Physics and chemistry of UV illuminated gas: The Horsehead case

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August 28

SCHISM

ANR grant: SCHISM
Structure and CHemistry of the InterStellar Medium

Structures
- Duration: 4 years starting on 2009-09-01.
- Partners: IRAM (J.Pety), LERMA-LRA (M.Gerin), LUTH-ISM (F.LePetit).
- Budget: 488 438 euros.

Goals
- Coupling solid and gas chemistry.
- Coupling chemistry and dynamics (MHD shocks and turbulence).
- Get benchmark observational datasets.

Relevancy
- State-of-the-art numerical developments.
- Use of the best (sub)-millimeter instruments (Herschel, ALMA, PdBI, 30m...).

A team of observers and theoreticians

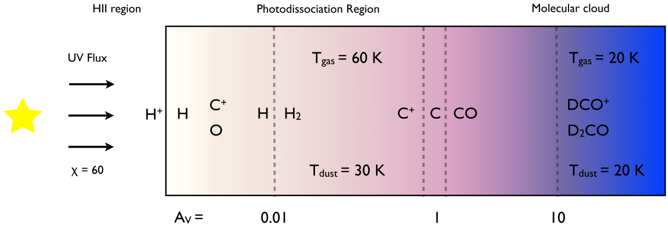
- IRAM: S.Bardeau, P.Gratier, V.Guzman, E.Reynier, N.Rodriguez-Fernandez.
- LERMA/LRA: S.Cabrit, M.DeLuca, E.Falgarone, B.Goddard, A.Gusdorf, P.Lesaffre.
- LUTH/ISM: J.LeBourlot, S.Miyake, E.Roueff.
- Additionals: P.Boissé, J.R.Goicoechea, H.Liszt, R.Lucas, G.Pineau des Forêts.

Results at 18 months from start

- 23 papers.
- 20 presentations in international conferences.

http://schism.ens.fr

PDR: Photo Dissociation Regions

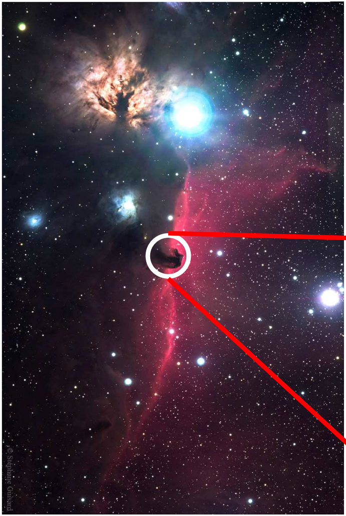


FUV photons ($<$ 13.6 eV) determine the physical and chemical properties.
Examples: diffuse clouds, starburst galaxies, surfaces of protoplanetary disks, ...
PDR models $\Rightarrow$ Understand evolution of FUV-illuminated matter.

Complex PDR models and chemical networks need well-defined observations to serve as basic references.

- Several species and many lines $\Rightarrow$ Radiative transfer models $\Rightarrow$ Column densities
- Spatial resolution $\Rightarrow$ resolve gradients predicted by models $\Rightarrow$ Interferometers (ALMA, NOEMA)

PDR template: the Horsehead nebula



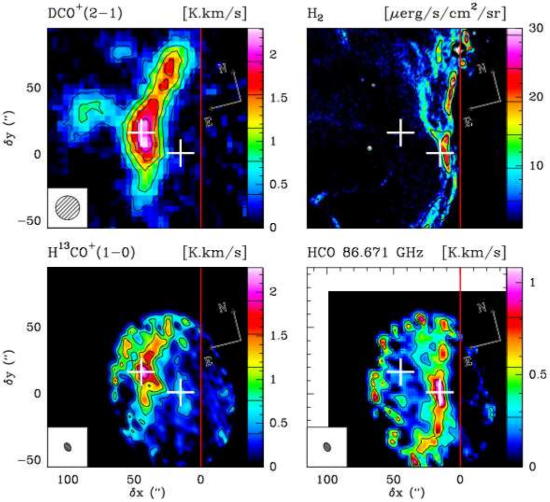
Credit: Ryan Steinberg & Family, Adam Block, NOAO, AURA, NSF

- Viewed nearly edge-on (Abergel et al. 2003)
- Nearby ($\sim$400 pc, 10'' $\leftrightarrow$ 0.02 pc).
- Illuminated by the O9.5 star σ Ori $\sim$ 3.5 pc away (Radiation field: $G_0 = 60$ in Draine units).
- Gas density is well constrained (Habart et al. 2005).

