomical literature. A questionable identification may be removed at a later date if circumstances warrant.

Jacque Crovisier has amassed a comprehensive **compilation** of species observed to date in the interstellar medium, in comets, or in non-terrestrial planetary atmospheres, plus additional ones which may prove to be found.



Linha do tempo das Descobertas

YEAR	SPECIES	CITATION	SOURCE(S)/LINES
1937	CH methylidyne <i>Astromolecule of the North</i> <a href="#">LMC</a>	<a href="#">Considerations Regarding Interstellar Molecules</a> P. Swings and L. Rosenfeld, <i>ApJ</i> 80:483-488 (1937) <a href="#">Evidence for the Molecular Origin of Some Hitherto Unidentified Interstellar Lines</a> A. McKellar, <i>Publ Astron Soc Pac</i> 52:187-192 (1940) <a href="#">Some Results with the COUDE Spectrograph of the Mount Wilson Observatory</a> W.S. Adams, <i>ApJ</i> 93:11-23 (1941) <a href="#">Radio Detection of Interstellar CH</a> O. E. H. Rydbeck, J. Eldler, and W.M. Irvine, <i>Nature</i> 246:246-248 (1973) <a href="#">Hubble Space Telescope Measurements of Vacuum Ultraviolet Lines of Interstellar CH</a> Y. Sheffer and S. R. Federman, <i>ApJ</i> 659:1353-1359 (2007)	$\zeta$ Oph vis lines at 3878.8, 3886.4, 3890.2, & 4300.3 Å; uv lines near 1271, 1368, 1369, 1370, 1549, & 1694 Å. Cas A and 4 dark clouds J = 1/2, $v_{10}$ (3263.794 MHz) J = 1/2, $v_{11}$ (3335.481 MHz) J = 1/2, $v_{10}$ (3349.193 MHz)
1940	CN cyano radical <i>Astromolecule of the North</i> <a href="#">NGC253</a>	<a href="#">Evidence for the Molecular Origin of Some Hitherto Unidentified Interstellar Lines</a> A. McKellar, <i>Publ Astron Soc Pac</i> 52:187-192 (1940) <a href="#">Some Results with the COUDE Spectrograph of the Mount Wilson Observatory</a> W.S. Adams, <i>ApJ</i> 93:11-23 (1941) <a href="#">Observation of the CN Radical in the Orion Nebula and W51</a> K. B. Jefferts, A. A. Penzios, and R. W. Wilson, <i>ApJ</i> 161:L87-L89 (1970)	$\zeta$ Oph lines at 3874.02 & 3874.61 Å Orion nebula, W51 J = 1 → 0 (113492 MHz)
1941	CH <sup>+</sup> methylidyne cation <i>Astromolecule of the North</i> <a href="#">LMC</a>	<a href="#">Note on CH<sup>+</sup> in Interstellar Space and in the Laboratory</a> A. E. Douglas and G. Herzberg, <i>ApJ</i> 94:381 (1941) <a href="#">OBSERVATIONS OF INTERSTELLAR NEUTRAL POLYSSIM AND NEUTRAL CALSIUM</a> T. Dunham, Jr., <i>Pub Astron Soc Pac</i> 49:26-28 (1937) <a href="#">Some Results with the COUDE Spectrograph of the Mount Wilson Observatory</a> W.S. Adams, <i>ApJ</i> 93:11-23 (1941)	$\zeta$ Oph, $\xi$ Per, $\chi^2$ Ori, 55 Oyg (0,0), (1,0), and (2,0) bands of the A <sup>1</sup> $\Pi$ - X <sup>1</sup> $\Sigma$ system at 4232.6, 3957.7, & 3745.3 Å
1963	OH hydroxyl radical <i>Astromolecule of the North</i> <a href="#">MB2</a>	<a href="#">Radio Observations of OH in the Interstellar Medium</a> S. Weinreb, A. H. Barrett, M. L. Meeks, and J. C. Henry, <i>Nature</i> 200:829-831 (1963)	Cas A F=2 → 2 (1667.5 / MHz) F=1 → 1 (1665.402 MHz)

# E) Alguns experimentos de astroquímica

1 Fase gasosa

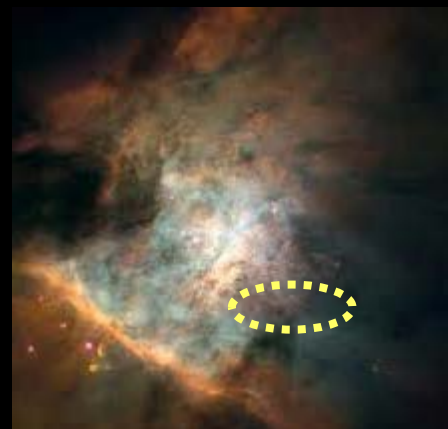
2 Fase condensada (gelos)



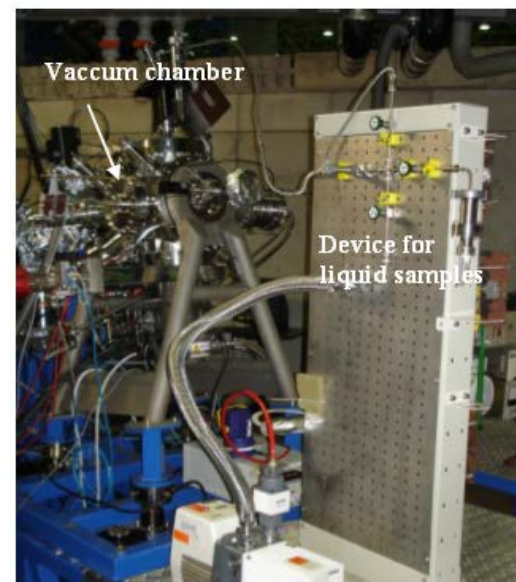
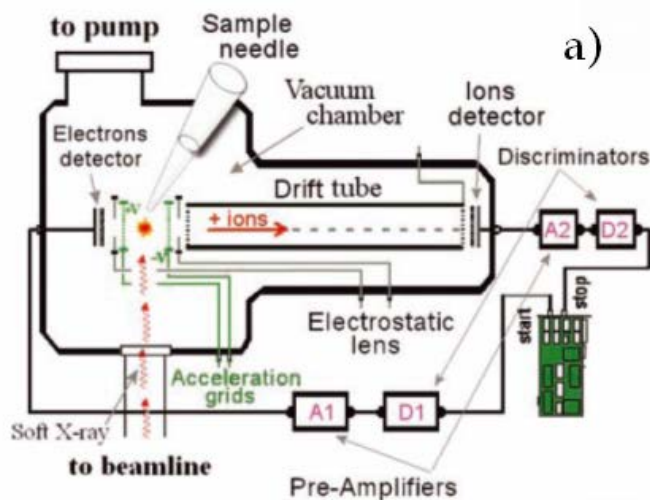


# 1 - Experimentos envolvendo a interação da radiação (fótons, elétrons, íons) com moléculas na fase gasosa.

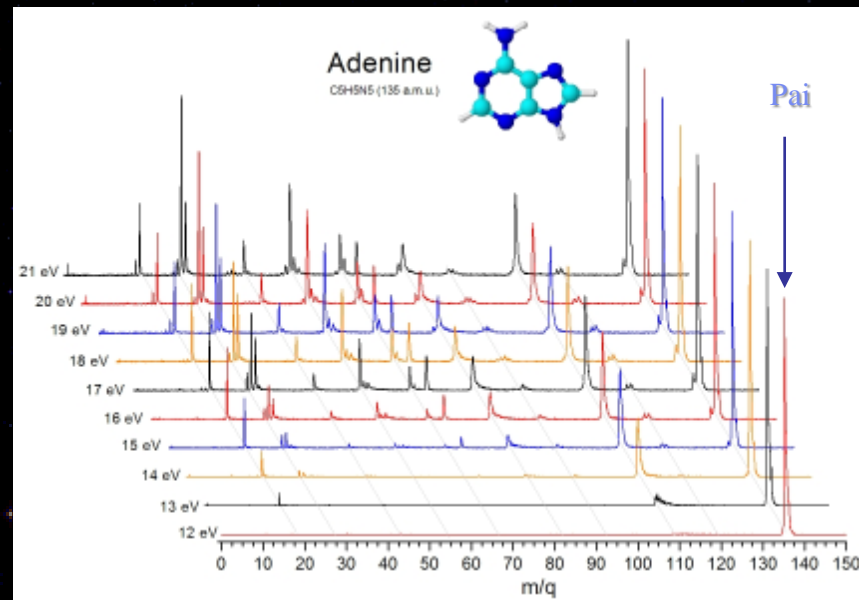
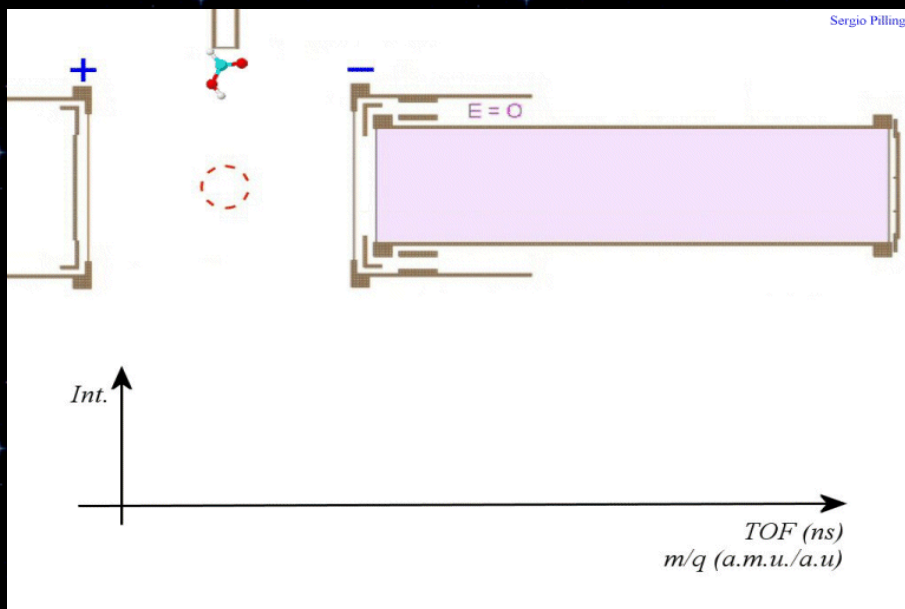
Resultados: Fragmentação, Canais de dissociação,  $\sigma$ ,  $\tau_{1/2}$



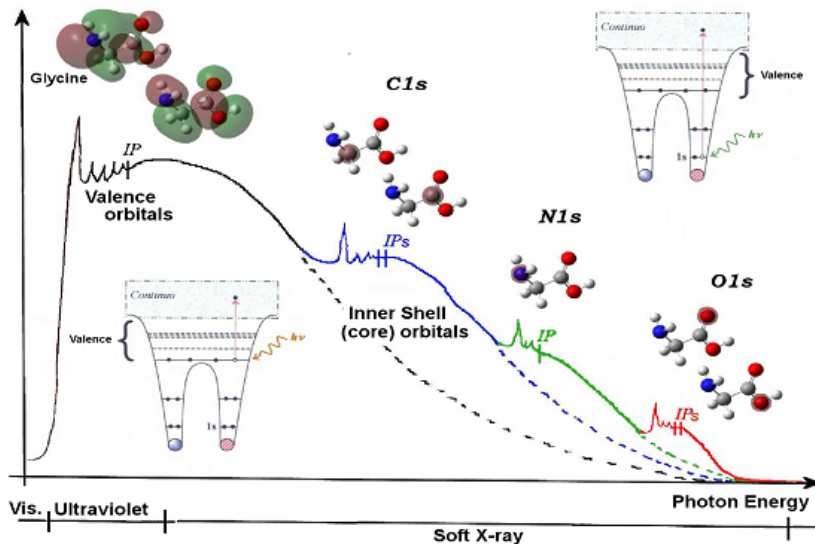
Ex. Fótons (LNLS)



- a) Schematic diagram of the experimental set-up employed in gas-phase experiments.  
b) Photography of equipment employed at the soft X-ray beamline of LNLS.

