Complex organics in the Horsehead PDR

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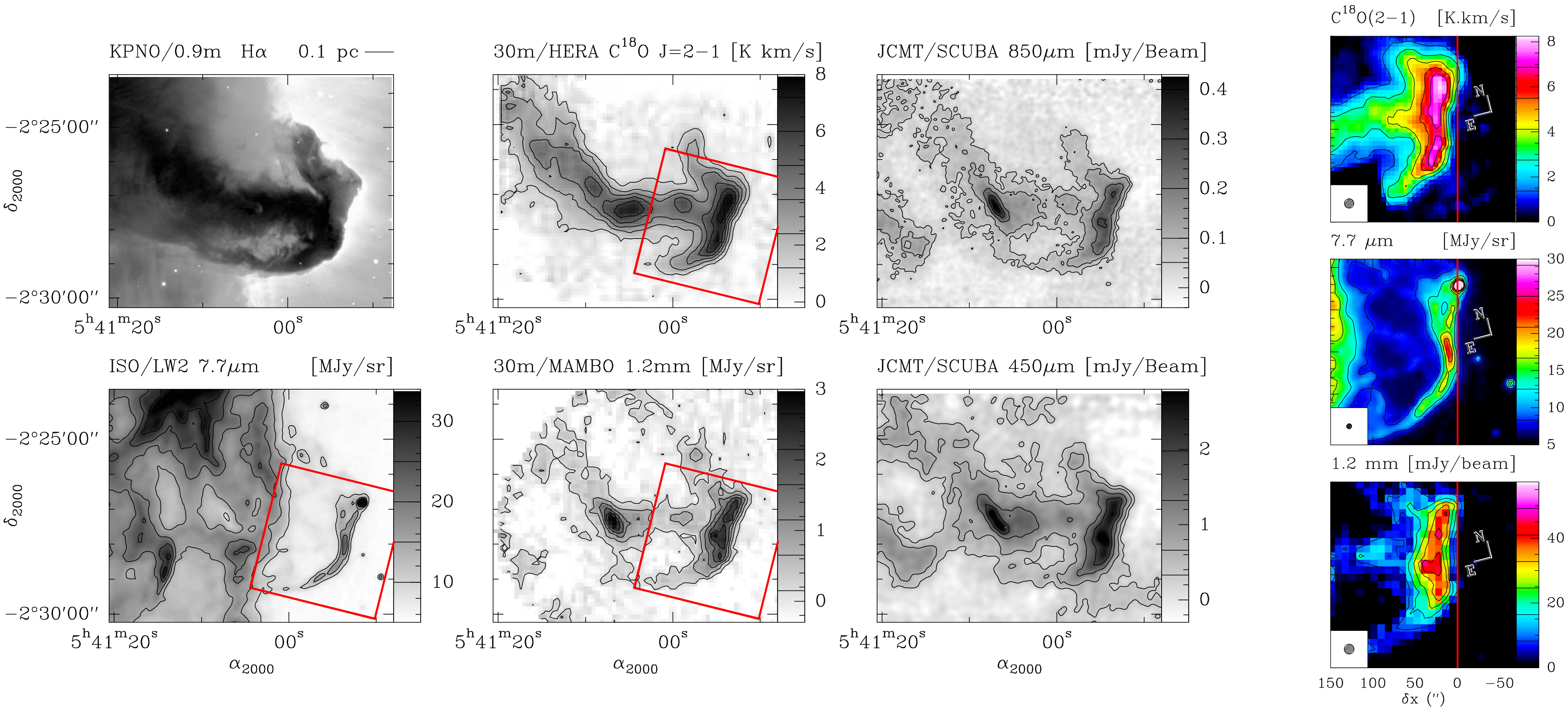
The Horsehead mane ID card: I. The environment
Credit: Rogelio Bernal Andreo

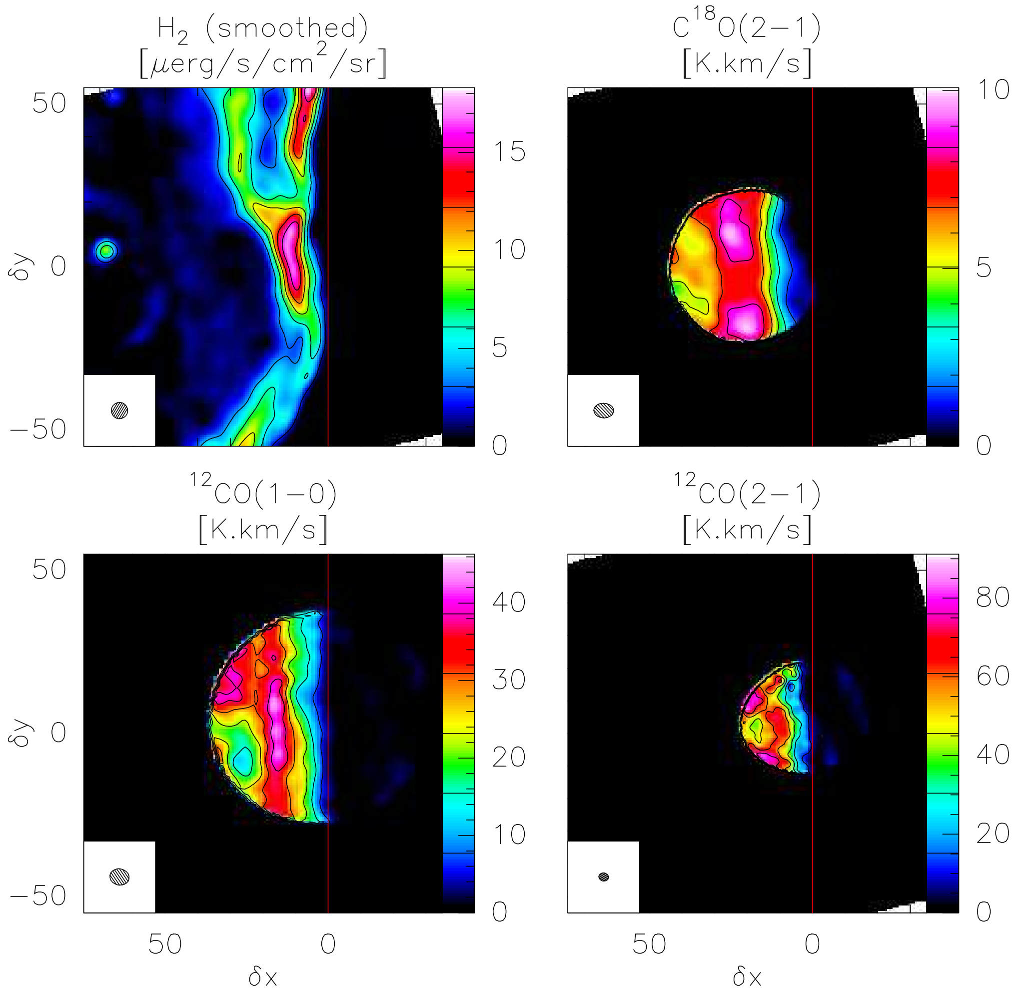
- Exciting star: σOri (O9.5V) at 0.5° (3.5 pc), PA 76°. ζOri either shadowed (Philipp et al. 2006) or in the foreground.
- Far–UV intensity: $G_0 = 100$ (Habing) or $\chi = 60$ (Draine).

The Horsehead mane ID card: II. The global structure

- KPNO Hα + BIMA ^{12}CO J=1–0 (Pound et al. 2003) $\Rightarrow$ Typical pillar;
- IRAM/30m C^{18}O J=2–1 (Hily-Blant et al. 2005) $\Rightarrow$ Neck in solid rotation;
- JCMT 850 μm and 450 μm continuum (Ward-Thompson et al. 2006) $\Rightarrow$ West condensation (2 M$_\odot$ in 0.31 $\times$ 0.13 pc) dynamics dominated by the ionisation front;
- ISO 7 μm continuum (Abergel et al. 2003) $\Rightarrow$ Edge-on structure, star in plane-of-sky.

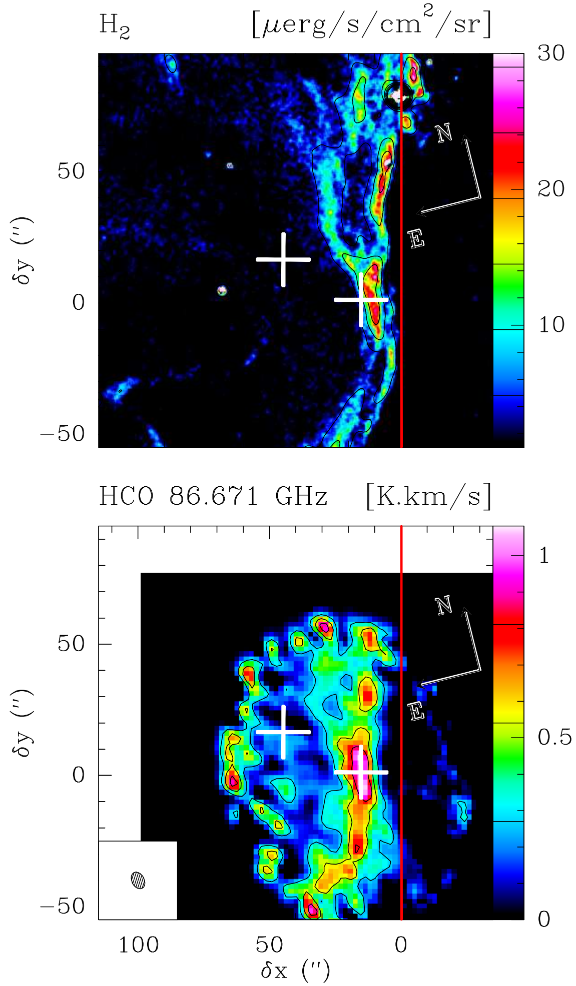


The Horsehead mane ID card: III. Density profile
NTT/SOFI H_2 2.1 μm + IRAM/PdBI ^{12}CO and C^{18}O
(Habart et al. 2005)



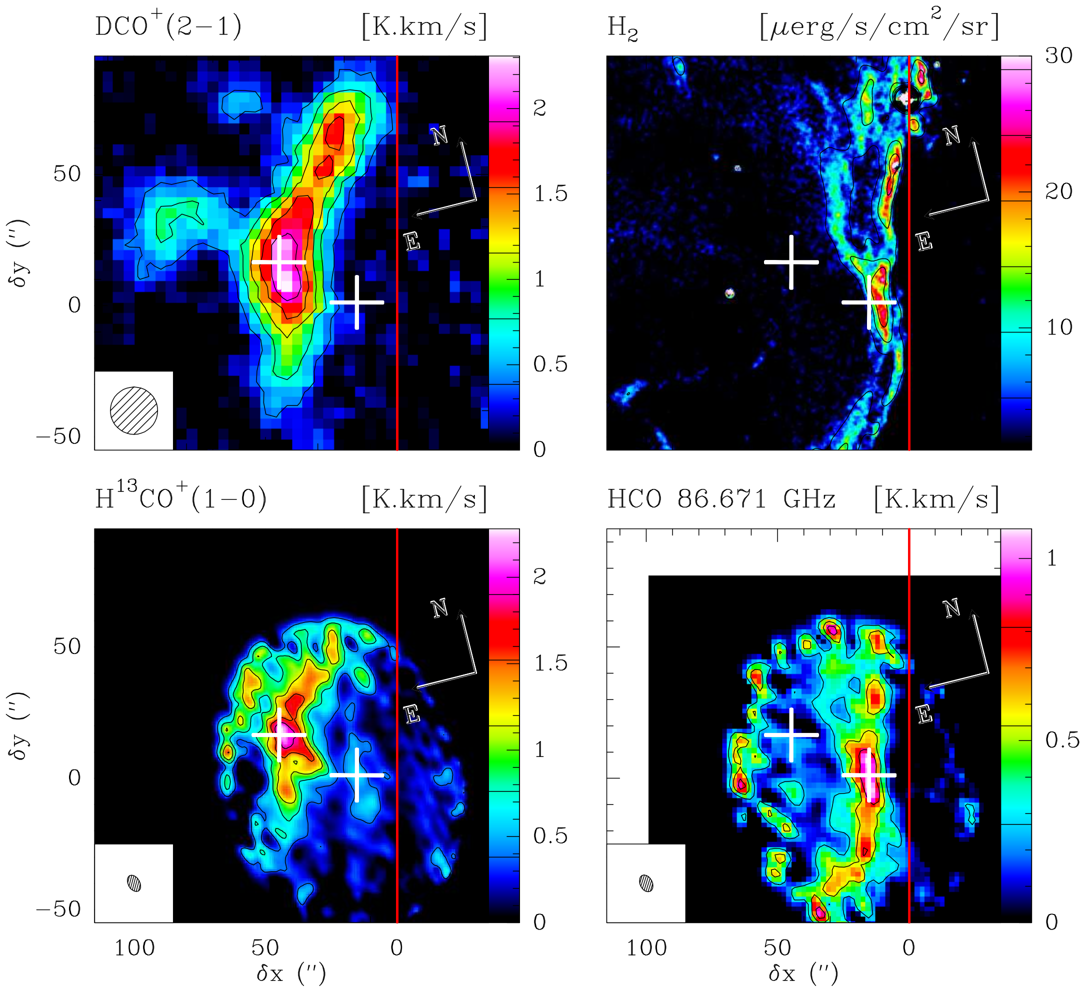
- H_2 filament width (∼5″)
  ⇒ PDR inclination on the plane-of-the-sky $< 5°$.
- Tracer stratification
  ⇒ Steep density gradient: $10^5\,\mathrm{cm}^{-3}$ in 10″ or 0.02 pc.
- Density + Thermal profiles
  ⇒ Roughly uniform thermal pressure: $\sim 4\,10^6\,\mathrm{K\,cm}^{-3}$.