$\Rightarrow$ Reference to chemical models.

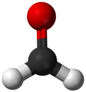
Credit: ESO

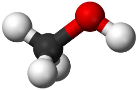
Two different environments less than 40” away



- A far-UV illuminated PDR HCO (Gerin et al. 2009)
  - $A_V \sim 1.5$
  - Warm $T_{\mathrm{kin}} \sim 60$ K
  - Relatively dense $n_{\mathrm{H}} \sim 6 \times 10^4 \mathrm{cm}^{-3}$
- A shielded, dense core DCO^+ (Pety et al. 2005)
  - $A_V \sim 20$
  - Cold $T_{\mathrm{kin}} \sim 20$ K
  - Dense $n_{\mathrm{H}} \sim 2 \times 10^5 \mathrm{cm}^{-3}$
  - High fractionation $[DCO^+]/[HCO^+] = 2\%$

(Complex) organic molecules: H_2CO and CH_3OH

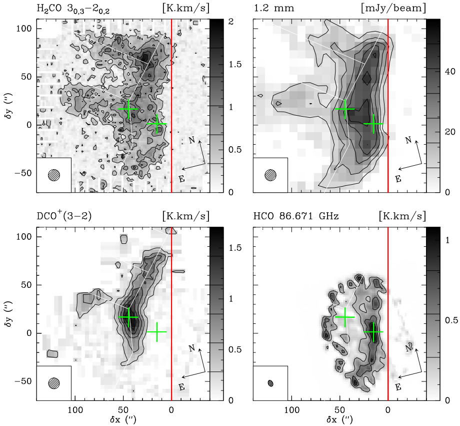




Importance: Synthesis of more complex organic molecules in the ISM
$\rightarrow$ protoplanetary diks?

- Both are observed in a wide range of interstellar environments (proto-stellar cores, YSOs, dark clouds, diffuse clouds, etc...)
- With high abundances ($10^{-6} - 10^{-7}$ in hot cores).
- H_2CO can form efficiently in both the gas-phase and on ices.
- CH_3OH is thought to be formed only in ices.
- $CO \xrightarrow{H} HCO \xrightarrow{H} H_2CO \xrightarrow{H} CH_3O \xrightarrow{H} CH_3OH$
- Evidence:
  - Methanol ices have been observed towards high- and low-mass protostars (abundances up to $\sim 30\%$ relative to water, Pontoppidan et al. 2003)
  - Laboratory experiments have shown this process is efficient (Watanabe et al. 2004, Fuchs et al. 2009)
- Thermal desorpion: evaporation temperature $\simeq 40$ K (H_2CO) and $\simeq 80$ K (CH_3OH)
- Photo-desorption (Öberg et al. 2009a,b; Muñoz Caro et al. 2010)

H_2CO: Photo-desorption of dust grain ice mantles (Guzmán et al. 2011)



IRAM-30m observations

- Abundance:
  - $[H_2CO] = 2.8 \times 10^{-10}$ PDR
  - $[H_2CO] = 2.0 \times 10^{-10}$ CORE

    Similar in PDR and dense core
- Ortho-to-para ratio
  - Core: $\sim$ 3 (equilibrium)
  - PDR: $\sim$ 2
- Dust temperature:
  - $T_{\rm dust} \simeq$ 30 K PDR
  - $T_{\rm dust} \simeq$ 20 K CORE

    $\rightarrow$ Clean environment to isolate the role of photodesorption.

H_2CO: Photo-desorption of dust grain ice mantles (Guzmán et al. 2011)

IRAM-30m observations ($\sim 16''$ resolution)

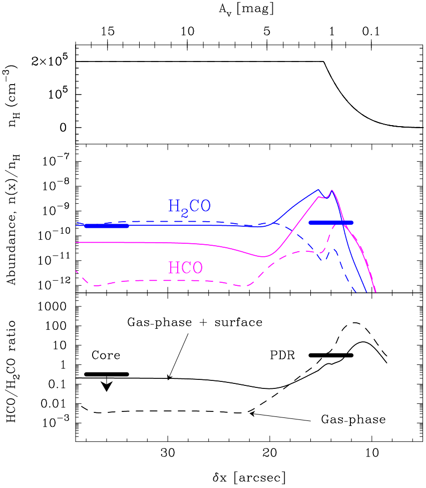
- Abundance:
  - $[H_2CO] = 2.8 \times 10^{-10}$ PDR
  - $[H_2CO] = 2.0 \times 10^{-10}$ CORE
- ortho-to-para ratio:
  - PDR: ~ 2
  - CORE: ~ 3 (equilibrium)