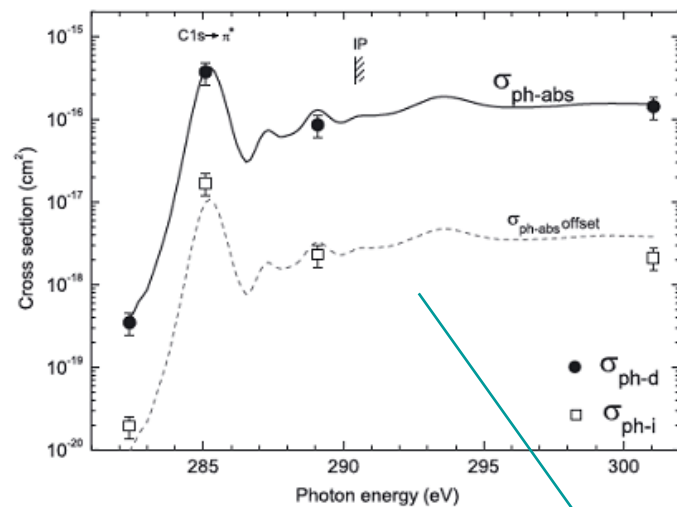
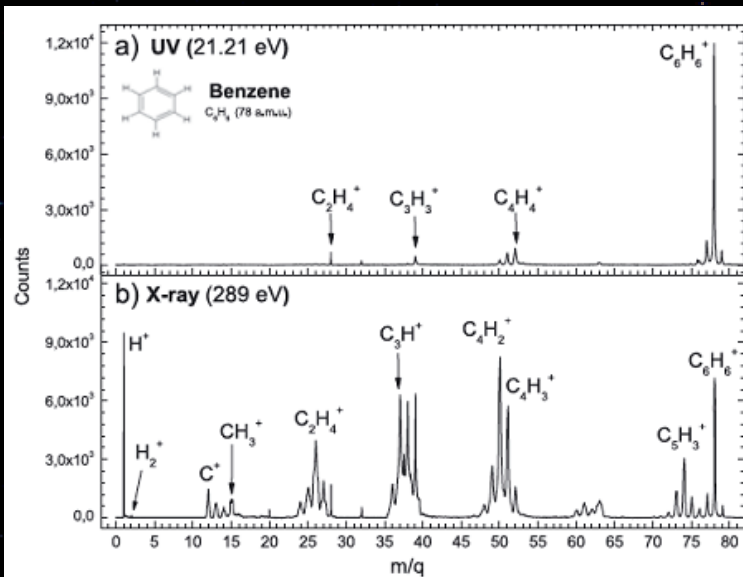
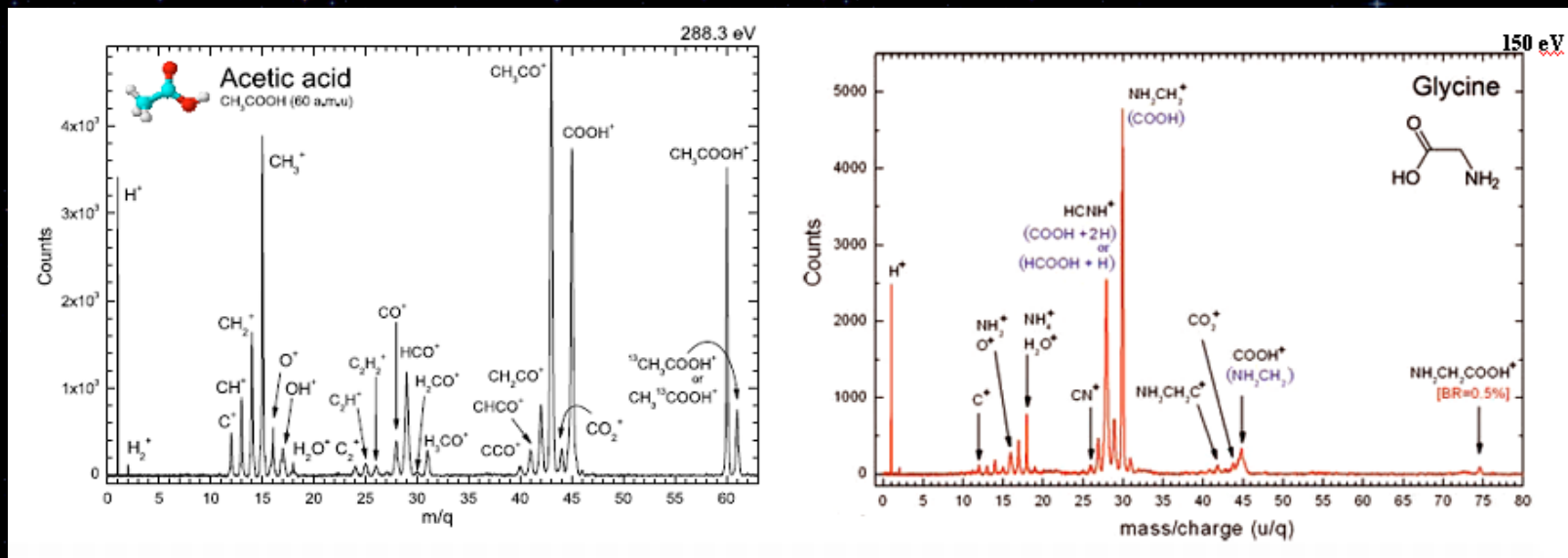


Absorption probability



Schematic view of absorption probability as a function of photon energy for polyatomic molecule (e.g. glycine). IP indicates the ionization potential of a given orbital.

# Outros exemplos

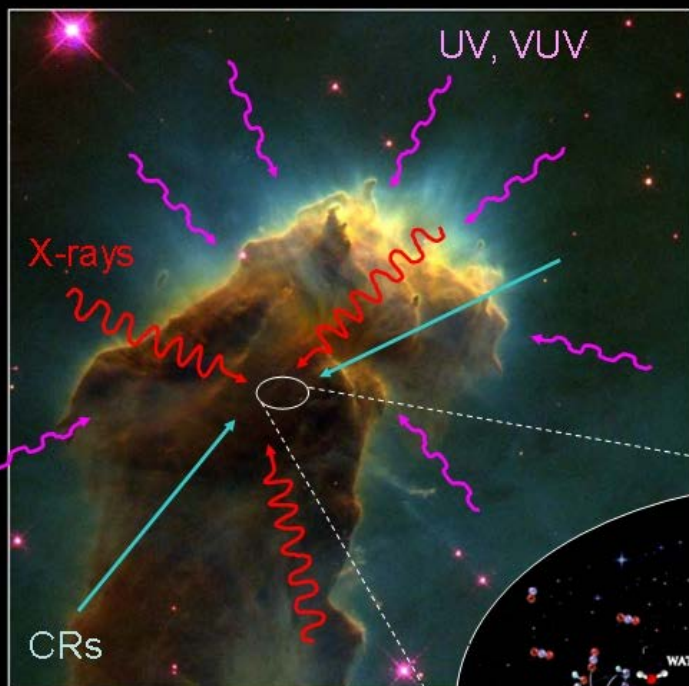
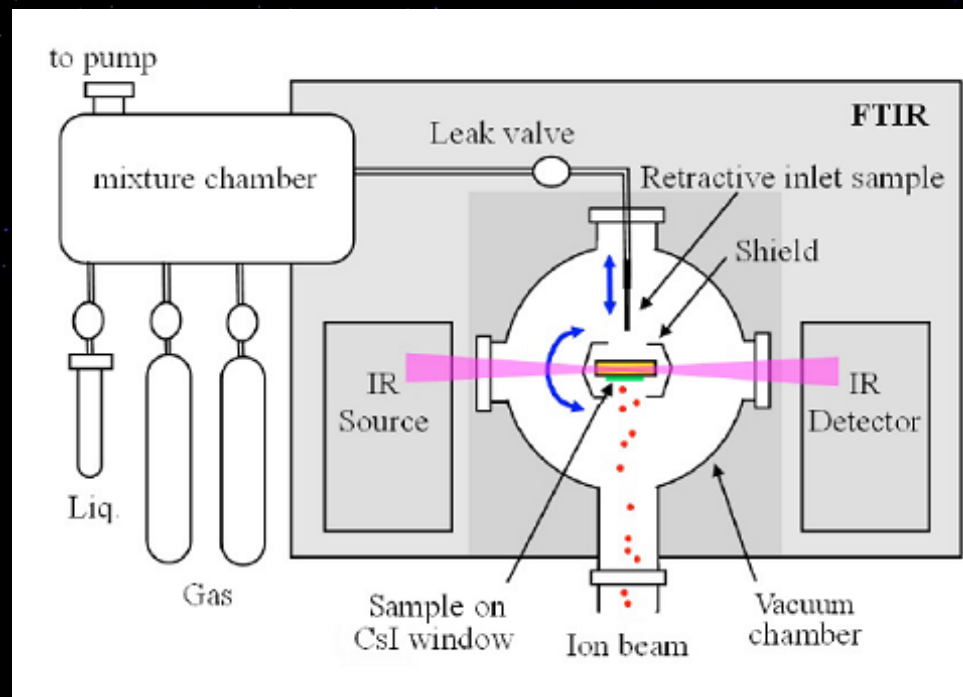


Taxa de Dissociação e tempo de meia-vida

$$R_i \approx \phi \times \sigma_{d,i} \quad [\text{s}^{-1}], \quad t_{1/2,i} = \frac{91n2}{R_i} \quad [\text{s}]$$

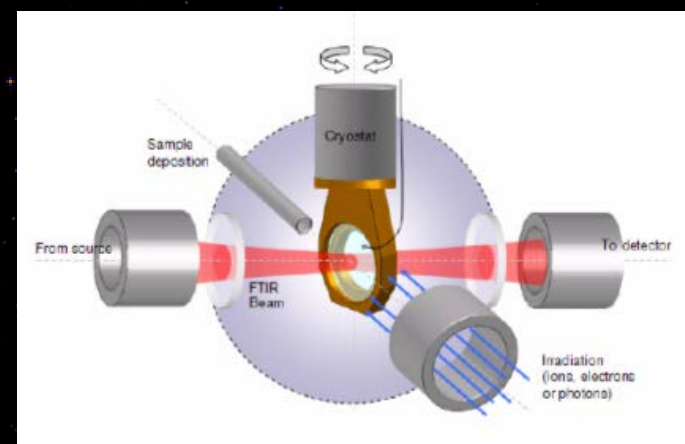
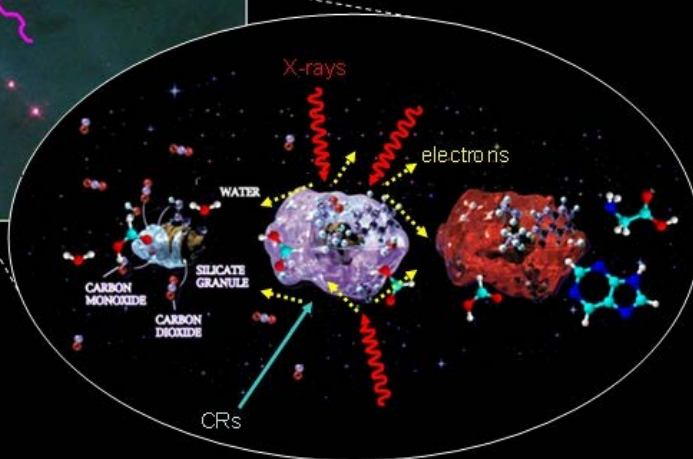
## 2- Experimentos de Radiólise/Fotólise de Gelos astrofísicos

- Criostato (10K);
- Câmara UHV ( $< 10^{-8}$  mbar);
- Agente ionizante (PUC-Rio, GANIL, LNLs)
- FTIR e QMS

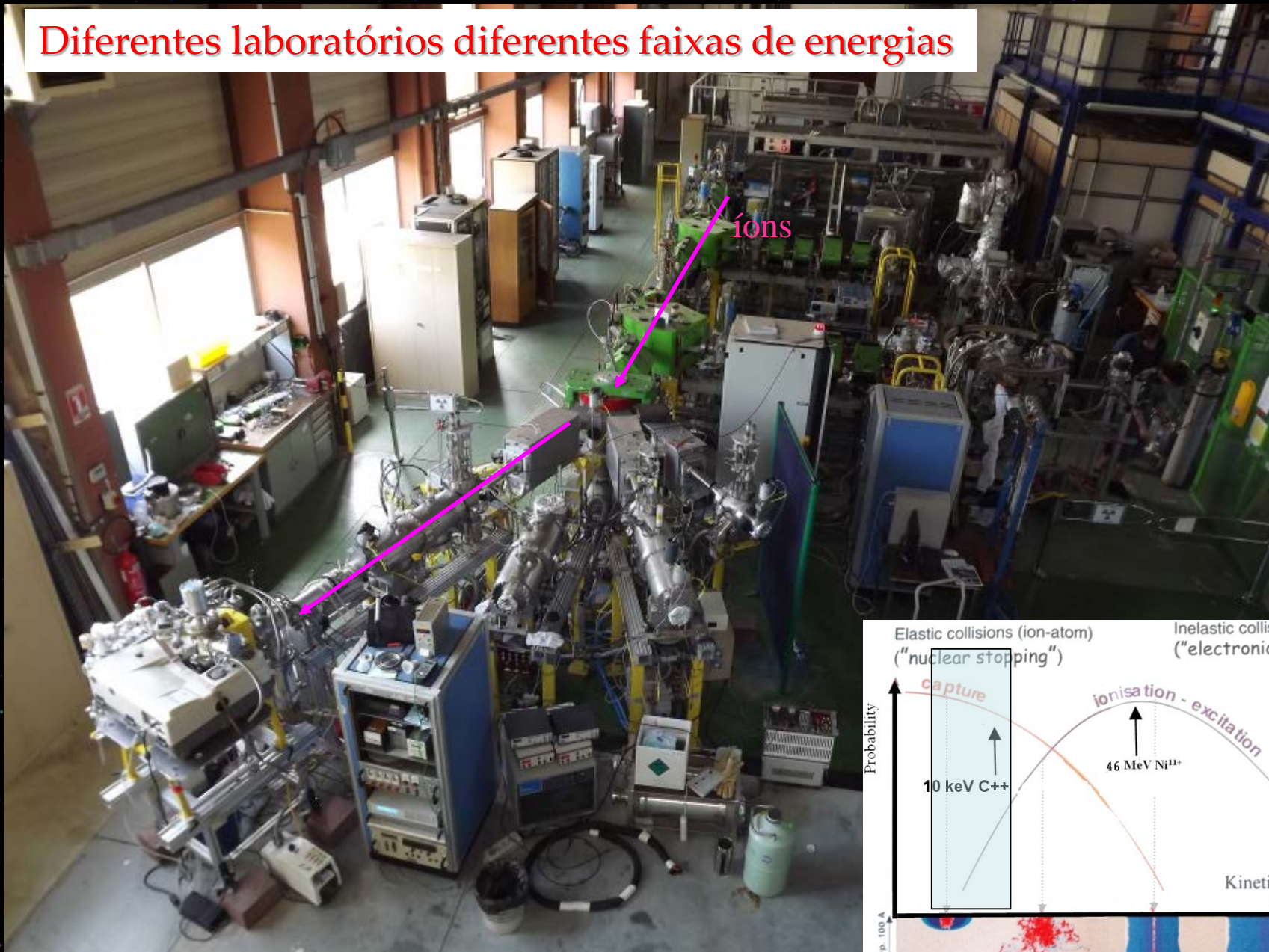


Star-Birth Clouds · M16  
PRC95-44b · ST ScI OPD · November 2, 1995  
J. Hester and P. Scowen (AZ State Univ.), NASA

