ROLE OF H/C INTERACTIONS IN THE EVOLUTION OF HYDROGENATED CARBON GRAINS IN THE ISM

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- Experimental results on H atom processing of carbon grain under simulated interstellar medium conditions

- The role of hydrogenated carbon grains in molecular hydrogen formation

Organic matter in the ISM

Diffuse Medium

3.4 μm band : features at 2955, 2925 e 2870 cm^{-1} characteristic of the C-H stretching modes in the CH_2 and CH_3 groups

The carrier is a widespread component of diffuse dust

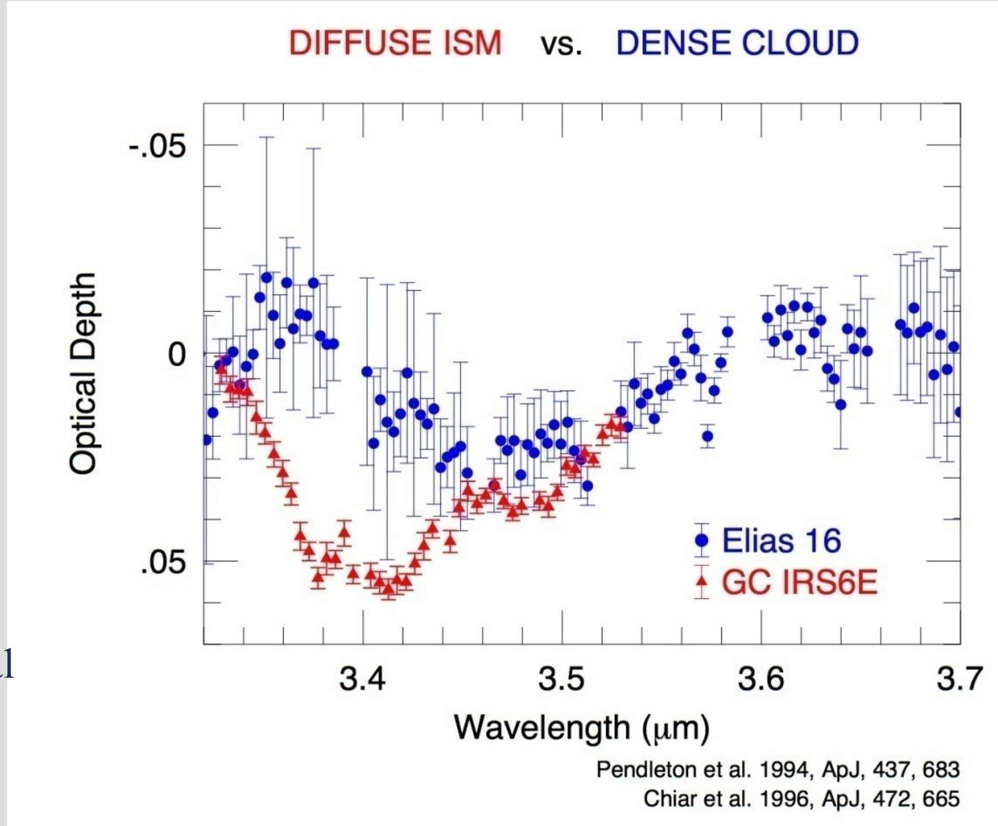
Dense Medium

No 3.4 μm band, 3.47 μm (2883 cm^{-1}) feature instead (Allamandola et al. 1992, Broke et al. 1996, 1999, Chiar et al. 1996)

The band intensity is better correlated with the 3.1 μm H_2O intensity than with the 10 μm silicate optical depth

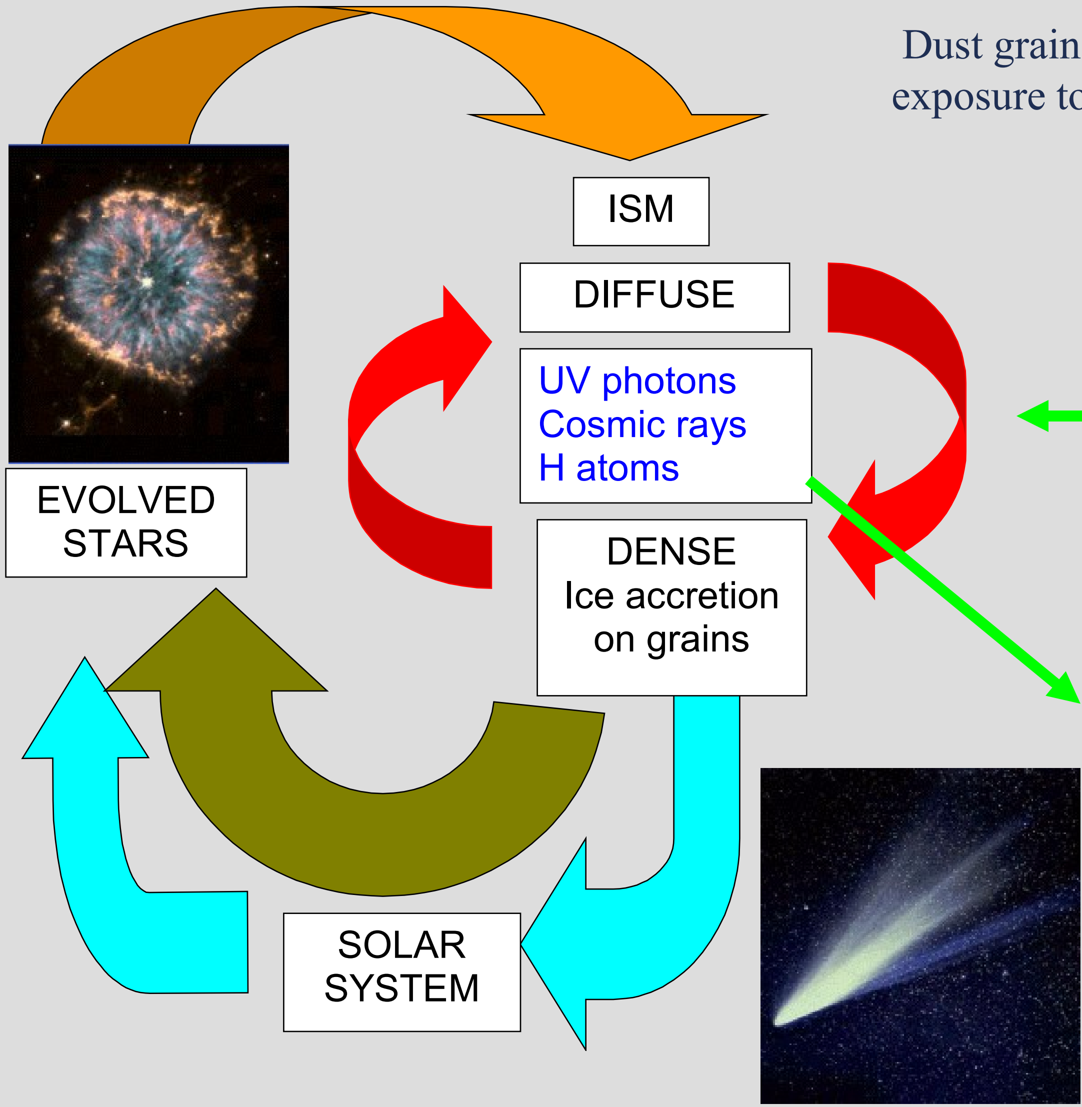
C-H stretching of hydrogen (solo) bonded to tertiary sp^3 carbon (Allamandola et al. 1992)

Vibrational mode due to N atom of NH_3 with an OH bond of the water molecule, forming an ammonia hydrate (Dartois et al. 2002)



Grain evolution in space

Dust grain composition in ISM evolves through exposure to UV photons, heat, gas, and cosmic rays.