PDR models: Meudon

Le Bourlot et al. (1993), Le Petit et al. (2006)

- Pure gas-phase chemistry
  - Core: OK
  - PDR: Underestimates abundance
- Gas-phase + Grain surface chemistry

  CO → HCO → H_2CO → CH_3O → CH_3OH
  - PDR: OK



⇒ Photo-desorption is needed to explain the observed H_2CO abundance in the PDR.

CH_3OH: (Guzmán et al. in prep)

IRAM-30m observations (16 – 29″ resolution)

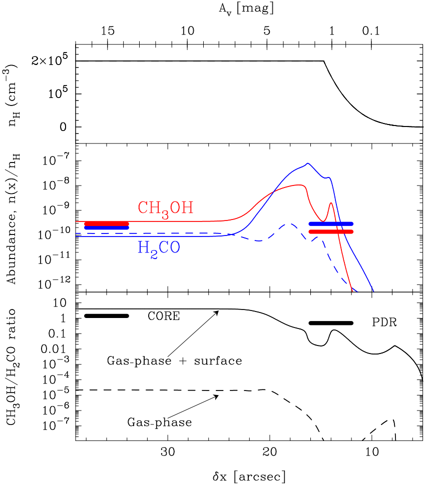
- Abundance:
  - $[CH_3OH] = (1.1 - 1.6) \times 10^{-10}$ PDR
  - $[CH_3OH] = (2.5 - 3.0) \times 10^{-10}$ CORE

PDR models: Meudon

Le Bourlot et al., to be submitted

- Pure gas-phase chemistry
  - Abundances underestimated by ~ 5 orders of magnitude
- Gas-phase + Grain surface chemistry

  $CO \rightarrow HCO \rightarrow H_2CO \rightarrow CH_3O \rightarrow CH_3OH$
  - PDR and CORE: OK

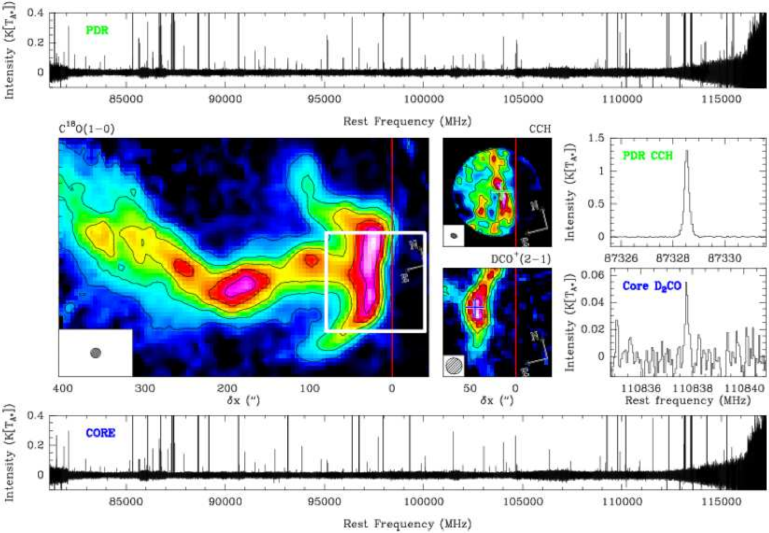


Unresolved peak at $\delta x \sim 15''$ $\Rightarrow$ Interferometric observations!

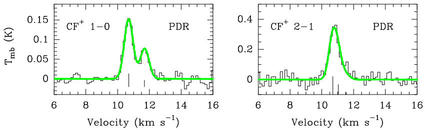
Horsehead WHISPER: 3, 2 and 1mm
(J. Pety, P. Gratier, V. Guzmán, et al.)

