

IV Escola de Inverno de Física

Programa de Pós-Graduação em Física

25 a 29 de julho de 2011 - Instituto de Física da UFBA - Salvador - Bahia



Minicurso:

Astroquímica e Astrobiologia

Sergio Pilling

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Aula 1:

A Evolução Química do Universo:

Nucleossínteses, Evolução estelar, Meio interestelar, Moléculas.

Aula 2:

Astroquímica:

Observações (IR e Radio) e experimentos.

Aula 3:

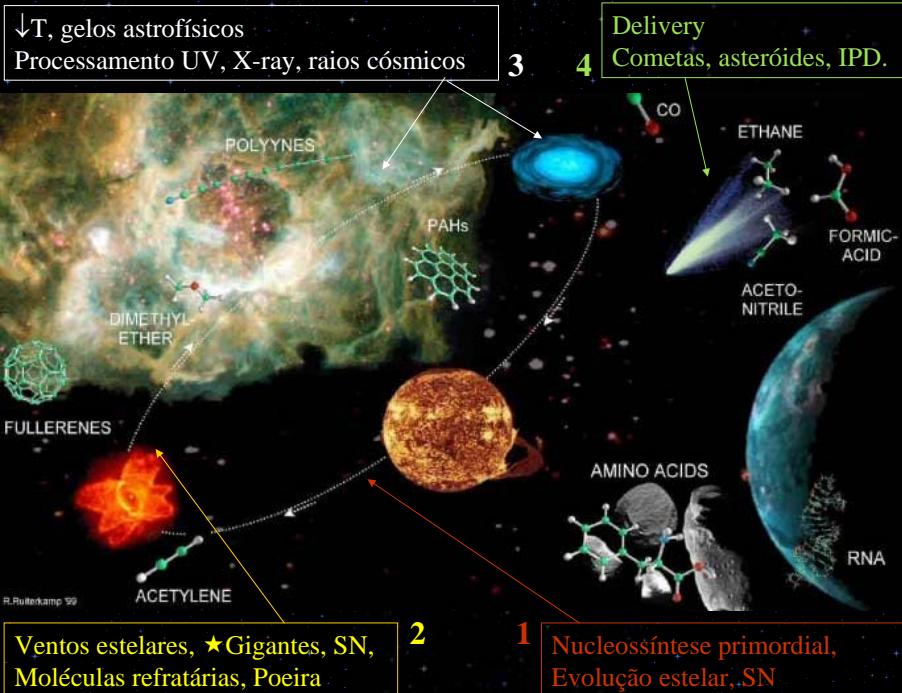
Astrobiologia:

Exoplanetas, habitabilidade, panspermia, extremofilos.

Aula 2:

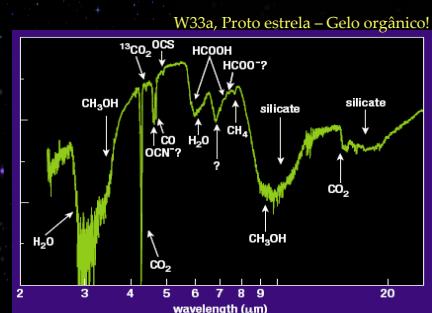
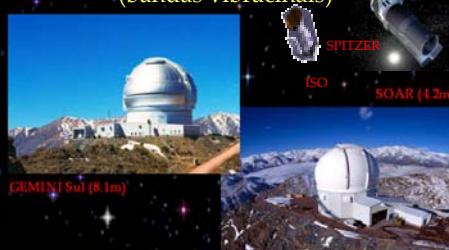
Astroquímica:

Observações (IR e Rádio) e experimentos.

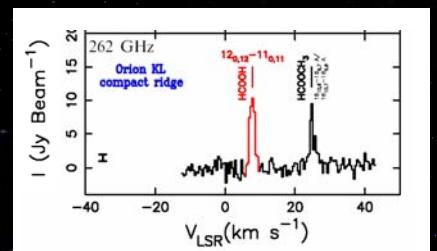


Como essas moléculas são detectadas?

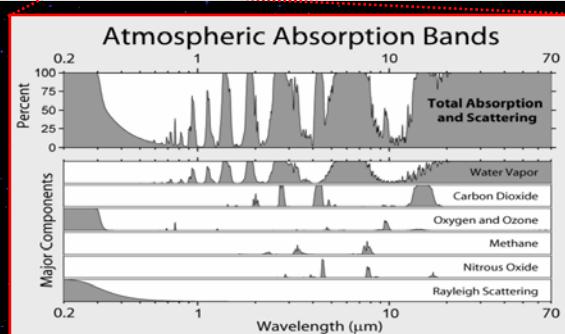
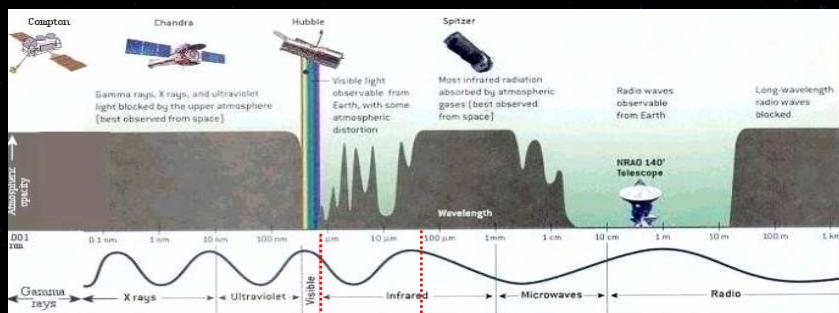
Telescopios Infravermelhos (bandas vibracionais)



Radiotelescopios (linhas rotacionais)



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)

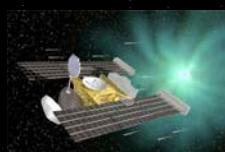
ISO (1995-1998)



Spitzer (2003-2009)



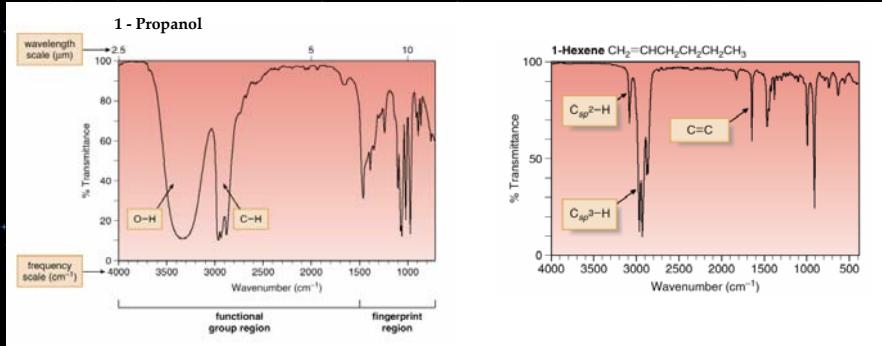
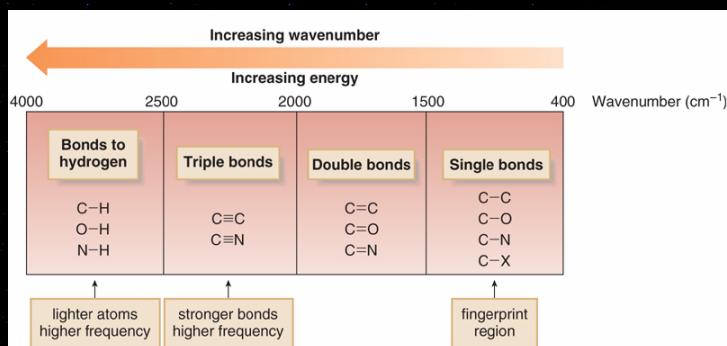
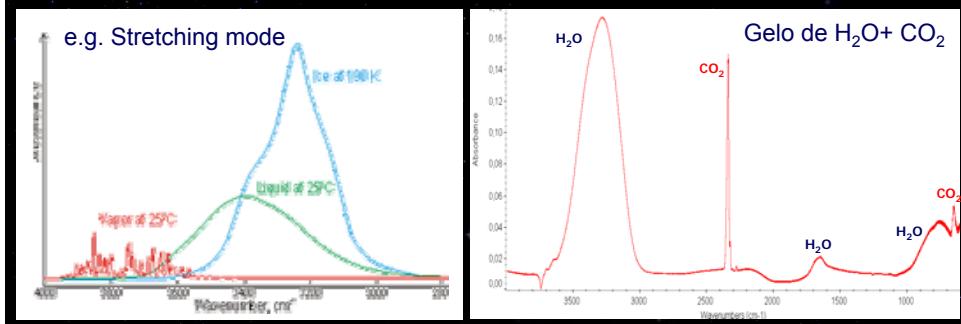
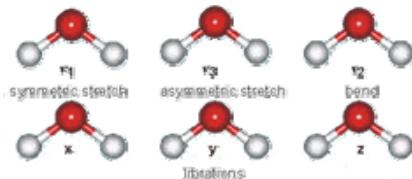
HST(1999, ...)



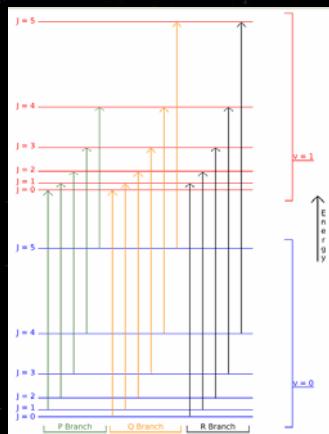
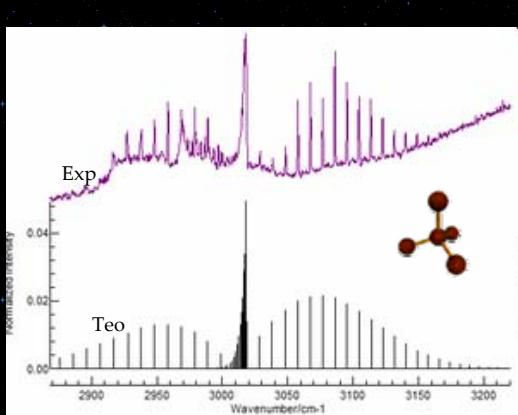
Ex. Stardust, Cassini, Mars Rovers

Spacecrafts

Espectroscopia Molecular no IR – Bandas vibracionais (GELO)



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



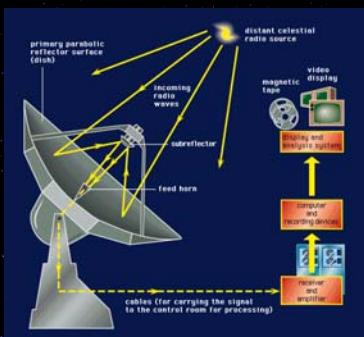
<http://web.mit.edu/5.33/www/lec/spec5.pdf>

http://www.ias.ac.in/initiat/sci_ed/resources/chemistry/rotational.pdf

Observatórios Microondas e Radio



Single Dishes



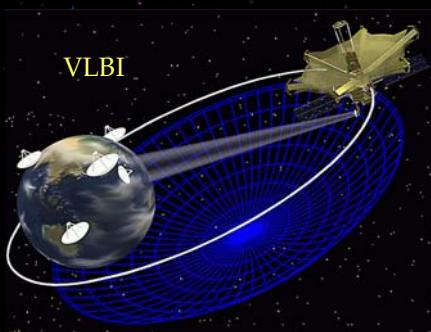
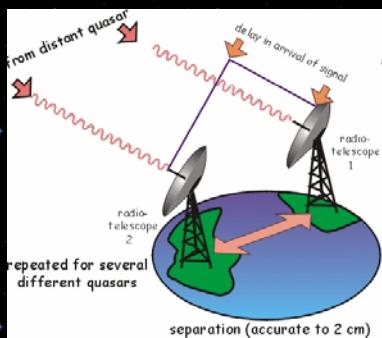
305-meter Arecibo



