# Diffusion effects in molecular clouds

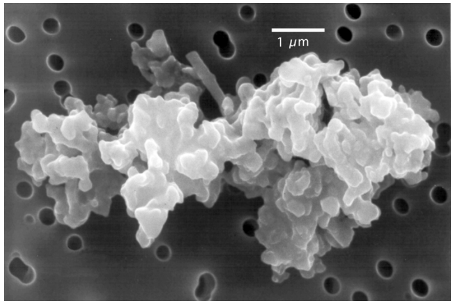
C1 Project

Aleena Baby
Doctoral student
I. Insititute of Physics,
University of Cologne
Germany

**Interstellar gas:**
Ions, atoms, and molecules in the gas phase.

**Cosmic rays:**
Ions and electrons with kinetic energies far greater than thermal.

**Electromagnetic radiation**




**Interstellar Magnetic field**

**The dark matter particles**

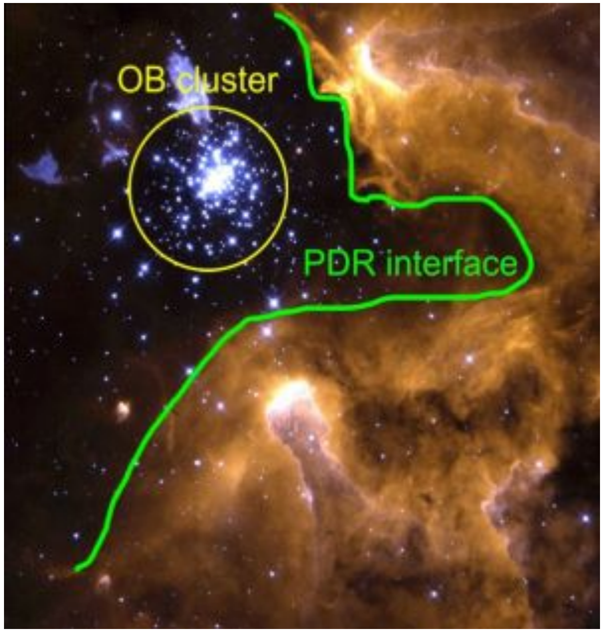
**The gravitational field**

**Interstellar dust:**
Small solid particles, mainly less than ~ 1μm in size, mixed with the interstellar gas.




baby@ph1.uni-koeln.de

- Space between stars is filled with very dilute gas with $T_{kin} \approx 10\text{-}\ 10^6$ K
- Molecules are found in the cold neutral gas
- Diffuse clouds: $T_{kin} \approx 100$ K, $n \approx 100\ cm^{-3}$
- Dense clouds: $T_{kin} \approx 10\text{-}100$ K, $n \approx 10^4\ \text{-}10^8\ cm^{-3}$




**Diffusion effects in molecular clouds**

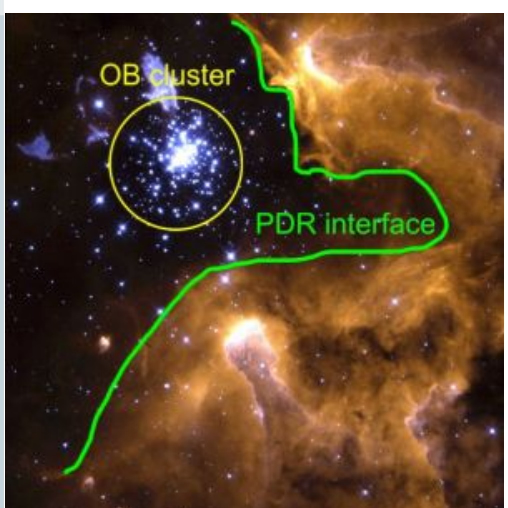
baby@ph1.uni-koeln.de

**Definition:** Neutral interstellar hydrogen gas where (6-13.6 eV) FUV radiation dominates the physical and chemical structure.

Interstellar PDRs include:

- The diffuse Warm and Cold neutral medium
- Translucent clouds: $A_v < 5$, $n_H < 1000\ cm^{-3}$ weak interstellar FUV fields.
- Dense molecular clouds: $A_v$ up to ~10, $n_H > 1000\ cm^{-3}$

  including intense FUV fields near OB stars




~90% of the Galactic molecular ISM may be "photon-dominated"

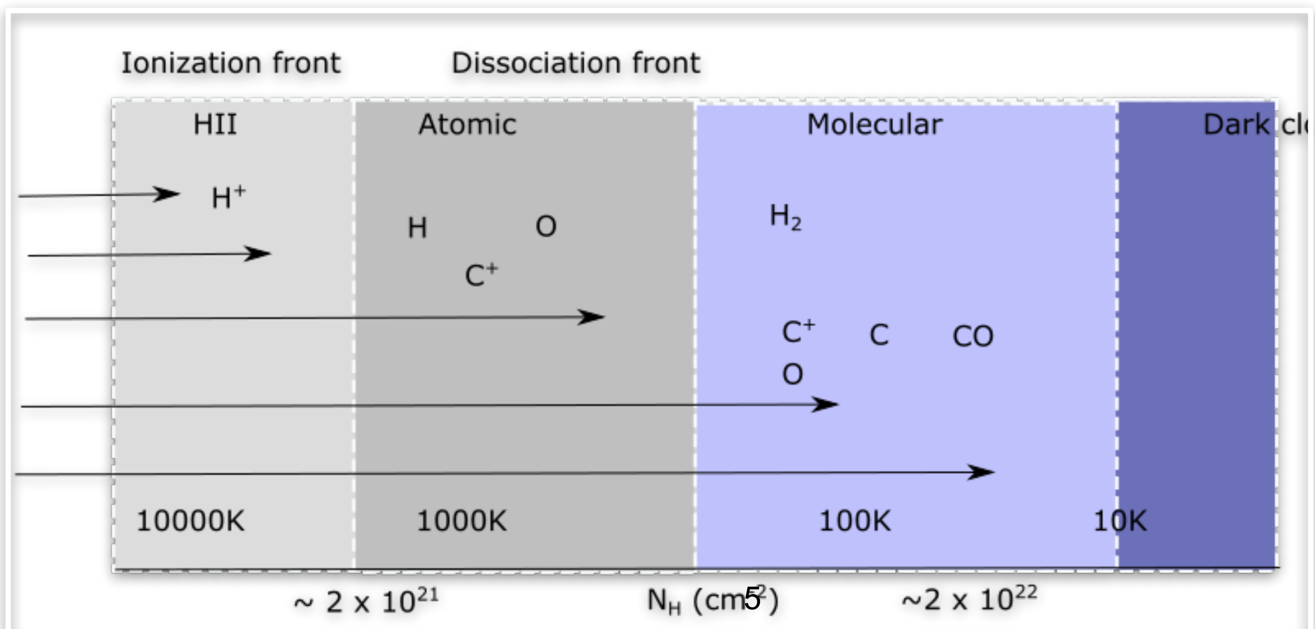




baby@ph1.uni-koeln.de

# PDR Structure:

- FUV photons penetrate a molecular cloud, ionizing, dissociating, and heating the gas.
- FUV photons with energies less than 13.6 eV will create a H/$C^+$ region.
- Once the flux of $H_2$ dissociating photons is substantially attenuated, the composition is dominated by $H_2$.
- deeper in the cloud(Av≃4) ionised carbon recombines and forms carbon monoxides.




Adapted from Hollenbach and Tielens (1999)

Diffusion effects in molecular clouds

baby@ph1.uni-koeln.de

# Important reactions

**Photoionization:**

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

**Photodissociation:**

$$AB + h\nu \rightarrow A + B$$

**Ion-neutral Exchange:**

$$\mathbf{AB^+ + C} \rightarrow \mathbb{AC}^+ + \mathbb{B}$$

**Neutral-neutral Exchange:**

$$\mathbf{AB + C} \rightarrow \mathbb{AC} + \mathbb{B}$$

**Radiative association Reactions:**

$$A + B \underset{k_d}{\overset{k_f}{\rightleftharpoons}} (AB)^* \xrightarrow{k_r} AB + h\nu$$

$K_f$ : formation reaction rate
$K_d$ : dissociation reaction rate
$K_r$ : reaction rate



baby@ph1.uni-koeln.de

# Important reactions

**Photoionization:**

$AB + h\nu \rightarrow \mathbb{AB}^{+} + e^{-}$

**Photodissociation:**

$AB + h\nu \rightarrow \mathbb{A} + \mathbb{B}$

Time scales:

$t_{coll} \approx$ 1 month at $n \approx 10^4\ cm^{-3}$

$t_{cheml} \approx 10^5 - 10^6$ yr

$t_{cloud} \approx 10^7 - 10^8$ yr

**Ion-neutral Exchange:**

$\mathbf{AB^{+} + C} \rightarrow \mathbb{AC}^{+} + \mathbb{B}$

**Neutral-neutral Exchange:**

$\mathbf{AB + C} \rightarrow \mathbb{AC} + \mathbb{B}$

**Radiative association Reactions:**

$$A + B \underset{k_d}{\overset{k_f}{\rightleftharpoons}} (AB)^{*} \xrightarrow{k_r} AB + h\nu$$

$K_f$ : formation reaction rate

$K_d$ : dissociation reaction rate

$K_r$ : reaction rate



baby@ph1.uni-koeln.de

# Interstellar clouds are very rich in chemistry!

**272 molecules**

Elemental abundances are not clearly known

~ 90%  hydrogen

~ 10%  helium

~ 0.1%  carbon, oxygen, nitrogen

< 0.01%  silicon, iron, calcium

~ $10^{-10}$ % dust (0.1 µm silicates, carbonaceous)

- ➢ Atoms & molecules
- ➢ Dust particles
- ➢ Cosmic ray particles
- ➢ Photons
- ➢ electron