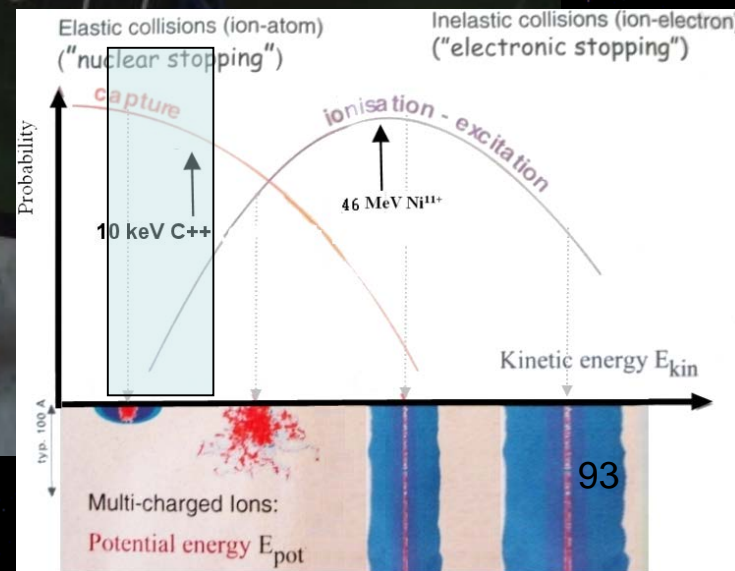
HST · WFPC2

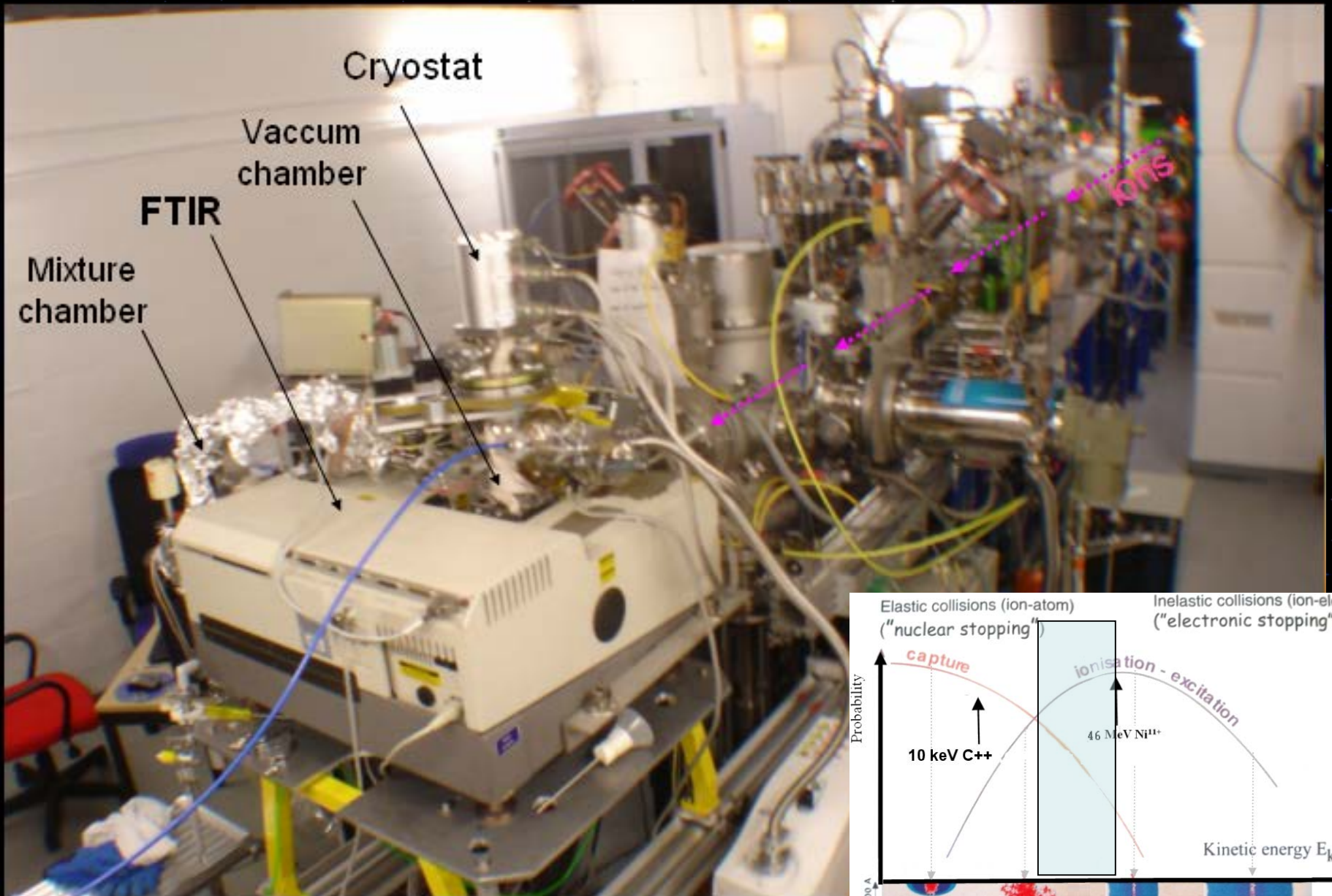


# Diferentes laboratórios diferentes faixas de energias



ARIBE/GANIL → Vento solar (implantação)  
 $E \sim 10 \text{ keV/u}$





IRRSUD/GANIL → Raios cósmicos pesados  
 $E \sim 0.1-10 \text{ MeV/u}$

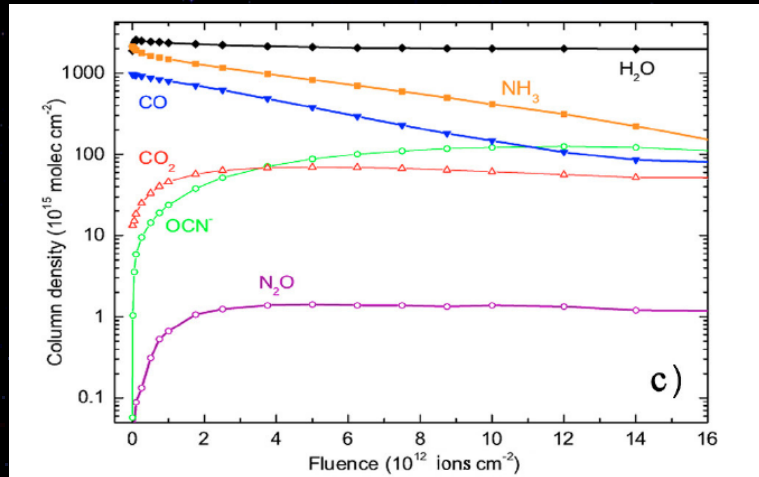
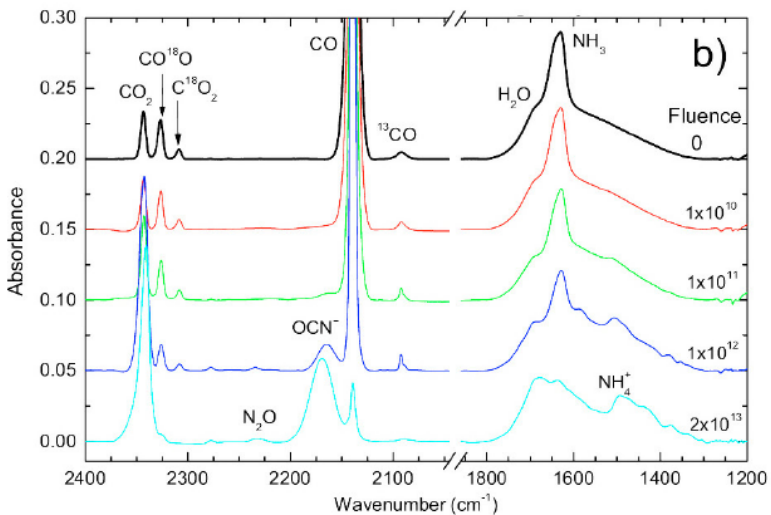
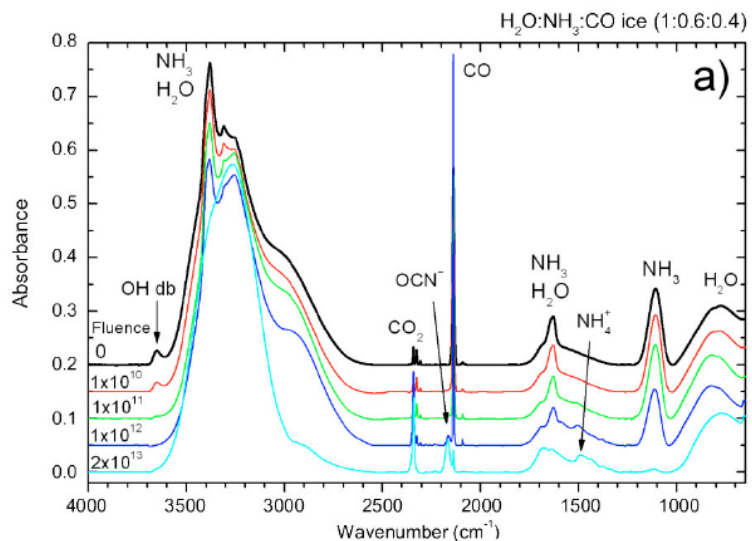
# 2.1: Bombardeamento de gelo interestelar contendo amonia com raios cósmicos

A&A 509, A87 (2010)  
 DOI: 10.1051/0004-6361/200912274  
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Astronomy  
&  
Astrophysics

## Radiolysis of ammonia-containing ices by energetic, heavy, and highly charged ions inside dense astrophysical environments

S. Pilling<sup>1,2</sup>, E. Seperuelo Duarte<sup>1,3,4</sup>, E. F. da Silveira<sup>1</sup>, E. Balanzat<sup>3</sup>, H. Rothard<sup>3</sup>, A. Domaracka<sup>3</sup>, and P. Boduch<sup>3</sup>

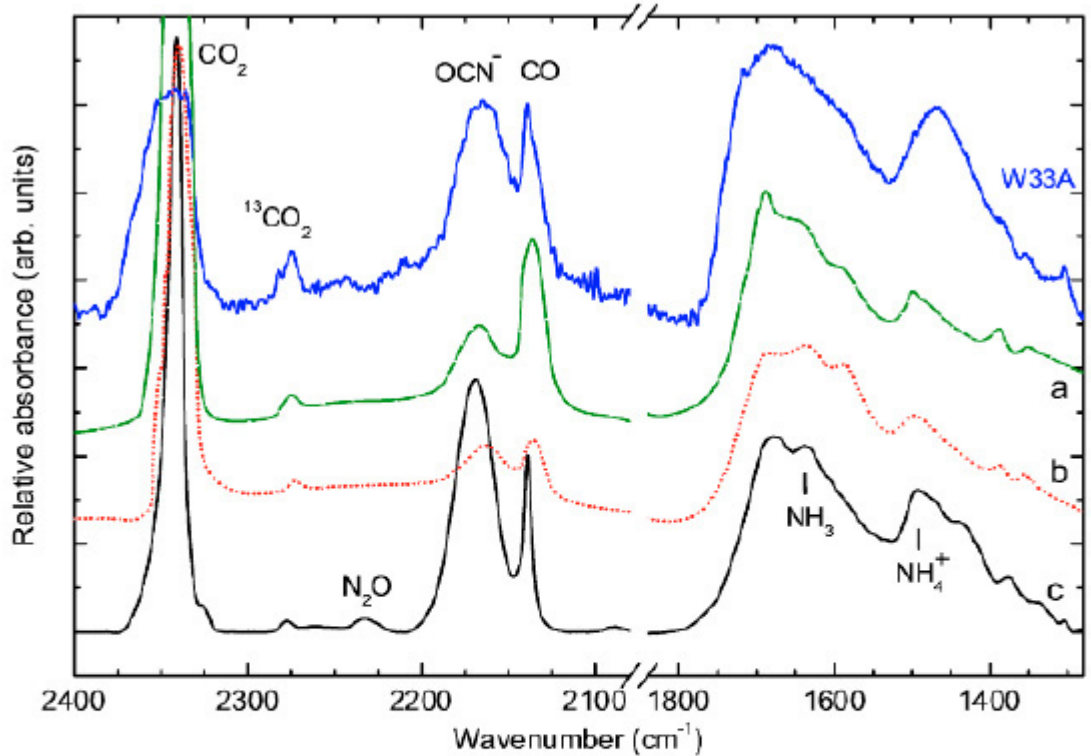


**Fig. 2.** a) Infrared spectra of H<sub>2</sub>O:NH<sub>3</sub>:CO ice (1:0.6:0.4) before (top dark line) and after different irradiation fluences. b) Expanded view from 2400 to 1200 cm<sup>-1</sup>. Each spectrum has an offset of 0.05 for better visualization. c) Molecular column density derived from the infrared spectra during the experiment.

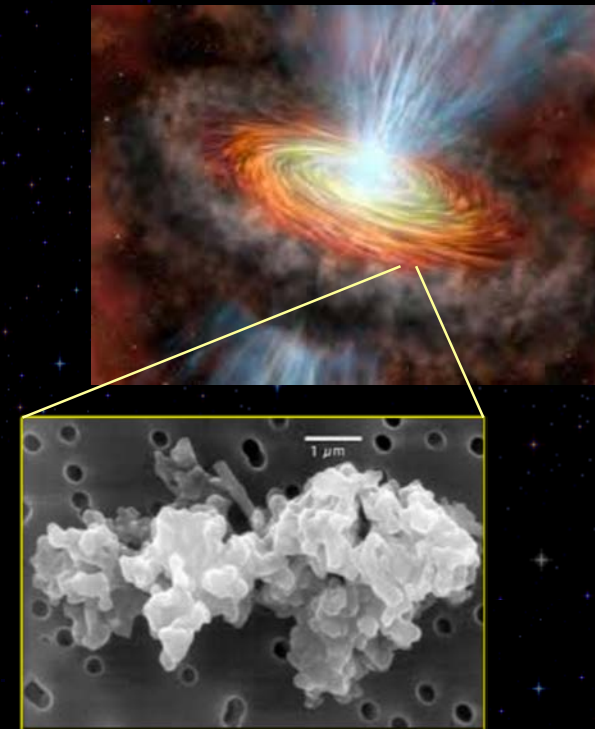
$$\frac{dN_i}{dF} = \sum_{j \neq i} \sigma_{f,ij} N_j + L_i - \sigma_{d,i} N_i - Y_i \Omega_i(F),$$

Table 3. Dissociation cross-sections of the studied molecular species for radiolysis of ammonia-containing ices by 46 MeV Ni ions

Species	Mixture (H <sub>2</sub> O:NH <sub>3</sub> :CO)	$\sigma_d$ (10 <sup>-13</sup> cm <sup>2</sup> )	$N_\infty$ (10 <sup>17</sup> molec cm <sup>-2</sup> )	$Y$ (10 <sup>4</sup> molec ion <sup>-1</sup> )	$L^f$ (10 <sup>4</sup> molec ion <sup>-1</sup> )	$N_0$ (10 <sup>17</sup> molec cm <sup>-2</sup> )
H <sub>2</sub> O	(1:0.5:0)	~2	23	1 <sup>a</sup>	38	29
	(1:0.6:0.4)	~2	19	1 <sup>a</sup>	35	24
NH <sub>3</sub>	(1:0.5:0)	1.3	NA <sup>e</sup>	0 <sup>b</sup>	0	2.0
	(1:0.6:0.4)	1.4	NA	0 <sup>b</sup>	0	1.7
CO	(1:0.6:0.4)	1.9	NA	0 <sup>b</sup>	0	1.0
	(1:0.6:0.4)	1.9	NA	0 <sup>b</sup>	1 <sup>d</sup>	1.0
	(1:0.6:0.4)	1.9	NA	1 <sup>c</sup>	0	1.0



**Fig. 5.** Comparison between IR spectra of interstellar and laboratory ices. The highest curve is the infrared spectra of protostellar source W33A obtained by the Infrared Space Observatory (ISO). Lower traces indicate laboratory spectra of H<sub>2</sub>O:NH<sub>3</sub>:CO ices after processing by: a) UV photons (Hudson & Moore 2000); b) 0.8 MeV protons (Hudson & Moore 2000), and c) 46 MeV Ni ions (this work).





