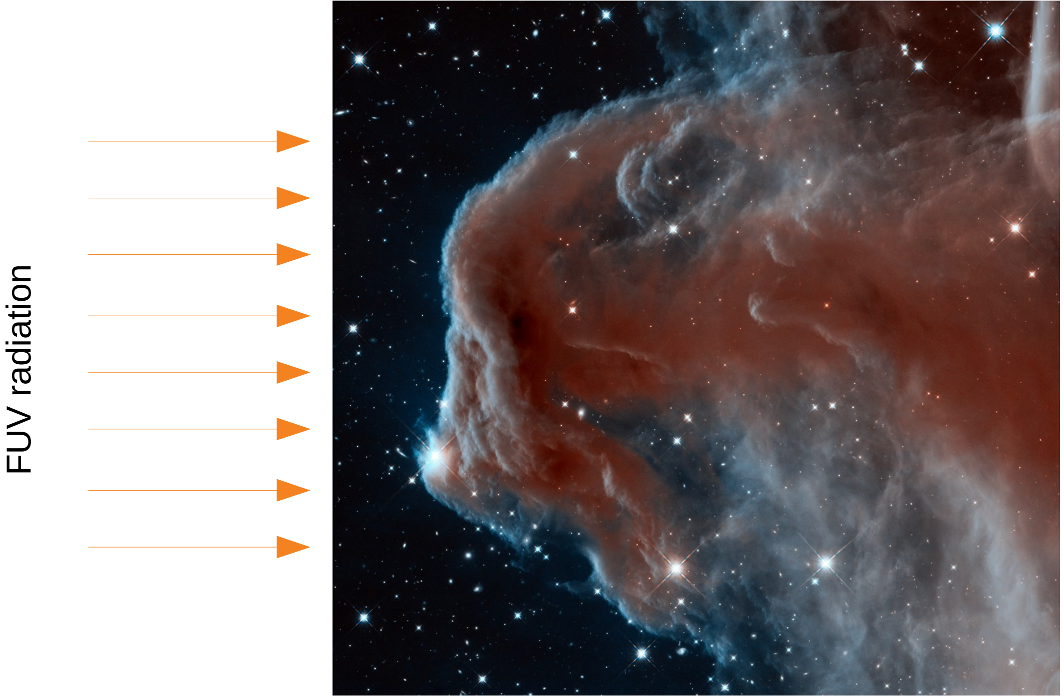
Photodissociation Regions

Photodissociation Regions

PDRs are predominantly neutral regions and where the transition between the atomic to molecular gas phase occurs.



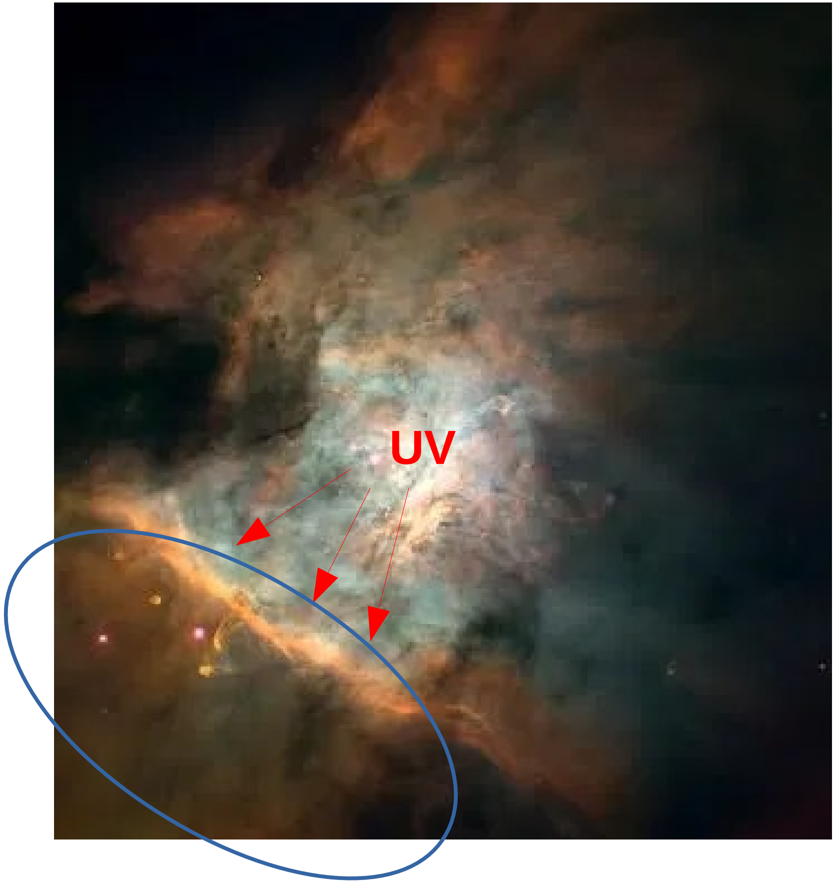
Studying PDRs and the interaction of the FUV radiation with the ISM is of significant importance to understand its physics and chemistry.

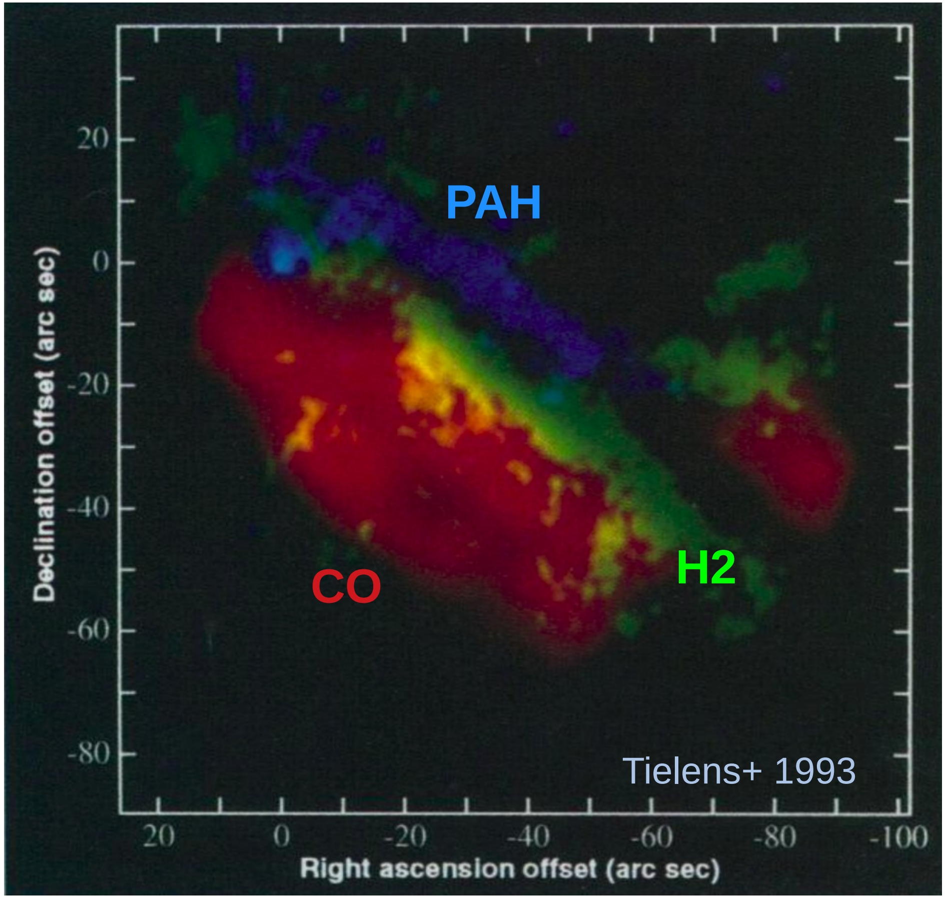
In a galaxy, most of the observed ISM is considered to be in PDR.

PDRs control the thermal balance in galaxies.

Photodissociation Regions

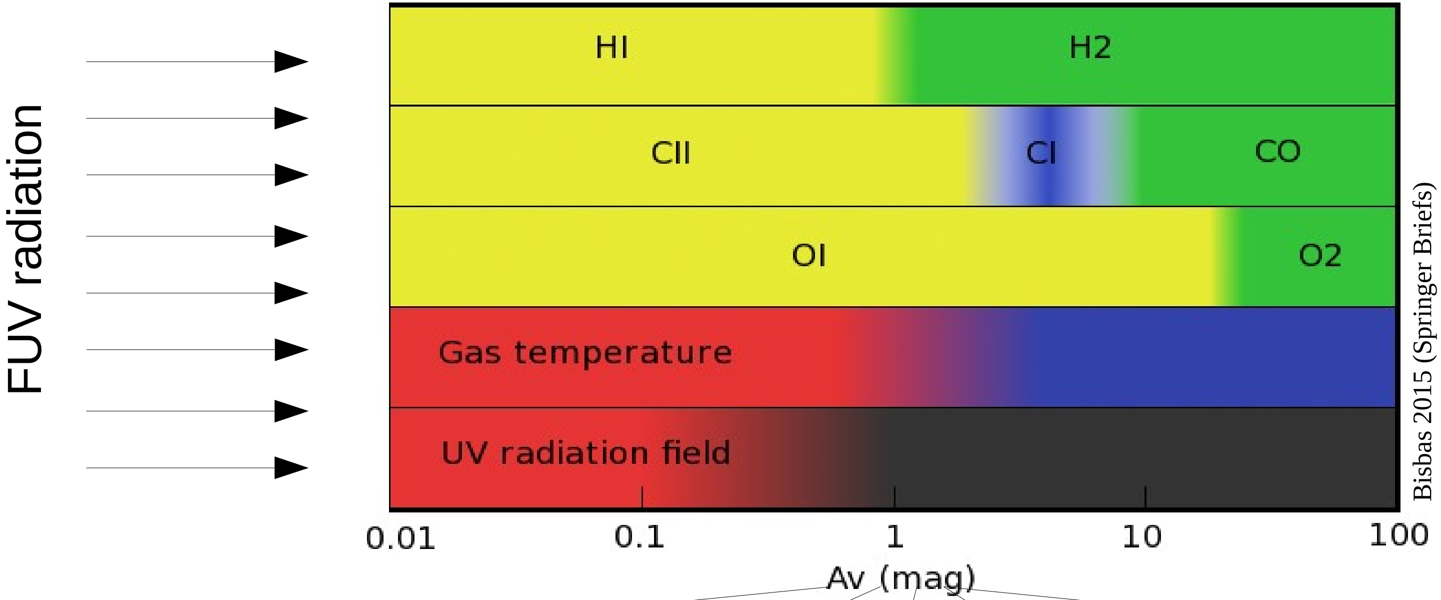
Orion Bar: the most famous PDR laboratory





Tielens+ 1993

The carbon cycle and the HI-to-H2 transition



Bisbas 2015 (Springer Briefs)

Age of cloud

van Dishoeck & Black (1988)
Sternberg & Dalgarno (1995)
Beuther et al. (2014)
Walch et al. (2015)
Clark et al. (2019)

X-rays

Maloney et al. (1996)
Meijerink et al. (2006)
Mackey et al. (2019)

Starlight (FUV)

van Dishoeck & Black (1988)
Bergin et al. (2004)
Langer et al. (2010)
Glover & Mac Low (2011)
Bisbas et al. (2021)

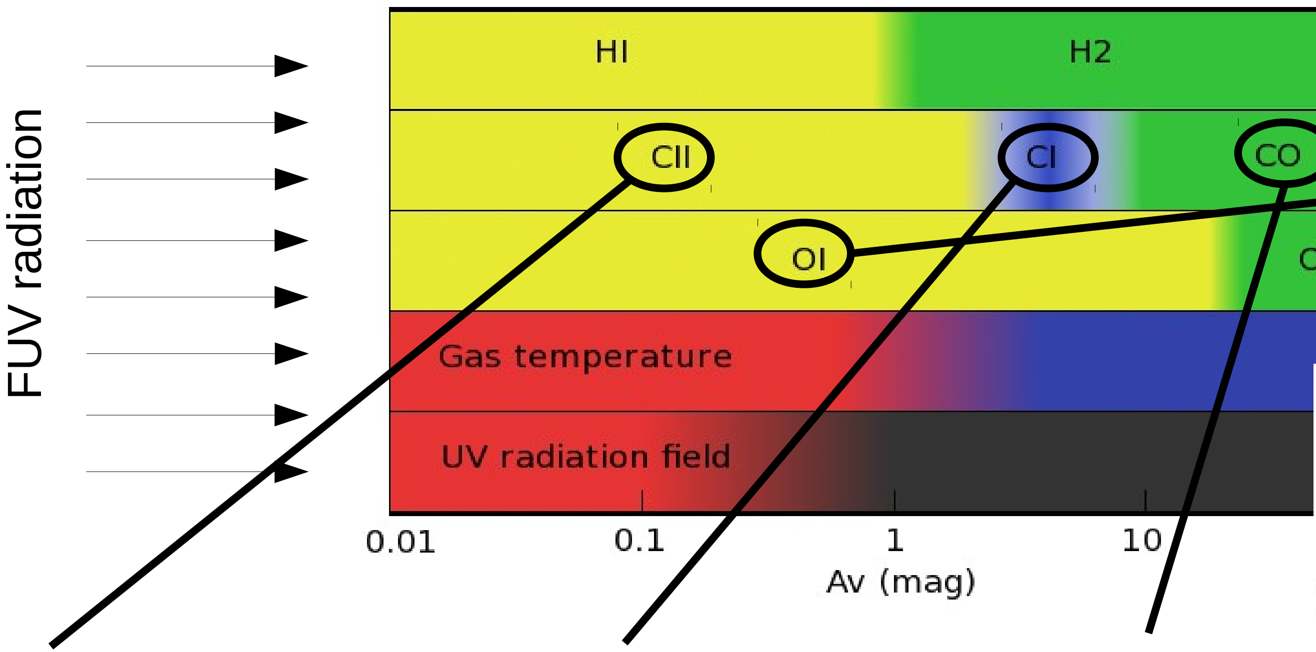
Cosmic-rays

Bisbas et al. (2015, 2017, 2021)
Papadopoulos et al. (2018)
Papadopoulos (2010)
Gaches et al. (2019a,b, 2021)

Metallicity (Z)

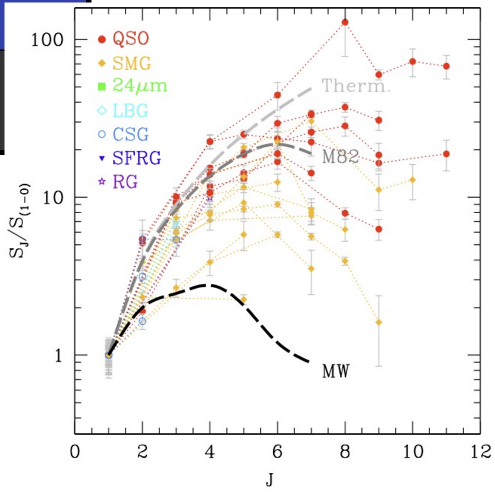
Maloney & Black (1988)
Wolfire et al. (1995)
Pak et al. (1998)
Madden et al. (2006)
Bialy & Sternberg (2015)
Bisbas et al. (2021)

The carbon cycle and the HI-to-H2 transition



[OI] 63 μm
[OI] 146 μm

CO ladder



Carilli & Walter (2013)

[CII] 158 μm

Important ISM coolant.
Ionized and atomic regions (HII, HI)

Ionization potential is 11.2eV, close to the 13.6eV of hydrogen.

