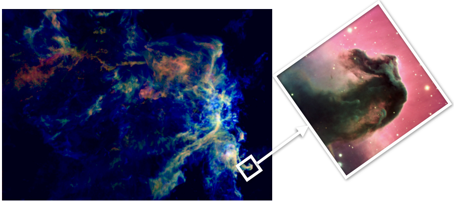
A statistical approach to infer molecular cloud conditions from multi-molecular line analysis of Horsehead nebula observations

PCMI - Oct. 29, 2024

Léontine Ségal[1, 2] **PH.D. supervisors**: Antoine Roueff[2] Jérôme Pety[1, 3]

[1] Institut de RadioAstronomie Millimétrique (IRAM), France [2] Univ.Toulon & IM2NP, France [3] LERMA, France



Introduction

Context

The **ORION-B** consortium

Studying the **Orion B** cloud to investigate the chemical & physical processes involve in **star formation** in Giant Molecular Clouds

- 90% of H $\rightsquigarrow$ H_2, 9% He

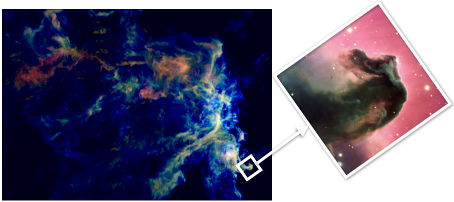
  < 0.01% of others (O, C...) $\rightsquigarrow$ CO, HCO^+...
- Dust grains

Estimate the gas properties

- The H_2 volume density n_{H_2} $[cm^{-3}]$
- The kinetic temperature T_{kin} [K]

✘ No ground truth

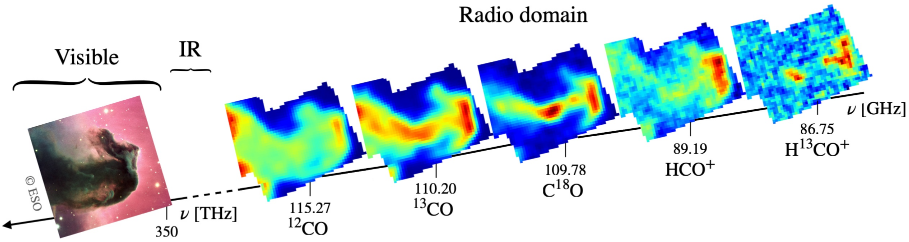
☞ **Statistical** methods & **Accuracy** analysis for **interpretable** results



The Orion B cloud observed at the $J = 1 \rightarrow 0$ of ^{12}CO (blue), ^{13}CO (green), $C^{18}O$ (red) (©J. Pety, the ORION-B Collaboration, IRAM), and the Horsehead nebula observed in the B, V, and R bands (©ESO).

The Horsehead nebula

An example of an heterogeneous cloud



Integrated intensities [$\mathrm{K\,km\,s^{-1}}$] around the $J = 1 \rightarrow 0$ frequency of the CO & HCO^+ isotopologues toward the Horsehead.

The **ORION-B Large Program**
(P.I.: J. Pety & M. Gerin)

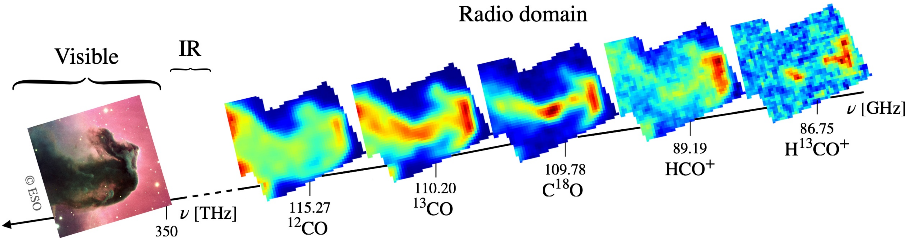
- **IRAM 30-meter** telescope
- $[72, 115]$ GHz
- The Horsehead portion ∼ 1500 pixels × 200 000 spectral channels

Representative physical regimes

- Dense & cold cores ($n_{H_2} \geq 10^{4-5}$ cm^{-3}, $T_{kin} \leq 20$ K)
- Diffuse & lukewarm gas ($n_{H_2} \sim 10^{3}$ cm^{-3}, $T_{kin} \geq 30$ K)
- Intermediate environments

The Horsehead nebula

An example of an heterogeneous cloud

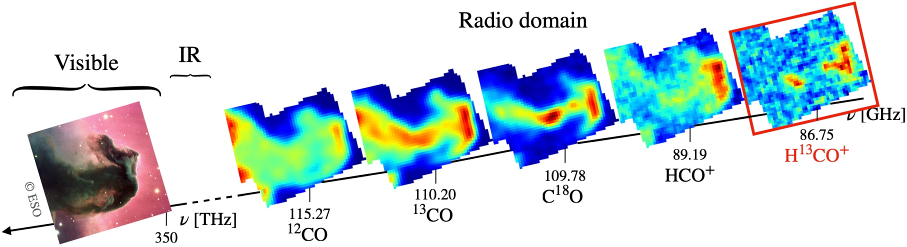


Integrated intensities [$\mathrm{K\,km\,s^{-1}}$] around the $J = 1 \rightarrow 0$ frequency of the CO & HCO^+ isotopologues toward the Horsehead.

Species	Transition	Frequency [GHz]
^{12}CO	$J = 1 \rightarrow 0$	115.271202
^{13}CO	$J = 1 \rightarrow 0$	110.201354
	$J = 2 \rightarrow 1$	220.398684
$C^{18}O$	$J = 1 \rightarrow 0$	109.782173
	$J = 2 \rightarrow 1$	219.560354
HCO^+	$J = 1 \rightarrow 0$	89.188525
$H^{13}CO^+$	$J = 1 \rightarrow 0$	86.754288

Representative physical regimes

- Dense & cold cores
  ($n_{H_2} \geq 10^{4-5}$ cm^{-3}, $T_{kin} \leq 20$ K)
- Diffuse & lukewarm gas
  ($n_{H_2} \sim 10^{3}$ cm^{-3}, $T_{kin} \geq 30$ K)
- Intermediate environments



Integrated intensities [K km s^{-1}] around the $J = 1 \rightarrow 0$ frequency of the CO & HCO^+ isotopologues toward the Horsehead.