The Horsehead mane ID card: IV.1 A far UV illuminated PDR
NTT/SOFI H_2 2.1 μm + IRAM/PdBI HCO
(Gerin et al. 2009)



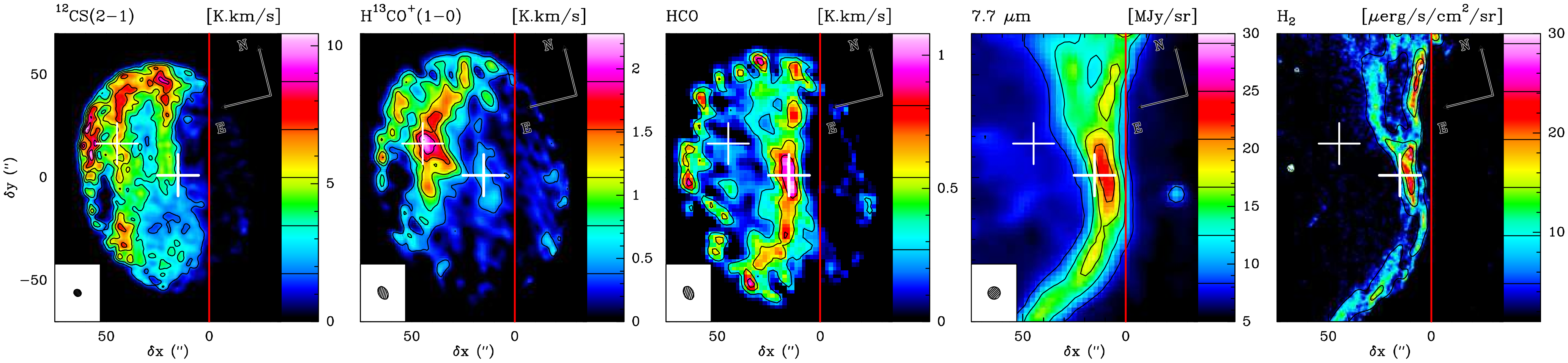
- 1.5 K HCO lines at 15″ from edge imply
  - Illuminated: $A_V \sim 1.5$,
  - Warm: $T_{gas} \sim 100 - 200\,K$,
  - Relatively dense: $n_H \sim 4 \times 10^4\,cm^{-3}$.
- HCO Abundances in PDR gas
  - $[HCO]/[H_2] \sim 1.7 \times 10^{-9}$,
  - $[HCO]/[H^{13}CO^+] \sim 55$,
  - $[HCO]/[HCO^+] \sim 1$.
- HCO: A surface tracer of dense FUV illuminated molecular gas.

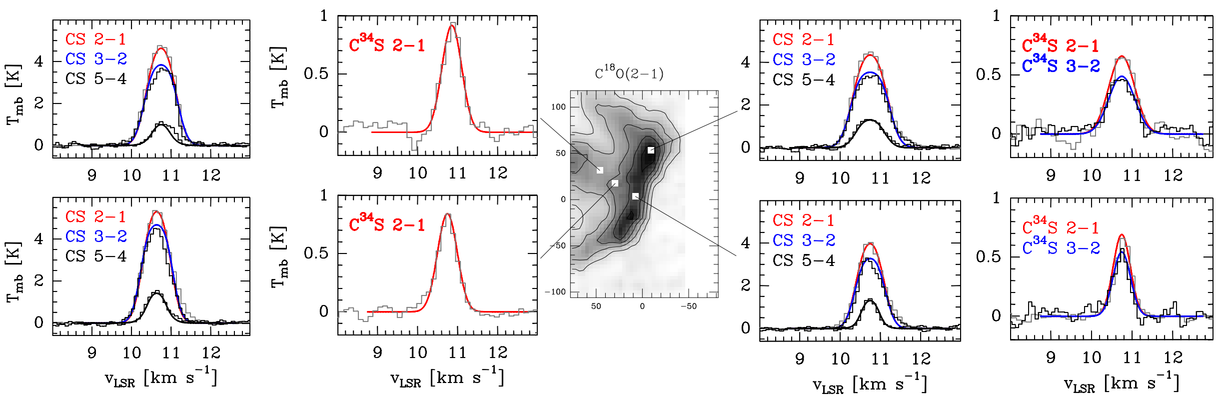
The Horsehead mane ID card: IV.2 In front of a shielded, dense core
IRAM/PdBI $H^{13}CO^+$ and DCO^+
(Pety et al. 2007)

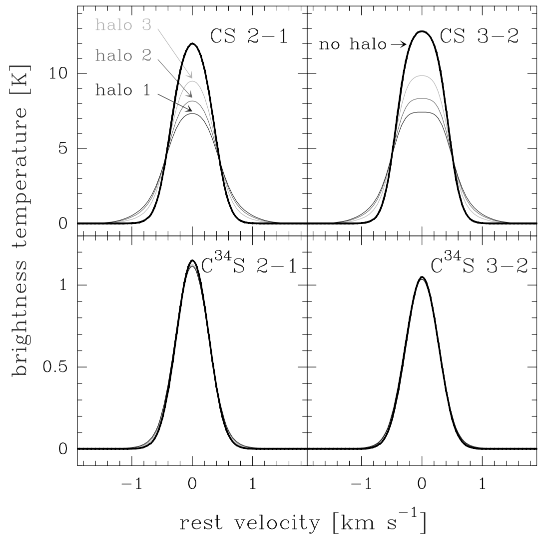


- 4 K DCO^+ lines less than 50″ from edge imply
  - Shielded: $A_v \geq 10$,
  - Cool: 10–20 K,
  - Dense: $n(H_2) \geq 2 \times 10^5\,cm^{-3}$.
- Fractionation levels
  - $[DCO^+]/[HCO^+] = 2\%$ in dense core.
  - $[DCO^+]/[HCO^+] < 0.1\%$ in PDR gas.

The Horsehead mane ID card: IV.3 Wrapped in a lower density halo
IRAM/PdBI CS J=2–1 + IRAM/30m CS, and $C^{34}S$
(Goicoechea et al. 2006)



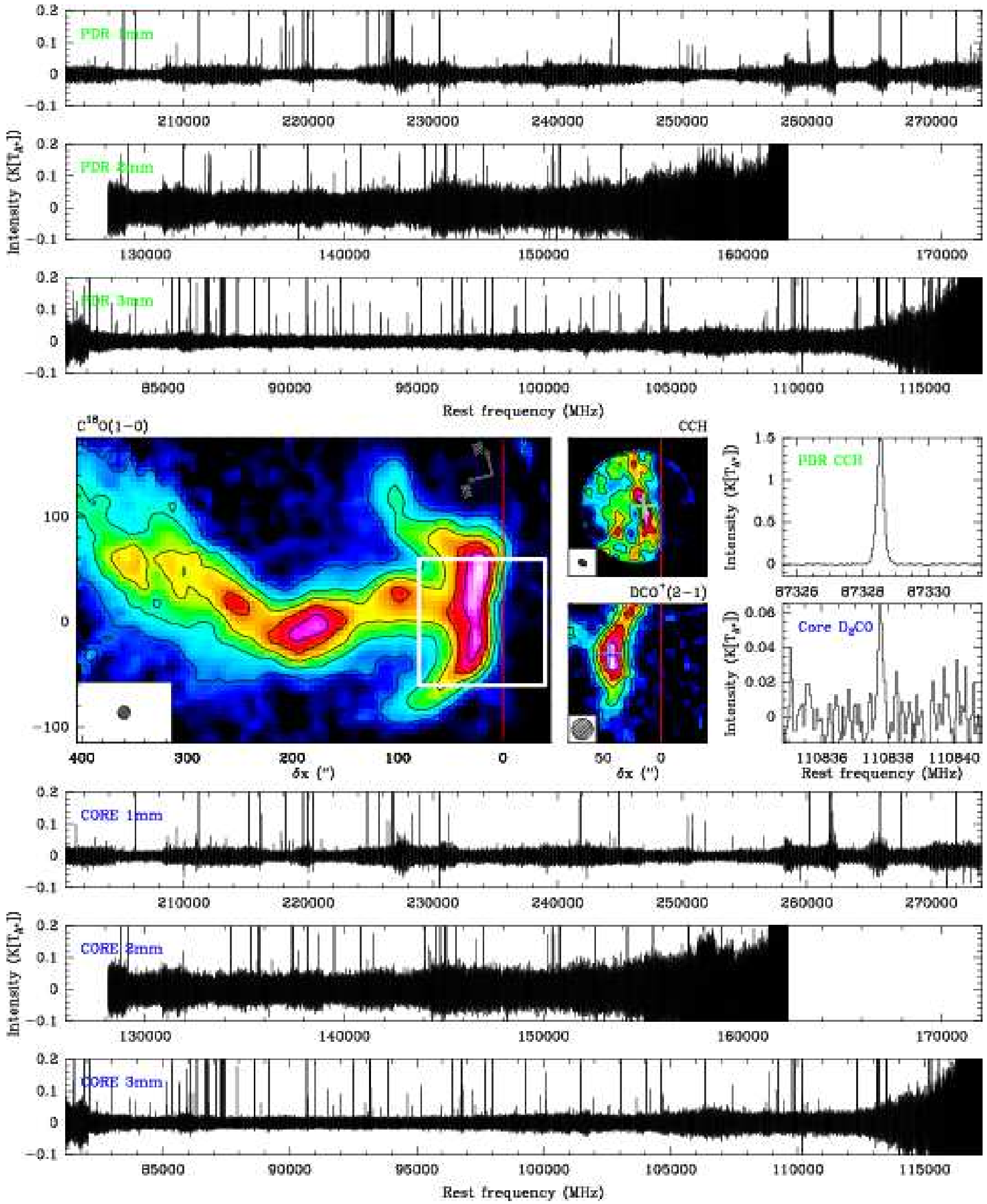




Presence of a $5 \times 10^4\,\mathrm{cm}^{-3}$ halo.

The Horsehead WHISPER line survey (PI: Pety, Guzmán, Gratier et al.)

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



IRAM-30m telescope
$\sim$ 75 hours per position

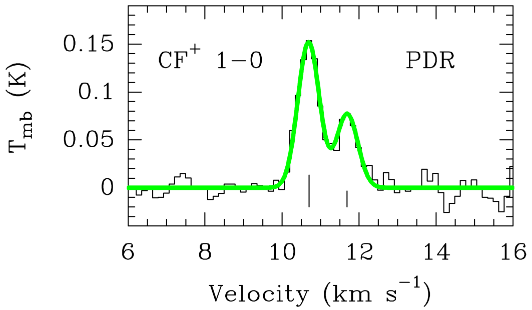
	1 mm	2 mm	3 mm
Bandwidth	73 GHz	34 GHz	36 GHz
Resolution	195 kHz	49 kHz	49 kHz
Sensitivity	8.6 mK	18.5 mK	8.1 mK

- 2 positions observed
  $\Rightarrow$ Detailed comparison of the chemistry of UV-illuminated and UV-shielded gas
- 30 species (plus their isotopologues) are detected with up to 7 atoms

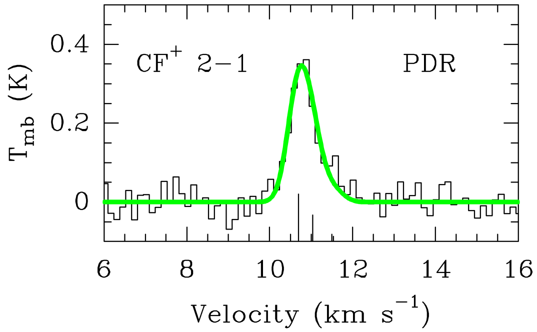
CF^+ emission in the Horsehead

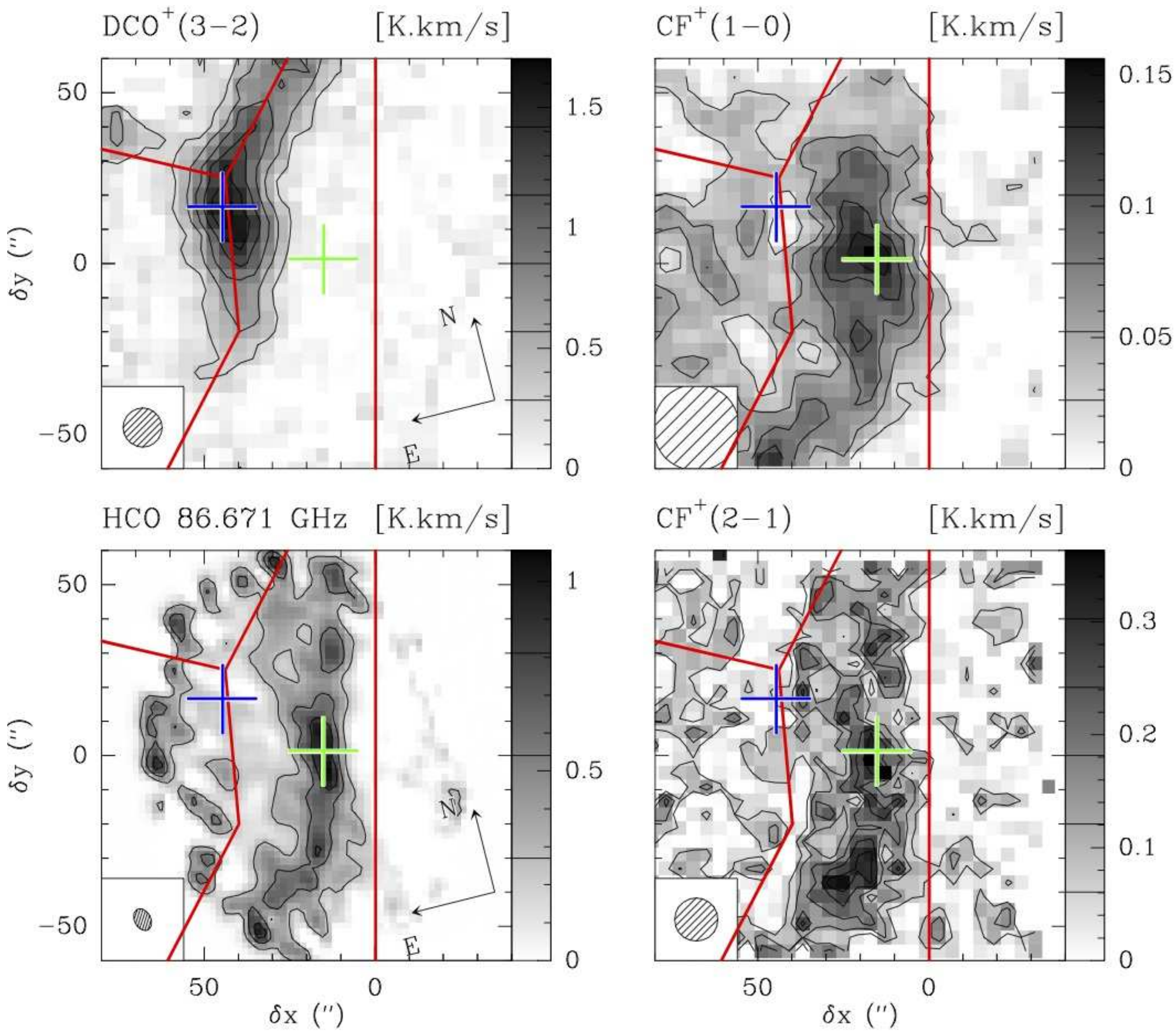
Guzmán et al. 2012a

$\nu = 102.587$ GHz



$\nu = 205.170$ GHz





Abundance:

- PDR: $4.9 - 6.5 \times 10^{-10}$

CF^+ emission arises from the UV-illuminated edge

CF^+: as a measure of the fluorine abundance

Guzmán et al. 2012a

Simple chemistry:

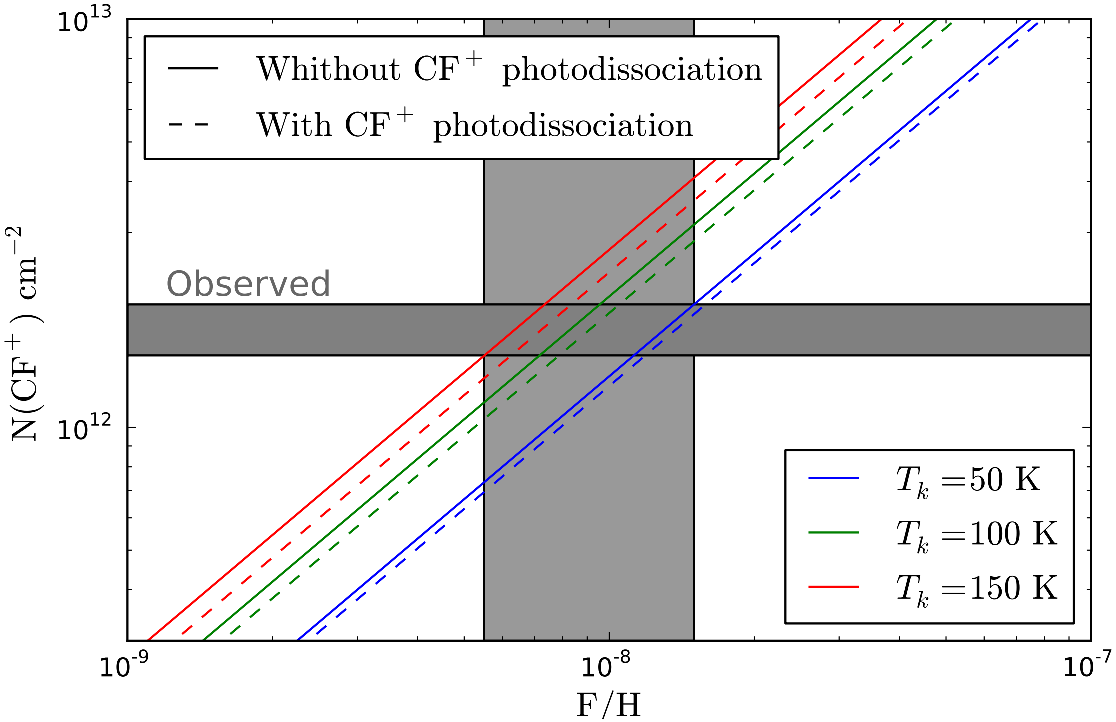
- Formation:
  $HF + C^+ \xrightarrow{k_1} CF^+ + H$
- Destruction:
  $CF^+ + e^- \xrightarrow{k_2} C + F$
  $CF^+ + h\nu \xrightarrow{k_{pd}} C^+ + H$

$$\Rightarrow N(CF^+) \simeq \frac{k_1}{(k_2+\chi k_{pd})} [F]\, n_H\, l \quad [\,cm^{-2}]$$

Horsehead: low UV field
$\rightarrow k_2 \gg \chi k_{pd}$

Fluorine abundance:

- Solar value
  F/H$= 2.6 \times 10^{-8}$
  (Asplund et al. 2009)
- Diffuse atomic gas
  F/H$= 1.8 \times 10^{-8}$
  (Snow et al. 2007)
- Diffuse molecular clouds
  F/H$= (0.5 - 0.8) \times 10^{-8}$
  (Sonnentrucker et al. 2010)



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

CF^+ as a proxy of C^+

Guzmán et al. 2012a

C^+ is a key species in the interstellar medium

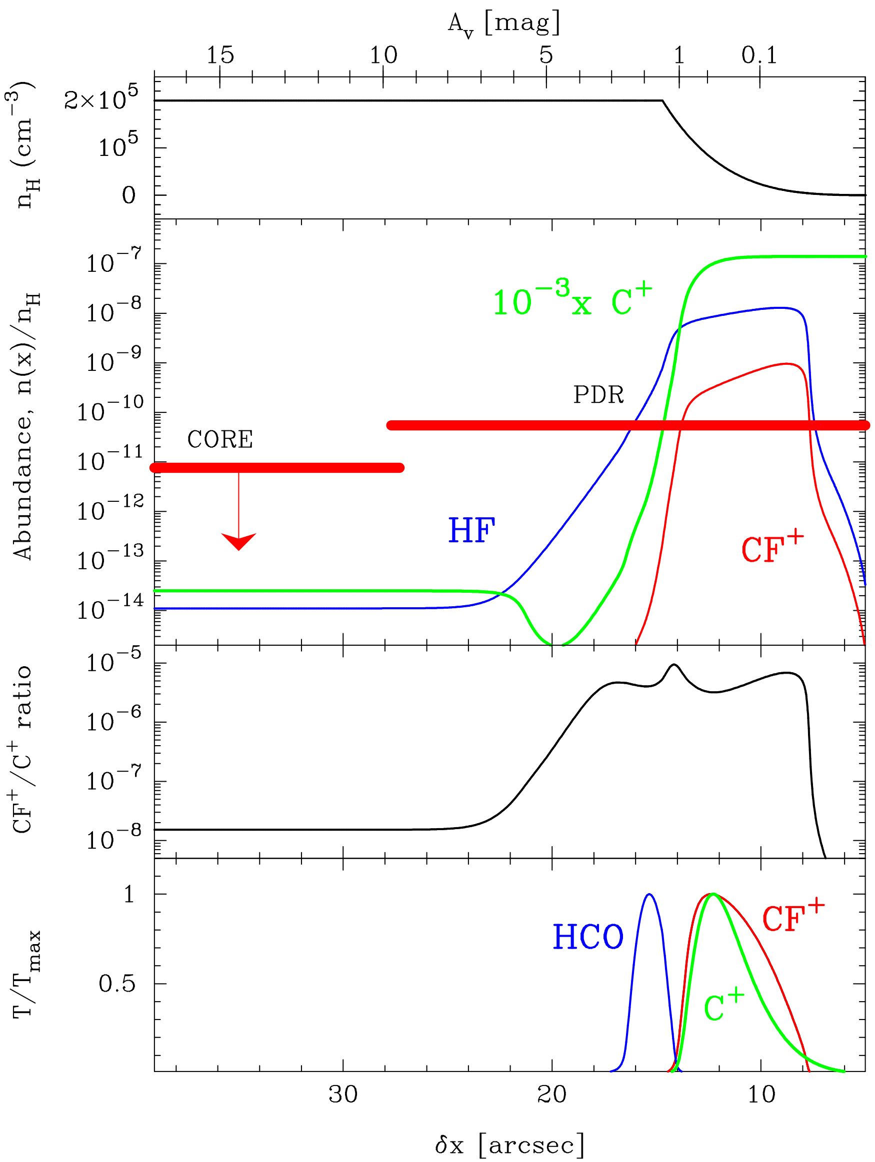
- Tracer of the neutral gas and the warm ionized medium (H II regions).
- Dominant gas phase reservoir of carbon in the diffuse ISM
- Its 1.9 THz (158 μm) fine structure transition is the main cooling mechanism of the diffuse gas.

But

- C^+ can only be observed from space at low angular resolution (Herschel at 12$''$, SOFIA at 15$''$)

Find tracers of C^+ that can be observed from the ground at much higher spatial resolution (ALMA and NOEMA)

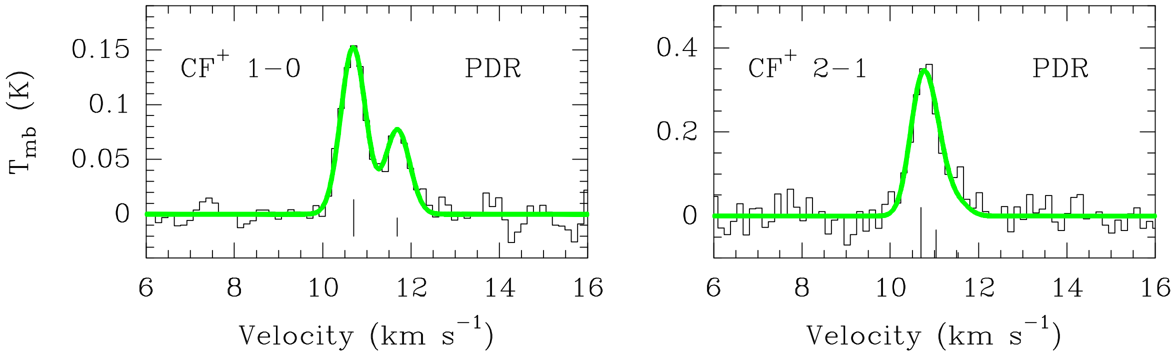
We propose CF^+ can be used as a tracer of C^+ associated to molecular gas that can be observed from the ground

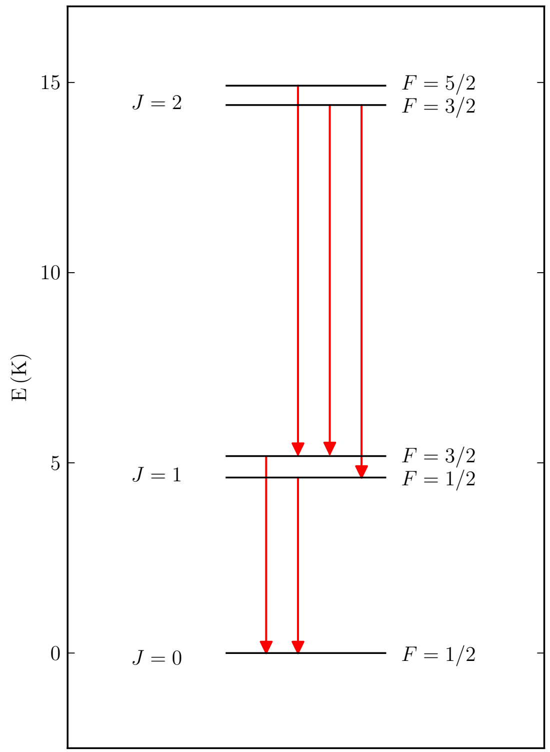


Significant overlap between CF^+ and C^+

Origin of the double peak in CF^+

Guzmán et al. 2012b





CF^+ is the only species detected in the survey showing a double peak line profile

- Kinematic origin?
- Hyperfine structure?