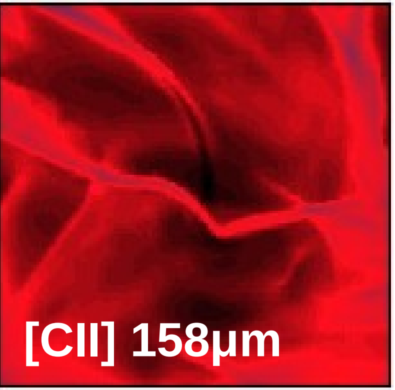
[CI](1-0) 609 μm
[CI](2-1) 370 μm

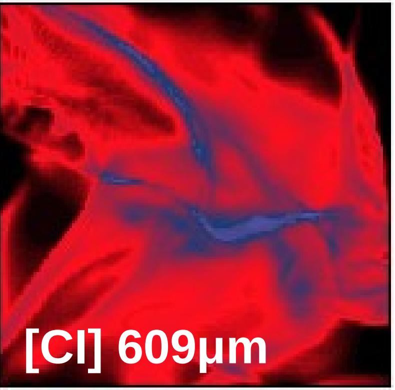
ISM coolant.
Molecular regions (H2). In normal conditions it is a “thin” layer.

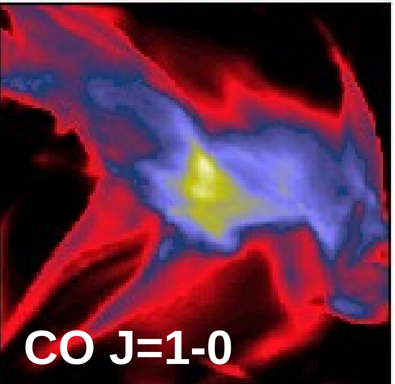
CO J=1-0
CO J=2-1
CO J=3-2 …

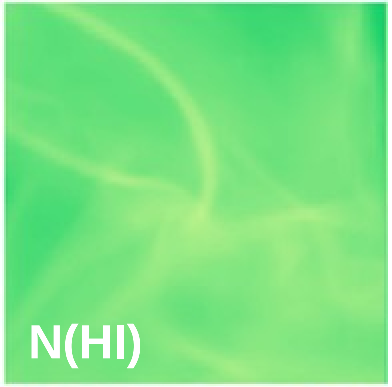
The higher the transition, the denser the ISM it traces. H2-rich clouds!

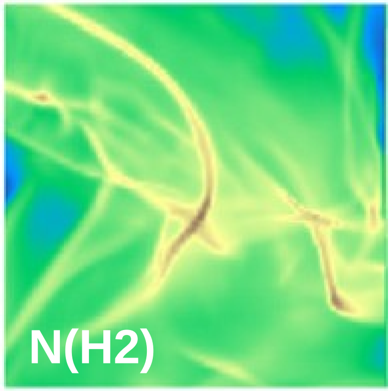
Understanding PDRs from simulations



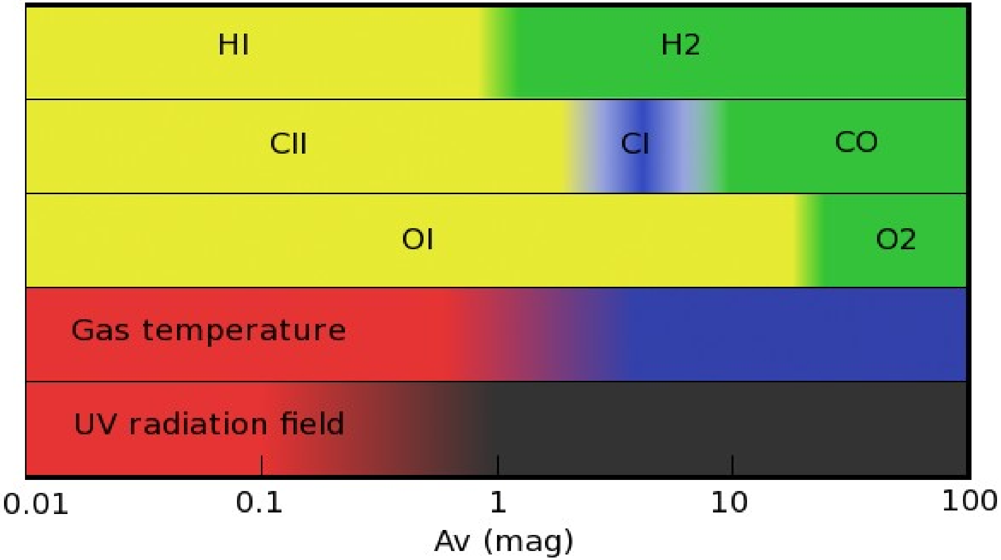








Bisbas et al. (2021)

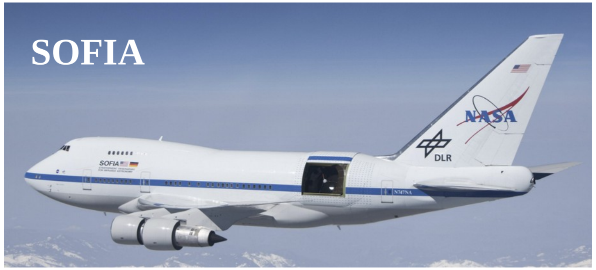


In the simulation, the stratification of the carbon cycle can be seen.

Outer layer: [CII] 158µm
Middle layer: [CI] 609µm
Inner part: CO *J*=1-0 (115 GHz)

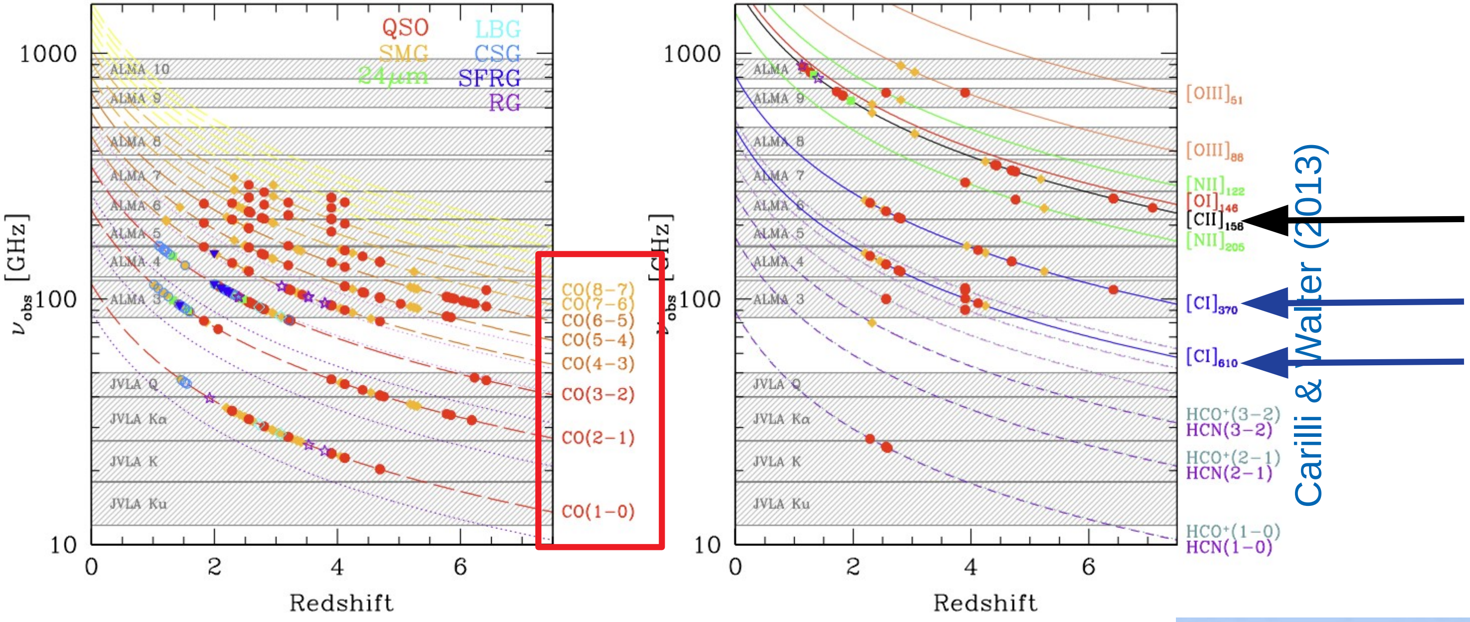
The column densities of HI and H2 are also shown.

Observing the carbon cycle


SOFIA


Herschel (archive)


ALMA



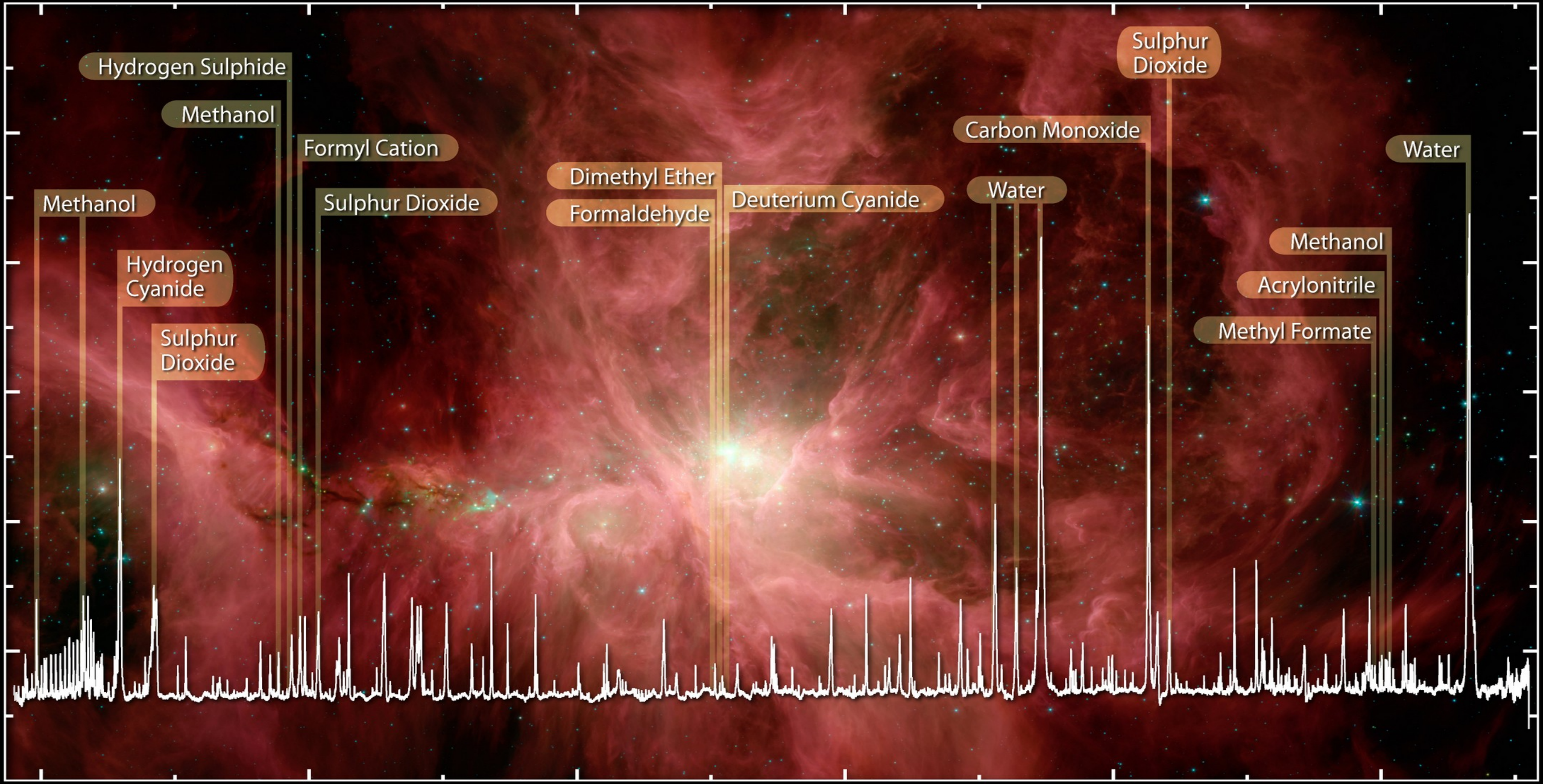
Carilli & Walter (2013)


JVLA


IRAM-30m


NOEMA


CCAT-prime

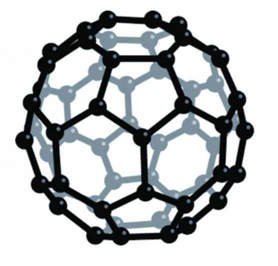


HIFI Spectrum of Water and
Organics in the Orion Nebula

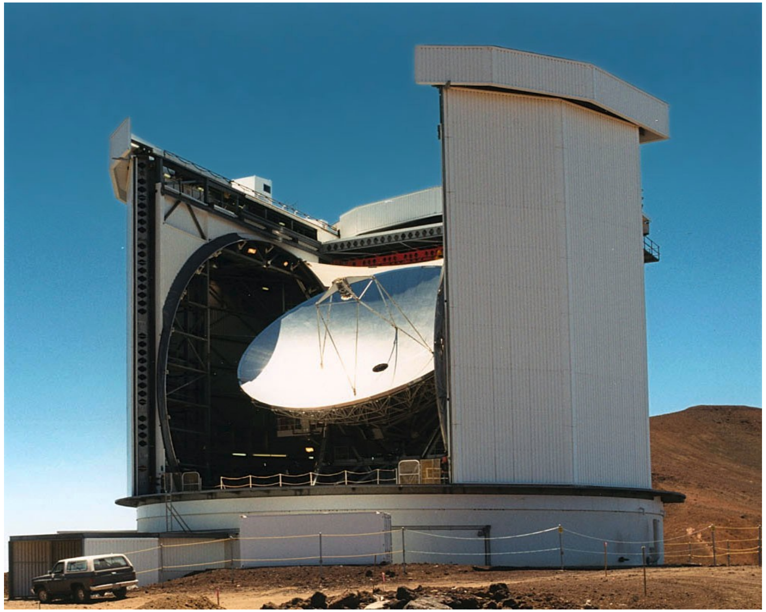
© ESA, HEXOS and the HIFI consortium
E. Bergin

Molecules discovered in ISM (so far, and not only...)