Dust cycling between dense and diffuse medium

Time scale 3×10^7 years

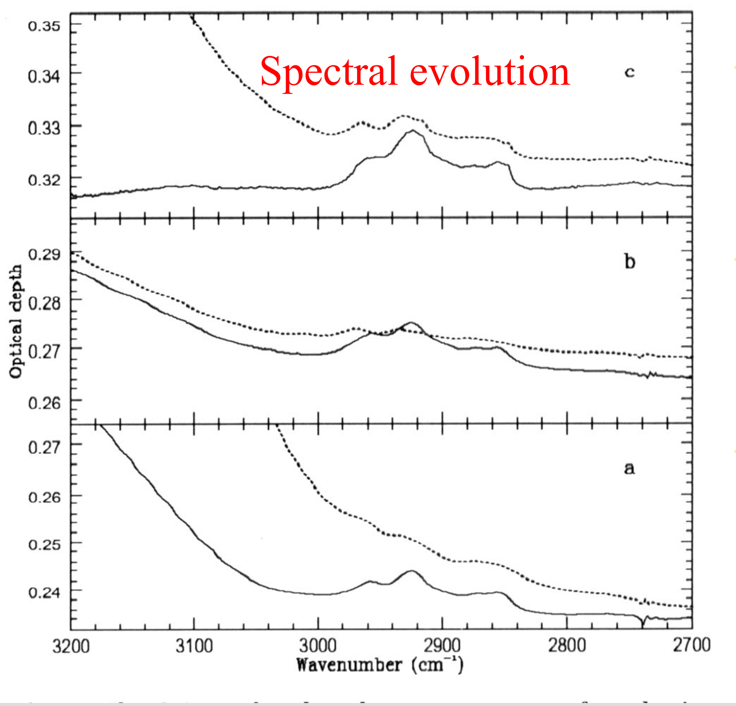
- UV photons: 8×10^7 photons cm $^{-2}$ s^{-1}
- Cosmic rays: 2 protons cm^{-2} s^{-1}

  (1 MeV protons)
- Interstellar gas: 8×10^6 H atoms cm $^{-2}$ s^{-1}

UV irradiation of carbonaceous materials under simulated diffuse and dense medium conditions

UV source: hydrogen flow discharge lamp

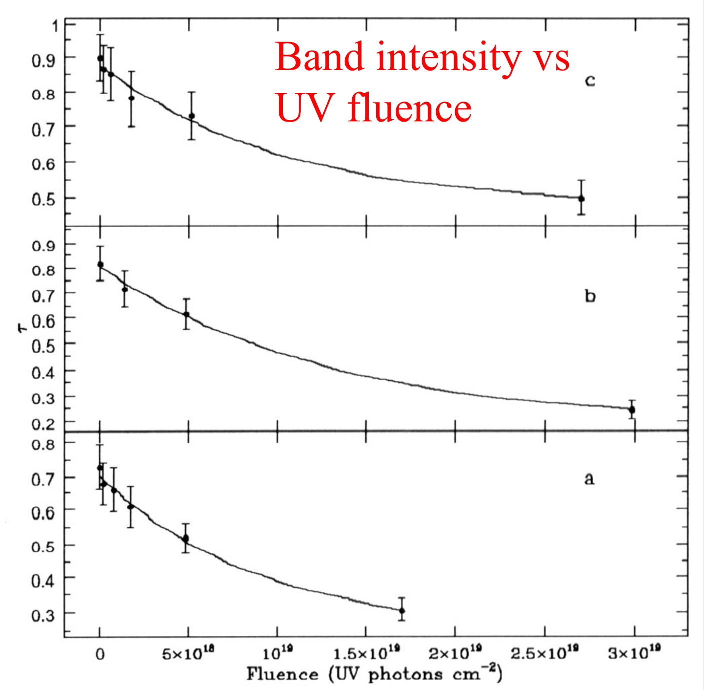
Samples: *hydrogenated carbon grains* produced by arc discharge in H_2 atmosphere (ACH2)



ACH2 + Ar ice layer (diffuse ISM)

ACH2 + H_2O:CO:NH3 ice mixture (dense clouds)

ACH2 + H_2O ice layer (dense clouds)



Mennella et al. 2001, collaboration with the group in Leiden

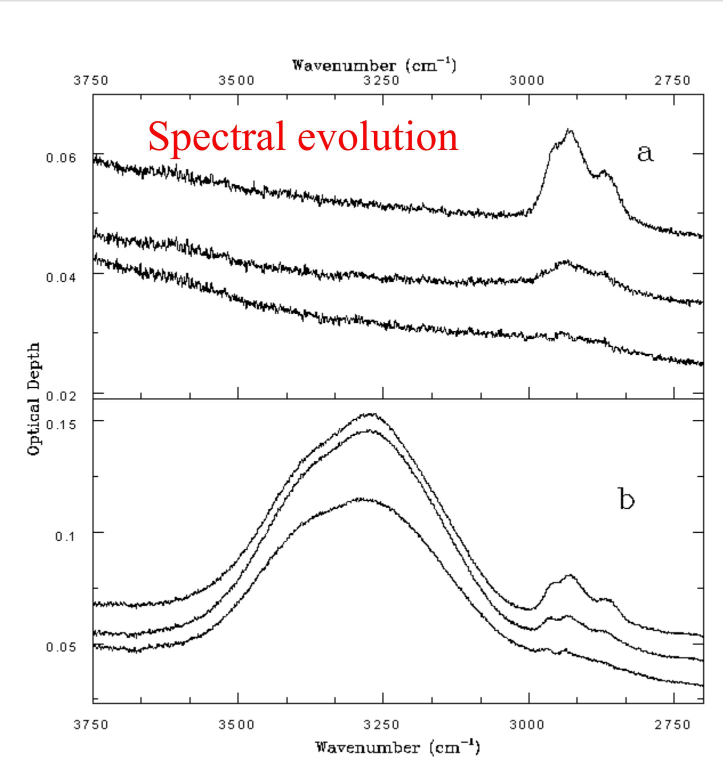
UV photodestruction cross section of C-H bonds:

$$\sigma_d = 1\times10^{-19}\ cm^2/\ photon$$

A similar result has been obtained for the cross section of hydrocarbon molecules (Munoz et al. 2001)

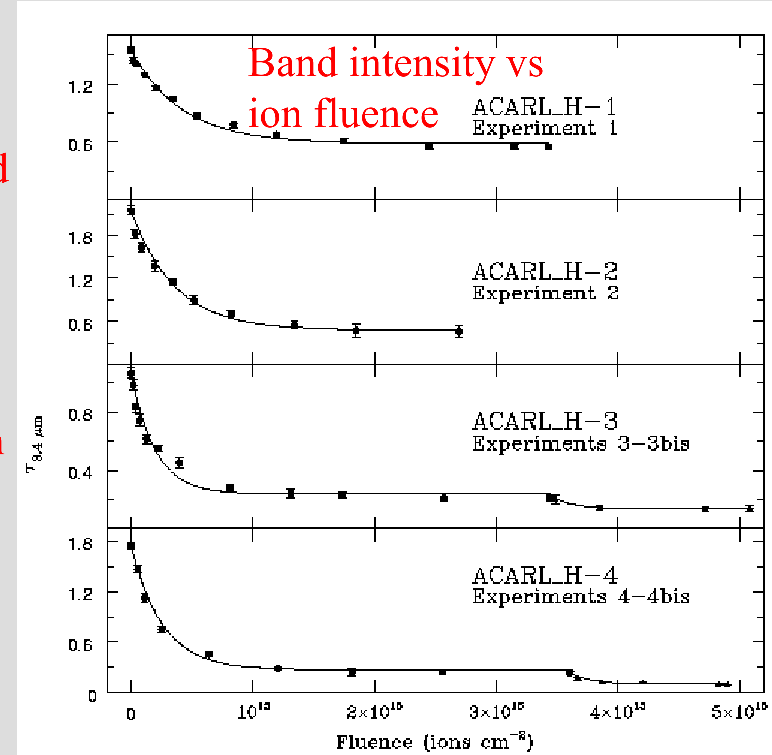
Ion irradiation of hydrogenated carbon grains