## Seção de Choque de Destruição e Sputtering

$$N = (N_0 + \frac{Y}{\sigma_d}) \exp(-\sigma_d F) - \frac{Y}{\sigma_d}$$

$$N_k \approx N_0 \sigma_{fk} \left[ F - \frac{\sigma_d + \sigma_{dk}}{2} F^2 \exp(-\sigma_d F) \right]$$

## Radiochemical yield

$$G_f = 100 \frac{\sigma_f}{S} \text{ molecule per 100 eV.}$$

## Taxa de Dissociação e tempo de meia-vida

$$R_i \approx \phi_{\text{HCR}} \times \sigma_{d,i} \quad [\text{s}^{-1}], \quad t_{1/2,i} = \frac{\ln 2}{R_i} \quad [\text{s}]$$

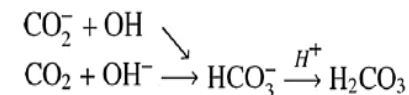
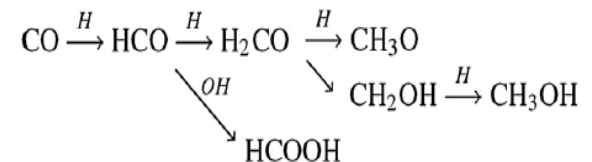
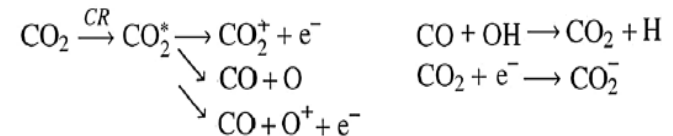
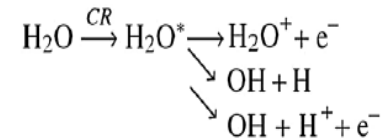
Valores médios empregando íons pesados  
( $E = 0.1-10 \text{ MeV/u}$ )

$$\sigma_d \sim 10^{-13} \text{ cm}^2; \quad G \sim 5-10; \quad Y \sim 10^4;$$

$$t_{1/2} \text{ (MI)} \sim 10^6 \text{ anos}$$

$$\sigma_f \sim 10^{-14} \text{ cm}^2;$$

## Exemplos de reações induzidas por CR



## 2.2 Destruição de aminoácidos em ambientes espaciais com raios cósmicos

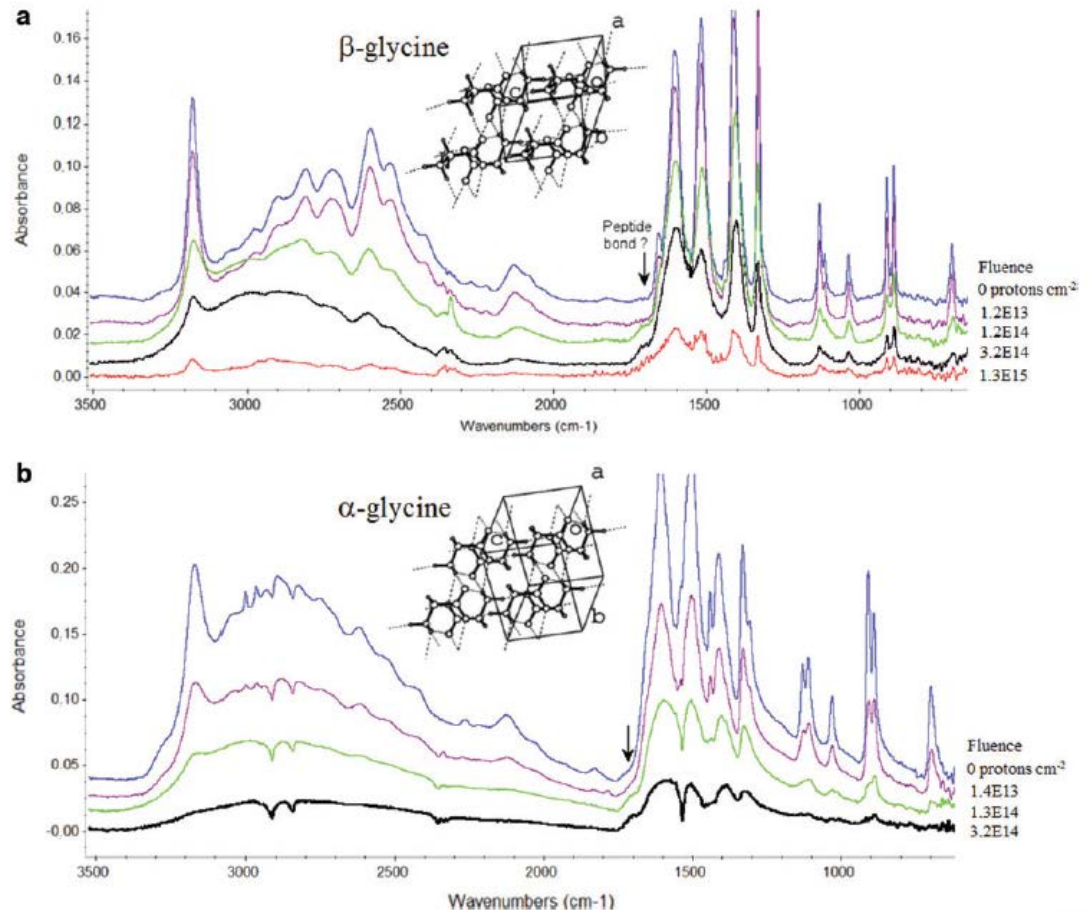
ASTROBIOLOGY  
Volume 13, Number 1, 2013  
© Mary Ann Liebert, Inc.  
DOI: 10.1089/ast.2012.0877

### The Influence of Crystallinity Degree on the Glycine Decomposition Induced by 1 MeV Proton Bombardment in Space Analog Conditions

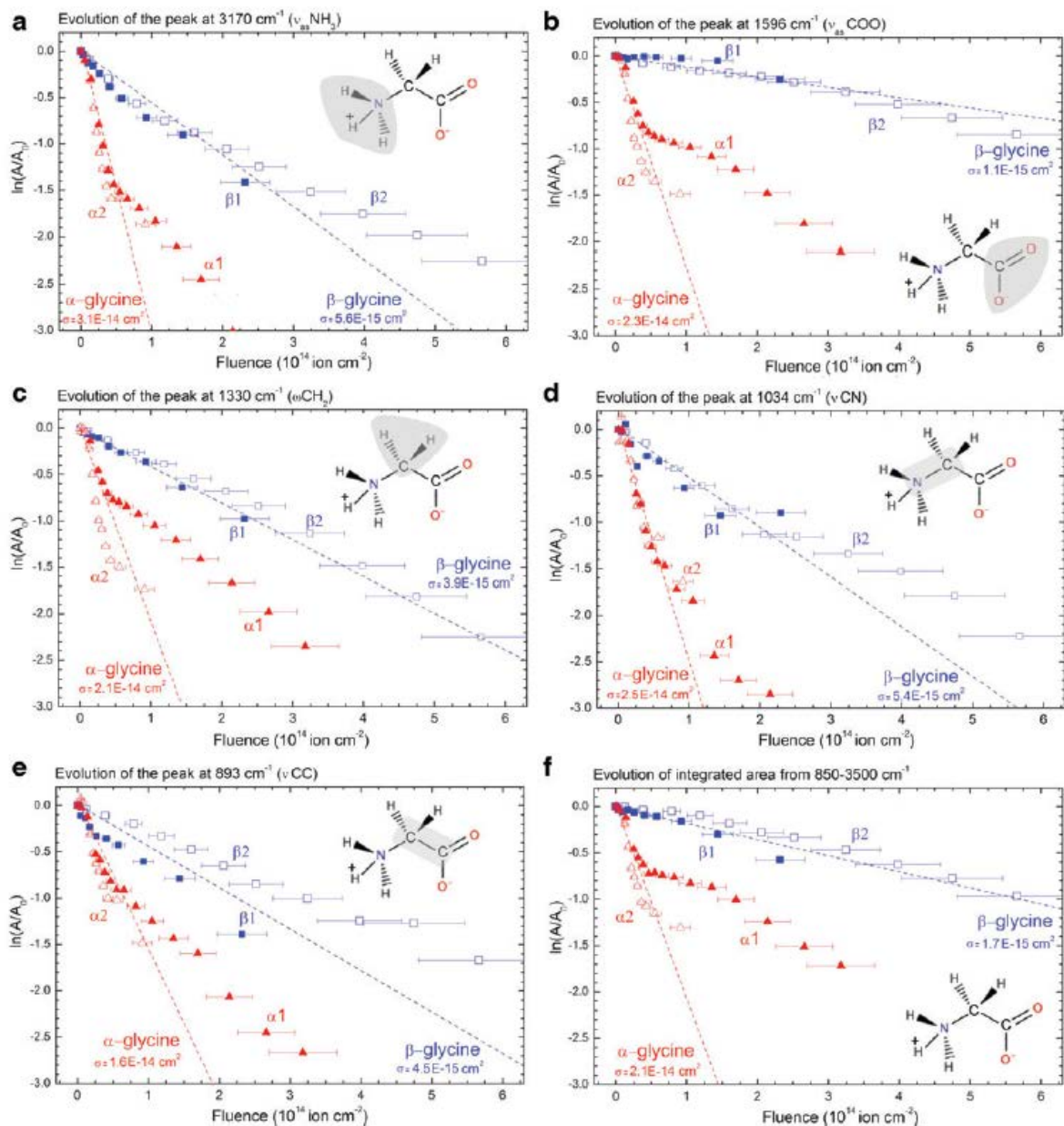
Sergio Pilling,<sup>1</sup> Luiz A.V. Mendes,<sup>2</sup> Vinicius Bordalo,<sup>3</sup> Christian F.M. Guaman,<sup>3</sup>  
Cássia R. Ponciano,<sup>3</sup> and Enio F. da Silveira<sup>3</sup>

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PILLING ET AL.



**FIG. 4.** Evolution of IR spectra of (a)  $\beta$ -glycine (from  $\beta 2$  experiment) as a function of proton fluence ( $0$ ,  $1.2 \times 10^{13}$ ,  $1.2 \times 10^{14}$ ,  $3.2 \times 10^{14}$ , and  $1.3 \times 10^{15}$  ions  $\text{cm}^{-2}$ ); (b)  $\alpha$ -glycine (from  $\alpha 1$  experiment) as a function of proton fluence ( $0$ ,  $1.4 \times 10^{13}$ ,  $1.3 \times 10^{14}$ , and  $3.2 \times 10^{14}$  ions  $\text{cm}^{-2}$ ). The absorption peaks around  $2910$ ,  $2850$ , and  $1550$   $\text{cm}^{-1}$  are artifacts from background subtraction. Crystal structures of glycine polymorphs were taken from Fábian and Kálmán (2004). Arrows indicate the position of an amide functional group around  $1650$ – $1700$   $\text{cm}^{-1}$ , suggesting the formation of peptide bonds in the sample. Color images available online at [www.liebertonline.com/ast](http://www.liebertonline.com/ast)



**FIG. 5.** Evolution of the normalized peak areas as a function of the proton fluence. The selected glycine IR bands are (a)  $3170\text{ cm}^{-1}$  ( $\nu_{\text{as}}\text{NH}_3$ ), (b)  $1596\text{ cm}^{-1}$  ( $\nu_{\text{as}}\text{COO}$ ), (c)  $1330\text{ cm}^{-1}$  ( $\omega\text{CH}_2$ ), (d)  $1034\text{ cm}^{-1}$  ( $\nu\text{CN}$ ), (e)  $893\text{ cm}^{-1}$  ( $\nu\text{CC}$ ), and (f) whole molecule using integrated area of IR spectra from  $850\text{ to }3500\text{ cm}^{-1}$ . The hatched site over zwitterionic glycine structural formulae shows the chemical bonds studied in each figure. The obtained values of the dissociation cross sections

## 2.3: Formação de aminoácidos, Hidrocarbonetos aromaticos e ligações peptidicas do espaço.

A&A 509, A87 (2010)  
DOI: 10.1051/0004-6361/200912274  
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Astronomy  
&  
Astrophysics