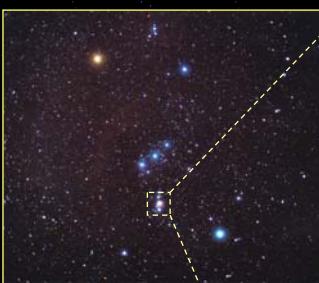
100-Meter Green Bank Radio Telescope

Observatórios Microondas e Radio

Multi-dishes Inferferometry



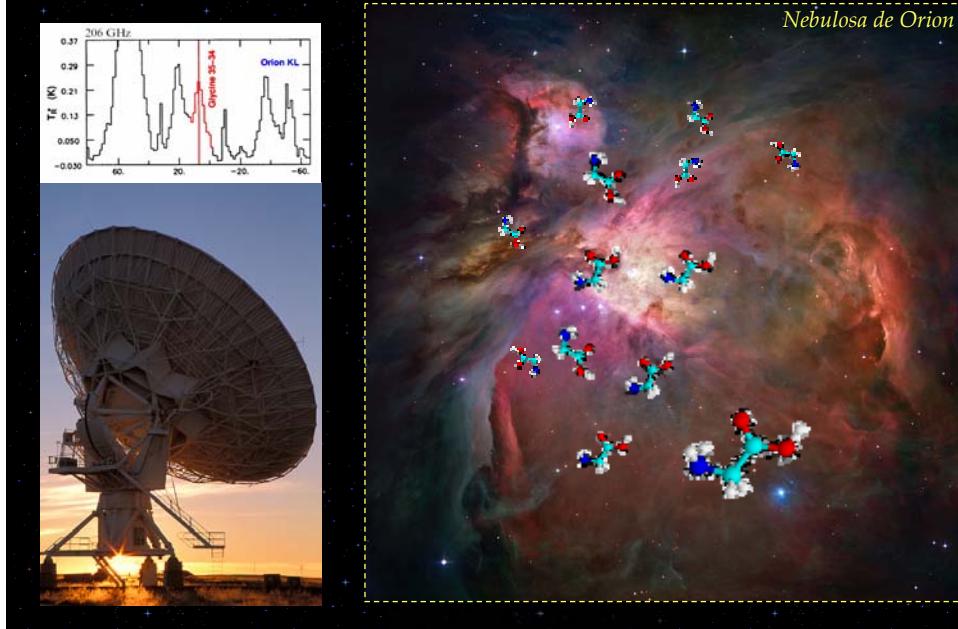
Nuvens moleculares: berçário estelar



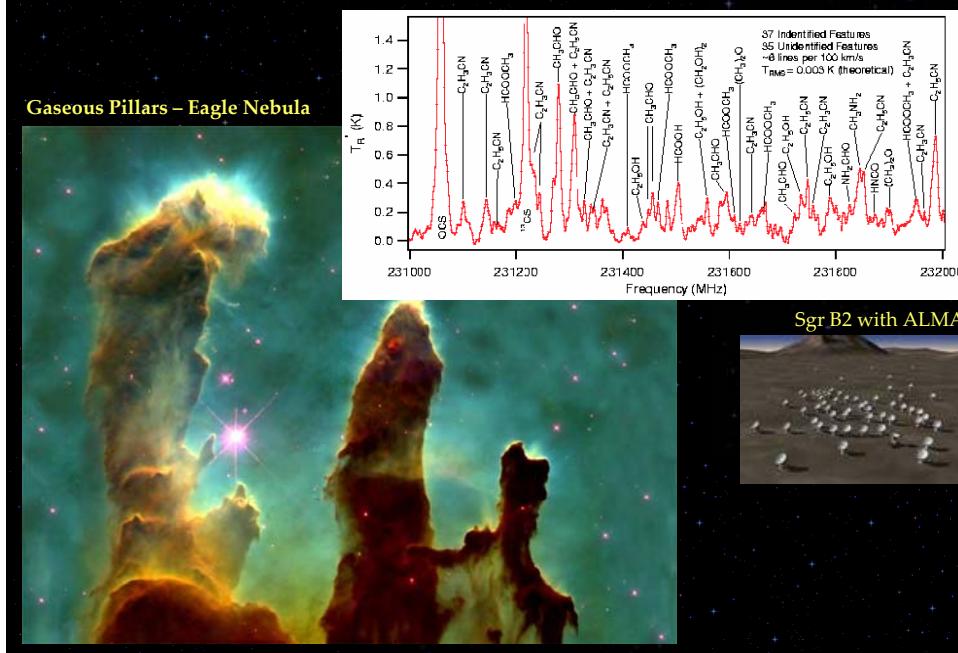
Nebulosa de Orion



Nuvens moleculares: berçário estelar

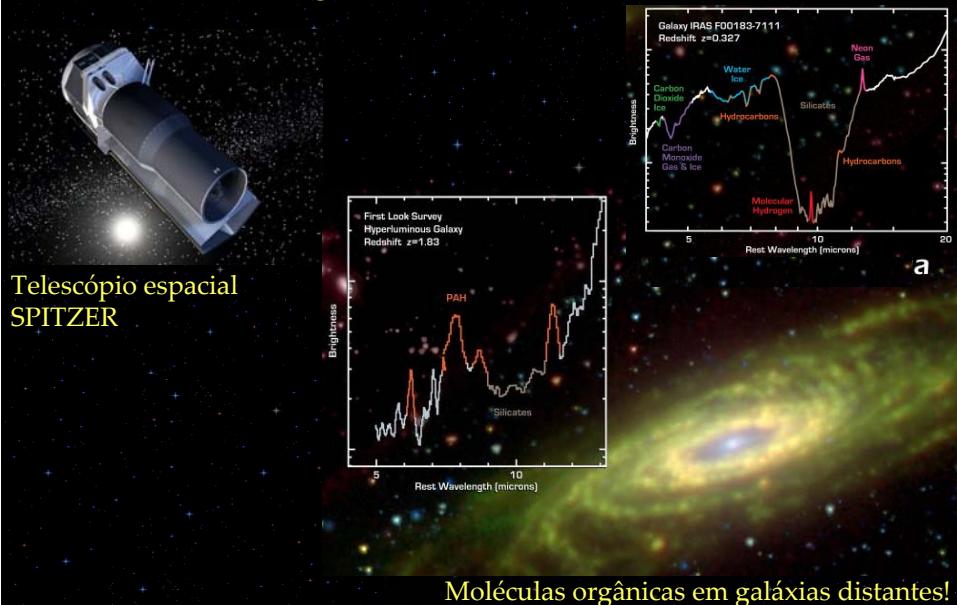


Aonde mais essas moléculas são encontradas?



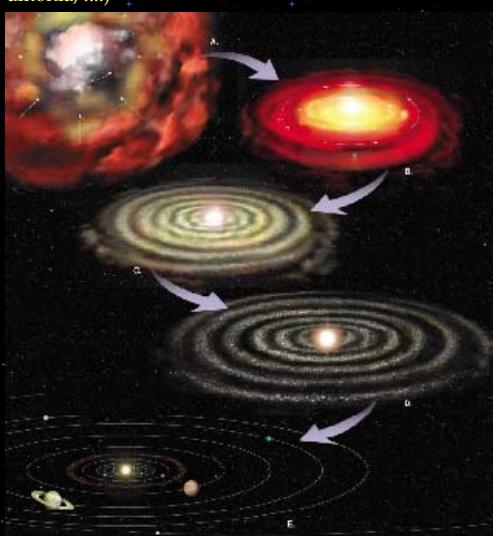
Moléculas em Galáxias distantes.

1ª moléculas orgânicas (~ 3.5 bi)



Moléculas em discos protoplanetários (gas e gelos)

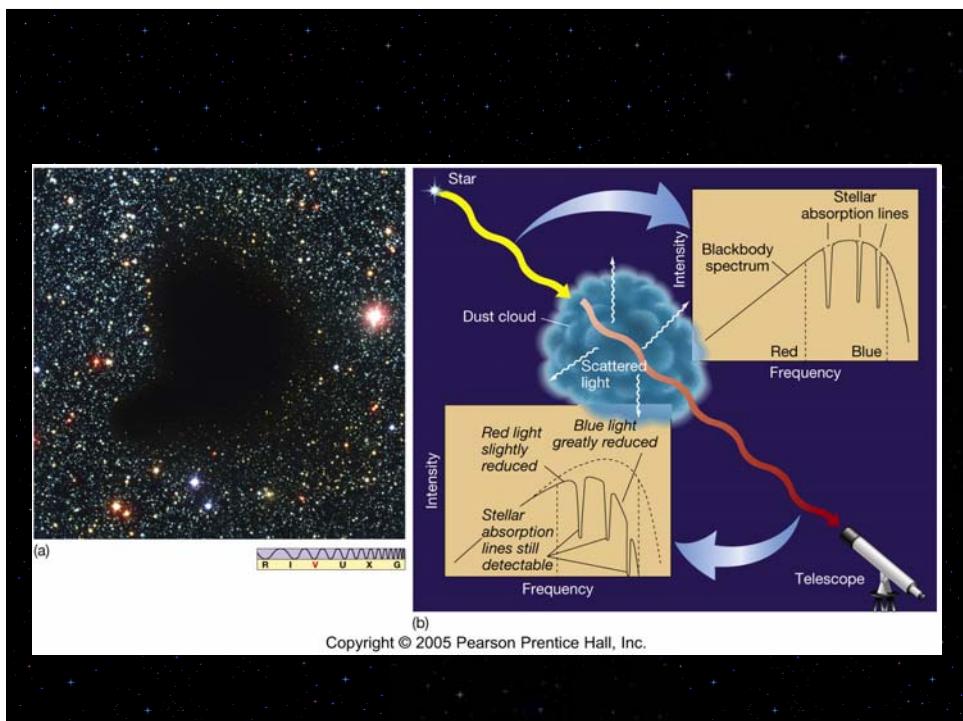
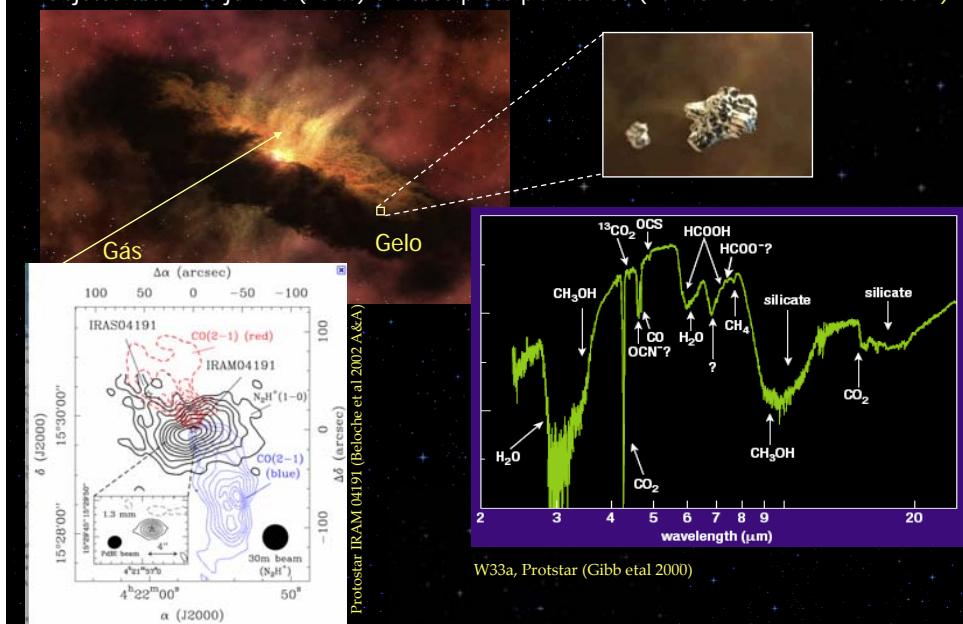
Nuvem de átomos (ex. H, He, C, N, O, ...) e moléculas (ex. H₂, silicatos, água, CO, CO₂, etanol, acetona, amônia, ...)