CF^+ nuclear spin $I = 1/2$
$\rightarrow \mathbf{F} = \mathbf{J} + \mathbf{I}$
$F = I + J, I + J - 1, ..., |I - J|$

The energy levels are given by

$$E = E_J + \frac{C_I}{2}[F(F+1) - I(I+1) - J(J+1)]$$

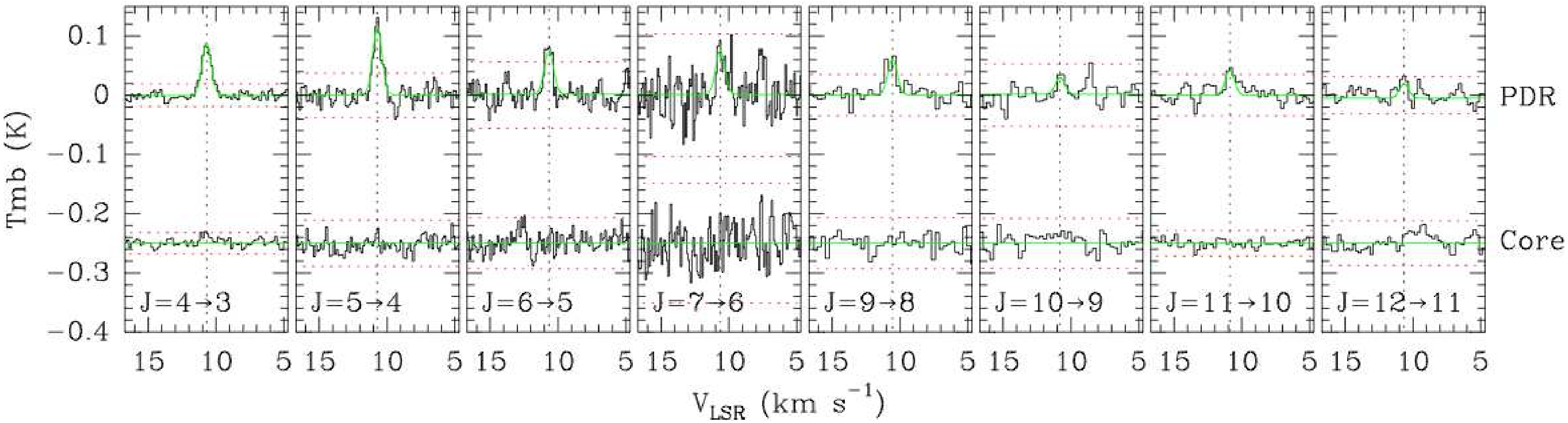
C_I : Spin rotation constant

Ab initio calculations by J. Gauss
$\rightarrow C_I = 229.2$ kHz

Consistent with observations

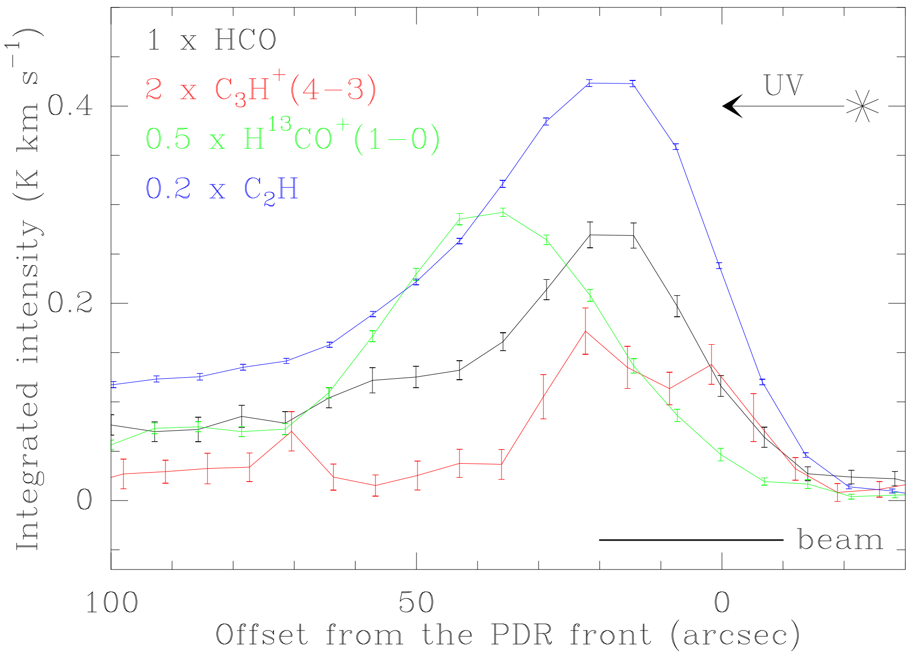
A new species in the ISM: Tentatively attributed to C_3H^+

Pety, Gratier, **Guzmán** et al. 2012

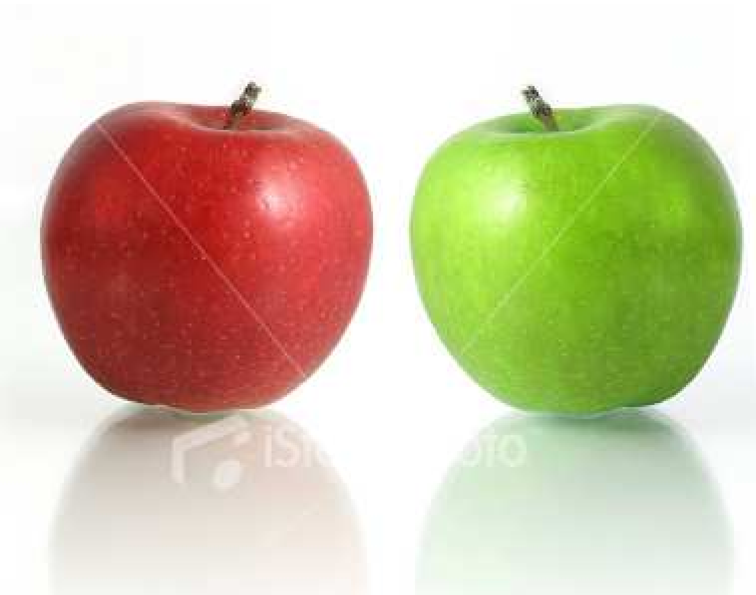


- Consistent set of 8 unidentified lines towards the PDR position.
- Linear rotor, with a $^1\Sigma$ electronic ground state.
- The deduced rotational constant is close to that of l-C_3H.
- Reactive molecule with a spatial distribution similar to small hydrocarbon chains.

$\Rightarrow$ Most probable candidate: C_3H^+



Controversy on the attribution: C_3H^+ or C_3H^-?



- Huang et al. 2013: High-accuracy quantum chemical calculations to compute the spectroscopic constants of C_3H^+
- Fortenberry et al. 2013 proposed that a more plausible candidate is the hydrocarbon anion C_3H^-

The lines are detected in emission in the Orion Bar (Cuadrado et al. in prep) and in absorption toward the Sgr B2(N) (McGuirre et al. 2013)
$\longrightarrow$ Confirms the presence of the carrier in the ISM

Problems:

1. No anions have detected in the Horsehead PDR (Agu\'ndez et al. 2008)
   - $C_4H^-/C_4H \leq 0.033$
   - $C_6H^-/C_6H \leq 8.9$
   - $CN^-/CN \leq 0.55$
2. $C_3H^-/C_3H \sim 57\%$, would be the highest anion to neutral ratio detected in the ISM so far!
3. The lines are not detected in the dark cloud TMC 1 and IRC+10216, where other anions have been already detected.

A direct measurement in the laboratory is necessary to provide a definitive assignment and close the controversy.

Laboratory, ab initio confirmations of the attribution to C_3H^+ and other detections

Laboratory confirmation

- Brünken et al., Laboratory Rotational Spectrum of l-C3H+ and Confirmation of its Astronomical Detection, 2014, *ApJ*, 783, 77.
- McCarthy et al., A Laboratory Study of C3H+ and the C3H Radical in Three New Vibrationally Excited 2Σ States Using a Pin-Hole Nozzle Discharge Source, 2015, *A&A*, 575, 82.

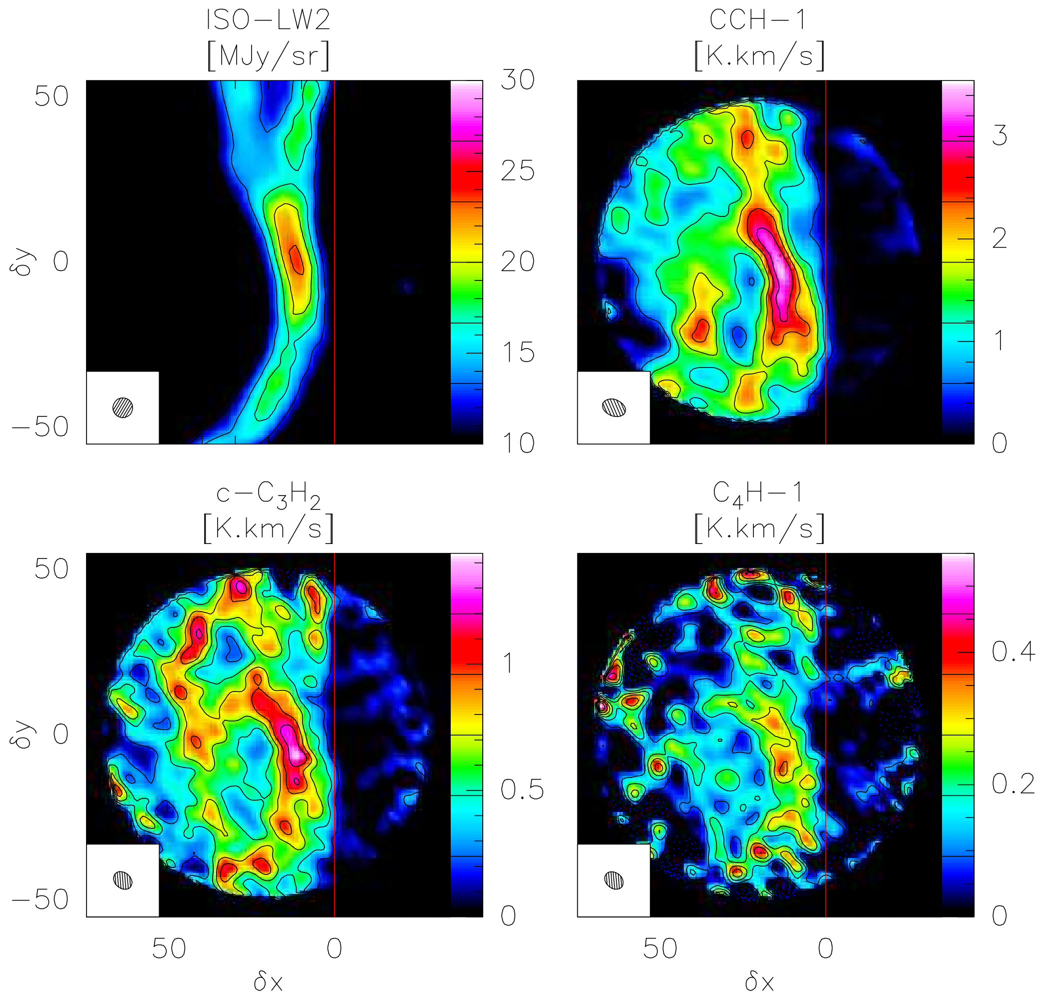
ab initio confirmation

- Botschwina et al., Strong Theoretical Support for the Assignment of B11244 to l-C3H+, 2014, *A&A*, 564, 64L.
- Mladenović, The B11244 story: Rovibrational calculations for C3H+ and C3H- revisited, 2014, *ApJ*, 796, 139.

Other detections

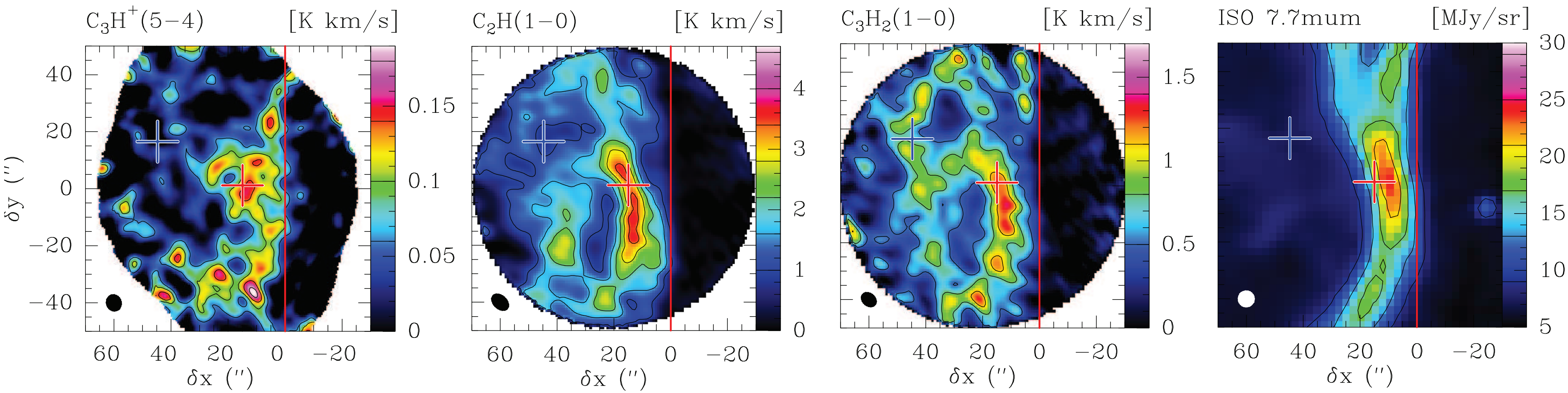
- Cuadrado et al., The chemistry and spatial distribution of small hydrocarbons in UV-irradiated molecular clouds: the Orion Bar PDR, 2015, *ApJ*, 800, 33.
- Mc Guire et al., in prep.

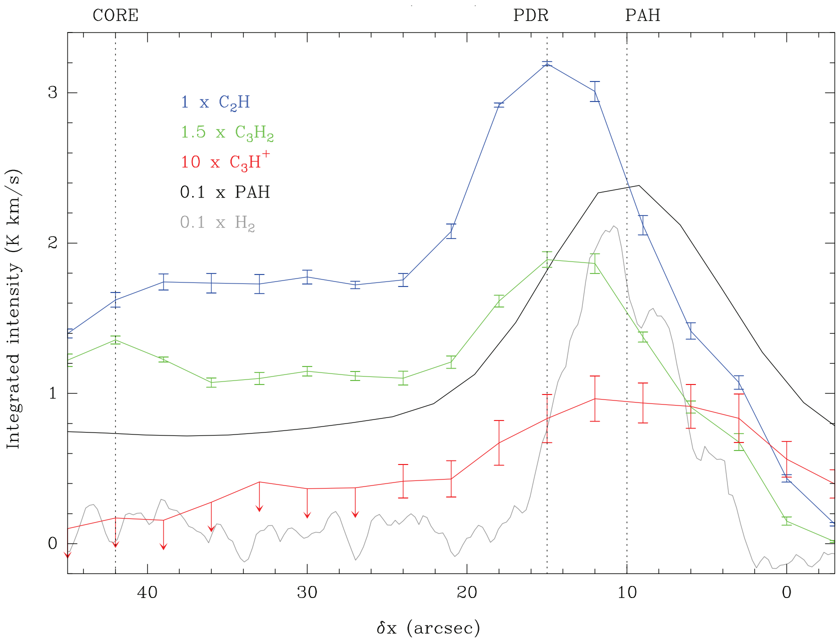
Small hydrocarbons and PAHs:
On the need of a Top-Down chemistry
IRAM/PdBI CCH, c-C_3H_2 and C_4H (Pety et al. 2005)



- Good spatial correlations of small hydrocarbon between them and with ISO 7 μm.
- Best PDR model fails to reproduce the abundances of the small hydrocarbon.
- Possible explanations:
  - Photo-erosion of PAHs (large C reservoirs).