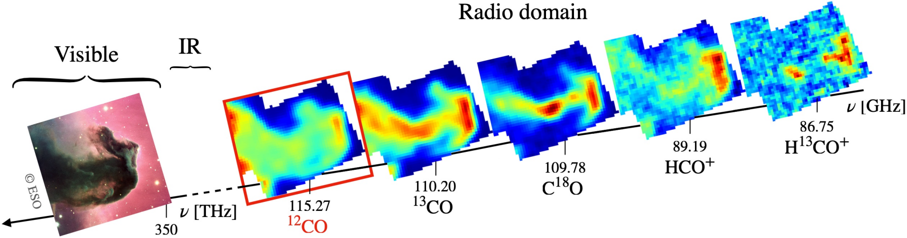
Species	Transition	Frequency [GHz]
^{12}CO	$J = 1 \rightarrow 0$	115.271202
^{13}CO	$J = 1 \rightarrow 0$	110.201354
	$J = 2 \rightarrow 1$	220.398684
$C^{18}O$	$J = 1 \rightarrow 0$	109.782173
	$J = 2 \rightarrow 1$	219.560354
HCO^+	$J = 1 \rightarrow 0$	89.188525
$H^{13}CO^+$	$J = 1 \rightarrow 0$	86.754288

Representative physical regimes

- Dense & cold cores
  ($n_{H_2} \geq 10^{4-5}$ cm^{-3}, $T_{kin} \leq 20$ K)
- Diffuse & lukewarm gas
  ($n_{H_2} \sim 10^3$ cm^{-3}, $T_{kin} \geq 30$ K)
- Intermediate environments

The Horsehead nebula

An example of an heterogeneous cloud



Integrated intensities [$K\,km\,s^{-1}$] around the $J = 1 \to 0$ frequency of the CO & HCO^+ isotopologues toward the Horsehead.

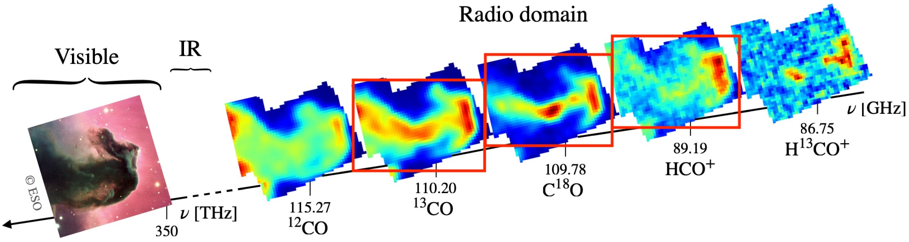
Species	Transition	Frequency [GHz]
^{12}CO	$J = 1 \to 0$	115.271202
^{13}CO	$J = 1 \to 0$	110.201354
	$J = 2 \to 1$	220.398684
$C^{18}O$	$J = 1 \to 0$	109.782173
	$J = 2 \to 1$	219.560354
HCO^+	$J = 1 \to 0$	89.188525
$H^{13}CO^+$	$J = 1 \to 0$	86.754288

Representative physical regimes

- Dense & cold cores
  ($n_{H_2} \geq 10^{4-5}$ cm^{-3}, $T_{kin} \leq 20$ K)
- Diffuse & lukewarm gas
  ($n_{H_2} \sim 10^3$ cm^{-3}, $T_{kin} \geq 30$ K)
- Intermediate environments

The Horsehead nebula

An example of an heterogeneous cloud

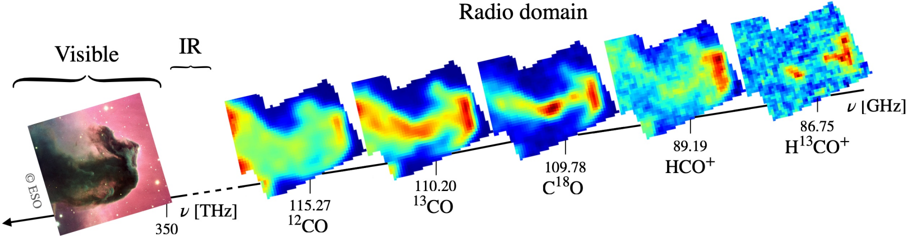


Integrated intensities [K km s^{-1}] around the $J = 1 \to 0$ frequency of the CO & HCO$^+$ isotopologues toward the Horsehead.

Species	Transition	Frequency [GHz]
^{12}CO	$J = 1 \to 0$	115.271202
^{13}CO	$J = 1 \to 0$	110.201354
	$J = 2 \to 1$	220.398684
C^{18}O	$J = 1 \to 0$	109.782173
	$J = 2 \to 1$	219.560354
HCO$^+$	$J = 1 \to 0$	89.188525
H^{13}CO$^+$	$J = 1 \to 0$	86.754288

Representative physical regimes

- Dense & cold cores
  ($n_{H_2} \geq 10^{4-5}$ cm^{-3}, $T_{kin} \leq 20$ K)
- Diffuse & lukewarm gas
  ($n_{H_2} \sim 10^3$ cm^{-3}, $T_{kin} \geq 30$ K)
- Intermediate environments



Integrated intensities [$K\,km\,s^{-1}$] around the $J = 1 \rightarrow 0$ frequency of the CO & HCO^+ isotopologues toward the Horsehead.

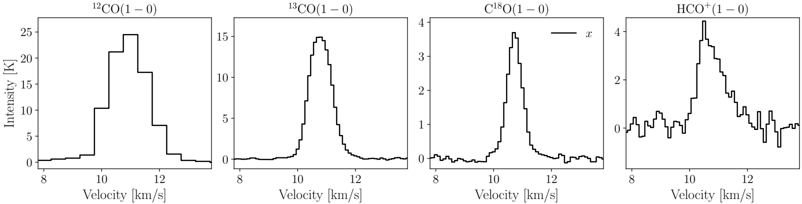
Species	Transition	Frequency [GHz]
^{12}CO	$J = 1 \rightarrow 0$	115.271202
^{13}CO	$J = 1 \rightarrow 0$	110.201354
	$J = 2 \rightarrow 1$	220.398684
$C^{18}O$	$J = 1 \rightarrow 0$	109.782173
	$J = 2 \rightarrow 1$	219.560354
HCO^+	$J = 1 \rightarrow 0$	89.188525
$H^{13}CO^+$	$J = 1 \rightarrow 0$	86.754288

Representative physical regimes

- Dense & cold cores
  ($n_{H_2} \geq 10^{4-5}$ cm^{-3}, $T_{kin} \leq 20$ K)
- Diffuse & lukewarm gas
  ($n_{H_2} \sim 10^3$ cm^{-3}, $T_{kin} \geq 30$ K)
- Intermediate environments

Multi-species data ⇝ Probing **different environments** along the LoS

⇝ Reaching **different** cloud **depths**



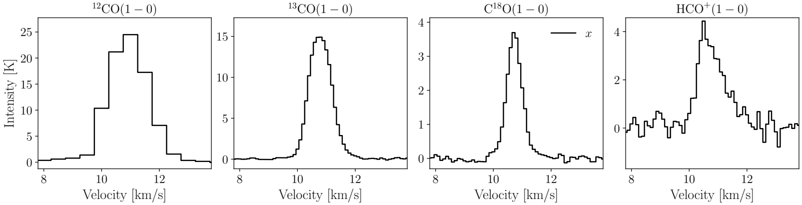
Spectra are sampled in **velocity** (Doppler effect $\frac{\nu}{\nu_l} = 1 - \frac{V}{c}$)

For each molecular line l,

$$\underbrace{\boldsymbol{x}_l}_{\textbf{Measures}} = \boldsymbol{s}_l(\boldsymbol{\theta}) + \underbrace{\boldsymbol{b}_l}_{\text{White Gaussian noise } \sigma_{b_l} \sim 100 \text{ mK}}$$

