

Physics and Chemistry of the Interstellar Medium



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OUTLINE of the LECTURE

1) Interstellar physics

ISM components
Heating and cooling
ISM 'phases' ...

2) Atomic/Molecular excitation & radiative transfer

The equation of radiative transfer
Approximations and models ...

3) Interstellar chemistry

Molecules in the ISM
Basic 'intro' to gas-phase chemistry
Public models...



Bibliography on Interstellar Medium (and credits to several slides)

- * “Physical Processes in the Interstellar Medium”

L. Spitzer, Jr., *New York: Wiley*, 1978.

- * “Interstellar Chemistry”

W.W. Duley and D.A. Williams, *Academic Press*, 1984.

- * “The Physics and Chemistry of the ISM” and “Molecular Astrophysics”

A.G.G.M. Tielens, *Cambridge University Press*, 2005 and 2021

- * “Physics of the Interstellar and Intergalactic Medium”

B. Draine, *Princeton University Press*, 2011.

- * “Master in Astrochemistry”

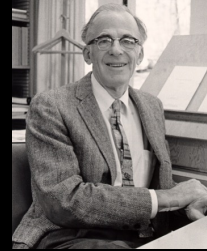
E. Van Dishoeck, 2010, Notes University of Leiden.



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Orion in the visible



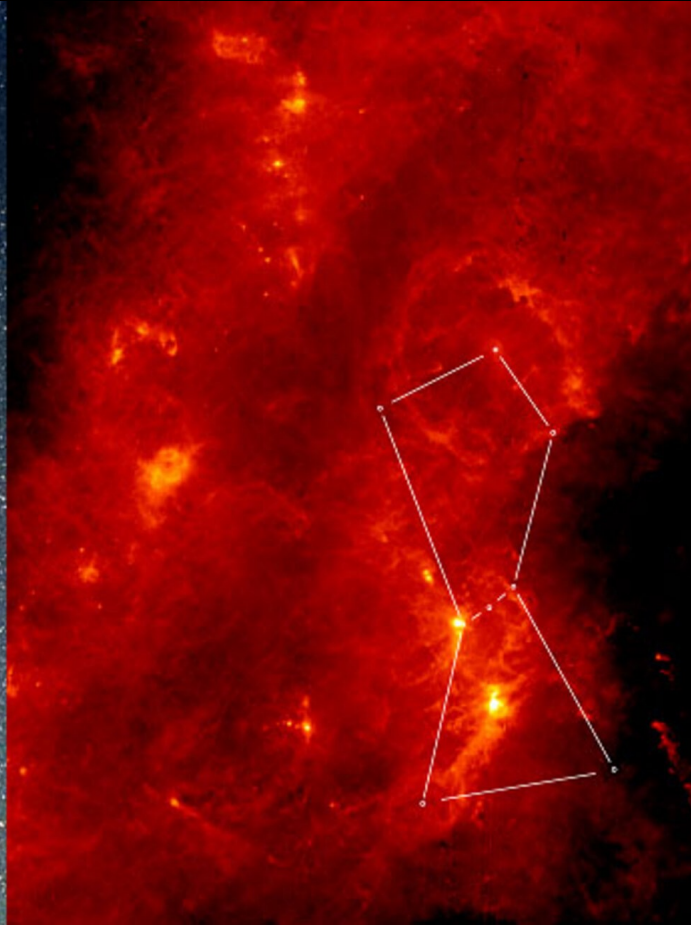
**Hot stars and
ionized gas (nebular)**

Orion in the visible



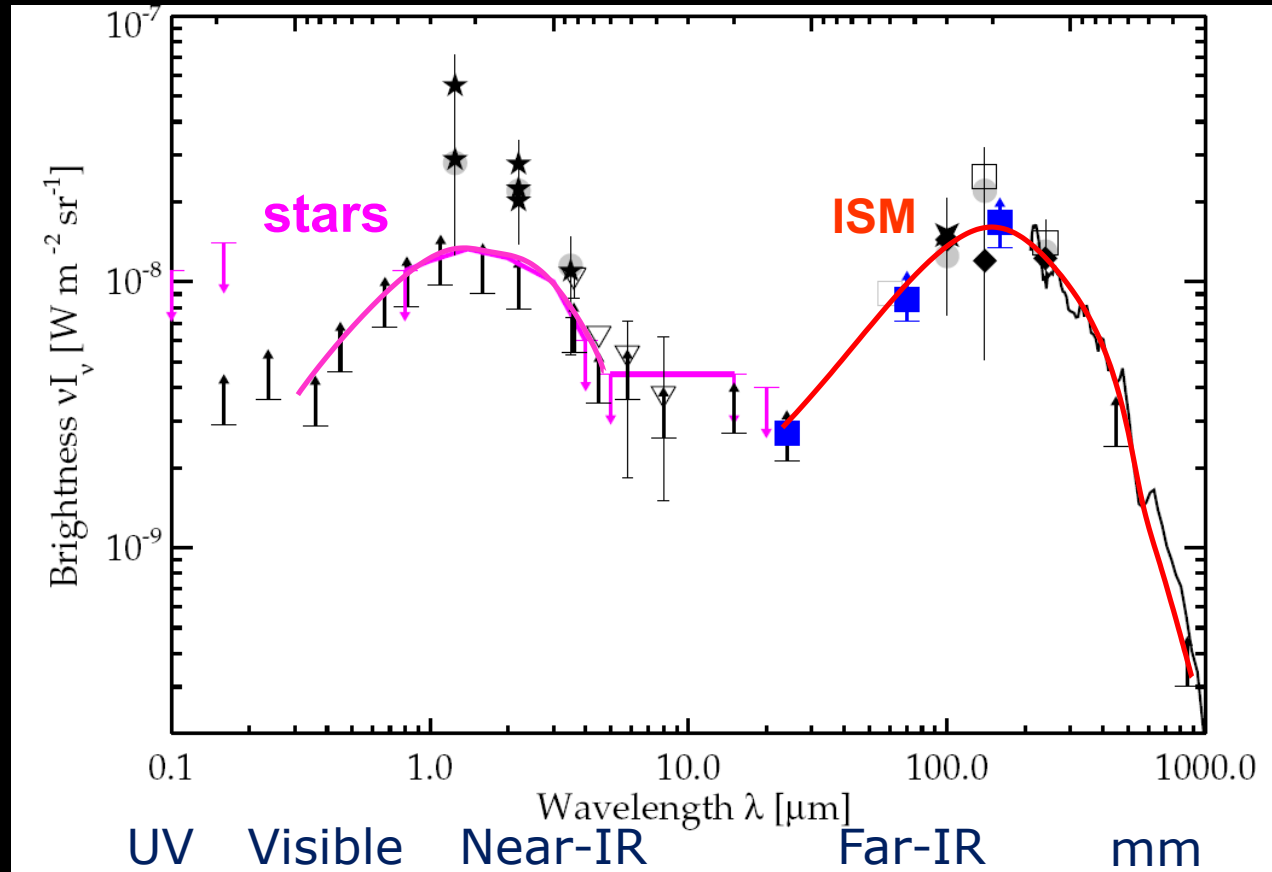
**Hot stars and
ionized gas (nebular)**

Far-IR dust emission



Cold ISM clouds

Half of the luminosity by the Universe is ISM dust (re)emission in the far-IR & submm



Starlight → ISM dust absorption

→ UV-heated dust re-emission



I. Interstellar Physics

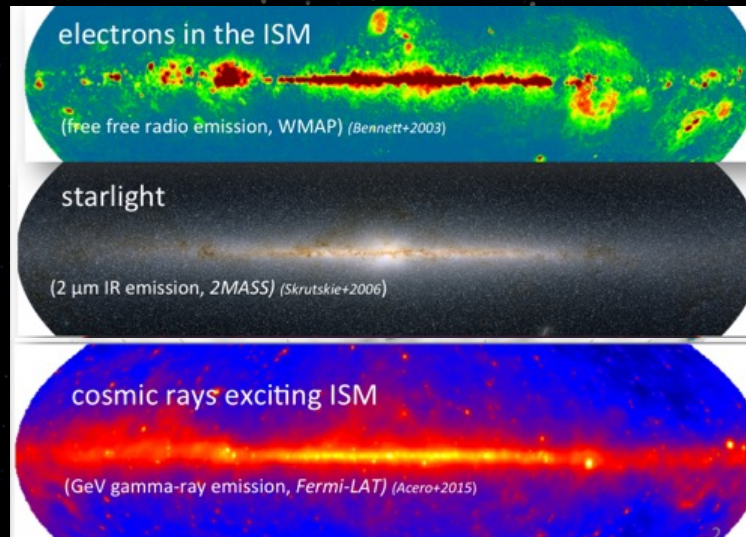


Galaxies are nearly empty ...

- Stars are separated by ≈ 2 pc (≈ 6.5 lyr)

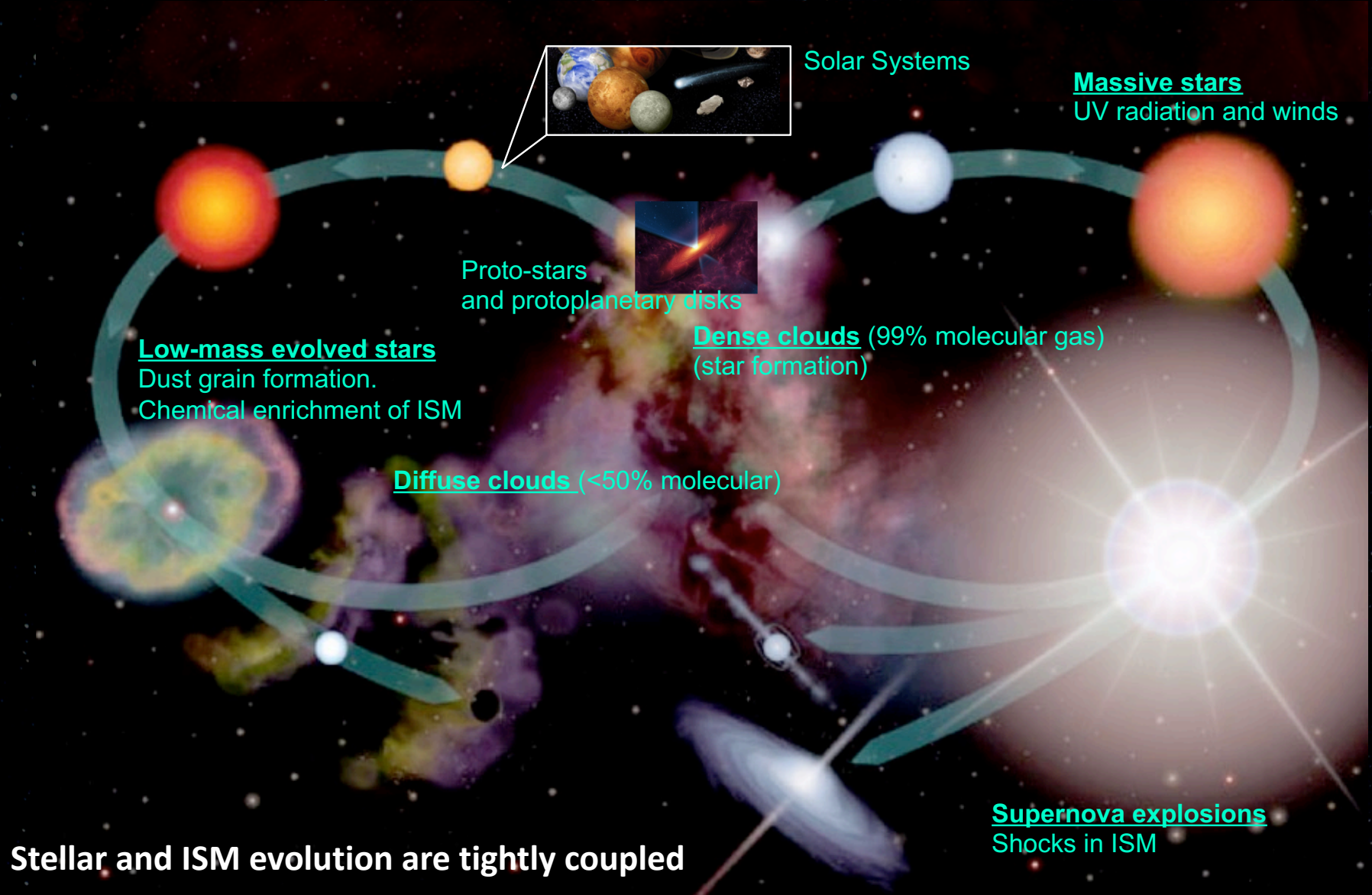
Interstellar Medium: *everything* between stars (matter, radiation, magnetic field ...)

- **Gas:** atoms, molecules, electrons, ...
- **Dust:** small solid grains, $\approx 0.1 \mu\text{m}$ in size, $\sim 1\%$ in mass wrt gas
- **Cosmic rays (particles):** energetic protons, nuclei, and e^- (1 MeV to 10^{20} eV ... ISM \sim GeV)
- **Radiation:** radio (plasmas), CMB (2.7 K), Far-IR to mm (dust thermal emission),
VISIBLE and UV (starlight), X-rays (hot gas in shocks), γ -rays ...



The ISM of the Milky Way as seen in **radio**, **IR**, and **γ -rays**

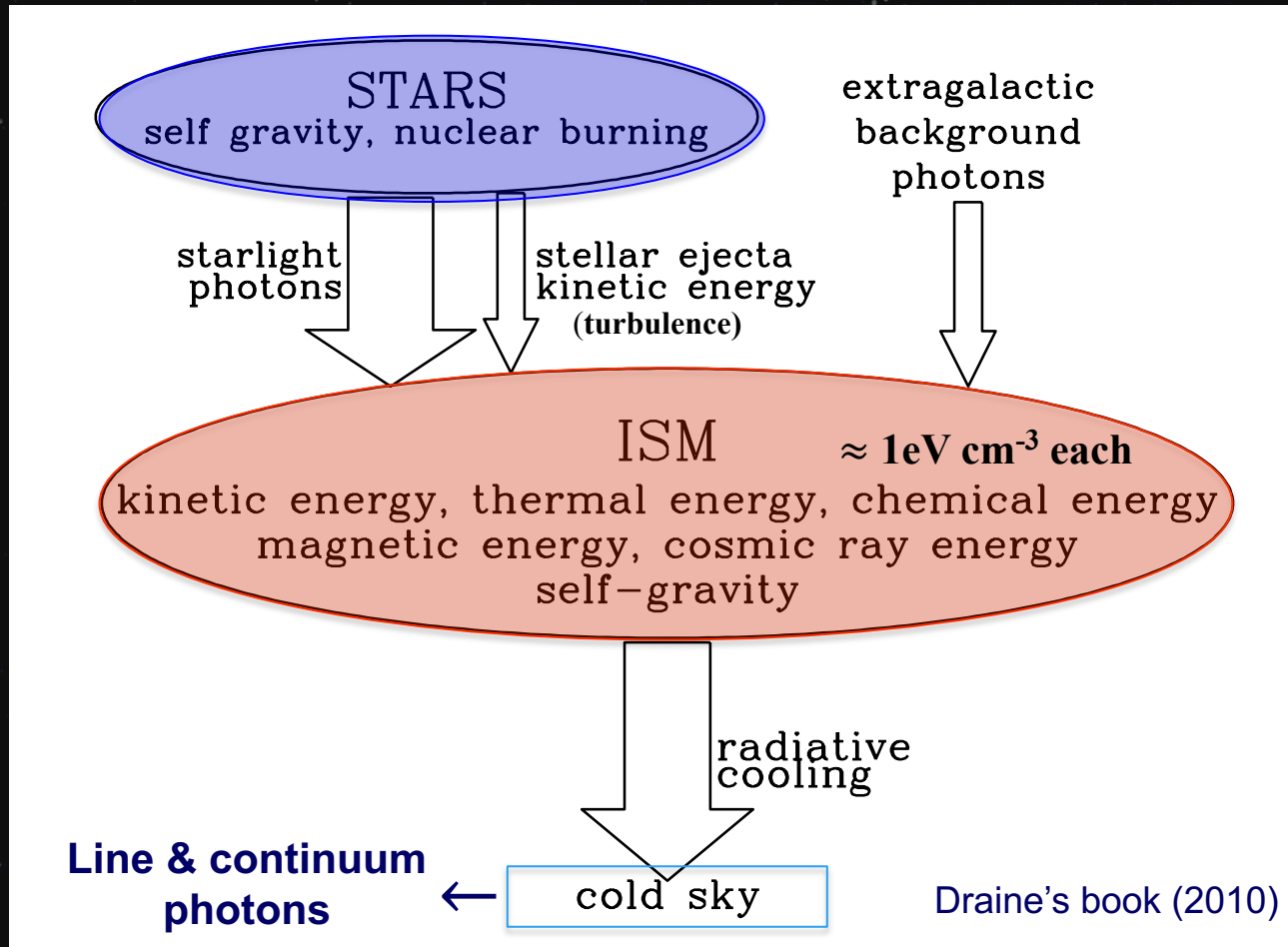
- As galaxies evolve, the ISM is slowly converted into new stars → **fuel for star formation**
- As stars die they return matter to the ISM → **chemical enrichment**
- 90 % of the baryons in the Milky Way are in stars ($\approx 5 \cdot 10^{10} M_{\text{Sun}}$) and **10% is in the ISM** ($\approx 7 \cdot 10^9 M_{\text{Sun}}$)



- **Stellar and ISM are tightly coupled** ← Stellar **UV**, **CRs** and **shocks** (*e.g.* winds and SNe) **heat** the ISM
- Most of the interstellar gas has temperatures and pressures *close* to be organized in “**phases**”:
 - 1) **Cold Neutral Medium (CNM)**: diffuse **HI** and denser molecular (**H₂**) “**CLOUDS**”
 - 2) **Warm Neutral Medium (WNM)** + Warm Ionized Medium (**WIM**) + Hot Ionized Medium (**HIM**)
→ “**INTERCLOUD**” component
- These “phases” depend on how the gas is heated & cooled → **Microphysical processes !**
- Chemical composition **determines** how the gas is cooled → **Chemistry and spectroscopy!**

SUMMARY: Much of the **ISM research** deals with understanding the (macro) **astrophysical processes** and also the **detailed microprocesses** that **form**, **destroy**, and **excite** atoms, molecules, and dust grains

Flow of Energy in normal Galaxies



CRUCIAL: Owing to very low gas densities and presence of UV, turbulence, and cosmic rays:

→ **ISM is NOT in equilibrium** → A single temperature DOES NOT describe all processes $T_k \neq T_{\text{ex}} \neq T_{\text{ionization}}$

→ One needs to **study** and **balance** all microprocesses using their **specific rates** and **cross-sections**:

Thermal balance, excitation & de-excitation, ionization & recombination ...

ISM “phases” in our Galaxy

H^+ (23% of mass) HI (60%) H_2 (17%)

Volume filling in the Milky Way

Phase	Density n_0^a (cm^{-3})	Temp. T^b (K)	Volume (%) ϕ_v^c (%)	M^d Mass ($10^9 M_\odot$)
Hot intercloud	0.003	10^6	~ 50.0	—
Warm neutral medium	0.5	8000	30.0	2.8
Warm ionized medium	0.1	8000	25.0	1.0
Cold neutral medium ^j	50.0	80	1.0	2.2
Molecular clouds	> 200.0	10	0.05	1.3
HII regions	$1-10^5$	10^4	—	0.05

^a Typical gas density for each phase.
^b Typical gas temperature for each phase.

~Pressure equilibrium

$$P_{\text{th}} / k = n T:$$

Field-Goldsmith-Habing+69 (CRs heating)
 Dalgarno & McRay 72 (review)
 Wolfire+95 (stellar FUV photons)

Tielens's book

The volume filling factor scales inversely with the density:

most of the **volume** is in the **hot & warm** phases, most of the **mass** is in the **cold neutral** ISM phases

→ PROPERTIES, MASSES, FILLING FACTORS... VERY UNCERTAIN NUMBERS.

→ HARD TO GET A GLOBAL PICTURE OF THE **ISM OF GALAXIES** AS A WHOLE → on-going research...