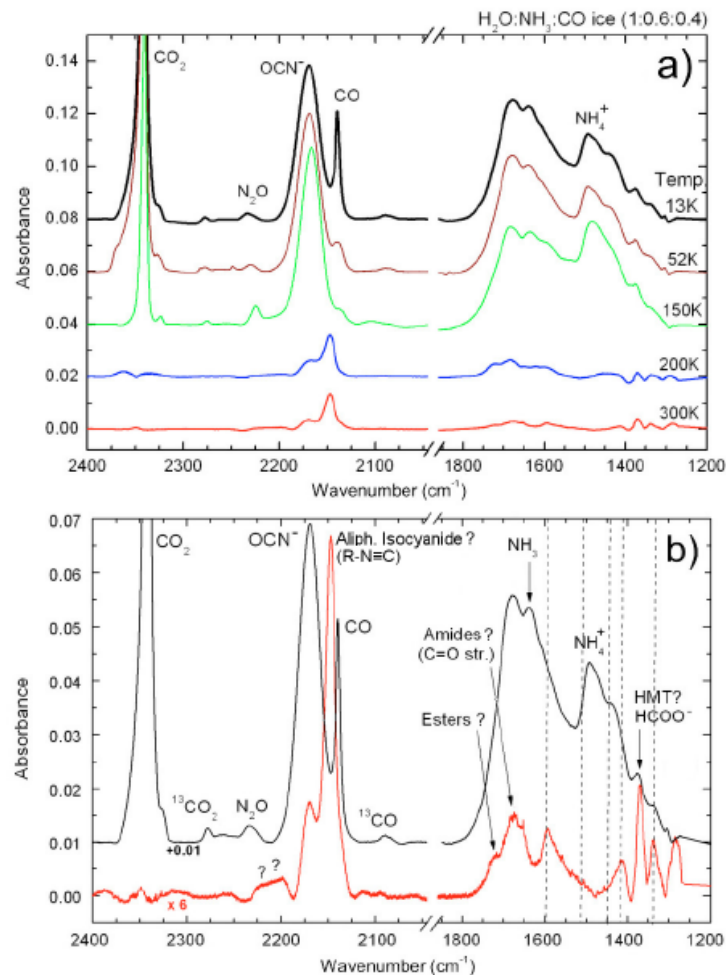
### Radiolysis of ammonia-containing ices by energetic, heavy, and highly charged ions inside dense astrophysical environments

S. Pilling<sup>1,2</sup>, E. Seperuelo Duarte<sup>1,3,4</sup>, E. F. da Silveira<sup>1</sup>, E. Balanzat<sup>3</sup>, H. Rothard<sup>3</sup>, A. Domaracka<sup>3</sup>, and P. Boduch<sup>3</sup>

**Table 4.** Assignment of infrared absorption features produced by the radiolysis of the H<sub>2</sub>O:NH<sub>3</sub>:CO ice (1:0.6:0.4) by 46 MeV Ni ions at 13 K and after warming to 300 K.

Frequency (cm <sup>-1</sup> )	Wavelength (μm)	Temp. (K)	Molecule	Notes
2233	4.48	13	N <sub>2</sub> O	[1,2]
2218–2200	4.51–4.54	300	nitriles <sup>†</sup>	[8]
2168	4.61	13, 300	OCN <sup>-</sup>	[1,3,4,7]
2147	4.66	300	aliph. isocyanide <sup>†</sup>	[8]
~2112	4.73	300	NCO <sub>2</sub> <sup>†</sup>	[2]
1725	5.80	300	ester <sup>†</sup>	[5]
1683	5.94	300	amides <sup>†</sup>	[5]
1652	6.05	300	asym-N <sub>2</sub> O <sub>3</sub> <sup>†</sup>	[2]
1637	6.11	13	?	
1593	6.28	300	NH <sub>3</sub> CH <sub>2</sub> COO <sup>-†</sup>	[6]
1558	6.42	300	?	
1533	6.52	300	?	
1506	6.64	300	NH <sub>3</sub> CH <sub>2</sub> COO <sup>-†</sup>	[6]
~1490	6.71	13	NH <sub>4</sub> <sup>+</sup>	[1,3,7]
1474	6.78	13	NO <sub>2</sub> <sup>†</sup>	[2]
1440	6.94	13	NH <sub>3</sub> CH <sub>2</sub> COO <sup>-†</sup>	[6]
1415	7.07	300	NH <sub>3</sub> CH <sub>2</sub> COO <sup>-†</sup>	[6]
~1370	7.30	13, 300	HMT <sup>†</sup>	[5]
			HCOO <sup>-</sup>	[5,9]
~1338	7.47	13, 300	NH <sub>3</sub> CH <sub>2</sub> COO <sup>-†</sup>	[6]
			NH <sub>2</sub> CH <sub>2</sub> COO <sup>-†</sup>	[6]
			HCOO <sup>-</sup>	[9]
1305	7.66	13	N <sub>2</sub> O <sub>2</sub> <sup>†</sup> ; N <sub>2</sub> O <sub>4</sub> <sup>†</sup>	[2]
1283	7.80	300	N <sub>2</sub> O <sub>3</sub> <sup>†</sup>	[2]

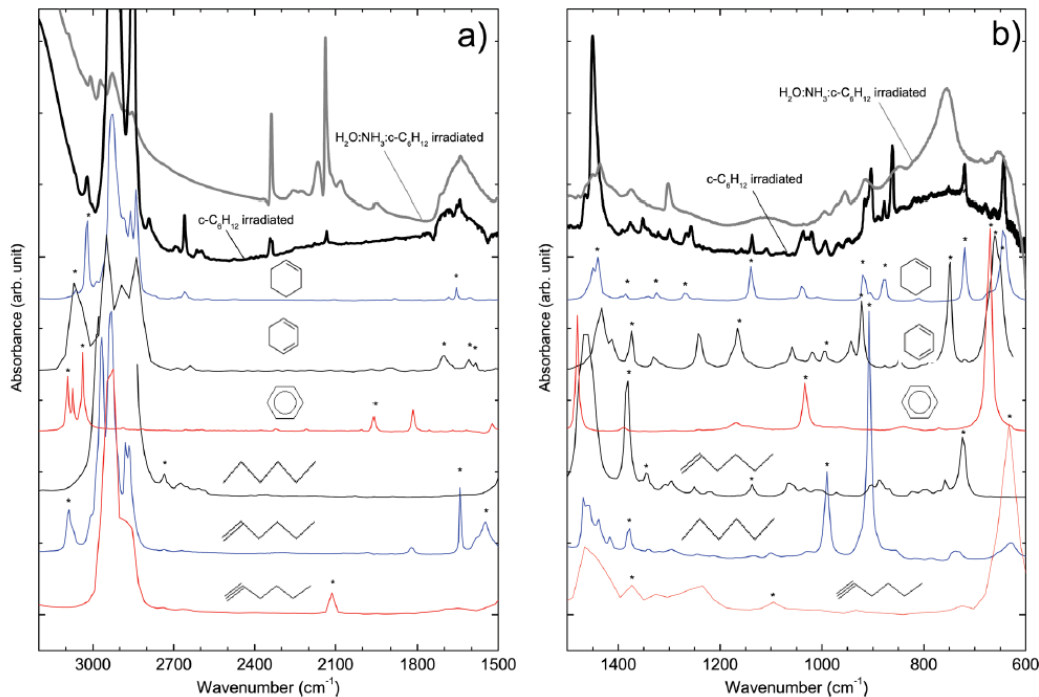
<sup>†</sup>Tentative assignment. [1] Proton bombardment of several ices (Hudson et al. 2001); [2] Electron bombardment of N<sub>2</sub>:CO<sub>2</sub> (Jamieson et al. 2005); [3] Hudson & Moore (2000); [4] van Broekhuizen et al. 2005; [5] UV photolysis of H<sub>2</sub>O:NH<sub>3</sub>:CH<sub>3</sub>OH:CO:CO<sub>2</sub> ice (Munoz Caro & Shutte 2003); [6] electron bombardment of CH<sub>3</sub>NH<sub>2</sub>:CO<sub>2</sub> ice (Holton et al. 2005); [7] UV photolysis of ammonia-containing ices (Demyk et al. 1998); [8] UV photolysis of N<sub>2</sub>:CH<sub>4</sub> ices at various pressures (Imanaka et al. 2004); [9] proton bombardment of H<sub>2</sub>O:NH<sub>3</sub>:CO ice (Hudson & Moore 2001).



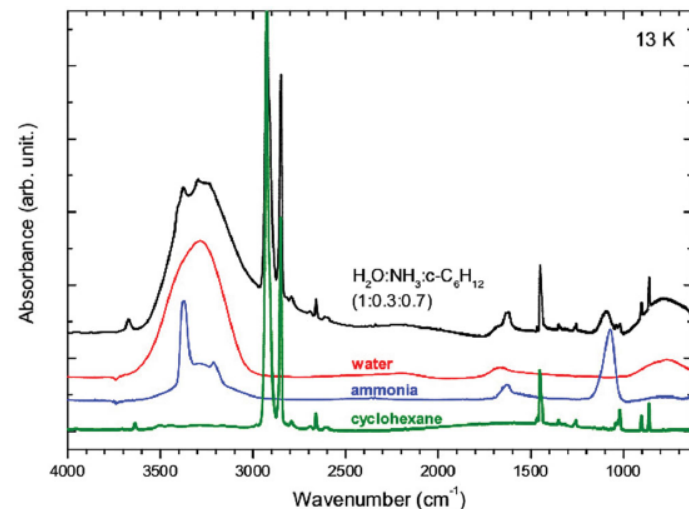
**Fig. 6.** a) Infrared spectra of H<sub>2</sub>O:NH<sub>3</sub>:CO ice (1:0.6:0.4) from 2400 to 1200 cm<sup>-1</sup> during heating to room temperature. The sample temperature of each spectrum is given. Each spectrum has an offset of 0.02 for clearer visualization. b) Comparison between the irradiated ice at 13 K (top spectrum) and the 300 K residue (bottom spectrum). Vertical dashed lines indicate the frequencies of some vibration modes of zwitterionic glycine (NH<sub>3</sub><sup>+</sup>CH<sub>2</sub>COO<sup>-</sup>).

## Formation of unsaturated hydrocarbons in interstellar ice analogues by cosmic rays

S. Pilling,<sup>1\*</sup> D. P. P. Andrade,<sup>1</sup> E. F. da Silveira,<sup>2</sup> H. Rothard,<sup>3</sup> A. Domaracka<sup>3</sup> and P. Boduch<sup>3</sup>

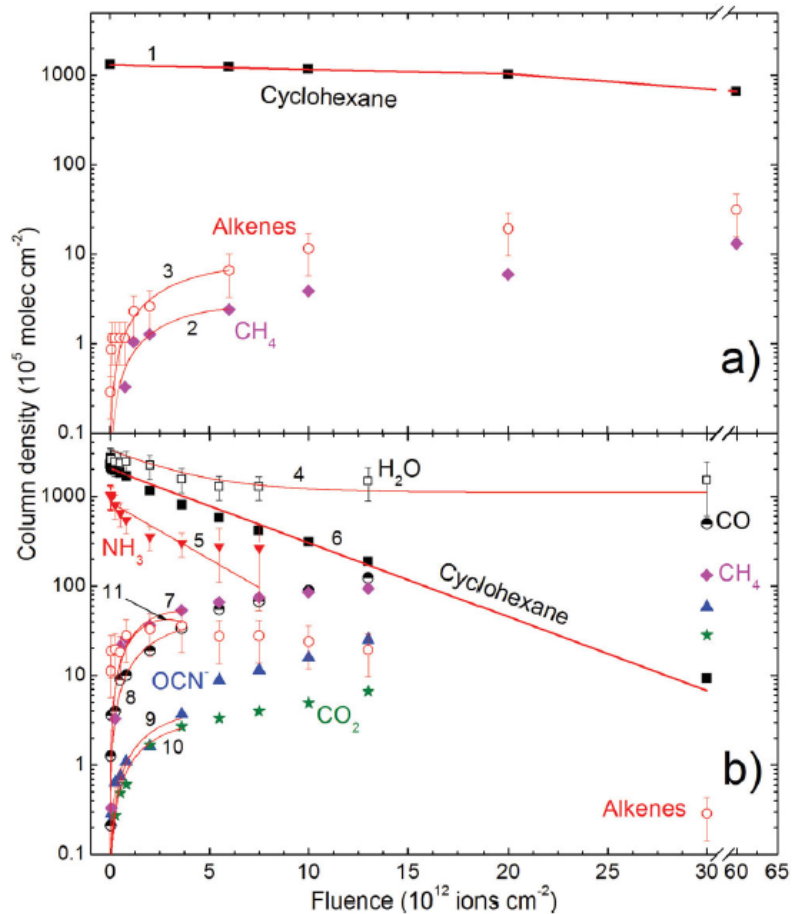


**Figure 5.** Comparison between the IR spectra of the two irradiated ices at highest fluences (this work) with IR spectra of different non-irradiated cyclic and aliphatic hydrocarbons from the NIST database (Lindstrom & Mallard 2005). Skeletal formulae of each species (cyclohexene, 1,3-cyclohexadiene, benzene, hexane, 1-hexene and 1-hexyne) are shown. Asterisks indicate the peaks that have possible identification in the spectra of irradiated ices. (a) From 3200 to 1500  $\text{cm}^{-1}$ . (b) From 1600 to 600  $\text{cm}^{-1}$ .