Kind	**Inorganic**		**Organic**	
Diatomic	H_2	**hydrogen**	CH	methylidyne radical
	OH	hydroxyl radical	CN	cyanogen radical
	SiO	silicon monoxide	C_2	carbon
	SO	sulphur monixide	CS	carbon monosulphide
	CO	**carbon monoxide**		
Triatomic	H_2O	**water**	CCH	ethynyl radical
	H_2S	hydrogen sulphide	HCN	hydrogen **cyanide**
	SO_2	sulphur dioxide	HCO	formyl radical
4-atomic	NH_3	**ammonia**	H_2CO	**formaldehyde**
			HNCO	hydrocyanic acid
			H_2CS	thioformaldehyde
5-atomic			CH_4	**methane**
			HCOOH	**formic acid**
…			…	…
13-atomic			$HC_{11}N$	cyanopentaacetylene
60-atomic	C_{60}	buckminsterfullerene		



Molecular hydrogen in the Universe



A major problem occurs when observing H2: due to its quantum mechanical properties, it does not emit radiation readily observable by (radio-)telescopes. The community therefore is widely using a technique in which H2 is traced by CO emission.

CO is *by far* the most abundant molecule in the Universe (~10^{-4}) after H2 itself. It is formed where H2 also forms. Its radiation (particularly the J=1-0 transition which has been considered to be the least bias for H2 detection) is easily captured by radiotelescopes (e.g. VLA, ALMA)

This CO-to-H2 technique has been found to work reasonably well for Milky Way clouds and has been therefore extensively used for determining the H2 gas mass.

However, during the last decade, there is growing evidence that CO-to-H2 may be biased in certain classes of extragalactic environments.

$$\mathrm{N}(\mathrm{H}_2) = X_{\mathrm{CO}} \underbrace{\int T_{\mathrm{A}}(\mathrm{CO})\,dv}_{\text{Radiotelescope observation (K km/s)}}$$

"X_{CO} – factor"

$$X_{\mathrm{CO}} \sim 2\times10^{20}\,\mathrm{cm}^{-2}\mathrm{K}^{-1}\mathrm{km}^{-1}\mathrm{s}$$

(Strong & Mattox 1996; Dame, Hartmann & Thaddeus 2001, Bolatto et al. 2013)

“CO-dark” molecular gas

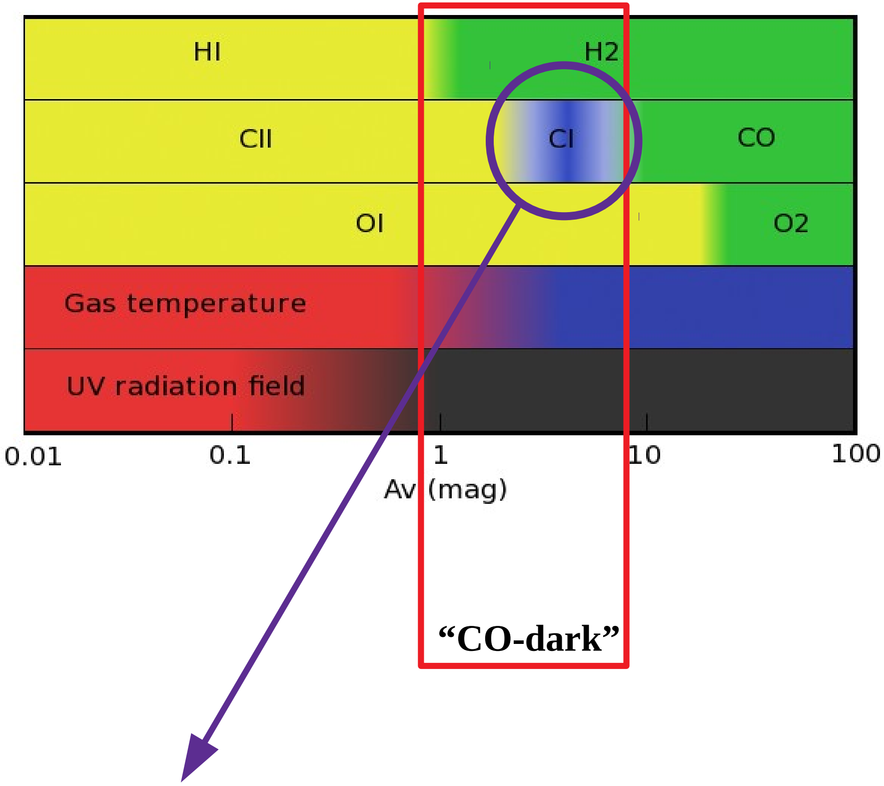
CO J=1-0 does not trace the entire extent of molecular gas.

There are layers, especially at the bounds of clouds, where carbon is in the form of CII, but hydrogen is in molecular form due to efficient self-shielding. This is the “CO-dark” molecular gas (term coined to van Dishoeck, 1992)

This molecular ISM phase is not traced by HI or CO.

Photoelectric heating by the interstellar radiation field increases the gas temperature to ~50K or even ~100K, making conditions appropriate for the survival of H2 molecule and carbon in the form of CII (and not CO).

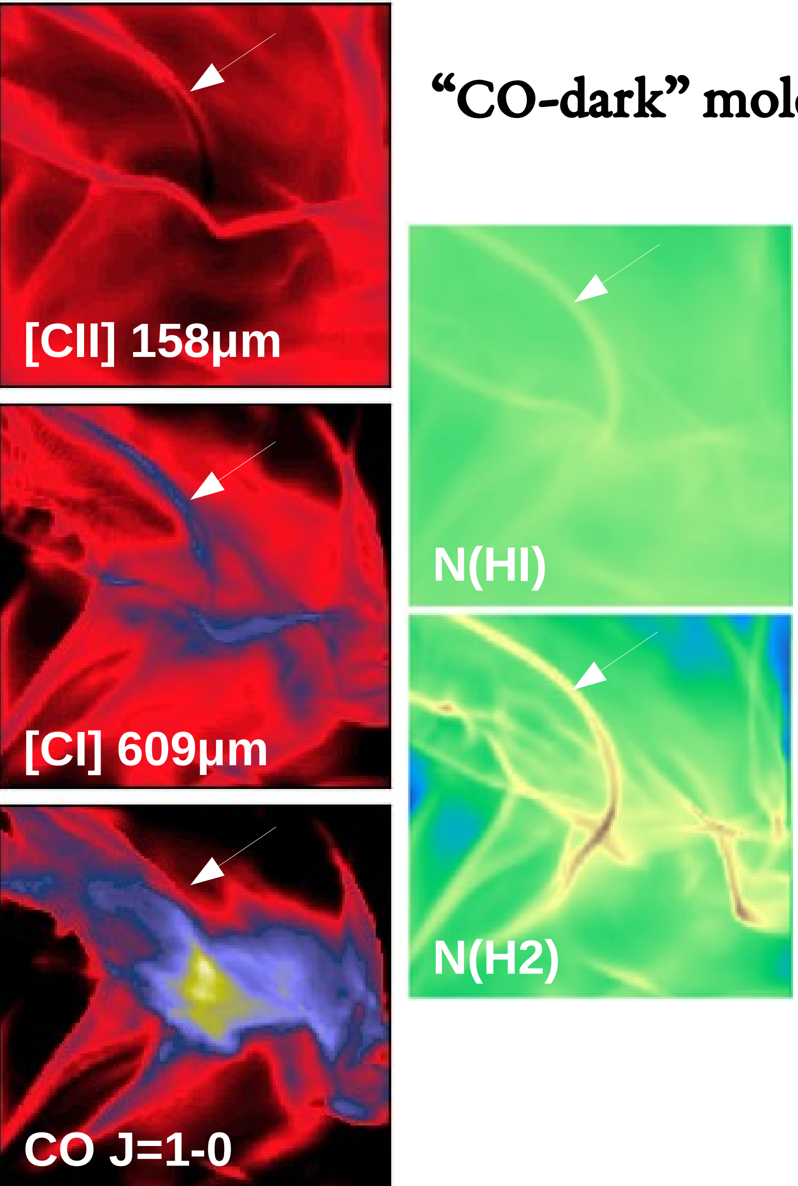
Since E = hν / k_B ~ 92.1 K for CII, it makes it a very good alternative tracer for regions with >50 K.



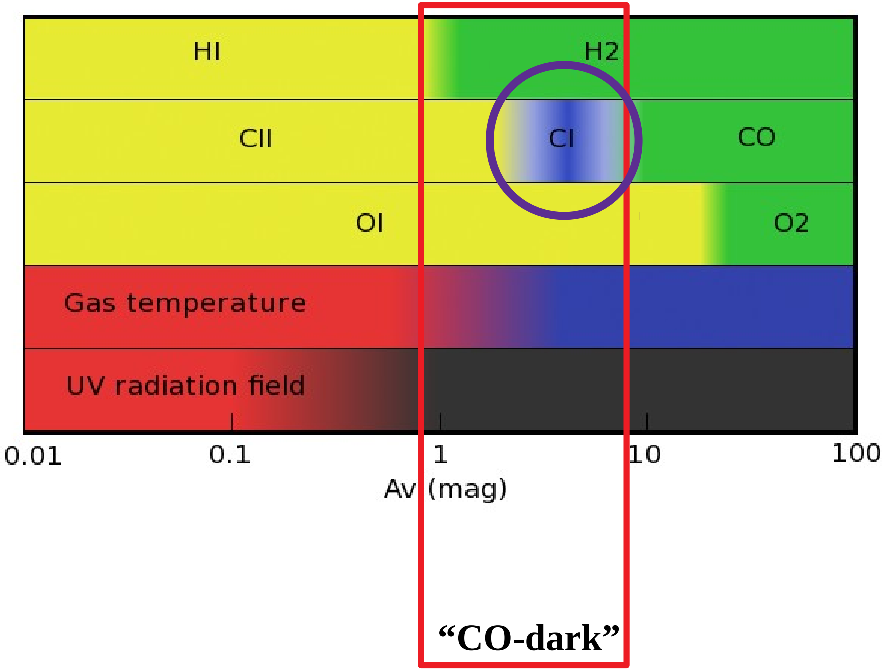
First paper to propose the CI(1-0) line as an H_2 gas tracer was published by Papadopoulos et al. (2004). Some first observations in the Vela Molecular Ridge cloud C supports its ability as H_2 proxy (Lo et al. 2014).

Thought to be a very thin layer, it was not favored as an alternative tracer for H_2 gas.

“CO-dark” molecular gas



Bisbas et al. (2021)



The filamentary structure is molecular, observable in [CII] and [CI] (1-0), but in CO(1-0) it is invisible. It’s “CO-dark” molecular gas.

Is the CO-to-H_2 method applicable everywhere?

There is a body of work demonstrates that the Xco-factor depends on:

- The average ISM metallicity (Pak et al. 1998; Wolfire et al. 1999)
- The ambient FUV radiation field (Pak et al. 1998; Wolfire et al. 2003 for a review)
- The average dynamical state of the gas (Papadopoulos et al. 2012)
- The CO-destruction due to CRs (Bisbas et al. 2015, 2017)

The destruction of CO is very sensitive to the average cosmic-ray energy density permeating the molecular clouds (Bisbas et al. 2015, 2017b)

Starburst galaxies with their high star-formation rates is where the average UV field and cosmic ray energy density is >1000x the average Milky Way value.

Also GMCs close to the Galactic Center may be prone to high CR ionization rates.

Is there an ideal H_2 tracer?

Other tracers include the most abundant isotopologues of CO (e.g. ^{13}CO) which are optically thin up to high column densities but are too weak to be observed in extragalactic objects.

The **ideal tracer** would have to:

1) be entirely connected with molecular gas
2) be optically thin under most ISM conditions
3) require a single transition to get its X-factor
4) be an emitter of strong lines
5) depend weakly on ambient ISM conditions
6) has an abundance high enough across the Universe

Papadopoulos+ (2004) has discussed the utility of CI as an alternative H_2 tracer (see also Offner+ 2014, Glover+ 2015).

Some first observations in the Vela Molecular Ridge cloud C supports its ability as H_2 proxy (Lo et al. 2014).

Molecular Astrophysics – reaction types in the ISM

Formation of molecules

Radiative association: $X^+ + Y \rightarrow XY^+ + hv$ (important for Early Universe chemistry)

Associative detachment: $X^- + Y \rightarrow XY + e^-$

Grain surface (gr): $X + Y{:}gr \rightarrow XY + gr$

Destruction of molecules

Photodissociation: $XY + hv \rightarrow X + Y$

Dissociative recombination: $XY^+ + e \rightarrow X + Y$

Collisional dissociation: $XY + M \rightarrow X + Y + M$

Charge exchange reactions

Ion-molecule reactions: $X^+ + YZ \rightarrow XY^+ + Z$

Charge-transfer reactions: $X^+ + YZ \rightarrow X + YZ^+$

Neutral-neutral reactions: $X + YZ \rightarrow XY + Z$

H2 formation in the Universe

We assume a cloud full of atomic gas in which there is no dust particles neither radiation field.

At t = 0, the density of atomic hydrogen is n = n(H) and the density of molecular hydrogen is $n(H_2) = 0$.

The H_2 formation then occurs through the following reactions:

~~$H + H \rightarrow H_2 + h\nu$~~

~~$H + H + H \rightarrow H_2 + H$~~

H_2 forms on dust grains!

(see later slides)

The first reaction needs some time to occur at which point the two H atoms won't be together.

For the second reaction to occur, we find the following relations between density and formation time:

n_H (cm^{-3})	10^5	10^{10}	10^{12}	10^{15}	10^{16}	10^{18}
t (years)	6×10^{14}	6×10^4	6	6×10^{-6} (600 s)	6×10^{-8} (6 s)	6×10^{-10} (0.0006 s)

So the second reaction can only by considered for densities $>10^{10}$ cm^{-3} which are very high for the ISM but realistic in YSOs.

However, H_2 is very abundant in the Universe...

H2 formation in the Universe

The formation of H_2 in the ISM of the Early Universe is difficult!

Reactions with H^+

$H + H^+ \rightarrow H_2^+ + h\nu$

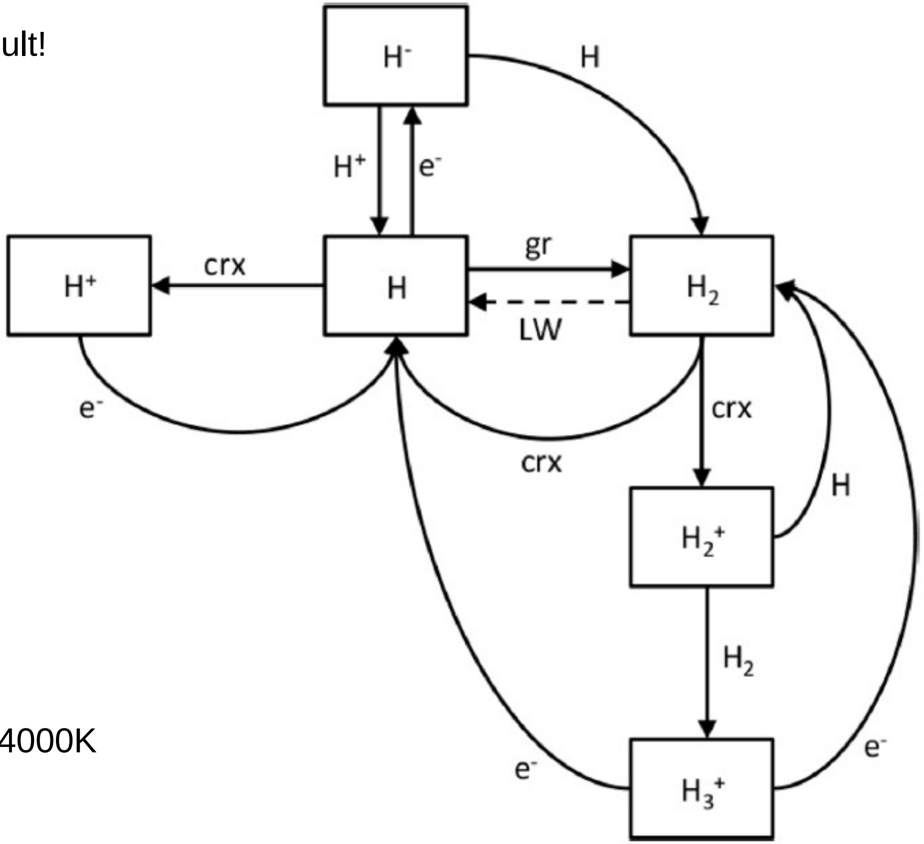
$H_2^+ + H \rightarrow H_2 + H^+$

H_2^+ is destroyed with photodissociation and dissociative recombination:

$H_2^+ + h\nu \rightarrow H + H^+$

$H_2^+ + e \rightarrow H + H$

H_2 formation becomes important when the temperature is <4000K at which point photodissociation ceases.