The neutral ISM

Hydrogen is atomic (HI) or molecular (H_2) but not ionized (H^+)

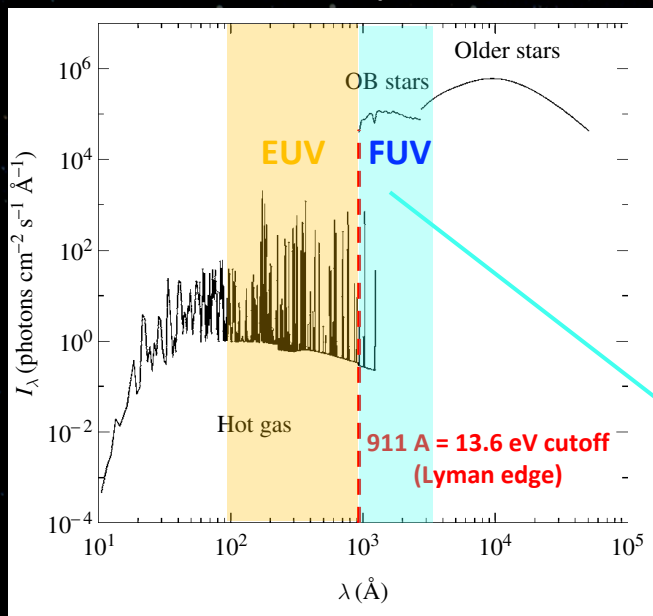


Dense molecular clouds, diffuse clouds (CNM), inter-cloud (WNM)

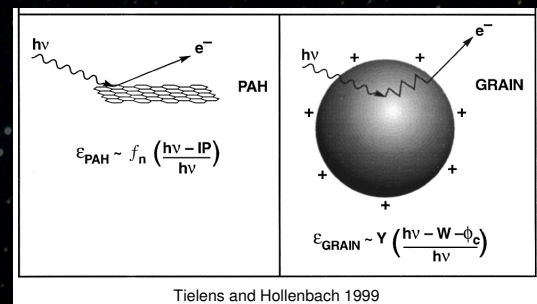
Heating of the neutral interstellar gas

- O- and B-type massive stars emit UV radiation fields:
 - **Extreme-UV (EUV)** photons with $100 \text{ eV} > h\nu > 13.6 \text{ eV}$ ionize H \rightarrow HII regions & WIM
 - Only **far-UV (FUV)** photons with $h\nu < 13.6 \text{ eV}$ propagate inside neutral HI and H₂ clouds
- IP(Hydrogen) = 13.6 eV; IP(Nitrogen) = 14.5 eV; IP(Carbon)=11.3 eV; IP(Sulfur)=10.4 eV

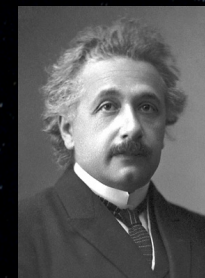
FUV photons impact dust grains and PAHs which eject energetic electrons through photo-electric effect \rightarrow 'photo-electrons' collide with atoms and molecules and **HEAT** the gas



Interstellar Radiation field



Photoelectric Heating on PAHs and Grains



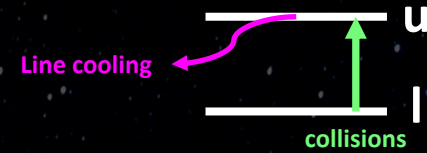
Nobel Prize
A. Einstein (1921)

$G_0 = 1$ Habing field = 10^8 FUV photons $\text{cm}^{-2} \text{s}^{-1}$

Examples: $G_0 \approx 1.7$ in solar neighborhood (mean ISRF)
 $G_0 \approx 10^{4-5}$ close to massive stars

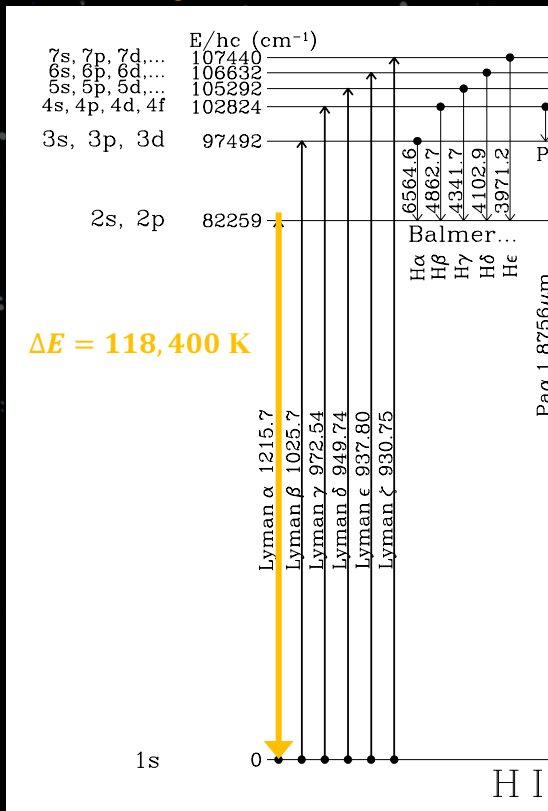
Cooling of the neutral interstellar gas

Ability of gas to cool itself sets the ISM "phases"

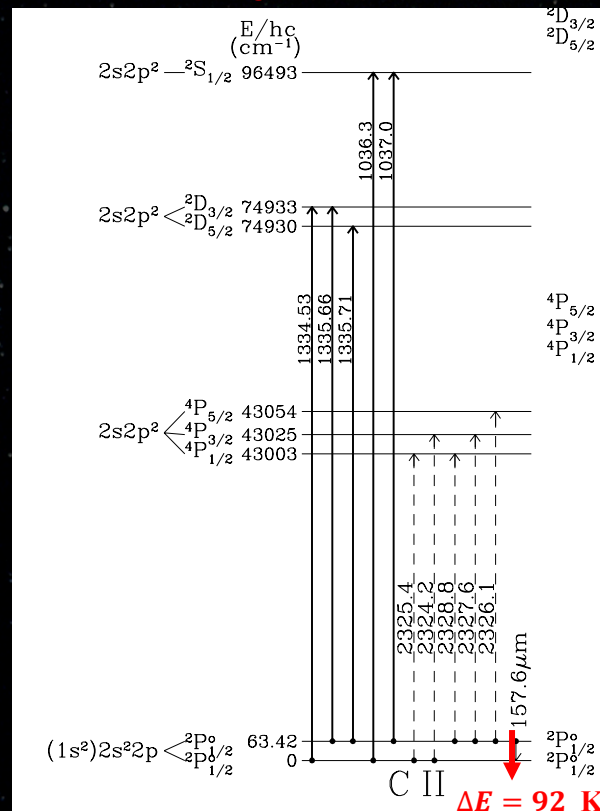


- **Collisions** of **HI atoms**, **C⁺ ions** and **CO molecules** with photo-electrons (and H₂ inside molecular clouds) EXCITE the *lowest energy* available levels (**electronic**, **fine-structure**, **rotational**)
- **Emission of a line photon** - escaping the cloud **COOLS** the gas (thermostats!).

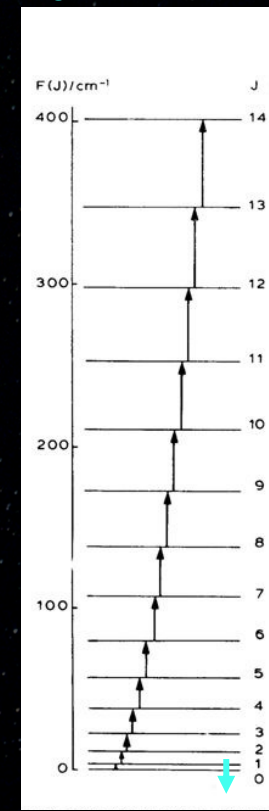
Ly α cooling (1216 Å)
of warm HI (WNM)
($T_{\text{gas}} \approx 8,000$ K)



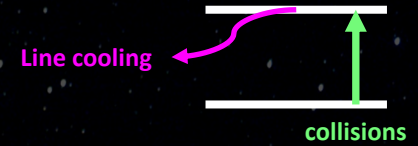
[CII] 158 μ m cooling
of diffuse clouds (CNM)
($T_{\text{gas}} \approx 80$ K)



CO cooling of
dense molecular gas
($T_{\text{gas}} \approx 10$ K)



Two-phases model of the neutral ISM



How do we determine T_{gas} ?

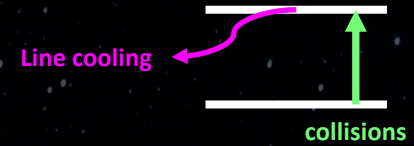
Thermal equilibrium \rightarrow Heating = Cooling

$\Gamma = n \Lambda \rightarrow$ gives T_{gas}

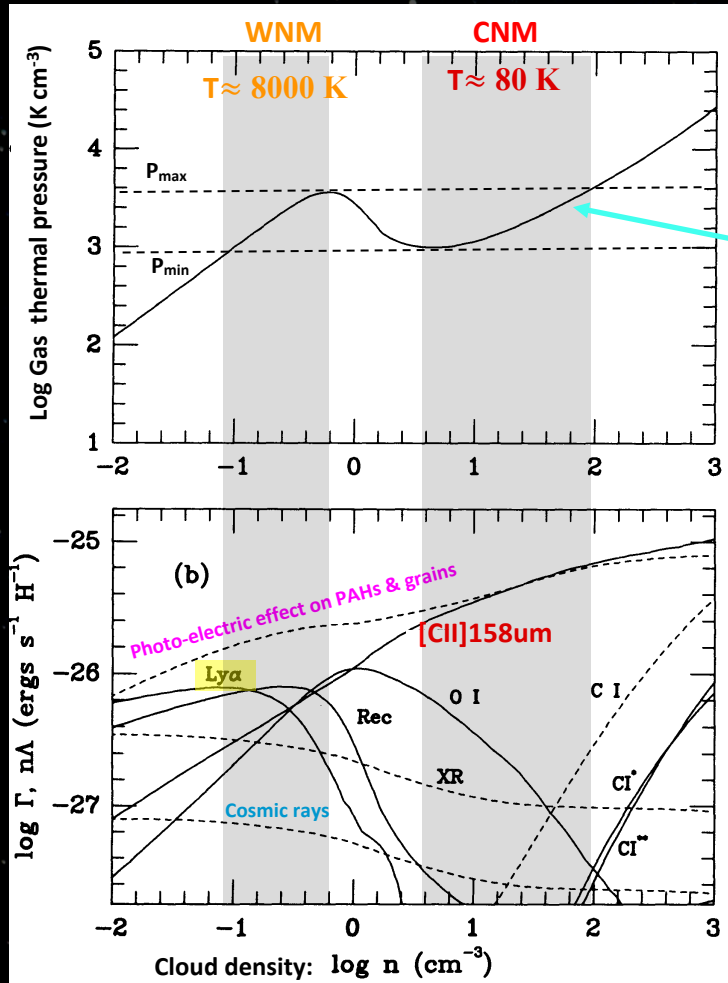
with n = gas density

$P_{\text{th}}/k = n T_{\text{gas}}$ = gas thermal pressure

Two-phases model of the neutral ISM



Two-phases can exist in **thermal pressure equilibrium**
 with $P_{\text{th}}/k = n T \approx 3000 \text{ K cm}^{-3}$
 “Thermally bi-stable”



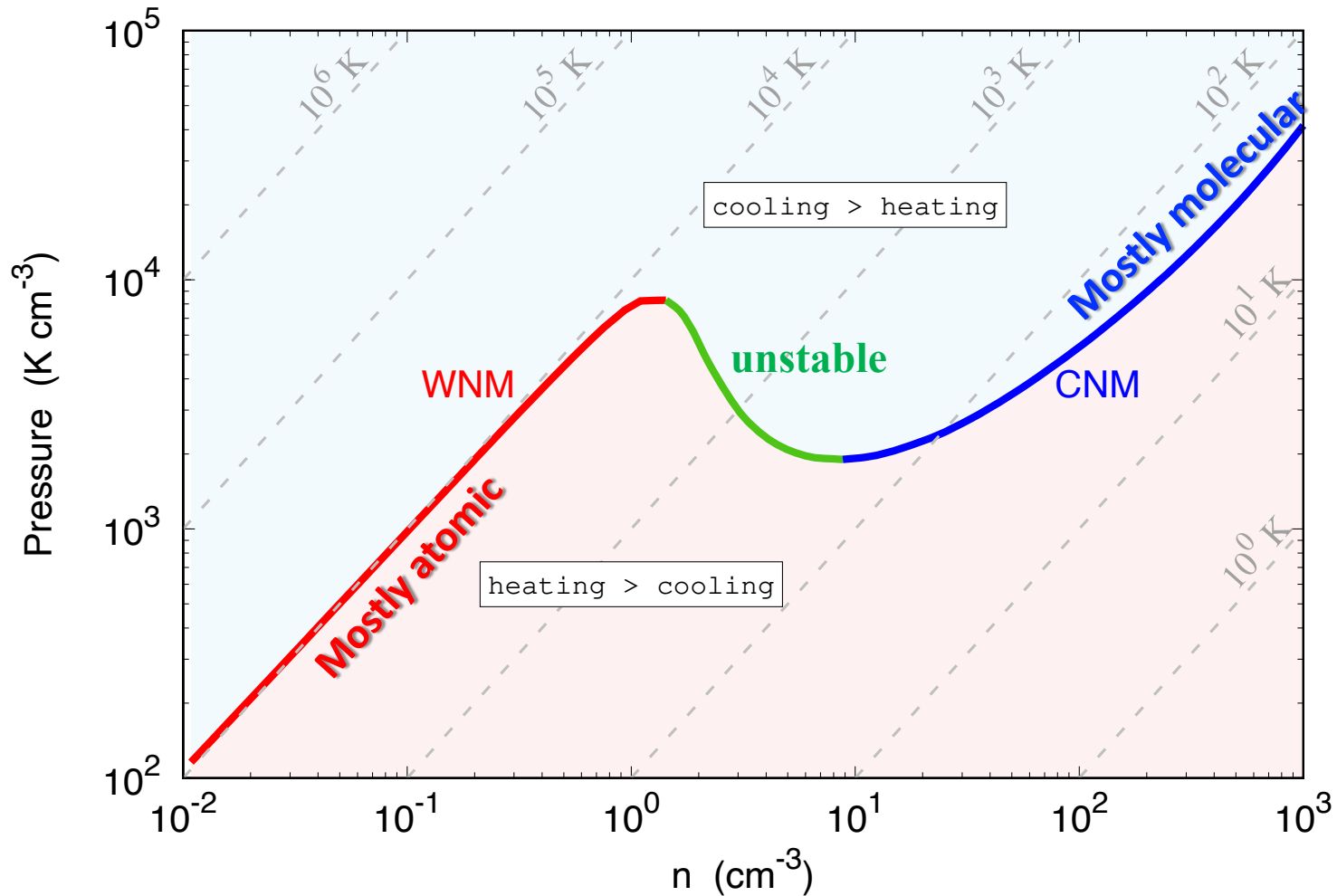
How do we determine T_{gas} ?
 Thermal equilibrium \rightarrow Heating = Cooling

$$\Gamma = n \Lambda \rightarrow \text{gives } T_{\text{gas}}$$

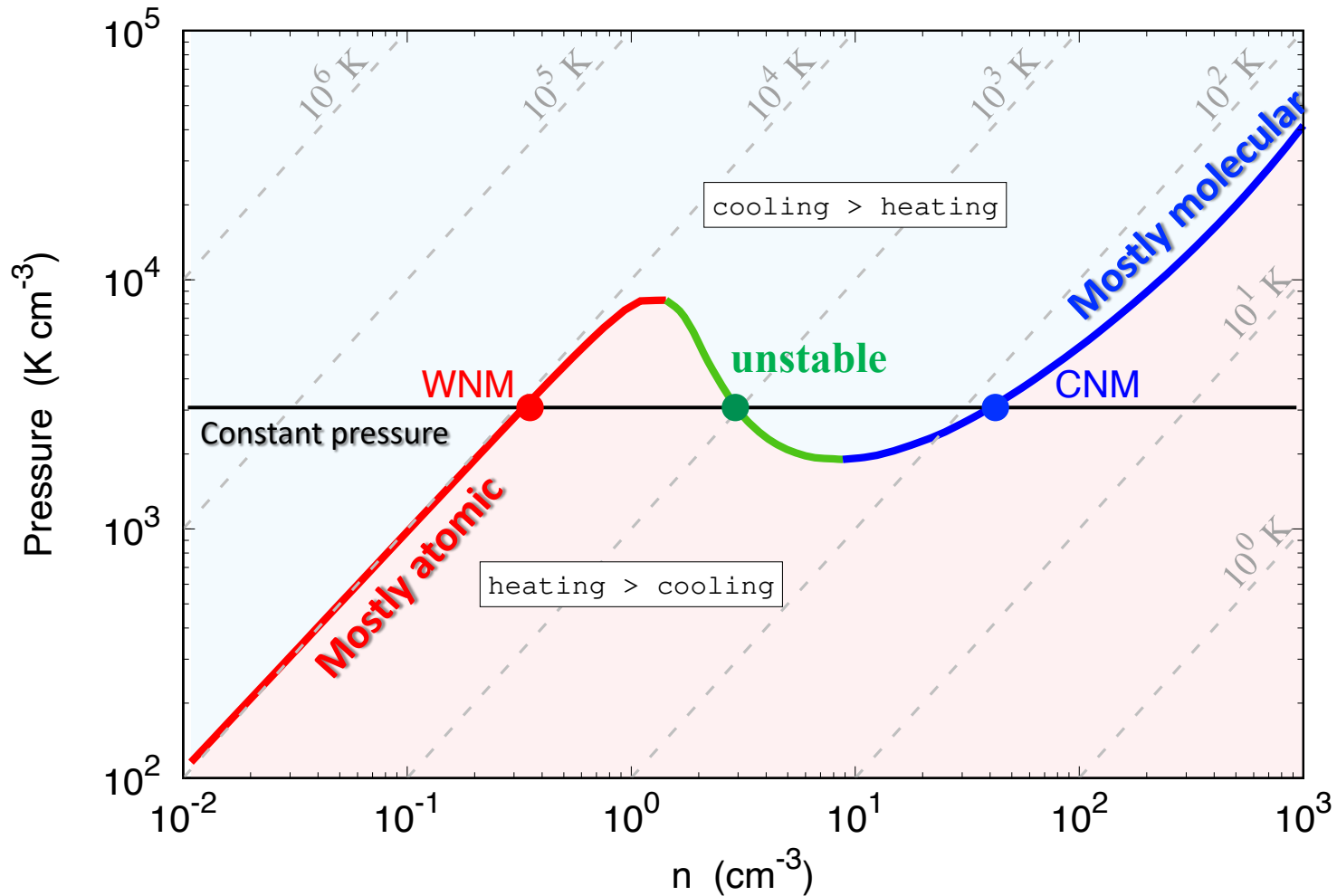
with n = gas density

$$P_{\text{th}}/k = n T_{\text{gas}} = \text{gas thermal pressure}$$

----- Heating processes
 ————— Cooling processes



Thermal bi-stability of the diffuse neutral gas
Adapted from Godard+2024



Thermal bi-stability of the diffuse neutral gas
Adapted from Godard+2024

Dense molecular clouds

$n(\text{H}_2) > 10^3 \text{ cm}^{-3}$ $M \sim 10^3\text{-}10^7 M_{\text{sun}}$ (those you see in CO & HCN emission with ALMA)

Dense molecular clouds are **self-gravitating** ($P_{\text{tot}} > P_{\text{amb}}$) rather than in pressure equilibrium with other phases in the ISM.

Cosmic Ray heating dominates

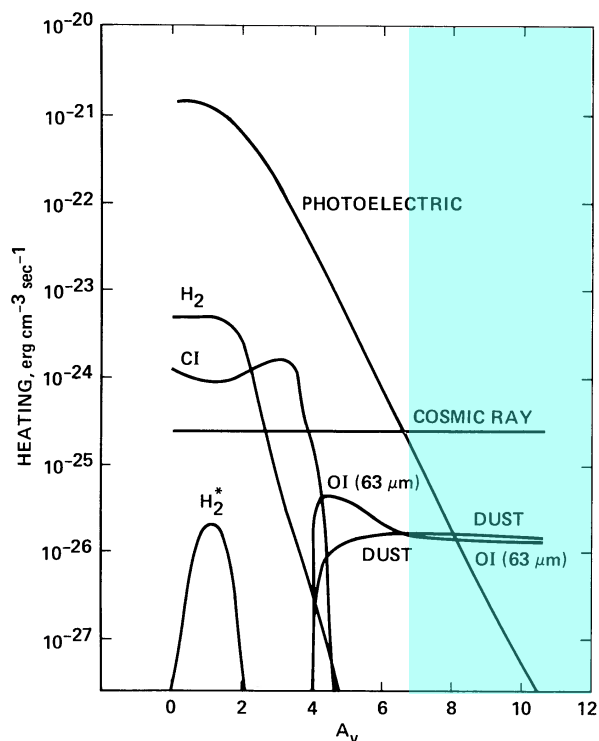


FIG. 1.—Different gas heating terms in the energy balance for the standard model, given as a function of the visual extinction A_v into the cloud. “Photoelectric” refers to the grain photoelectric heating mechanism; “ H_2 ” refers to photodissociation of H_2 ; “ H_2^* ” is the collisional de-excitation of FUV-pumped H_2^* ; “C I” is the photoionization of atomic carbon; “O I (63 μm)” is the collisional de-excitation of IR-pumped neutral oxygen; “dust” refers to the collisions with warm dust.