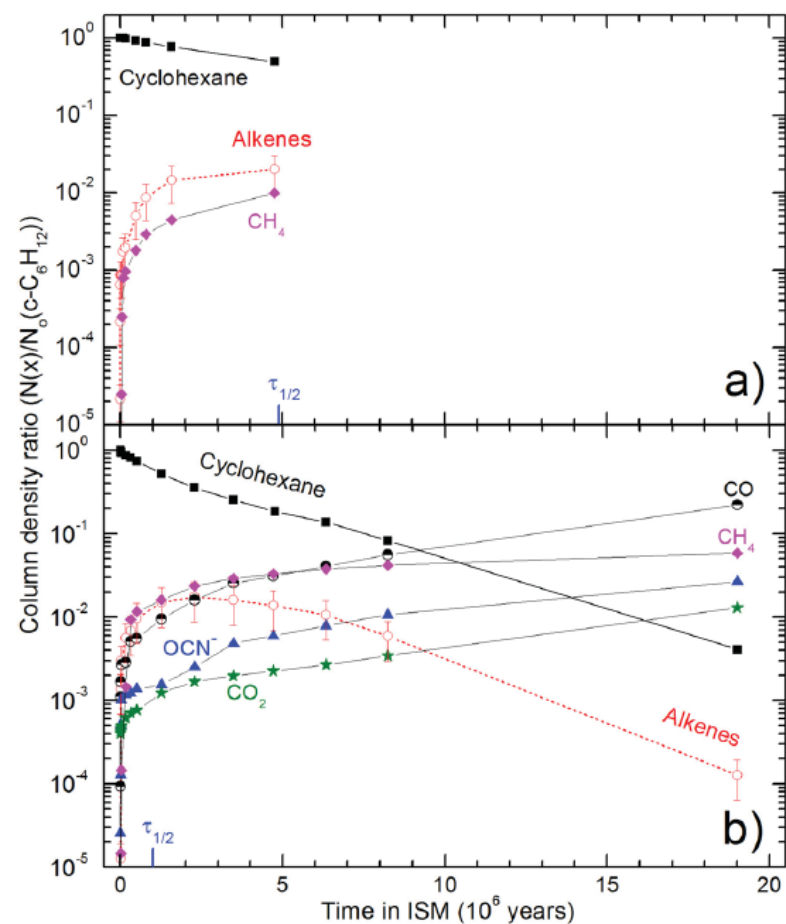
**Figure 2.** FTIR spectra from 4000 to 600  $\text{cm}^{-1}$  of non-irradiated ices at 13 K: mixed  $\text{H}_2\text{O}:\text{NH}_3:\text{c-C}_6\text{H}_{12}$  (1:0.3:0.7) ice (top) and pure  $\text{c-C}_6\text{H}_{12}$  ice (bottom). For comparison, spectra of pure  $\text{H}_2\text{O}$  ice and pure  $\text{NH}_3$  ice are also shown.

No Lab.



**Figure 6.** (a) Variation of the column density of cyclohexane and selected daughter species ( $\text{CH}_4$ ) in pure ice experiment as function of ion (219-MeV O) fluence. (b) Variation of the column density of cyclohexane, water and ammonia and selected daughter species ( $\text{CO}$ ,  $\text{CO}_2$ ,  $\text{CH}_4$  and  $\text{OCN}^-$ ) in mixed ice experiment as a function of ion (632-MeV Ni) fluence. The lines indicate the fittings using equation (4) (pure cyclohexane), equation (5) (cyclohexane and ammonia in mixed ice), equation (6) (water in mixed ice) and equation (7) (products). The model parameters are given in Table 3.

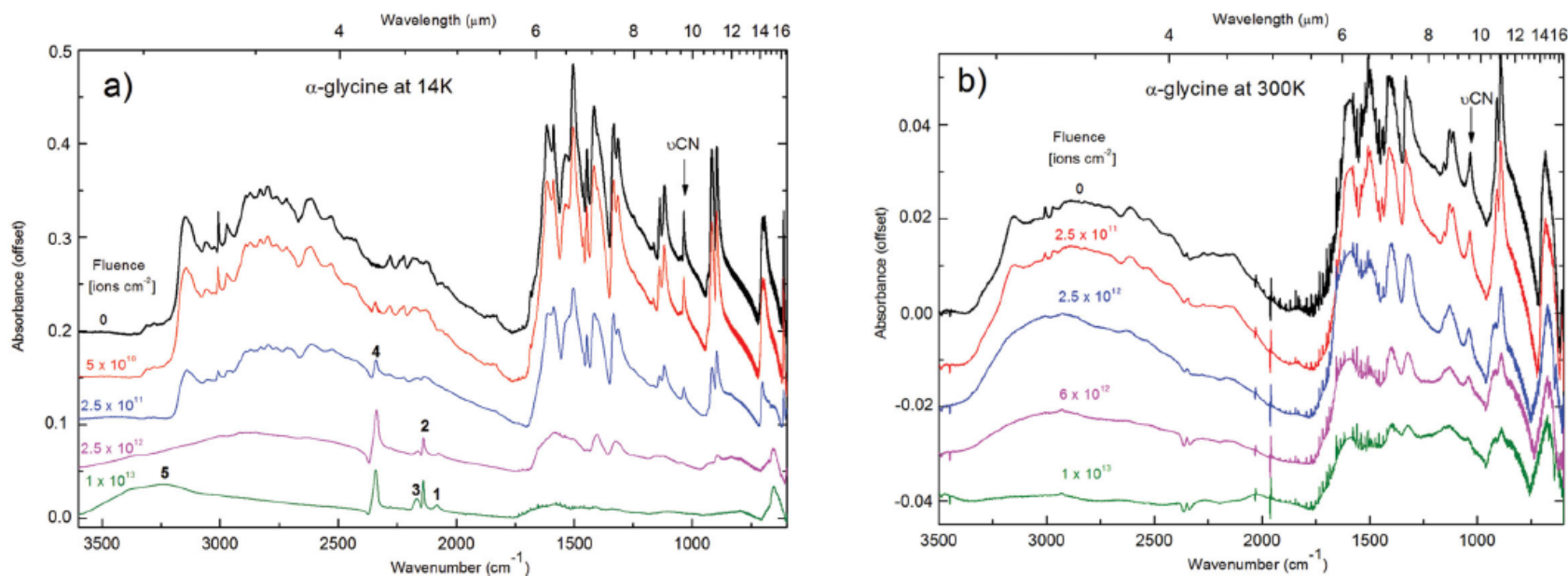
No espaço



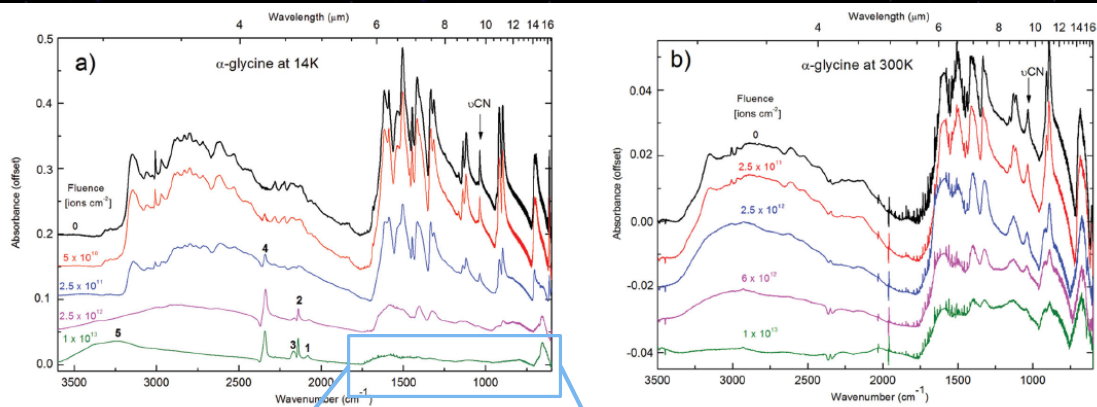
**Figure 7.** Column density ratios of cyclohexane and some radiolysis products over initial cyclohexane column density as function of equivalent cosmic ray exposure time at ISM. (a) Pure  $\text{c-C}_6\text{H}_{12}$  ice at 13 K irradiated by 219-MeV O ions (medium-mass cosmic ray analogue). (b) Mixed  $\text{H}_2\text{O}:\text{NH}_3:\text{c-C}_6\text{H}_{12}$  (1:0.3:0.7) ice at 13 K irradiated by 632-MeV Ni ions (heavy cosmic ray analogue). In each figure, the half-life of cyclohexane ( $t_{1/2}$ ) in ISM as a result of cosmic ray bombardment is indicated. Lines are only to guide the eyes.

## Radiolysis of amino acids by heavy and energetic cosmic ray analogues in simulated space environments: $\alpha$ -glycine zwitterion form

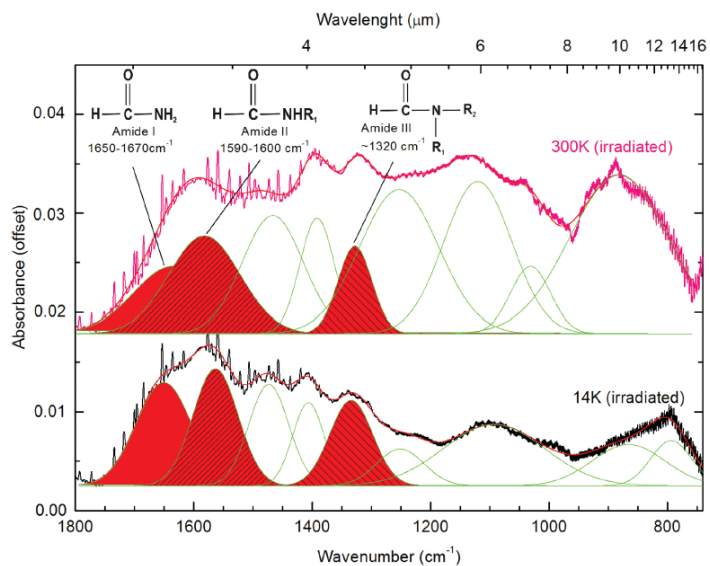
Williamary Portugal,<sup>1</sup> Sergio Pilling,<sup>1\*</sup> Philippe Boduch,<sup>2</sup> Hermann Rothard<sup>2</sup> and Diana P. P. Andrade<sup>1,2</sup>



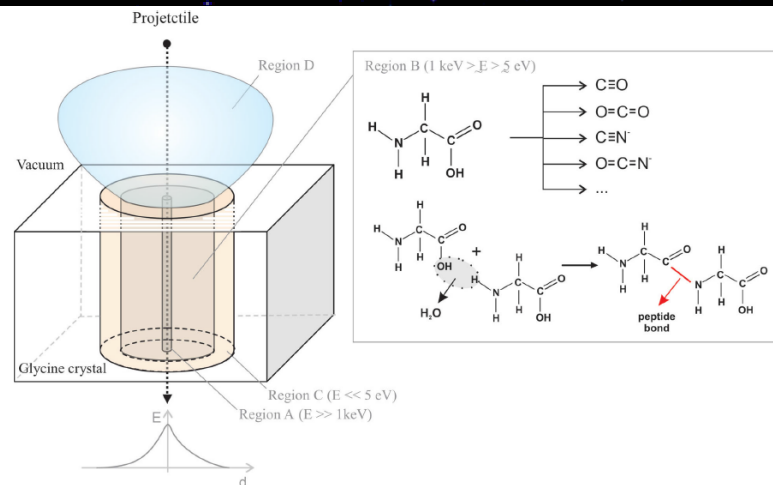
**Figure 2.** Infrared spectra of  $\alpha$ -glycine ( $^+\text{NH}_3\text{CH}_2\text{COO}^-$ ) before (top dark line) and after different irradiation fluences. The arrow on the peak at  $1034\text{ cm}^{-1}$  indicates the location of the CN stretching mode employed to quantify the sample. The peaks of daughter species formed on the irradiated sample at 14 K are indicated by numbers: (1)  $\text{CN}^-$  ( $2080\text{ cm}^{-1}$ ); (2)  $\text{CO}$  ( $2137\text{ cm}^{-1}$ ); (3)  $\text{OCN}^-$  ( $2165\text{ cm}^{-1}$ ); (4)  $\text{CO}_2$  ( $2336\text{ cm}^{-1}$ ); (5)  $\text{H}_2\text{O}$  ( $3280\text{ cm}^{-1}$ ). Samples at (a) 14 K and (b) 300 K.



**Figure 2.** Infrared spectra of  $\alpha$ -glycine ( $^+NH_3CH_2COO^-$ ) before (top dark line) and after different irradiation fluences. The arrow on the peak at  $1034\text{ cm}^{-1}$  indicates the location of the CN stretching mode employed to quantify the sample. The peaks of daughter species formed on the irradiated sample at 14 K are indicated by numbers: (1)  $CN^-$  ( $2080\text{ cm}^{-1}$ ); (2)  $CO$  ( $2137\text{ cm}^{-1}$ ); (3)  $OCN^-$  ( $2165\text{ cm}^{-1}$ ); (4)  $CO_2$  ( $2336\text{ cm}^{-1}$ ); (5)  $H_2O$  ( $3280\text{ cm}^{-1}$ ). Samples at (a) 14 K and (b) 300 K.



**Figure 8.** Expanded view of infrared spectra of the residues produced after the bombardment employing  $1 \times 10^{13}\text{ Ni ion cm}^{-2}$ . Filled curves present tentative assignments of amide bands obtained from a spectral deconvolution employing nine Gaussian profiles, in the range  $1800\text{--}750\text{ cm}^{-1}$ .



**Figure 7.** Schematic diagram of the three different physical-chemical regions surrounding the ion track during the bombardment of the glycine sample (named as regions A, B, C and D). Selected reaction pathways for some daughter species that can occur in region B and a schematic plot of the energy delivered within the sample as a function of the distance of the ion track are also shown. A tentative reaction for eventual production of the peptide bond is also illustrated. See details in the text.



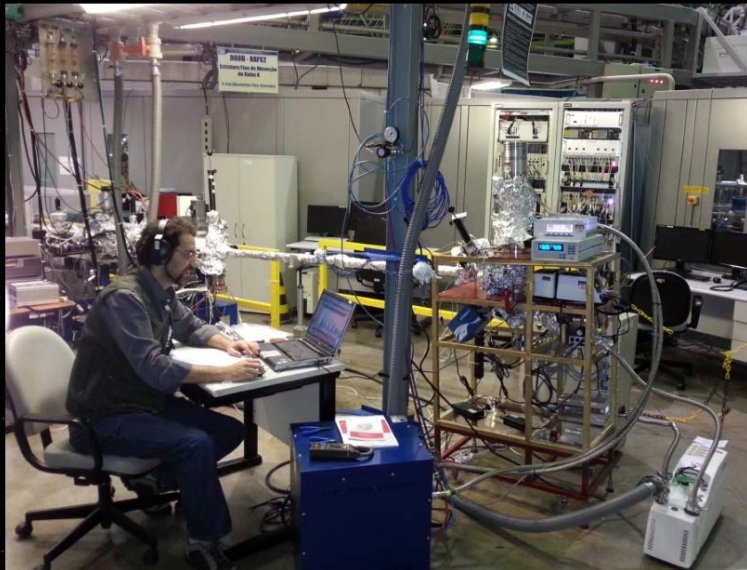
## 2.4 - Experimentos de fotólise com luz Síncrotron (UV, Raios X)

The measurements were performed inside a high vacuum chamber from Astrochemistry and Astrobiology Univap's laboratory (LASA) coupled to SGM beamline at the Brazilian Synchrotron light Source LNLs at Campinas in June of 2013.