Bialy+ 2015

H2 formation in the Universe

In the gas phase and when the metallicity is low (e.g. during the first steps of galaxy formation), H_2 forms according to the following **reactions with H^-:**

$H + e^- \rightarrow H^- + h\nu$

$H^- + H \rightarrow H_2 + e^-$

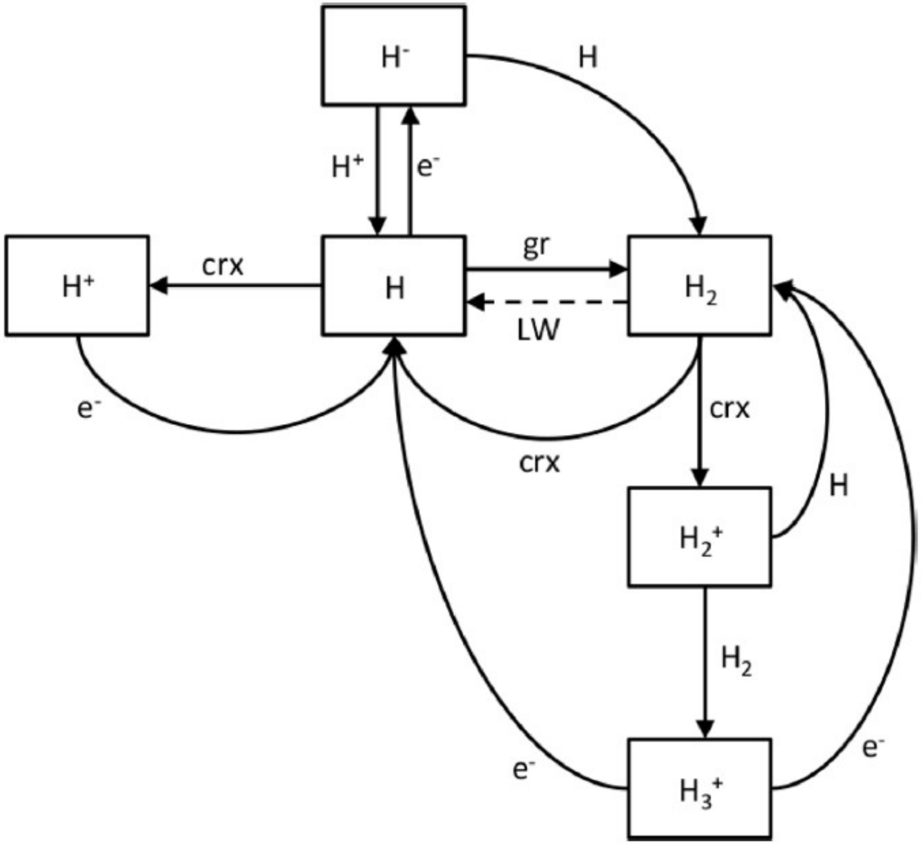
The reaction:

$H^- + H^+ \rightarrow H + H$

mitigates the $H^- + H \rightarrow H_2 + e^-$

In addition, $H^- + h\nu \rightarrow H + e^-$

We need gas temperatures of <1000K



Bialy+ 2015

H2 formation in the Universe

Both chemical networks with H^+ and H^- are catalytic, because they return H^+ and e^-.

Therefore, H_2 is being destroyed according to the reactions:

$$H_2 + H^+ \rightarrow H_2^+ + H$$

$$H_2 + e \rightarrow H + H^-$$

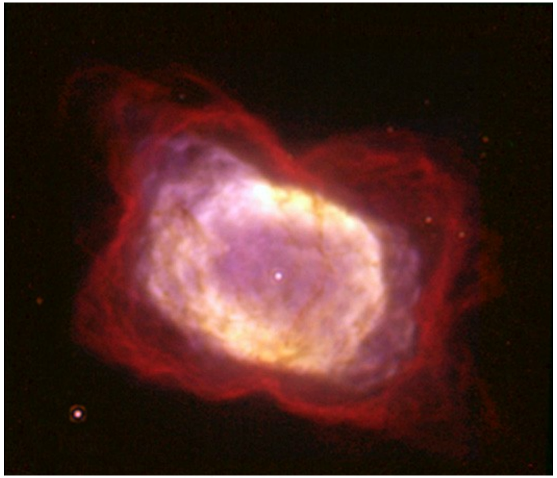
As a result, molecular hydrogen forms at an abundance of 10^{-6}.

H_2 formation in the Early Universe is therefore difficult! However, this small amount of H_2 is very important for the formation period of first stars to begin.

The chemistry in the Early Universe is therefore much different compared to the chemistry of the local Universe!

Formation of the first molecules in the Universe: He_2^+ and HeH^+

HeH^+ (helium hydride) is formed from reactions of H and He (radiative reactions), which are the first atoms formed in the Universe.



Formed when temperature of the Universe ~4000K.

Discovered in NGC 7027 in 2019.

Ionization potential:

He++ → 54.5eV
He+ → 24.6eV
H+ → 13.6eV

The above means that first He atom will form and then H, as the Universe cools down (He forms at 110kyr and H at 320kyr age of the Universe)

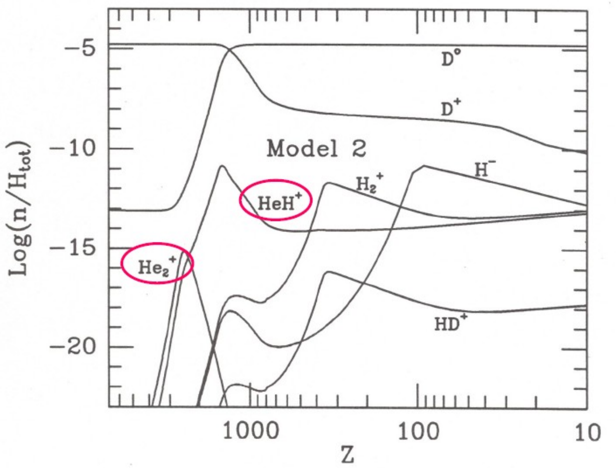
HeH^+ forms from the reaction:

$$He + H^+ \rightarrow HeH^+ + hv$$

HeH^+ is destroyed through the reaction:

$$HeH^+ + H \rightarrow He + H_2^+$$

This reaction paves the way of H_2 formation in the Universe, marking the start of Molecular Epoch.



Formation of gas-phase carbon monoxide (CO)

CO is the most abundant molecule in the Universe, after H_2. Its abundance is ~10^{-4} compared to H.
CO is formed through three main chemical channel pathways: through **OH**, through **CH**, and through $\mathbf{O_2}$

Formation of CO through OH (dominant mechanism at low metallicities and important at high CR rates)

$C + OH \rightarrow \mathbf{CO} + H$ or
$C^+ + H \rightarrow CO^+ + H$ and CO^+ reacts either with H or H_2:
$CO^+ + H \rightarrow \mathbf{CO} + H^+$ or
$CO^+ + H_2 \rightarrow HCO^+ + H$ and then $HCO^+ + e^- \rightarrow \mathbf{CO} + H$

Formation of CO through CH (dominant mechanism at high metallicities)

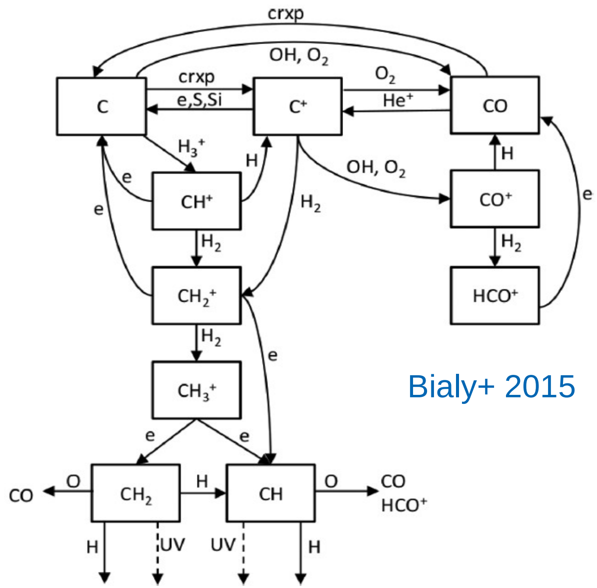
$O + CH \rightarrow \mathbf{CO} + H$
In addition $O + CH \rightarrow HCO^+ + e^-$ and then $HCO^+ + e^- \rightarrow \mathbf{CO} + H$
But also $O + CH_2 \rightarrow \mathbf{CO} + H_2$ and $\mathbf{CO} + H + H$

Formation of CO through O_2 (dominant mechanism in regions of high CR rates)

$O_2 + C \rightarrow \mathbf{CO} + O$
$O_2 + C^+ \rightarrow \mathbf{CO} + O^+$ but also $CO^+ + O$. In the second case CO^+ reacts with H or H_2 forming CO as above.

Destruction of CO

$He^+ + CO \rightarrow He + O + C^+$



Bialy+ 2015

Thermal balance

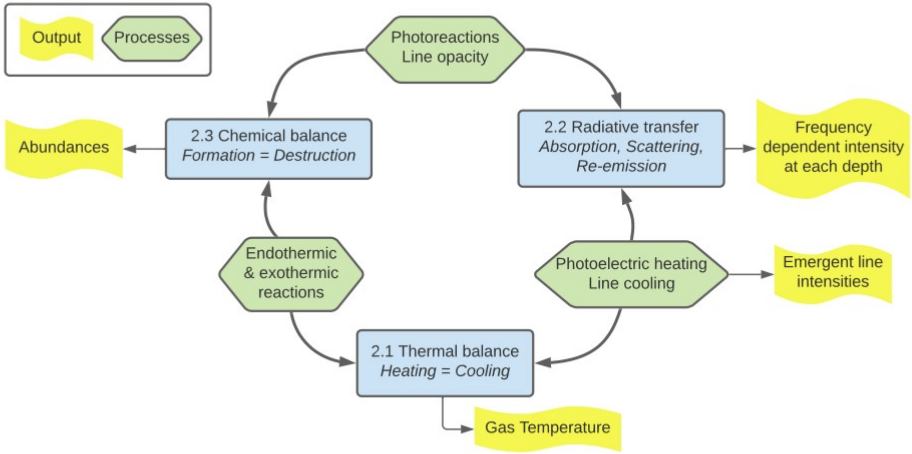
In short, the gas temperature is obtained by balancing the total heating with the total cooling.
Numerically, this condition occurs to within a user-defined tolerance parameter controlling the accuracy.
For a stationary PDR, the thermal balance equation is:

$$\Gamma(T_{\rm gas}, ...) = \Lambda(T_{\rm gas}, ...)$$

The above are in units of [*erg cm*$^{-3}$ *s*$^{-1}$] (rate of energy per volume).

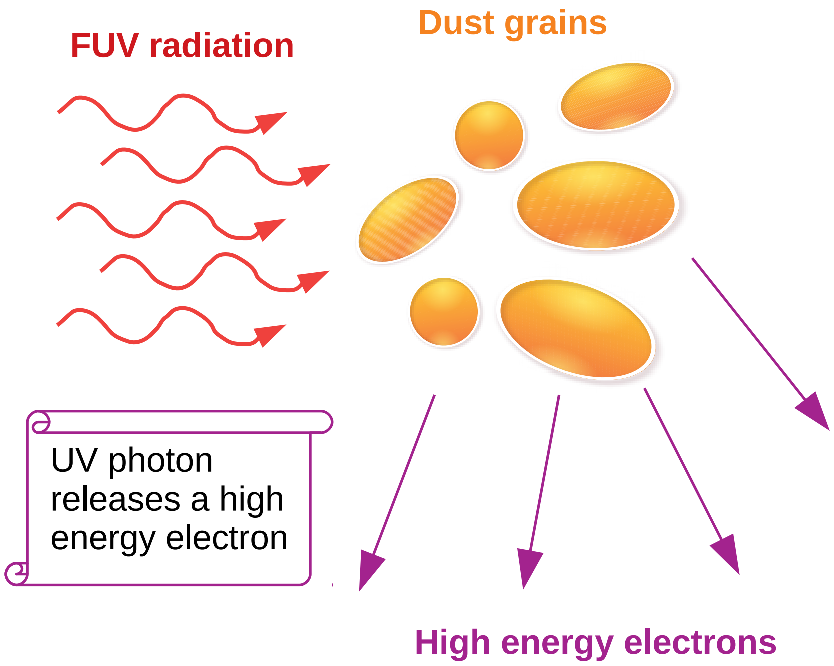
Another notation of the above: $n_{\rm H}\Gamma(T_{\rm gas}, ...) = n_{\rm H}^2\Lambda(T_{\rm gas}, ...)$

Heating functions	Cooling functions
Photoelectric heating H_2 deexcit. & FUV pumping H_2 formation heating Cosmic-ray heating Carbon photoionization heating Exothermic chemical reactions Dust heating Turbulent heating	Line emission: e.g. [CII], [CI], [OI], CO Dust-gas collisions



Wolfire et al. (2022)

Photoelectric heating



UV photon releases a high energy electron

- Assumption 1: specific spectral shape for the UV field
- Assumption 2: standard MRN grain size distribution.
- Depends on the charge of the grain.
- Expression should be used generally for low intensities of radiation fields.
- $\Gamma_{\rm PE}$ is not known until thermal balance convergence.