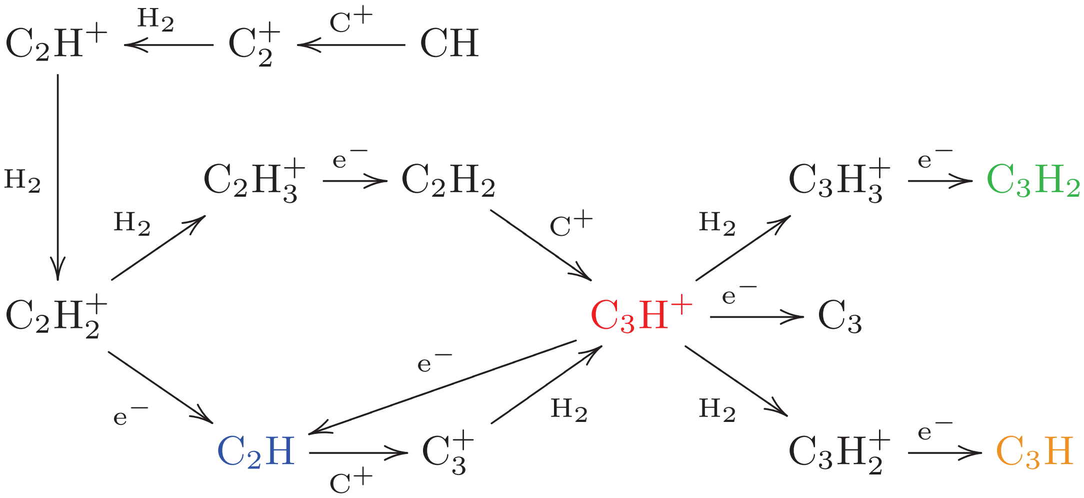
Small hydrocarbons and PAHs:
On the need of a Top-Down chemistry
IRAM/PdBI C_3H^+ (Guzmán et al., 2015)

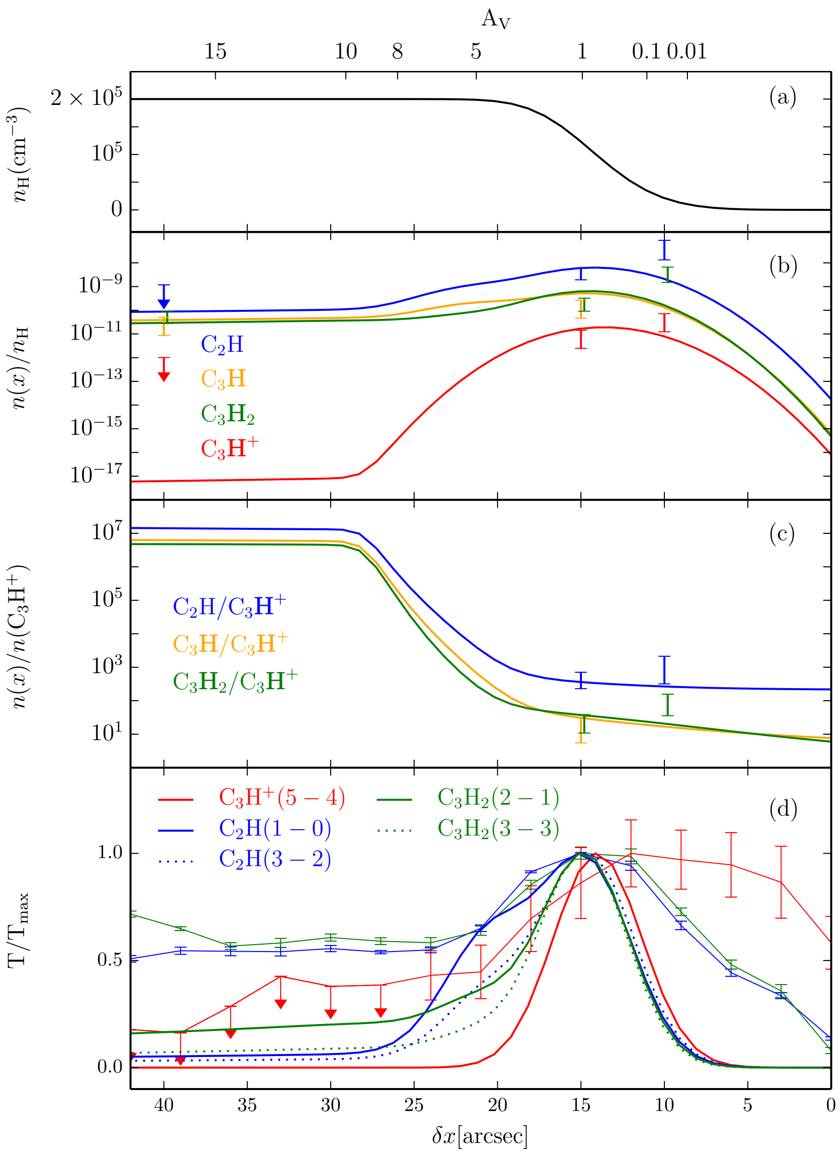




- C_3H^+ peaks before than CCH and C_3H_2.
- C_3H^+ cut is a mixture of the PAH and the small hydrocarbon emission profiles.

Small hydrocarbons and PAHs:
On the need of a Top-Down chemistry
IRAM/PdBI C_3H^+ (Guzmán et al., 2015)

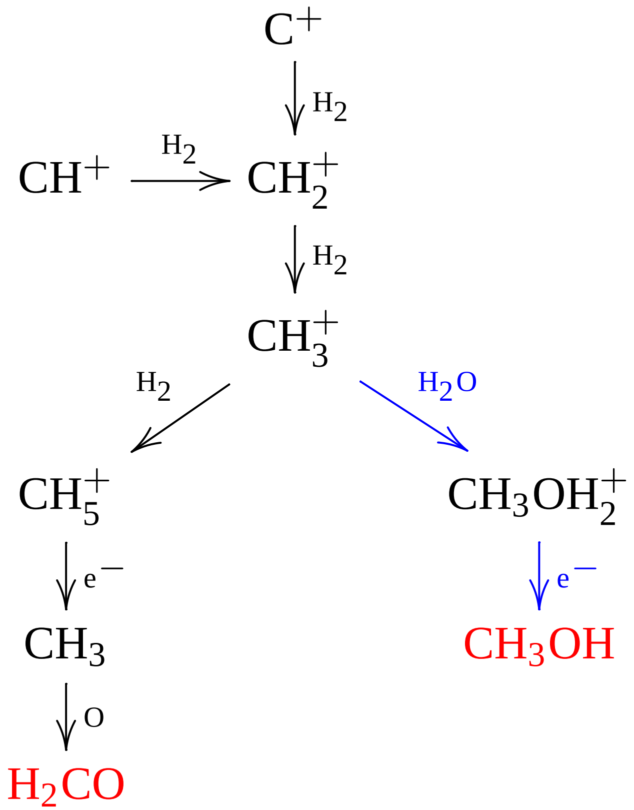




- C_3H^+ is a key intermediate species in the hydrocarbon chemistry.
- The abundances of C_3H^+ are closer to models than the CCH and C_3H_2 ones, but the brightness profile is not well reproduced by the models.

Formation of H_2CO and CH_3OH

Gas-phase:



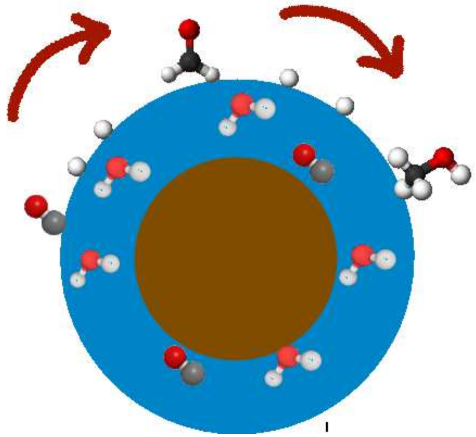
Efficient Inefficient

Garrod et al. 2006
Geppert et al. 2006

Grain surface chemistry:

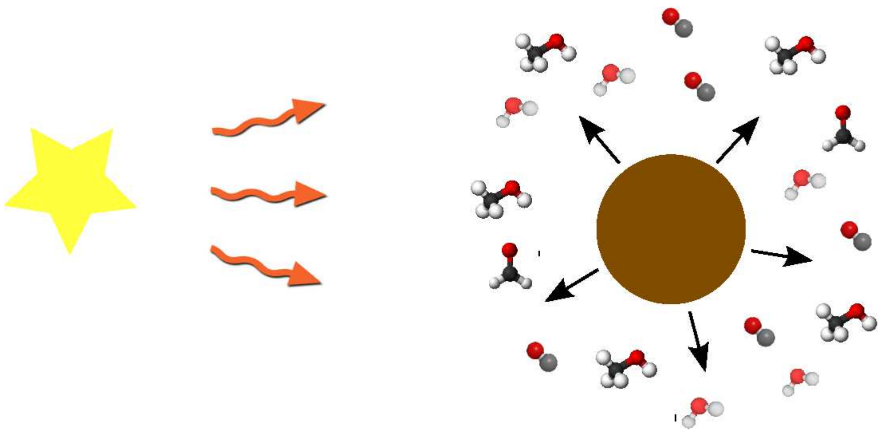
CO → HCO → H_2CO → CH_3O → CH_3OH

- Lab. experiments: Both species can be formed efficiently in the ices (Watanabe et al. 2004, Fuchs et al. 2009)
- ISO and Spitzer observations: dust grains are covered by ice mantles (Öberg et al. 2008, Bottinelli et al. 2010)
  - $[CH_3OH_{ice}/H_2O_{ice}] \sim 1 - 30\%$
  - $[H_2CO_{ice}/H_2O_{ice}] \sim 6\%$



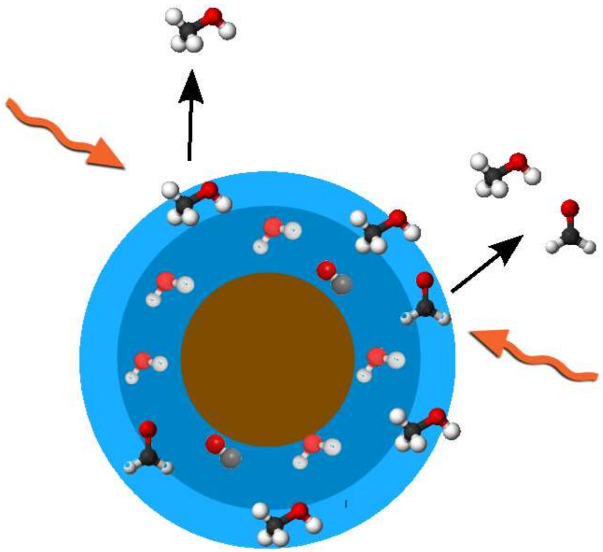
Formation of H_2CO and CH_3OH: Grain surface chemistry

Thermal desorption



- Hot cores
- Hot corino
- High UV illuminated PDRs
- $T_{\mathrm{sublimation}} \simeq 40$ K (H_2CO)
- $T_{\mathrm{sublimation}} \simeq 80$ K (CH_3OH)