Sistemas planetários, cometas, etc.

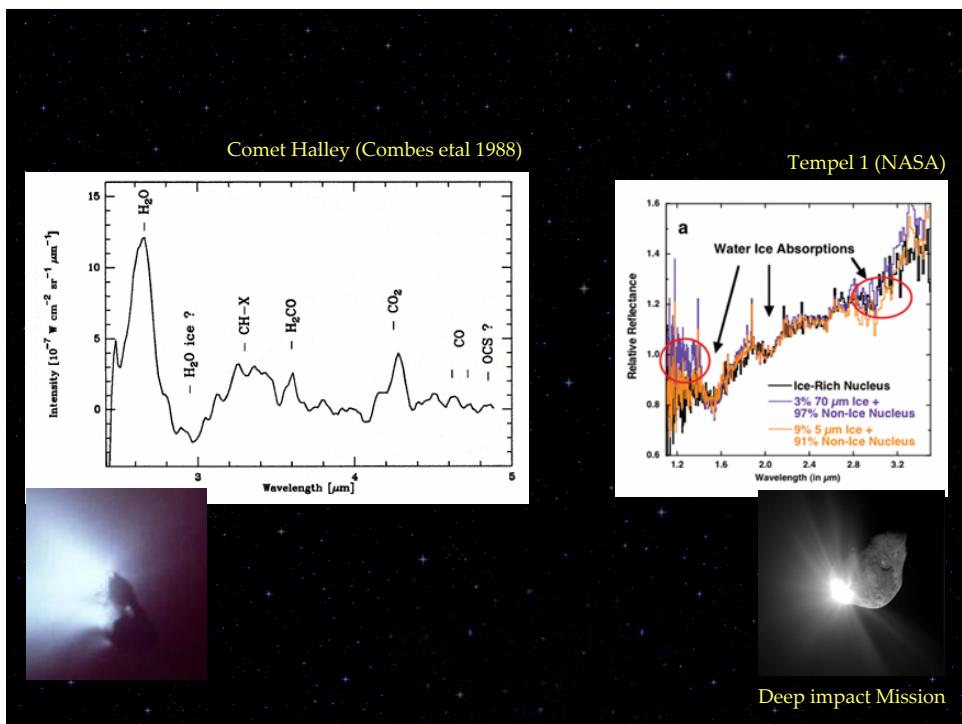
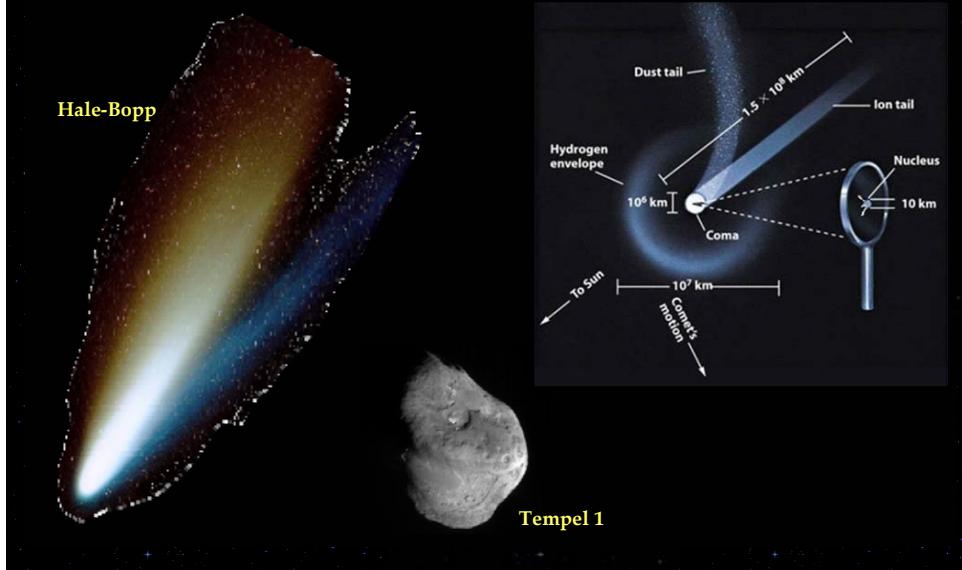
Moléculas em discos protoestelares

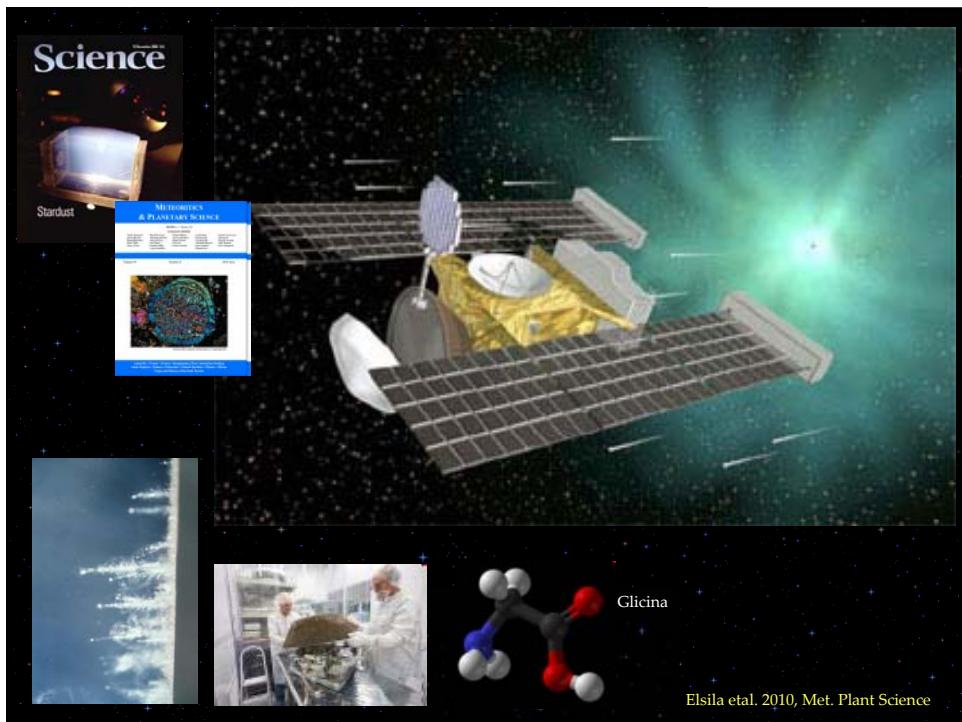
• Objetos estelares jovens (YSOs) e discos proto planetários ($N \sim 10^4\text{-}10^8 \text{ cm}^{-3}$; $T \sim 10\text{-}50 \text{ K}$)



Moléculas em cometas

- Cometas (~80% água, CO, CO₂, CH₄, ...)





Moléculas e gelos extraterrestres: outras evidências observacionais

- Luas e Planetas.

Artist impressions of Enceladus



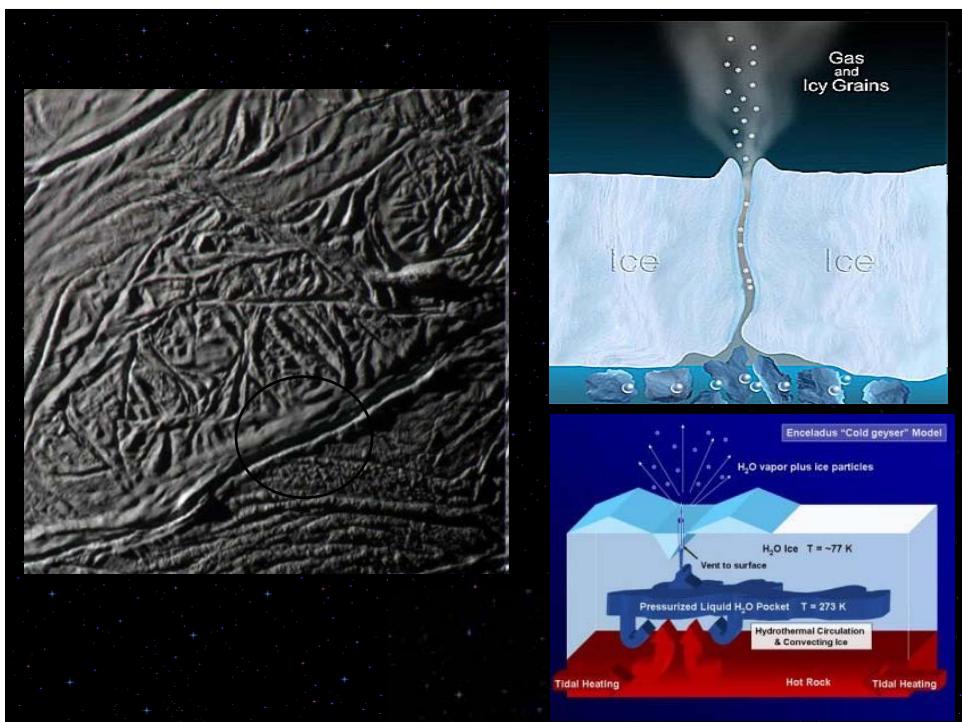
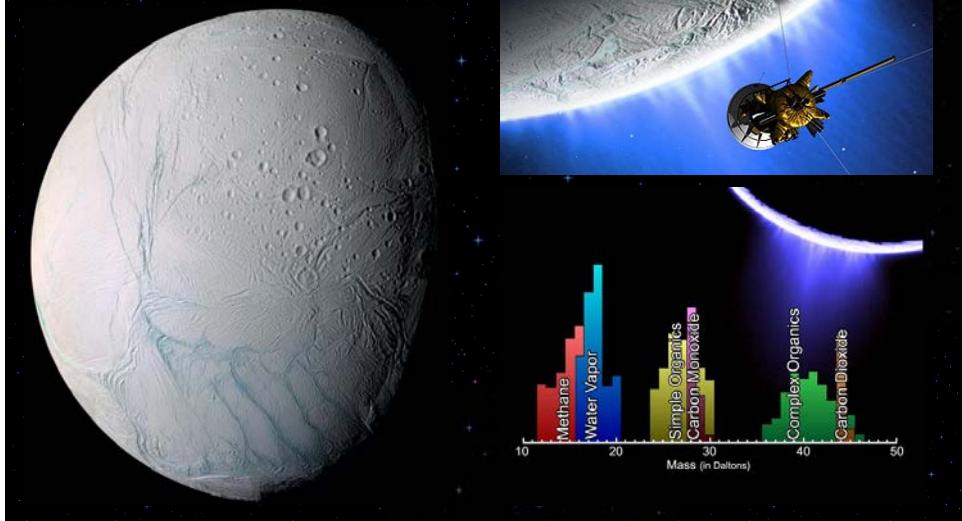
Table 1. Ices in the Solar System.