IONS: 30 keV He^+



Bare hydrogenated carbon grains (diffuse ISM)

Hydrogenated carbon grains + H_2O ice layer (dense ISM)



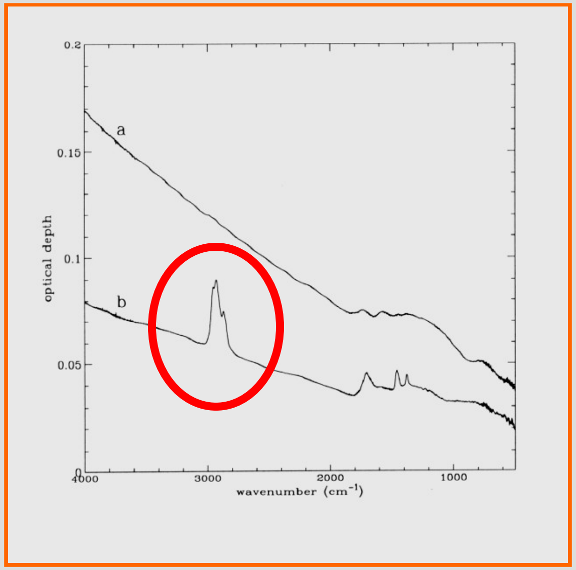
Mennella et al. 2003, collaboration with the group in Catania

Destruction cross section of C-H bonds for 1 MeV protons:

$$\sigma_d = 9.4\times10^{-16}\ \mathrm{cm}^2$$

The presence of the 3.4 µm band in the spectrum of diffuse clouds implies that a mechanism able to form C-H bonds must be active.

H atom processing of carbon particles

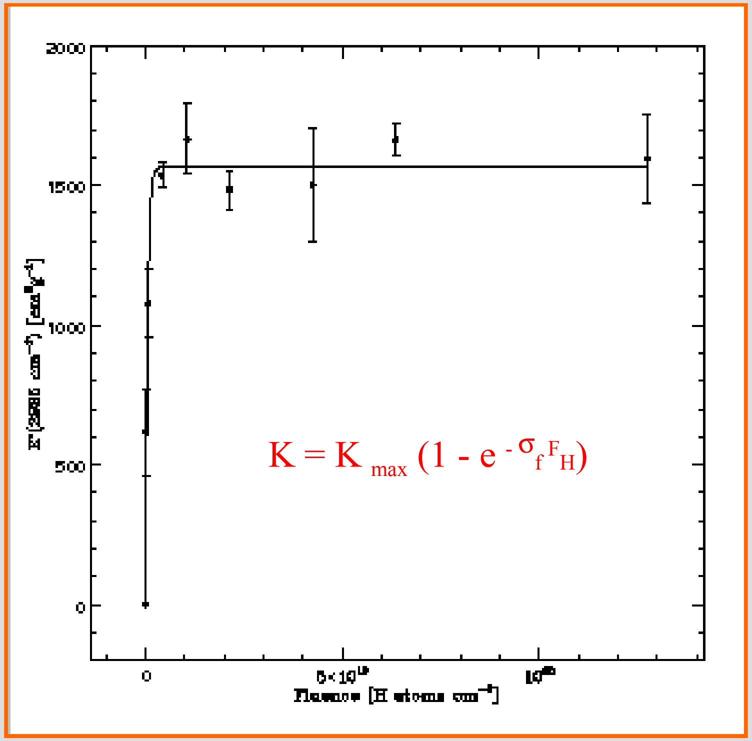


Activation of the aliphatic C-H stretching and bending modes

The band intensity increases with H atom fluence up to a constant value of $K_{max} = 1.6\times10^3$ cm^2/g, indicating saturation of the hydrogenation process.

Formation cross section of C-H bonds by H atoms:

$$\sigma_f = 1.9\times10^{-18}\ \text{cm}^2/\ \text{H atom}$$

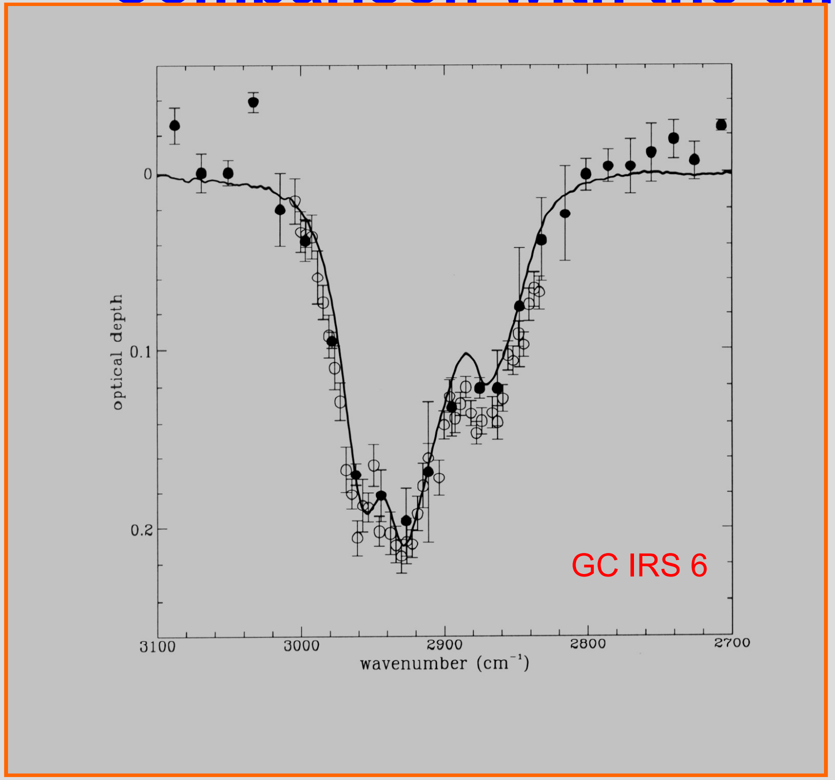


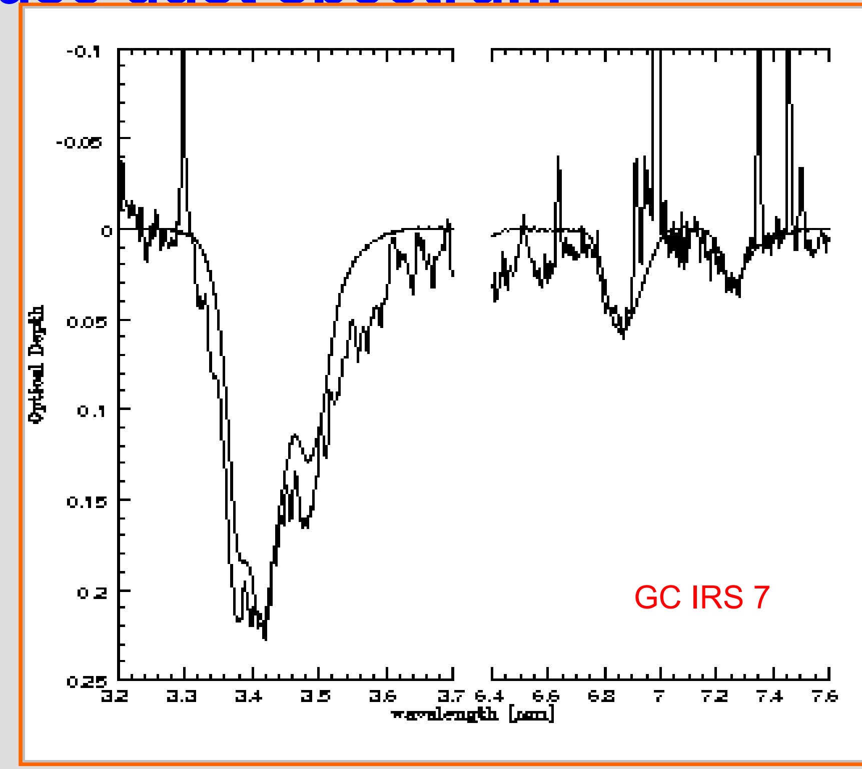
The amount of carbon necessary to reproduce the interstellar feature intensity is 60 ppm relative to hydrogen.

The upper limit estimation for H/C is 0.66 in the saturation region.

The aliphatic mass fraction of C atoms is 25%.

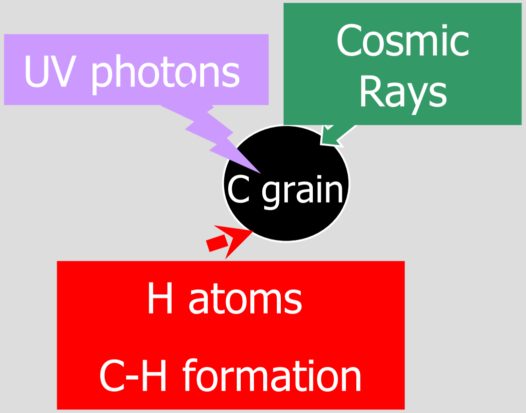
Comparison with the diffuse dust spectrum



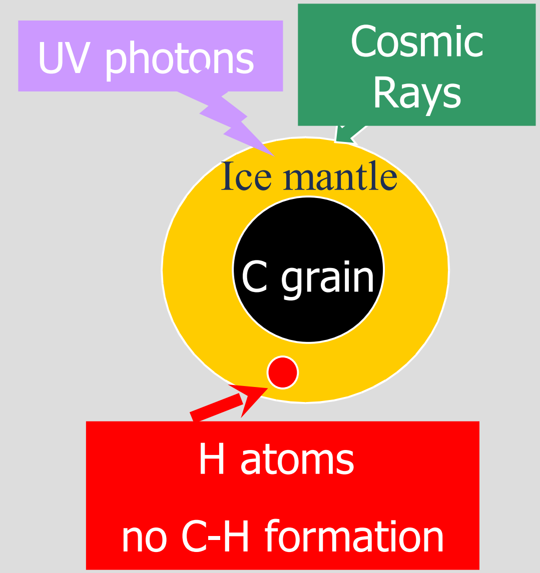


- The C-H stretching and bending features are reproduced very well in terms of peak position and relative intensities

Evolutionary model



Diffuse medium



Dense medium

Quantitative model based on the results of simulation experiments

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Destruction and formation cross sections

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Evolution of C-H bonds – first order kinetic process

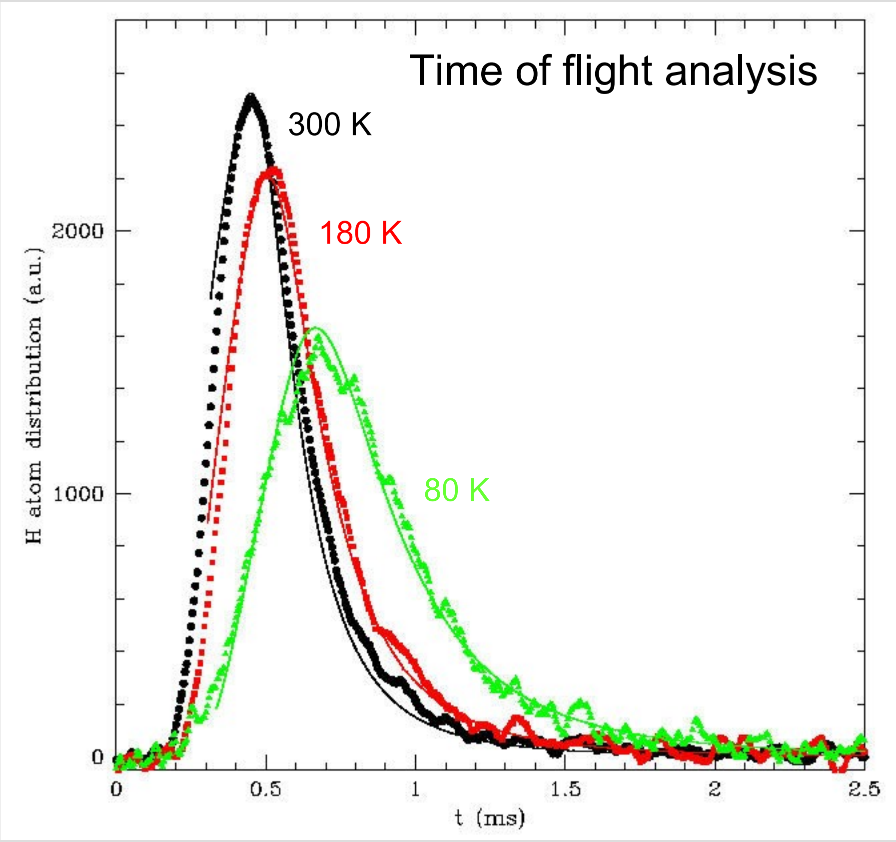
A systematic study of the interaction of H atoms with carbon grains with a water ice cap is lacking

