The Horsehead nebula: a beautiful PDR case

M. Gerin, J. Goicoechea, P. Gratier, V. Guzman, J. Pety, F. Le Petit, J. Le Bourlot, E. Roueff
The Horsehead nebula: a beautiful case

The Horsehead nebula has been a great source of speculation and inspiration for the last century. We give a brief discussion of why that is as well as summarizing our recent observations using SOFI on the NTT.

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The Horsehead nebula: a beautiful PDR case

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Ah, to softly slip behind the scene,
One clear and snow-draped, silent winter night,
To pierce the density which seems to screen,
Obstruct the splendour of that cosmic light,
To pass beyond that dark and mystic cloud,
Which looms like portal in a garden wall,
The ancient loveliness within to shroud,
How it ones fancy does inspire, enthrall,
In that great starlit garden of the sky,
Where light eternal dwells in calm repose,
Who knows what beauty there might greet the eye,
What undreamed truth a brief glimpse there disclose,
As strange as thought, to thought there is no space,
At will, ones thoughts the universe may embrace.

Lisa Odland
Popular Astronomy 48, 1940
Outline

H$_2$ infrared emission in the Horsehead nebula: the trigger of Malcolm’s interest
Constraining the physical structure through PDR modeling
New observations

The chemical surprises and challenges from the WHISPERS spectral survey and interferometric mapping at IRAM led by J. Pety: a very peculiar PDR
Detection of CF$^+$
A new molecular ion : C$_3$H$^+$
Complex Organic molecules
The first doubly sulfuretted molecule S$_2$H

Summary
Determination of the Horsehead density structure (1)

ESO VLT, H\(\alpha\)

CO(3-2) CSO

C\(^{18}\)O(2-1) IRAM

1.2mm dust continuum IRAM

ESO VLT composite image with contour of the H\(_2\) (1-0) S(1) transition emission

Habart, Abergel, Walmsley et al. A&A 437, 177, 2005
Determination of the Horsehead density structure (2)

Interpretation of the \( \text{H}_2 \) (1-0) S(1) observations with the Meudon PDR code

- steep density gradient required at the edge of the PDR with concomitant temperature variation
- \( P \approx 4 \times 10^6 \text{ cm}^{-3} \text{ K} \)

Habart, Aberge, Walmsley et al. A&A 437, 177, 2005

Illumination by \( \sigma \) Ori O9.5V star at about 4pc

\[ \approx 100 \text{ UV Habing radiation field} \]

UV spatial stratification: Edge On PDR located at \( d \approx 400 \text{ pc} \),

\[ 1' \approx 0.12 \text{ pc} \]

“moderate” PhotoDissociation Region (PDR)

PDR

Physics and chemistry controlled by UV photons with \( \lambda > 912 \text{ Å} \)

Atomic to molecular transition, predominantly neutral medium

Specific role of \( \text{H}_2 \)

Transformation of UV photons to I.R. - mm: thermal balance of dust

Molecular region: \( \text{CO} \), \( \text{C} \), \( \text{C}^+ \), \( \text{H}_2 \), \( \text{H} \)

Gas (\( \text{H, H}_2, \ldots \))

Cosmic rays

Radiation field

Dust grains
The physical processes at work in PDRs

Radiative transfer

- UV induced photo processes (gas + dust) continuum + lines
- Radiation energy density as a function of $\lambda$
- Compute photorates and photoelectric effects

IR - submm - mm: discrete transitions

Chemistry: $\frac{d[X]}{dt} = F - D[X] = 0$

Gas phase: reaction rate coefficients are radiation field and temperature dependent

Dust and gas/solid interface: at least for $H_2$ formation

Thermal balance: $\Delta G = H - C = 0$

Heating: photoelectric effect, collisional de-excitation of pumped $H_2$, cosmic rays, chemical formation through exothermic reactions

Cooling: radiative emission following collisional excitation

kinetic energy $\Rightarrow$ radiative energy

Solve the detailed balance (collisional excitation, radiative emission/pumping) endothermic chemical reactions

Gas-grain coupling
The physical processes at work in PDRs

Radiative transfer

UV induced photo processes (gas + dust) continuum + lines
Radiation energy density as a function of $\lambda$

Compute photorates and photoelectric effects

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Solve the detailed balance (collisional excitation, radiative emission/pumping)
endothermic chemical reactions
Gas-grain coupling
The two steps in numeric PDR chemical codes

1. Determination of local quantities, within a chosen geometry (plane parallel, spherical)
   - Abundances = f(x)
   - Level populations of selected atoms and molecules (H2, CO, C+, C, O, CS, H2O, …)
   - Temperature (gas + dust)

Iterative process

Computer time consuming

2. Post-processing
   - Column densities
   - Line emissivities (local + integrated)

_allow comparison with observations_

robust tool within “simple“ assumptions (e.g. fixed T, n)


Extreme sensitivity to H2 formation efficiency, dust properties (size distribution), recombination on grains, ...