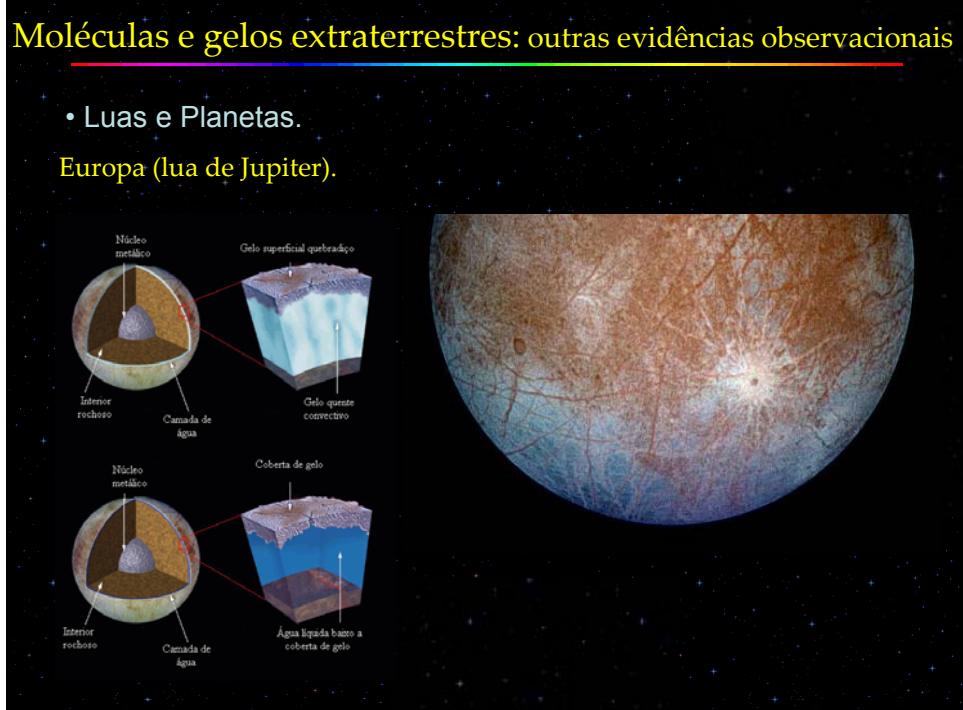
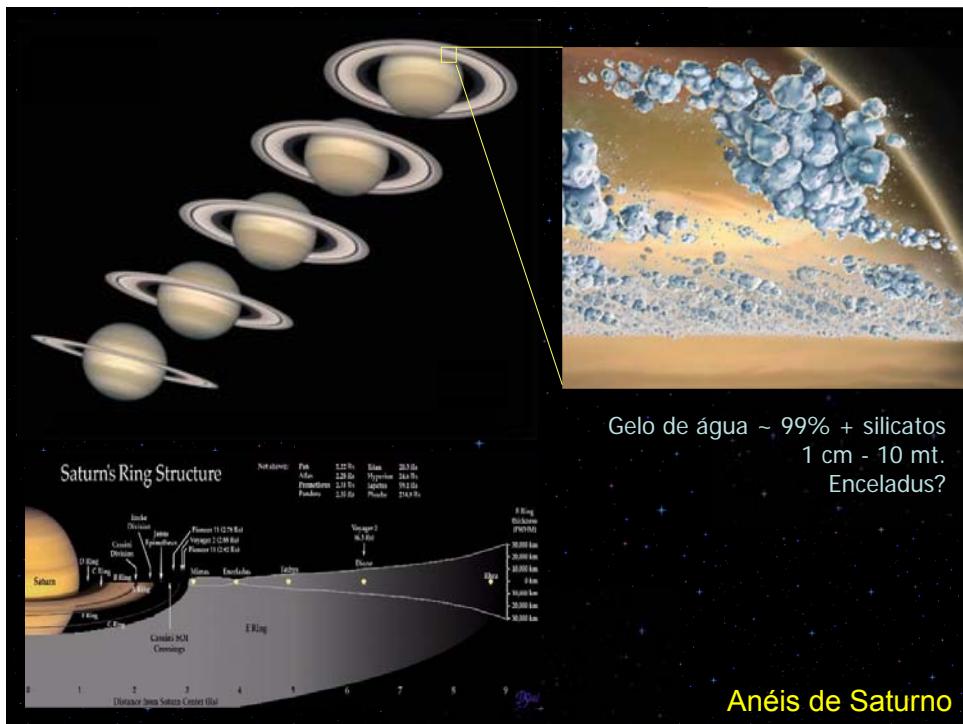
Planet (Ref.)	Observed Species
Jupiter	
Io	SO ₂ , H ₂ S, H ₂ O
Europa	H ₂ O, SO ₂ , CO ₂ , H ₂ O ₂
Ganimede	H ₂ O, O ₂ , O ₃ , CO ₂
Callisto	H ₂ O, SO ₂ , CO ₂
(Cahen et al. 1995; Nash and Betts 1995)	
Saturn	
Mimas	H ₂ O
Enceladus	H ₂ O
Tetis	H ₂ O
Dione	H ₂ O, O ₃
Rhea	H ₂ O, O ₃
Hyperion	H ₂ O
Iapetus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

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

- Luas e Planetas.

Enceladus (lua de Saturno).

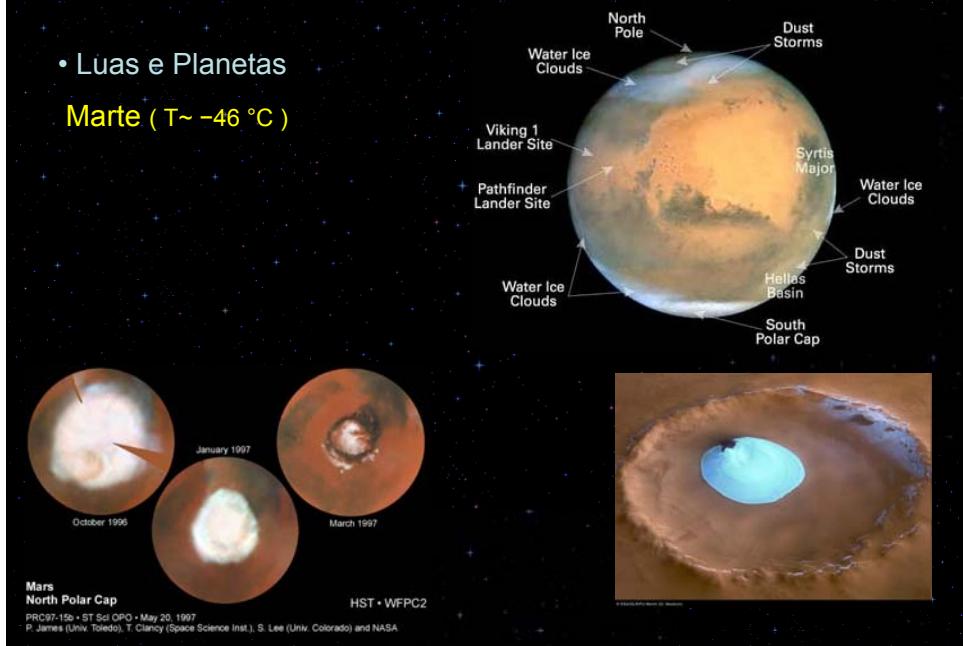




Moléculas e gelos extraterrestres: outras evidências observacionais

- Luas e Planetas

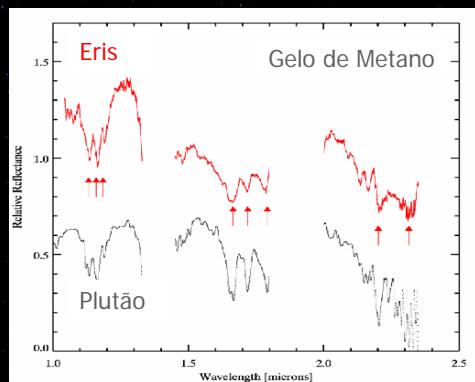
Marte ($T \sim -46^{\circ}\text{C}$)



Moléculas e gelos extraterrestres: outras evidências observacionais

- Planetas anões

Plutão e Eris

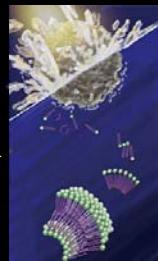


Aonde mais essas moléculas são encontradas?

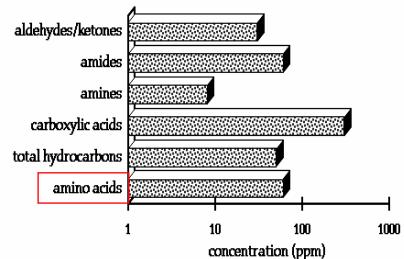


Murchison meteorite

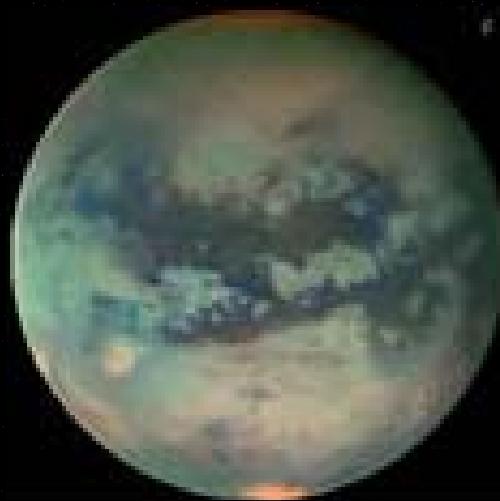
- Aminoácidos
- Bases de DNA.
- Açúcares
- Precursores de Fosfolipídios →



	Sugars	Sugar Alcohols	Sugar Acids	Dicarboxylic Sugar Acids
3C	CH_2OH $\text{H}=\text{C}-\text{OH}$ CH_2OH	CH_2OH $\text{H}=\text{C}-\text{OH}$ CH_2OH	CO_2H $\text{H}=\text{C}-\text{OH}$ CH_2OH	—
4C	—	CH_2OH $\text{H}=\text{C}-\text{OH}$ $\text{H}=\text{C}-\text{OH}$ CH_2OH	CO_2H $\text{H}=\text{C}-\text{OH}$ $\text{HO}-\text{C}-\text{H}$ CO_2H	$\text{HO}-\text{C}-\text{H}$
5C	—	CH_2OH $\text{H}=\text{C}-\text{OH}$ $\text{H}=\text{C}-\text{OH}$ CH_2OH	CO_2H $\text{H}=\text{C}-\text{OH}$ $\text{H}=\text{C}-\text{OH}$ CH_2OH	Tetrahydro & Hexahydro Monocarboxylic acid
	Ethylenetriol & Threitol	Ethylenetriol & Threitol		
	Ribitol isomers	Ribitol isomers		2,3,4-Trihydroxy Pentenoic acid

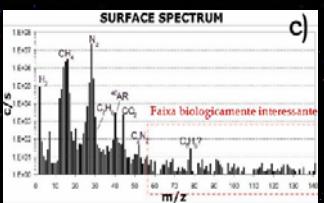
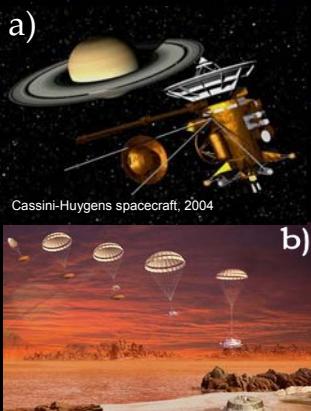


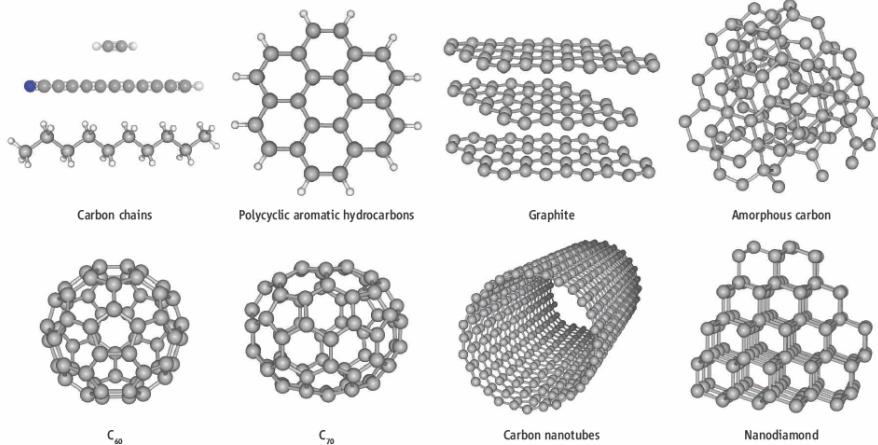
Moléculas em outros planetas



Titã

Metano e gelo de água fazem o papel da água e silicatos na terra.
 $T_{\text{sup}} \sim 100\text{K}$, $P_{\text{sup}} \sim 1.5\text{ atm}$.