Photo-desorption

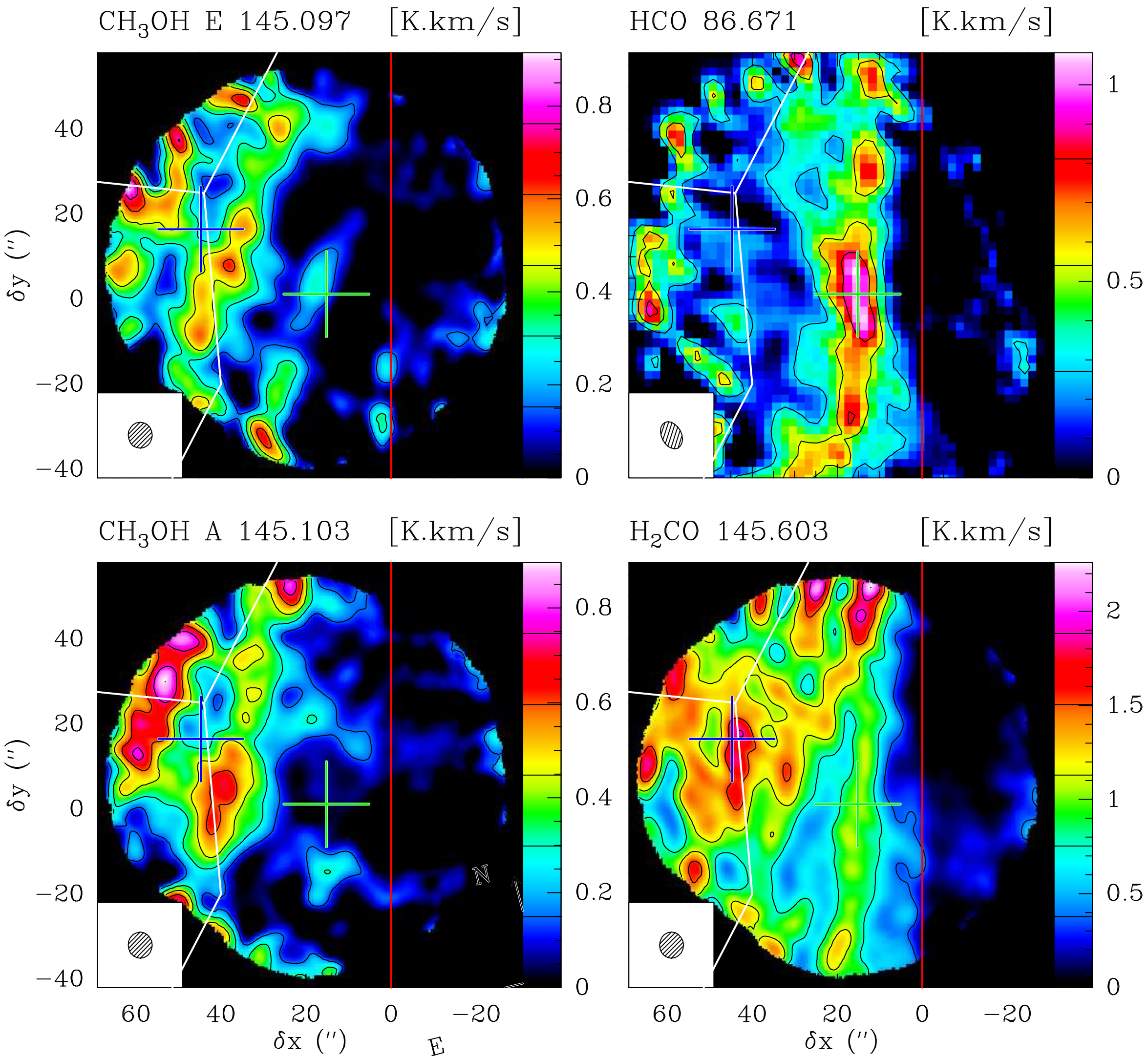


- UV-shielded dense cores (secondary photons)
- Low UV illuminated PDRs

In the Horsehead $T_{\mathrm{dust}} \simeq 20 - 30$ K

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

Different H_2CO formation mechanism



Guzmán et al. 2013

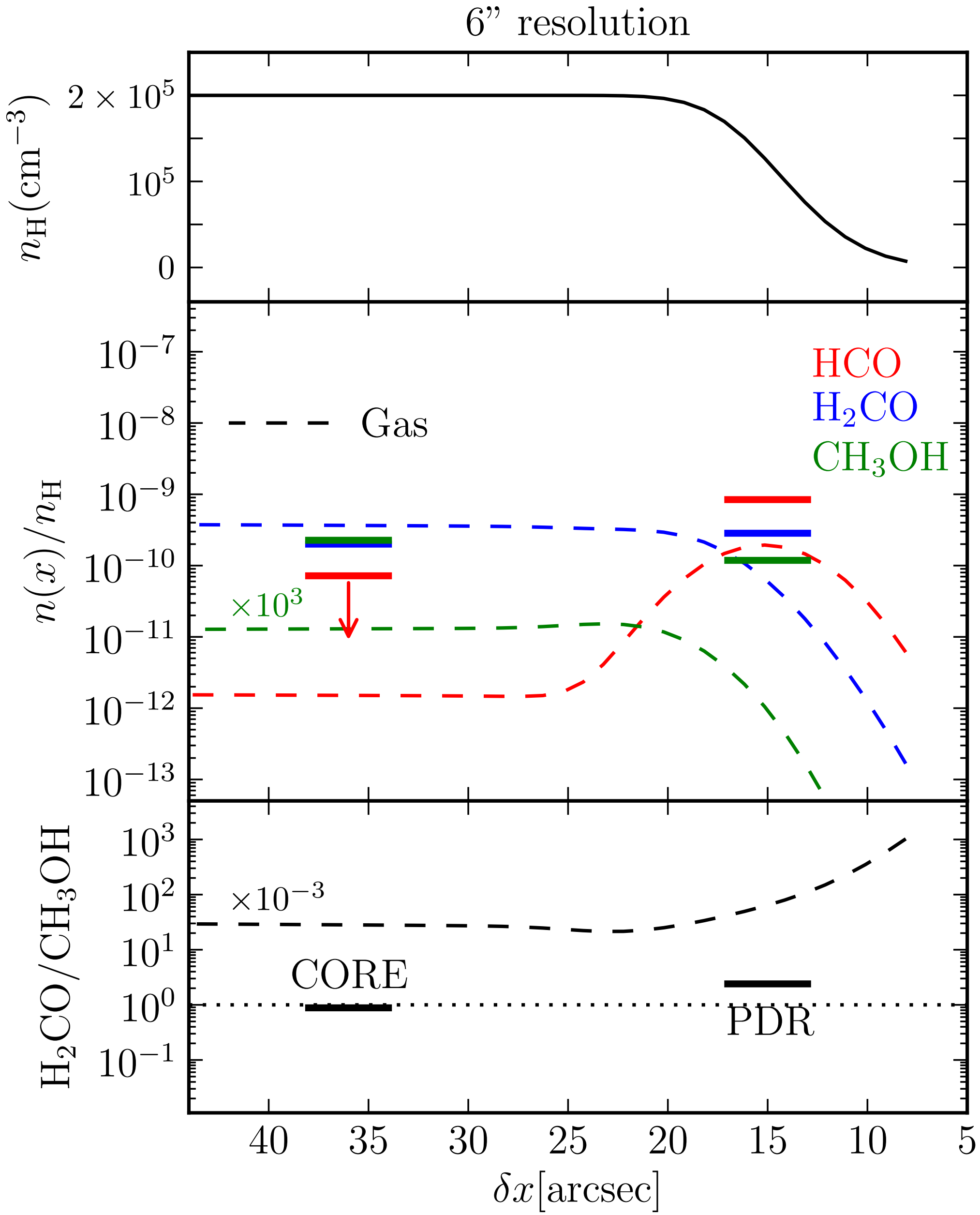
PDR: grain surface
Dense core: gas-phase

Evidence:

- Different ortho-to-para ratio (2 in the PDR, 3 in the core)
- Spatial distribution $\rightarrow$ CH_3OH depletion at core
- Radiative transfer analysis of CH_3OH yields lower gas density at core
- Pure gas-phase model can reproduce H_2CO abundance at the dense core

CH_3OH:
$\rightarrow$ **envelope around dense core**
H_2CO:
$\rightarrow$ **envelope and dense core itself**

Gas-phase vs. Grain surface chemistry



Guzmán et al. 2013

PDR models: Meudon PDR Code

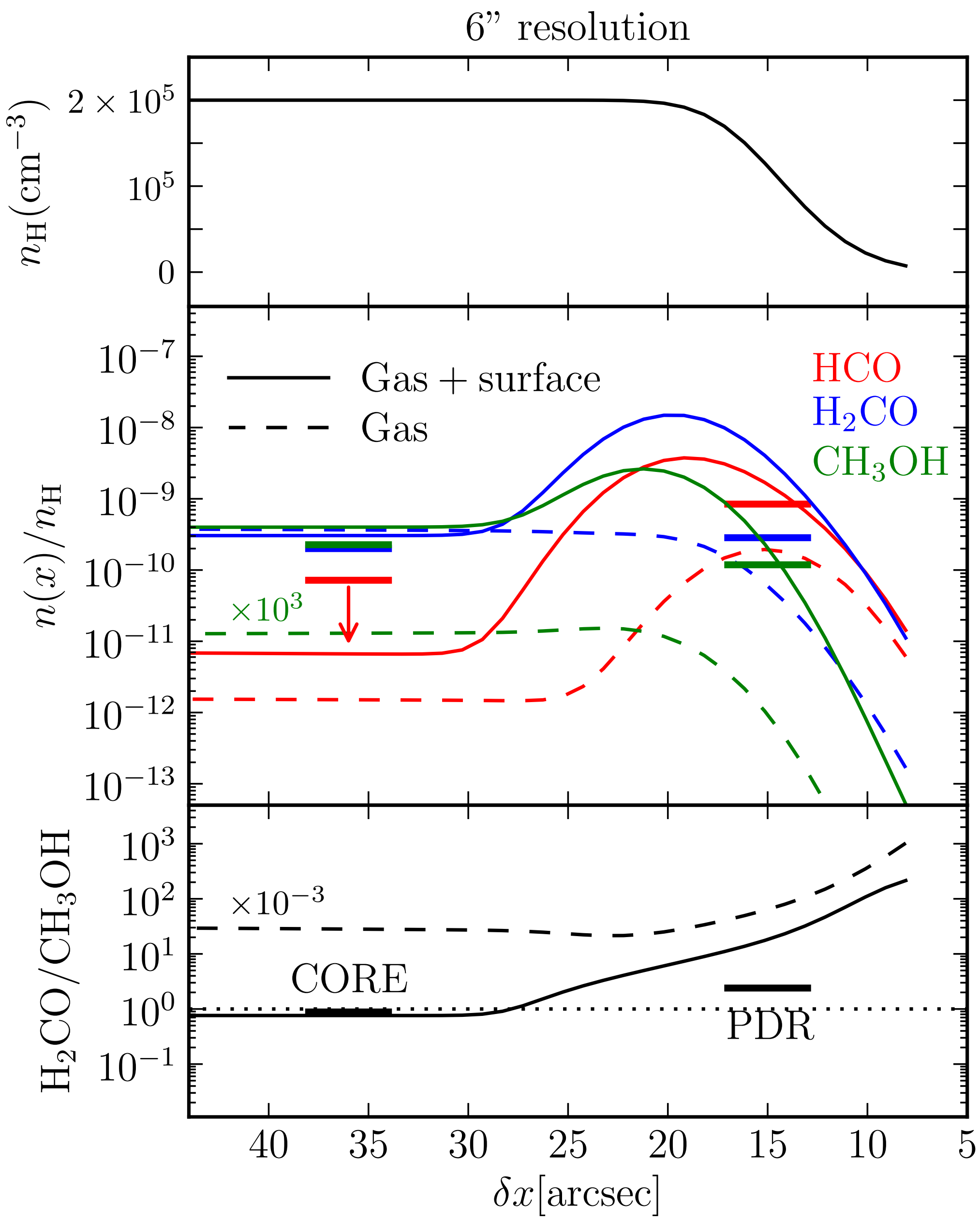
Evelyne Roueff

Le Petit et al. (2006)

Le Bourlot et al. (2012)

- Pure gas-phase
  H_2CO: CORE ✓, PDR ✗
  CH_3OH: CORE: ✗, PDR ✗

Gas-phase vs. Grain surface chemistry



Guzmán et al. 2013

PDR models: Meudon PDR Code

Evelyne Roueff

Le Petit et al. (2006)

Le Bourlot et al. (2012)

- Pure gas-phase
  H_2CO: CORE ✓, PDR ✗
  CH_3OH: CORE: ✗, PDR ✗
- Gas-phase + grain surface

⇒ Photo-desorption is needed to explain the observed H_2CO and CH_3OH abundance in the PDR.

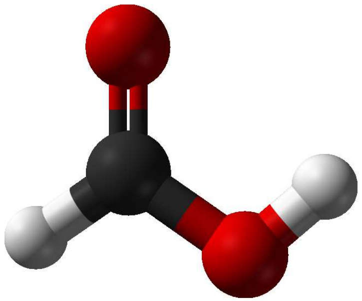
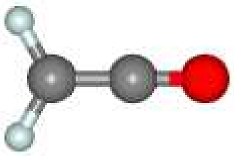
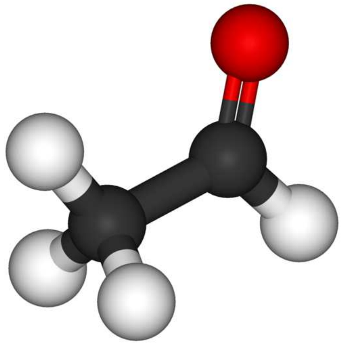
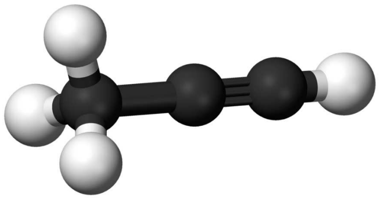
Complex molecules: HCOOH, CH_2CO, CH_3CHO, CH_3CCH

Present high abundances in:

- Hot cores (high-mass stars)
- Hot corino (low-mass stars)
- Shocked gas

Regions where $T_{\rm kin} > 100$ K $\rightarrow$ evaporation of ices or sputtering

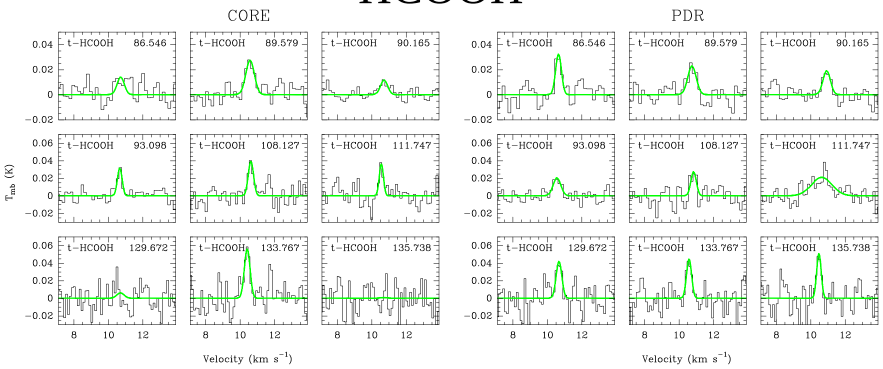
- Also detected in a cold prestellar core (Bacmann et al. 2012)
  $\rightarrow$ Challenged the current formation scenario of complex molecules on dust grains
- And now we detect them in a PDR