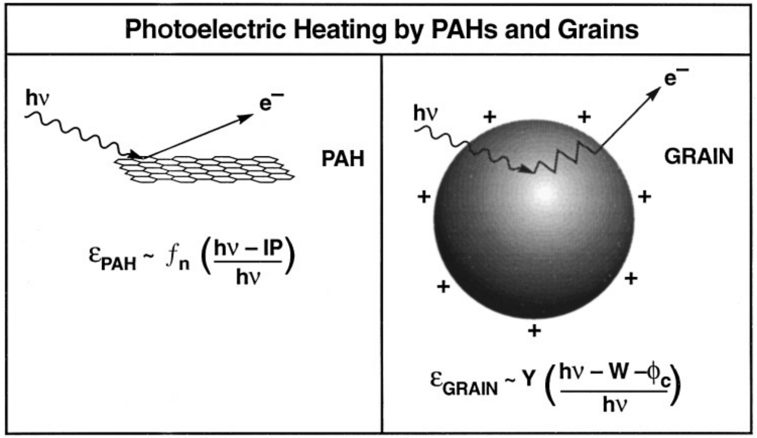
- Dominant heating mechanism near the PDR surface.
- Photoelectric ejection of electrons from small dust grains and polycyclic aromatic hydrocarbons (PAHs).
- At high gas temperatures it is countered by cooling due to recombination of electrons with grains/PAHs.

$$\Gamma_{\rm PE} = 10^{-24}\epsilon G_0 n_{\rm H}$$

[erg cm^{-3} s^{-1}] (Bakes & Tielens 1994)

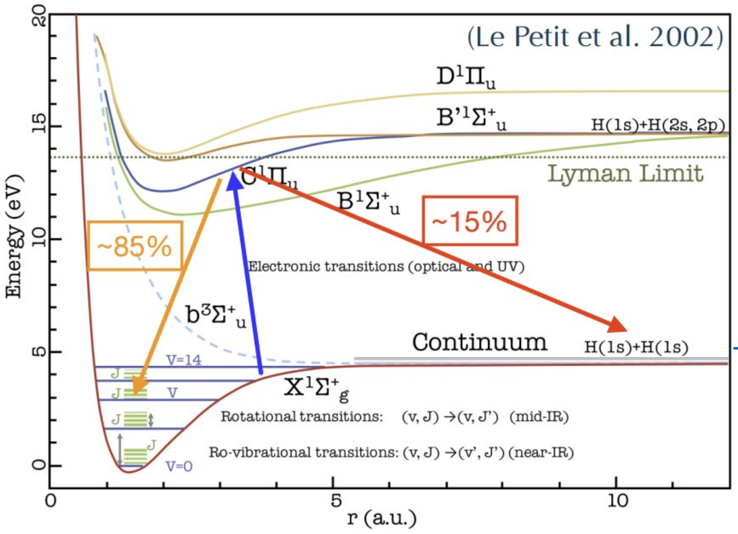
$$\epsilon = \frac{4.87\times10^{-2}}{[1+4\times10^{-3}(G_0T^{1/2}/n_{\rm e})^{0.73}]} + \frac{3.65\times10^{-2}(T/10^4)^{0.7}}{[1+2\times10^{-4}(G_0T^{1/2}/n_{\rm e})]}$$

Photoelectric heating efficiency



Tielens & Hollenbach (1999)

H2 de-excitation following FUV pumping



From E. Bron's presentation

- The collisional de-excitation of vibrationally excited H_2 following FUV pumping is important heating mechanism in dense gas near the cloud surface.

- Assumption: single excited pseudo-vibrational level of H_2, denoted as H_2^*
- Assumption is to effectively account for the full distribution of H_2 molecules in vibrationally excited levels.

$$\Gamma_{\mathrm{H}_2^*} = [n(\mathrm{H})\gamma_{*0}^{\mathrm{H}} + n(\mathrm{H}_2)\gamma_{*0}^{\mathrm{H}_2}]n(\mathrm{H}_2^*)E_*$$

[erg cm^{-3} s^{-1}] (Tielens & Hollenbach 1985)

Energy of the single excited pseudo-vibrational level (2.6eV)

$$\gamma_{*0}^{\mathrm{H}_2} = 1.4 \times 10^{-12} T^{1/2} \mathrm{e}^{-18100/(T+1200)}$$

[cm^{3} s^{-1}]

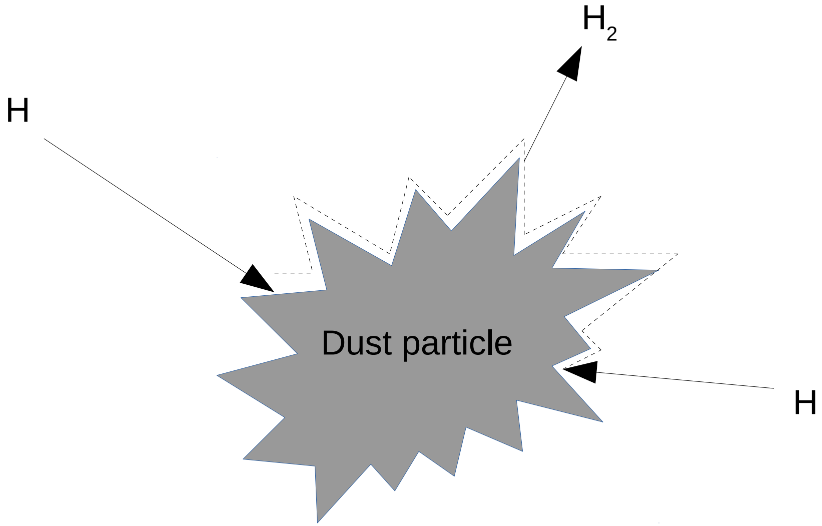
$$\gamma_{*0}^{\mathrm{H}} = 10^{-12} T^{1/2} \mathrm{e}^{-1000/T}$$

[cm^{3} s^{-1}]

Collisional de-excitation rate coefficients from the excited to the ground vibrational level

Number densities

H2 formation on dust grains



$H + H \rightarrow H_2 + h\nu$ $h\nu = 4.5 eV$

- Dust heating
- Breaks the dust-molecule bind and liberates H_2 in ISM
- Vibrational energy

$$\left(\frac{dn(\mathrm{H_2})}{dt}\right)_{\mathrm{form}} = R\, n_{\mathrm{H}}\, n(\mathrm{H})$$

Rate at which H atoms colliding with grains are turned into H_2

$$R = \frac{1}{2}\underbrace{\left(\frac{8kT}{\pi m_{\mathrm{H}}}\right)^{1/2}}_{\text{Thermal velocity}} \langle\epsilon_{\mathrm{gr}}\rangle \Sigma_{\mathrm{gr}}$$

General expression

Dust surface

Average efficiency

H_2 formation heating: $\Gamma_{\mathrm{H2,form}} = 1.5\,\mathrm{eV} \times R n_{\mathrm{H}} n(\mathrm{H})$

Energy liberated as heat during H_2 formation

For theoretical/numerical studies, *R* is usually approximated with $R = 3 \times 10^{-17}\ \mathrm{cm^3\,s^{-1}}$ based on observations (Jura 1975)

Formation of other molecules on dust grains

H atoms move fast on the dust surface

The most common reactions are with C, N, O and H_2 in **atomic clouds (rich in H)**

$$C \Rightarrow CH_4: \quad \text{methane}$$
$$N \Rightarrow NH_3: \quad \text{ammonia}$$
$$O \Rightarrow H_2O: \quad \text{water}$$

In atomic clouds, the above molecules as well as CO that comes from the gas phase, create icy mantles around the dust.

In clouds poor in H, there are more complex molecules formed:

$$O + H \Rightarrow OH \xrightarrow{+C} COH \xrightarrow{+3H} CH_3OH: \ \text{methanol}$$
$$CH + H \Rightarrow CH_2 \xrightarrow{+O} H_2CO: \ \text{formaldehyde}$$
$$C + H \Rightarrow CH \xrightarrow{+COH+4H} CH_3CH_2OH: \ \text{ethanol}$$

In clouds with no H, the icy mantles consist of C, N, O which form O_2, CO and maybe NO.

Other heating mechanisms

Photoionization of neutral carbon

Photoionization of neutral carbon liberates about 1 eV per photoelectron (Black 1987)

Cosmic-ray heating

Deeper within the cloud, cosmic-rays do most of the heating of the gas.

$$\Gamma_{\rm CR} = 1.5 \times 10^{-11} \zeta n(\mathrm{H_2})$$

Cosmic-ray ionization rate [*s^{-1}*]
Average MW value **10^{-16} s^{-1}**

Exothermic reactions (chemical heating)

Exothermic reactions that are due to recombinations of HCO^+, H_3^+, H_3O^+ and ion-neutral reactions of $He^+ + H_2$ become important when the cosmic-ray ionization rate increases.

Turbulence heating

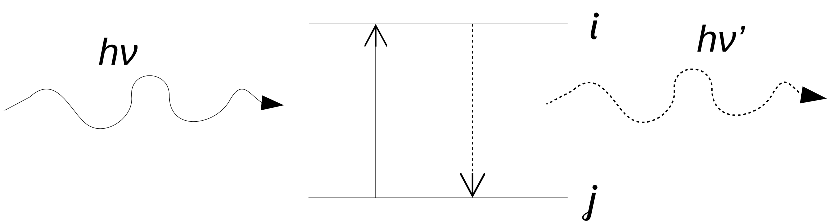
Also, deep in the cloud gas is heated due to dissipation of supersonic turbulence

$$\Gamma_{\rm TURB} = 3.5 \times 10^{-28} v_{\rm TURB}^3 / l_{\rm TURB} n_{\rm H}$$

Turbulent scale length [*pc*]
Typical value **5 pc**

Turbulent velocity [*km/s*]
Typical values **1-2 km/s**

Cooling mechanisms: Line emission



Statistical equilibrium:

$$\overbrace{n_i(p)\sum_{j\neq i} R_{ij}(p)}^{\text{Emission}} = \overbrace{\sum_{j\neq i} n_j(p) R_{ji}(p)}^{\text{Absorption}}$$

Population densities of levels *i*, *j*

$$R_{ij}(p) = \begin{cases} A_{ij} + B_{ij}\langle J_{ij}(p)\rangle + C_{ij}(p), & i > j \\ B_{ij}\langle J_{ij}(p)\rangle + C_{ij}(p), & i < j \end{cases}$$

A_{ij} and B_{ij} are the Einstein coefficients, C_{ij} is the collisional rate for excitation (i<j) and de-excitation (j>i) and $\langle J_{ij}(p)\rangle$ is the mean integrated intensity received at *p* from all solid angles dΩ.

The **escape probability approach** is all about calculating $\langle J_{ij}(p)\rangle$. This approach approximates <J> as

$$\langle J_{ij}(p)\rangle = [1 - \beta_{ij}(p)]S_{ij}(p) + \beta_{ij}(p)\mathcal{B}(\nu_{ij}).$$

(Sobolev 1960; Castor 1970; de Jong et al. 1975; Poelman & Spaans 2005)

Cooling mechanisms: Line emission

$$S_{ij}(p) = \frac{2h\nu_{ij}^3}{c^2}\frac{n_i(p)g_j}{n_j(p)g_i - n_i(p)g_j}$$

Source function due to transitions between levels *i* and *j*
ν_{ij} is the photon frequency
g_i, g_j are the statistical weights of n_i and n_j

$$\langle J_{ij}(p)\rangle = [1-\beta_{ij}(p)]S_{ij}(p) + \beta_{ij}(p)\mathcal{B}(\nu_{ij}).$$

$B(\nu_{ij})$ is the total background radiation valid at FIR and submm wavelengths, including CMBR blackbody emission at 2.7K and dust emission approximated as a modified blackbody at T_{dust}.

$$\beta_{ij} = \int_0^{4\pi}\frac{\mathrm{d}\Omega}{4\pi}\left[\frac{1-\mathrm{e}^{-\tau_\mathrm{L}}}{\tau_\mathrm{L}}\right]$$

Escape probability: describes the probability that a photon of frequency ν_{ij} escapes from the element *p* **without interacting** with the rest of the cloud.

The emissivity will then be given by $j_{\mathrm{emis}} = A_{ij}h\nu_{ij}n_i\beta_{ij}\frac{S_{ij}-\mathcal{B}_{ij}}{S_{ij}}$ [erg cm^{-3} s^{-1}]. This will be plotted with 3D-PDR.

Example: two-level atom

In some cases, such as the one of CO, we can adopt the two-level approximation to understand better the line emission of the coolant. In this example we will consider that all electrons are in *only two* states: the ground one (denoted as 0) and the excited one (denoted as 1).

Another assumption for this example, is that CO is excited through collisions and de-excited through collisions and photon emission. We also denote with n_c the number density of the colliding partner (e.g. electrons).

The equation describing the population density at the excited level is

$$\frac{dn_1}{dt} = n_c n_0 q_{01} - n_c n_1 q_{10} - n_1 A_{10}$$

where q_{01} and q_{10} are the rates at which the electrons change state through collisions and A_{10} is the Einstein coefficient.

We assume that the cloud is static, so $dn_1/dt = 0$. Therefore, the above equation takes the form:

$$\boxed{\frac{n_1}{n_0} = \frac{n_c q_{01}}{n_c q_{10} + A_{10}}}$$

In the above, the q rates are related through $q_{01} = \frac{g_1}{g_0} q_{10} e^{-E_{10}/k_B T_{\rm gas}}$ where E_{10} is the energy that is emitted in the form of electromagnetic radiation of the J=1-0 transition.

Radiative transfer equation

The radiative transfer equation for radiation of frequency ν along dz (line-of-sight), is given by:

$$\frac{dI_\nu}{dz} = -\alpha_\nu I_\nu + \alpha_\nu S_\nu$$

where α_ν is the absorption coefficient and S_ν is the source function. For the transition $i \rightarrow j$, α_ν and S_ν are given by:

$$\begin{aligned} S_\nu &= \frac{2h\nu_0^3}{c^2}\frac{n_i g_j}{n_j g_i - n_i g_j} \\ \alpha_\nu &= \frac{c^2 n_i A_{ij}}{8\pi\nu_0^2}\left(\frac{n_j g_i}{n_i g_j} - 1\right)\phi_\nu \end{aligned}$$

ν_0 is the frequency at line center

φ_0 is the line profile

For a Maxwellian distribution, the line profile is given by:

$$\phi_\nu = \frac{1}{\sqrt{2\pi\sigma_\nu^2}}\boxed{\exp\left\{-\frac{[(1+v_{\rm los}/c)\nu - \nu_0]^2}{2\sigma_\nu^2}\right\}}$$

This term is 0 for a stationary cloud

where $v_{\rm los}$ is the gas velocity along the line of sight (positive for red-shifted, negative for blue-shifted) and

$$\sigma_\nu = \frac{\nu_0}{c}\sqrt{\frac{k_{\rm B}T_{\rm gas}}{m_{\rm mol}} + \frac{v_{\rm turb}^2}{2}}$$

Velocity dispersion due to thermal and turbulent components

$m_{\rm mol}$ is the molecular mass of the coolant.