Hollenbach +1991

CO line cooling dominates $\rightarrow T_k = 10\text{-}20 \text{ K}$

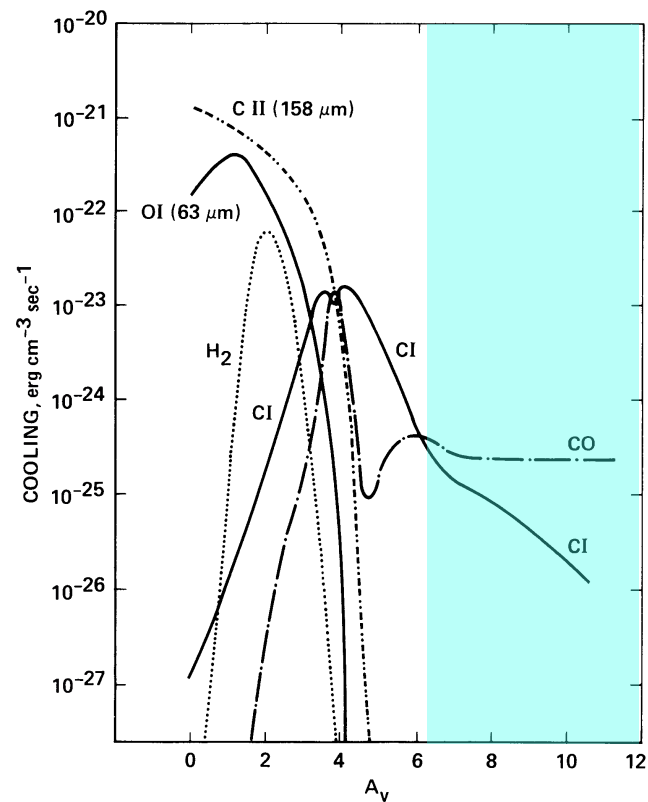
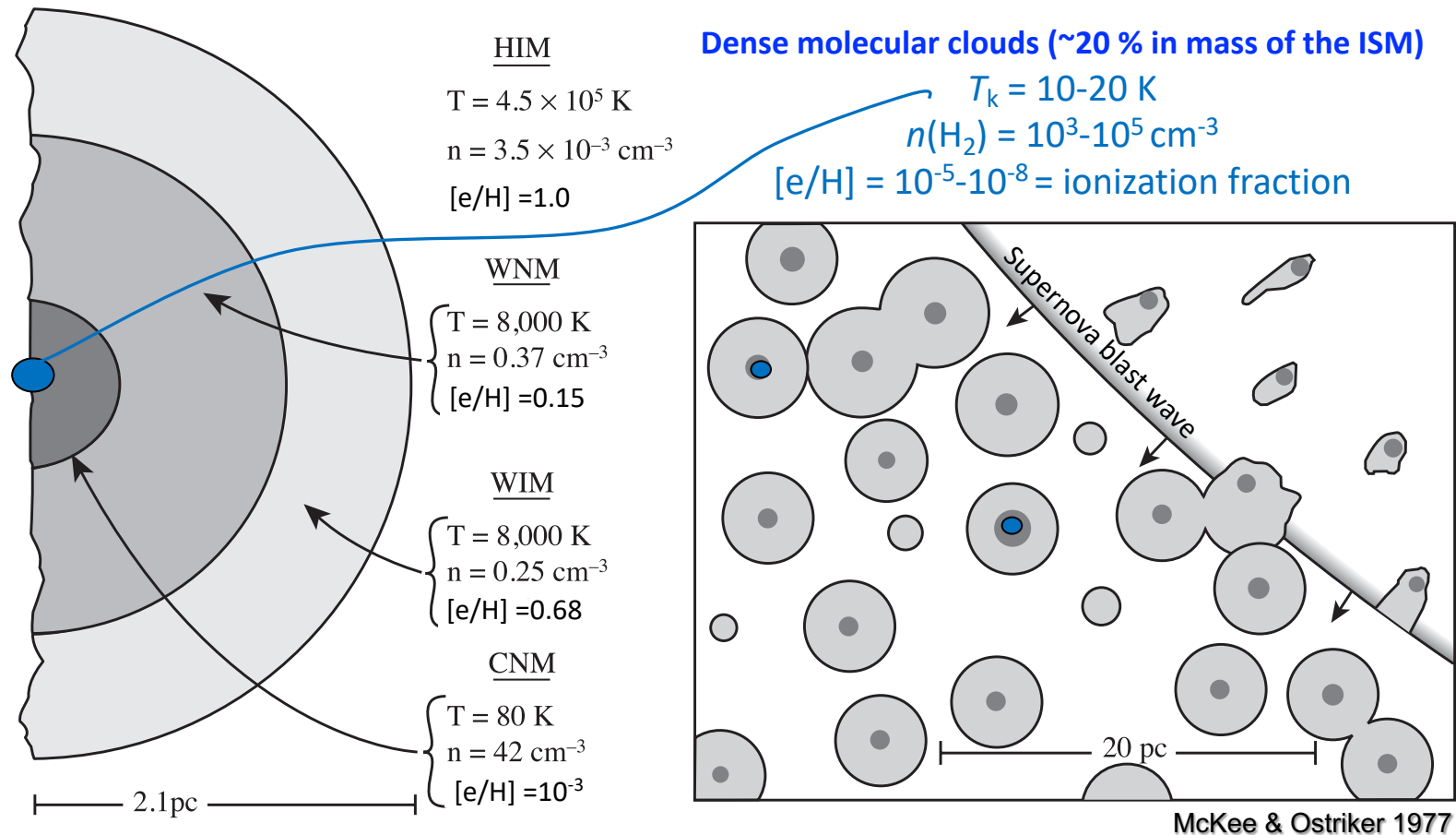


FIG. 2.—Different gas cooling terms in the energy balance for the standard model, given as a function of the visual extinction A_v into the cloud. “C I” is the sum of [C I] 370 μm and [C I] 609 μm ; “ H_2 ” and “CO” are the total cooling by rotational and vibrational transitions of these molecules.

The *classical* multi-phase model of the ISM

cloud = CNM inter-cloud medium = WNM and WIM + HIM



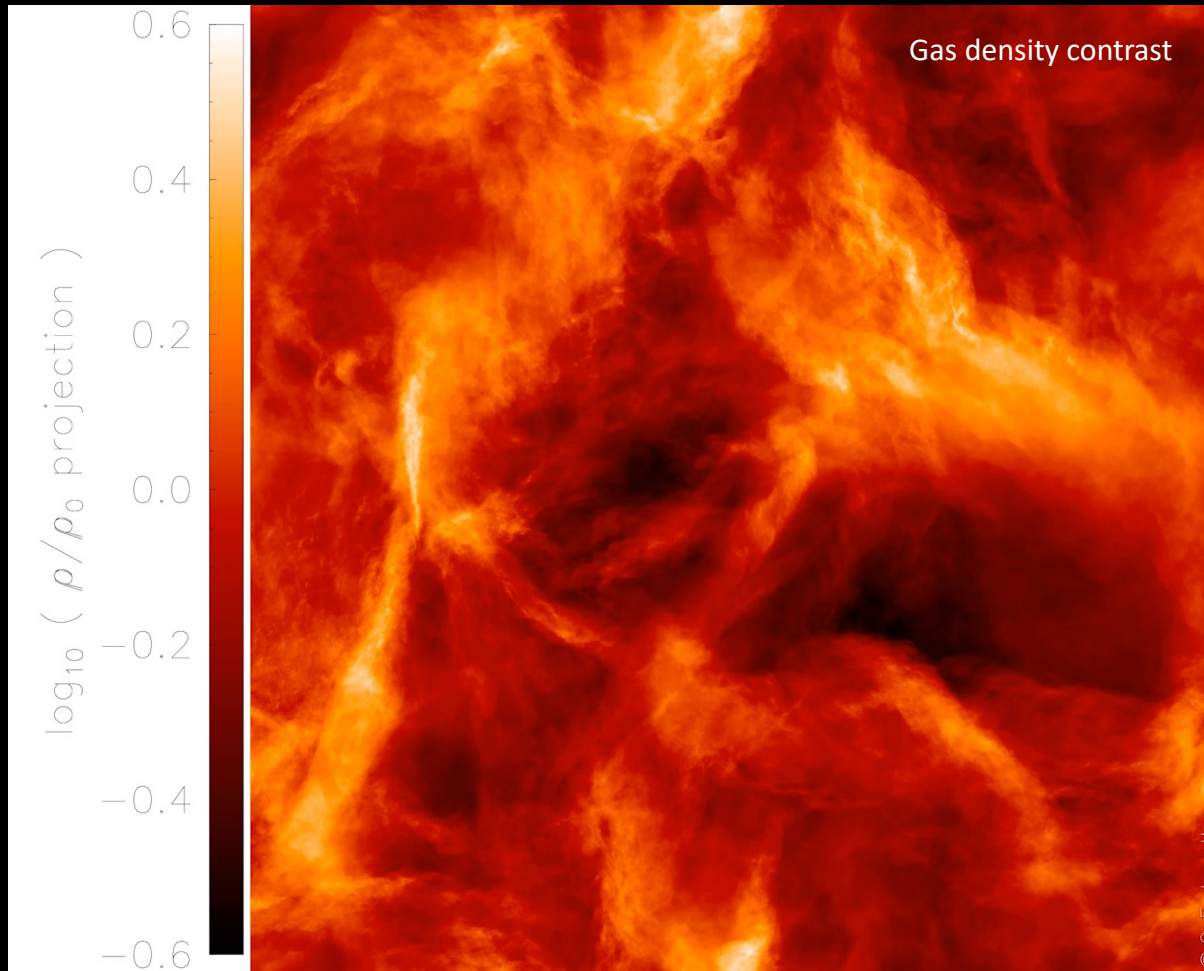
But the ISM is **dynamic & turbulent ...** changes of 'phase' or 'mixing' occur,
observations show WNM HI clouds in the **thermally unstable regime** ($T \neq 8000 \text{ K}$), etc.

Today: hydrodynamic simulations of the turbulent (+ shocks) and magnetized ISM

Modern-day simulations of the turbulent ISM

Complicated problem: **turbulence is injected at very large scales but dissipated at very small scales**

Hennebelle & Falgarone 2012 for a review.



**Shocks can induce
phase transitions
between WNM and CNM**

Godard+2024

**Turbulence in molecular
clouds can be supersonic
→ shocks...**

Federrath et al. 2021,

Nature Astronomy, **FLASH Code**

**Supersonic to sonic turbulence transition at ~ 0.1 pc
(gravity overcomes turbulence. *e.g.*, P. André+2010)**

Interstellar extinction by ISM dust

For **standard** diffuse ISM grains in the Milky Way:

$$N_{\text{H}} = N(\text{H}) + 2N(\text{H}_2) \approx 1.9 \cdot 10^{21} \cdot A_V \text{ cm}^{-2} \text{ mag}^{-1} \quad \text{Bohlin et al. (1978, ApJ)}$$

- A_V = magnitudes of **extinction in the visible range** ($V = \lambda_V = 0.55 \mu\text{m} = 5500 \text{ Armstrongs}$) ...

A_V defines a useful “scale” to classify ISM neutral clouds:

- * $A_V \leq 1 \text{ mag} \rightarrow$ “**Diffuse cloud**” : Visible- and FUV photons from stars are not attenuated

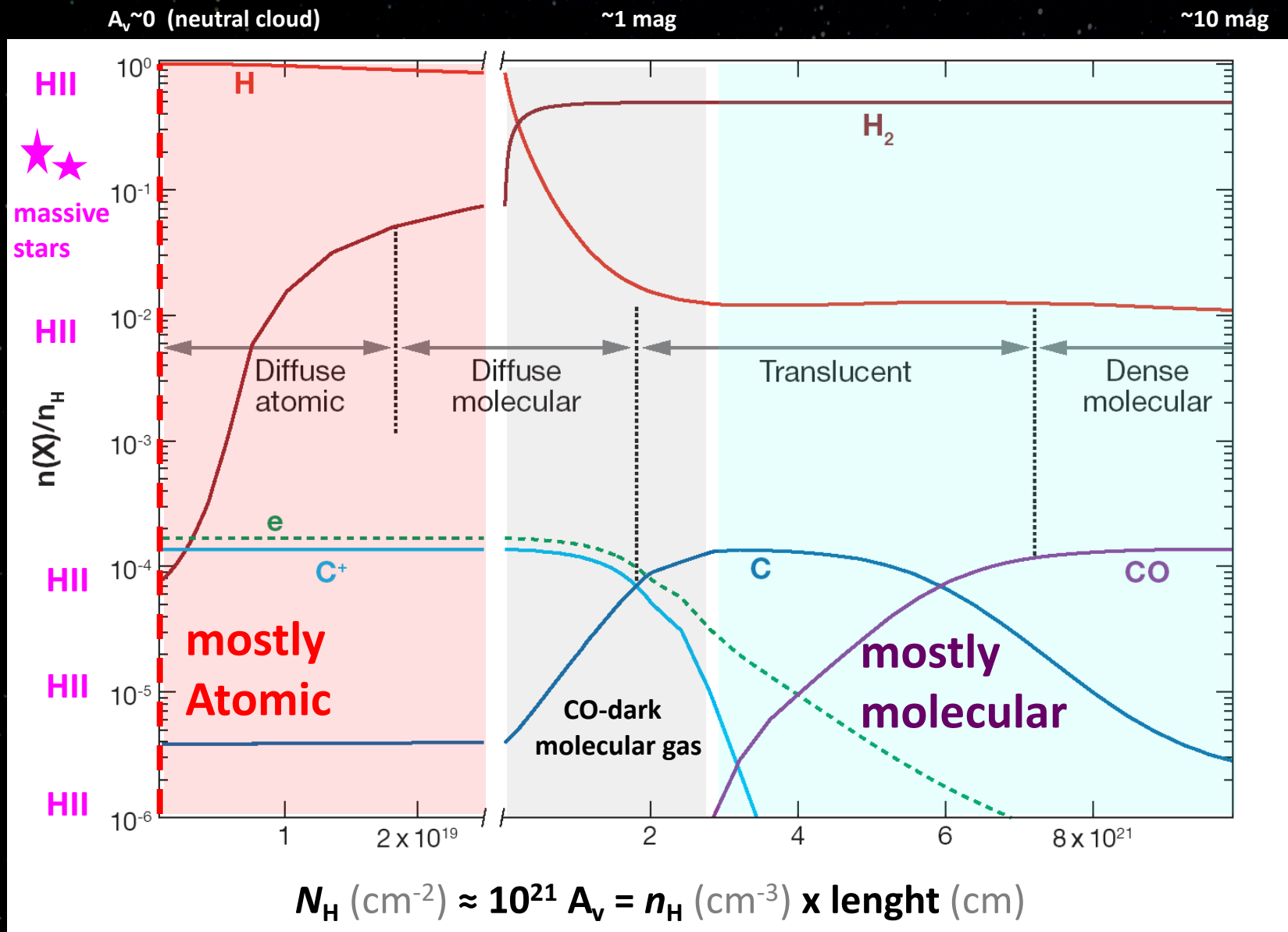
\rightarrow gas is neutral but large fraction of hydrogen is in HI atoms

- * $1 \leq A_V \leq 4 \text{ mag} \rightarrow$ “**Translucent molecular cloud**”: FUV flux is still significant

\rightarrow most hydrogen is molecular H_2

- * $A_V > 4 \text{ mag} \rightarrow$ “**Dense Molecular cloud**”: mostly shielded from stellar FUV radiation

Model of the neutral ISM

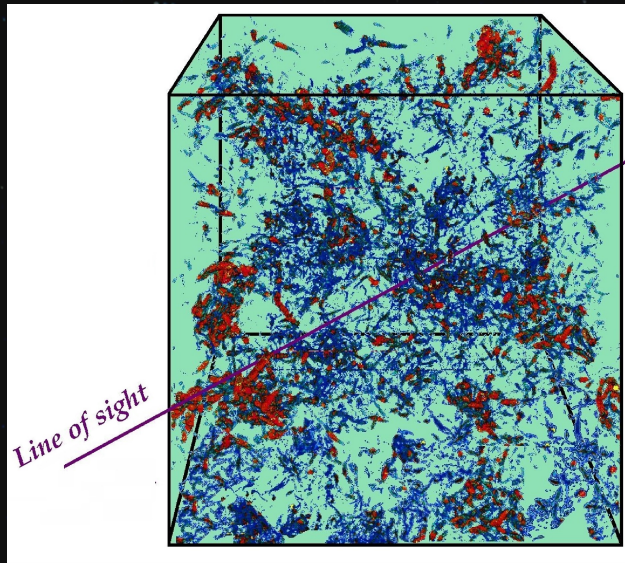


Only $E < 13.6 \text{ eV}$ photons penetrate neutral clouds \rightarrow far-UV photons, below Lyman limit ($\lambda > 911 \text{ \AA}$)

Remember, $\text{IP}(\text{Carbon}) = 11.3 \text{ eV}$

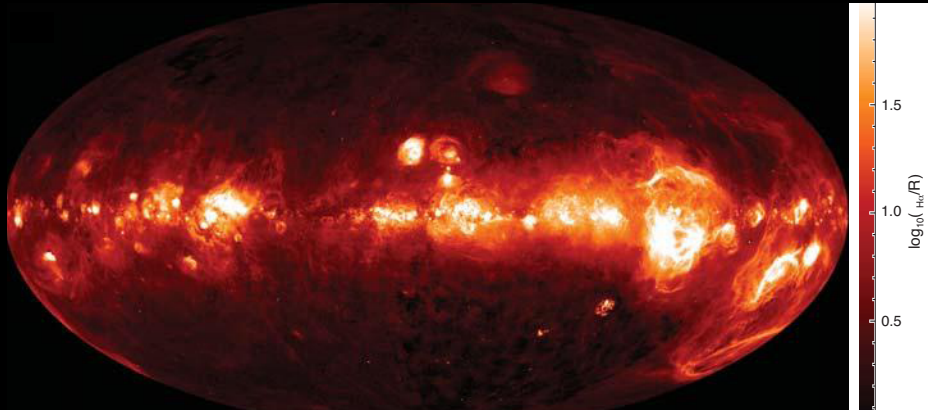
Open big questions

- How are ISM clouds assembled from diffuse gas and how do they ultimately form stars?
- How do the different **energy sources** (UV, thermal, CRs, turbulence, magnetic fields, gravity) contribute to the dynamical properties and evolution of the ISM ? **Feedback processes?**
- What are the limits of chemical complexity in the ISM ? → How are molecules formed?
What do different molecules trace?



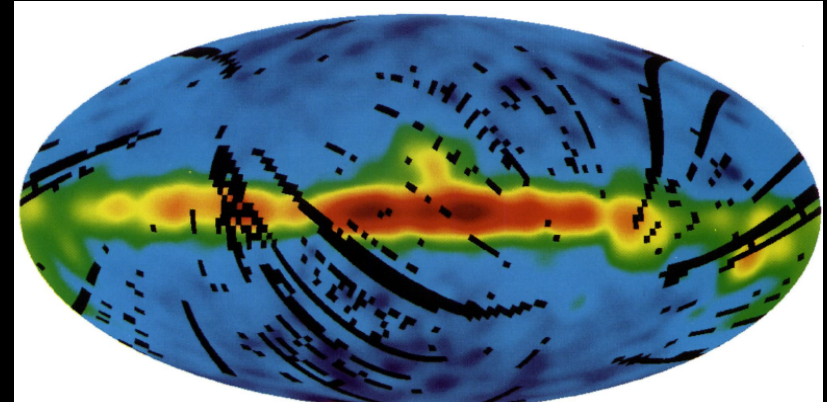
Answers: Observations and models !