**Molecules in the Interstellar Medium or Circumstellar Shells (as of 06/2022)**

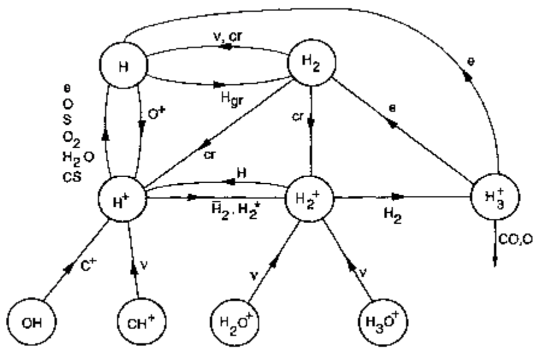
| 2 atoms | 3 atoms | 4 atoms | 5 atoms | 6 atoms | 7 atoms | 8 atoms | 9 atoms | 10 atoms | 11 atoms | 12 atoms |
|---|---|---|---|---|---|---|---|---|---|---|
| $H_2$ | $C_3$* | c-$C_3H$ | $C_5$* | $C_5H$ | $C_6H$ | $CH_3C_3N$ | $CH_3C_4H$ | $CH_3C_5N$ | $HC_9N$ | c-$C_6H_6$* |
| AlF | $C_2H$ | l-$C_3H$ | $C_4H$ | l-$H_2C_4$ | $CH_2CHCN$ | $HC(O)OCH_3$ | $CH_3CH_2CN$ | $(CH_3)_2CO$ | $CH_3C_6H$ | n-$C_3H_7CN$ |
| AlCl | $C_2O$ | $C_3N$ | $C_4Si$ | $C_2H_4$* | $CH_3C_2H$ | $CH_3COOH$ | $(CH_3)_2O$ | $(CH_2OH)_2$ | $C_2H_5OCHO$ | i-$C_3H_7CN$ |
| $C_2$** | $C_2S$ | $C_3O$ | l-$C_3H_2$ | $CH_3CN$ | $HC_5N$ | $C_7H$ | $CH_3CH_2OH$ | $CH_3CH_2CHO$ | $CH_3OC(O)CH_3$ | $C_2H_5OCH_3$ |
| CH | $CH_2$ | $C_3S$ | c-$C_3H_2$ | $CH_3NC$ | $CH_3CHO$ | $C_6H_2$ | $HC_7N$ | $CH_3CHCH_2O$ | $CH_3C(O)CH_2OH$ | 1-c-$C_5H_5CN$ (2021) |
| $CH^+$ | HCN | $C_2H_2$* | $H_2CCN$ | $CH_3OH$ | $CH_3NH_2$ | $CH_2OHCHO$ | $C_8H$ | $CH_3OCH_2OH$ | c-$C_5H_6$ (2021) | 2-c-$C_5H_5CN$ (2021) |
| CN | HCO | $NH_3$ | $CH_4$* | $CH_3SH$ | c-$C_2H_4O$ | l-$HC_6H$* | $CH_3C(O)NH_2$ | c-$C_6H_4$ (2021) | $HOCH_2CH_2NH_2$ (2021) | $CH_3C_7N$ (?) (2022) |
| CO | $HCO^+$ | HCCN | $HC_3N$ | $HC_3NH^+$ | $H_2CCHOH$ | $CH_2CHCHO$ | $C_8H^-$ | $H_2CCCHC_3N$ (2021) | | n-$C_3H_7OH$ (2022) |
| $CO^+$ | $HCS^+$ | $HCNH^+$ | HCCNC | HCCCHO | $C_6H^-$ | $CH_2CCHCN$ | $C_3H_6$ | $C_2H_5NCO$ (2021) | | i-$C_3H_7OH$ (2022) |
| CP | $HOC^+$ | HNCO | HCOOH | $NH_2CHO$ | $CH_3NCO$ | $H_2NCH_2CN$ | $CH_3CH_2SH$ | $C_2H_5NH_2$ (?) (2021) | | |
| SiC | $H_2O$ | HNCS | $H_2CNH$ | $C_5N$ | $HC_5O$ | $CH_3CHNH$ | $CH_3NHCHO$ | $HC_7NH^+$ (2022) | | |
| HCl | $H_2S$ | $HOCO^+$ | $H_2C_2O$ | l-$HC_4H$* | $HOCH_2CN$ | $CH_3SiH_3$ | $HC_7O$ | | | |
| KCl | HNC | $H_2CO$ | $H_2NCN$ | l-$HC_4N$ | HCCCHNH | $H_2NC(O)NH_2$ | HCCCHCHCN (2021) | | | |
| NH | HNO | $H_2CN$ | $HNC_3$ | c-$H_2C_3O$ | $HC_4NC$ | $HCCCH_2CN$ | $H_2CCHC_3N$ (2021) | | | |
| NO | MgCN | $H_2CS$ | $SiH_4$* | $H_2CCNH$ | c-$C_3HCCH$ (2021) | $HC_5NH^+$ | $H_2CCCHCCH$ (2021) | | | |
| NS | MgNC | $H_3O^+$ | $H_2COH^+$ | $C_5N^-$ | l-$H_2C_5$ (2021) | $CH_2CHCCH$ (2021) | HOCHCHCHO (?) (2022) | | | |
| NaCl | $N_2H^+$ | c-$SiC_3$ | $C_4H^-$ | HNCHCN | $MgC_5N$ (2021) | $MgC_6H$ (2021) | | | | |
| OH | $N_2O$ | $CH_3$* | HC(O)CN | $SiH_3CN$ | $CH_2C_3N$ (2021) | $C_2H_3NH_2$ (2021) | | | | |
| PN | NaCN | $C_3N^-$ | HNCNH | $C_5S$ | | $(CHOH)_2$ (2022) | | | | |
| SO | OCS | $PH_3$ | $CH_3O$ | $MgC_4H$ | | | | | | |
| $SO^+$ | $SO_2$ | HCNO | $NH_4^+$ | $CH_3CO^+$ (2021) | | | | | | |
| SiN | c- | HOCN | $H_2NCO^+$ | [illegible] | | | | | | |

**Diffusion effects in molecular clouds**

baby@ph1.uni-koeln.de

July 14, 2022

# PDR chemistry: Chemical networks



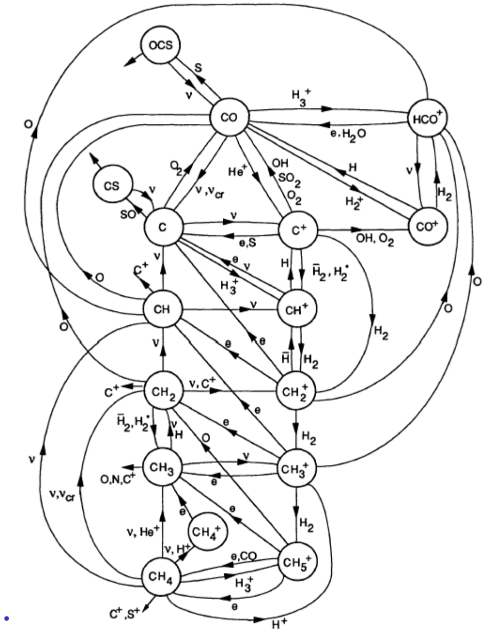




FIG. 3.—Carbon network

- Lead to the synthesis of the atomic and molecular species.
- Vary with the cloud depth as the local radiation field, and gas temperature varies.

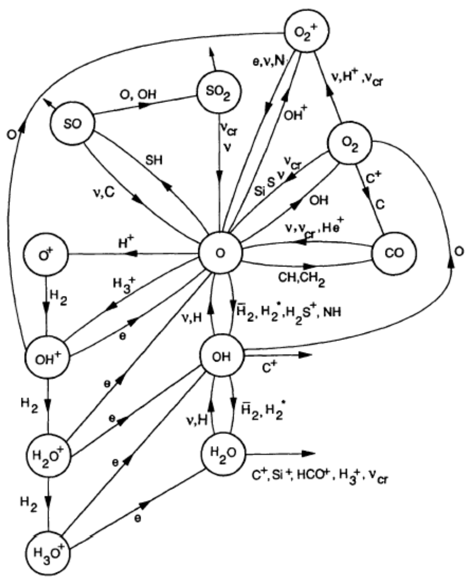
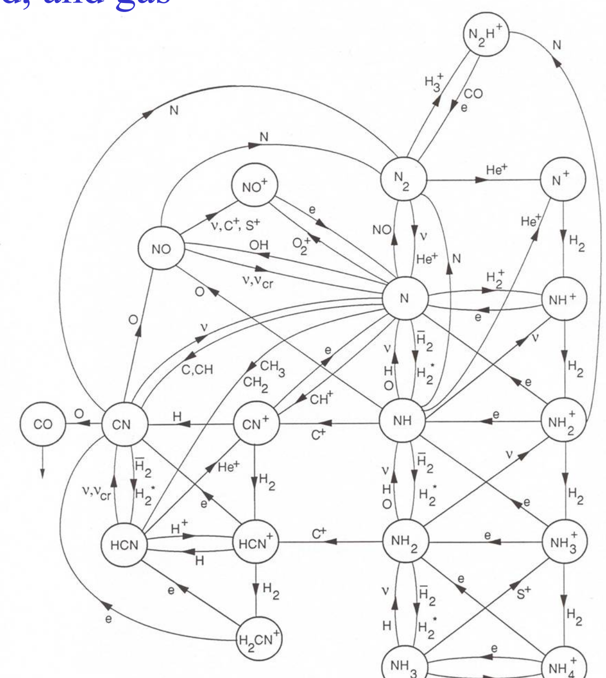



FIG. 2.—Oxygen network




NITROGEN

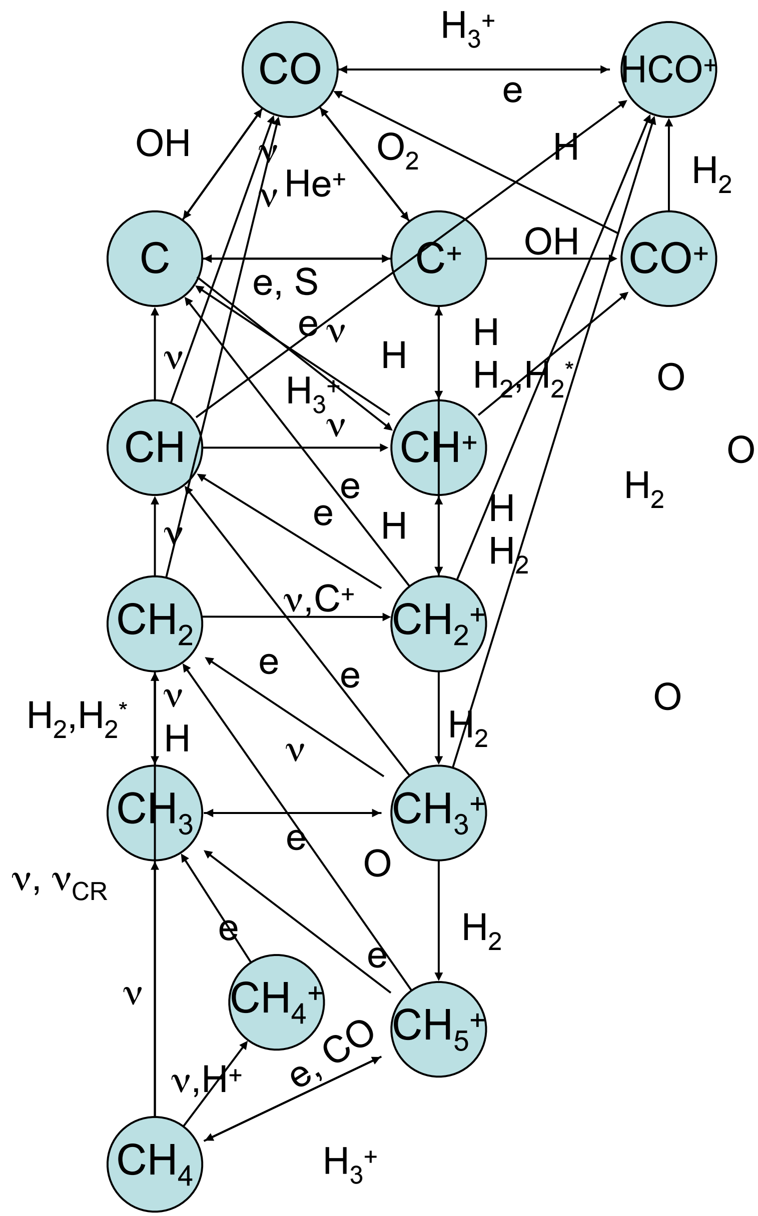
**Diffusion effects in molecular clouds**

baby@ph1.uni-koeln.de

July 14, 2022

# The carbon road map

- How to get from A to B
- Some points are quick some are slow
- Unlike any normal road map, some slow paths may become very quick under certain conditions




baby@ph1.uni-koeln.de

**Diffusion effects in molecular clouds**

July 14, 2022

Example: **Diffuse Cloud**

starting point: $C^+$

collision with $H_2$:

ΔE=4600K

$\cancel{C^+ + H_2 \rightarrow CH^+ + H}$

k ≈ $10^{-15}$ $cm^3s^{-1}$

instead:

$C^+ + H_2 \rightarrow CH_2^+ + \nu$

k ≈ $10^{-9}$ $cm^3s^{-1}$

$CH_2^+ + H_2 \rightarrow CH_3^+ + H$

then:

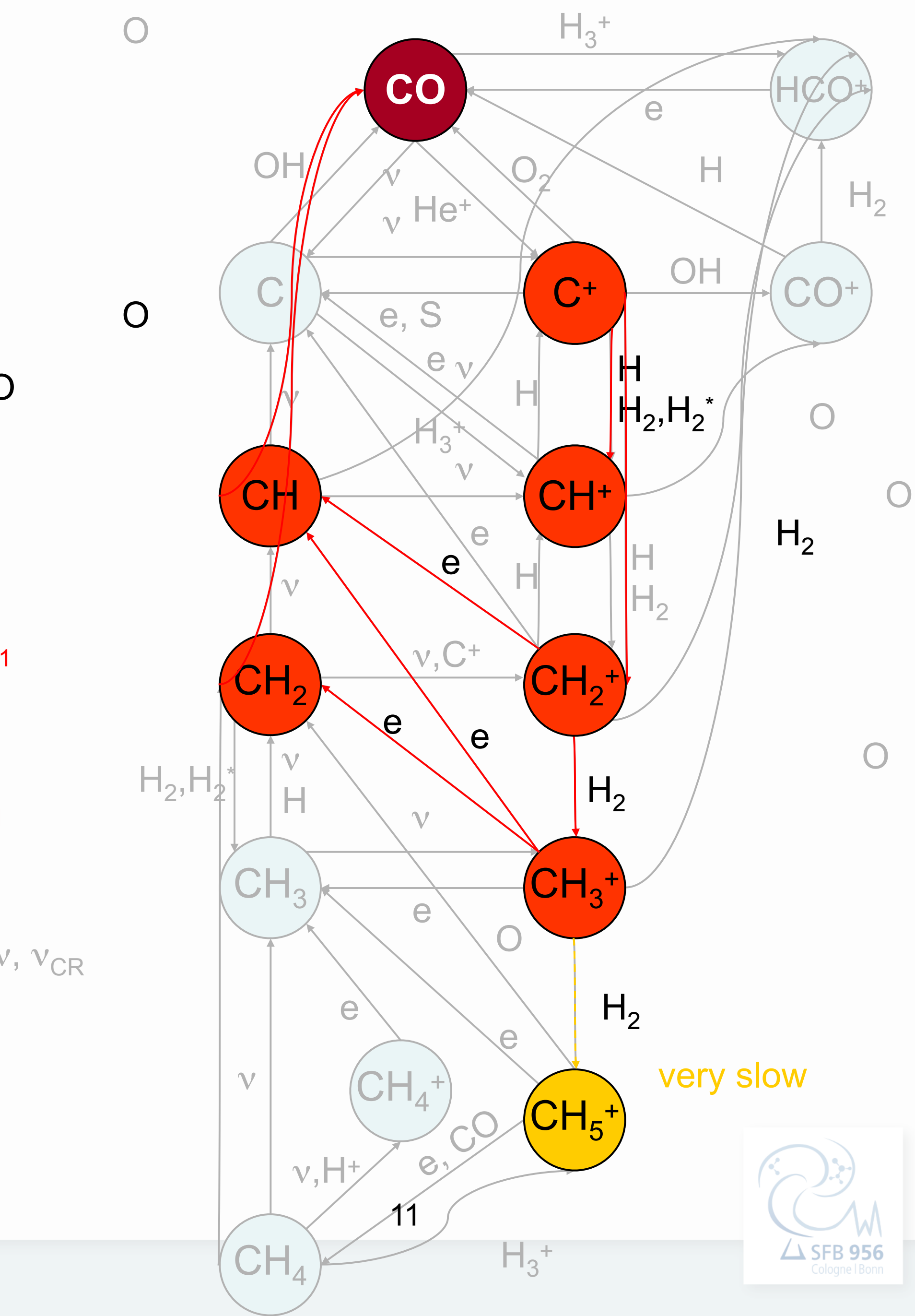
k ≈ $10^{-7}$ $cm^3s^{-1}$

$CH_n^+ + e \rightarrow CH_{n-1} + H$

and:

k ≈ $10^{-10}$ $cm^3s^{-1}$

$CH_n + O \rightarrow CO + n\,H$



# Example: **PDR**

high FUV intensity heats

the gas at the surface

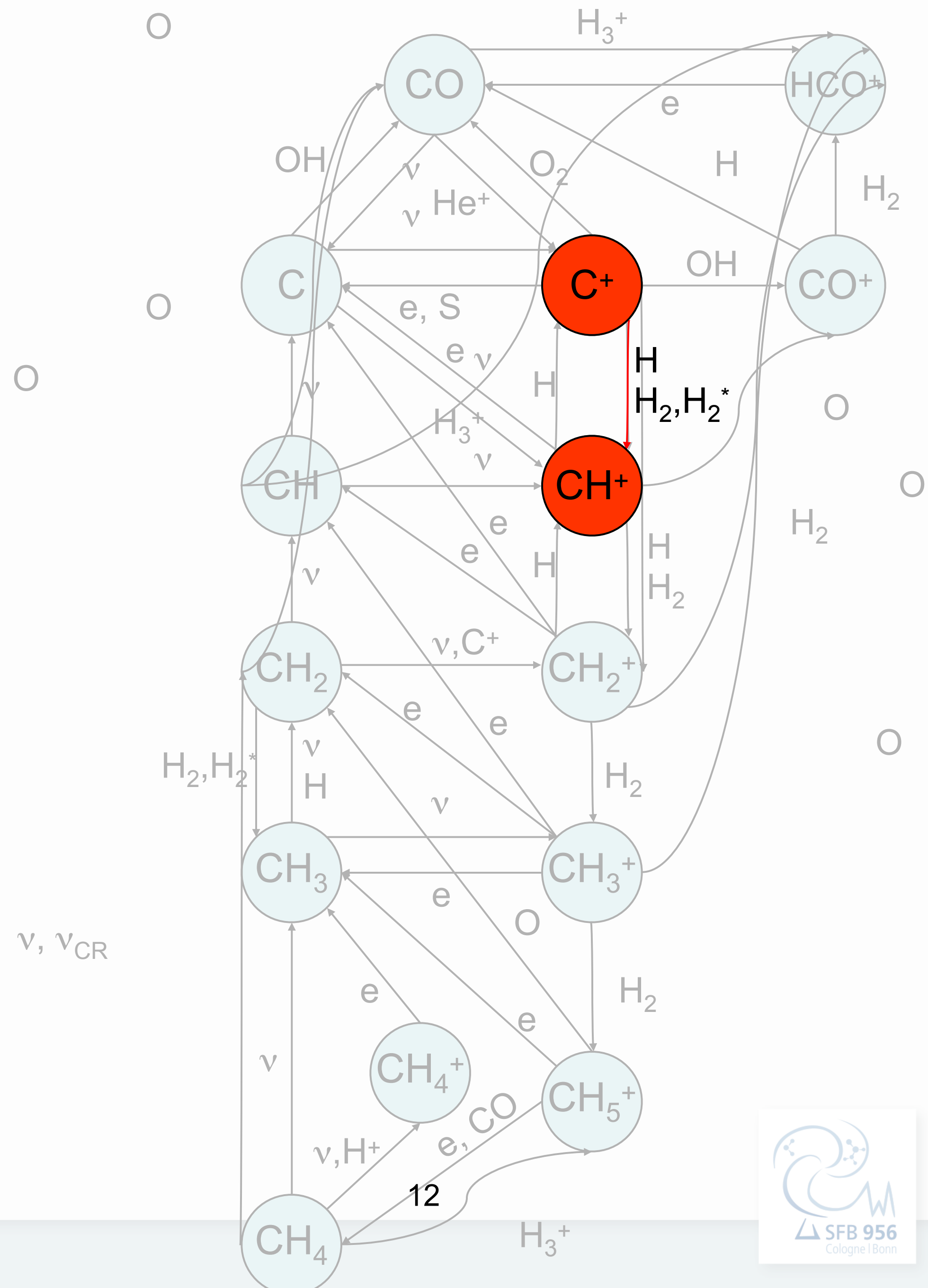
→ some slow routes become quick

$C^+ + H_2 \rightarrow CH^+ + H$

$C^+ + H_2^* \rightarrow CH^+ + H$

endothermic reactions become possible

activation energy barriers become surmountable



# Example: **Dark Cloud**

# cold and dense:

$T = 10$ K, $n = 10^4$-$10^5$ cm$^{-3}$

carbon locked in CO

$He + c.r \rightarrow He^+ + e$

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

FUV fully absorbed

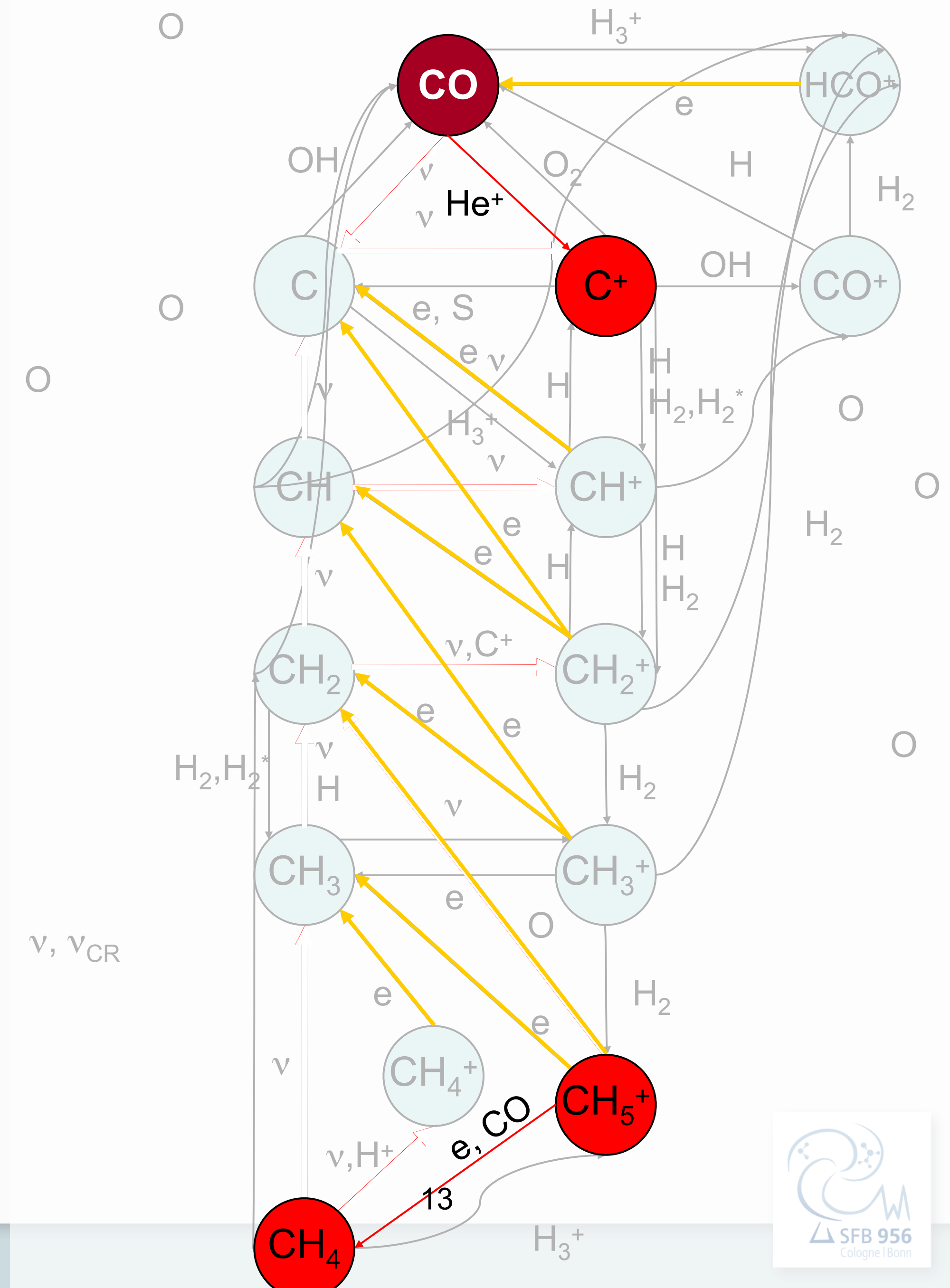
some roads vanish

some roads become slow

e.g. reactions with e$^-$

but:

$CH_5^+ + CO \rightarrow CH_4 + HCO^+$



$CH^+$ was one of the first interstellar molecules discovered

$$\mathbf{C^+ + H_2 \rightarrow CH^+ + H - 4600\ K}$$

(suppressed at low temperature of diffuse clouds)

$$\mathbf{C^+ + H \rightarrow CH^+ + h\nu}$$

(too weak $k \sim 10^{-16}\ cm^{-3}\ s^{-1}$ )