Radiative transfer equation

So the expression $\frac{dI_\nu}{dz} = -\alpha_\nu I_\nu + \alpha_\nu S_\nu$ takes the form:

$$\boxed{I_\nu(z) = I_\nu(0)e^{\tau_\nu(z)} + \int_0^{\tau_\nu(z)} S_\nu e^{\tau'_\nu - \tau_\nu(z)} d\tau'_\nu \, [\mathrm{erg\,cm^{-2}}]}$$

After solving it, we can determine the brightness (or antenna) temperature. The latter is given by:

$$T_\mathrm{A} = \frac{c^2 I_\nu}{2k_\mathrm{B}\nu^2} \, [\mathrm{K}]$$

This is the general expression for the brightness temperature at frequency *ν*. Integrating this in all velocity channels, we obtain the **velocity integrated emission** measured in [K km/s]:

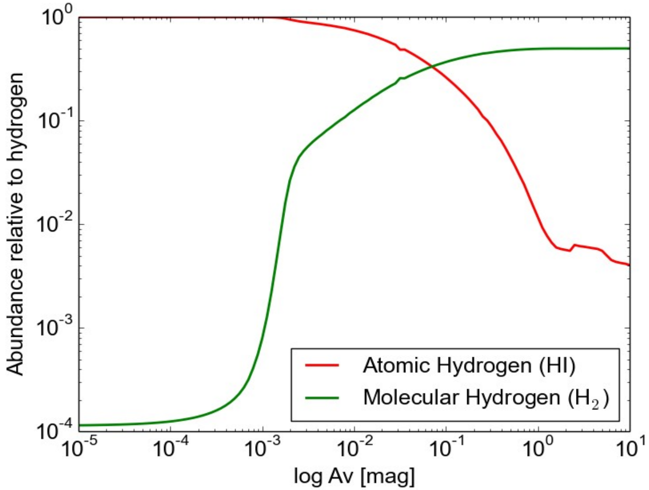
$$W = \int T_\mathrm{A} dv_\mathrm{los} \, [\mathrm{K\,km\,s^{-1}}]$$

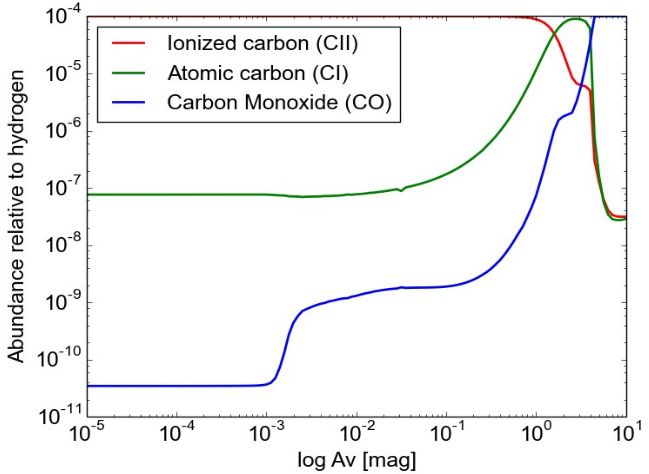
This is the emission captured by radio-telescopes. Therefore, making velocity integrated emission maps from our simulations allows us to have a ***direct*** comparison with observations.

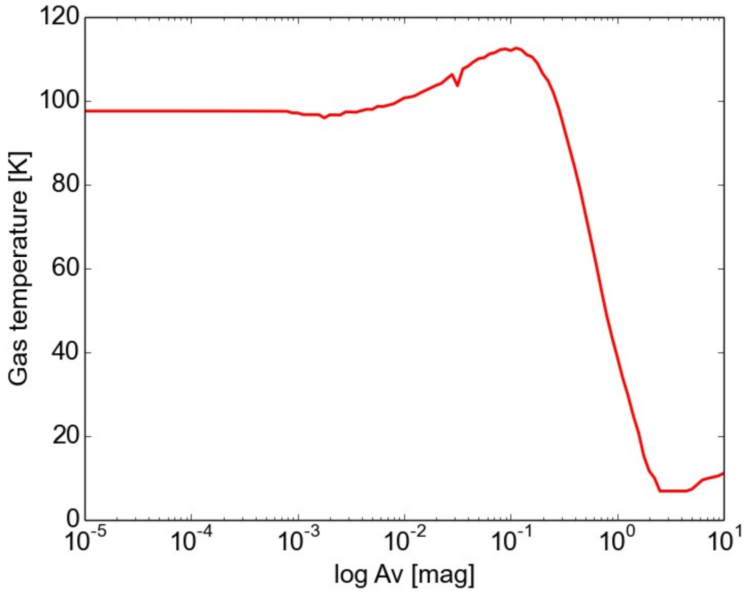
A quick and very easy script to use for RT, is **RADEX**, which can be used online:
http://var.sron.nl/radex/radex.php

Results from simulations

One-dimensional PDR simulations







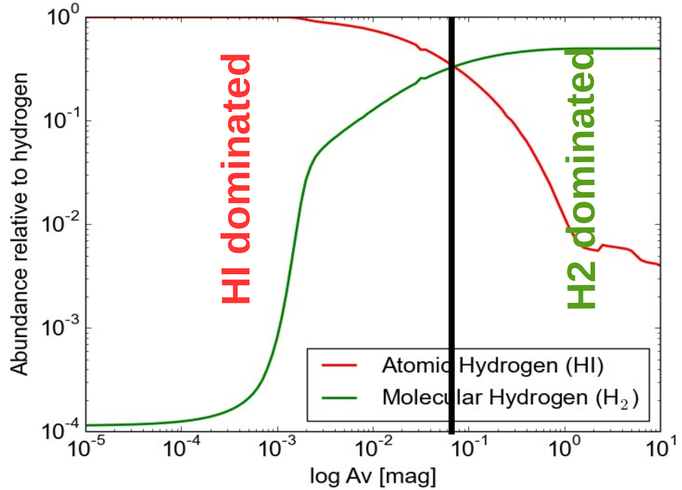
Density: n=10^3 cm^{-3}

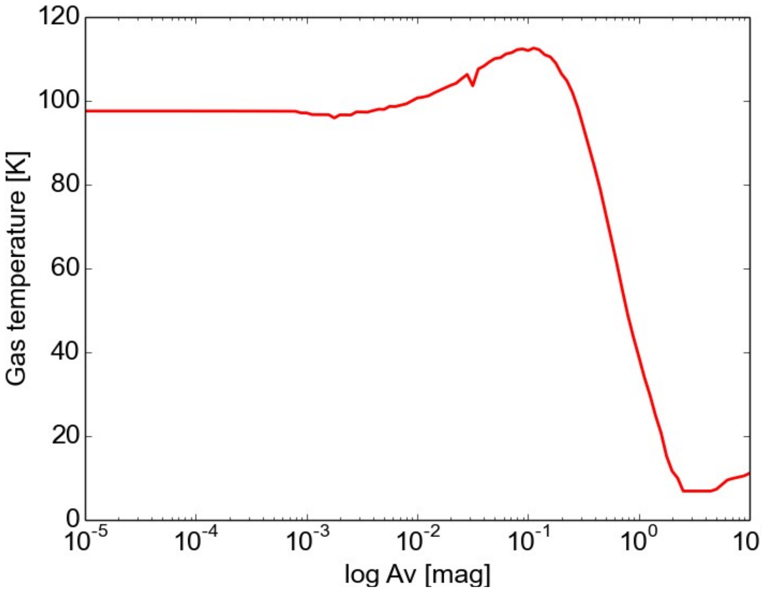
Radiation field: χ/χ_0=10 (Draine)

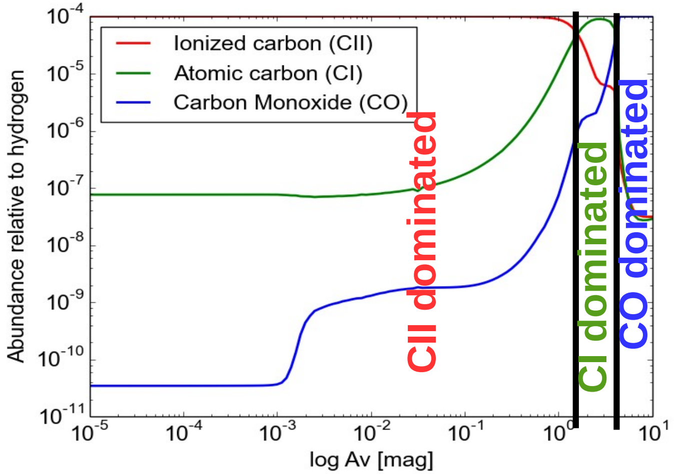
Cosmic-ray ζ_{CR}=10^{-17} s^{-1}

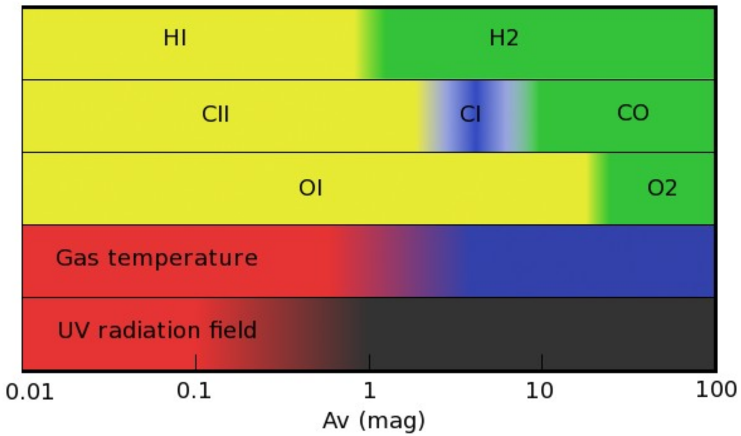
Metallicity = 1 Z_O (solar)