Legenda: a) Acondicionamento da câmara STARK para seu transporte para realização de experimentos no LNLs em Campinas, SP; b) Chegada dos equipamentos no LNLs; c) Desempacotamento da câmara STARK dentro do Hall experimental do LNLs; d) Câmara STARK montada na linha SGM do LNLs pronta para início dos experimentos; e) Cilindros de amostras e detectores de gases do LASA acoplados a câmara STARK; f) Teste da linha de gás da câmara STARK; g) Equipe do LASA realizando os experimentos no LNLs; h) Eletrônica dos controladores de pressão e temperatura da câmara

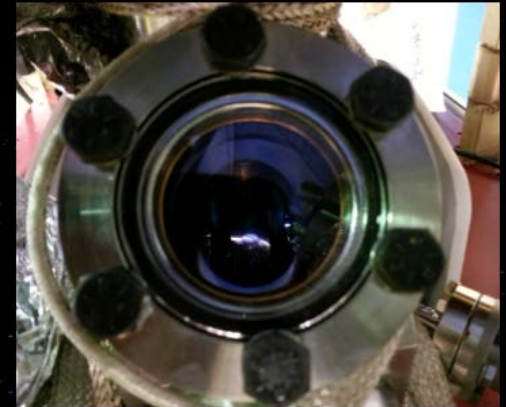
## 2.4.1 Simulação da lua Europa



Sample preparation



Sample irradiation



The gas samples were deposited onto a ZnSe substrate at 13 K and then heated (when was the case) to specific temperatures to be irradiated. *In-situ* analysis were performed by a **Fourier transform infrared (FTIR)** spectrometer at different photon fluences. Cross section, photolysis yield and half-lives of the produced species were quantified.

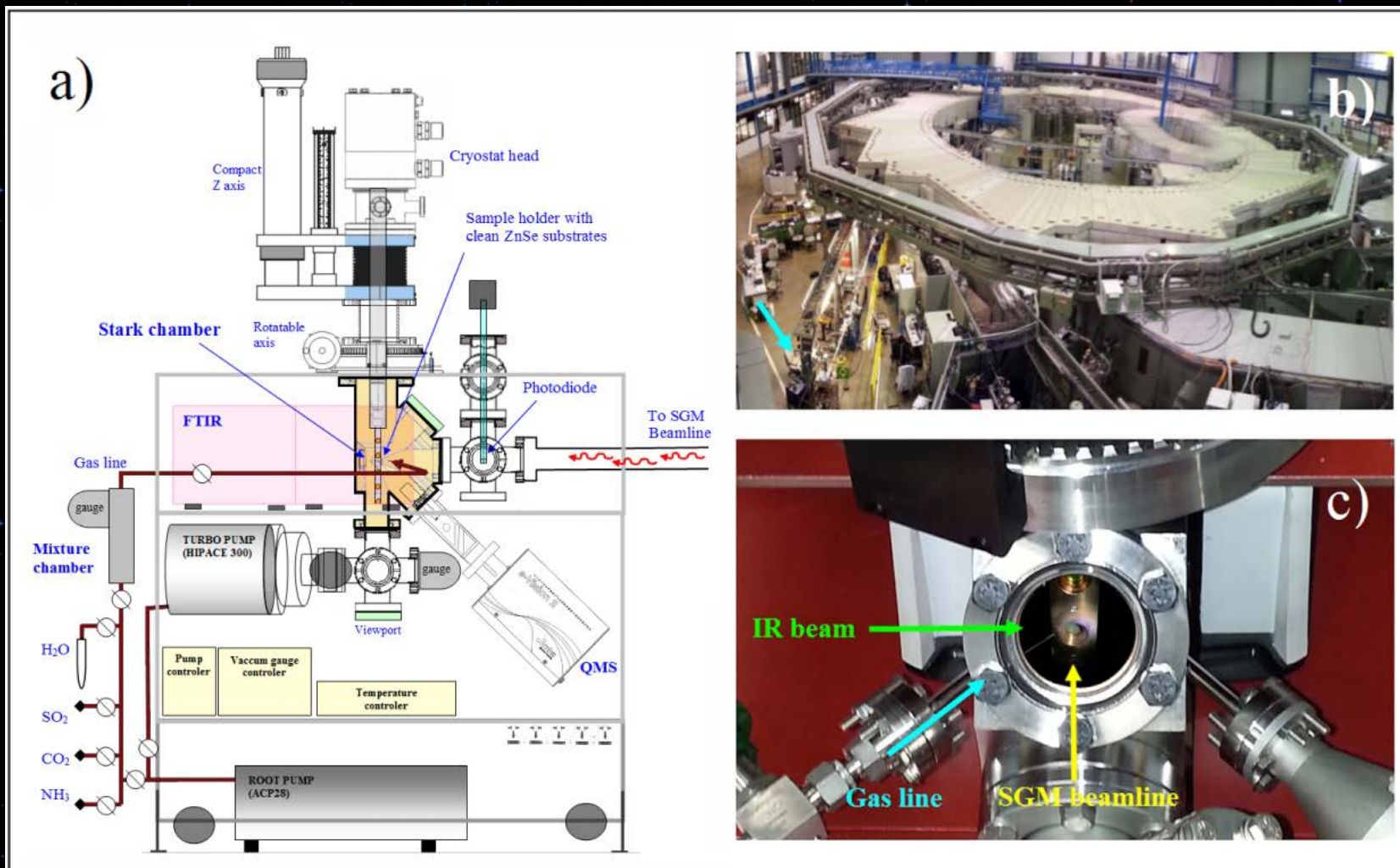


Figure 1. a) Diagram of the experimental setup (Stark chamber). b) Picture of the experimental hall of the Brazilian synchrotron source (LNLS) with the experimental chamber coupled at the SGM beam line (arrow). c) Picture showing the Europa surface analog inside the chamber ready to be irradiated by synchrotron light.

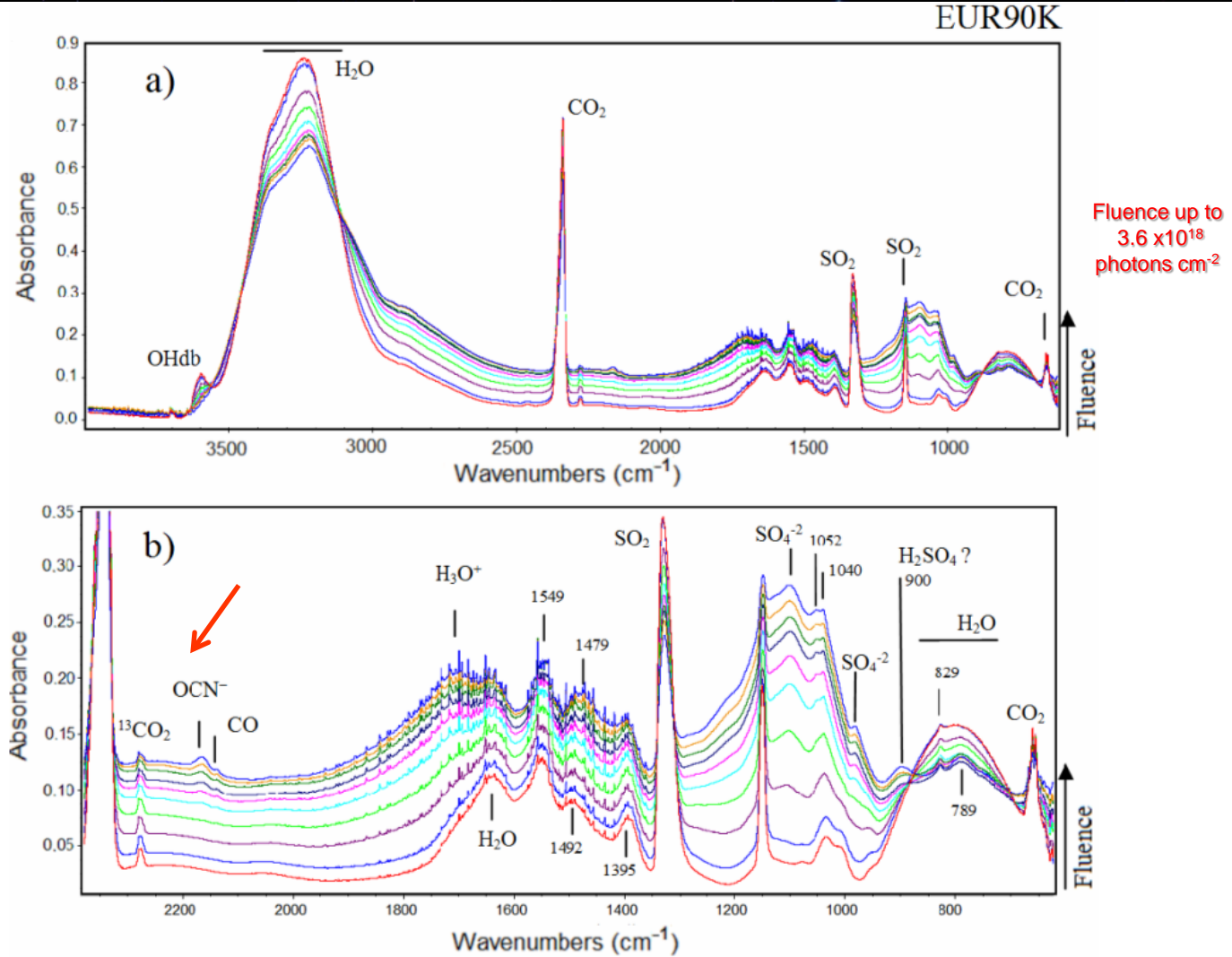
# Irradiation of the Europa surface analog by X-rays.

doi:10.1088/0004-637X/811/2/151

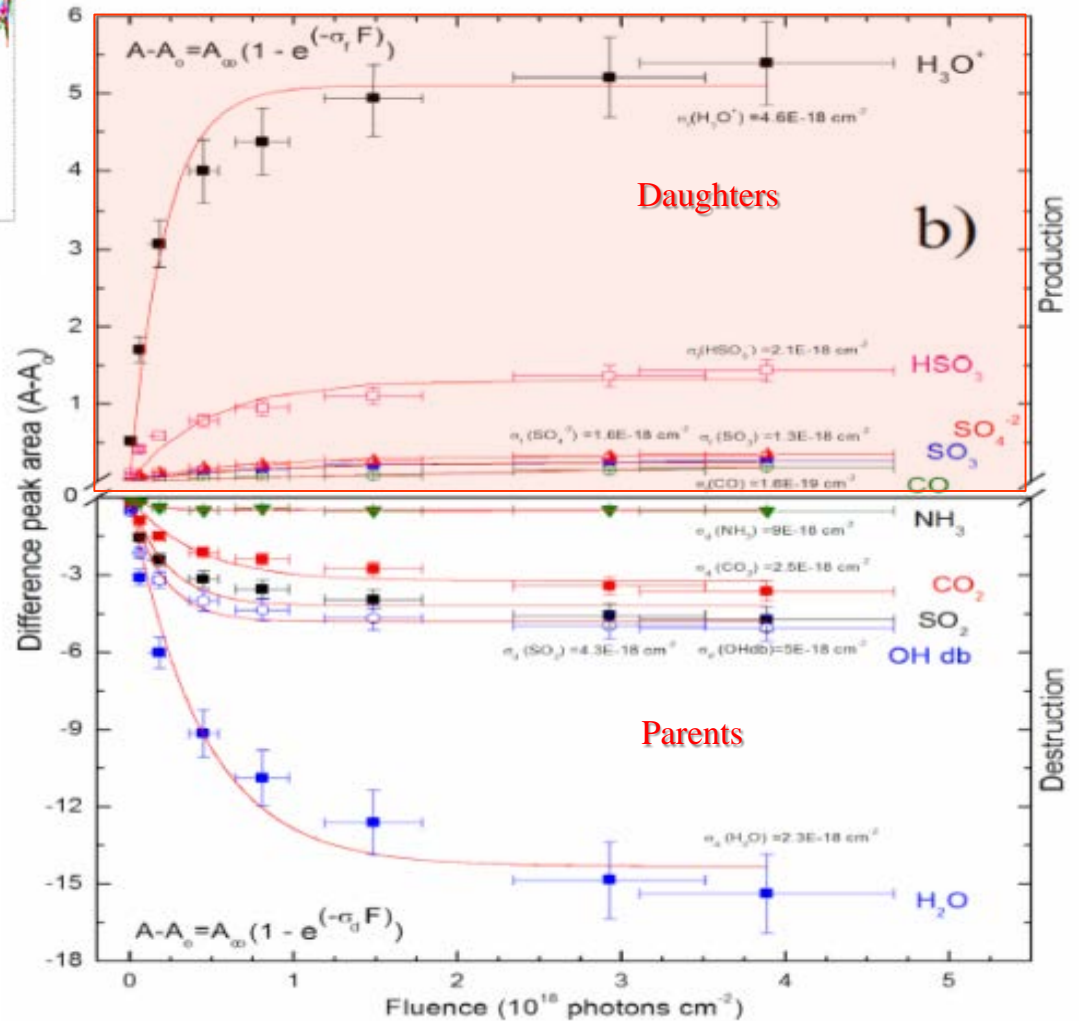
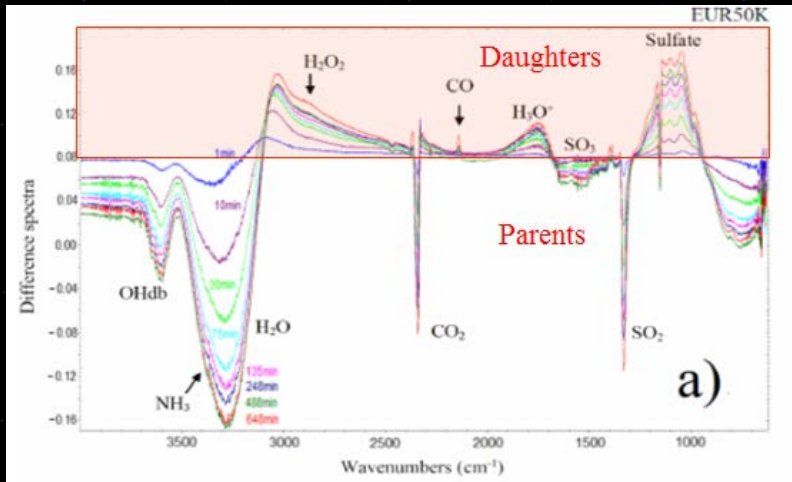
THE ASTROPHYSICAL JOURNAL, 811:151 (22pp), 2015 October 1  
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## THE EFFECT OF BROADBAND SOFT X-RAYS IN SO<sub>2</sub>-CONTAINING ICES: IMPLICATIONS ON THE PHOTOCHEMISTRY OF ICES TOWARD YOUNG STELLAR OBJECTS