? Formation of $H_2$ is not fully understood

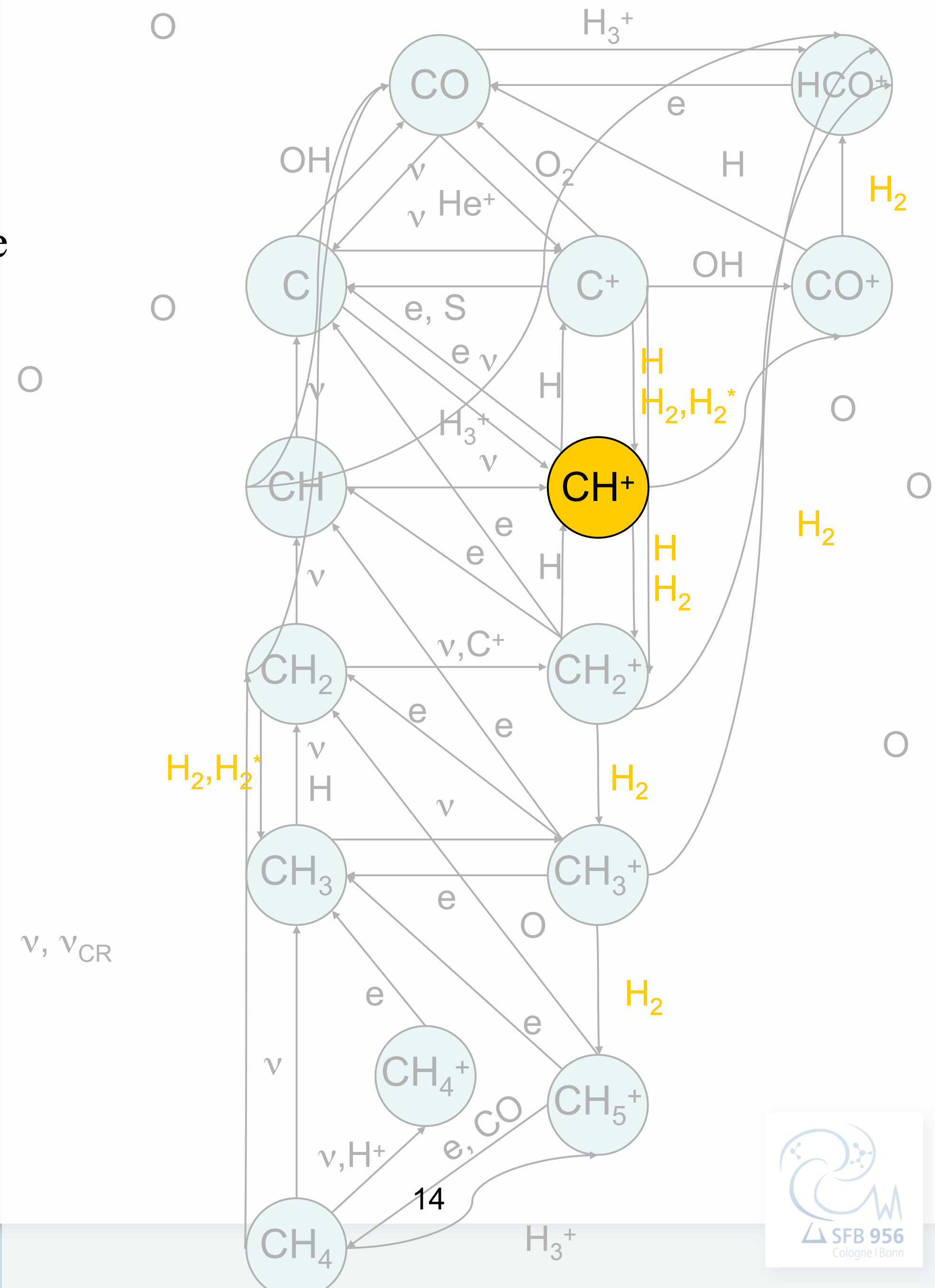
? C/$C^+$/CO stratification is not fully understood

? Effect of cosmic-ray ionization rate

? larger molecules see at mm wavelengths

? Effect of transport of molecules

**and many more…**



How do we model these regions?

# 1. Basic, 1D Plane parallel model

Controlling parameters:

a) Cloud density/pressure

b) FUV density

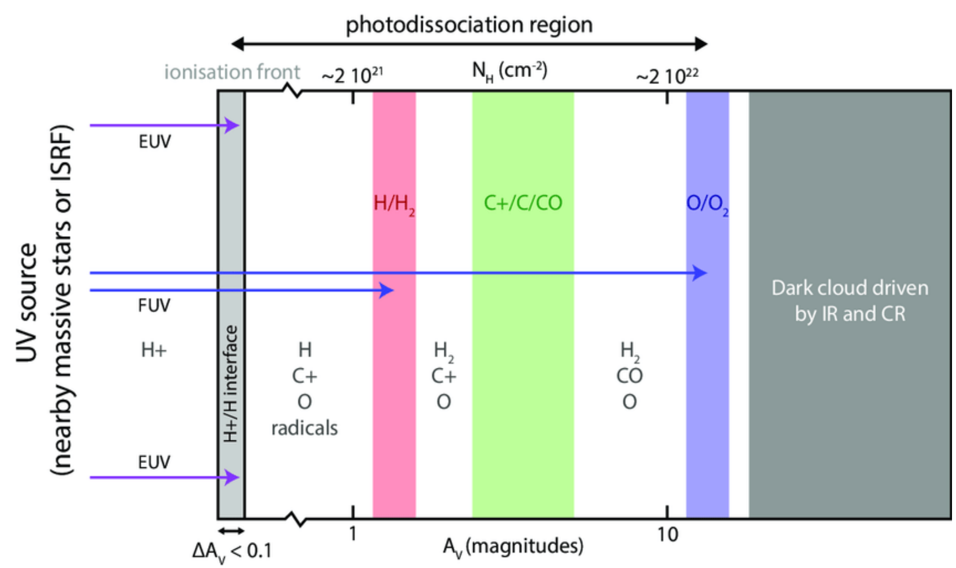
c) Grain scattering properties

d) $H_2$ formation rate coefficient

e) geometry/clumpiness

f) Gas phase abundances

g) Magnetic field



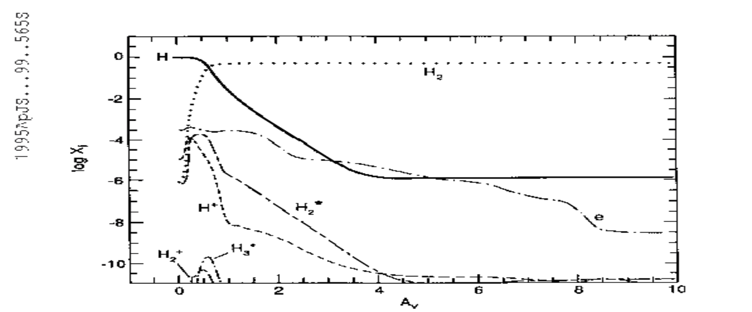
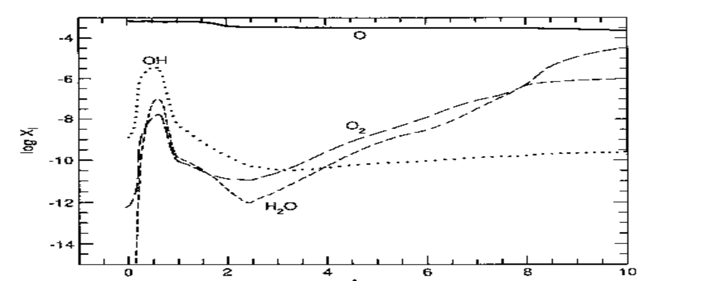



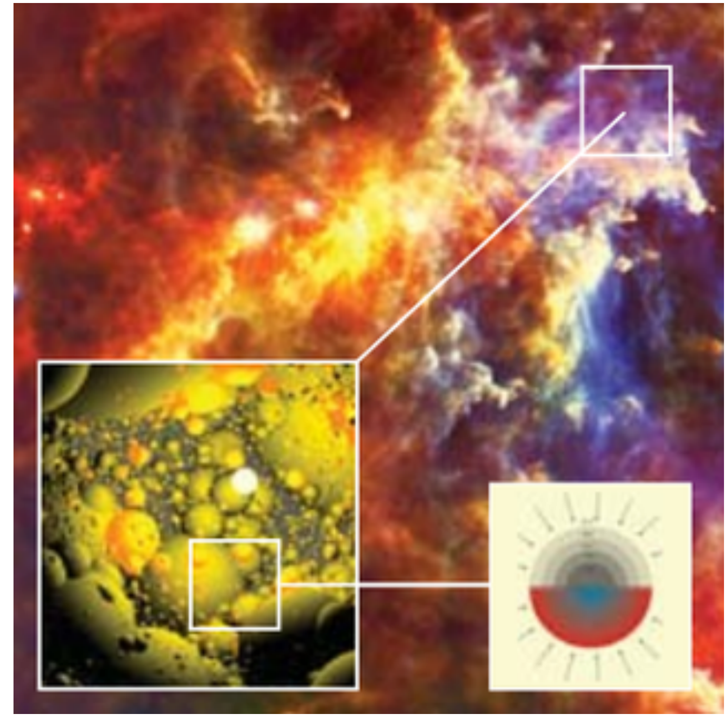

FIG. 8a

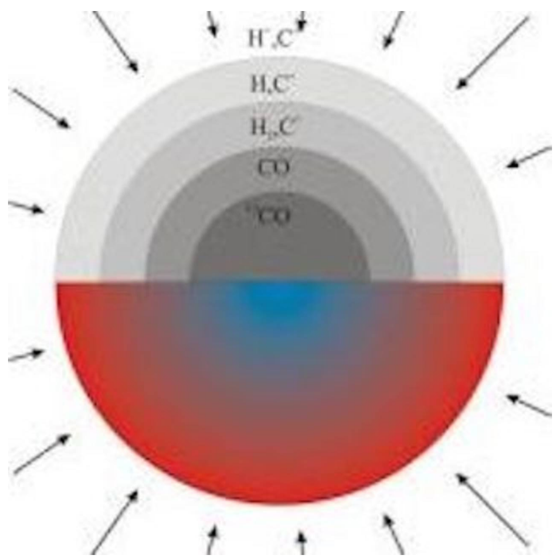
FIG. 8.—(a) Abundances $x_i = n_i/n$ (where $n$ is the density of hydrogen nuclei
Integrated column densities $N_i$ ($cm^{-2}$) of H, $H_2$, $H_2^*$, $H^+$, $H_2^+$, $H_3^+$, and $e$.