Study of the interaction of carbon grains + H_2O with H atoms

Atomic hydrogen beam produced by microwave excited dissociation of H_2

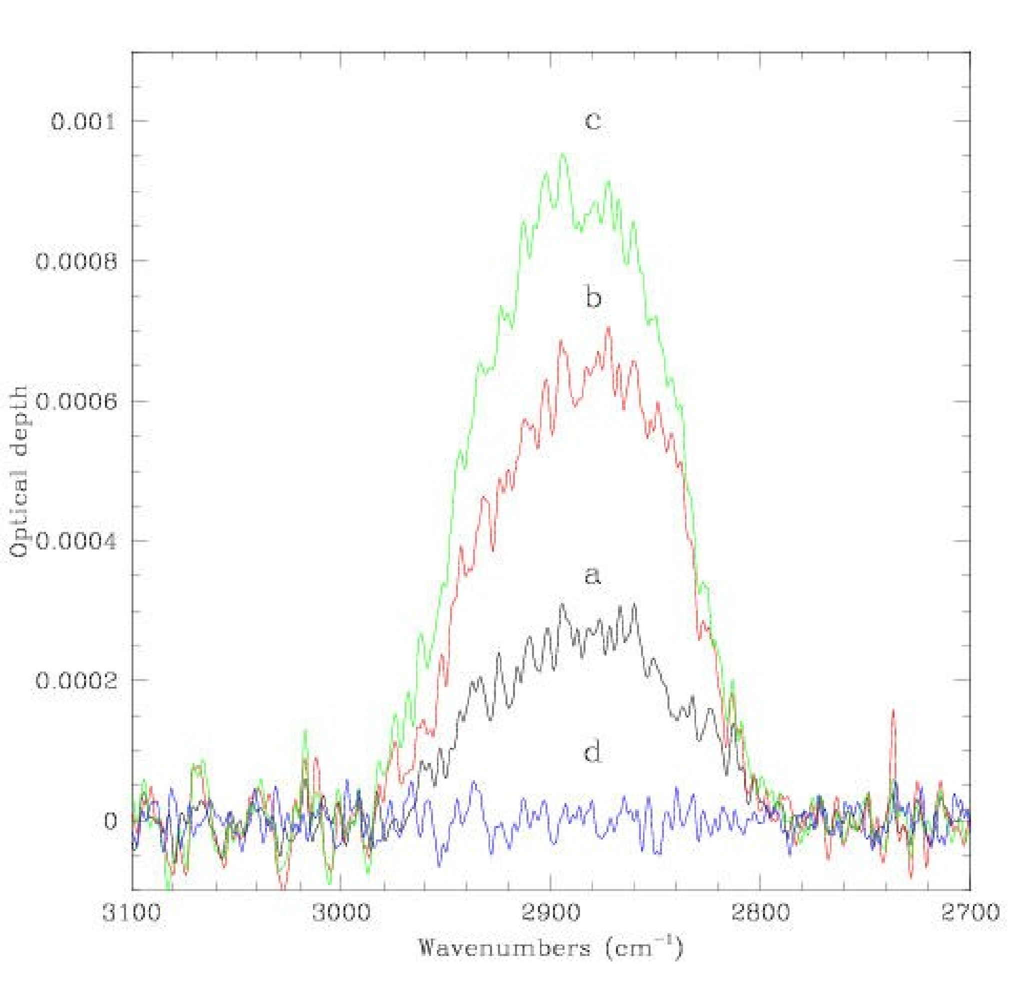
Base pressure < 10^{-9} mbar

- Carbon grains produced by laser ablation of carbon rods in Ar atmosphere
- Water ice layer at 12 K
- H atoms at 80 K
- IR spectroscopy



Results

Carbon grains + H_2O layer (22 nm thick) at 12 K
+
exposure to H atoms at 80 K



No activation of aliphatic CH_2 and CH_3 bands

Activation of a band at 2883 cm^{-1}

The band intensity increases with H atom exposure

Hydrogenation is selective with respect to the C bonding configuration

H atoms pass through the water layer and reac with carbon grains forming hydrogen solo C-H bonds with tertiary sp^3 C.

The water ice layer adsorbs part of H atoms an it lowers the temperature of those reaching grains below the activation temperature (70 K) of C-H bonds in the CH_2 and CH_3 groups

The formation of hydrogen solo CH bonds has negligible activation energy

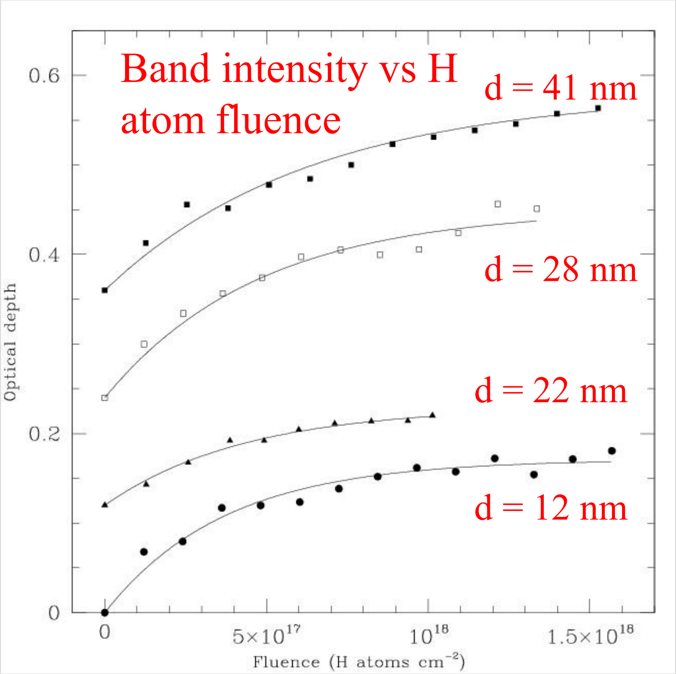
FORMATION CROSS SECTION

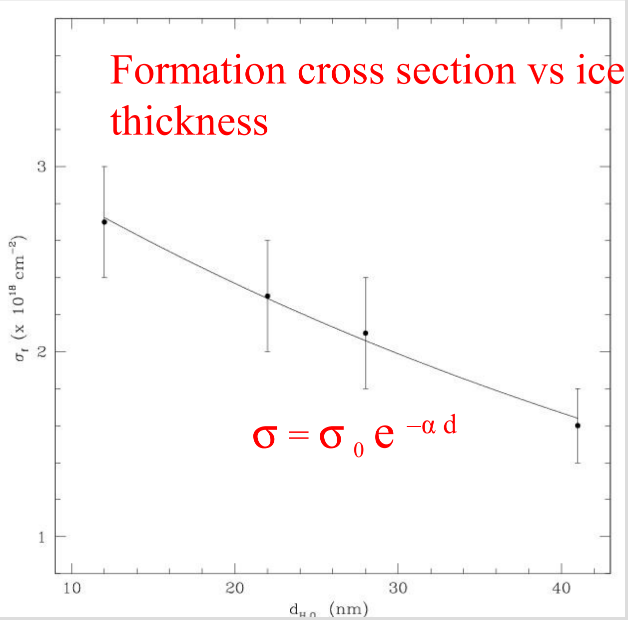
Cross section derived from the increase of the band intensity with H atom fluence