Methods

Model of multi-spectral observations (one sight-line)



Spectra are sampled in **velocity** (Doppler effect $\frac{\nu}{\nu_l} = 1 - \frac{V}{c}$)

For each molecular line l,

$$\boldsymbol{x}_l = \boldsymbol{s}_l(\boldsymbol{\theta}) + \boldsymbol{b}_l$$

Measures — $\boldsymbol{x}_l$

White Gaussian noise $\sigma_{b_l} \sim 100$ mK — $\boldsymbol{b}_l$

Vector of **unknowns** — $\boldsymbol{\theta}$

Physical & chemical

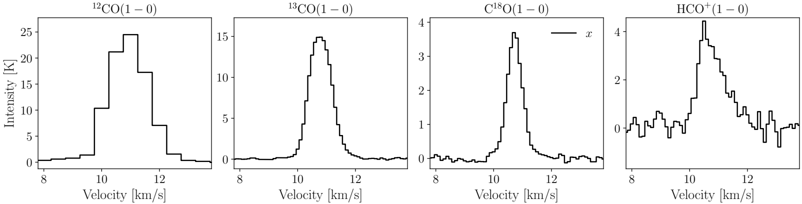
- T_{kin} [K] : Kinetic temperature
- n_{H_2} [cm^{-3}] : H_2 volume density
- $N_l = \int n_l dz$ [cm^{-2}] : Column density of species l

Kinematics

- C_V [km s^{-1}] : Centroid velocity
- FWHM [km s^{-1}] : Full Width at Half Maximum

Methods

Model of multi-spectral observations (one sight-line)



Spectra are sampled in **velocity** (Doppler effect $\frac{\nu}{\nu_l} = 1 - \frac{V}{c}$)

For each molecular line l,

Model

$$\boldsymbol{x}_l = \boldsymbol{s}_l(\boldsymbol{\theta}) + \boldsymbol{b}_l$$

Measures — White Gaussian noise $\sigma_{b_l} \sim 100$ mK

Vector of **unknowns**

Physical & chemical

- T_{kin} [K] : Kinetic temperature
- n_{H_2} [cm^{-3}] : H_2 volume density
- $N_l = \int n_l dz$ [cm^{-2}] : Column density of species l

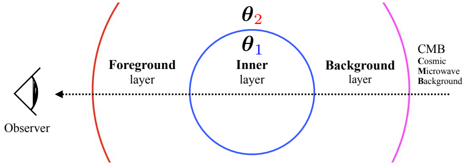
Kinematics

- C_V [$\text{km}\,\text{s}^{-1}$] : Centroid velocity
- FWHM [$\text{km}\,\text{s}^{-1}$] : Full Width at Half Maximum

Methods

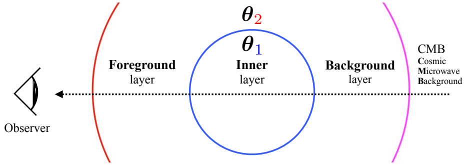
Model of multi-spectral observations (one sight-line)

Multilayer model



$$\boldsymbol{\theta} = \{\boldsymbol{\theta}_1, \boldsymbol{\theta}_2\} \text{ where } \boldsymbol{\theta}_i = \{\log T_{\text{kin},i}, \log n_{\text{H}_2,i}, \log N_{l,i}, \text{FWHM}_i, C_{V,i}\}, \text{ for } i \in \{1, 2\}$$

Multilayer model



$$\boldsymbol{\theta} = \{\boldsymbol{\theta}_1, \boldsymbol{\theta}_2\} \text{ where } \boldsymbol{\theta}_i = \{\log T_{\mathrm{kin},\,i}, \log n_{\mathrm{H}_2,\,i}, \log N_{l,i}, \mathrm{FWHM}_i, C_{V,\,i}\}, \text{ for } i \in \{1, 2\}$$

Radiative Transfer Equation (RTE)

$$s_l = s_{l,\mathrm{fore}}$$

$$s_{l,\mathrm{fore}} = \mathcal{J}(T_{\mathrm{ex},1})\left[1 - \exp\left(-\Psi_1\right)\right]$$

Intensity [K]

$$\mathcal{J}(\boldsymbol{T}_{\mathbf{ex}}) = \frac{h\nu}{k} \frac{1}{\exp\left(\frac{h\nu}{k\boldsymbol{T}_{\mathbf{ex}}}\right) - 1}$$

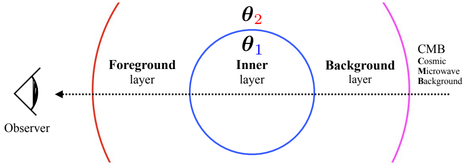
Opacity profile [-]

$$\Psi = \boldsymbol{\tau} \exp\left(\frac{-\left(\mathrm{v} - C_V\right)^2}{2\sigma_V^2}\right)$$

where $\sigma_V = \mathrm{FWHM}/\sqrt{8 \ln 2}$

$$\boldsymbol{\theta} \rightarrow \boxed{\text{RADEX}} \rightarrow \{\boldsymbol{T}_{\mathbf{ex}}, \boldsymbol{\tau}\}$$

Multilayer model



$$\boldsymbol{\theta} = \{\boldsymbol{\theta}_1, \boldsymbol{\theta}_2\} \text{ where } \boldsymbol{\theta}_i = \{\log T_{\mathrm{kin},\,i}, \log n_{\mathrm{H_2},\,i}, \log N_{l,i}, \mathrm{FWHM}_i, C_{V,\,i}\}, \text{ for } i \in \{1, 2\}$$

Radiative Transfer Equation (RTE)

$$s_l = s_{l,\mathrm{fore}} + s_{l,\mathrm{inner}}$$

$$s_{l,\mathrm{fore}} = \mathcal{J}(T_{\mathrm{ex},1})\,[1 - \exp(-\Psi_1)]$$

$$s_{l,\mathrm{inner}} = \mathcal{J}(T_{\mathrm{ex},2})\,[1 - \exp(-\Psi_2)]\exp(-\Psi_1)$$

Intensity [K]

$$\mathcal{J}(\boldsymbol{T}_{\mathbf{ex}}) = \frac{h\nu}{k}\frac{1}{\exp\left(\frac{h\nu}{k\boldsymbol{T}_{\mathbf{ex}}}\right) - 1}$$

Opacity profile [-]

$$\Psi = \boldsymbol{\tau}\exp\left(\frac{-(\mathrm{v} - C_V)^2}{2\sigma_V^2}\right)$$

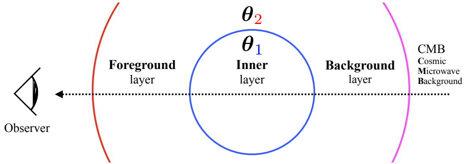
where $\sigma_V = \mathrm{FWHM}/\sqrt{8\ln 2}$

$$\boldsymbol{\theta} \rightarrow \boxed{\text{RADEX}} \rightarrow \{\boldsymbol{T}_{\mathbf{ex}}, \boldsymbol{\tau}\}$$