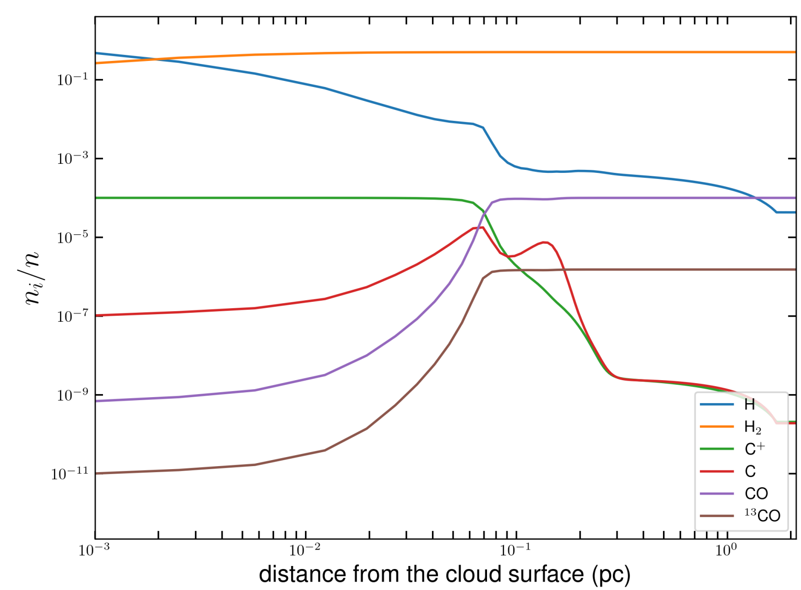


# 1D spherical model
## Example: KOSMA-τ

- Power-law density geometry
- Isotropic illumination
- Self-consistent solution of
  - Energy balance(local)
  - Chemical balance (local)
  - Radiative transfer (global)





SFB 956
Cologne | Bonn

ph1 Universität zu Köln

# How do we solve numerically?

**Solve chemical network**

$$n_i\left\{\tilde{\varsigma}_i + \sum_q n_q \cdot k_{qi}(T)\right\} = \sum_r \sum_s k_{rs}(T) \cdot n_r \cdot n_s + \sum_t n_t \cdot \tilde{\varsigma}_{ti}$$

destruction — formation

$n_i(\vec{r})$

**Solve energy balance**

$$\sum_i \Gamma_i(\vec{r}, \vec{n}, \chi, T) = \sum_i \Lambda_i(\vec{r}, \vec{n}, \chi, T)$$

heating — cooling

$T(\vec{r})$

**Solve level population**

$$0 = \frac{dn_\mu}{dt} = \sum_{\kappa \neq \mu} n_\kappa(\vec{r}) R_{\kappa\mu}(\vec{r}) - n_\mu(\vec{r}) \sum_{\kappa \neq \mu} R_{\mu\kappa}(\vec{r})$$

populating — depopulating

$S_\nu$

**Solve radiative transfer**

$$I_\nu(\vec{r}, \vec{n}) = I_\nu(\vec{r}_0, \vec{n}) e^{-\tau_\nu^*} + \int_0^{\tau_\nu^*} S_\nu(\tau_\nu) e^{-\tau_\nu} d\tau_\nu$$

absorption — absorption & emission

$I_\nu(\vec{r}, \vec{n}) = I_\nu$

**Diffusion effects in molecular clouds**

baby@ph1.uni-koeln.de

# Solving chemical network

- Solving a system of rate equations
- This includes all the formation and destruction reactions of every species

Solve chemical network

$$n_i \left\{ \tilde{\varsigma}_i + \sum_q n_q \cdot k_{qi}(T) \right\} = \sum_r \sum_s k_{rs}(T) \cdot n_r \cdot n_s + \sum_t n_t \cdot \tilde{\varsigma}_{ti}$$

destruction formation

$I_\nu(\vec{r},\vec{n}) = I_\nu$

$n_i(\vec{r})$

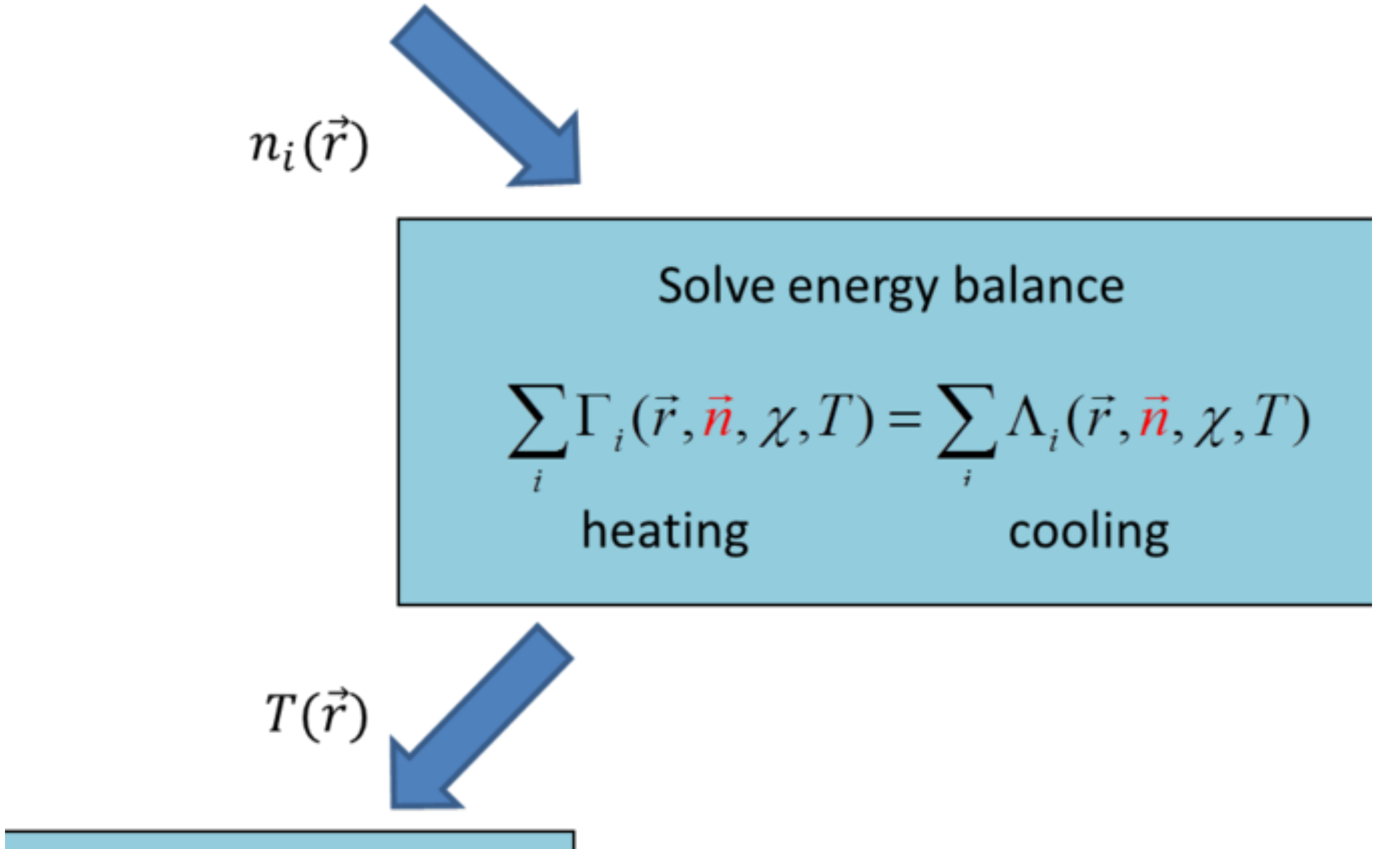
**Diffusion effects in molecular clouds**

baby@ph1.uni-koeln.de

July 14, 2022

# Energy Balance

- Balancing all the heating and cooling processes to derive the local kinetic gas and dust temperature.






Diffusion effects in molecular clouds

baby@ph1.uni-koeln.de

July 14, 2022

# Level population

compute the energy level population of species that are relevant for the energy balance and for the emission of the model clump.

$S_\nu$ $T(\vec{r})$

Solve level population

$$0 = \frac{dn_\mu}{dt} = \sum_{\kappa \neq \mu} n_\kappa(\vec{r}) R_{\kappa\mu}(\vec{r}) - n_\mu(\vec{r}) \sum_{\kappa \neq \mu} R_{\mu\kappa}(\vec{r})$$

populating depopulating

**Diffusion effects in molecular clouds**

baby@ph1.uni-koeln.de

July 14, 2022

# Radiative transfer

The radiative transfer computes the emission and absorption processes along a line-of-sight through the model cloud.

$I_\nu(\vec{r},\vec{n})=I_\nu$

Solve radiative transfer

$$I_\nu(\vec{r},\vec{n})=I_\nu(\vec{r}_0,\vec{n})e^{-\tau_\nu{}^*}+\int_0^{\tau_\nu{}^*} S_\nu(\tau_\nu)e^{-\tau_\nu}d\tau_\nu$$

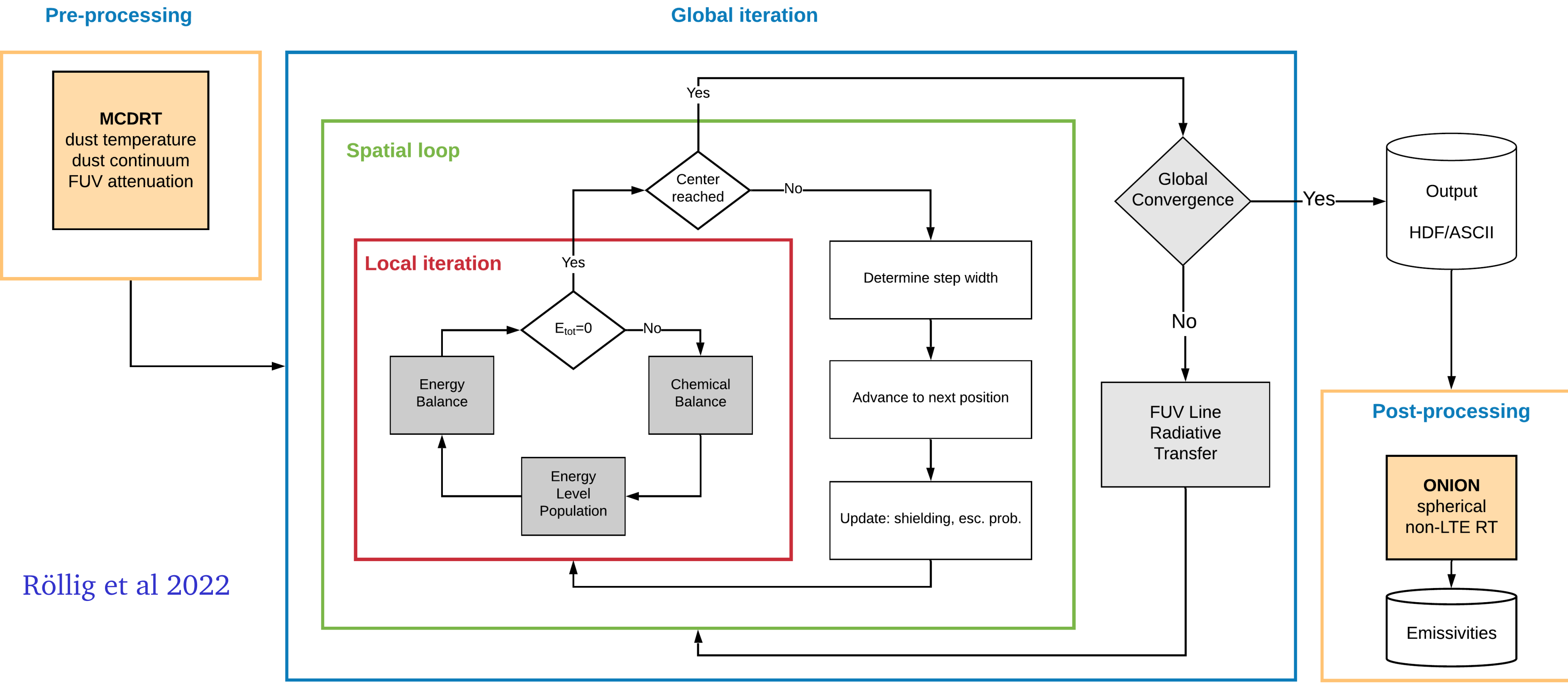
absorption absorption & emission

$S_\nu$

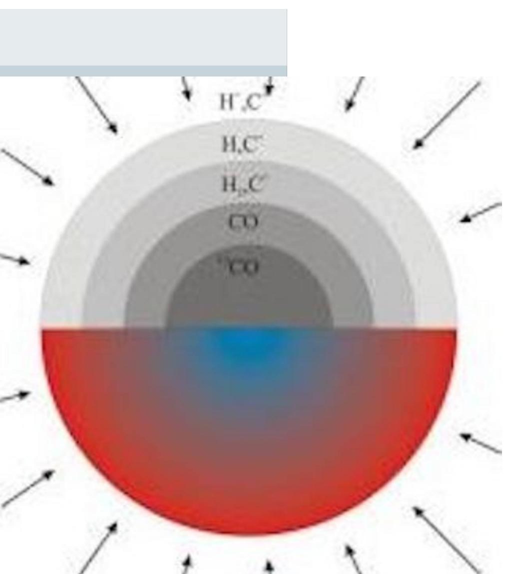
**Diffusion effects in molecular clouds**

baby@ph1.uni-koeln.de

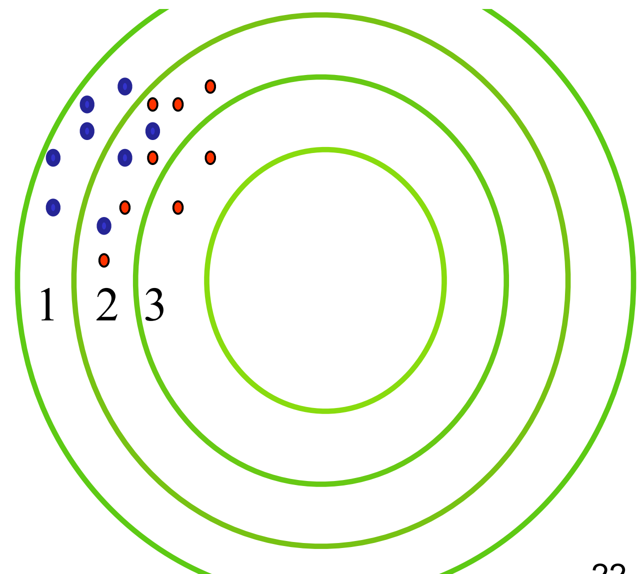
July 14, 2022




Röllig et al 2022



KOSMA - $\tau$ PDR Model




Aleena et al 2022 (in prep)

# DIFFUSION

Net movement, for example, atoms, ions, and molecules from a region of higher concentration to a region of lower concentration.