H α survey WIM



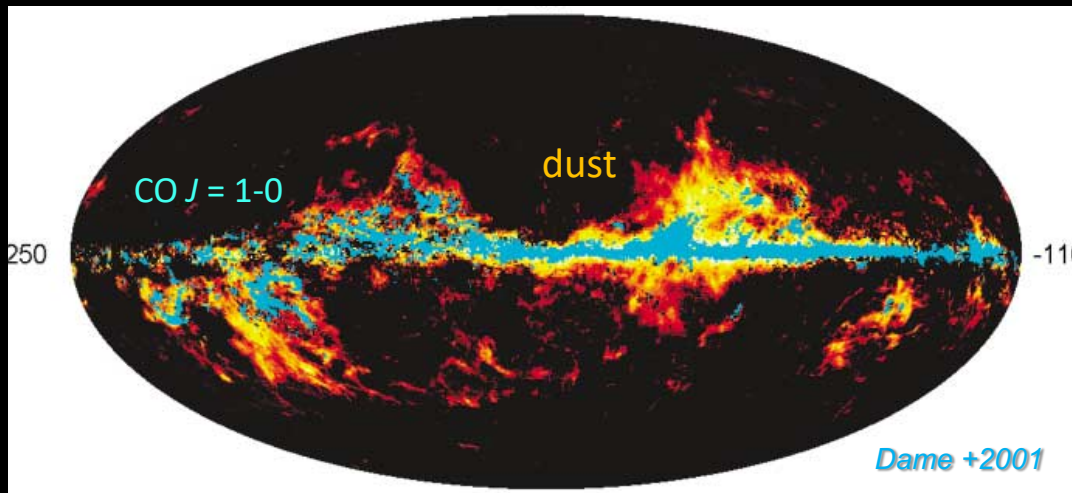
Finkbeiner +2003

[CII]158 μ m (C⁺) Most important coolant of the CNM



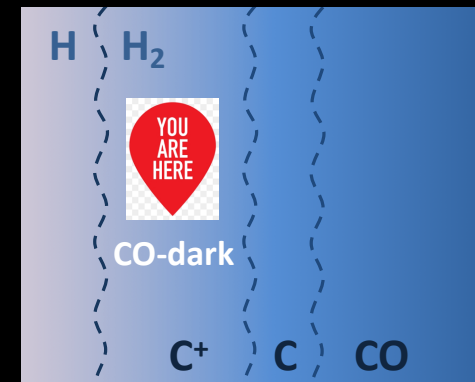
Bennett +1994, COBE

Molecular ISM

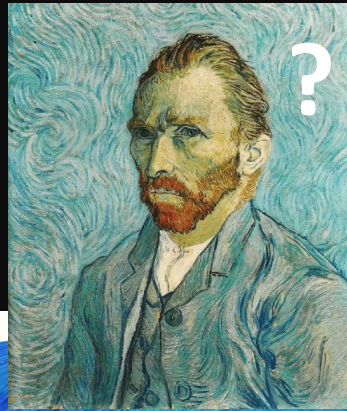


Dame +2001

Excess of dust emission over CO and HI column density
Planck collaboration+11 (*dust*) & Grenier+15 (*γ -rays*)
→ **Missing baryons** 20-80% of molecular gas in galaxies?

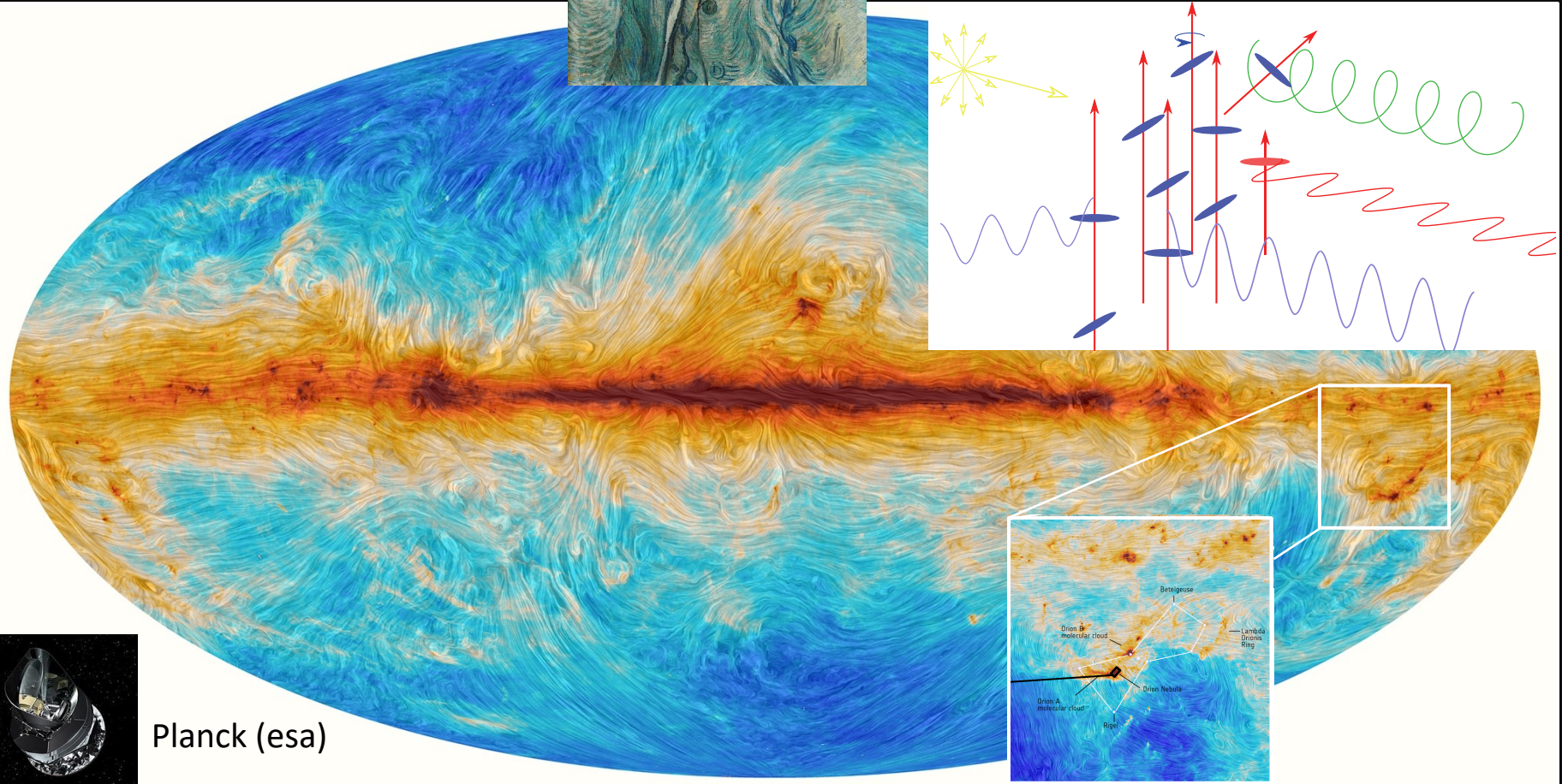


Magnetic field



Wavelength-dependent polarization of light
→ grains are not spherical

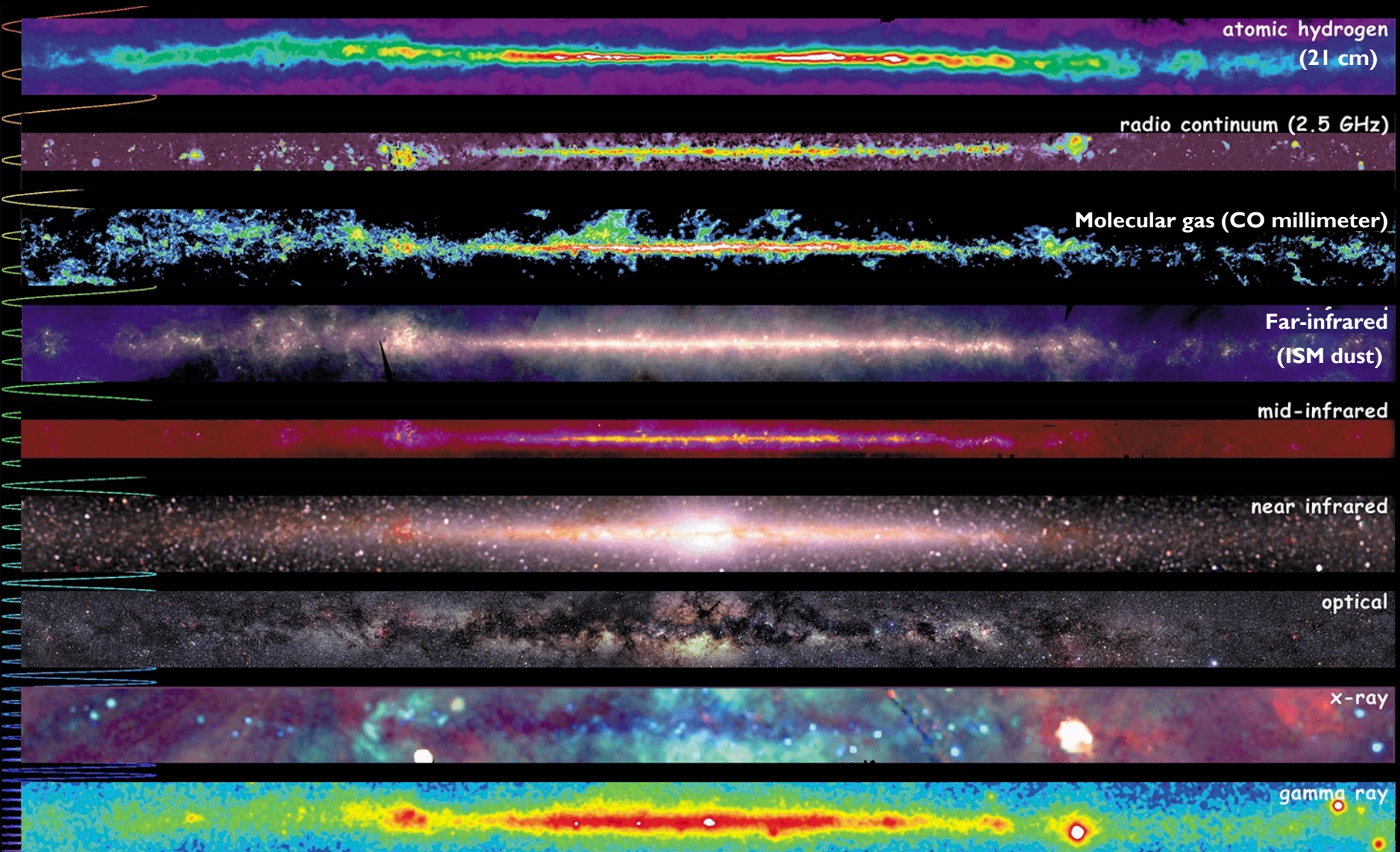
If polarization degree and angle are measured
→ B field orientation can be estimated.



Planck (esa)

Sub(mm) dust thermal emission and polarization Magnetic field orientation
(texture)

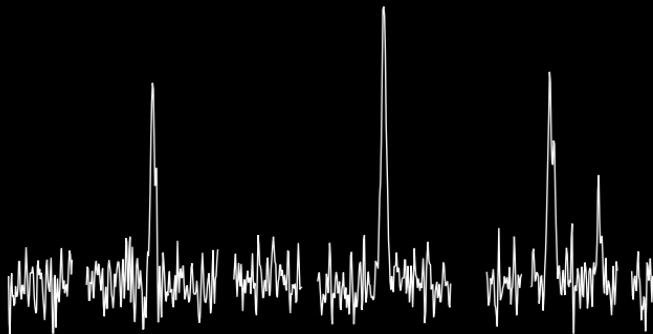
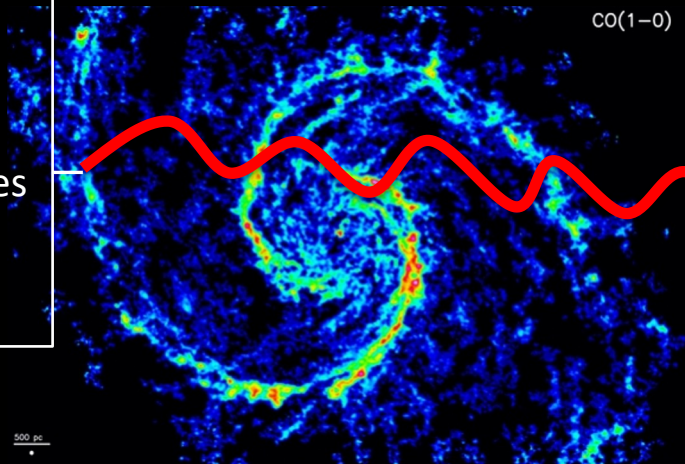
Most λ 's carry specific information about the ISM



The Milky Way at kpc scales

II. Atomic/Molecular excitation and radiative transfer

n
 T
Abundances
 σ_{vel}
...



The equation of radiative transfer

$$I_\nu = \text{energy time}^{-1} \text{area}^{-1} \text{frequency}^{-1} \text{solid angle}^{-1} = \text{erg s}^{-1} \text{cm}^{-2} \text{Hz}^{-1} \text{sr}^{-1}$$

$$\frac{dI_\nu}{ds} = -\alpha_\nu I_\nu + j_\nu$$

defining τ_ν and S_ν as:

$$d\tau_\nu = \alpha_\nu ds \quad S_\nu = \frac{j_\nu}{\alpha_\nu}$$

$$\frac{dI_\nu}{d\tau_\nu} = -I_\nu + S_\nu$$

s path length of propagation of ray (=) cm

α_ν local absorption coefficient (=) cm^{-1}

j_ν local emission coefficient (=) $\text{erg s}^{-1} \text{cm}^{-3} \text{Hz}^{-1} \text{sr}^{-1}$

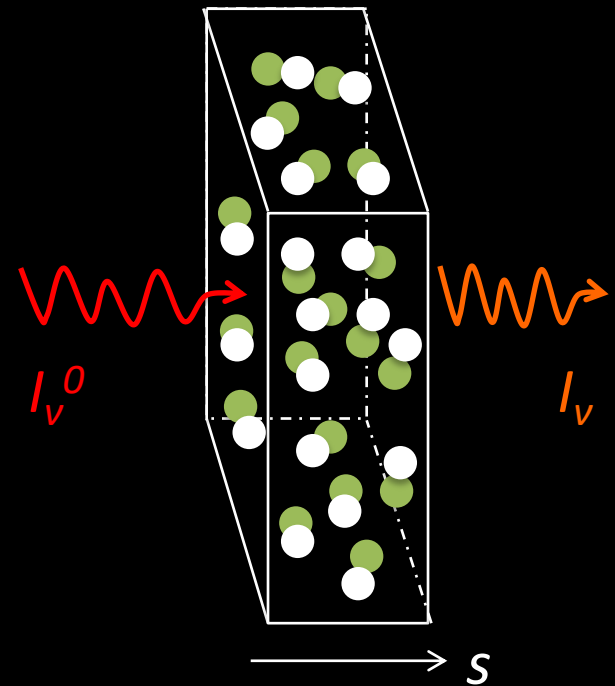
$1/\alpha_\nu$ ~mean free path (=) cm

Formal solution of the equation of radiative transfer:

$$I_\nu(\tau_\nu) = I_\nu^0 e^{-\tau_\nu} + \int_0^{\tau_\nu} S_\nu(\tau_\nu') e^{-(\tau_\nu - \tau_\nu')} d\tau_\nu'$$

Solution for an homogeneous medium:

$$I_\nu = I_\nu^0 e^{-\tau_\nu} + S_\nu(1 - e^{-\tau_\nu})$$

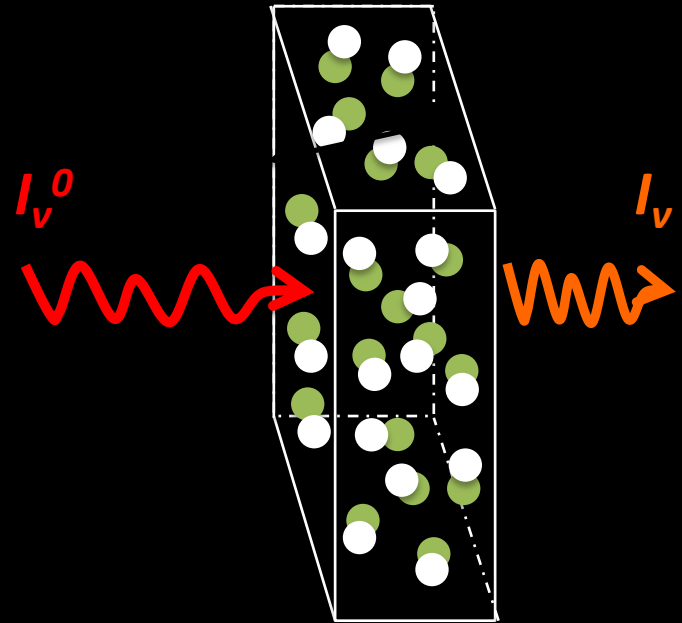


Limiting cases (τ_ν)

radiative transfer equation
for an homogeneous medium

$$I_\nu = I_\nu^0 e^{-\tau_\nu} + S_\nu(1 - e^{-\tau_\nu})$$

→ It shows the effects of matter on radiation.



$$\tau_\nu \rightarrow 0 \quad \rightarrow \quad I_\nu = I_\nu^0 + [S_\nu - I_\nu^0] \tau_\nu$$

optically “thin” emission

$$\tau_\nu \rightarrow \infty \quad \rightarrow \quad I_\nu = S_\nu$$

optically “thick” emission

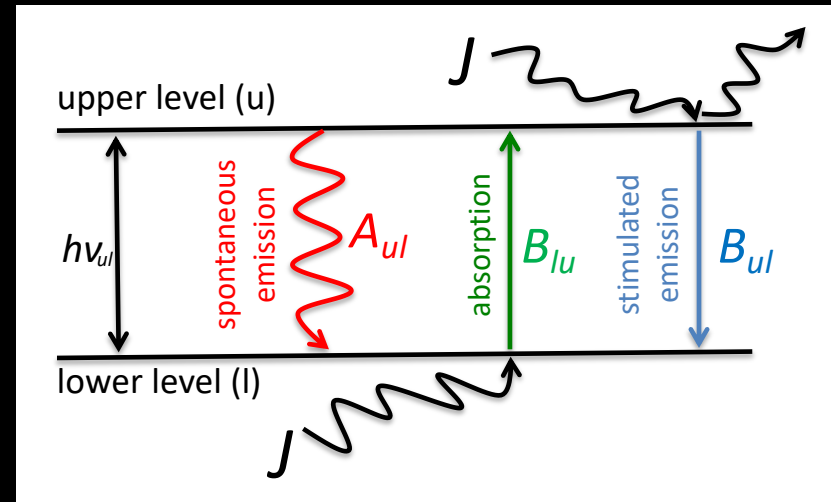
From macroscopic (α_ν, j_ν) to microscopic quantities

two-level system

A_{ul} *spontaneous emission rate* [=] s^{-1}

$J \cdot B_{lu}$ *absorption rate* [=] s^{-1}

$J \cdot B_{ul}$ *stimulated emission rate* [=] s^{-1}



Relations between Einstein coefficients

$$A_{ul} = \frac{2h\nu^3}{c^2} B_{ul} \text{ (s}^{-1}\text{)} \quad g_l B_{lu} = g_u B_{ul}$$

g_l, g_u statistical weight of lower and upper level

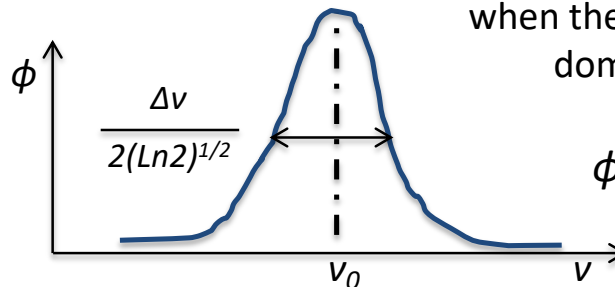
Average intensity J (over angle and line profile):

$$J = \frac{1}{4\pi} \int_{4\pi} d\Omega \int_0^\infty I_\nu \phi(\nu) d\nu$$

Intrinsic line profile function $\phi(\nu)$ in terms frequency [=] Hz^{-1}

normalized such as:

$$\int_0^\infty \phi(\nu) d\nu = 1$$



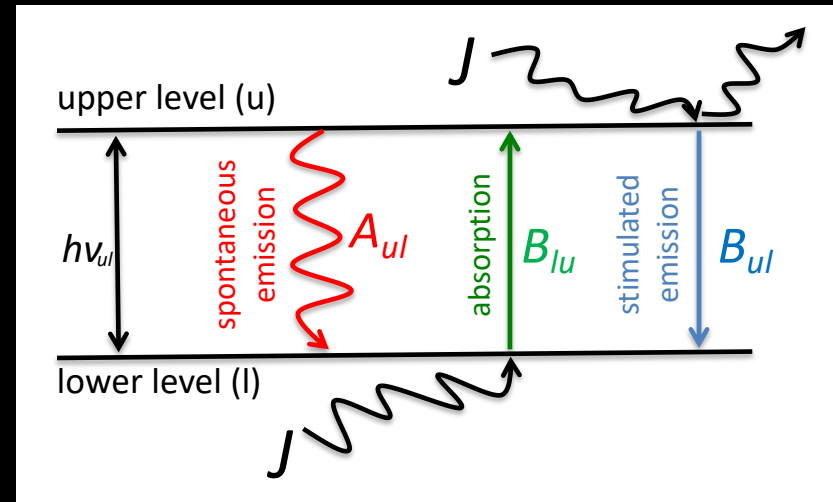
when thermal motions or microturbulence dominate \rightarrow gaussian line profile

$$\phi(\nu) = \frac{1}{\Delta\nu \pi^{1/2}} \exp\left\{-\left(\frac{\nu - \nu_0}{\Delta\nu}\right)^2\right\}$$