Methods

Model of multi-spectral observations (one sight-line)

Multilayer model



$$\boldsymbol{\theta} = \{\boldsymbol{\theta}_1, \boldsymbol{\theta}_2\} \text{ where } \boldsymbol{\theta}_i = \{\log T_{\text{kin},\,i}, \log n_{\text{H}_2,\,i}, \log N_{l,i}, \text{FWHM}_i, C_{V,\,i}\}, \text{ for } i \in \{1, 2\}$$

Radiative Transfer Equation (RTE)

$$s_l = s_{l,\text{fore}} + s_{l,\text{inner}} + s_{l,\text{back}}$$

$$s_{l,\text{fore}} = \mathcal{J}(T_{\text{ex},\,1})\,[1 - \exp(-\Psi_1)]$$

$$s_{l,\text{inner}} = \mathcal{J}(T_{\text{ex},\,2})\,[1 - \exp(-\Psi_2)]\exp(-\Psi_1)$$

$$s_{l,\text{back}} = \mathcal{J}(T_{\text{ex},\,1})\,[1 - \exp(-\Psi_1)]\exp(-\Psi_1 - \Psi_2)$$

Intensity [K]

$$\mathcal{J}(\boldsymbol{T}_{\mathbf{ex}}) = \frac{h\nu}{k}\frac{1}{\exp\left(\frac{h\nu}{k\boldsymbol{T}_{\mathbf{ex}}}\right) - 1}$$

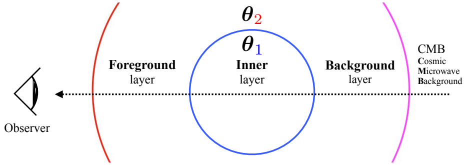
Opacity profile [-]

$$\Psi = \boldsymbol{\tau}\exp\left(\frac{-(\mathrm{v} - C_V)^2}{2\sigma_V^2}\right)$$

where $\sigma_V = \text{FWHM}/\sqrt{8\ln 2}$

$$\boldsymbol{\theta} \longrightarrow \boxed{\textbf{RADEX}} \longrightarrow \{\boldsymbol{T}_{\mathbf{ex}}, \boldsymbol{\tau}\}$$

Multilayer model



$$\boldsymbol{\theta} = \{\boldsymbol{\theta}_1, \boldsymbol{\theta}_2\} \text{ where } \boldsymbol{\theta}_i = \{\log T_{\mathrm{kin},\,i}, \log n_{\mathrm{H}_2,\,i}, \log N_{l,i}, \mathrm{FWHM}_i, C_{V,\,i}\}, \text{ for } i \in \{1, 2\}$$

Radiative Transfer Equation (RTE)

$$s_l = s_{l,\mathrm{fore}} + s_{l,\mathrm{inner}} + s_{l,\mathrm{back}} + s_{l,\mathrm{CMB}}$$

$$s_{l,\mathrm{fore}} = \mathcal{J}(T_{\mathrm{ex},1})\left[1 - \exp\left(-\Psi_1\right)\right]$$

$$s_{l,\mathrm{inner}} = \mathcal{J}(T_{\mathrm{ex},2})\left[1 - \exp\left(-\Psi_2\right)\right]\exp\left(-\Psi_1\right)$$

$$s_{l,\mathrm{back}} = \mathcal{J}(T_{\mathrm{ex},1})\left[1 - \exp\left(-\Psi_1\right)\right]\exp\left(-\Psi_1 - \Psi_2\right)$$

$$s_{l,\mathrm{CMB}} = \mathcal{J}(T_{\mathrm{CMB}})\left[\exp\left(-2 \times \Psi_1 - \Psi_2\right)\right] - \mathcal{J}(T_{\mathrm{CMB}})$$

where $T_{\mathrm{CMB}} = 2.73\,\mathrm{K}$

Intensity [K]

$$\mathcal{J}(\boldsymbol{T}_{\mathbf{ex}}) = \frac{h\nu}{k}\,\frac{1}{\exp\left(\frac{h\nu}{k\boldsymbol{T}_{\mathbf{ex}}}\right) - 1}$$

Opacity profile [-]

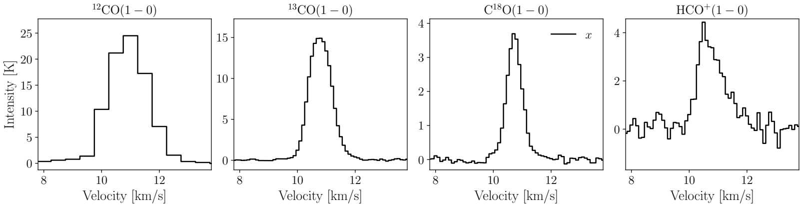
$$\Psi = \boldsymbol{\tau}\exp\left(\frac{-(\mathrm{v} - C_V)^2}{2\sigma_V^2}\right)$$

where $\sigma_V = \mathrm{FWHM}/\sqrt{8\ln 2}$

$$\boldsymbol{\theta} \rightarrow \boxed{\textbf{RADEX}} \rightarrow \{\boldsymbol{T}_{\mathbf{ex}}, \boldsymbol{\tau}\}$$

Methods

Fitting multi-spectral observations (one sight-line)

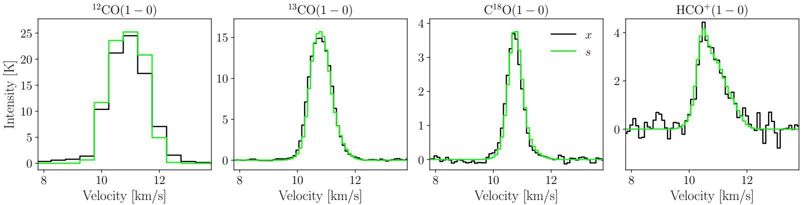


For each molecular line l,

$$\boldsymbol{x}_l = \boldsymbol{s}_l(\boldsymbol{\theta}) + \boldsymbol{b}_l$$

Methods

Fitting multi-spectral observations (one sight-line)



For each molecular line l,

$$\boldsymbol{x}_l = \boldsymbol{s}_l(\widehat{\boldsymbol{\theta}}) + \boldsymbol{b}_l$$

Find
$$\widehat{\boldsymbol{\theta}} = \{\log T_{\mathrm{kin},1}, \log n_{\mathrm{H}_2,1}, \log N_{l,1}, \mathrm{FWHM}_1, C_{V,1}, \log T_{\mathrm{kin},2}, \log n_{\mathrm{H}_2,2}, \log N_{l,2}, \mathrm{FWHM}_2, C_{V,2}\}$$

such as

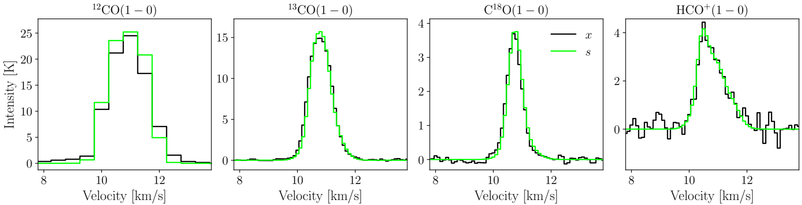
$$\widehat{\boldsymbol{\theta}} = \arg\min_{\theta} \left[-\log \mathscr{L}(\boldsymbol{\theta}) \right] \quad (1)$$

where $-\log \mathscr{L}(\boldsymbol{\theta})$ is the **N**egative **L**og-**L**ikelihood (NLL)

$$-\log \mathscr{L}(\boldsymbol{\theta}) = \frac{1}{2} \sum_{l} \frac{\|\boldsymbol{x}_l - \boldsymbol{s}_l\|^2}{\sigma_{b,l}^2} + \mathrm{cte} \quad (2)$$