Wideband High-resolution Iram-30m Surveys at two Positions with Emir Receivers

3mm: Median noise: 8 mK at 49 kHz resolution → 2 x 740000 channels

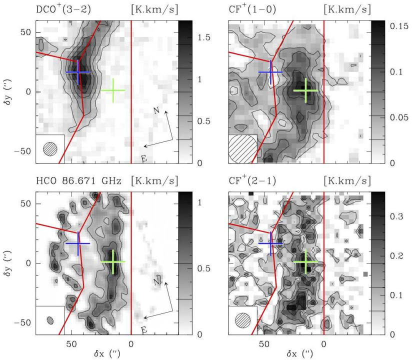


I. CF^{+}: as a proxy of C^{+} (Guzmán et al. 2012)

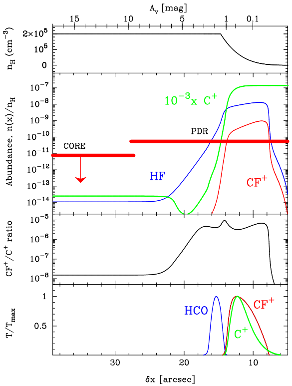


Hyperfine structure resolved!

Guzmán et al. submitted to A&A



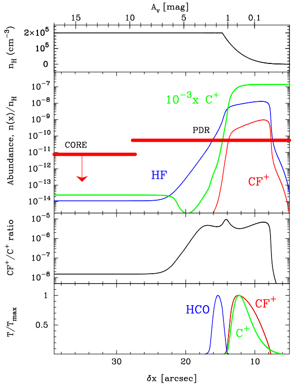
- Second detection in the ISM.
- Abundances:
  - PDR: $4.9 - 6.5 \times 10^{-10}$



→ Significant overlap between CF^{+} and C^{+}

I. CF^+: as a measure of the fluorine abundance (Guzmán et al. 2012)

- Second detection in the ISM.
- Abundances:
  - PDR: $4.9 - 6.5 \times 10^{-10}$



→ Significant overlap between CF^+ and C^+

- Simple chemistry:
  - Formation:

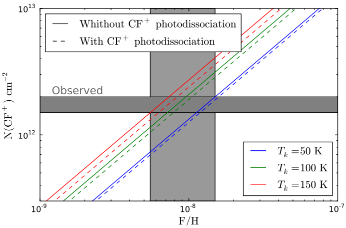
    $HF + C^+ \xrightarrow{k_1} CF^+ + H$
  - Destruction:

    $CF^+ + e^- \xrightarrow{k_2} C + F$

    $CF^+ + h\nu \rightarrow C^+ + H$

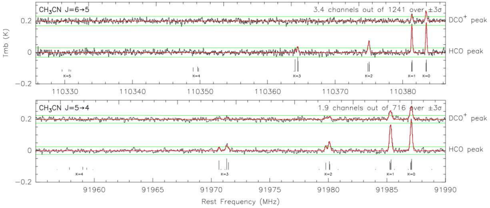
$\Rightarrow N(CF^+) \simeq \frac{k_1}{k_2}[\mathrm{F}]\, n_\mathrm{H}\, l \quad [\mathrm{cm}^{-2}]$

F/H $\simeq (0.6 - 1.5) \times 10^{-8}$

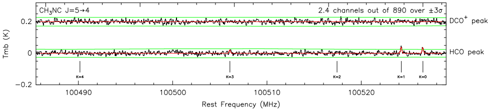


II. Relatively complex (iso-)nitriles: CH_3CN (Gratier et al. in prep)

CH_3CN hyperfine structure resolved



First firm detection of CH_3NC at mm wavelength



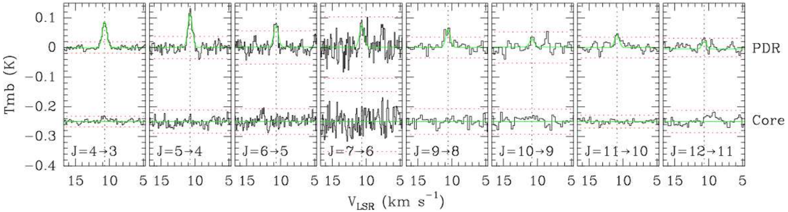
- Good thermometer for large densities ($\geq 10^6 \mathrm{cm}^{-3}$).
- Abundances:
  - PDR
    $[CH_3CN] = (1.6 - 6.3) \times 10^{-10}$
  - Core
    $[CH_3CN] = (0.5 - 1.3) \times 10^{-11}$