From macroscopic (α_ν, j_ν) to microscopic quantities

$$j_\nu = \frac{h\nu}{4\pi} n_u A_{ul} \phi(\nu)$$

$$\alpha_\nu = \frac{h\nu}{4\pi} (n_l B_{lu} - n_u B_{ul}) \phi(\nu)$$



j_ν emission coefficient

α_ν absorption coefficient

(=) $\text{erg s}^{-1} \text{cm}^{-3} \text{Hz}^{-1} \text{sr}^{-1}$

(=) cm^{-1}

A_{ul} Einstein coefficient of spontaneous emission

[=] s^{-1}

B_{ul} and B_{lu} Stimulated emission/absorption coefficients

[=] $\text{cm}^2 \text{erg}^{-1} \text{s}^{-1}$

g_l g_u Statistical weight of lower and upper level

$\phi(\nu)$ Line profile function

[=] Hz^{-1}

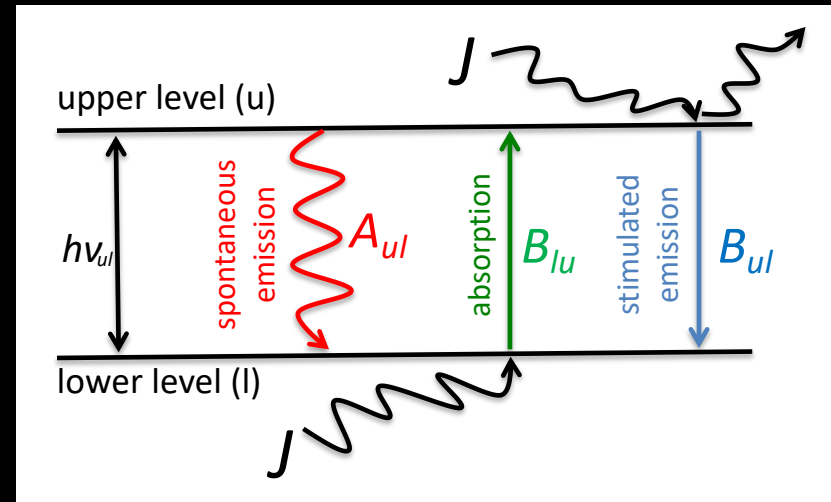
n_l n_u Population of lower and upper level

[=] cm^{-3}

The excitation temperature

$$j_\nu = \frac{h\nu}{4\pi} n_u A_{ul} \phi(\nu)$$

$$\alpha_\nu = \frac{h\nu}{4\pi} (n_l B_{lu} - n_u B_{ul}) \phi(\nu)$$



we define T_{ex} as in Boltzmann law

$$\frac{n_u/g_u}{n_l/g_l} = \exp(-h\nu/kT_{ex})$$

$$n_l/g_l > n_u/g_u \Rightarrow T_{ex} > 0 \Rightarrow \alpha_\nu > 0 \Rightarrow \tau_\nu > 0$$

“normal” populations
thermal emission

$$n_u/g_u > n_l/g_l \Rightarrow T_{ex} < 0 \Rightarrow \alpha_\nu < 0 \Rightarrow \tau_\nu < 0$$

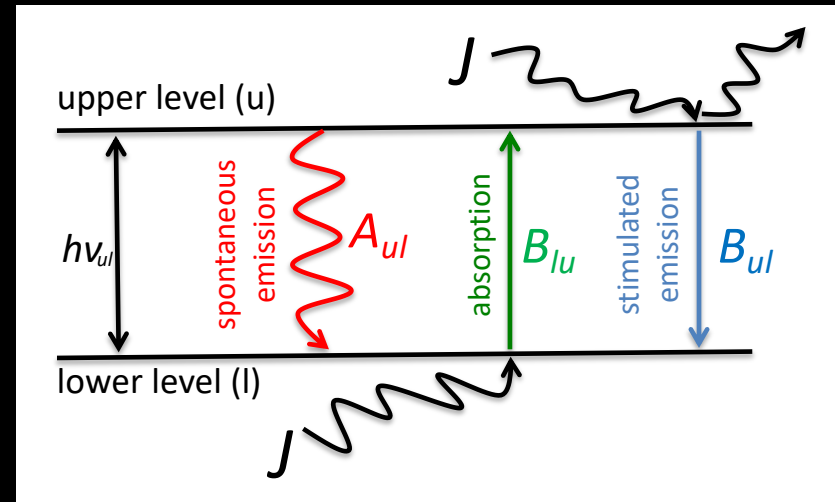
inverted populations
maser emission

The Source function S_ν

$$I_\nu = I_\nu^0 e^{-\tau_\nu} + S_\nu(1 - e^{-\tau_\nu})$$

$$j_\nu = \frac{h\nu}{4\pi} n_u A_{ul} \phi(\nu)$$

$$\alpha_\nu = \frac{h\nu}{4\pi} (n_l B_{lu} - n_u B_{ul}) \phi(\nu)$$



$$S_\nu = \frac{j_\nu}{\alpha_\nu} =$$

...

$$\frac{n_u/g_u}{n_l/g_l} = \exp(-h\nu/kT_{ex})$$

$$= \underbrace{\frac{2h\nu^3}{c^2} \frac{1}{\exp(h\nu/kT_{ex}) - 1}}_{\text{Planck law at } T=T_{ex}}$$

Blackbody
at T_{ex}

$$S_\nu = B_\nu(T_{ex})$$

But T_{ex} is not known ...

Brightness temperature, $h\nu \ll kT$



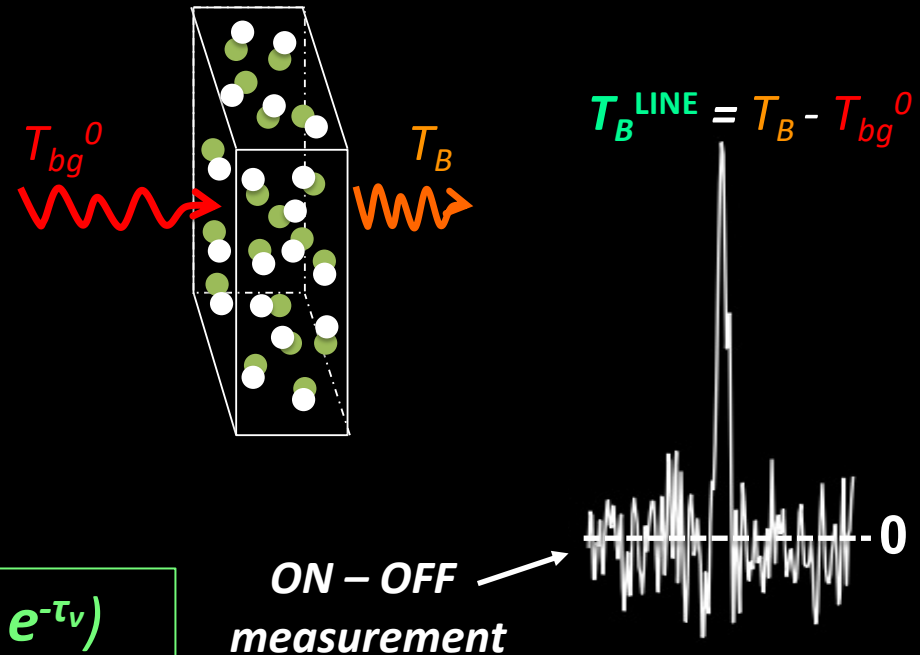
radiative transfer equation
for an homogeneous medium

$$I_\nu = I_\nu^0 e^{-\tau_\nu} + S_\nu (1 - e^{-\tau_\nu})$$

When $h\nu \ll kT$ we can use the Rayleigh–Jeans law:

$$T_b = \frac{I_\nu c^2}{2k\nu^2} \quad \text{Expanding the Planck law for small } h\nu/k \text{ values ...}$$

$$T_B = T_{bg}^0 e^{-\tau_\nu} + T_{ex} (1 - e^{-\tau_\nu})$$



$$T_B^{\text{LINE}} = T_B - T_{bg}^0 = (T_{ex} - T_{bg}^0) \cdot (1 - e^{-\tau_\nu})$$

$$\tau_\nu \rightarrow 0 \quad \Rightarrow \quad T_B^{\text{LINE}} \sim (T_{ex} - T_{bg}^0) \cdot \tau_\nu \sim T_{ex} \cdot N \quad \text{optically 'thin' emission}$$

$$\tau_\nu \rightarrow \infty \quad \Rightarrow \quad T_B^{\text{LINE}} \sim T_{ex} - T_{bg}^0 \sim T_{ex} \quad \text{optically 'thick' emission}$$

How are level populations (n_u n_l) - **thus** T_{ex} - determined?

Rotational population diagram (or 'Boltzmann plot')

Hands-on Project 3: *Tracing the physical properties of warm molecular gas through observations and models of the submillimeter CO rotational ladder*
Wait until Thursday...

Statistical equilibrium equations

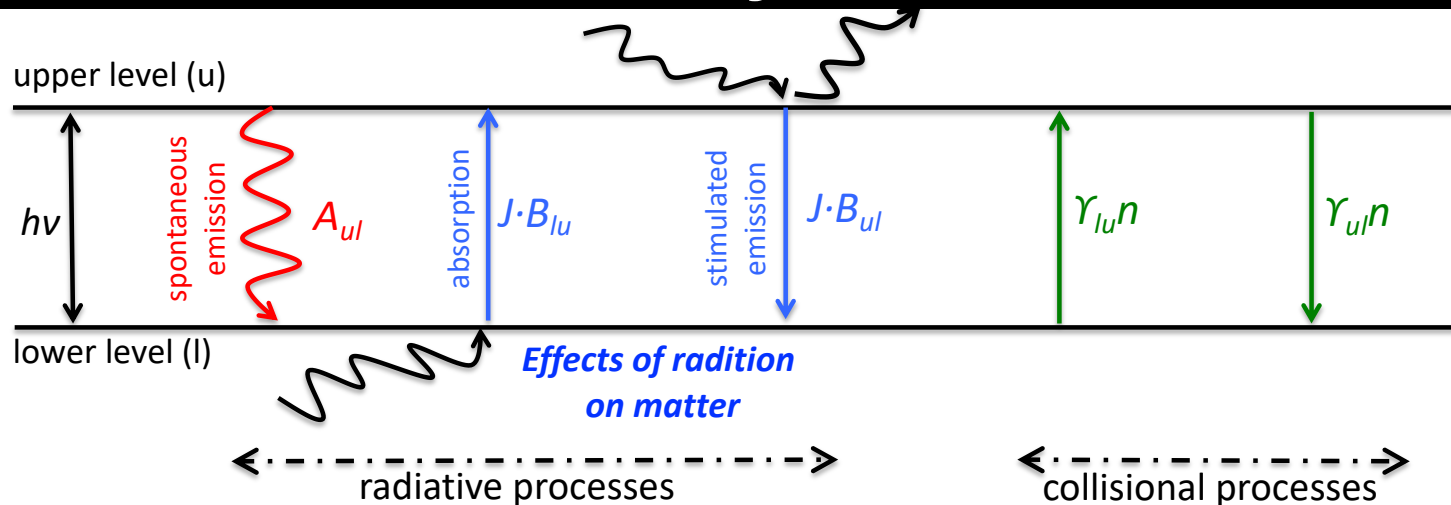
$$\frac{dn_i}{dt} = \sum_{j \neq i} n_j \underbrace{(J \cdot B_{ji} + \gamma_{ji} n)}_{\text{Populate upper level } i} + \sum_{j > i} n_j A_{ji} - n_i \sum_{j \neq i} \underbrace{(J \cdot B_{ij} + \gamma_{ij} n)}_{\text{De-populate upper level } i} - n_i \sum_{j < i} A_{ij} = 0$$

γ_{ul} collisional rate coefficient for transition $u \rightarrow l$ [=] $\text{cm}^3 \text{s}^{-1}$

n colliders density (H_2 , e^- , ...) [=] cm^{-3}

$\gamma_{ul} \cdot n$ collisional excitation rate for transition $u \rightarrow l$ per unit time [=] s^{-1}

Two-level system



Limiting case: collisional rates \gg radiative rates \rightarrow LTE

$$\frac{dn_i}{dt} = \sum_{j \neq i} n_j \left(\cancel{J_{ji}} \cancel{B_{ji}} + \gamma_{ji} n \right) + \sum_{j > i} n_j \cancel{A_{ji}} - n_i \sum_{j \neq i} \left(\cancel{J_{ij}} \cancel{B_{ij}} + \gamma_{ij} n \right) - n_i \sum_{i < j} \cancel{A_{ij}} = 0$$

$\gamma_{lu} g_l = \gamma_{ul} g_u \exp(-h\nu/kT_{kin})$ collisional rate coefficients must fulfil detailed balance

$$n_u \gamma_{ul} n - n_l \gamma_{lu} n = 0 \rightarrow \frac{n_u/g_u}{n_l/g_l} = \exp(-h\nu/kT_{kin})$$

Boltzmann population distribution at T_{kin}
 “LTE”

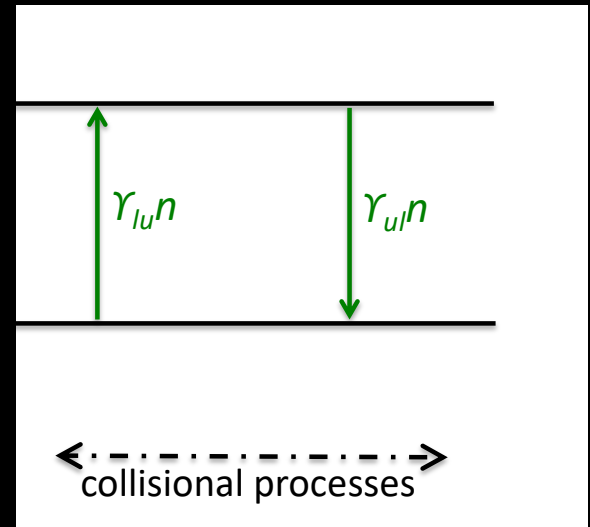
Collisional rate coefficients (e.g. CO + H₂):

$$\gamma_{ul} \sim \sigma_{ul} \cdot v [=] \text{cm}^3 \text{s}^{-1}$$

$$\gamma_{ul}(T) = \int \sigma_{ul}(v) v f_v dv$$

Cross-section [cm²]
 (computed by quantum methods)

Maxwell distribution
 of thermal velocities [cm/s]

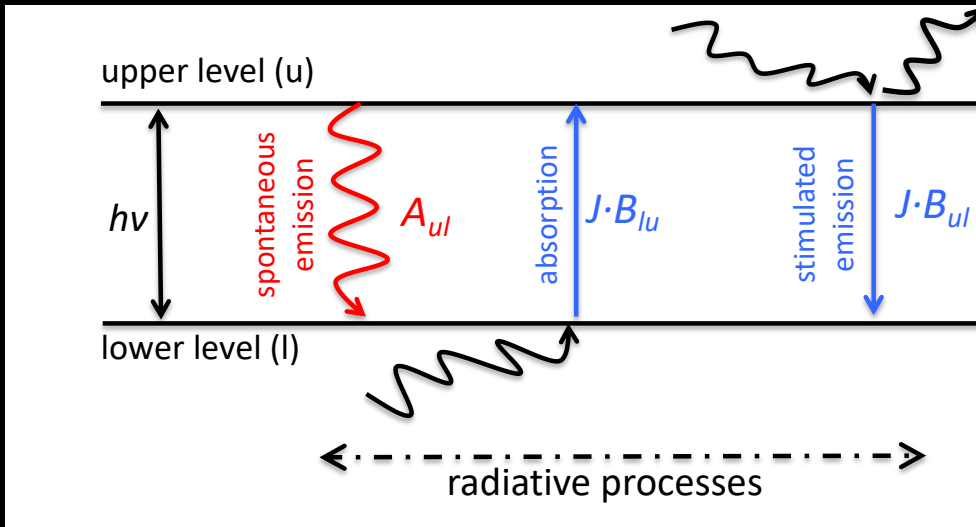


Limiting case: collisional rates \ll radiative rates

$$\frac{dn_i}{dt} = \sum_{j \neq i} n_j (J \cdot B_{ji} + \cancel{\gamma_{ji} n_j}) + \sum_{j > i} n_j A_{ji} - n_i \sum_{j \neq i} (J \cdot B_{ij} + \cancel{\gamma_{ij} n_i}) - n_i \sum_{j < i} A_{ij} = 0$$

if $J \sim B_\nu(T_{bg})$ \rightarrow uniform blackbody radiation field at T_{bg}

$$n_u J \cdot B_{ul} + n_u A_{ul} - n_l J \cdot B_{lu} = 0 \rightarrow \frac{n_u/g_u}{n_l/g_l} = \exp(-h\nu/kT_{bg}) \quad \text{Boltzmann population distribution at } T_{bg}$$



Radiative transfer models

$$\frac{dn_i}{dt} = \sum_{j \neq i} n_j (J \cdot B_{ji} + \gamma_{ji} n) + \sum_{j > i} n_j A_{ji} - n_i \sum_{j \neq i} (J \cdot B_{ij} + \gamma_{ij} n) - n_i \sum_{j < i} A_{ij} = 0$$

Different methods depend on how J is computed

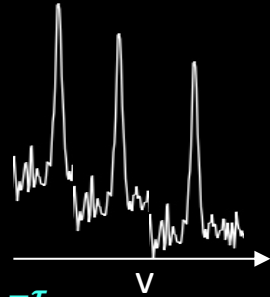
NON-LTE BUT LOCAL EXCITATION AND RADIATIVE TRANSFER MODELS:

- **LVG & escape probability:**
One slab with $J \sim S_{ij} (1 - \beta)$

Sobolev 1960 and Castor 1970, *MNRAS*

RADEX: van der Tak et al. 2007, *A&A*

$\beta = \text{The probability that a photon escapes} \sim \frac{1 - e^{-\tau}}{\tau}$



NON-LOCAL & NON-LTE EXCITATION AND RADIATIVE TRANSFER MODELS:

- **Monte Carlo** (solving Eq. RT):
(flexible geometries and velocity fields)

Bernes 1979, A&A Hogerheijde & van der Tak 2000, *A&A*

González-Alfonso & Cernicharo 1993, *A&A*

Goicoechea et al. 2006, 2022, *A&A*

Brinch & Hogerheijde 2010 (**LIME**)

- **Accelerated Λ Iteration (ALI):**

Rybicki & Hummer 1991, A&A

- **Coupled escape probability (CEP):**
(multi slabs)

Elitzur & Asensio Ramos 2006, MNRAS

Asensio Ramos & Elitzur 2018, *A&A* **MOLPOP-CEP**

Critical density of a transition

$$n_{\text{cr}} \sim \frac{A_{ul}}{\gamma_{ul}} \quad [\text{cm}^{-3}]$$

$$\text{with } Y_{ul} = \sigma v \quad [\text{cm}^3 \text{ s}^{-1}]$$

USEFUL LIMITS:

If $n \gg n_{\text{cr}} \rightarrow$ collisions dominate excitation $\rightarrow T_{\text{ex}} \approx T_{\text{kin}} \sim \text{LTE}$

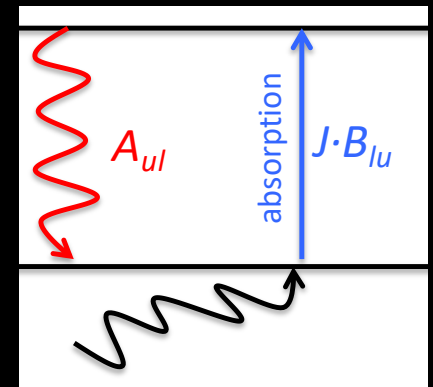
If $n \ll n_{\text{cr}} \rightarrow$ radiative excitations dominate $\rightarrow T_{\text{ex}} < T_{\text{kin}}$

(‘subthermal’ emission)

‘Line trapping’ as τ increases:

$$n_{\text{cr,eff}} \sim \frac{A_{ul} \cdot \beta}{\gamma_{ul}} \sim \frac{A_{ul}}{\gamma_{ul} \cdot \tau} \sim \frac{n_{\text{cr}}}{\tau} \rightarrow T_{\text{ex}} \uparrow$$

Optically thick lines thermalize at lower densities

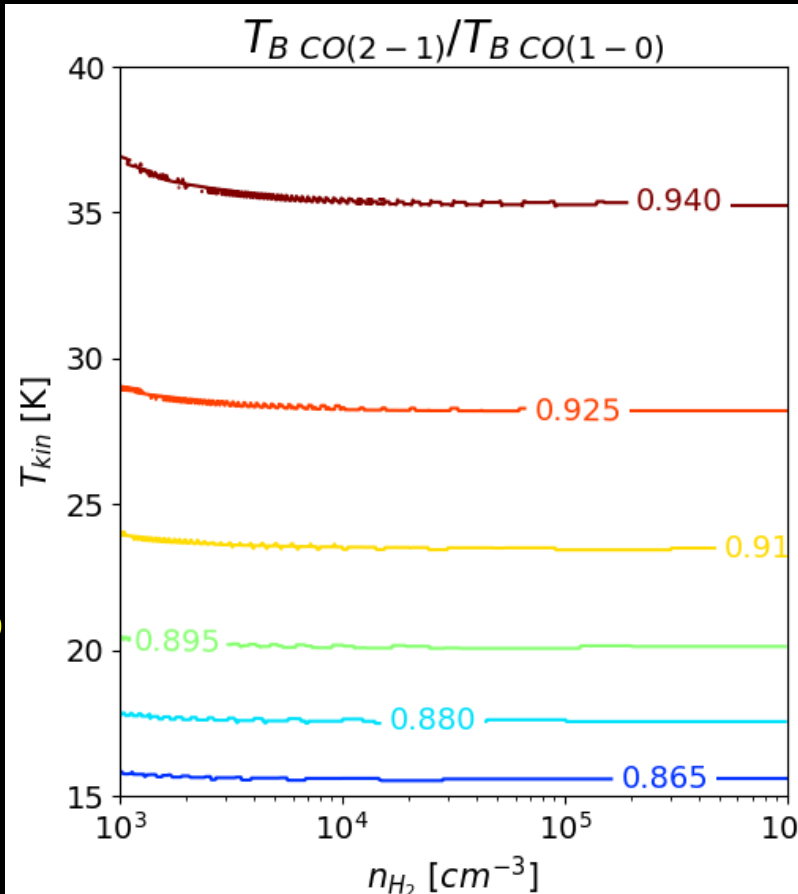


In most cases, **one must solve the statistical equilibrium equations with a model ...**