The cross section decreases when the thickness of the water ice increases

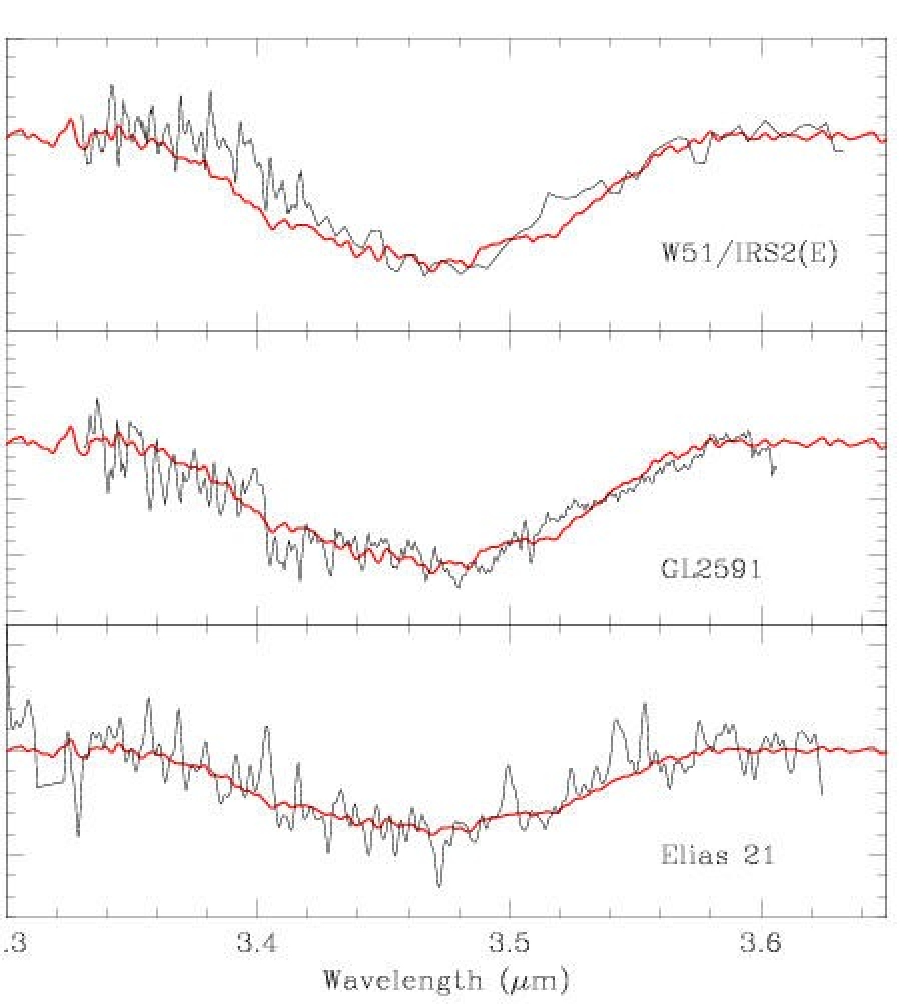
Estimation of the mean free path of H atoms:

$$L = 1 / \alpha = 56 \text{ nm}$$





Comparison with observations



The lab spectrum reproduces that of interstellar sources

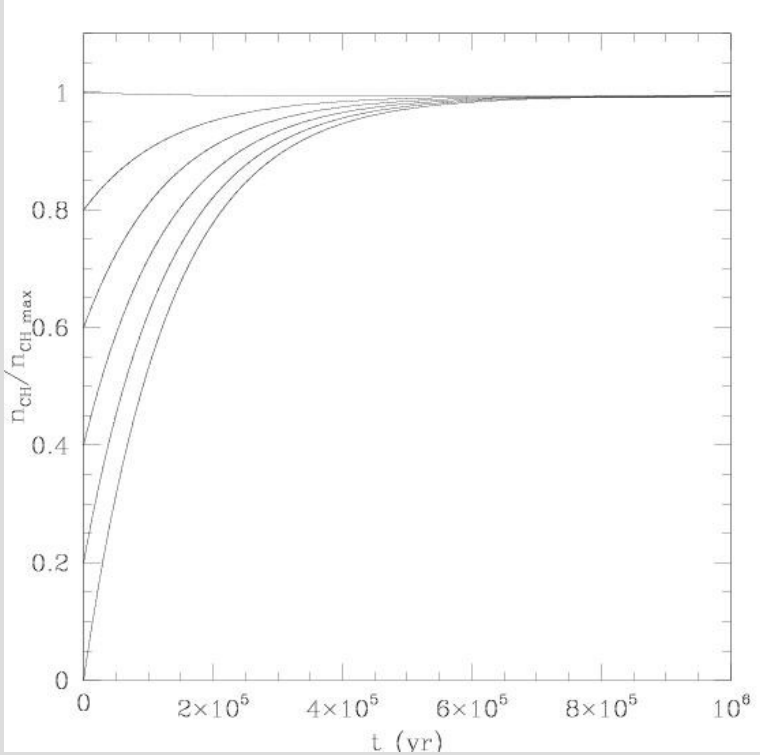
This nice spectral match should be considered a first step for a solid assignment of the feature

Interstellar spectra from Brooke et al. (1999) black lines

Lab spectrum red lines

EVOLUTION OF THE 3.47 μm BAND

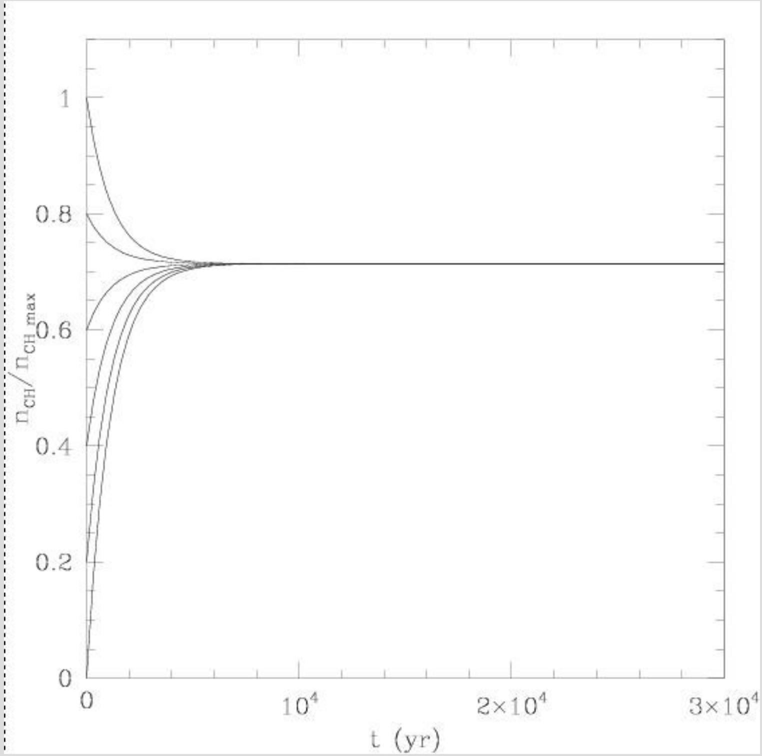
Dense Medium



The equilibrium between formation and destruction is obtained in 6 × 10^5 yr

The presence of the C-H bonds absorbing at 3.47 μm is compatible with the conditions expected in dense clouds

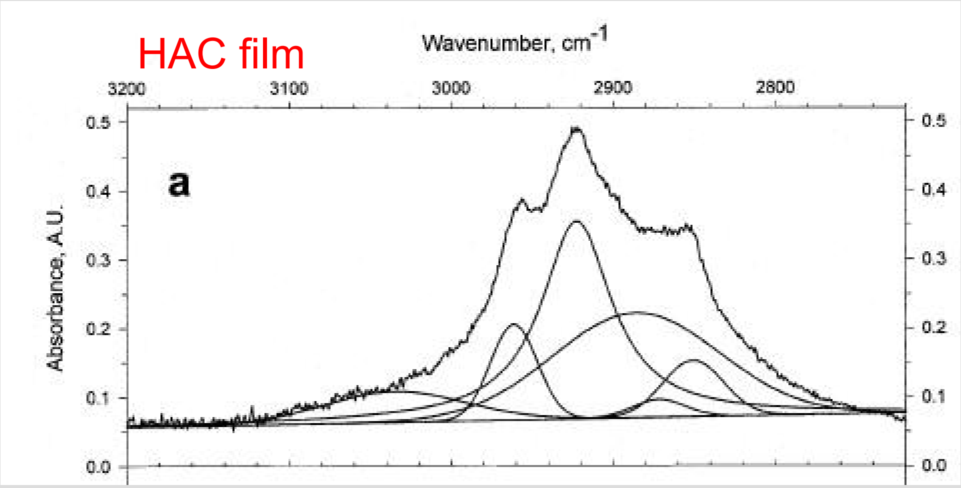
Diffuse Medium



Hydrogen solo C-H bonds should also be present in diffuse interstellar regions.