Carbon in space. The evidence for interstellar C_{60}^+ and detection of neutral C_{60} and C_{70} fullerene compounds in T_c 1 boosts the number of carbon allotropes present in space. Nanodiamonds and graphite are found in meteorites. Amorphous carbon may represent the main component of the solid-state carbon fraction in low-density interstellar regions. Future

observations and laboratory data may lead to the identification of other fullerene compounds, such as carbon nanotubes or carbon onions. Polyynes (carbon chains) and polycyclic aromatic hydrocarbons (PAHs) are observed ubiquitously in space and are likely involved in the process of fullerene formation.

Universo Molecular!

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

Diatomeric	Tratomic	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms	13 atoms
H ₂	C ₃	c-C ₂ H	C ₆	C ₆ H	C ₆ H	CH ₂ C ₂ N	CH ₃ C ₂ H	CH ₃ C ₃ N	HC ₃ N	HC ₁₁ N
AlF	C ₂ H	I-C ₂ H	C ₆ H	I-H ₂ C ₄	CH ₂ CHCN	HC ₂ COOH	CH ₃ CH ₂ CN	(CH ₂) ₂ O	CH ₃ CH ₂ COOH	
AlCl	C ₂ O	C ₃ N	C ₆ Si	C ₂ H ₄	CH ₃ C ₂ H	CH ₃ COOH	(CH ₂) ₂ O	NH ₂ CH ₂ COOH		
C ₂	C ₂ S	C ₃ O	I-C ₃ H	CH ₂ CN	HC ₃ N	C ₂ H	CH ₃ CH ₂ OH			
CH	CH ₂	C ₃ S	c-C ₃ H ₂	CH ₂ NC	HCOCH ₃	CH ₂ OHCHO	HC ₃ N			
CH ⁺	HCN	C ₂ H ₂	CH ₂ CN	CH ₂ OH	NH ₂ CH ₃	CH ₂ OHCHO	C ₂ H			
CN	HCO	CH ₂ D ⁺	CH ₄	CH ₂ SH	c-C ₂ H ₆ O					
CO	HCO ⁺	HCCN	HC ₃ N	HC ₃ NH ⁺	CH ₂ CHO					
CO ⁺	HCS ⁺	HCCN ⁺	HC ₂ NC	HC ₂ CHO						
CP	HOC ⁺	HNCO	HCOOH	NH ₂ CHO						
CSI	H ₂ O	HNCs	H ₂ CHN	C ₂ N						
HCl	H ₂ S	HOCO ⁺	H ₂ C ₂ O							
KCl	HNC	H ₂ CO	H ₂ NCN							
NH	HNO	H ₂ CN	HNC ₃							
NO	MgCN	H ₂ CS	SIH ₄							
NS	MgNC	H ₂ CO ⁺								
NaCl	NH ₃ ⁺	NH ₃								
OH	N ₂ O	SIC ₃								
PN	NaCN									
SO	OCS									
SO ⁺	SO ₂									
SIN	c-SiC ₂									
SIO	CO ₂									
SIS	NH ₂									
CS	H ₃ ⁺									
HF	SiCN									
SH										

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

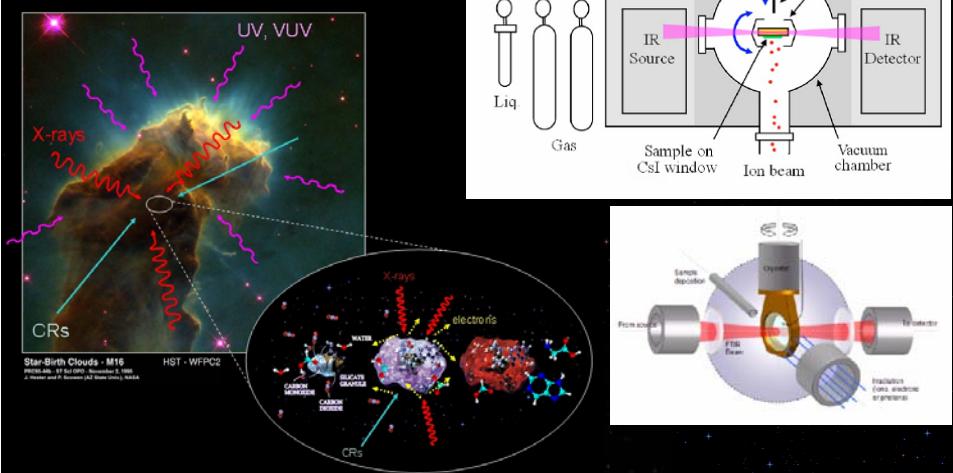
Hidrocarbonetos, PAHs,

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

Alguns Experimentos de Astroquímica.

1. Experimentos de Radiólise/Fotólise de Gelos astrofísicos

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



Vento solar (íons baixa energia)

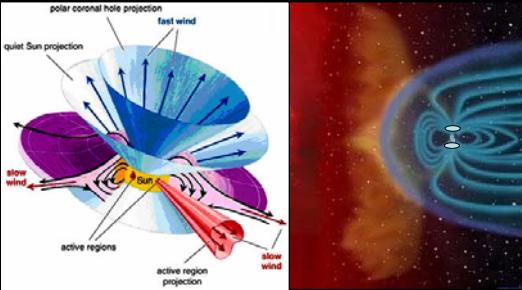


Table 1. Averaged properties of solar wind at 1 au (adapted from Kroll & Trivelpiece 1973, Toptygin 1985 and Zirin 1988).

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

^a95 per cent H⁺, 4 per cent He⁺⁺, and traces of C, N, O, Ne, Mg, Si and Fe ions.

Pilling et al. 2006, MNRAS, 372, 1379,

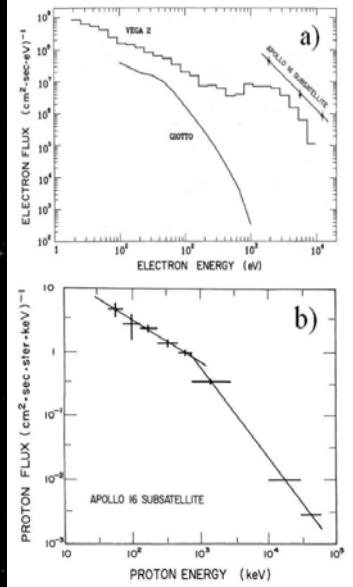


Figure 1. (a) Electron fluxes in comet Halley measured by the Vega 2 (Gringauz et al. 1986), Giotto (D'Uston et al. 1989) and at lunar orbit measured by APOLLO 16 subsatellite (adapted from Lin et al. 1974). (b) The proton energy spectrum due to solar wind at lunar orbit measured by APOLLO 16 subsatellite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

Raios cósmicos e partículas enérgicas do vento solar

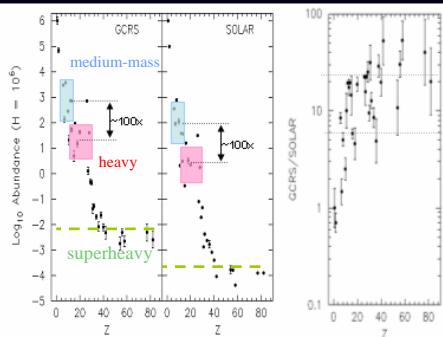


Table 1. Galactic cosmic-ray (GCR) source abundances compared to the Solar abundances (normalized to H = 1.0 × 10⁶).

Z	Elem	GCRs ¹	Solar ²	$E_{\max}(\text{MeV/nuc})^3$
1	H	1.0×10^6	1.0×10^6	—
2	He	6.9×10^4	9.8×10^4	1.4
6	C	3000.	355.	22.5
8	O	3720.	741.	45.8
12	Mg	734.	38.0	132.6
14	Si	707.	36.3	209.8
26	Fe	713.	31.6	∞

1 – Meyer et al. (1998); 2 – Grevesse et al. (1996).

3 – E_{\max} is the maximum energy which can heat a 0.1 μm grain up to 27 K by a cosmic ray ion.

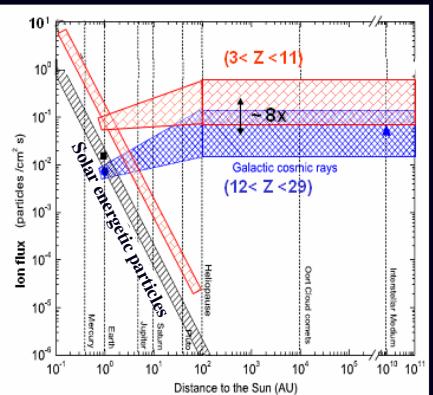
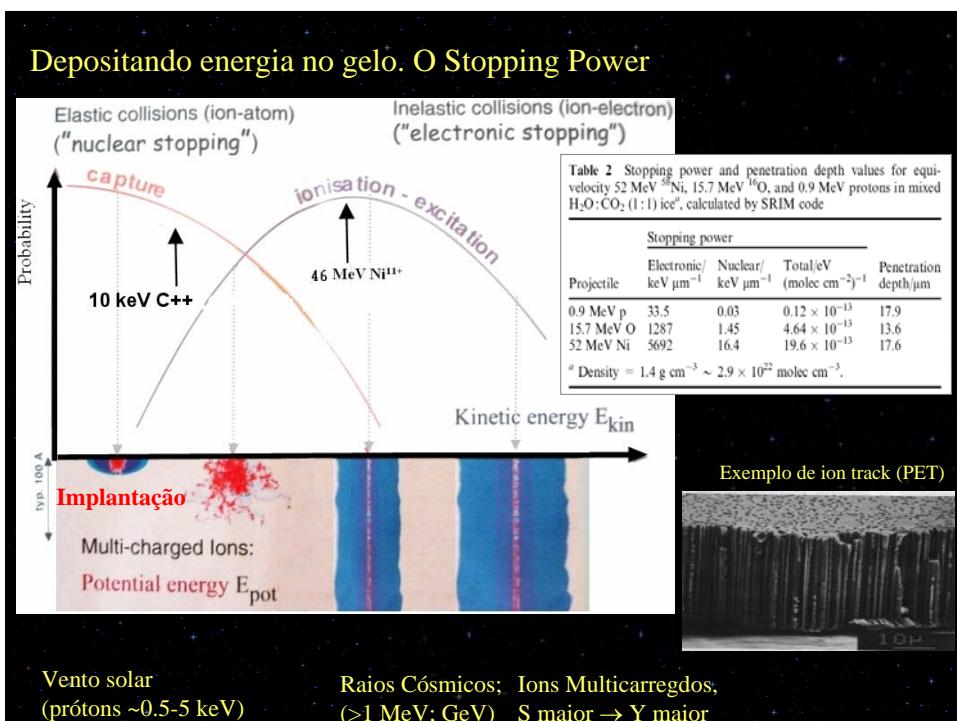
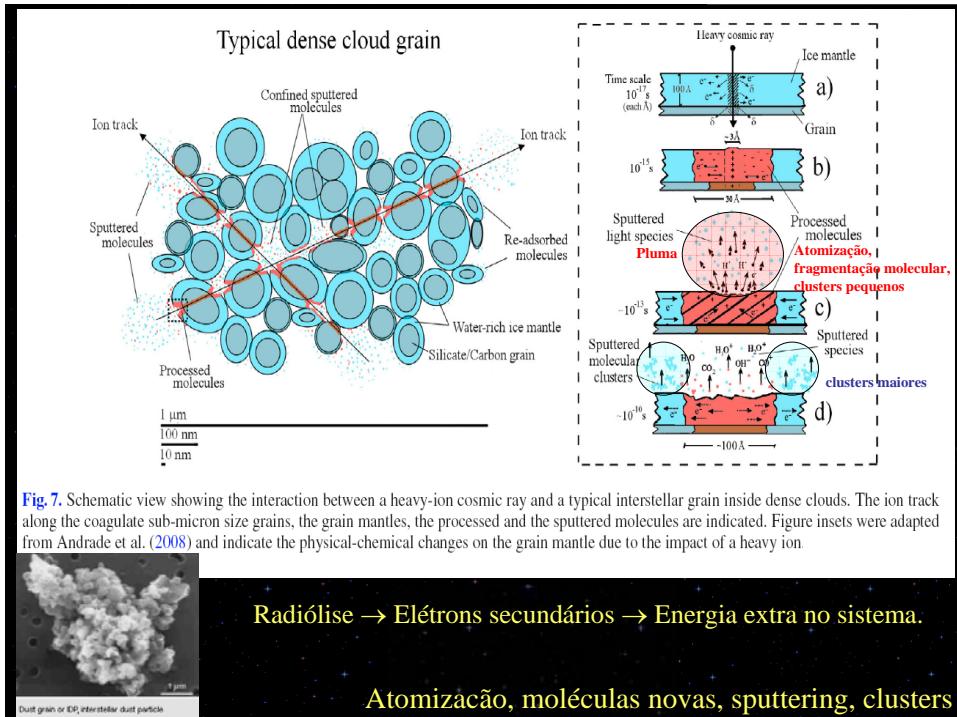
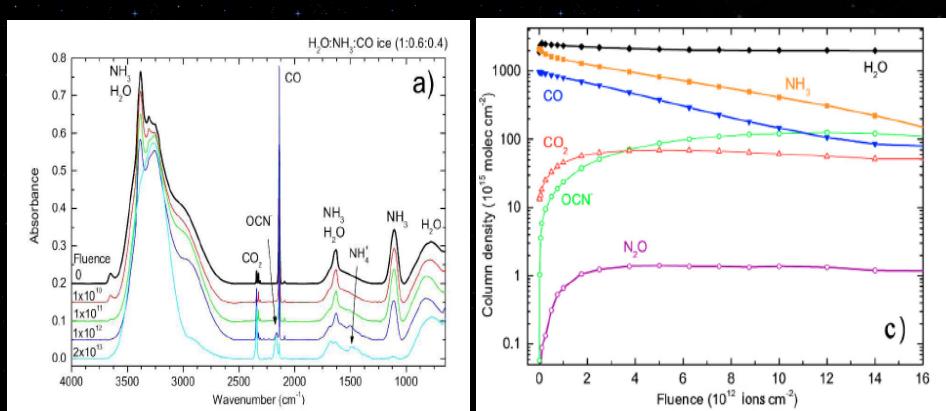