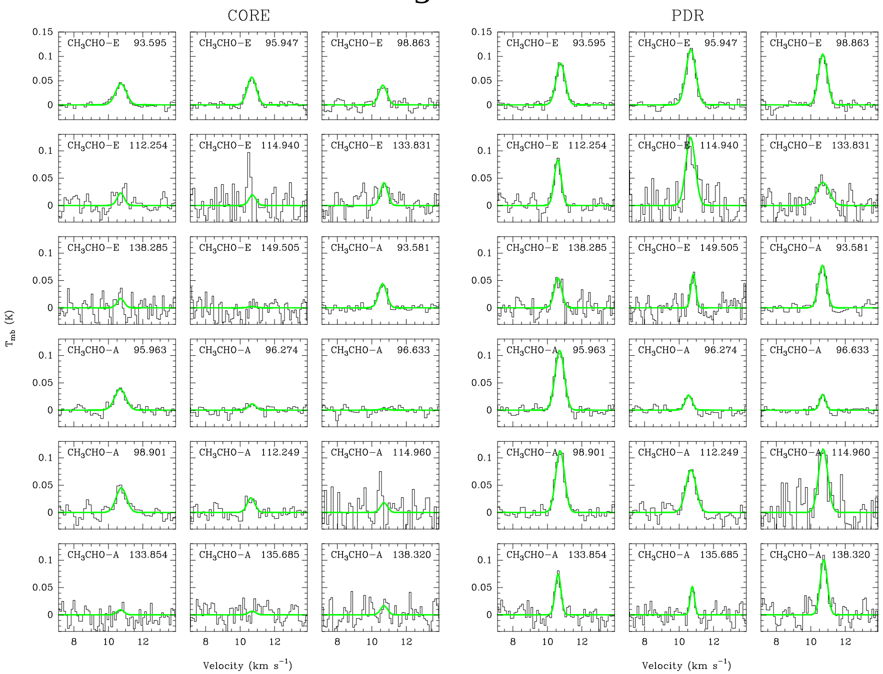
Complex molecules in the Horsehead

Guzmán et al. accepted for the Faraday Discussions

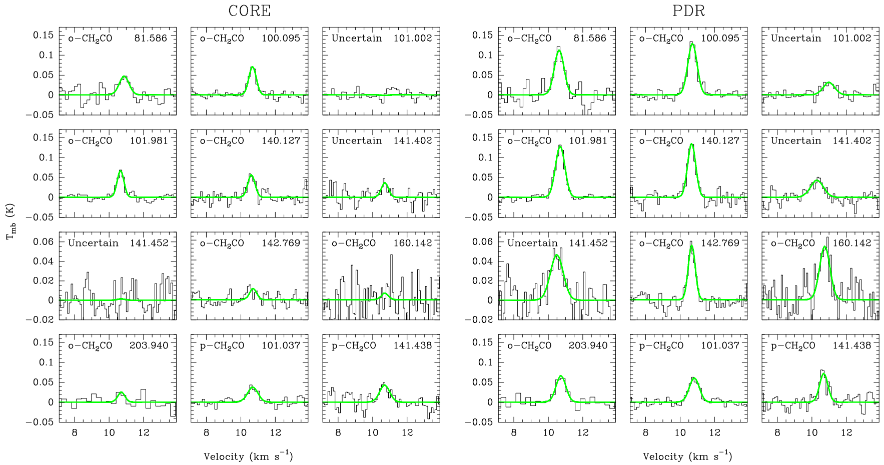
HCOOH



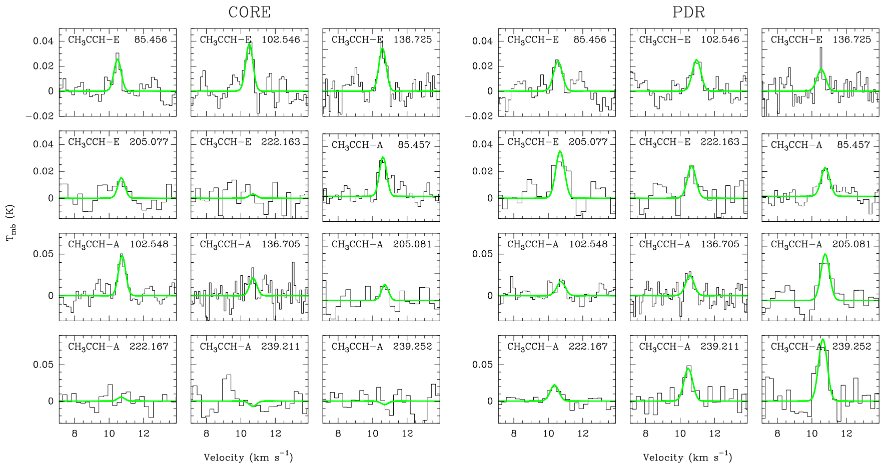
CH_3CHO



CH_2CO



CH_3CCH



Rotational temperatures

Guzmán et al. accepted for the Faraday Discussions

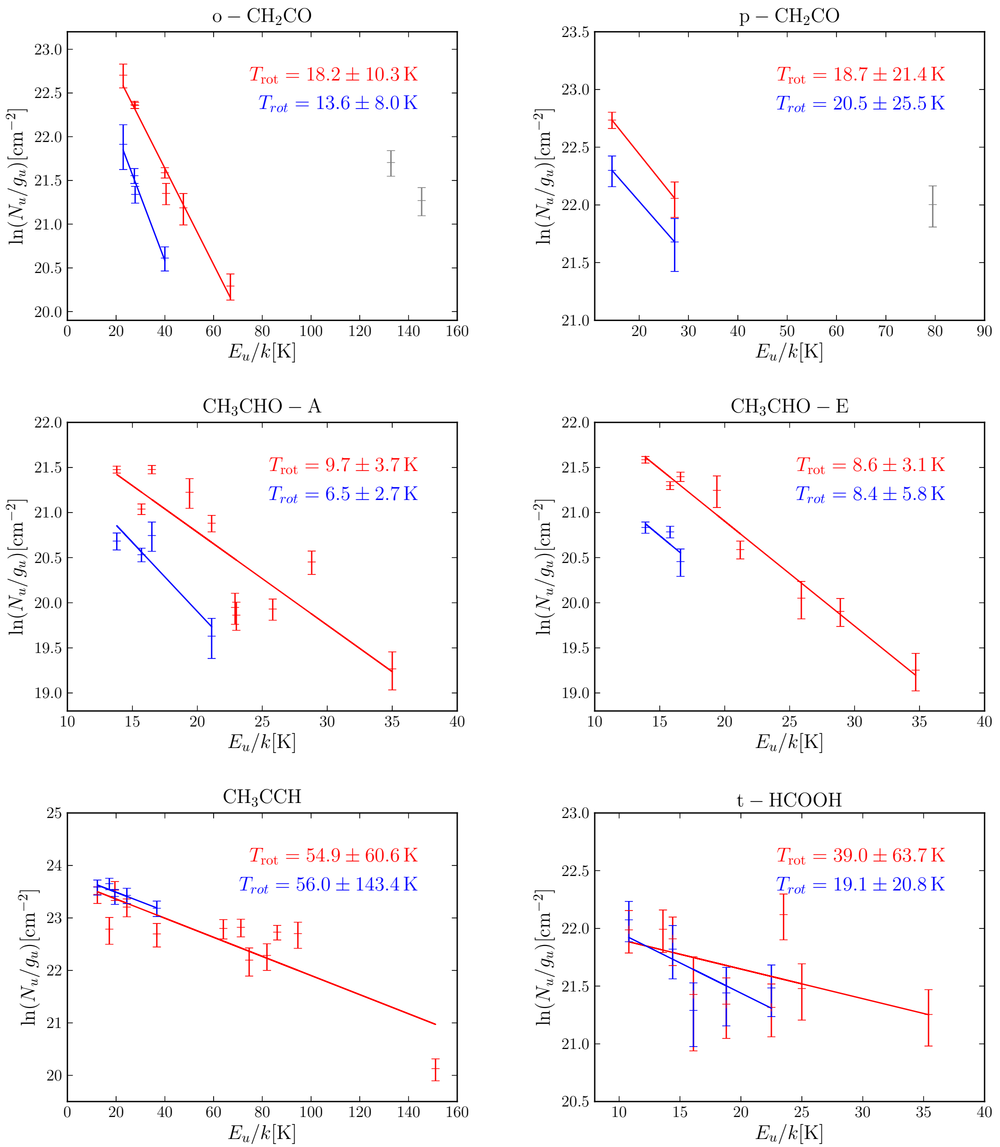
Rotational temperatures

- CH_2CO and CH_3CHO: $T_{rot} \leq 20$ K
- CH_3CCH: $T_{rot} \sim 50$ K

$\rightarrow$ 'Cold' molecules

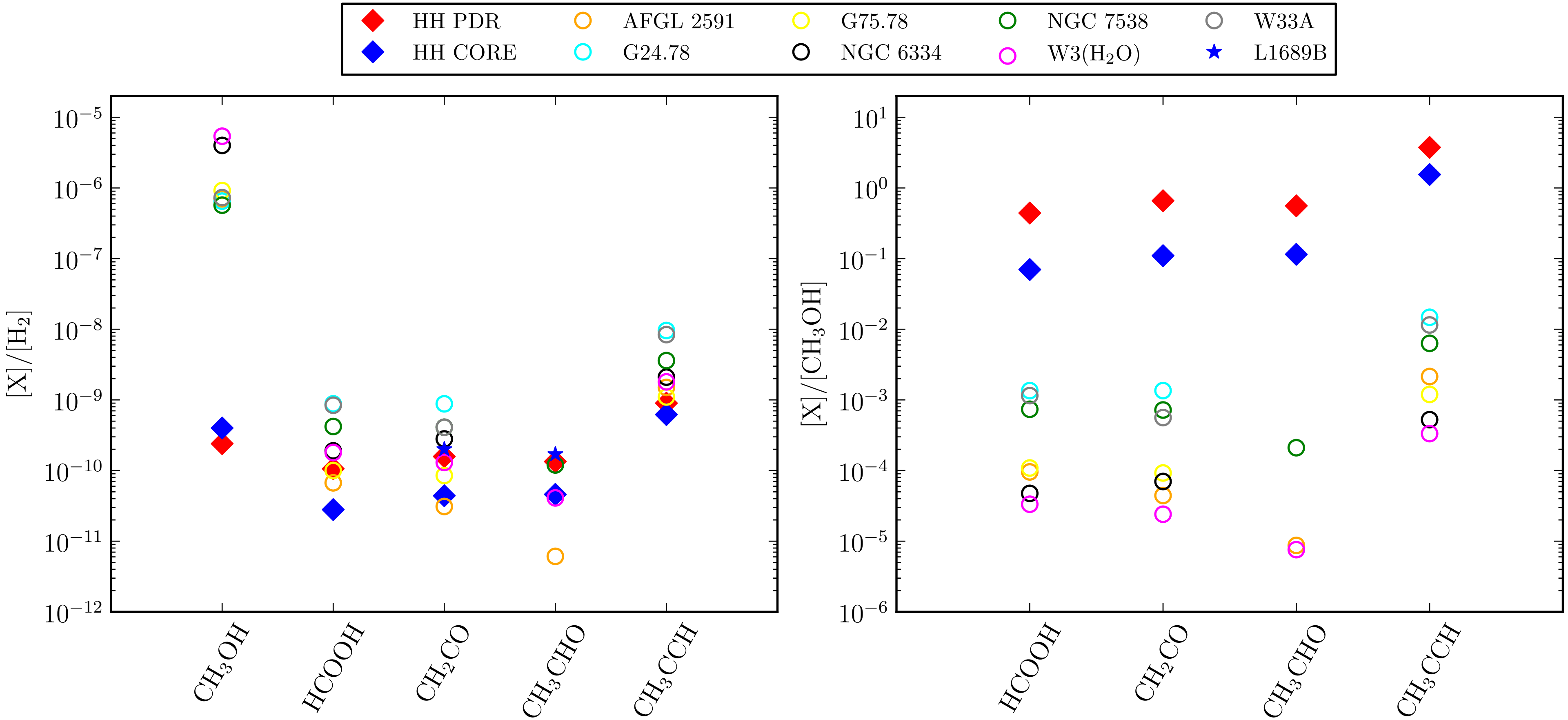
Abundances:

- $10^{-11} - 10^{-10}$
- [HCOOH], [CH_2CO], and [CH_3CHO] are 3 – 4 times larger in the PDR than in the dense core
  $\rightarrow$ Enhanced due to UV-field?
- $[CH_3CCH]_{PDR} \simeq 1.5[CH_3CCH]_{core}$



Abundances

Open circles: **Hot core sources** from Bisschop et al. 2007
Diamonds: **Horsehead PDR and dense core**



- $[X/H_2]$ are similar in the Horsehead and in hot cores
- $[X/CH_3OH]$ are higher in the Horsehead
  $\rightarrow$ In hot cores, CH_3OH and other molecules trace different regions