CO: low $n_{\text{cr}} \sim 10^{2-3} \text{ cm}^{-3}$

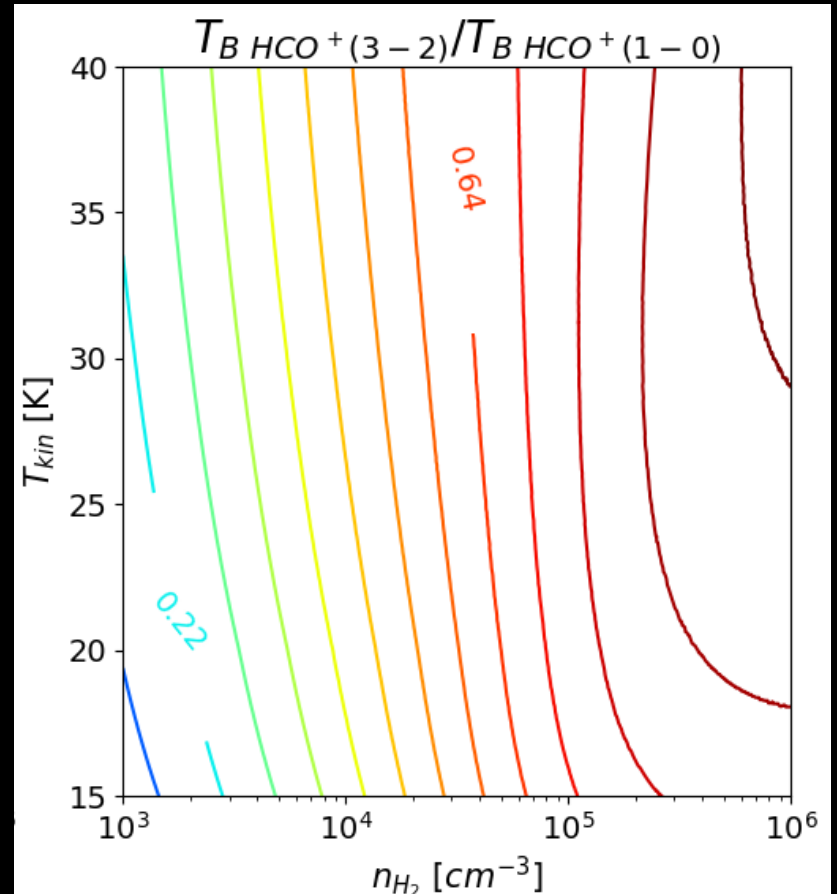
HCO⁺: high $n_{\text{cr}} \sim 10^5 \text{ cm}^{-3}$

L. Segal & A. Roueff 2022,
using a non-LTE model



$$T_{\text{ex}} \sim T_{\text{kin}}$$

CO line intensity ratios
trace the gas temperature



$$T_{\text{ex}} \ll T_{\text{kin}} \text{ (subthermal)}$$

HCO⁺ line intensity ratios
trace the gas density

Spectroscopic & Collisional data

$$\frac{dn_i}{dt} = \sum_{j \neq i} n_j (J \cdot B_{ji} + \gamma_{ji} n) + \sum_{j > i} n_j A_{ji} - n_i \sum_{j \neq i} (J \cdot B_{ij} + \gamma_{ij} n) - n_i \sum_{j < i} A_{ij} = 0$$

The **C**ologne **D**atabase for **M**olecular **S**pectroscopy
CDMS

<https://cdms.astro.uni-koeln.de/classic/entries/>

LAMDA

Leiden Atomic and Molecular Database

[Data format](#) | [RADEX](#)

<https://home.strw.leidenuniv.nl/~moldata/>



Jet Propulsion Laboratory
California Institute of Technology

+ View

JPL HOME

EARTH

SOLAR SYSTEM

Molecular Spectroscopy
Jet Propulsion Laboratory
California Institute of Technology

<https://spec.jpl.nasa.gov>

[Browse collisions](#)

[Search collisions](#)

[Search articles](#)

Basecol

Ro-Vibrational Collisional Excitation
Database and Utilities

<https://basecol.vamdc.eu/index.html>

**Try to thank the papers with the
specific calculations too... !**

Radiative transfer models

(extra ingredients...)

$$\boxed{\frac{dl_v}{ds} = -\alpha_v l_v + j_v} \rightarrow \boxed{\begin{array}{l} \text{defining } \tau_v \text{ and } S_v \text{ as:} \\ d\tau_v = \alpha_v ds \quad S_v = \frac{j_v}{\alpha_v} \end{array}} \rightarrow \boxed{\frac{dl_v}{d\tau_v} = -l_v + S_v}$$

A) Gas and dust coexist, affecting the excitation of molecular lines:

$$\alpha_v = \alpha_{\text{gas}} + \alpha_{\text{dust}}$$

with α_{dust} = dust absorption coefficient

e.g., Draine & Lee 84, Ossenkopf & Henning 94

$$j_v = j_{\text{gas}} + j_{\text{dust}}$$

with $j_{\text{dust}} = \alpha_{\text{dust}} \cdot B(T_{\text{dust}})$ = dust emissivity

B) When chemical formation & destruction processes are comparable to collisional processes:

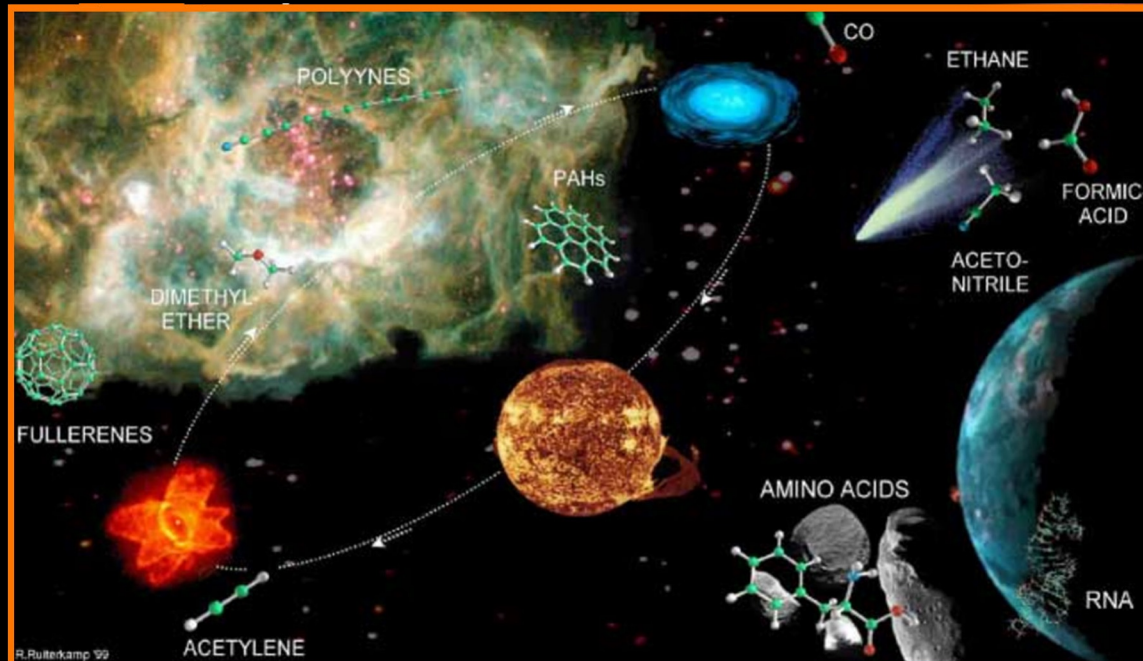
$$\frac{dn_i}{dt} = 0 = \mathcal{F}_i - n_i \mathcal{D}_i,$$

J. H. Black 1998

$$\begin{aligned} \sum_{j>i} n_j A_{ji} + \sum_{j\neq i} n_i (B_{ji} \bar{J}_{ji} + C_{ji}) + F_i \\ = n_i \left(\sum_{j<i} A_{ij} + \sum_{j\neq i} (B_{ij} \bar{J}_{ij} + C_{ij}) + D_i \right) \end{aligned}$$

+Chemical formation and destruction rates

III. Interstellar Chemistry



**Where do interstellar molecules come from?
How are they formed?**

Molecules in the ISM? Typical Scales...

“Size” of a diatomic molecule, $r \approx 2 \text{ \AA} = 2 \cdot 10^{-8} \text{ cm}$

Cross-section (surface) $\sigma = \pi r^2 \approx 10^{-15} \text{ cm}^2$

Typical speeds $v \approx 0.1 \text{ km s}^{-1} = 10^4 \text{ cm s}^{-1}$

Reactive collision rate $\gamma (\text{cm}^3 \text{ s}^{-1}) = \sigma \cdot v = 10^{-11} \text{ cm}^3 \text{ s}^{-1}$

H_2 density in dense clouds $n(\text{H}_2) \approx 10^5 \text{ cm}^{-3}$

Time between collisions of two molecules $t (\text{s}) \approx 1 / (\gamma n_{\text{H}_2}) \approx 2 \text{ weeks} !!$

Distance between collisions $d = v t \approx 100,000 \text{ km} !!$

SLOW chemistry,

Astrophysicists did not expect many molecules in space...

(SHORT) HISTORY OF INTERSTELLAR CHEMISTRY



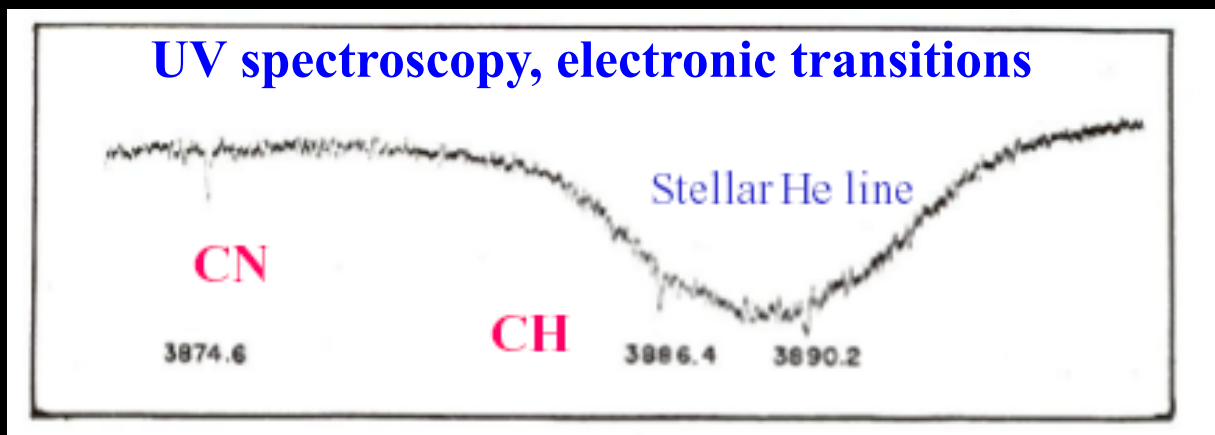
* 1926 – **A. Eddington**

It is difficult to admit the existence of **molecules** in interstellar **space** because when once a molecule becomes dissociated there seems **no** chance of the atoms joining up again.²⁸

“Atoms are physics, but molecules are chemistry...”

* In 1930-1940 **three** molecules were observed in the line-of-sight toward slightly reddened stars in the near-UV: **CN**, **CH** and **CH⁺**

Swing &
Rosenfeld 1937



MOLECULAR SPECTRA and MOLECULAR STRUCTURE

I. SPECTRA OF DIATOMIC MOLECULES

By

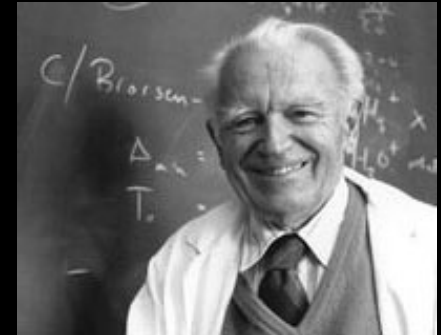
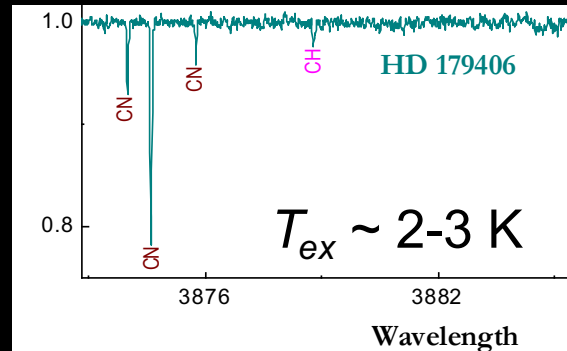
GERHARD HERZBERG, F.R.S.

National Research Council of Canada

With the co-operation, in the first edition, of
J. W. T. SPINKS, F.R.S.C.

SECOND EDITION

CN line absorption toward diffuse ISM clouds



Nobel prize in chemistry
in 1971

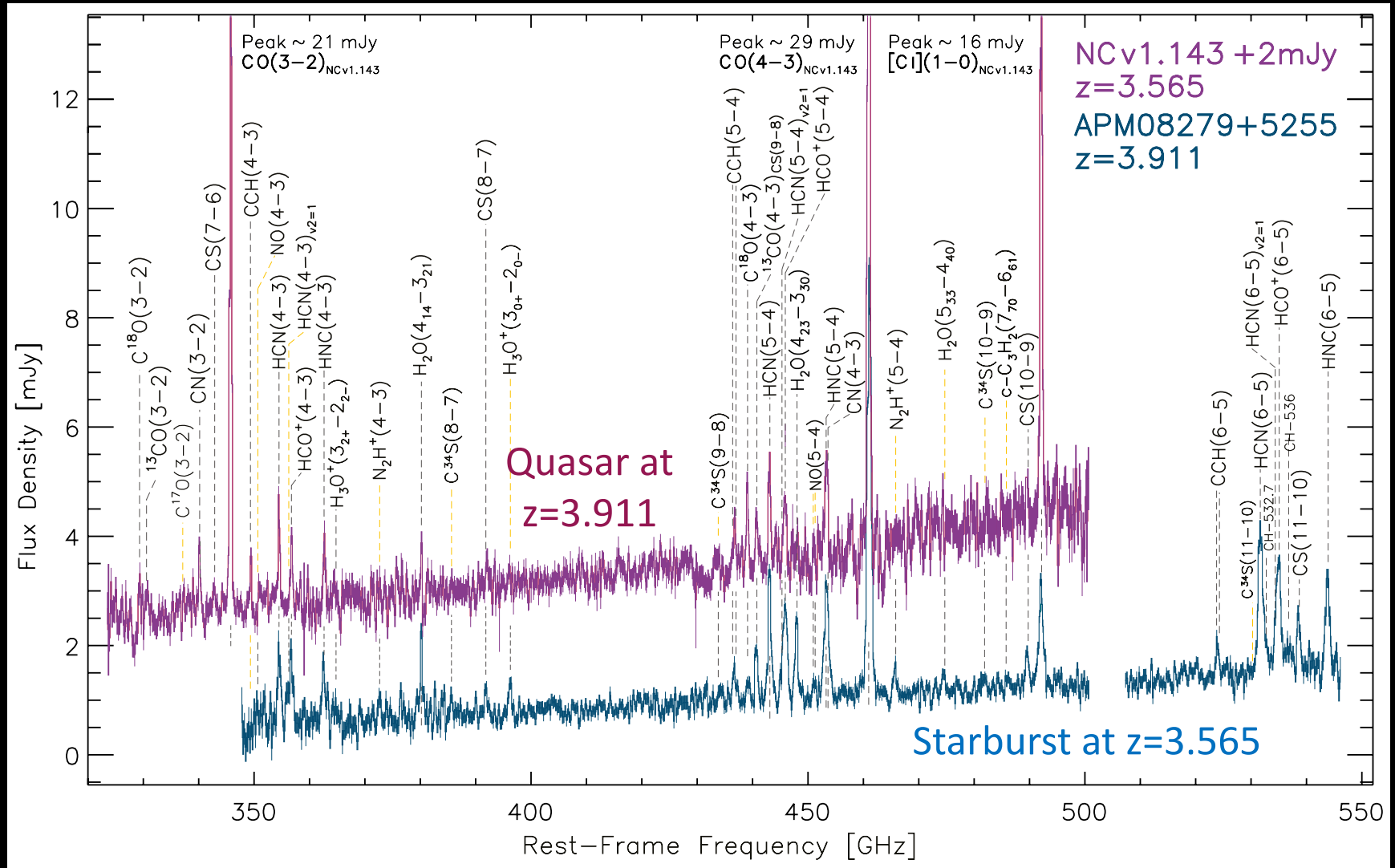
but he did not know
about Cosmology

At the low gas densities of diffuse clouds, collisional
excitation is negligible, thus $T_{\text{ex}} (\text{molecules}) \approx T_{\text{background}}$

The observation that in interstellar space only the very lowest rotational levels of CH, CH⁺, and CN are populated is readily explained by the depopulation of the higher levels by emission of the far infrared rotation spectrum (see p. 43) and by the lack of excitation to these levels by collisions or radiation. The intensity of the rotation spectrum of CN is much smaller than that of CH or CH⁺ on account of the smaller dipole moment as well as the smaller frequency [due to the factor ν^4 in (I, 48)]. That is why lines from the second lowest level ($K = 1$) have been observed for CN. From the intensity ratio of the lines with $K = 0$ and $K = 1$ a rotational temperature of 2.3° K follows, which has of course only a very restricted meaning. **1950**

Nearly 15 years before Penzias & Wilson discovery of the CMB in the radio (Nobel Prize) ...

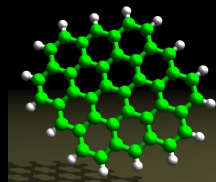
Yes, molecules are there, everywhere !



Yang+2023 with IRAM's NOEMA interferometer

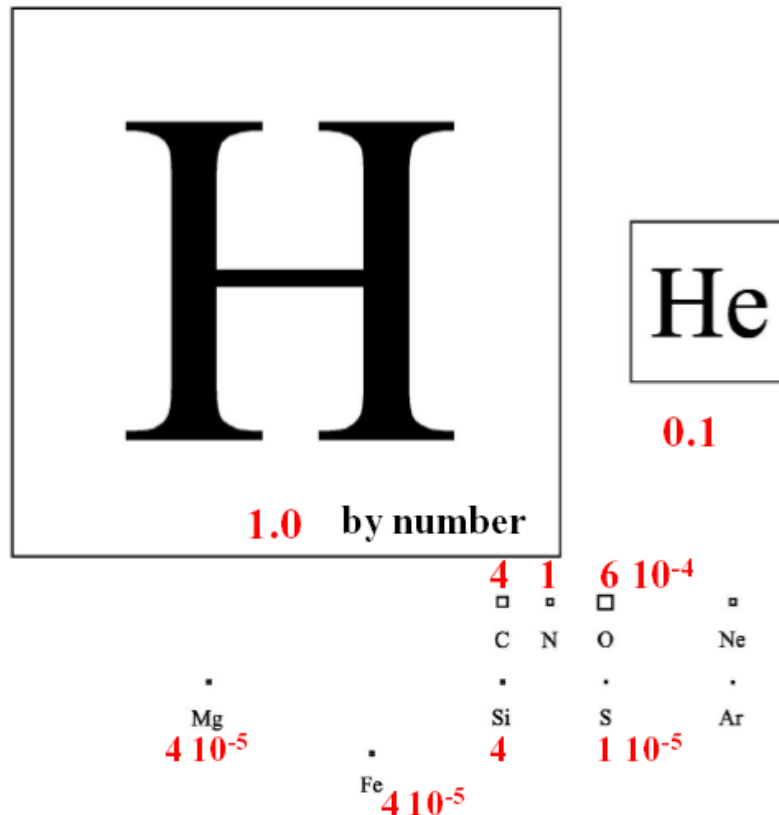
$$\text{freq}_{\text{obs}} = \text{freq}_{\text{rest-frame}} \cdot (1+z)^{-1}$$

Molecules in Space

- **About 330 molecules found in Space** (~75 in galaxies)
- **H₂** most abundant species (... **CO**)
- **H₂O, CH⁺, ...** simple hydrides → first steps of ISM chemistry
- **Polycyclic Aromatic Hydrocarbons** 
- **HCOCH₂OH** glycolaldehyde, simplest sugar + **COMs** ...