Our philosophy: try to include as much physics as possible

Continuous increments (new cooling transitions, new photodissociation cross-sections (Heays + 2017), ...) but also new processes (stochastic effects linked to grain, state to state chemistry, ...)
Spitzer observations: a test of H$_2$ excitation

Habart et al. 2011, A&A 527, A122

Interpretation with Meudon PDR

significant rotational excitation of H$_2$ in this moderate PDR
H$_2$, J=0 and J=1 mainly probe the bulk of the molecular gas at moderate temperatures
(1-0) S(1) probe the UV excitation

+ other excitation diagnostics


+ probing the role of PAH photoelectric heating : PACS Herschel + SPITZER
(Okada+ 2013, A&A553, A2)

IRS low resolution spectra (Compiègne et al. 2008, AA408, 797)
New observations constraining H$_2$ excitation

PV diagram thumbnails

K. Kaplan PhD Dissertation, U. Texas, 2017

Immersion Grating INfrared Spectrometer (IGRINS)
Collaboration between Texas University (Austin) and Korea Astronomy Space Science Institute (KASI)
High spectral resolution R=45,000
Simultaneous coverage of H and K band
Observations performed on the 2.7m telescope at McDonald observatory

Other studied PDRs: Orion Bar, NGC7023, S140, IC63
New observations constraining H$_2$ excitation

Comparison with Cloudy models (Ferland) with a grid of constant density and constant temperature models

Significant discrepancy between modeled and observed excited rotational levels

A nice challenge for future work
Chemical signatures in the Horsehead mane (1)

Whisper project: PI J. Pety
Wideband High-resolution IRAM-30m Survey at two Positions with Emir Receivers

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<tr>
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<th>1mm</th>
<th>2mm</th>
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<tbody>
<tr>
<td>Bandwidth (GHz)</td>
<td>76</td>
<td>25</td>
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<tr>
<td>Resolution (kHz)</td>
<td>195</td>
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<td>Sensitivity (mK)</td>
<td>8.4</td>
<td>18.5</td>
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2 positions
≈ 145 hours
≈ 31 species + isotopologues
Chemical signatures in the Horsehead mane (2)

Two different environments less than 40" away

IRAM PdB Observations (PI J. Pety)
Chemical signatures in the Horsehead mane (2)

Two different environments less than 40" away

A far-UV illuminated PDR: HCO (Gerin et al. A&A 494, 977, 2009)
Av ∼ 1.5
Warm $T_{\text{kin}}$ ∼ 60K
Relatively dense $n_H$ ∼ $2 \times 10^4$ cm$^{-3}$

A shielded, dense core DCO$^+$ (Pety et al. 2007)
Av ∼ 20
Cold $T_{\text{kin}}$ ∼ 20K
Dense $n_H$ ∼ $2 \times 10^5$ cm$^{-3}$
High fractionation $[\text{DCO}^+]/[\text{HCO}^+] = 2\%$
Chemical signatures in the Horsehead mane (2)

Two different environments less than 40" away

A far-UV illuminated PDR : HCO (Gerin et al. A&A 494, 977, 2009)
A\textsubscript{V} \sim 1.5

**warm** $T_{\text{kin}} \sim 60$K
Moderately dense $n_{\text{H}} \sim 2 \times 10^4$ cm\(^{-3}\)

A **shielded**, dense core DCO$^+$
A\textsubscript{V} \sim 20

**Cold** $T_{\text{kin}} \sim 20$K
dense $n_{\text{H}} \sim 2 \times 10^5$ cm\(^{-3}\)
High fractionation $[\text{DCO}^+]/[\text{HCO}^+] = 2\%$

IRAM PdB Observations (PI J. Pety)
Detection of CF$^+$ in the PDR

Guzman et al. 2012, A&A 543, L1

\[ \text{DCO}^+ (3-2) \quad \text{CF}^+ (1-0) \]

\[ \text{HCO}(86.671\text{GHz}) \quad \text{CF}^+ (2-1) \]

\[ \begin{align*}
F + H_2 & \rightarrow HF + H \quad k_1 \\
C^+ + HF & \rightarrow CF^+ + H \quad k_2 \quad \text{(Denis-Alpizar 2018, MNRAS)} \\
CF^+ + e & \rightarrow C + F \quad k_3 : 1.95 \times 10^{-7} \quad (T/300)^{-0.276} \quad \text{(Novotny 2012)}
\end{align*} \]

\[ \frac{n(\text{CF}^+)}{n(C^+)} = \frac{k_2}{k_3} \frac{n(\text{HF})}{n(e)} \]