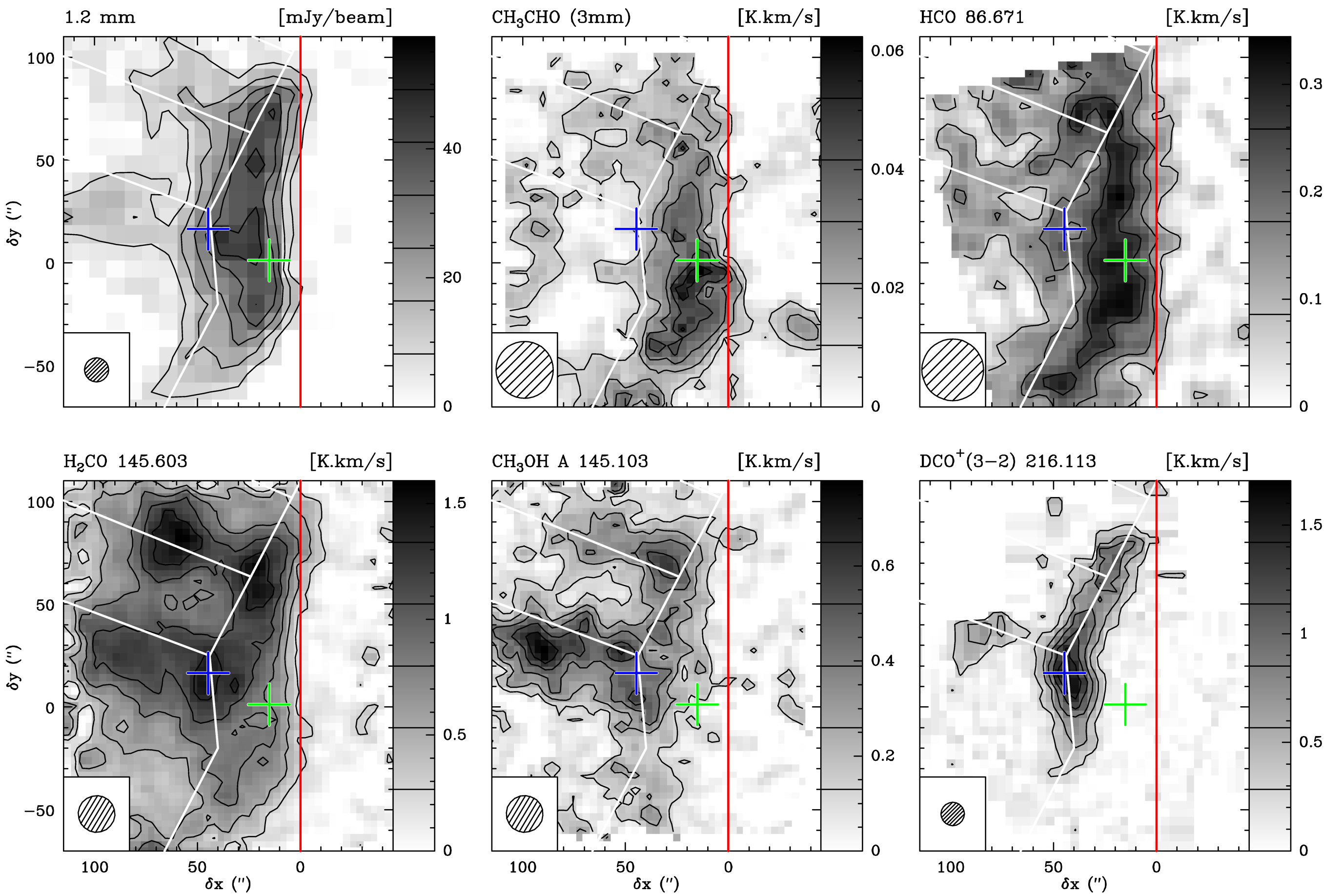
Formation on grains

- CH_2CO and CH_3CHO are thought to form on the surface of dust grains

$$CO \xrightarrow{H} HCO \xrightarrow{C} HCCO \xrightarrow{H} CH_2CO \xrightarrow{2H} CH_3CHO$$

- HCOOH ices have been observed in star-forming regions (Keane et al. 2001)

In the Horsehead, the enhanced abundances towards the PDR compared to the dense core suggests that their formation is more efficient in the presence of far-UV photons.



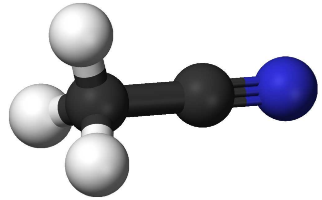
Consistent with photodesorption

Relatively complex nitriles: CH_3CN,CH_3NC, HC_3N

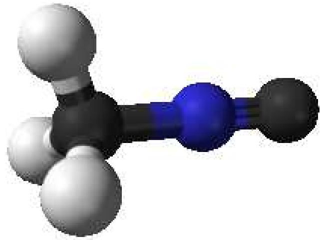
- Important for pre-biotic chemistry → parent molecules of many amino acids (Hudson et al. 2008)
- CH_3CN → good thermometer for high densities ($\geq 10^5$ cm^{-3})
- CH_3CN emission is enhanced in star forming regions containing ultracompact H II regions (Purcell et al. 2006)
- Tracers of hot cores and hot corinos
- Tracers of shocked gas (Codella et al. 2009)

Formation: Gas-phase or grain surface chemistry?

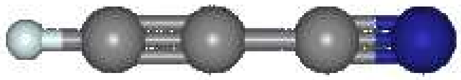
CH_3CN



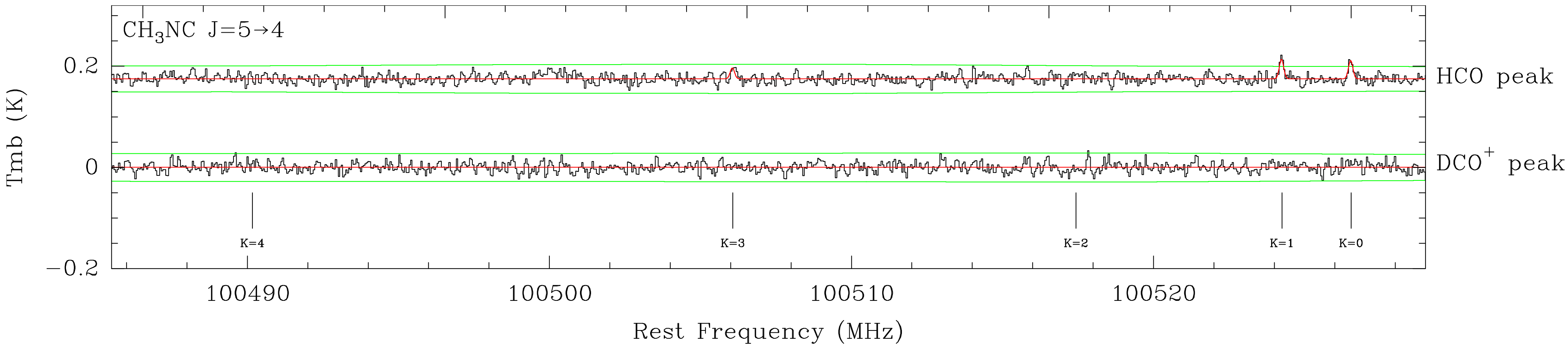
CH_3NC



HC_3N



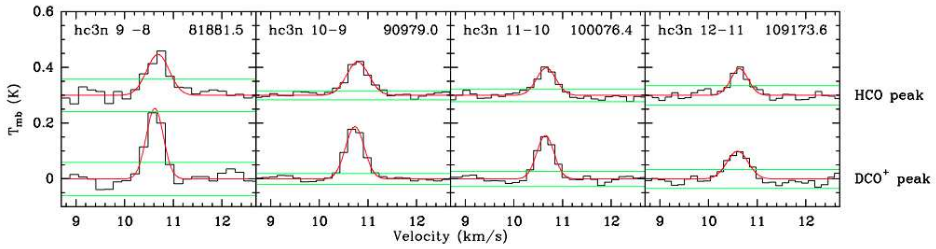
First clear detection of CH_3NC at mm waves:
$\Rightarrow [CH_3NC]/[CH_3CN] = 0.15 \pm 0.02$
(Gratier et al., 2013)



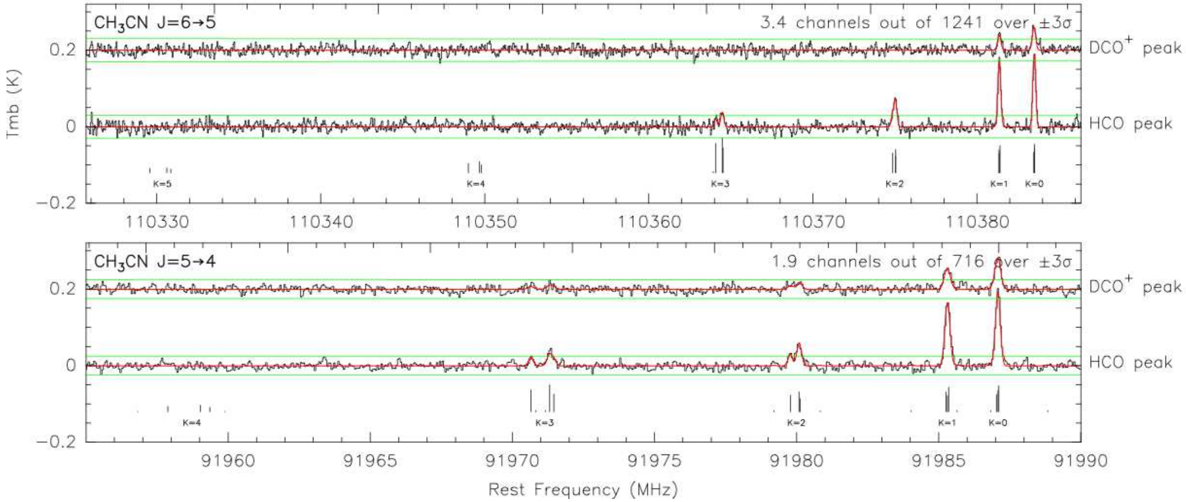
Nitriles in the Horsehead: CH_3CN and HC_3N

Gratier, Pety, **Guzmán** et al. 2013

HC_3N



CH_3CN



HC_3N

- $[HC_3N]_{PDR} \simeq [HC_3N]_{Core}$

CH_3CN

- $[CH_3CN]_{PDR} \simeq 2.5 \times 10^{-10}$
- $[CH_3CN]_{PDR} \simeq 30\ [CH_3CN]_{Core}$

$\longrightarrow$ Different chemistry

Gas-phase model predicts CH_3CN abundance $\sim$ 2400 times lower

$\longrightarrow$ Enhanced abundance due to FUV field?

- Enhanced abundance of precursors in the PDR
- UV photo-processing of N bearing ices ($C_2H_5NH_2$) followed by photodesorption (Danger et al. 2011)

The Horsehead nebula is a good benchmark for PDR modeling and astrochemistry

CF^+ A new diagnostic of UV illuminated gas and a potential proxy of the C^+ emission associated to molecular gas (Guzmán et al. 2012a,b).

Detection of a new species in the ISM
Recently confirmed to be C_3H^+, it supports the top-down scenario of formation of the small hydrocarbons from PAHs and small grains (Pety et al. 2012, Guzmán et al. 2015).

Formaldehyde and methanol are as abundant in the PDR as in the dense core
Photo-desorption of ices is an efficient mechanism to release molecules into the gas phase (Guzmán et al. 2011, 2013)

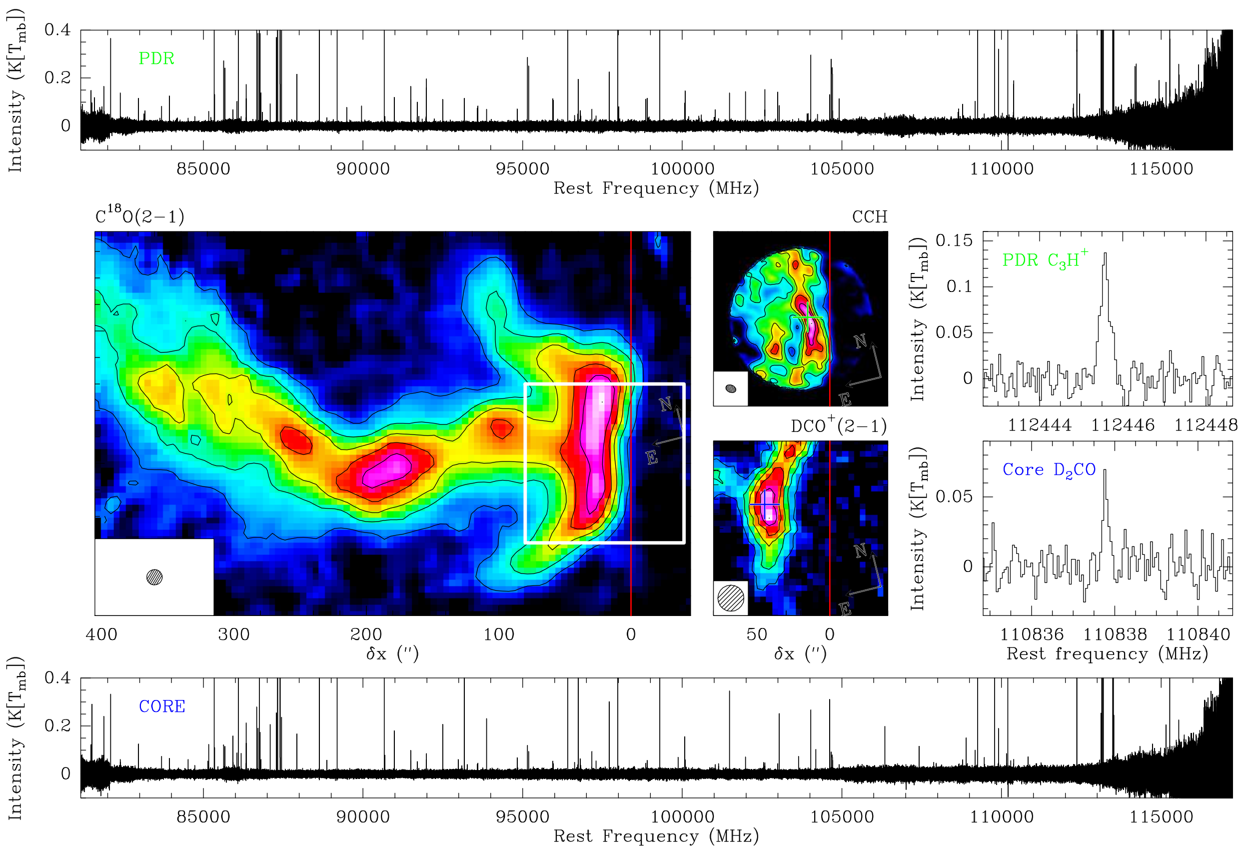
The first detection of the complex organic molecules in a PDR HCOOH, CH_2CO, CH_3CHO, and CH_3CCH reveal the degree of chemical complexity reached in the UV illuminated neutral gas (Guzmán et al. 2014).

CH_3CN as a special case 30 times more abundant in the PDR than in the dense core
⇒ A specific mechanism, related to the presence of FUV photons, to produce it (Gratier et al. 2013).
- Gas phase?
- Ice photo-processing?
- Top-down chemistry, e.g., photo-destruction of DIB carriers?

Next step:
Deep $3''$ imaging of complex organic molecules with ALMA.

The Horsehead WHISPER 3mm line survey

http://www.iram-institute.org/~horsehead/



Guzman et al. 2012a, 2012b, 2013, 2014, and 2015

Gratier et al. 2013

Pety et al. 2013

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