- Molecular diffusion
- Thermal diffusion
- Turbulent diffusion

$$\boxed{\frac{\partial n}{\partial t} = -\frac{\partial \phi}{\partial x} = -\frac{\partial \phi_{turb}}{\partial x} - \frac{\partial \phi_{mol}}{\partial x} + \frac{\partial \phi_{thermal}}{\partial x}}$$

$\phi_{turb} \rightarrow$ turbulent diffusion

$\phi_{mol} \rightarrow$ molecular diffusion

$\phi_{thermal} \rightarrow$ thermal diffusion

Aleena et al 2022

SFB 956 Cologne | Bonn

ph1 Universität zu Köln

**Diffusion effects in molecular clouds**

baby@ph1.uni-koeln.de

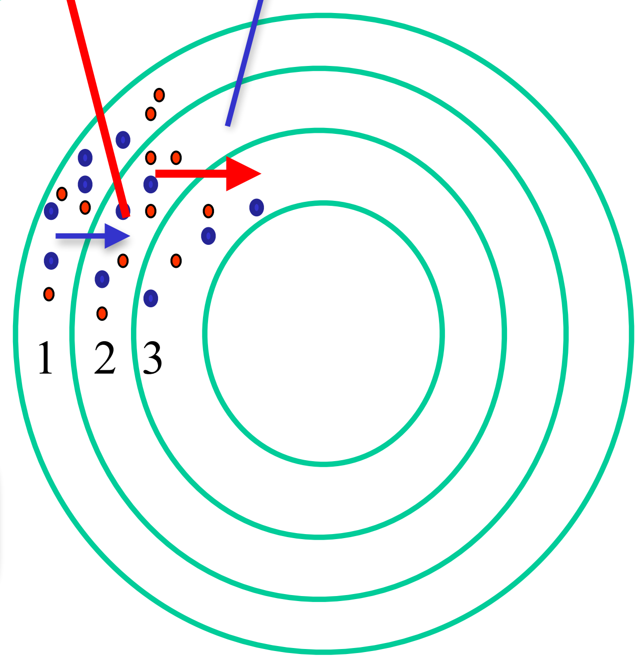
Solve chemical network

$$n_i\left\{\tilde{\varsigma}_i+\sum_q n_q\cdot k_{qi}(T)\right\}=\sum_r\sum_s k_{rs}(T)\cdot n_r\cdot n_s+\sum_t n_t\cdot\tilde{\varsigma}_{ti}$$

destruction formation

Rate of particles moving out of the current shell

Rate of particles moving into the current shell




Chemistry is no longer a local problem!

Aleena et al 2022(in prep)

Diffusion effects in molecular clouds

baby@ph1.uni-koeln.de

$$\phi_{turb} = -\, n\, K_{turb} \frac{\partial n_i}{\partial x}$$

$$K_{turb} = < V_t L >$$

Xie et al 1995

$V_t = 1$ Km/s
**L = 0.1 - 0.5 pc**

$$\phi_{mol} = -\, n\, K_{mol} \frac{\partial n_i}{\partial x}$$

$$K_{mol} = < V_i \lambda > = \sqrt{\frac{5kT}{3\mu_i}} \frac{1}{\sigma n}$$

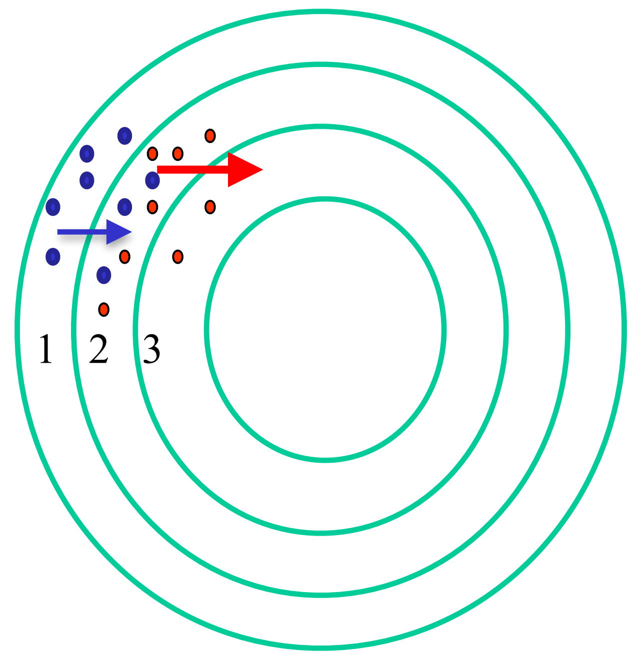
$$\sigma = 10^{-15} \mathrm{cm}^2$$

Lesaffre et al 2007

$$\phi_{thermal} = -\, n\, K_{thermal} \frac{n}{T} \frac{\partial n_i}{\partial x}$$

$$K_{thermal} = K_{mol} k_T$$
$$= K_{mol} \alpha n_i n_j$$

Chapman 1985



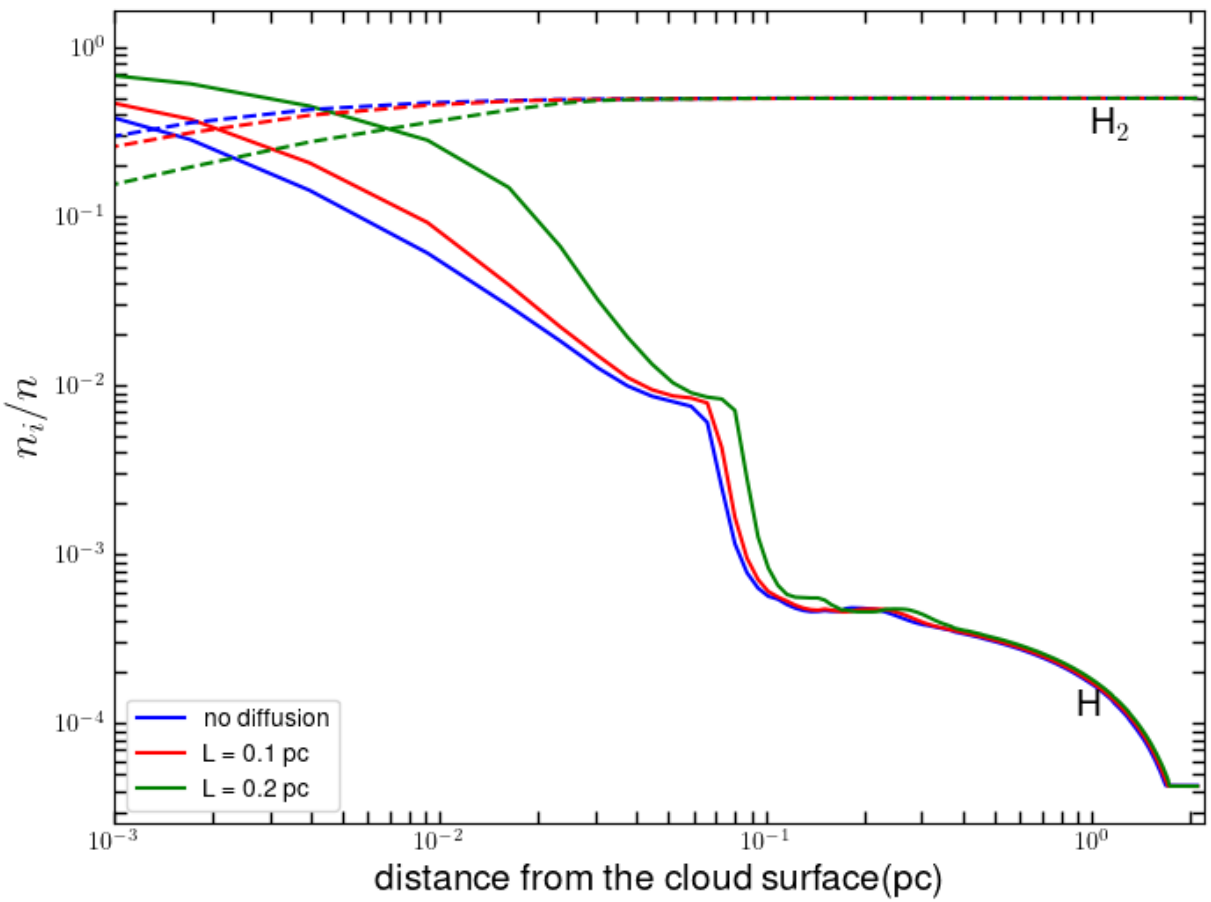

Aleena et al 2022 (in prep)

$K = 10^{15} - 10^{23}\ \mathrm{cm^2 s^{-1}}$

$n_i$ : fractional number density　　T : Temperature
$\mu_i$ : average molecular weight　$n$ : total number density ($\mathrm{cm}^{-3}$)

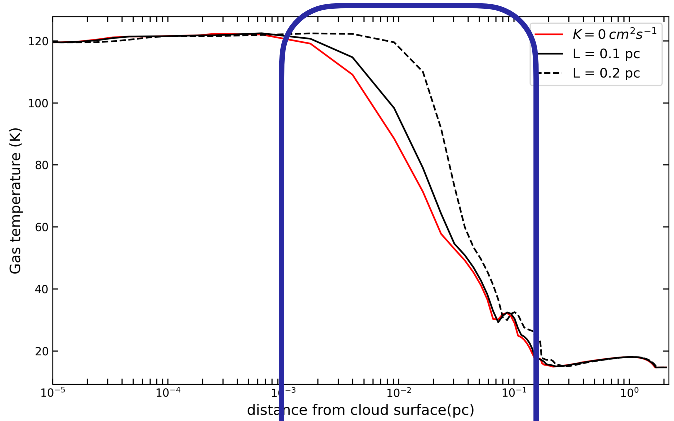
baby@ph1.uni-koeln.de

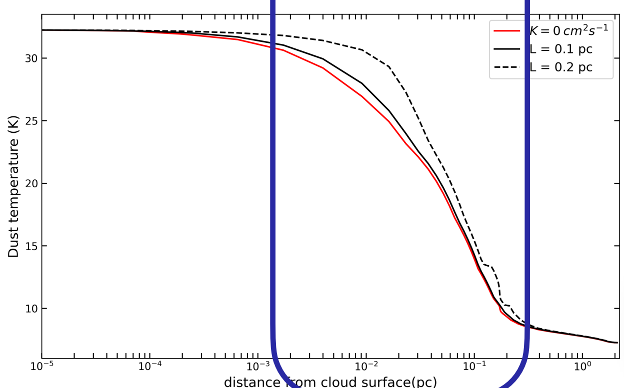
## H-$H_2$ transition shifted deeper into the cloud