Fig. Estimated value of the integrated ion flux ($3 \leq Z \leq 11$) and ($12 \leq Z \leq 29$) with energy between 0.1–10 MeV/u inside solar system and at interstellar medium as a function of distance to the Sun. Both Galactic cosmic rays and solar wind particles are displayed. Square: integrated flux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

Pilling et al. 2011, PCCP

Shen et al 2004; Drury et al 1999





Densidade de Coluna

$$N = \frac{1}{A} \int \tau_y d\nu = \frac{2.3}{A} \int Abs_y d\nu \quad [\text{molec cm}^{-2}],$$

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

Seção de Choque de Destrução e Sputtering

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

Seção de Choque de Formação

$$N_k \approx N_0 \sigma_{f,k} \left[F - \frac{\sigma_d + \sigma_{d,k}}{2} F^2 \exp(-\sigma_d F) \right]$$

Seção de Choque de Destrução e Sputtering

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

$$N_k \approx N_0 \sigma_{f,k} \left[F - \frac{\sigma_d + \sigma_{d,k}}{2} F^2 \exp(-\sigma_d F) \right]$$

Radiochemical yield

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

Taxa de Dissociação e tempo de meia-vida

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

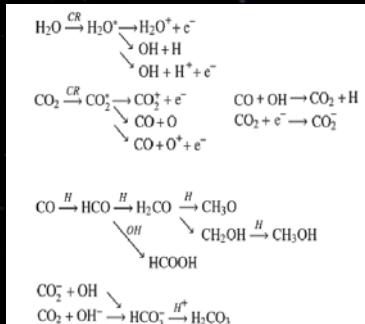
Exemplos de reações induzidas por CR

Valores médios empregando íons pesados
(E = 0.1-10 MeV/u)

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

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

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

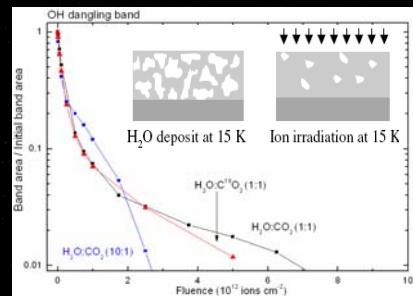


Outros resultados:

Física da Matéria condensada (Morfologia e estrutura cristalina)

Compactação do gelo (microporos) devido ao bombardeio (OH db $\sim 3650 \text{ cm}^{-1}$).

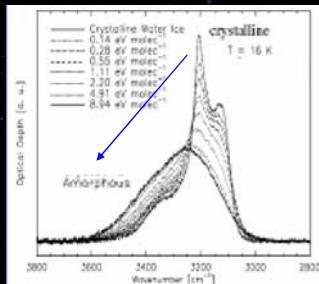
Não acontece no caso de fôtons!



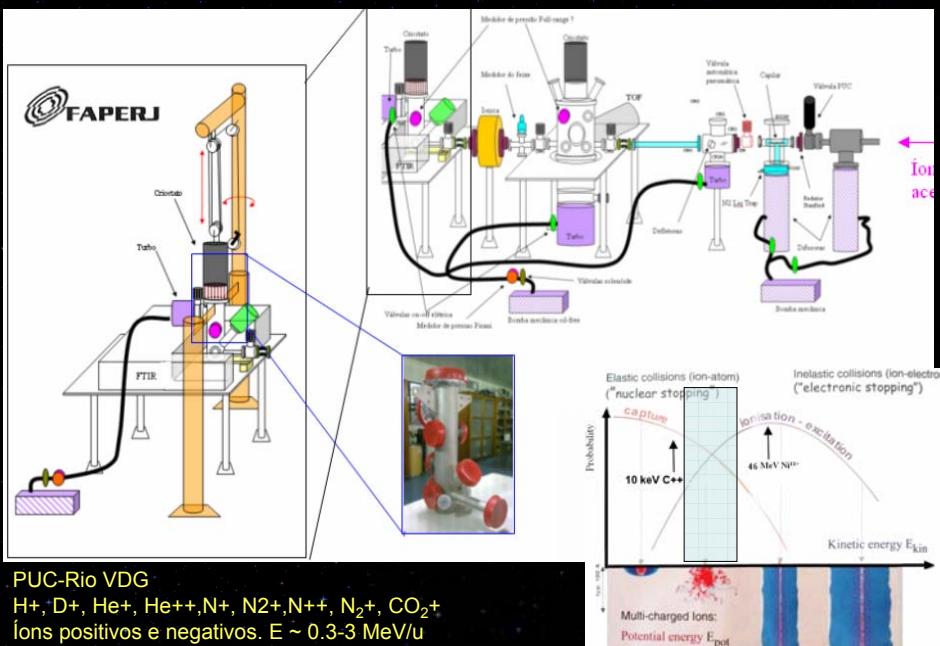
Alteração da estrutura cristalina devido a irradiação.

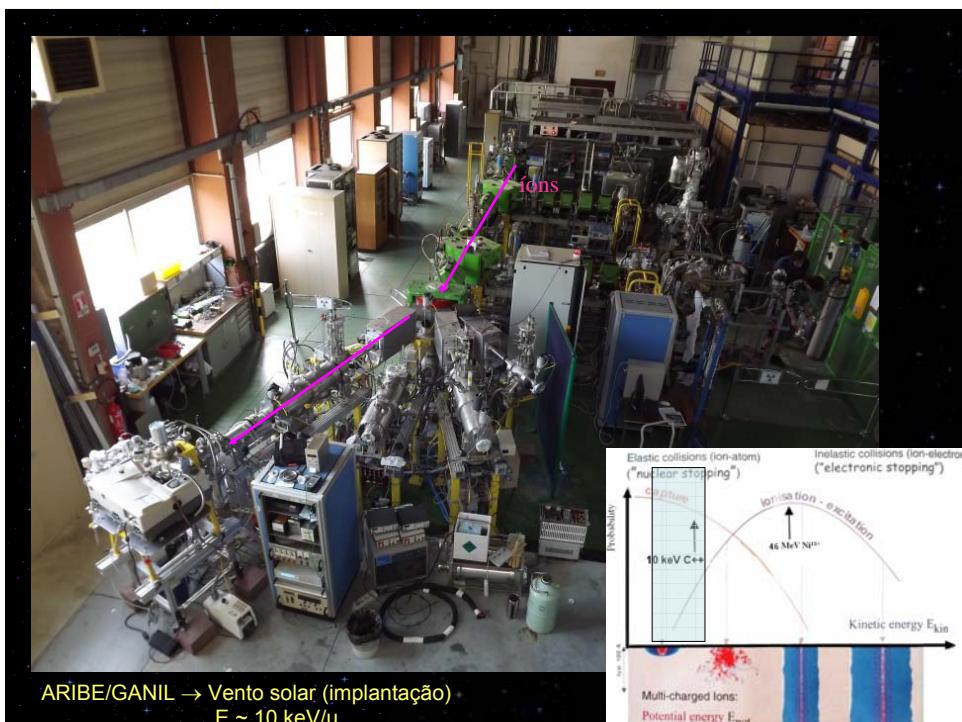
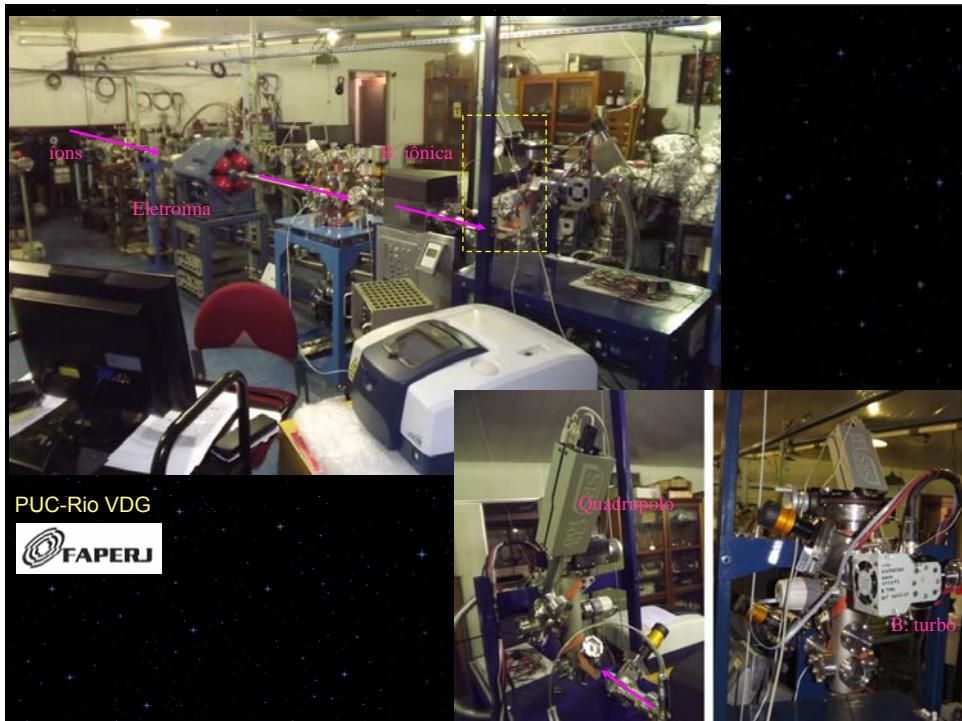
(cristalino \rightarrow amorfico)