Elemental abundances in Universe

The Astronomers' Periodic Table



The number of C, N, O, S ... atoms represents
< 0.1% of H atoms.

I'm sorry Dr. Eddington ...

Molecules are very important !

- Exotic chemistry and unique laboratory
 - Chemical composition evolves with time
- } *Astrochemistry*
-
- Molecules as diagnostics (T_{kin} , n_{H} , σ_{ν} , B , ζ_{CR} , ...)
 - Gas coolants (gravitational collapse, shocks...)
- } *Astrophysics*

Interstellar chemistry is peculiar ...

- Diffuse H₂ clouds: $n_{\text{H}_2} \sim 100 \text{ cm}^{-3}$, $T_{\text{kin}} \sim 100 \text{ K}$
- Dense molecular clouds: $n_{\text{H}_2} \sim 10^5 \text{ cm}^{-3}$, $T_{\text{kin}} \sim 10\text{-}20 \text{ K}$
- Compare with this room: $T_{\text{kin}} \sim 300 \text{ K}$ $n \sim 10^{19} \text{ cm}^{-3}$
- Best laboratory ultra-vacuum chambers: $P = 2.5 \cdot 10^{-11} \text{ mbar} \rightarrow n \sim 10^5 \text{ cm}^{-3}$

ISM = very low densities, very low temperatures \rightarrow conditions very different compared to Earth !!

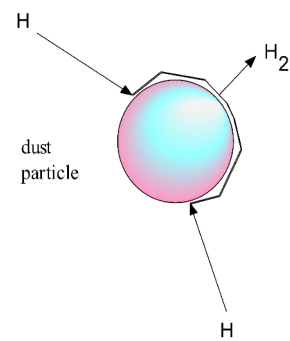
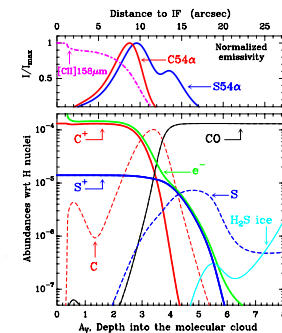
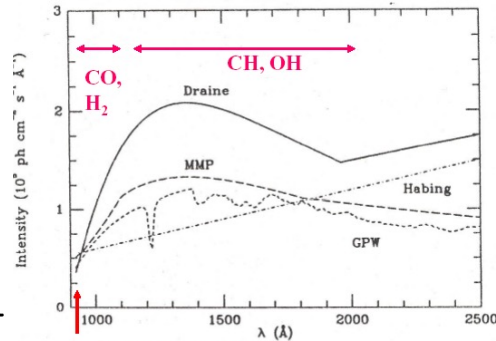
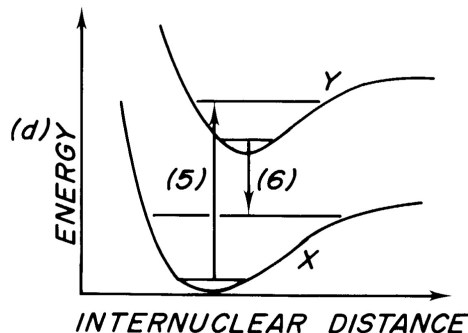
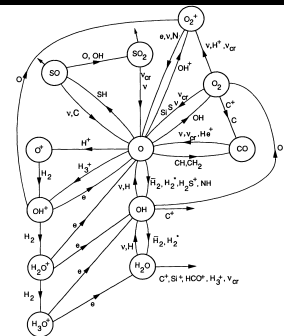
+ chemistry affected by presence of UV-photons, X-rays, Cosmic Rays, turbulence, magnetic fields...

\rightarrow ISM chemistry is NEVER in 'thermo-chemical equilibrium'
 \rightarrow solve two body reaction kinetics: $\mathbf{A + BC = AB + C}$
(+ many quantum effects)

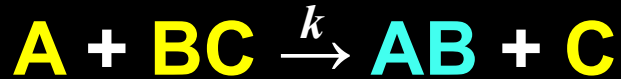
Summarized Interstellar chemistry

- 1) Need to form the basic molecule $\text{H}_2 \rightarrow$ dust grain surfaces
- 2) We need atomic (C^+ , S^+ , O^+ ,) and molecular ions ($\text{H}_2 + \text{O}^+ \rightarrow \text{OH}^+ + \text{H}$):
 - FUV-photons from massive OB-type stars
 - Cosmic-ray particles

Gas-phase molecules are (predominantly) synthesised in exothermic reactions in the gas and on the surfaces of tiny grains (many exceptions!).



BIMOLECULAR REACTIONS IN THE ISM



$k(T)$ = “reaction rate coefficient”

$$[k] = \text{cm}^3 \text{ s}^{-1} \sim \sigma (\text{cm}^2) \cdot v (\text{cm s}^{-1})$$

β = “photodissociation rate”

$$[\beta] = (\text{molecules}) \text{ s}^{-1}$$

$$F = \text{Formation rate of AB} = k \cdot n(\text{A}) \cdot n(\text{BC}) \quad [\text{cm}^{-3} \text{ s}^{-1}]$$

$$D = \text{Destruction rate of AB} = \beta \cdot n(\text{AB}) \quad [\text{cm}^{-3} \text{ s}^{-1}]$$

$n(\text{AB})$ as function of time ?

$$d/dt \ n(\text{AB}, t) = F - D = k \ n(\text{A}, t) \ n(\text{BC}, t) - \beta \ n(\text{AB}, t)$$

$$\text{Steady-state} \rightarrow d/dt \ n(\text{AB}) = 0 \rightarrow n(\text{AB}) = k \ n(\text{A}) \cdot n(\text{BC}) / \beta$$

(time to reach steady-state is $\sim 1/\beta$, $\beta \sim 10^{-10} \text{ s}^{-1}$ $1/\beta \sim 300 \text{ yr}$)

Astrochemical models contain thousands of reactions but only a few reaction types:

■ Formation of bonds reaction rate $k(T) \sim \sigma \cdot v$:

- Radiative association: $10^{-13} \text{ cm}^3 \text{ s}^{-1}$ $X^+ + Y \rightarrow XY^+ + h\nu$
- Associative detachment $X^- + Y \rightarrow XY + e$
- Grain surface: $3 \cdot 10^{-17} \text{ cm}^3 \text{ s}^{-1}$ (e.g. H_2) $X + Y:g \rightarrow XY + g$

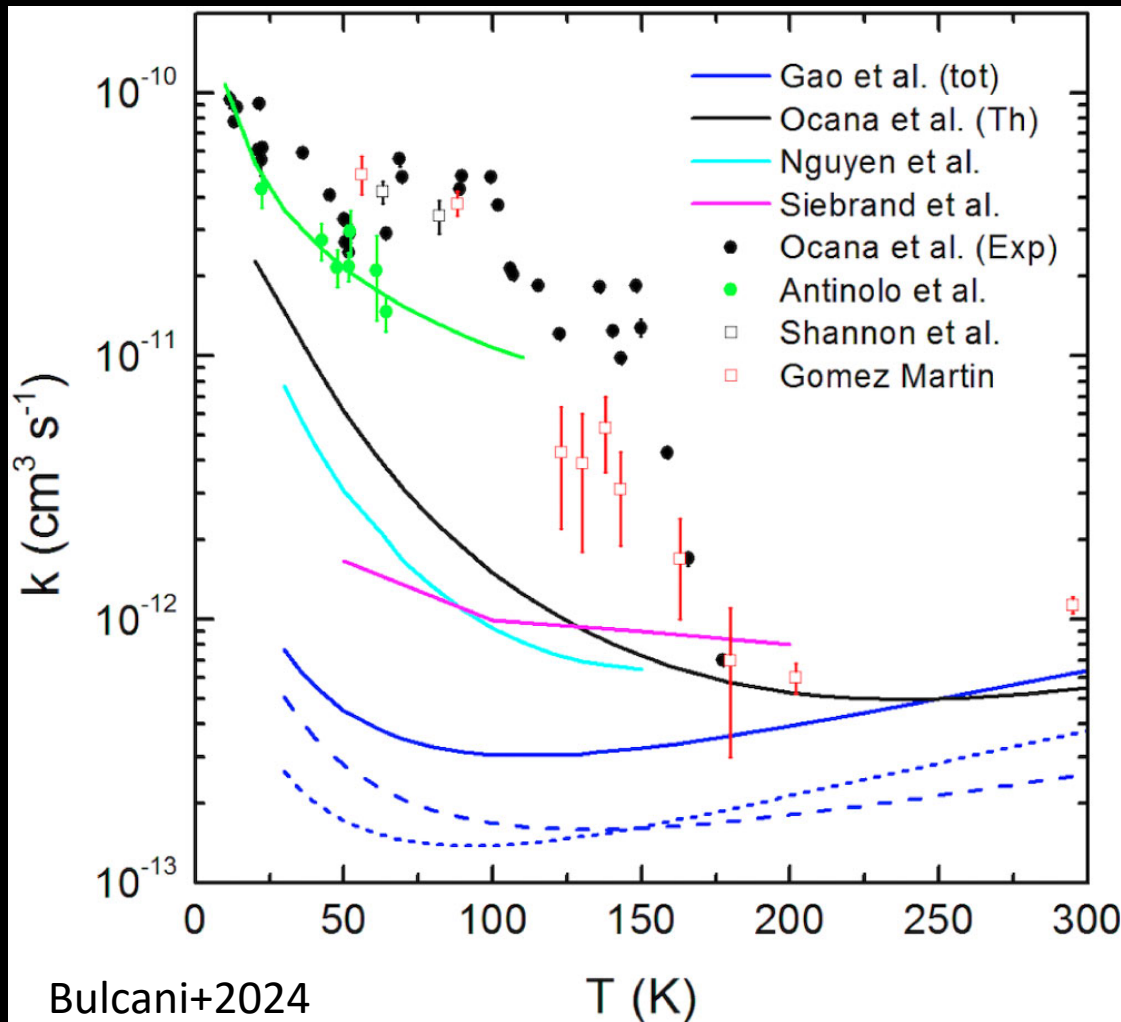
■ Destruction of bonds

- Photo-dissociation: $10^{-9} - 10^{-12} \text{ s}^{-1}$ $XY + h\nu \rightarrow X + Y$
- Dissociative recombination: $10^{-6} \text{ cm}^3 \text{ s}^{-1}$ $XY^+ + e \rightarrow X + Y$
- Collisional dissociation: $XY + M \rightarrow X + Y + M$

■ Rearrangement of bonds

- Ion-molecule reactions: $10^{-9} \text{ cm}^3 \text{ s}^{-1}$ $X^+ + YZ \rightarrow XY^+ + Z$
- Charge-transfer reactions: $10^{-9} \text{ cm}^3 \text{ s}^{-1}$ $X^+ + YZ \rightarrow X + YZ^+$
- Neutral-neutral reactions: $10^{-12} \text{ cm}^3 \text{ s}^{-1}$ $X + YZ \rightarrow XY + Z$
 $+ E_{\text{barrier}}$

Negative temperature dependence of many reactions



$$k(T) = a(T/300)^b \exp(-c/kT) \quad [\text{cm}^3 \text{s}^{-1}]$$

Arrhenius-law fit

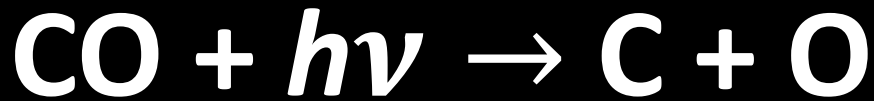


**FAST COLD INTERSTELLAR
CHEMISTRY !**



PHOTO-DISSOCIATION of MOLECULAR GAS:

- Stellar FUV photons dissociate molecules:



$$\beta_{\text{CO}} = G_0 \cdot 2.4 \cdot 10^{-10} \text{ (s}^{-1}\text{)}$$

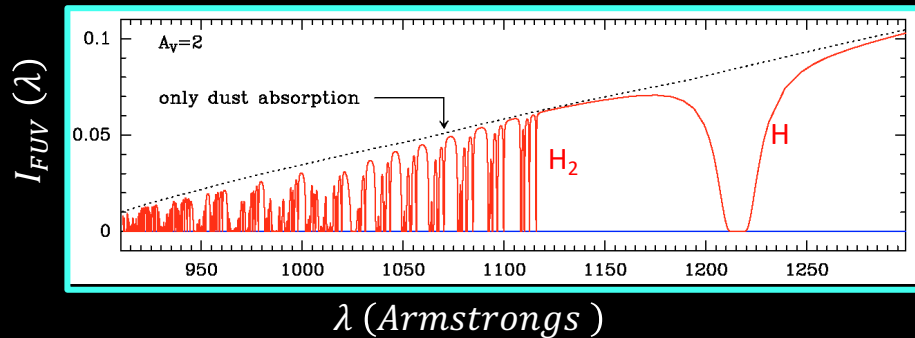
Photodissociation rate β :

$$\beta \text{ (dissociation s}^{-1}\text{)} = \int_{911\text{\AA}}^{2400\text{\AA}} I_{\text{FUV}}(\lambda) \sigma_{\text{dissociation}}(\lambda) d\lambda$$

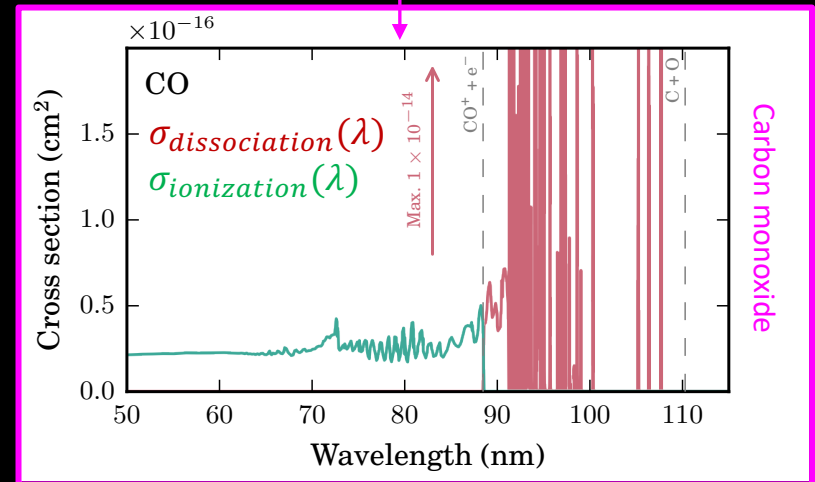
Stellar physics &
FUV propagation

Molecular Physics

FUV radiation field inside a molecular cloud



Goicoechea & Le Boulot 2007



Heays, Bosman, van Dishoeck 2017

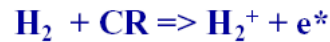
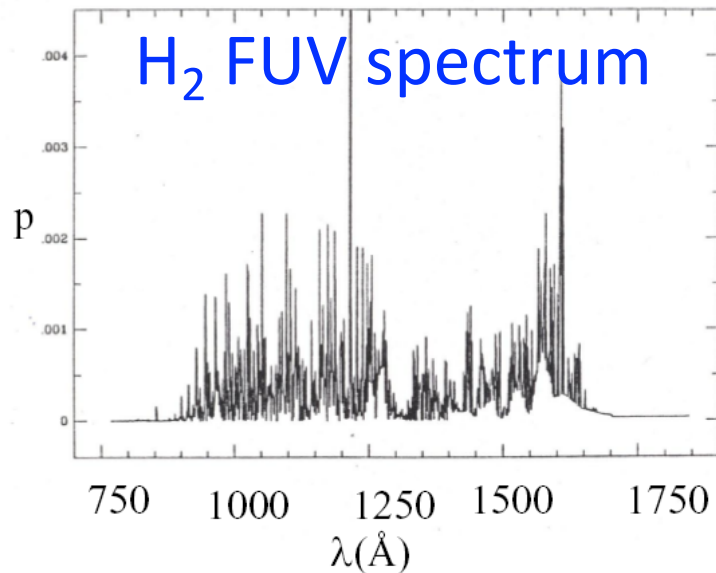
$I_{\text{FUV}}(\lambda)$ = FUV radiation field in photons $\text{cm}^{-2} \text{s}^{-1}$ at each λ and each cloud-depth position

$\sigma_{\text{dissociation}}(\lambda)$ = photodissociation cross-section in $\text{cm}^2 \rightarrow$ experiments or quantum calculations

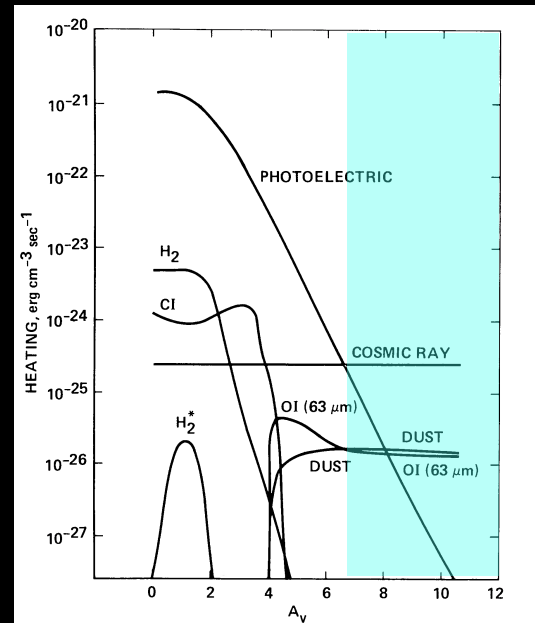
Dark molecular clouds are not completely dark

Molecular clouds with $n(\text{H}_2) > 10^3 \text{ cm}^{-3}$

Cosmic-ray induced FUV radiation ("secondary FUV photons")



Prasad & Tarafdar 1983
Gredel et al. 1987



$G_0 = 10^{-4}$ deep inside molecular clouds

(May affect the chemistry of grain ice mantles in cloud interiors)

(Astro)chemical reaction data bases

Gas-phase chemical reactions:

Typical models contain ~5000 reactions between ~450 species up to 13 atoms

<https://umistdatabase.uk> (UMIST-UDFA, T. Millar et al.)

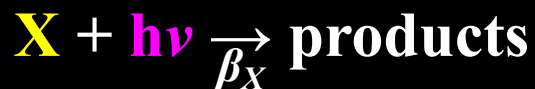
<http://kida.obs.u-bordeaux1.fr> (KIDA-Bordeaux, Wakelam, Herbst, et al.)