  CH_3CN is 40 times more abundant in the PDR than in the dense core!
- Pure gas-phase models fail:

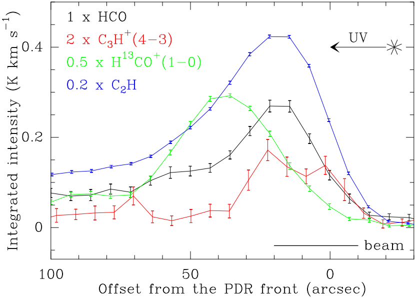
  $$HCN \xrightarrow{CH_3^+} CH_3HCN^+ \xrightarrow{e^-} CH_3CN$$

  - photo-desorption?
  - UV photo-processing on ices?
- Isomeric ratio in PDR
  $[CH_3NC]/[CH_3CN] = 0.1$

III. First detection of C_3H^+ in the ISM (Pety et al. submitted to A&A)



- Consistent set of 8 unidentified lines towards the PDR position.
- Linear rotor, with a $^1\Sigma$ electronic ground state.
- The deduced rotational constant is close to l-C_3H.
- Reactive molecule with a spatial distribution similar to small hydrocarbon chains.



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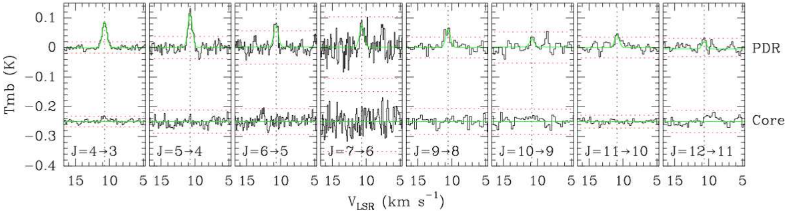

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- Linear rotor, with a $^1\Sigma$ electronic ground state.
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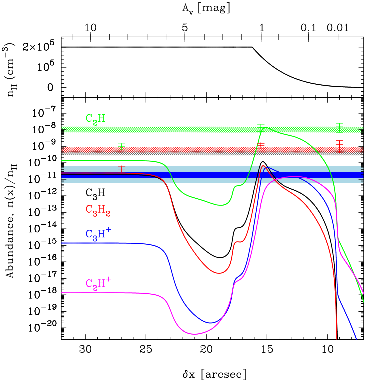
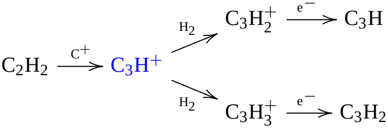
⇒ Most probable candidate: C_3H^+

- Right electronic state.
- Computed rotational constant (Cooper & Murphy 1988) close to deduced value .
- Dipole moment: 2.97 Debye (ab inito calculations by D. Talbi, private comunication)
- Experimental spectroscopic confirmation is on-going at the PhLAM lab in Lille (Bailleux & Margules, priv. comm.)

III. First detection of C_3H^+ in the ISM (Pety et al. submitted to A&A)



- Importance: Ion-molecule reactions with C_3H^+ $\rightarrow$ most important channels to form hydrocarbons.



- Abundance: $[C_3H^+] = 2 \pm 0.7 \times 10^{-11} \mathrm{cm}^{-2}$
- Spatial structure: 2 peaks
  - Narrow filament at the edge
  - Lower abundance Plateau at dense core

  Need high resolution observations!
- C_2H and C_3H_2 High-resolution observations (Pety et al. 2005)

Summary

- Organic molecules:
  - Photo-desorption of dust grain ice mantles is needed to explain the observed H_2CO abundance in the PDR (Guzmán et al. 2011).
  - CH_3OH is efficiently photo-desorbed in both the PDR and dense core.
  - On-going PdBI interferometric observations to resolve the peak at the edge of the PDR.
- Horsehead WHISPER: 3, 2 and 1mm
  - CF^+ can be used as a proxy of C^+ and a measure of the fluorine abundance (Guzmán et al. 2012).
  - CH_3CN is 40 times more abundant in the PDR than in the shielded dense core (Gratier et al. in prep).
  - First detection of C_3H^+ in the ISM (Pety et al. submitted to A&A).
- Approximately 30 species (+ their isotopologues) detected in the PDR and the dense core $\Rightarrow$ This enables a detailed comparison of the chemistry of UV-illuminated and UV-shielded gas.

Thank you!