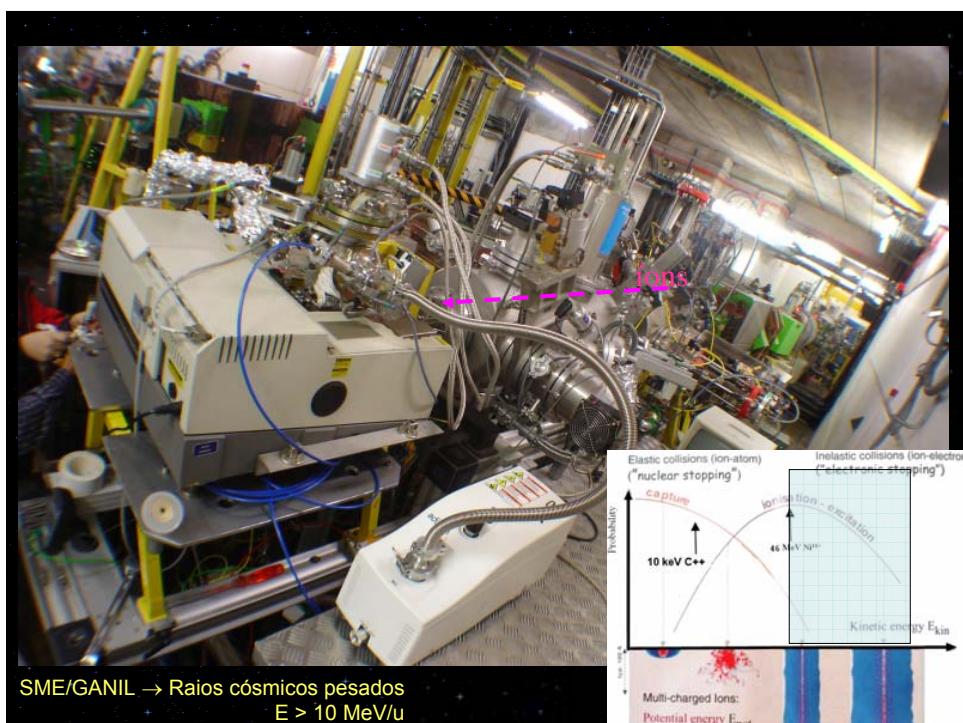
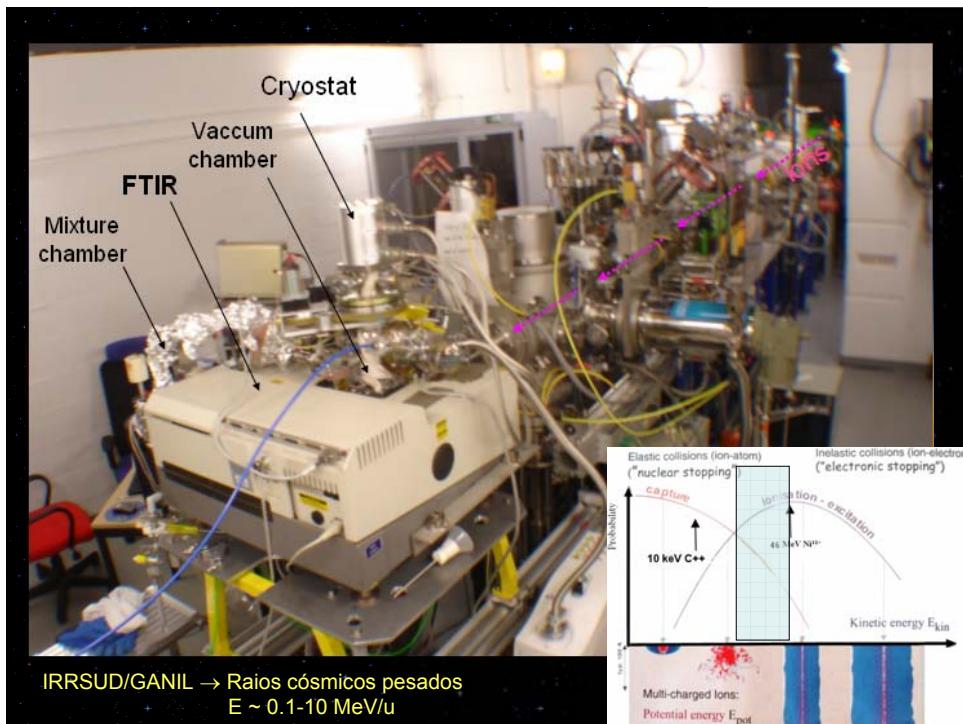
Acontece com fôtons e íons.



Metodologia Experimental (galeria de fotos)







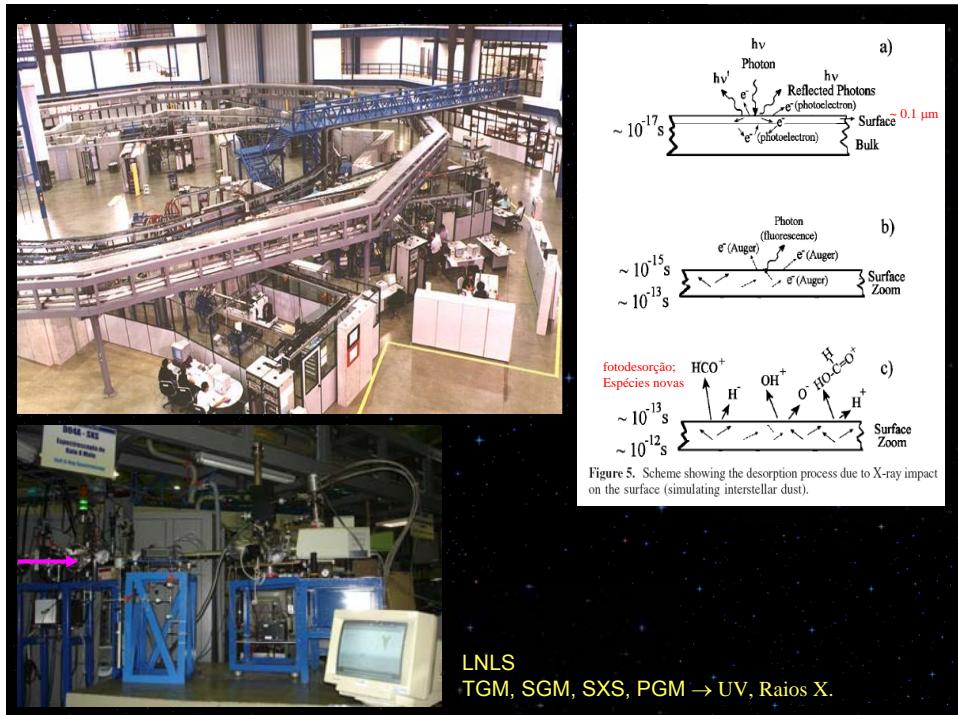
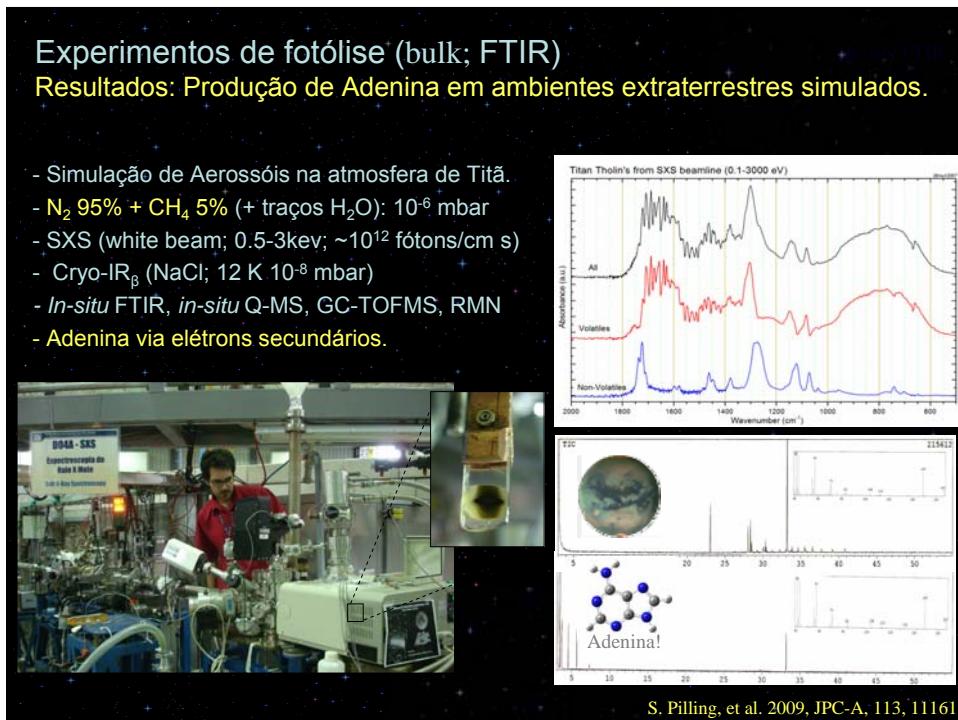


Figure 5. Scheme showing the desorption process due to X-ray impact on the surface (simulating interstellar dust).



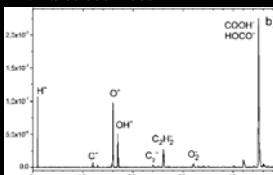
Experimentos de radiólise/fotólise de superfície (TOF)

Resultados: Clusters (íons), Moléculas novas, Sputtering yield, $\tau_{1/2}$

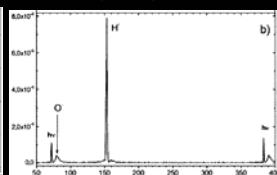
-Íons: VDG ou Califórnio (PDMS ^{252}Cf)

-Fótons: LNLS (PSID)

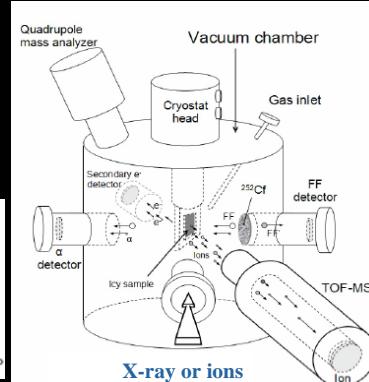
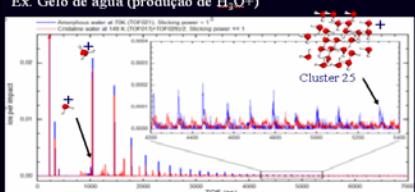
Ex. Raios cósmicos



Ex. Fótons (535eV)



Ex. Gelo de água (produção de H_2O^+)

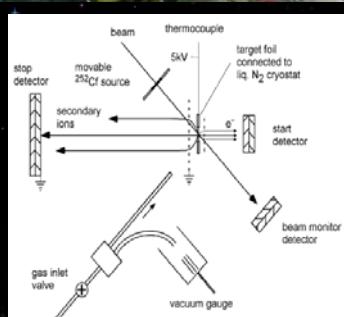


Câmara PDMS LNLS (UHV) e
Nova câmara PDMS PUC-Rio (UHV)

Andrade et al. H. M., 2008, J. of Phy. Chem. C, 112, 11954
Andrade et al., 2009, Surface Science, 603, 3301,
Bordalo et al. 2011, in Prep.