Methods

Fitting multi-spectral observations (one sight-line)



For each molecular line l,

$$x_l = s_l(\widehat{\theta}) + b_l$$

Find
$$\widehat{\theta} = \{\log T_{\text{kin},1}, \log n_{H_2,1}, \log N_{l,1}, \text{FWHM}_1, C_{V,1}, \log T_{\text{kin},2}, \log n_{H_2,2}, \log N_{l,2}, \text{FWHM}_2, C_{V,2}\}$$

such as

$$\widehat{\theta} = \arg\min_{\theta} \left[-\log \mathscr{L}(\theta)\right] \quad (1)$$

where $-\log \mathscr{L}(\theta)$ is the Negative Log-Likelihood (NLL)

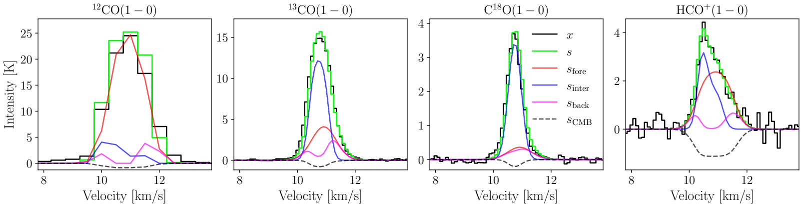
$$-\log \mathscr{L}(\theta) = \frac{1}{2} \sum_l \frac{\|x_l - s_l\|^2}{\sigma_{b,l}^2} + \text{cte} \quad (2)$$

$\widehat{\theta}$ + few constraints on chemistry ⇒ **14 unknowns**

1. **Random walk** in a **14-D** gridded space
   ✓ Avoiding local minima ⇒ rough $\widehat{\theta}$
2. **Gradient descent** ⇒ refined $\widehat{\theta}$

Methods

Fitting multi-spectral observations (one sight-line)



For each molecular line l,

$$\boldsymbol{x}_l = \boldsymbol{s}_l(\widehat{\boldsymbol{\theta}}) + \boldsymbol{b}_l$$

Find

$$\widehat{\boldsymbol{\theta}} = \{\log T_{\mathrm{kin},1}, \log n_{\mathrm{H}_2,1}, \log N_{l,1}, \mathrm{FWHM}_1, C_{V,1}, \log T_{\mathrm{kin},2}, \log n_{\mathrm{H}_2,2}, \log N_{l,2}, \mathrm{FWHM}_2, C_{V,2}\}$$

such as

$$\widehat{\boldsymbol{\theta}} = \underset{\theta}{\arg\min} \left[-\log \mathscr{L}(\boldsymbol{\theta}) \right] \quad (1)$$

where $-\log \mathscr{L}(\boldsymbol{\theta})$ is the **N**egative **L**og-**L**ikelihood (NLL)

$$-\log \mathscr{L}(\boldsymbol{\theta}) = \frac{1}{2} \sum_l \frac{\|\boldsymbol{x}_l - \boldsymbol{s}_l\|^2}{\sigma_{b,l}^2} + \mathrm{cte} \quad (2)$$

$$\boldsymbol{s}_l = \boldsymbol{s}_{l,\mathrm{fore}} + \boldsymbol{s}_{l,\mathrm{inner}} + \boldsymbol{s}_{l,\mathrm{back}} + \boldsymbol{s}_{l,\mathrm{CMB}}$$

$$\boldsymbol{s}_{l,\mathrm{fore}} = \mathcal{J}(T_{\mathrm{ex},1}) \left[1 - \exp\left(-\Psi_1\right)\right]$$

$$\boldsymbol{s}_{l,\mathrm{inner}} = \mathcal{J}(T_{\mathrm{ex},2}) \left[1 - \exp\left(-\Psi_2\right)\right] \exp\left(-\Psi_1\right)$$

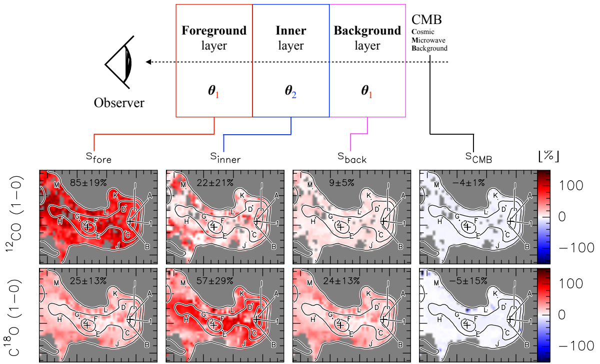
$$\boldsymbol{s}_{l,\mathrm{back}} = \mathcal{J}(T_{\mathrm{ex},1}) \left[1 - \exp\left(-\Psi_1\right)\right] \exp\left(-\Psi_1 - \Psi_2\right)$$

$$\boldsymbol{s}_{l,\mathrm{CMB}} = \mathcal{J}(T_{\mathrm{CMB}}) \left[\exp\left(-2 \times \Psi_1 - \Psi_2\right)\right] - \mathcal{J}(T_{\mathrm{CMB}})$$

Results

Distribution of the integrated intensity (full field of view)

☞ Pixel-wise analysis without spatial *a priori* or constraints between the outer and inner layer



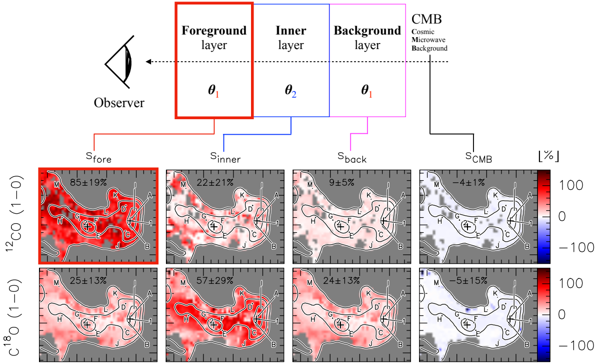
Contributions of the different layers to the integrated intensity of the $J = 1 \rightarrow 0$ line of ^{12}CO (top) and $C^{18}O$ (bottom); The foreground layer, inner layer, background layer and CMB (from the left to the right).