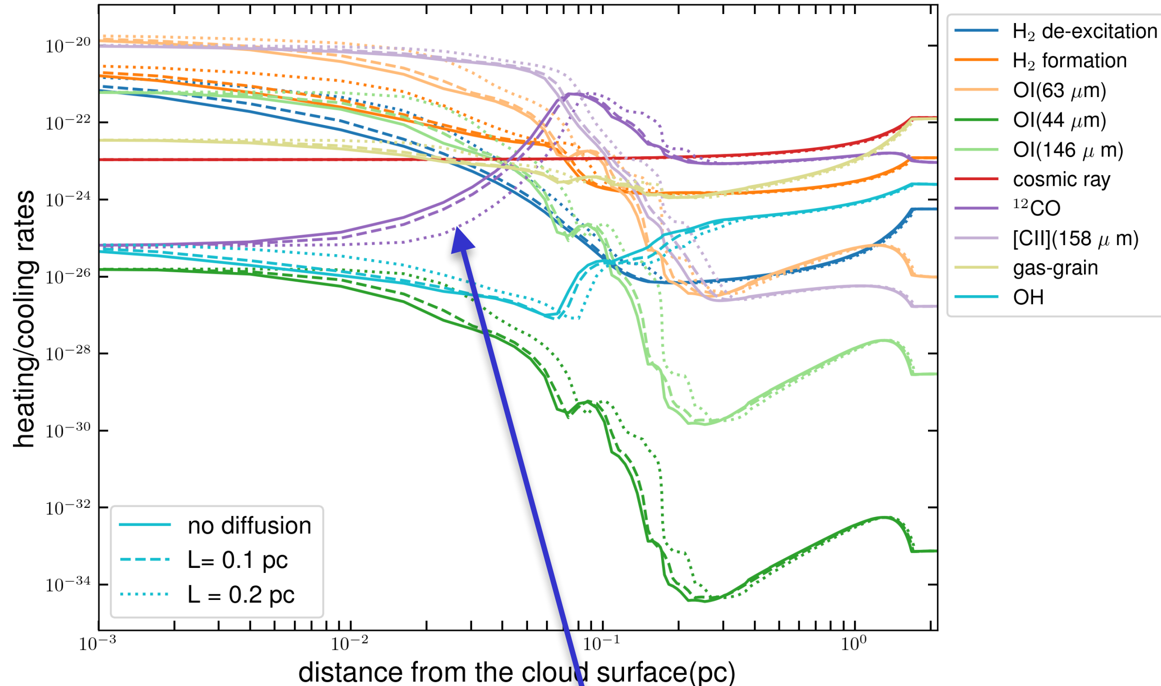



**$H_2$ formation is reduced because H is diffused into the cloud!**

Aleena et al 2022 (in prep)




Aleena et al 2022

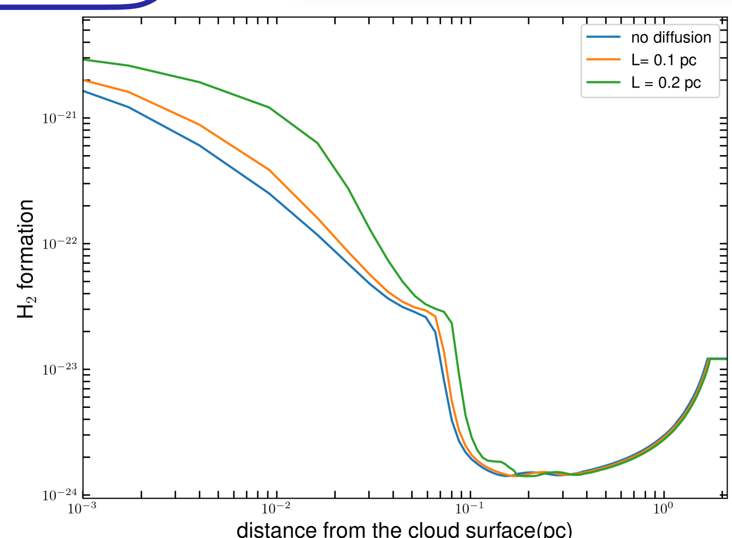
Increase in temperature

Heating rates: ↑

- Photo-dissociation
- $H_2$ formation
- Collisional de-excitation of vibrationally excited $H_2$

Cooling rates:

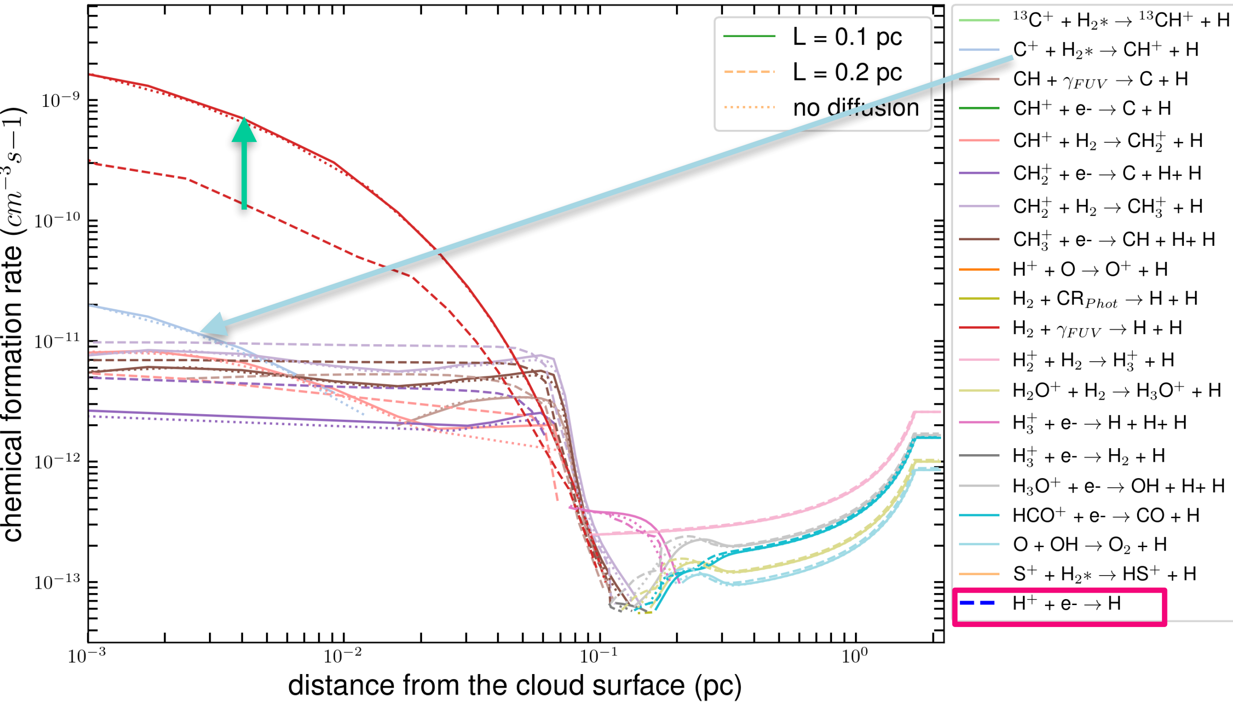
- $^{12}$CO line ↓
- [OI] line cooling ↑
- $C^+$ line ↑




**Diffusion effects in molecular clouds**

baby@ph1.uni-koeln.de

July 14, 2022



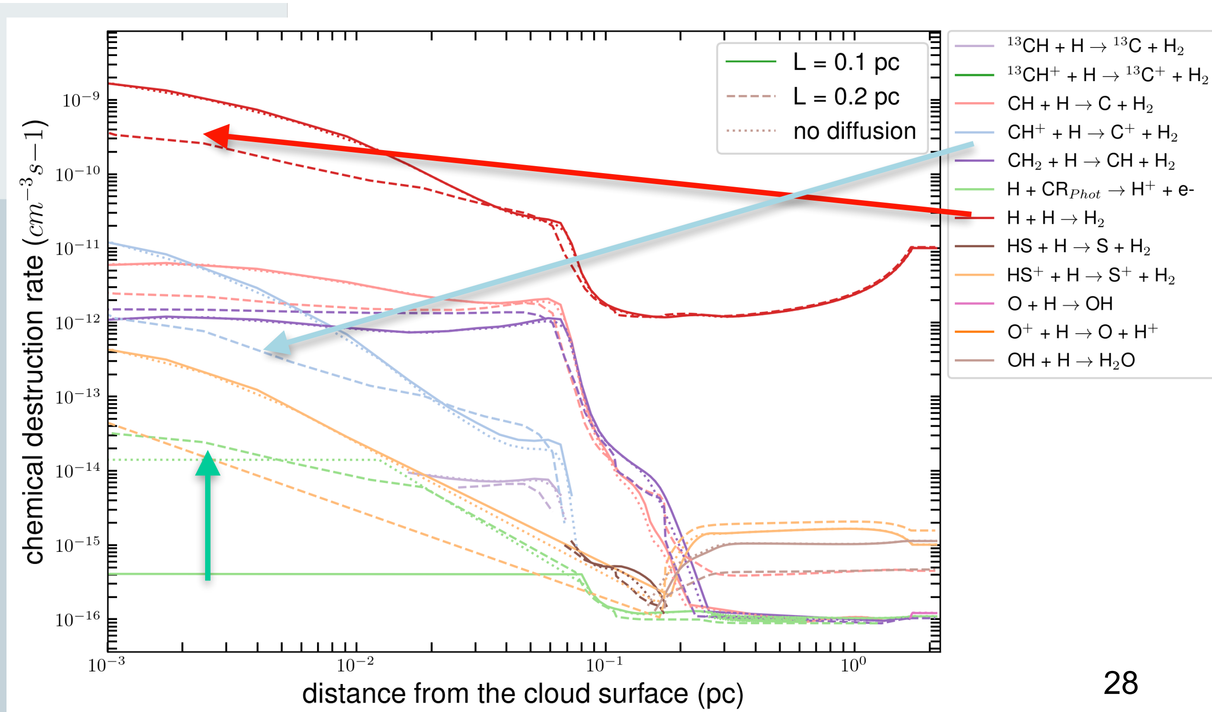

New chemical pathway:

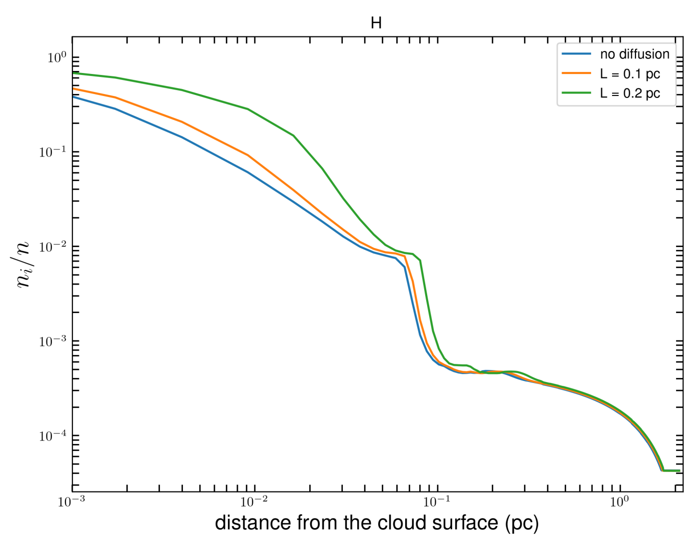
$$H^+ + e^- \rightarrow H$$

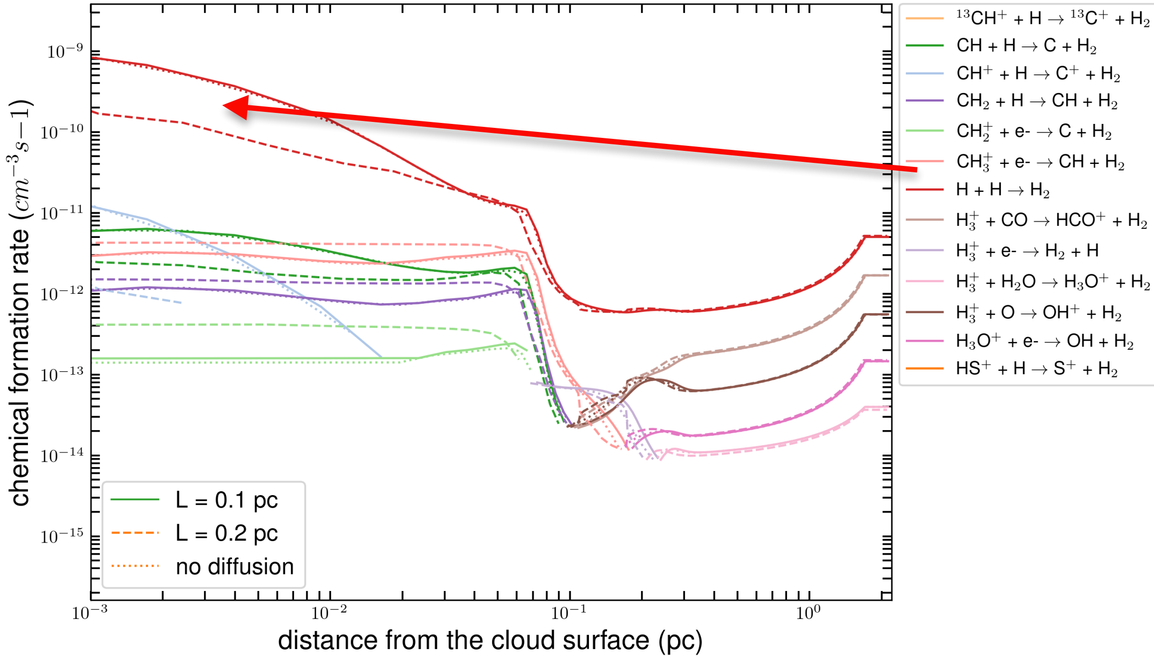
Removed pathway:

$$C^+ + H_2{*} \rightarrow CH^+ + H$$

Aleena et al 2022



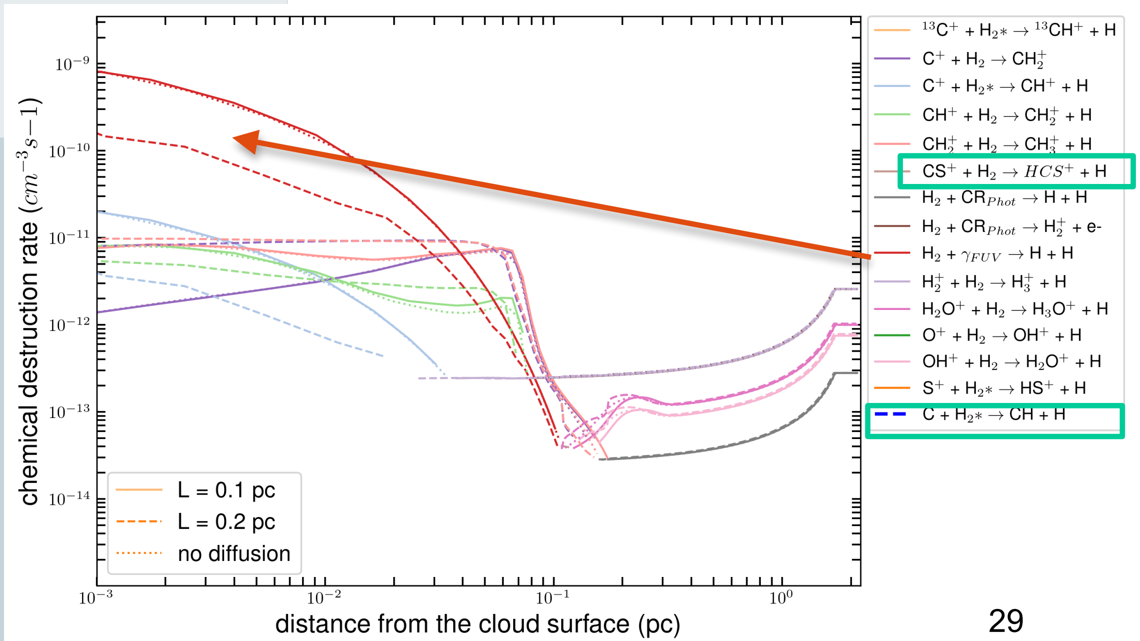


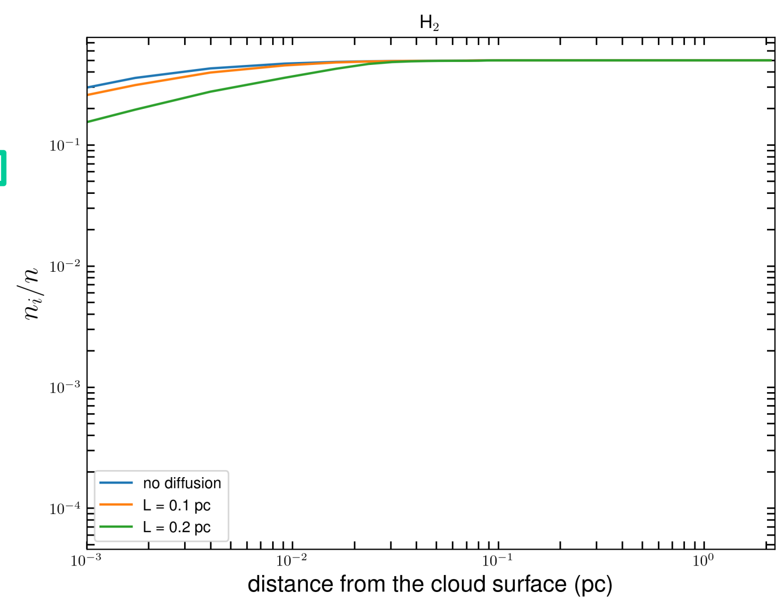

New chemical pathway:

$$C + H_2{}^* \rightarrow CH + H$$

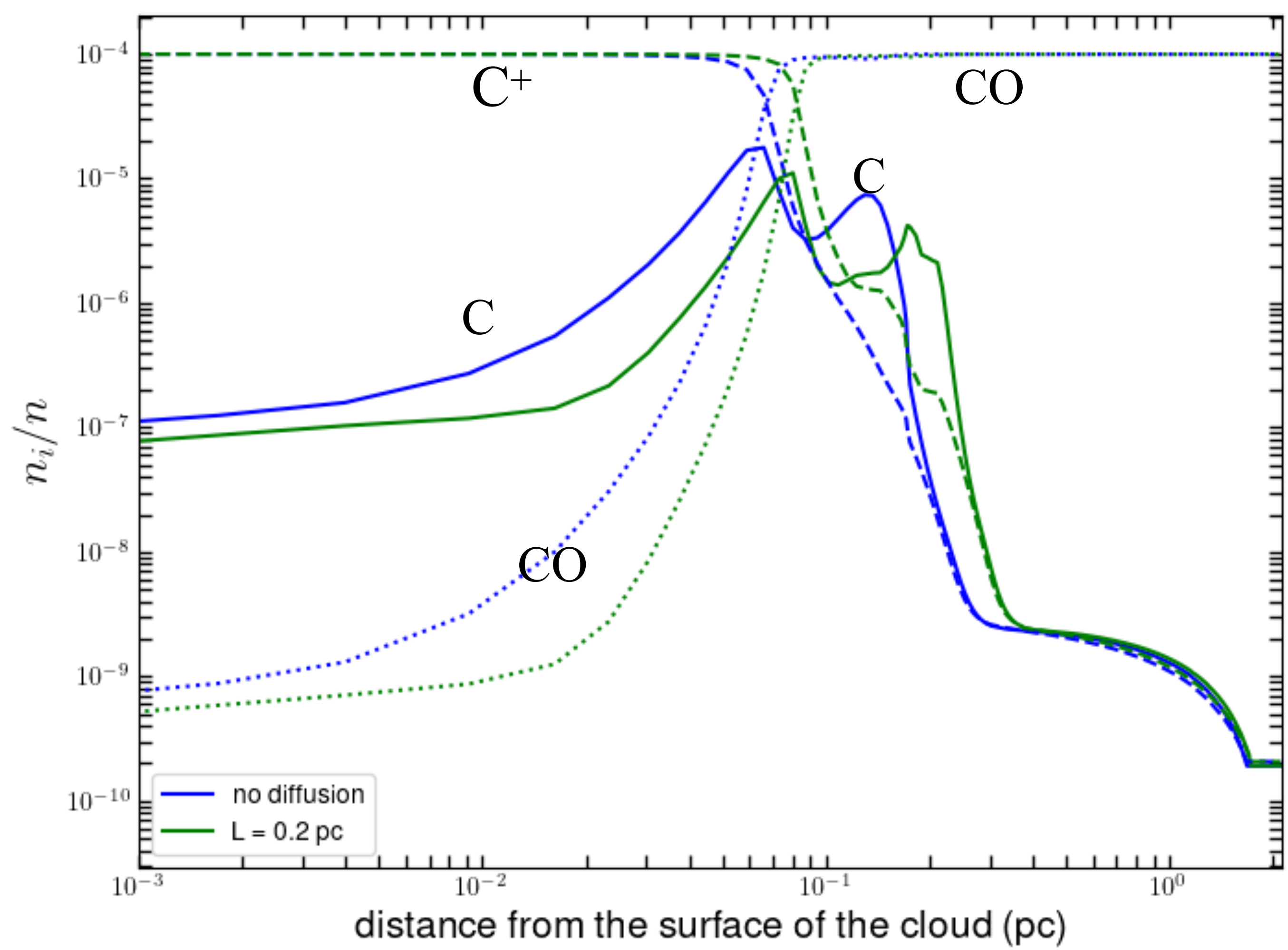
$$CS^+ + H_2 \rightarrow HCS^+ + H$$

Aleena et al 2022



# C/C+/CO stratification




**Diffusion effects in molecular clouds**

baby@ph1.uni-koeln.de

July 14, 2022

# Conclusion:

The atomic region is expanding into the molecular region

Observational confirmation of Diffusion

on the surface: H and $H_2$

deeper in the cloud: C and CO, and CH

towards the core: $C^+$

Higher J values show less deviation from the no diffusion case.

Aleena et al 2022



baby@ph1.uni-koeln.de

# Reference


Andree-Labsch et al. (2017), A&A, 598, A2

Sydney Chapman 1958 Proc. Phys. Soc. 72 353

Chieze JP, Pineau Des Forets G. 1989. Astronomy and Astrophysics. 221:89–94

Chieze J-P, Pineau des Forets G, Herbst E. 1991. The Astrophysical Journal.373:110–22

Gierens, K., Stutzki, J., and Winnewisser, G 1992, A&A, 259,271

Nagy, Z., Van der Tak, F. F. S., Ossenkopf, V., et al. 2013, A&A, 550, A96

Röllig M, Abel NP, Bell T, Bensch F, Black J, et al. 2007. A&A. 467(1):187–206

Röllig M, Ossenkopf V. 2013. Astronomy and Astrophysics. 550:A56

Singh, ashok kumar & Bhadauria, Beer. (2009). Finite Difference Formulae forUnequal Sub-Intervals Using Lagrange's Interpolation Formula. Journal ofMath. Analysis. 3. 815-827.

Sternberg, A. and A. Dalgarno, Astrophysics. J.,338:197, (1989)

Sternberg, A. and A. Dalgarno, Astrophysics. J., Suppl. Ser 99, 565(1995)

The Physics and Chemistry of the Interstellar Medium,A. G. G. M. Tielens

Willacy K, Langer WD, Allen M. 2002. . 573:4

Xie, Allen and Langer, Astrophysics. J.,440:674(1995)


SFB 956
Cologne | Bonn

ph1 Universität zu Köln

**Diffusion effects in molecular clouds**

baby@ph1.uni-koeln.de

**Diffusion effects in molecular clouds**

baby@ph1.uni-koeln.de