Câmara PDMS PUC-Rio (HV)



L.S. Ferreira et al. / International Journal of Mass Spectrometry 243 (2005) 85–93

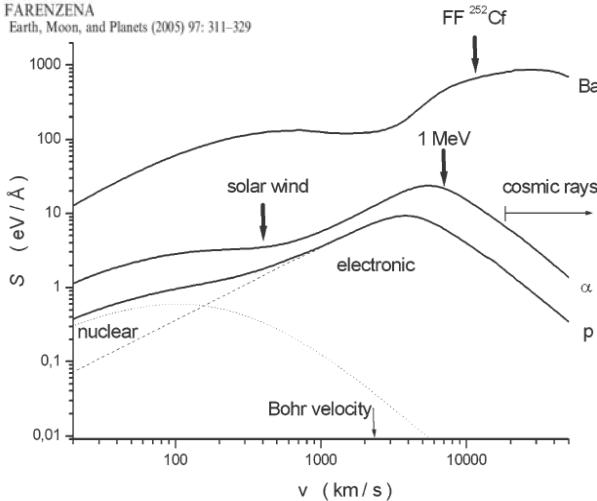


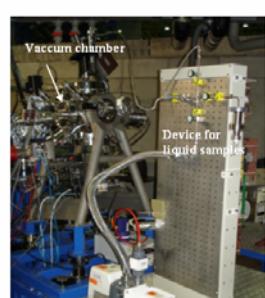
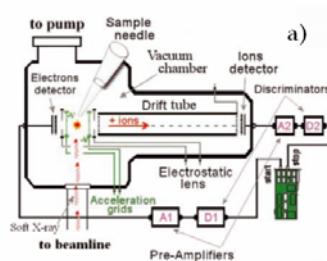
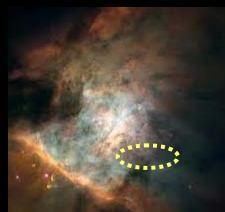
Figure 1. The total stopping power of protons, α particles and barium projectiles on water ice. For protons, the dot and dash lines represent the nuclear and the electronic stopping power, respectively. Ba is a common fission fragment (FF) of the ^{252}Cf ; its velocity (energy of ~ 65 MeV) after leaving the radioactive source employed is indicated by the arrow. Velocities of 1 MeV α particles and of a typical solar wind are also indicated. Note that the electronic stopping power values of the solar wind and cosmic rays are much greater than the corresponding nuclear stopping power values.

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

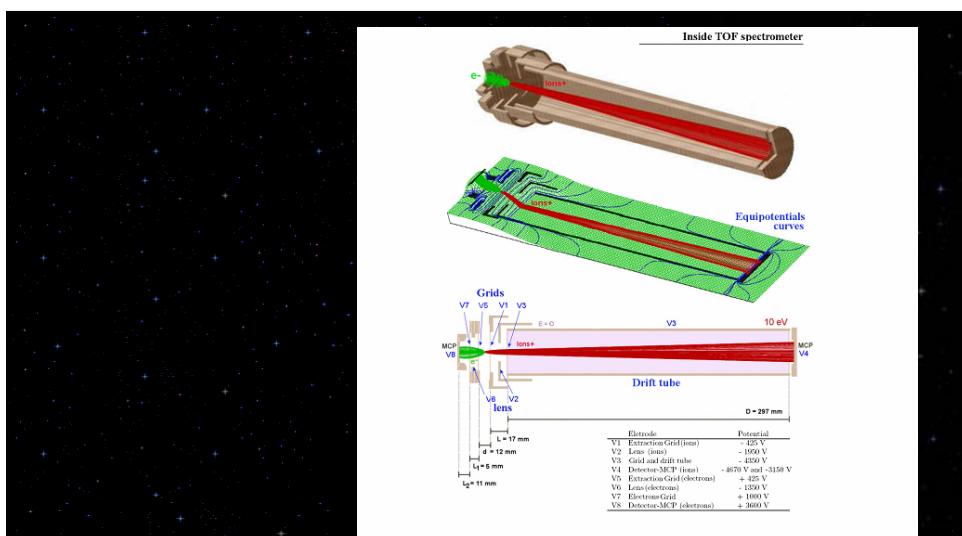
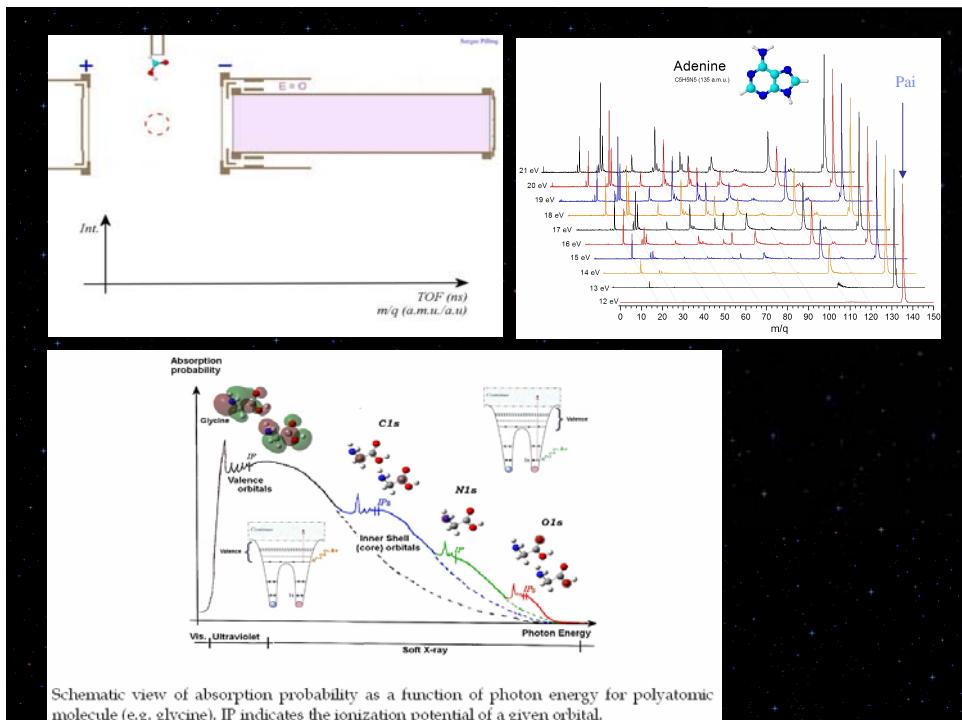
Resultados: Fragmentação, Canais de dissociação, σ , $\tau^{1/2}$



Ex. Fótons (LNLS)



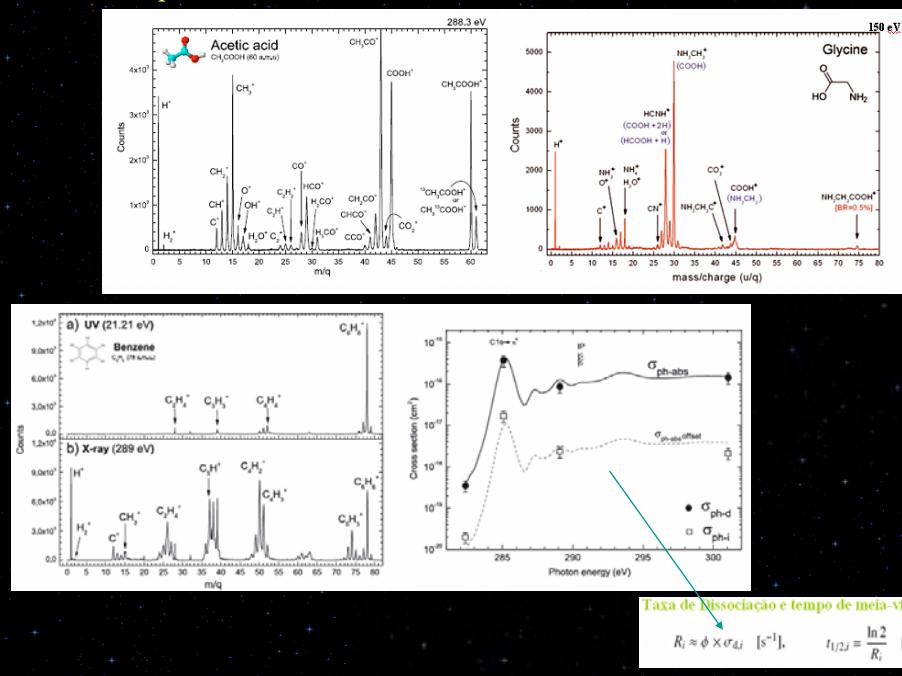
a) Schematic diagram of the experimental set-up employed in gas-phase experiments.
b) Photography of equipment employed at the soft X-ray beamline of LNLS.



Referências bibliográficas:

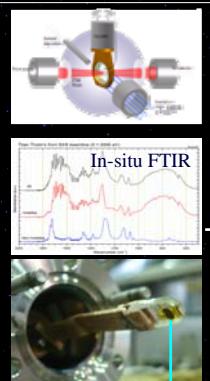
- Boechat-Roberty et al. 2005, A&A, 438, 915; Pilling et al. 2006, A&A, 449, 1289; Pilling et al., 2006, Brazilian Journal of Physics, 36, 2B; Pilling et al. N. V. 2006, MNRAS, 372, 1379; Pilling et al., 2007, J El. Spect. Rel. Phen., 156-158, 139; Cavasso-Filho et al., 2007, J El. Spect. Rel. Phen., 156-158, 168; Pilling et al., 2007, J El. Spect. Rel. Phen., 155, 70; Pilling et al., 2007, MNRAS, 375, 1488; Pilling et al. A&A, 464, 393; Pilling et al., Rapid Comm. on Mass Spectrometry, 21, 3646; Boechat-Roberty et al. 2009, MNRAS, 394, 810; Pilling S., Baptista L., et al., 2010, Astrobiology, In Press.

Outros exemplos



Ligando observações com experimentos

Simulação de gelo astrofísico
com fótons, íons, elétrons.

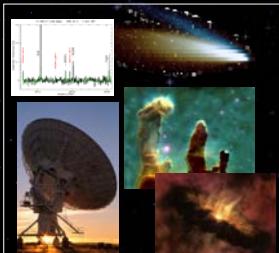


Observações IR



Comparação direta

Observações Radio



Calculo das freqüências Radio
(ou busca na literatura)

Predição de novas espécies.
- pouco abundantes (S/N baixa)
- aminoácidos, bases, açúcares....

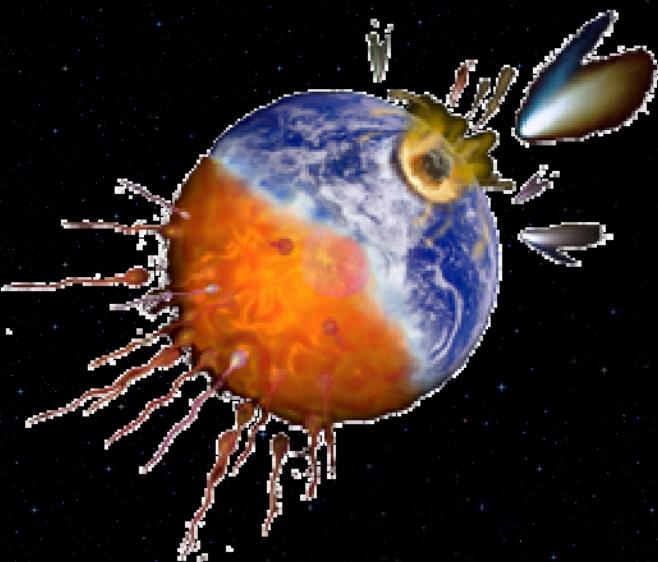
Resíduos orgânicos: Cromatografia e RMN

Artigos Sugeridos Para leitura

- Bergin et al. 2009, Earth Plant Astr, Chemical evolution of PPD.
- Gibb et al. 2004, AJSS, 151, 35, *Observations of YSOs with ISO*.
- Van Dishoeck and Blake, 1998, ARAA, Chemical evolution of SFRs
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- Galvin and Dworkin, PNAS, 2009, *Amino acids excess in CM meteorites*.
- Ehrenfreund et al 2001, AJ, 550, L95, *Photo stability of amino acids in space*.
- Ehrenfreund & Charnley, ARAA, 2000, *Organic molecules in the IM*.
- Pilling et al 2009, JPC A, 113, 11161, *Adenine in Titan simulation*.
- Pilling et al 2009, A&A, *in press* Radiolysis of astrophysical ice analogs.

Sites recomendados

- <http://www1.univap.br/~spilling/AQ/AO.htm>
- http://www.strw.leidenuniv.nl/events/phdtheses/oberg/oberg_thesis.pdf
- <http://www.gps.caltech.edu/~gab/ge128/ge128.html>
- <http://www.strw.leidenuniv.nl/~wehres/astrochem/>
- <http://www.gps.caltech.edu/~gab/ge132/ge132.html>



Continuamos na próxima aula.