One-dimensional PDR simulations

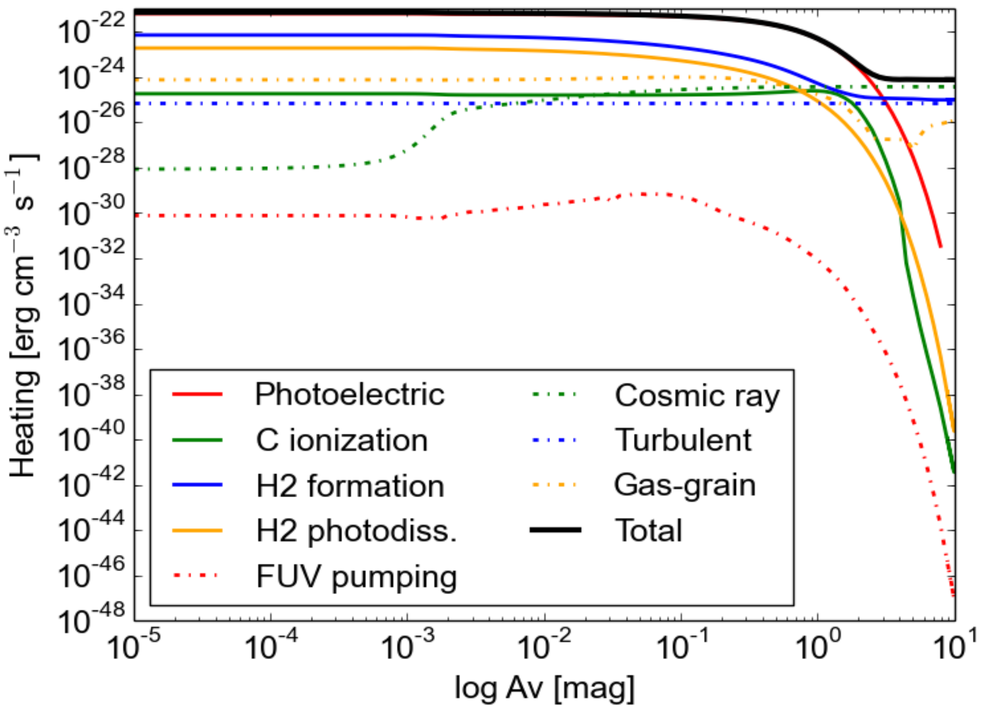




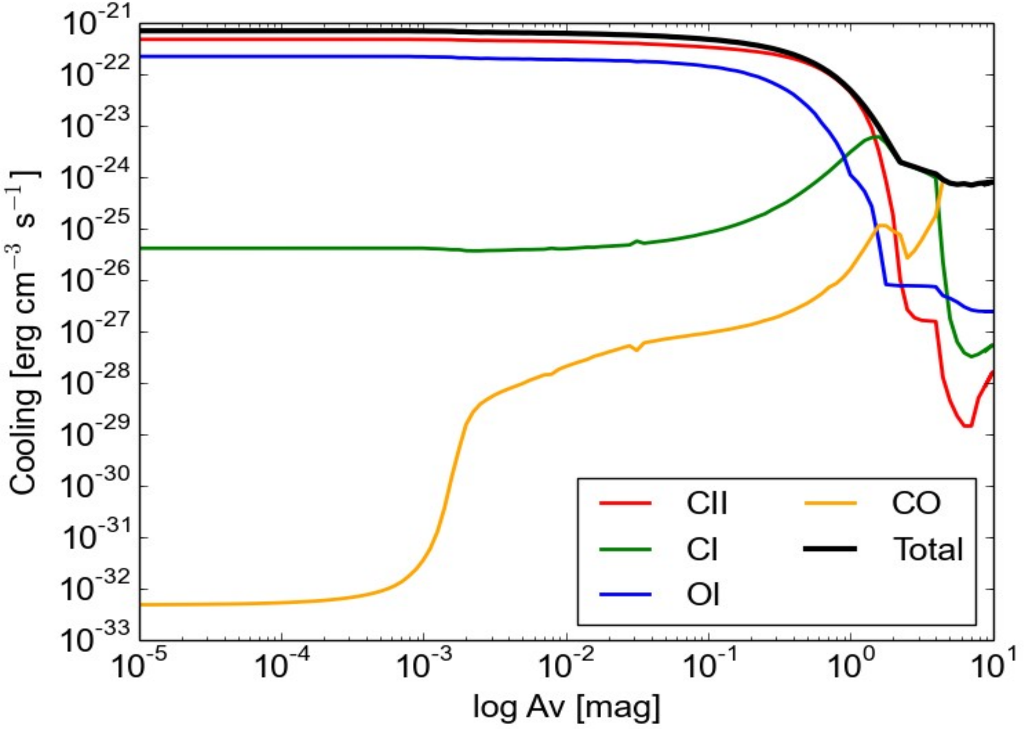




One-dimensional PDR simulations



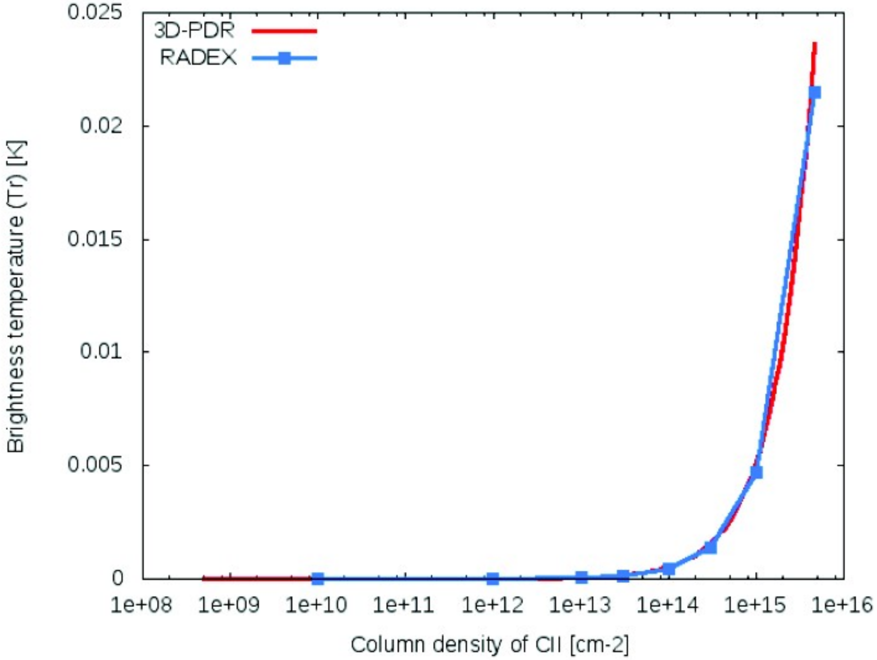
Heating functions



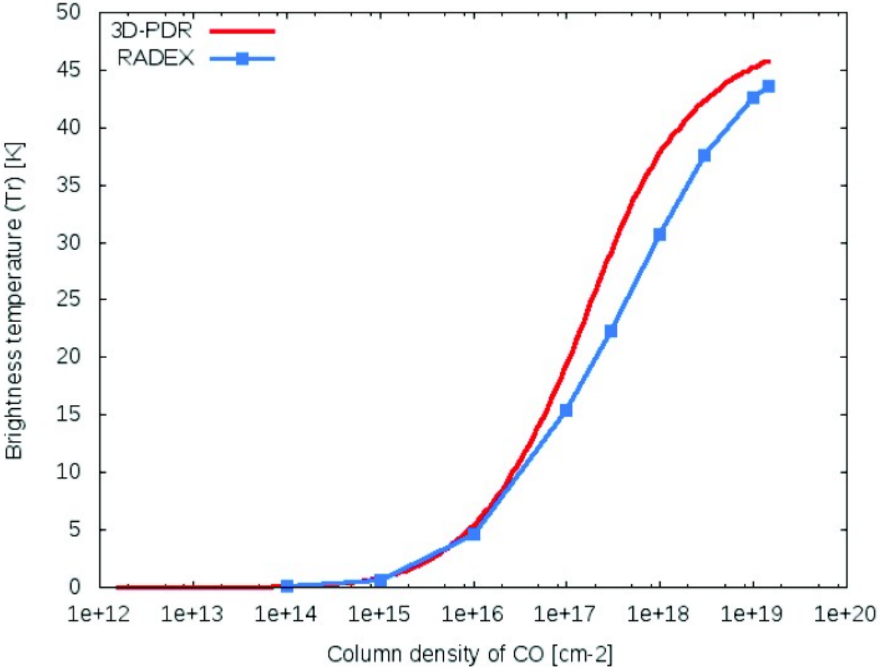
Cooling functions

Radiative transfer

[CII] is generally optically thin

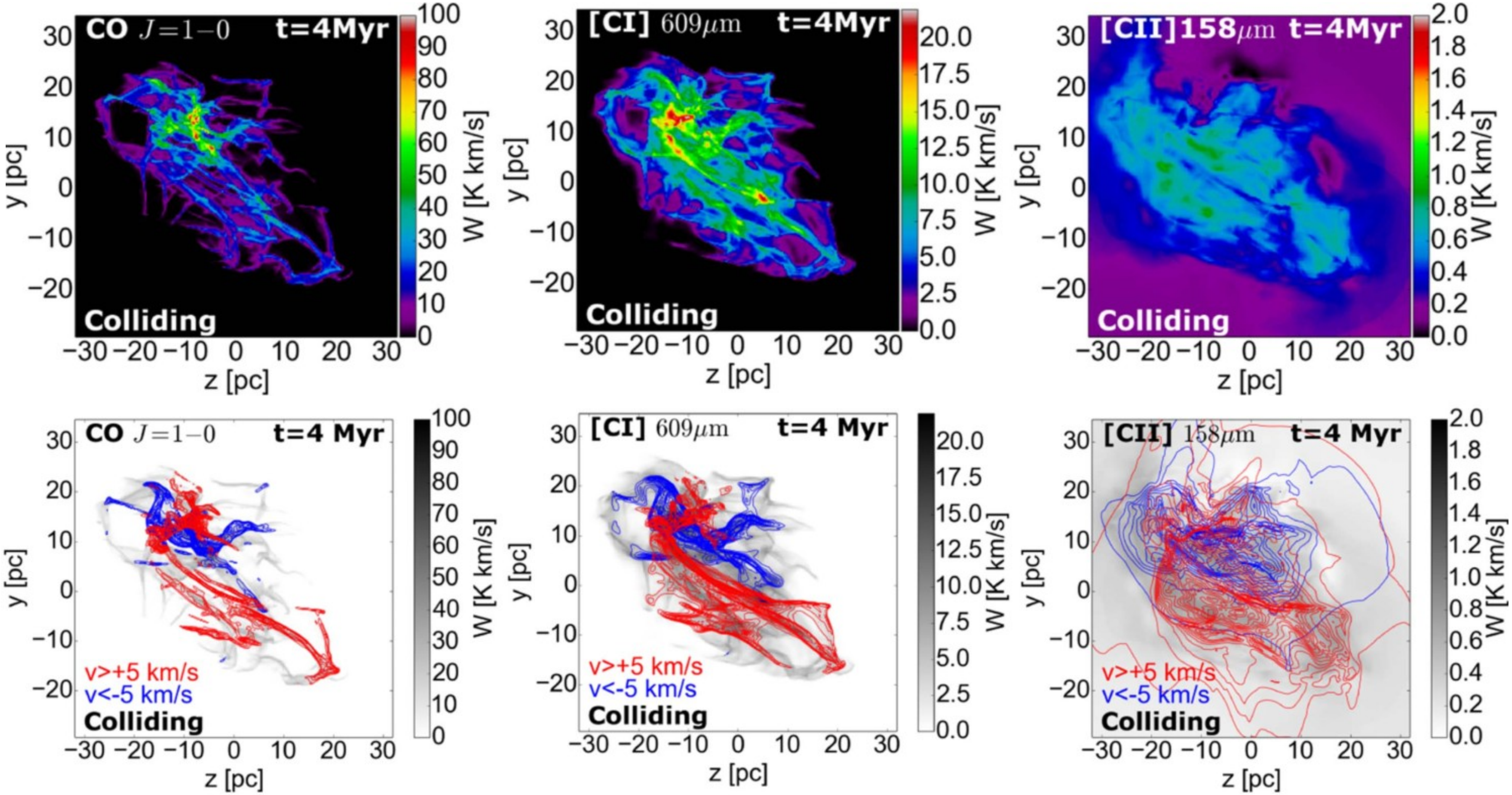


CO is generally optically thick



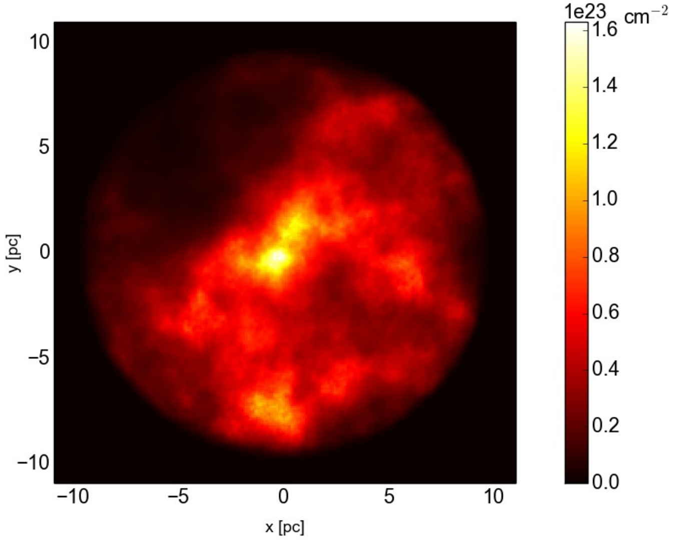
Three-dimensional PDRs (from Bisbas+ 2017a)

Radiative transfer calculations of a cloud-cloud collision event

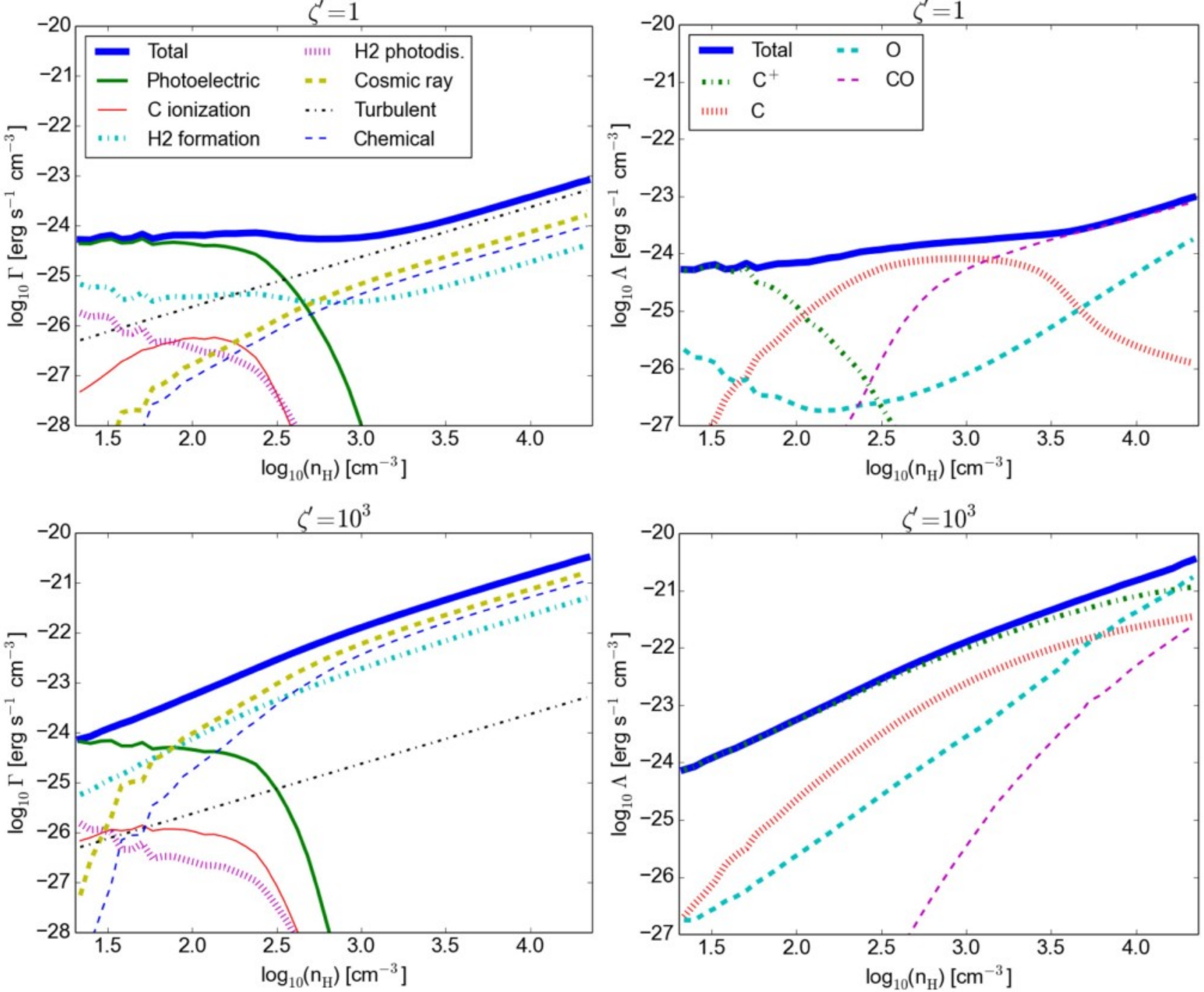


Three-dimensional simulations (from Bisbas+ 2017b)

In a 3D cloud, we increased the cosmic-ray ionization rate by 1000 times and compared the heating and cooling functions



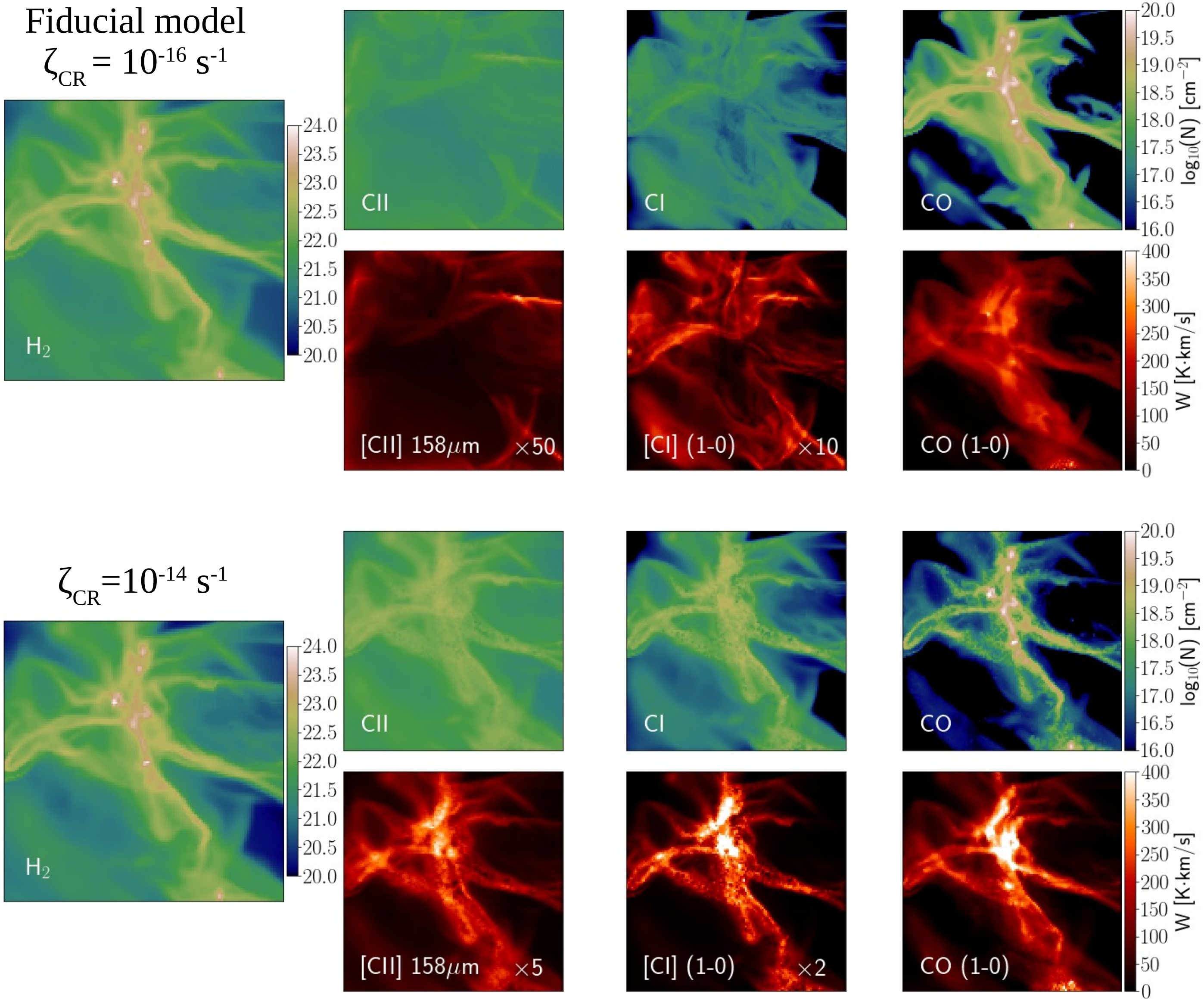
Heating functions **Cooling functions**



Effect of cosmic-rays

Bisbas et al. (2021)

- $N(H_2)$ remains nearly unchanged
- N(CII) and N(CI) are increased due to destruction of CO by cosmic-rays
- W(CII) and W(CI) are rapidly increased and they trace H_2 gas
- W(CO) decreases in the outer parts but increases at high column densities


Fiducial model

$\zeta_{CR} = 10^{-16}\ s^{-1}$

$\zeta_{CR}=10^{-14}\ s^{-1}$

Why do we need numerical astrochemistry?