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Received 2015 May 12; accepted 2015 August 31; published 2015 September 30



# Absolute formation and dissociation cross sections (e.g. EUR 50K).



# Absolute formation and dissociation cross sections.

**Table 4 - Dissociation cross sections and dissociation rate for parental species in Europa surfaces simulation considering photons between 6 to 1200 eV (mostly soft X-rays). Half-life obtained in the lab are also given. The uncertainty was estimated to be around 20%**

	EUR50K			EUR90K		
	$\sigma_d$ (cm <sup>2</sup> )	$k_{lab}$ (s <sup>-1</sup> )	$t_{1/2}$ (lab) <sup>a</sup> [10 <sup>3</sup> s]	$\sigma_d$ (cm <sup>2</sup> )	$k_{lab}$ (s <sup>-1</sup> )	$t_{1/2}$ (lab) <sup>a</sup> [10 <sup>3</sup> s]
H <sub>2</sub> O <sup>b</sup>	3E-18	3E-4	2.3	7.0E-18	7.0E-4	9.9
CO <sub>2</sub>	2.2E-18	2.2E-4	3.1	3.0E-18	3.0E-4	2.3
NH <sub>3</sub>	~6E-18	~6E-4	~1	~2E-18	~2E-4	~3
SO <sub>2</sub>	4.3E-18	4.3E-4	1.6	4.0E-18	4.0E-4	1.7

<sup>a</sup>Considering the half-life  $t_{1/2} = \ln(2)/k$ , where  $k$  is the photodissociation rate in units of s<sup>-1</sup> (see Table 4).

<sup>b</sup>For OHdb the destruction cross sections are  $5 \times 10^{-18}$  cm<sup>2</sup> and  $8 \times 10^{-18}$  cm<sup>2</sup> for exp EUR50K and EUR90K, respectively.

**Table 5 - Formation cross sections and formation rate for selected parental species in Europa surfaces simulation considering photons between 6 to 1200 eV. The uncertainty was estimated to be around 20%.**

$$k = \sigma \times \phi \quad [s^{-1}]$$

	EUR50K		EUR90K	
	$\sigma_f$ (cm <sup>2</sup> )	$k_{lab}$ (s <sup>-1</sup> )	$\sigma_f$ (cm <sup>2</sup> )	$k_{lab}$ (s <sup>-1</sup> )
H <sub>3</sub> O <sup>+</sup>	4.6E-18	4.6E-04	4E-18	4E-04
H <sub>2</sub> O <sub>2</sub>	-	-	9E-19	9E-05
HSO <sub>3</sub> <sup>-</sup>	2.1E-18	2.1E-04	4E-18	4E-04
SO <sub>3</sub>	1.3E-18	1.3E-04	-	
SO <sub>4</sub> <sup>-2</sup>	1.6E-18	1.6E-04	2E-17	2E-03
CO	1.6E-19	1.6E-05	9E-19	9E-05
OCN <sup>-</sup>	-	-	7E-20	7E-06
1470 cm <sup>-1</sup>	-	-	9E-19	9E-05

# 2.4.2 Destruição de aminoácidos e bases nitrogenadas em ambientes espaciais

## Photostability of gas- and solid-phase biomolecules within dense molecular clouds due to soft X-rays

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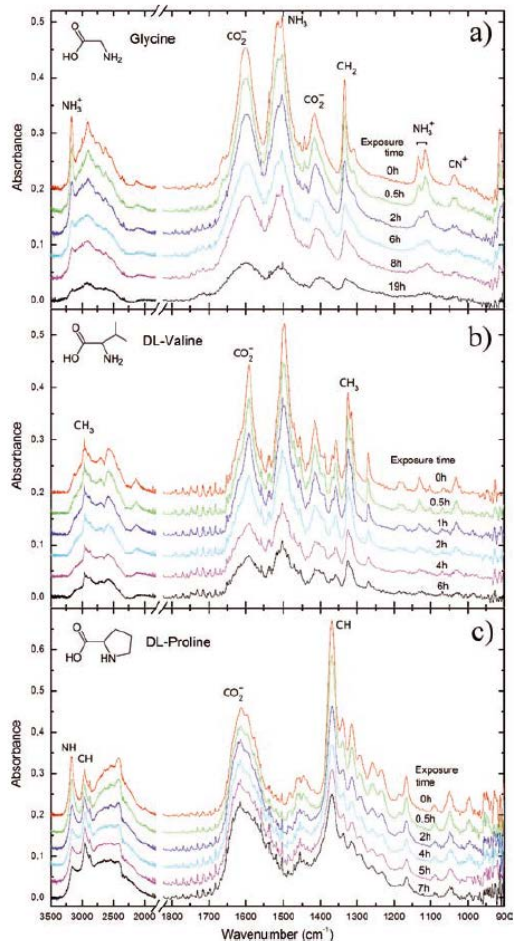


Figure 3. Photostability of the solid-phase amino acids due to the exposure of 150-eV soft X-rays photons as a function of time.

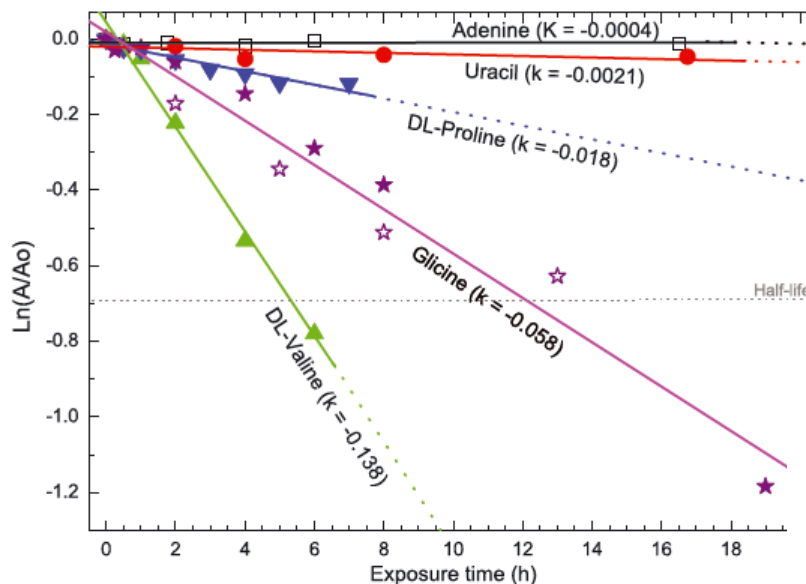


Figure 5. Integrated absorbance spectra of the solid-phase samples as a function of irradiation time. For each compound, the photodissociation rate  $k$ , is also indicated.

Table 2. Comparison between the half-lives values of solid-phase amino acids and nucleobases in dense clouds due to UV cosmic ray induced flux and soft X-ray flux.

Samples	Half-life in dense clouds (Myr)	
	UV <sup>a</sup>	Soft X-rays <sup>b</sup>
Glycine	1.84 <sup>c</sup>	0.7 <sup>d</sup>
DL-Valine	–	0.3
DL-Proline	–	2
Adenine	8.27 <sup>c</sup>	90 <sup>d</sup>
Uracil	2.03 <sup>c</sup>	20 <sup>d</sup>

<sup>a</sup> Assuming a cosmic ray induced UV flux of  $10^3$  photons  $\text{cm}^{-2} \text{s}^{-1}$  (Prasad & Tarafdar 1983).

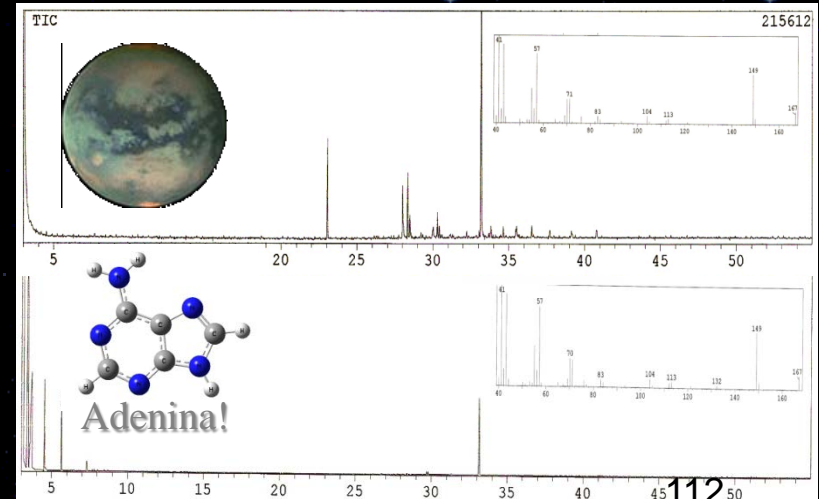
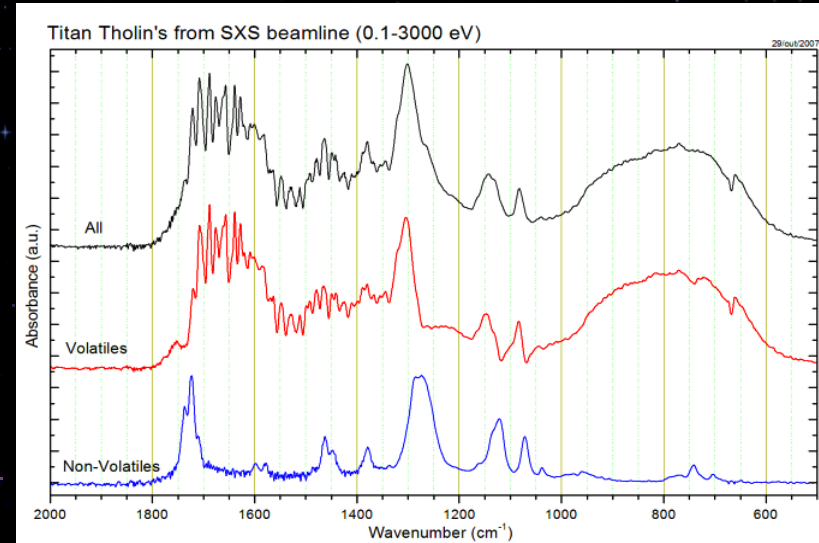
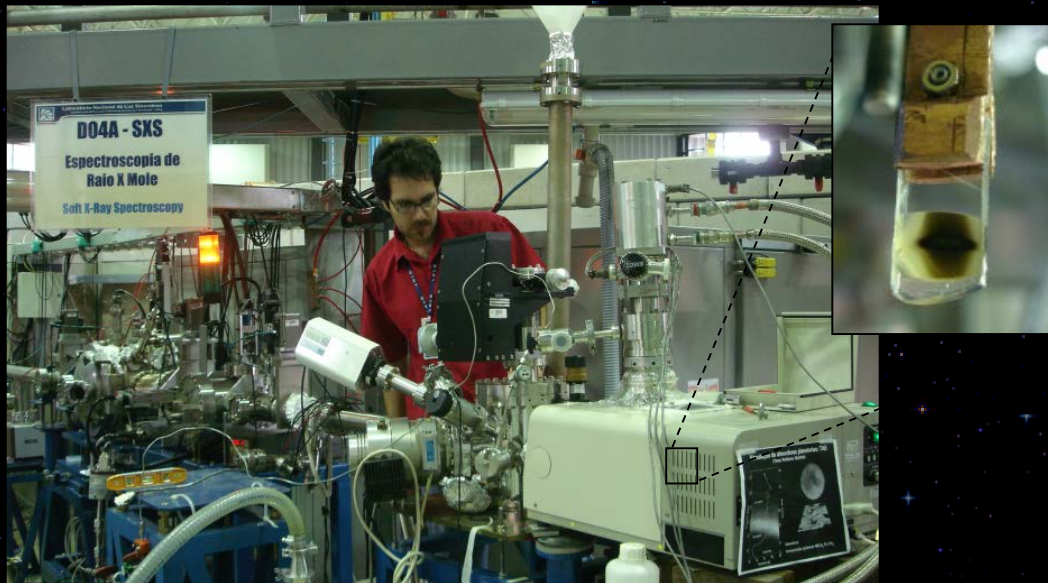
<sup>b</sup> Assuming a 150 eV photon flux of  $3 \times 10^6$  photon  $\text{cm}^{-2} \text{s}^{-1}$  (for AFGL 2591, at 200 au from the X-ray source; Stauber et al. 2005).

<sup>c</sup> Pure compounds at 12 K in Argon matrix; Peeters et al. (2003).

<sup>d</sup> Pure compounds at room temperature; this work.

## 2.4.3 - Produção de Adenina em ambientes extraterrestres simulados (Lua Titã)

- Simulação de Aerossóis na atmosfera de Titã.
- $N_2$  95% +  $CH_4$  5% (+ traços  $H_2O$ ):  $10^{-6}$  mbar
- SXS (white beam; 0.5-3keV;  $\sim 10^{12}$  fótons/cm s)
- Cryo-IR $_{\beta}$  (NaCl; 12 K  $10^{-8}$  mbar)
- *In-situ* FTIR, *in-situ* Q-MS, GC-TOFMS, RMN
- Adenina via elétrons secundários.

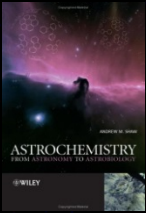




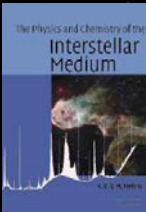
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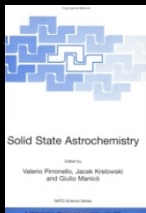


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Continuamos na próxima aula.