Assuming \( n(C^+) = n(e) \) and \([F] \approx HF\), one can derive the \([F]\) elemental abundance from CF$^+$ observations

\[ \frac{n(\text{CF}^+)}{n(C^+)} \]

Double peak: signature of HFS, \( I(F) = 1/2 \)

anomalously large spin rotation constant:
\( C = 229.2 \text{ kHz} \) computed through QM (CFour package, Gauss et al 1998, JCP105, 2804)

\( ^{13}\text{CO}: C = 32.6\text{kHz} \)

Consistent with the non-experimental detection of HFS by Cazzoli et al. 2010, A&A 509, A1)
Chemical signatures in the Horsehead mane (4)

A new molecular ion

A new molecular ion: $\text{C}_3\text{H}^+$


Harmonic progression of transition frequencies suggesting $1\Sigma^+$ electronic state with $B \sim 11.24$ GHz

− several heavy atoms, close to $B(\text{C}_3\text{H}) = 11.189$ GHz

Value compatible with ab-initio calculations of most stable geometry: $B \sim 11.045$ GHz (Ikuta, JCP 106, 4536, 1997)

predicted to be more stable than $\text{c-C}_3\text{H}^+$

vibrational spectrum predicted by Wang et al in JPCA 111, 4056, 2007

No experimental spectroscopic data
Chemical signatures in the Horsehead mane (4)

A new molecular ion : \( C_3H^+ \)


\[
\nu(J \rightarrow J - 1) = 2B \times J - 4D \times J^3
\]

\[B = 11\,244.9474 \pm 0.0007 \text{ MHz}\]
\[D = 7.652 \pm 0.011 \text{ kHz}\]


Searching for the carrier of \( B11244 \) in HH, SgB2 (N), TMC1, IRC+10216

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Chemical signatures in the Horsehead mane (4)

A new molecular ion : C$_3$H$^+$


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$B = 11 \, 244.9474 \pm 0.0007 \, \text{MHz}$

$D = 7.652 \pm 0.011 \, \text{kHz}$


*Debate amongst quantum chemists in ApJ and JCP*
Chemical signatures in the Horsehead mane (4)

A new molecular ion : C$_3$H$^+$

PdB observations : checking the spatial distribution

possibility of top down hydrocarbon chemistry in the PDR

Yet photo-erosion of PAHs and small carbonaceous grains should be quantified
Chemical signatures in the Horsehead mane (5)

Complex organic molecules
Guzman et al. 2013, A&A 560, A73
Guzman et al. 2014, Faraday Discussions 168, 103

H$_2$CO formation

**PDR**
H$_2$CO-ice photo-desorption

**Core**
Gas phase formation
CH$_3$ + O -> H$_2$CO + H
or photo-desorption
Chemical signatures in the Horsehead mane (5)

Complex organic molecules
Guzman et al. 2013, A&A 560, A73
Guzman et al. 2014, Faraday Discussions 168, 103

CH$_3$OH formation

PDR CH$_3$OH-ice photo-desorption by prim. UV
Core CH$_3$OH-ice photo-desorption by second. UV

Other COMs
Chemical signatures in the Horsehead mane (5)

Complex organic molecules
Guzman et al. 2013, A&A 560, A73
Guzman et al. 2014, Faraday Discussions 168, 103

New ACA + IRAM 30m maps courtesy of V. Guzman
Unexpected detection of $S_2H$ in the Horsehead nebula carefully searched in other surveys: without success

However, present in two different physical environments, both in the PDR and in the core!
A very specific S/H ratio?
Outstanding environment that was pinpointed by Malcolm

- well defined geometry, constrained illumination
- edge on PDR, moderate radiation field, variable density profile

**Test of the cooling / heating mechanisms**

- $\text{H}_2$
- $\text{C}^+, \text{OI}, \text{PAH}$

**Surprising chemistry**

- Two different chemical probes at less than 40” away
- PDR signatures: HCO, CF$^+$, C$_3$H$^+$, carbon chains
- Presence of COMs: role of photodesorption and/or surface reaction
desorption
- The puzzling $\text{S}_2\text{H}$ present in the PDR and in the shielded environment

*Still much to do…*