<http://home.strw.leidenuniv.nl/~ewine/photo/> (Photo-rates, E. van Dishoeck)

$$k(T)=a(T/300)^b \exp (-c/kT) \text{ [cm}^3 \text{ s}^{-1}] \quad \textit{Arrhenius law}$$

$$k_{photo}(A_v)=G_0 \cdot \beta \exp (-\alpha A_v) \text{ [s}^{-1}]$$

Computational chemistry



One differential equation per species in the network:

$$d/dt \, n_X = F - D = \sum_A \sum_B k_{AB} n_A n_B - (\sum_C k_{XC} n_C + \beta_X) n_X$$

+ Conservation equations:

$$\text{Carbon } n_C = n(C^+) + n(C) + n(CO) + n(CH) \dots + 2n(C_2) + 2n(C_2H) + \dots$$

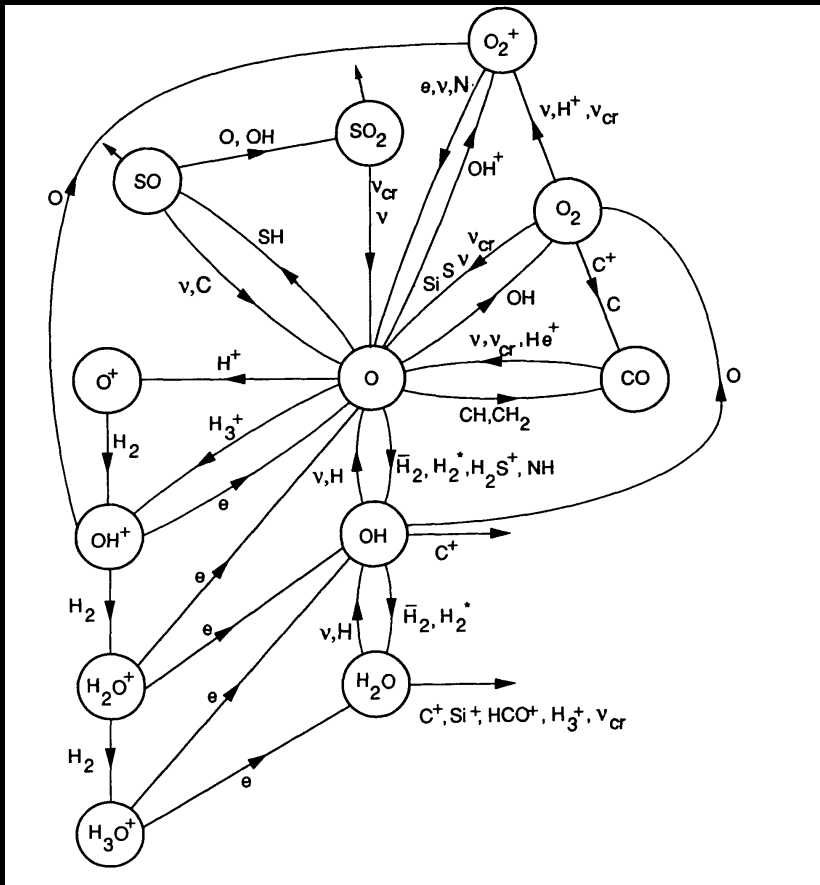
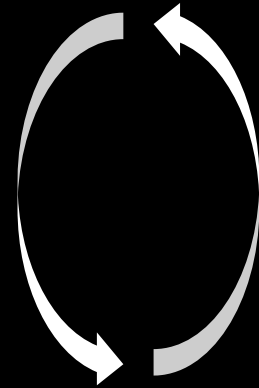
$$\dots$$
$$\text{Charge } n_e = n(C^+) + n(H^+) + n(H_3^+) + \dots$$

SOLVED ITERATIVELY

(eg. Netwon-Raphson techniques
when $dn/dt = 0$ steady-state)

Ideal astrochemical models

- Input radiation field (UV) → output atomic/molecular line emission
- Gas heating & cooling → T_{gas} (depends on composition!) + T_{dust}
- Chemistry (gas + grain surface) → abundances (depend on T)



Several iterations
needed

But remember, reaction rates
are often uncertain...,
→ **Model predictions are
uncertain (factors ~2 to 10)**
e.g. Wakelam et al. 2005

The *Meudon* PDR code (public)

[CODES](#)[ISMDB](#)[TOOLS](#)[TECHNOLOGIES](#)[PARTNERS](#)[REGISTER](#)[PDR Code](#)[Download](#)[Tools](#)

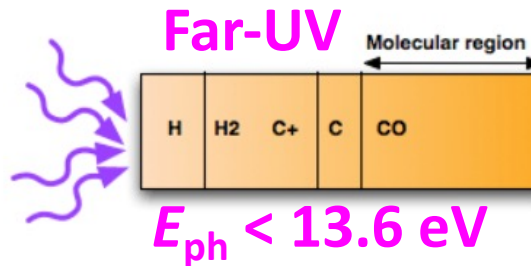
<https://pdr.obspm.fr>

PDR Code FUV-dominated Photodissociation regions

The code considers a stationary plane-parallel slab of gas and dust illuminated by a radiation field coming from one or both sides of the cloud. The incident radiation field can be the Interstellar Standard Radiation Field (ISRF) and/or a star.

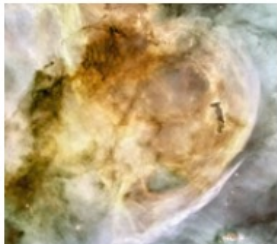
It solves at each point in the cloud, the radiative transfer in the UV taking into account the absorption in the continuum by dust and in discrete transitions of H and H₂. The model computes the thermal balance taking into account heating processes such as the photoelectric effect on dust, chemistry, cosmic rays, etc. and cooling resulting from infrared and millimeter emission of the abundant species.

Chemistry is solved for any number of species and reactions.



Once abundances of atoms and molecules and level excitation of the most important species have been computed at each position in the cloud, line intensities and column densities can be deduced by a post-processor code.

The Meudon PDR code can be used to study the physics and chemistry of diffuse clouds, photodissociation regions (PDRs), dark clouds, ...



LERMA - Paris Observatory

Scientists and engineers

Emeric Bron (*scientist*)
David Languignon (*engineer*)
Jacques Le Bourlot (*scientist*)
Franck Le Petit (*scientist*)
Nicolas Moreau (*engineer*)
Evelyne Roueff (*scientist*)

References

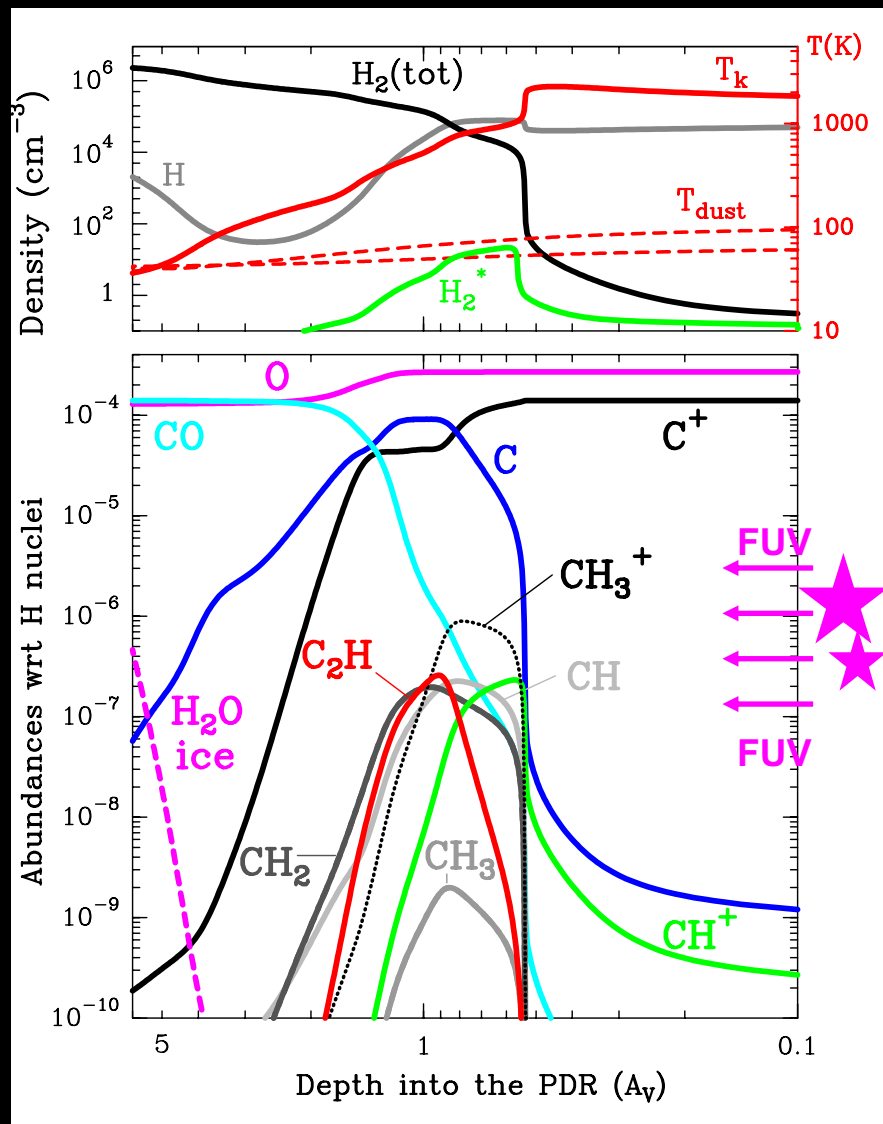
- Le Petit et al., 2006, ApJS, 164, 506
- Goicoechea et al., 2007, A&A, 467, 1
- Gonzalez Garcia et al., 2008, A&A, 485, 127
- Le Bourlot et al., 2012, A&A, 541, 76
- Bron E., 2014, Thesis
- Bron et al., 2014, A&A, 569, 100
- Bron et al., 2016, A&A, 588, 27

G_0
 P_{th}

γ_{CRs}
 M^+
...

FUV radiative transfer + heating/cooling + chemistry + molecular excitation

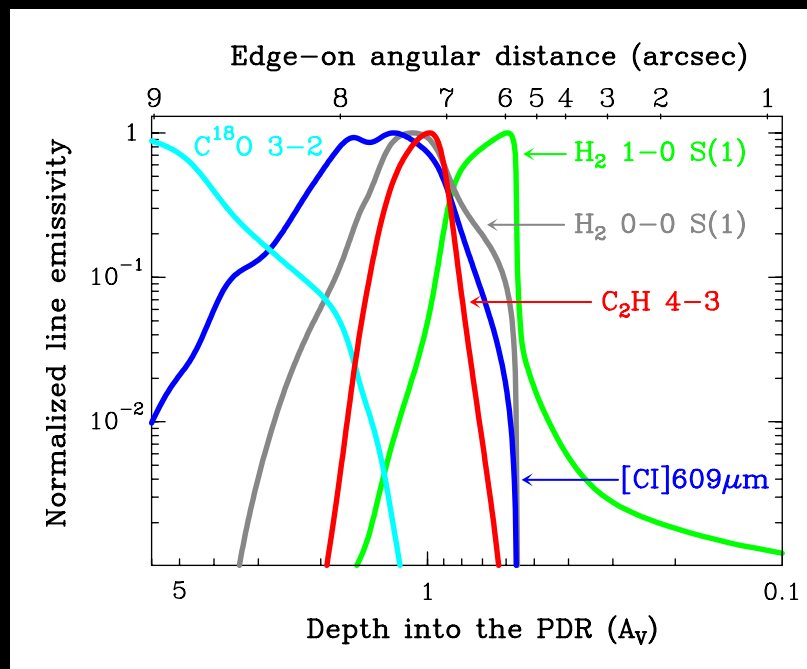
Typical output



Physical structure

Chemical abundances

Line emission stratification:



Example from Goicoechea +2025, A&A

The Orion Bar PDR, $G_0 = 2 \cdot 10^4$, $P_{\text{th}} = 10^8 \text{ K cm}^{-3}$

The InterStellar Medium DataBase (ISMDB) allows quick and easy access to precalculated theoretical models for various ISM conditions and objects. ISMDB includes models produced by the [Meudon PDR code](#) and the [Paris-Durham shock code](#).

Presently, ISMDB gives access to several thousands [PDR 1.5.4](#) models covering different astrophysical conditions. Later, it will also contains [shock](#) models produced by the Paris-Durham shock code and it will be extended to other astrophysical conditions.

Prepare and interpret observations

To prepare and interpret observations, ISMDB provides an inverse search service to allow:

- queries on observables to find the best models that match observations
- access to line intensity maps in a parameter space (ex: density, UV flux) to prepare observations
- download model results without running the code

Search models in ISMDB

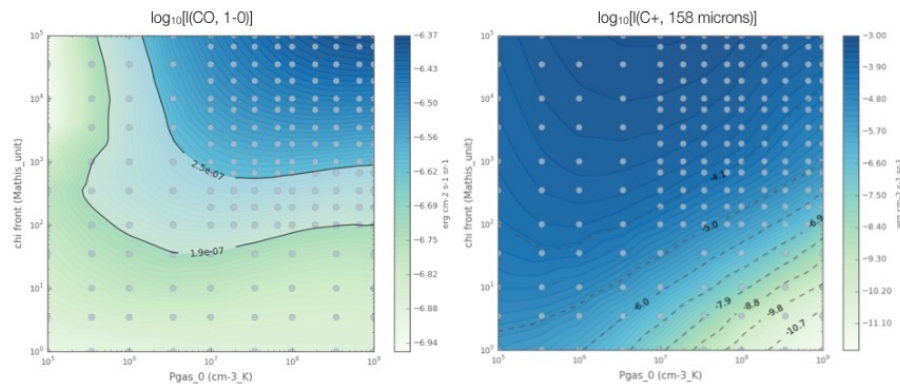
Examples

To find the best models that have $I(\text{CO } 1-0)$ between $2.4\text{E-}9$ and $7.2\text{E-}8 \text{ erg cm}^{-2} \text{ s}^{-1} \text{ sr}^{-1}$ for a face on PDR, enter in ISMDB:

- $I(\text{CO } v=0, J=1 \rightarrow v=0, J=0 \text{ angle } 00 \text{ deg}) > 1.9\text{e-}7$
- $I(\text{CO } v=0, J=1 \rightarrow v=0, J=0 \text{ angle } 00 \text{ deg}) < 2.5\text{e-}7$

To get estimations of the C^+ 158 microns line intensity, enter in ISMDB:

- $I(\text{C}^+ \text{ El}=2\text{P}, J=3/2 \rightarrow \text{El}=2\text{P}, J=1/2 \text{ angle } 00 \text{ deg})$



Content of ISMDB

October 2021

- PDR 1.5.4 – isochoric PDR models
- PDR 1.5.4 – isobaric PDR models

December 2016

- PDR 1.5.2 – isochoric PDR models
- PDR 1.5.2 – isobaric PDR models

Pre-run PDR models & quick diagnostic plots

Shock models coming soon...

The PDR toolbox

PhotoDissociation Region Toolbox

TOOLS MODELS DOCUMENTS ABOUT CONTACT

<https://dustem.astro.umd.edu/tools.html>

M. Wolfire & M. Pound



Ultraviolet photons from O and B stars strongly influence the structure and emission spectra of the interstellar medium. The UV ionize hydrogen $h\nu > 13.6\text{eV}$ will create the H II region around the star, but lower energy UV photons escape. These far-UV photons $6\text{ eV} < h\nu < 13.6\text{ eV}$ are still energetic enough to photodissociate molecules and to ionize low ionization-potential atoms such as sulfur. They thus create a *photodissociation region* (PDR) just outside the H II region. In aggregate, these PDRs dominate the heating of the interstellar medium. The gas is heated by photo-electrons from grains and cools mostly through far-infrared fine structure lines.

The **PDR Toolbox** is an open-source, science-enabling tool for the community, designed to help astronomers determine the physical conditions of photodissociation regions from observations. Typical observations of both Galactic and extragalactic PDRs come from ground-based submillimeter, and far-infrared telescopes such as ALMA, SOFIA, JWST, Spitzer, and Herschel. Given a set of observations of spectral intensities, PDR Toolbox can compute best-fit FUV incident intensity and cloud density based on our models of PDR emission. Or, given physical conditions, it can compute emission excitation diagrams to determine temperature, column density, and ortho-to-para ratio.

The current version is **2.4.4** (released Feb 07, 2025)

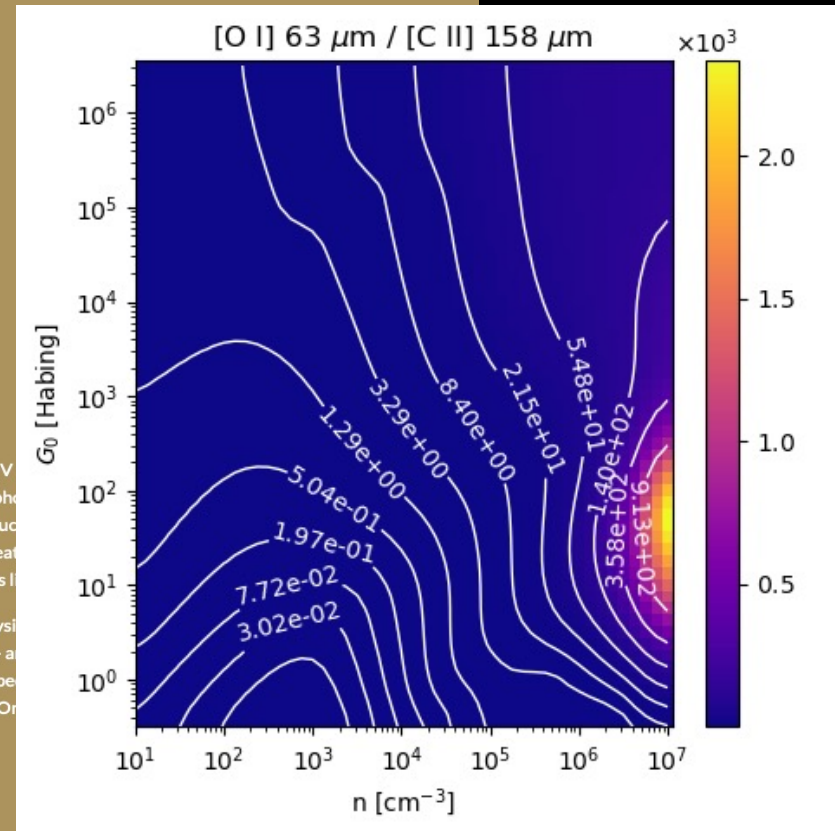
Release Highlights

- **[O I] 1.316 μm Diagnostic Diagram**

We provide guidance to help take into account viewing inclination angle when interpreting measured [O I] 1.316 μm emission line (e.g., with JWST).

- **LMC metallicity surface temperature**

We have computed models for surface temperature at the metallicity of the Large Magellanic Cloud ($z=0.5$).



Quick diagnostic plots

Cloudy photoionization code (public)

README.md

<https://gitlab.nublado.org/cloudy/cloudy>

Cloudy

HII regions and more

Cloudy is an *ab initio* spectral synthesis code designed to model a wide range of interstellar "clouds", from H II regions and planetary nebulae, to Active Galactic Nuclei, and the hot intracluster medium that permeates galaxy clusters.

Cloudy has been in continuous development since 1978, led by Gary Ferland, and in close collaboration with a number of scientists -- see the [list of contributors](#).

Version

Includes extreme-UV (EUV) with $E_{\text{ph}} > 13.6$ eV

The current version of Cloudy is C23, released in 2023. A summary of what is new is available [here](#).

If you used Cloudy in your research, please cite our most recent [release paper](#)

Q_{Ly}
 U
 n_e
 T_e

EUV + FUV + heating/cooling + HII region ionization + chemistry

There are other models of PDRs, shocks, HII regions ...

Interstellar chemistry makes this...

Diffuse clouds



Low densities, warm gas ~ 100 K
FUV heating & CR ionization

Simple reactive molecules:
 OH^+ , CH^+ , CH, ...

Cold & dense clouds

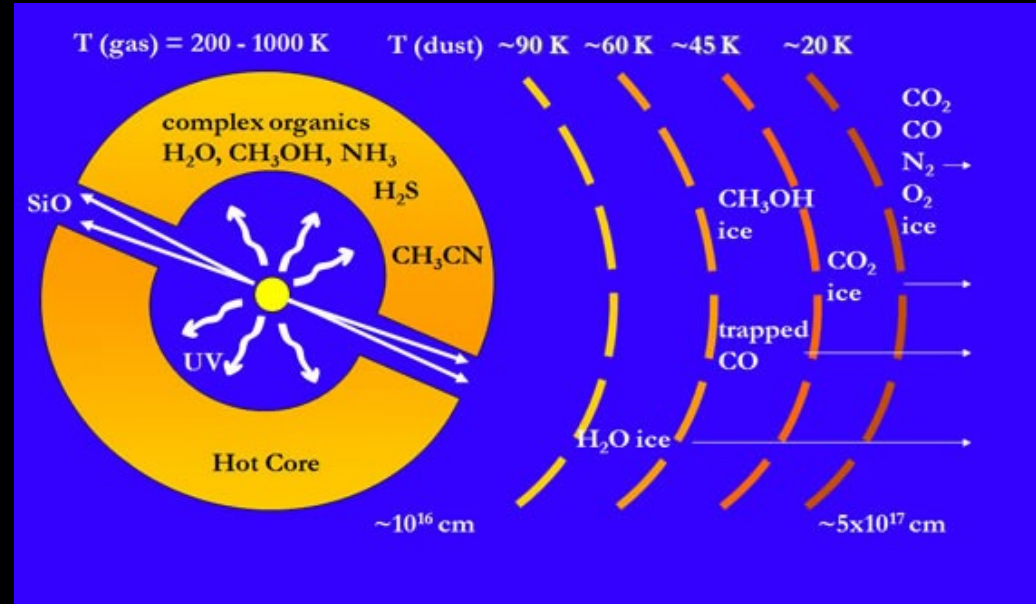


High densities, cold gas,
depletion, CR ionization...

H_2O and even CO freeze out
Deuterated species: N_2D^+ ...

Outflows and shocks

Hot Cores around massive protostars



Ice-mantle evaporation
Warm-temperature chemistry
 CH_3OH , and saturated COMs

High-Temperature chemistry
Grain sputtering

High- J CO, H_2O , OH, SiO ...

Photodissociation regions



Photochemistry,
UV dissociation and gas heating
IR emission from PAHs & H₂
Reactive molecular ions ...

Circumstellar envelopes around evolved stars



High densities, dust formation

with metals: NaCl...
refractory: TiO, SiC₂...

Take home messages

- **ISM** = A very important component of galaxies ...
- The ISM is slowly converted into stars. As the die, they return enriched matter back.
- UV , cosmic rays and shocks heat the ISM → Stellar and ISM evolution are tightly coupled
- Fascinating physical and chemical (micro) processes → collaborate with quantum chemists and experimentalists
- New developments: magnetic fields and turbulence → more sophisticated MHD simulations
- Bright future: ALMA, NOEMA, IRAM30m, JWST, SKA, ... be a multiwavelength astronomer !



THANK YOU !!