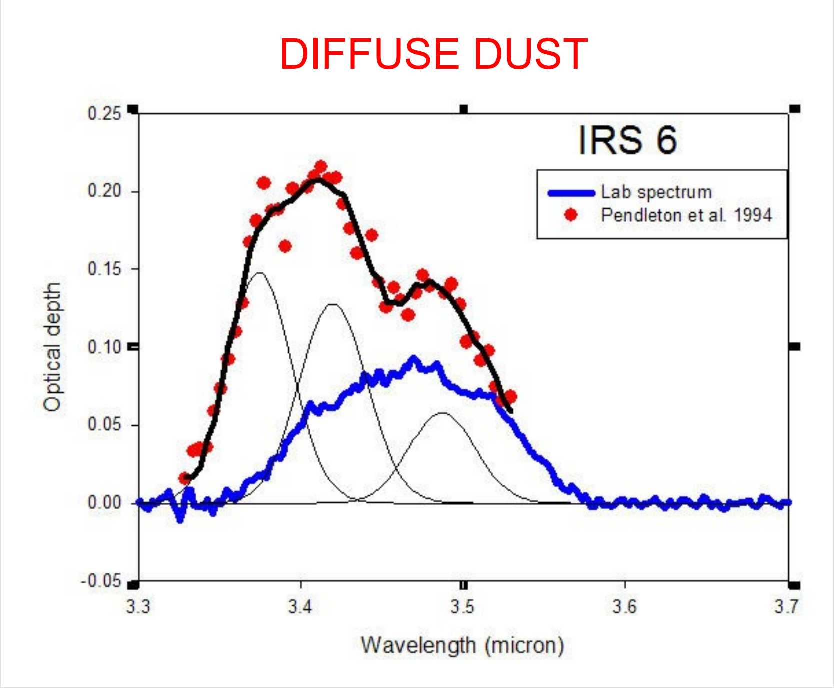
Activation of aliphatic C-H bonds masks hydrogen solo C-H bonds

The 3.47 µm band as component of the 3.4 µm feature



Gaussian line shape fitting analysis of the 3.4 µm band

Band at 2886 cm^{-1} assigned to CH of tertiary sp^3 carbon
(Grishko & Duley 2000)



Fit with three gaussian profiles plus the lab profile of the 3.47 um band.

The presence of the hydrogen solo C-H bonds in diffuse interstellar regions is compatible with the spectroscopic observations

Conclusions

- Based on a complete simulation activity of grain processing occuring in space, a solid interpretation of the evolution of the aliphatic interstellar component is proposed.
- For the first time the band proposed by Allamandola et (1992) as responsible for the 3.47 μm has been reproduced in the lab through experiments simulating dense cloud conditions.
- There is no need to invoke two separate grain populations for the bands observed in diffuse and dense clouds.
- Carbon grains responsible for the 3.4 μm band in the diffuse ISM can give rise to the absorption band at 3.47 μm in dense clouds.

The two features are the result of evolutionary transformations of carbon grains caused by processing.

H_2 formation

H_2 molecules form on interstellar grains

H atom recombination on silicates, carbon grains and water ice has been studied in lab (e.g. Pirronello et al. 1997, 1999; Hornekaer et al. 2003, Perets et al. 2005)

The recombination efficiency is high only at low grain temperatures ($T_g < 20$ K)

Laboratory results fail to explain the formation of H_2 molecules at higher grain temperatures (PDRs)

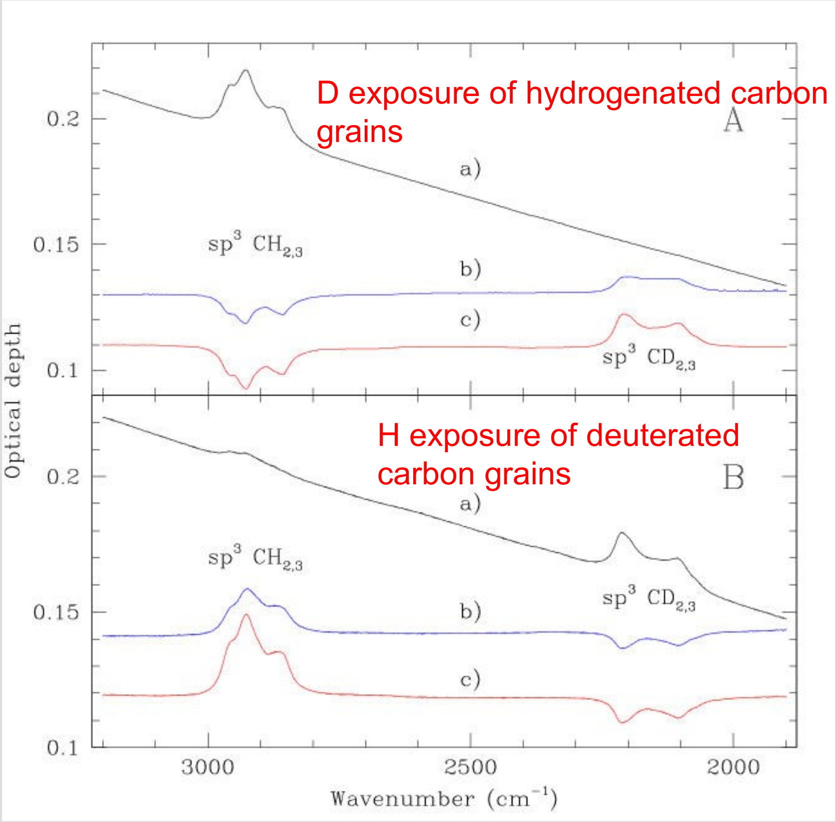
Theoretical studies suggest that H_2 formation takes place at higher grain temperatures if chemisorbed H atoms on carbon particles are considered (Cazaux &Tielens 2004)

Aliphatic C-H bonds neglected

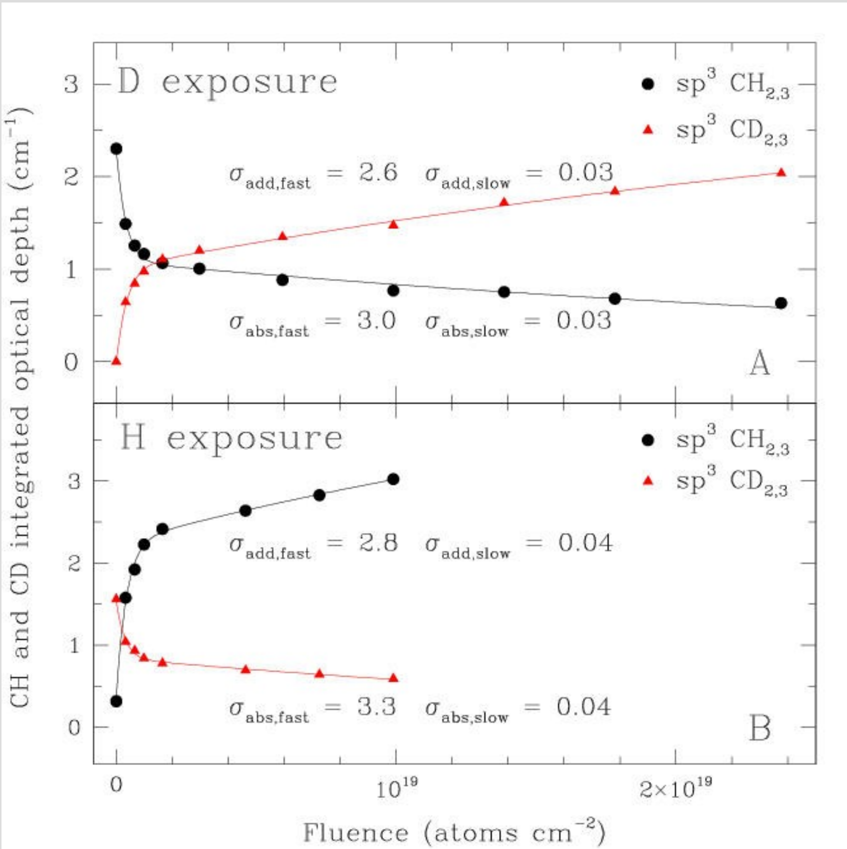
There is no experimental evidence for H_2 formation for grain and H atom temperatures relevant to PDRs conditions