⇒ Check & **quantify** conjectures drawn from observations

Results

Distribution of the integrated intensity (full field of view)

☞ Pixel-wise analysis without spatial *a priori* or constraints between the outer and inner layer



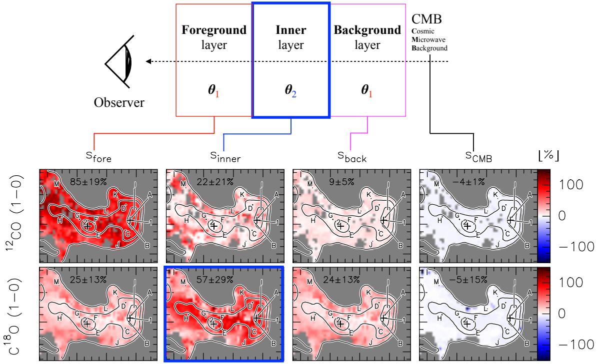
Contributions of the different layers to the integrated intensity of the $J = 1 \rightarrow 0$ line of ^{12}CO (top) and $C^{18}O$ (bottom);
The foreground layer, inner layer, background layer and CMB (from the left to the right).

⇒ Check & **quantify** conjectures drawn from observations

Results

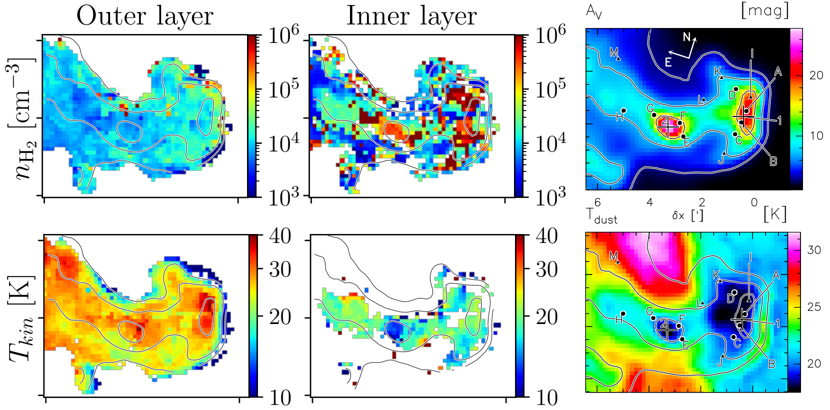
Distribution of the integrated intensity (full field of view)

☞ Pixel-wise analysis without spatial *a priori* or constraints between the outer and inner layer



Contributions of the different layers to the integrated intensity of the $J = 1 \rightarrow 0$ line of ^{12}CO (top) and C^{18}O (bottom); The foreground layer, inner layer, background layer and CMB (from the left to the right).

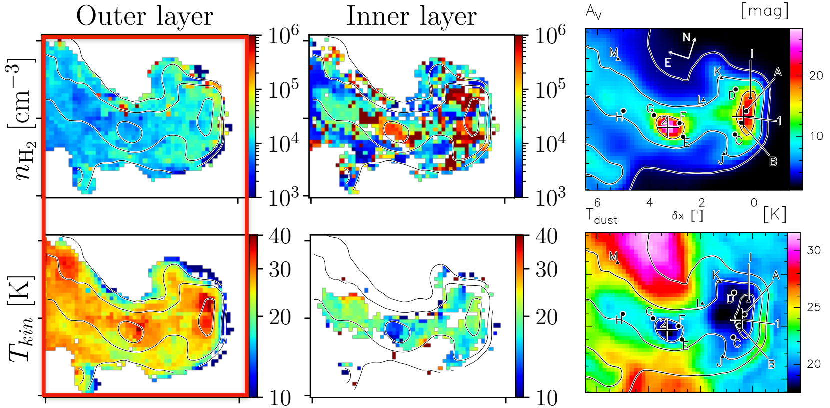
⇒ Check & **quantify** conjectures drawn from observations



Left and middle columns : Estimation maps of $\boldsymbol{n}_{\mathbf{H_2}}$ (first row) and $\boldsymbol{T}_{\mathbf{kin}}$ (second row). Right column : **Visual extinction** A_V [mag] (top) and **dust temperature** T_{dust} [K] (bottom). Contours of $A_V \in [3, 6, 16]$ mag are overlaid on each panel. White pixels correspond to filtered out estimations.

Results

Distribution of n_{H_2} and T_{kin}

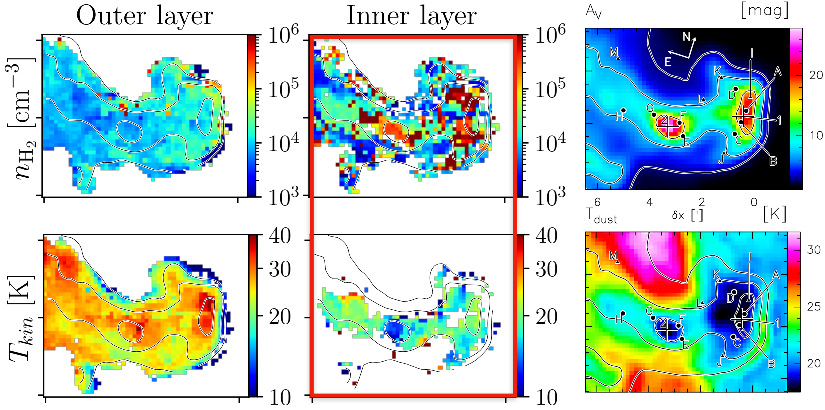


Left and middle columns : Estimation maps of $\boldsymbol{n_{H_2}}$ (first row) and $\boldsymbol{T_{kin}}$ (second row). Right column : **Visual extinction** A_V [mag] (top) and **dust temperature** T_{dust} [K] (bottom). Contours of $A_V \in [3, 6, 16]$ mag are overlaid on each panel. White pixels correspond to filtered out estimations.