Hydrodynamics

Astrochemistry

Observations

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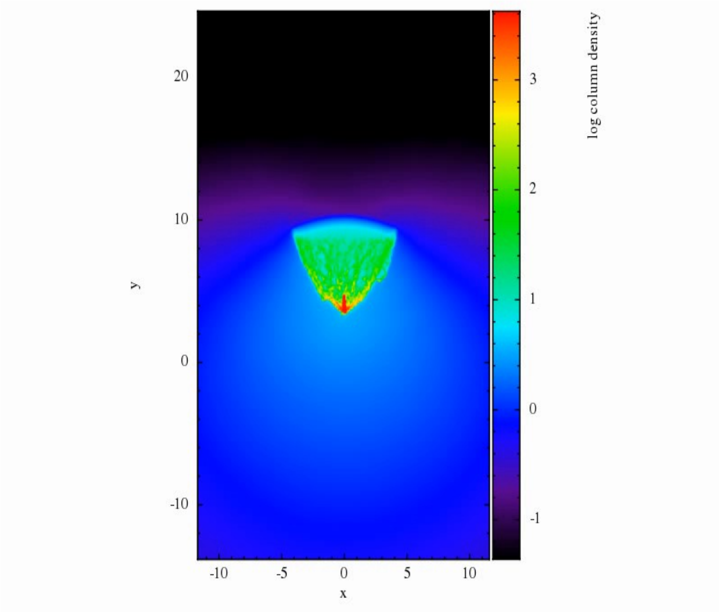
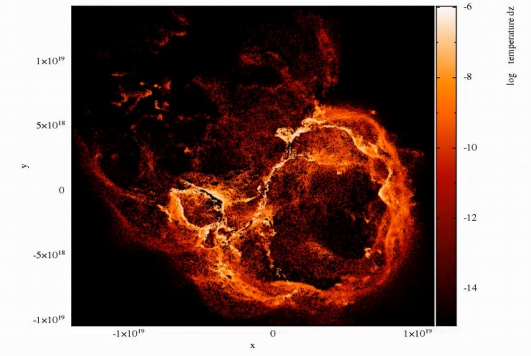
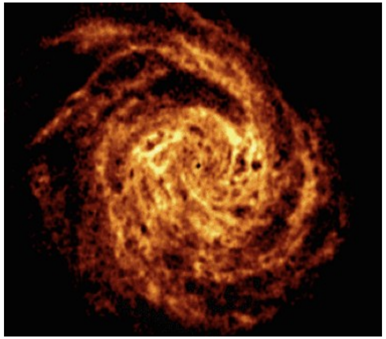
Hydrodynamics

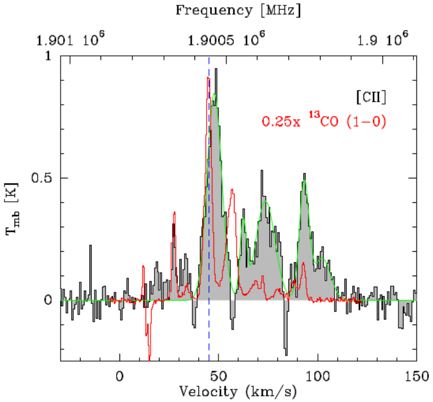
Astrochemistry

Observations

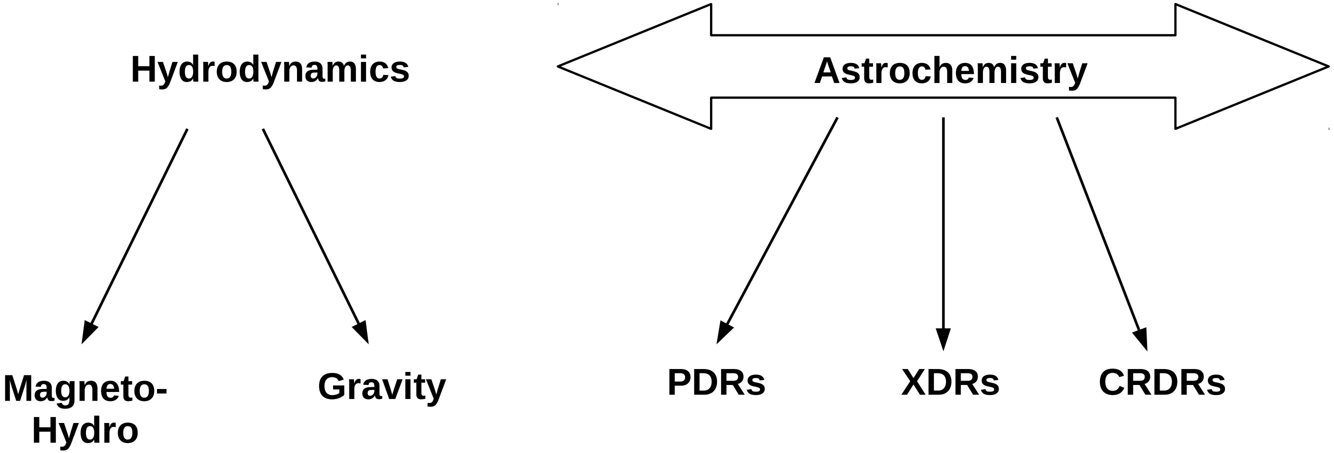








Why do we need numerical astrochemistry?



Hydrodynamics

Astrochemistry

Observations

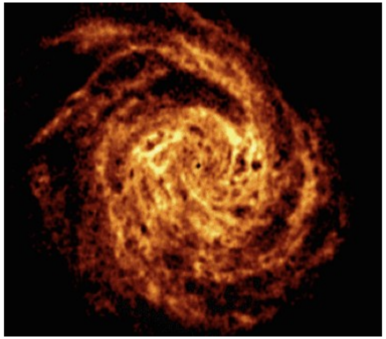
Magneto-Hydro

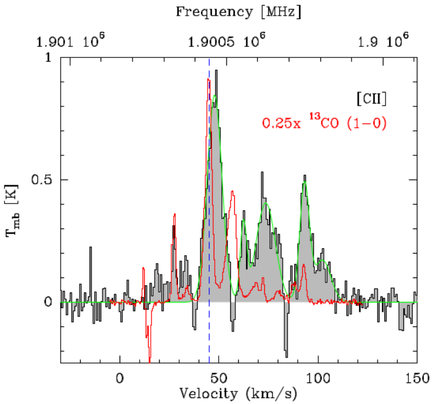
Gravity

PDRs

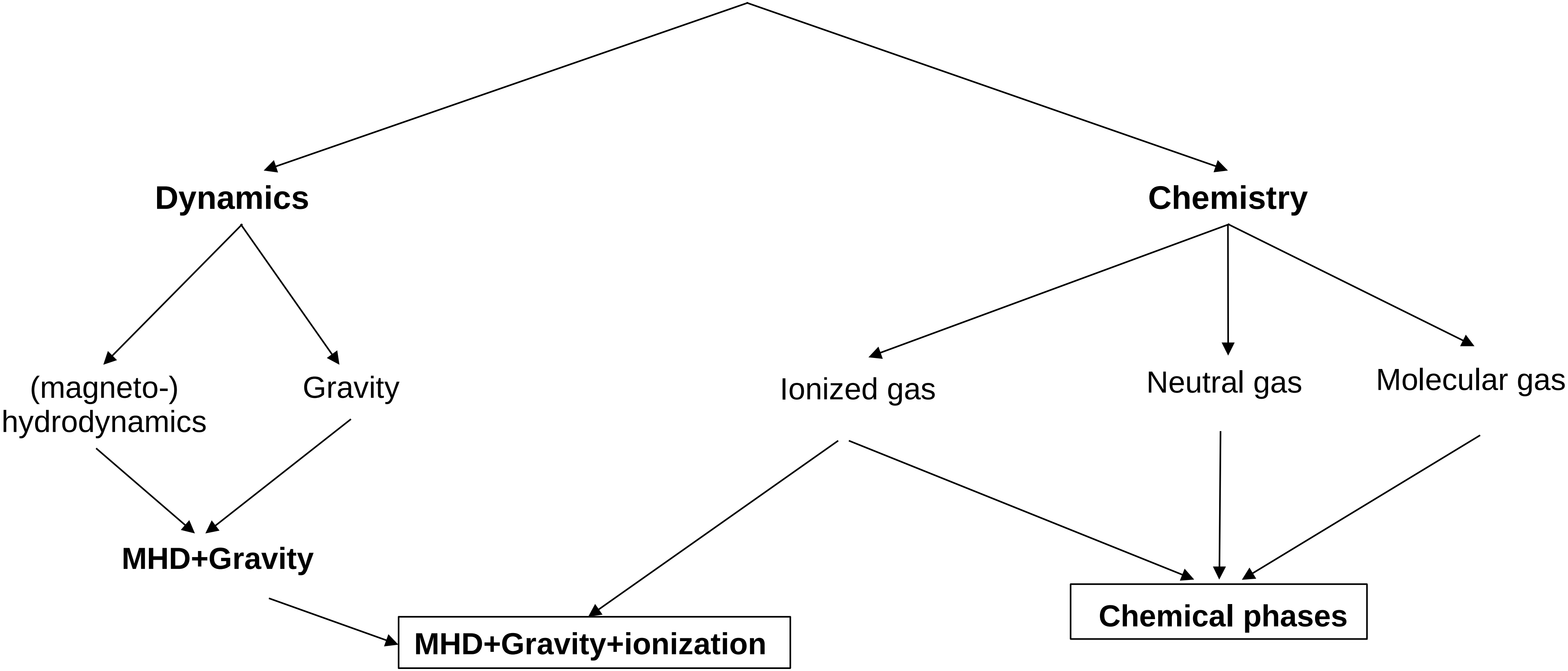
XDRs

CRDRs





Simulating the interstellar medium



Dynamics

Chemistry

(magneto-)
hydrodynamics

Gravity

Ionized gas

Neutral gas

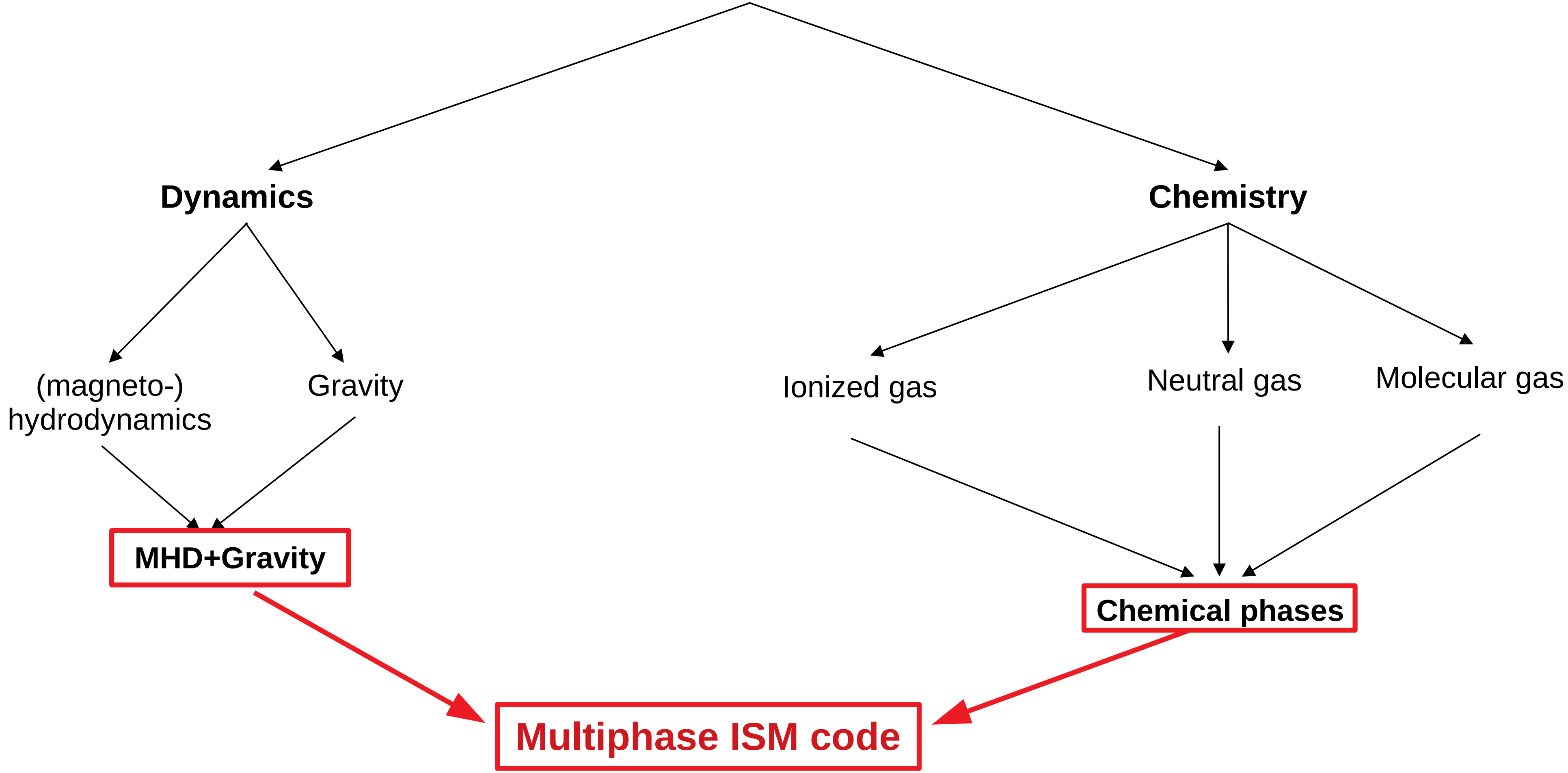
Molecular gas

MHD+Gravity

MHD+Gravity+ionization

Chemical phases

Simulating the interstellar medium



Dynamics

(magneto-)
hydrodynamics

Gravity

MHD+Gravity

Chemistry

Ionized gas

Neutral gas

Molecular gas

Chemical phases

Multiphase ISM code

Take home messages

1. Astrochemistry is the bridge connecting (magneto-)hydrodynamical simulations with observations

2. Photodissociation regions are the regions where the gas transitions from its atomic to molecular phase. Studying PDRs help understand the emission lines captured from radiotelescopes.

3. Several heating and cooling processes occur and many hundreds of chemical reactions, on top of radiative transfer equations need to be considered to obtain good models to understand the ISM. Numerical astrochemistry is, thus, difficult.

3. Molecular gas is traced using (usually) CO. Alternative tracers, such as CI, are now more frequently used with great success. Measuring molecular gas across cosmic time is of fundamental importance for studying the cosmic star formation history.