HD formation by abstraction of hydrogen chemisorbed in aliphatic sites carbon grains

IR spectroscopy



Cross sections



There is no isotope effect in the cross sections

The small values of the abstractions cross section are indicative of an Eley-Rideal process driving HD formation

Abstraction and addition cross sections are equal suggesting that dehydrogenation is the rate-limiting step of the reaction sequence

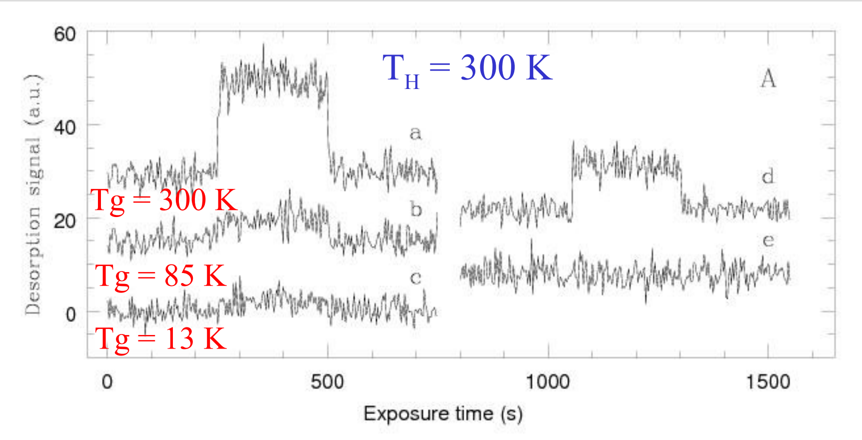
1) Dehydrogenation via H abstraction:

$$CH_n + D \rightarrow CH_{n-1} + HD_{gas}$$

2)Deuteration via D addition:

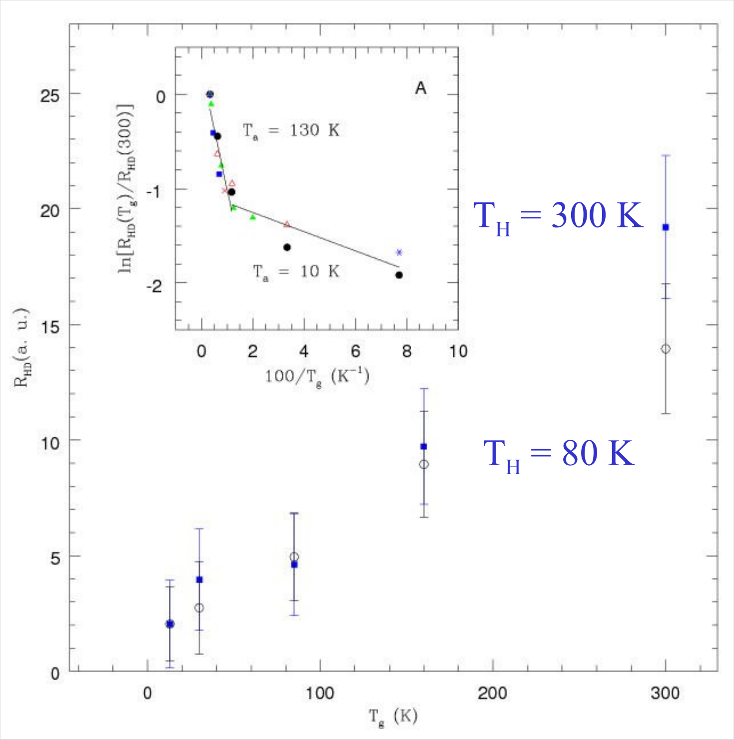
$$CH_{n-1} + D \rightarrow CH_{n-1}D$$

Mass spectroscopy



HD desorption rate measured in real-time during H atom irradiation of deuterated carbon grains

HD molecules are produced by H atoms of the beam and D atoms of deuterated carbon grains

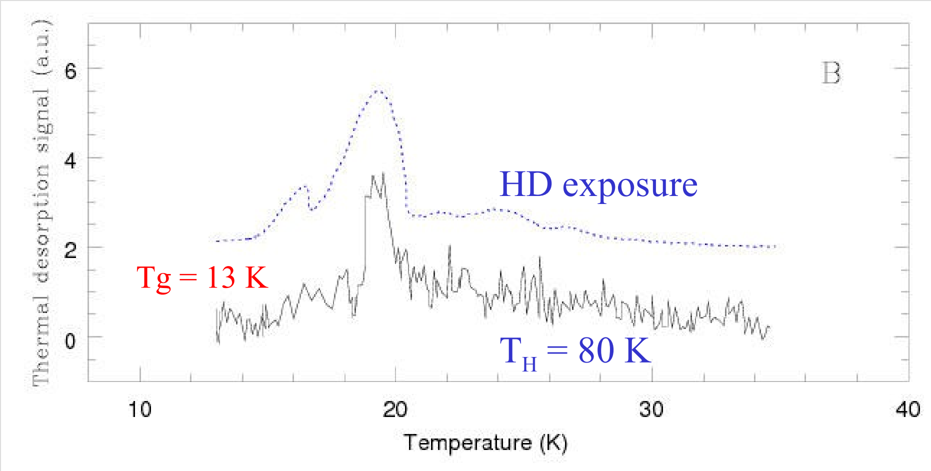


No activation barrier for HD formation

$$R_{HD} = \sigma \, \Phi \, n_{CD}$$

The desorption rate depends on the grain temperature

Thermal programmed desorption



TPD spectrum: main peak at 19 K

The integrated TPD signal is a factor 1.4 higher than the real-time desorption signal

HD molecules are produced by H atoms at low T. Desorption is thermally activated

Contribution to H_2 formation in space

$$R_{H2} = v_H \sigma n_{CH} / n_0 = 1.5\times10^4 T_H^{0.5} \sigma n_{CH} / n_0 \ (cm^3\ s^{-1})$$

$$\sigma = \sigma_{abs\ HD} = 1\times10^{-18}\ cm^2$$

DISM

$T_H = 100$ K

$n_{CH} / n_0 = 3.7\times10^{-5}$ (Mennella et al. 2002) $R_{H2} = 5.6\times10^{-18} (cm^3\ s^{-1})$

50-19 % of R_{H2} derived from observations: $(1\text{-}3) \times10^{-17} (cm^3\ s^{-1})$

(e.g. Duley & Williams 1984)

PDRs

$T_H = 500$ K

$n_{CH} / n_0 = 3.7\times10^{-5}$

$R_{H2} = 1.2\times10^{-17} (cm^3\ s^{-1})$

40-8 % of R_{H2} derived from observations: 3×10^{-17}- 1.5×10^{-16} $(cm^3\ s^{-1})$ (Habart et al. 2004)

- H_2 formed in chemisorbed sites of carbon grains should not be in highly excited states and should not contribute to interstellar gas heating