Outer layer ~ lukewarm & moderately dense gaz

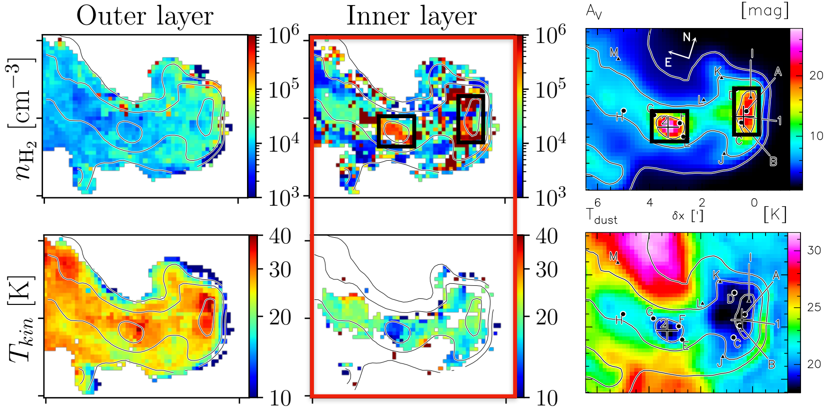
Results

Distribution of n_{H_2} and T_{kin}



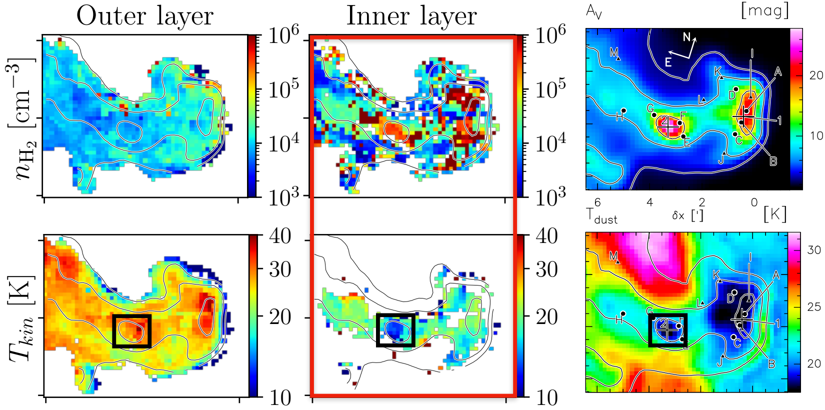
Left and middle columns : Estimation maps of $\boldsymbol{n_{H_2}}$ (first row) and $\boldsymbol{T_{kin}}$ (second row). Right column : **Visual extinction** A_V [mag] (top) and **dust temperature** T_{dust} [K] (bottom). Contours of $A_V \in [3, 6, 16]$ mag are overlaid on each panel. White pixels correspond to filtered out estimations.

Inner layer ∼ steep n_{H_2} and T_{kin} gradients



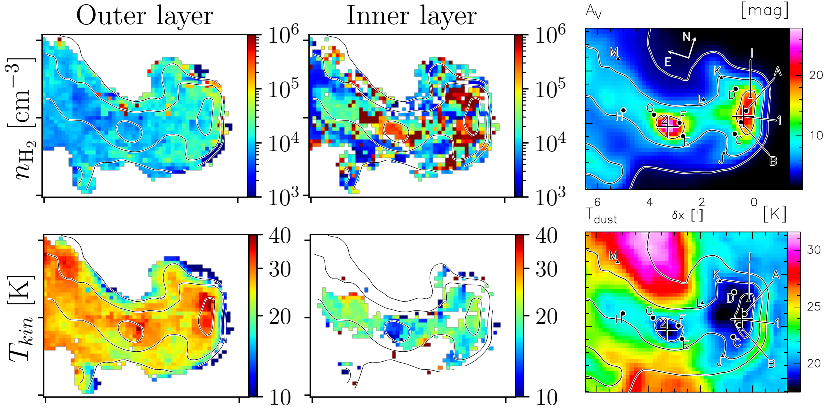
Left and middle columns : Estimation maps of $\boldsymbol{n_{H_2}}$ (first row) and $\boldsymbol{T_{kin}}$ (second row). Right column : **Visual extinction** A_V [mag] (top) and **dust temperature** T_{dust} [K] (bottom). Contours of $A_V \in [3, 6, 16]$ mag are overlaid on each panel. White pixels correspond to filtered out estimations.

Dense cores in a **less dense** filament



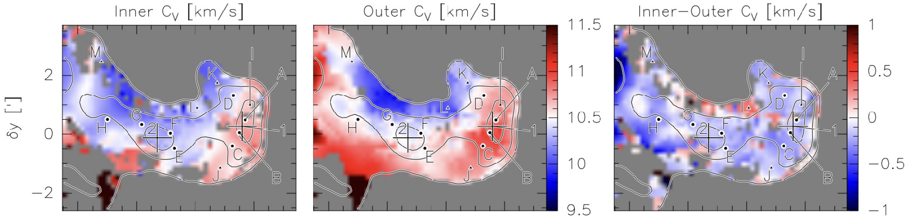
Left and middle columns : Estimation maps of $\boldsymbol{n_{H_2}}$ (first row) and $\boldsymbol{T_{kin}}$ (second row). Right column : **Visual extinction** A_V [mag] (top) and **dust temperature** T_{dust} [K] (bottom). Contours of $A_V \in [3, 6, 16]$ mag are overlaid on each panel. White pixels correspond to filtered out estimations.

Cold core in a **warmer** filament



Left and middle columns : Estimation maps of $\boldsymbol{n_{H_2}}$ (first row) and $\boldsymbol{T_{kin}}$ (second row). Right column : **Visual extinction** A_V [mag] (top) and **dust temperature** T_{dust} [K] (bottom). Contours of $A_V \in [3, 6, 16]$ mag are overlaid on each panel. White pixels correspond to filtered out estimations.

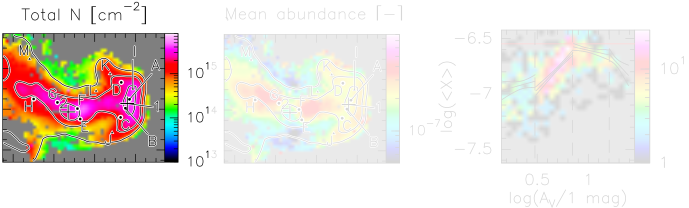
⇒ **Unmix** the **different environments** with complementary observations



- Doppler effect $\frac{\nu}{\nu_l} = 1 - \frac{V}{c}$
  Blue-shift → **Forward** motion
  Red-shift → **Inward** motion
- **Rotation** around the east-west axis Hily-Blant et al. 2005
- **Accretion** of the **foreground** by the **inner** layer

Results

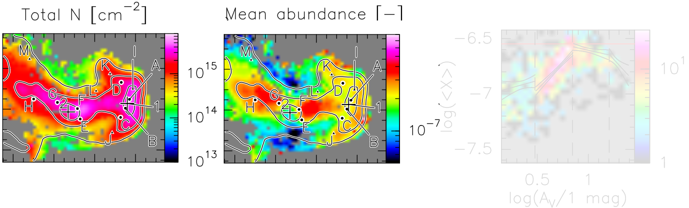
Quantitative analysis of the $C^{18}O$ depletion at { $A_V > 16$ mag, $T_{kin} < 15$ K }



Left panel : Map of the **total column density** N_{tot} of $C^{18}O$. Middle panel : Map of the **mean abundance** $\langle X \rangle$ of $C^{18}O$. Contours of $A_V \in [3, 7, 16]$ mag are overlaid on the two first panels. Right panel : **joint histogram of the mean abundance** of $C^{18}O$ vs $\boldsymbol{A_V}$. The black lines show the piecewise power-law fits of the scatter points within each range of $A_V \in [3, 7, 16]$ mag.

- With $X = C^{18}O$, $\langle X \rangle = N_{tot}(X) / N_{tot}(H_2)$, where $N_{tot}(X) = 2\, N_{ou}(X) + N_{in}(X)$
- **Highest** A_V & **lowest** T_{dust} : **Depletion** in the **gas phase** of a factor of 2.2

$\rightsquigarrow$ Molecular freezing onto dust grains Kramer et al. 1998, Tafalla et al. 2004



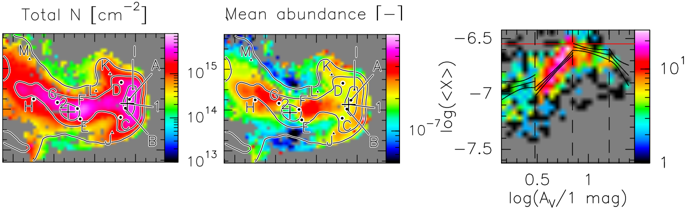
Left panel : Map of the **total column density** N_{tot} of $C^{18}O$. Middle panel : Map of the **mean abundance** $\langle X \rangle$ of $C^{18}O$. Contours of $A_V \in [3, 7, 16]$ mag are overlaid on the two first panels. Right panel : **joint histogram of the mean abundance** of $C^{18}O$ vs $\boldsymbol{A_V}$. The black lines show the piecewise power-law fits of the scatter points within each range of $A_V \in [3, 7, 16]$ mag.

- With $X = C^{18}O$, $\langle X \rangle = N_{tot}(X) / N_{tot}(H_2)$, where $N_{tot}(X) = 2\, N_{ou}(X) + N_{in}(X)$
- **Highest** A_v & **lowest** T_{dust} : **Depletion** in the **gas phase** of a factor of 2.2

$\rightsquigarrow$ Molecular freezing onto dust grains Kramer et al. 1998, Tafalla et al. 2004

Results

Quantitative analysis of the $C^{18}O$ depletion at { $A_v > 16$ mag, $T_{kin} < 15$ K }



Left panel : Map of the **total column density** N_{tot} of $C^{18}O$. Middle panel : Map of the **mean abundance** $\langle X \rangle$ of $C^{18}O$. Contours of $A_v \in [3, 7, 16]$ mag are overlaid on the two first panels. Right panel : **joint histogram of the mean abundance** of $C^{18}O$ vs $\boldsymbol{A_v}$. The black lines show the piecewise power-law fits of the scatter points within each range of $A_v \in [3, 7, 16]$ mag.

- With $X = C^{18}O$, $\langle X \rangle = N_{tot}(X) / N_{tot}(H_2)$, where $N_{tot}(X) = 2\,N_{ou}(X) + N_{in}(X)$
- **Highest** A_v & **lowest** T_{dust} : **Depletion** in the **gas phase** of a factor of 2.2

⇝ Molecular freezing onto dust grains Kramer et al. 1998, Tafalla et al. 2004

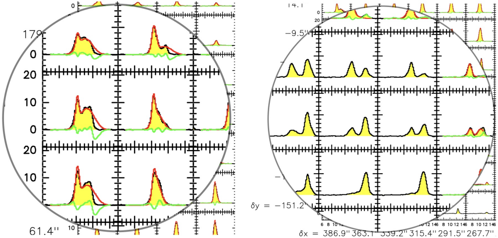
Conclusion & Perspectives

Approximate gradient of the gas properties

- Multilayer model extended to **random number of layers**
  - ⤳ For analyzing other GMCs
  - ⤳ The fitting procedure will be in **open access**
- Method and results detailed in *Toward a robust physical and chemical characterization of heterogeneous lines of sight: The case of the Horsehead nebula*, Ségal et al., accepted sept. 2024, A&A https://arxiv.org/abs/2409.20074v2

Next step

- Extend the model to spectra with **multiple velocity components**



References

- *A computer program for fast non-LTE analysis of interstellar line spectra. With diagnostic plots to interpret observed line intensity ratios*, Van der Tak et al., A&A, 2007
- Mather, J. C., Cheng, E. S., & Cottingham, D. A., e. a. 1994, The Astrophysical Journal, 420, 439
- Hily-Blant, P., Teyssier, D., Philipp, S., & Güsten, R. 2005, A&A, 440, 909
- C. Kramer, J. Alves, C.J. Lada, E.A. Lada, A. Sievers, H. Ungerechts, and C.M. Walmsley, A&A, 342, 257–270 (1999)
- *L1521E: The first starless core with no molecular depletion*, M. Tafalla and J. Santiago, A&A 414, L53–L56 (2004)
- *Toward a robust physical and chemical characterization of heterogeneous lines of sight: The case of the Horsehead nebula*, Ségal et al., [A&A, accepted in sept. 2024]

Methods

Accuracy analysis with the Cramér-Rao bound

The Cramér-Rao bound (CRB) provides a **lower bound of the variance** on estimations for any **unbiased** estimator (Garthwaite et al., 1995).

$$\mathrm{var}(\widehat{\theta}_i) \geq [\mathrm{CRB}(\boldsymbol{\theta})]_{ii} \quad \text{for} \quad \widehat{\theta}_i \in \widehat{\boldsymbol{\theta}} \tag{3}$$

For **efficient** estimator,

$$\mathrm{var}(\widehat{\theta}_i) = [\mathrm{CRB}(\boldsymbol{\theta})]_{ii} \quad \text{for} \quad \widehat{\theta}_i \in \widehat{\boldsymbol{\theta}} \tag{4}$$

Unbiased & **Efficient** estimator ⇒ CRB provides **error bars** on estimations

where $\mathrm{CRB}^{-1} = \boldsymbol{I}_F$, $\boldsymbol{I}_F$ is the Fisher information matrix defined by

$$\forall (i,j) \quad [\boldsymbol{I}_F(\boldsymbol{\theta})]_{ij} = \mathbb{E}\left[\frac{\partial \log \mathscr{L}(\boldsymbol{\theta})}{\partial \theta_i} \frac{\partial \log \mathscr{L}(\boldsymbol{\theta})}{\partial \theta_j}\right] \tag{5}$$

Chemical assumptions & model constraints

- ^{12}CO($J = 1 \rightarrow 0$) optically **thick** & **LTE** $\rightsquigarrow$ fitting the **peak intensity** only
- Constraints on relative column densities:

We write X/Y the column density ratio $N(X)/N(Y)$, for each couple of species $\{X, Y\}$. Intervals correspond of the explored ranges when estimating the corresponding ratios. $N(^{13}CO)/N(H^{13}CO^+)$ is deduced from $N(^{13}CO)/N(H^{13}CO^+) = N(^{12}CO)/N(HCO^+)$.

Column density ratio		Model	
		Inner layer	Outer layer
Assumed	$^{12}CO/^{13}CO$	$10^{1.8} \sim 63$	$[10^{1.3}, 10^{1.9}] \sim [20, 80]$
	$^{13}CO/C^{18}O$	$10^{0.9} \sim 7.9$	$[10^{0.75}, 10^{1.4}] \sim [5.6, 25.1]$
	$^{13}CO/HCO^+$	$[10^{2.88}, 10^{3.78}]$	$[10^{2.88}, 10^{3.78}]$
	$^{13}CO/H^{13}CO^+$	$^{12}CO/HCO^+$	$^{12}CO/HCO^+$
Derived	$^{12}CO/C^{18}O$	$10^{2.7} \sim 500$	$[10^{2.05}, 10^{3.3}]$
	$C^{18}O/H^{13}CO^+$	$[10^{3.78}, 10^{4.68}]$	$[10^{2.78}, 10^{4.93}]$
	$^{12}CO/HCO^+$	$[10^{4.68}, 10^{5.58}]$	$[10^{4.18}, 10^{5.68}]$