



# PDR Modelling

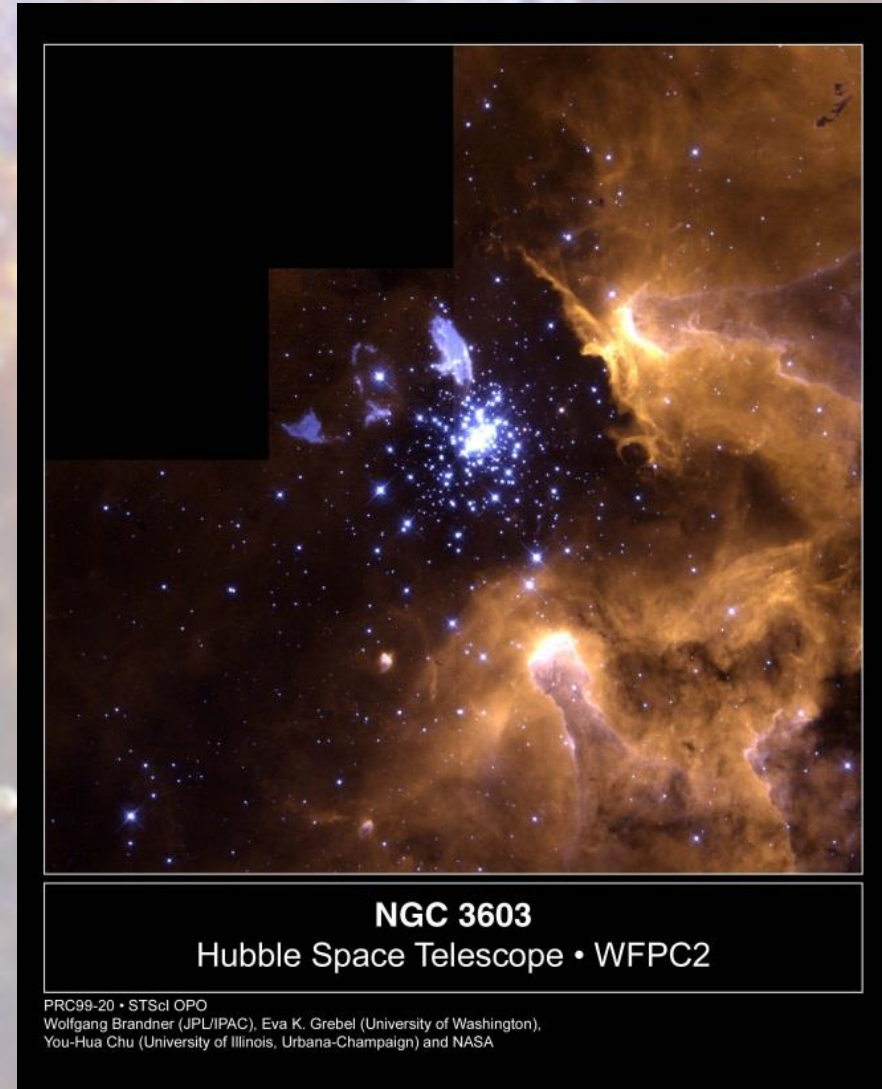
M. Röllig

I. Physikalisches Institut, Universität zu Köln



# Introduction

- PDR is short for
  - **P**hoto-**D**issociation **R**egion
  - **P**hoton **D**ominated **R**egion



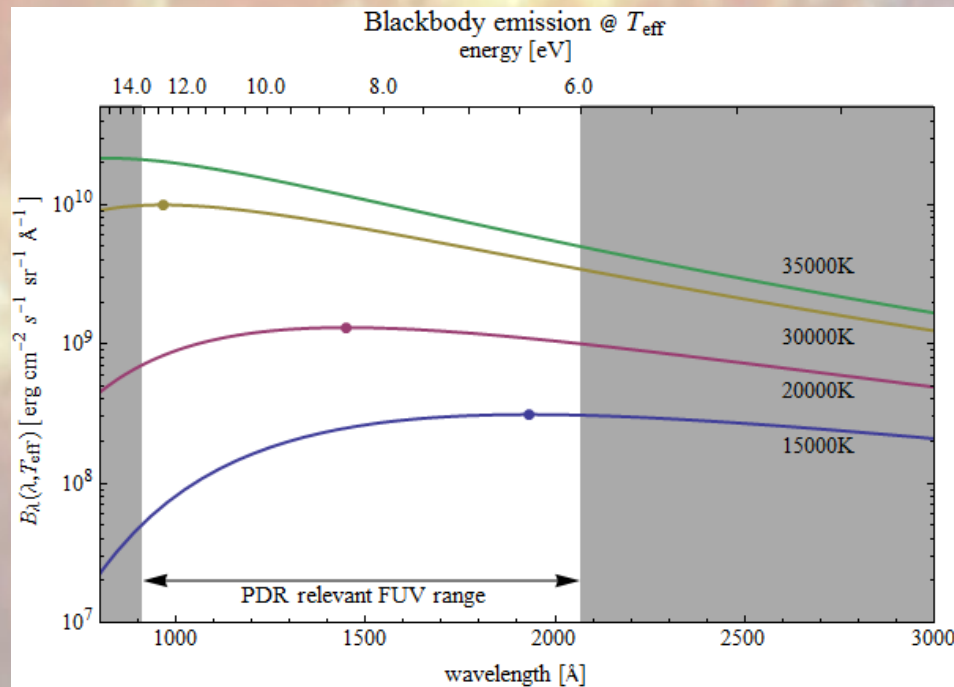


# Introduction

- A region where far-ultraviolet (FUV: **6-13.6 eV**) photons from young, massive stars dominate the physics and the chemistry of the interstellar medium.
  - **6 eV (2066 Å)**      ~ionization potential of dust/PAHs
  - 11.1 eV (1117 Å)      dissociation energy of CO
  - 11.3 eV (1097 Å)      ionization potential of C
  - **13.598 eV (912 Å)**      ionization potential of H
  - 13.618 eV              ionization potential of O
  - 14.5 eV (855 Å)        ionization potential of N

# Introduction

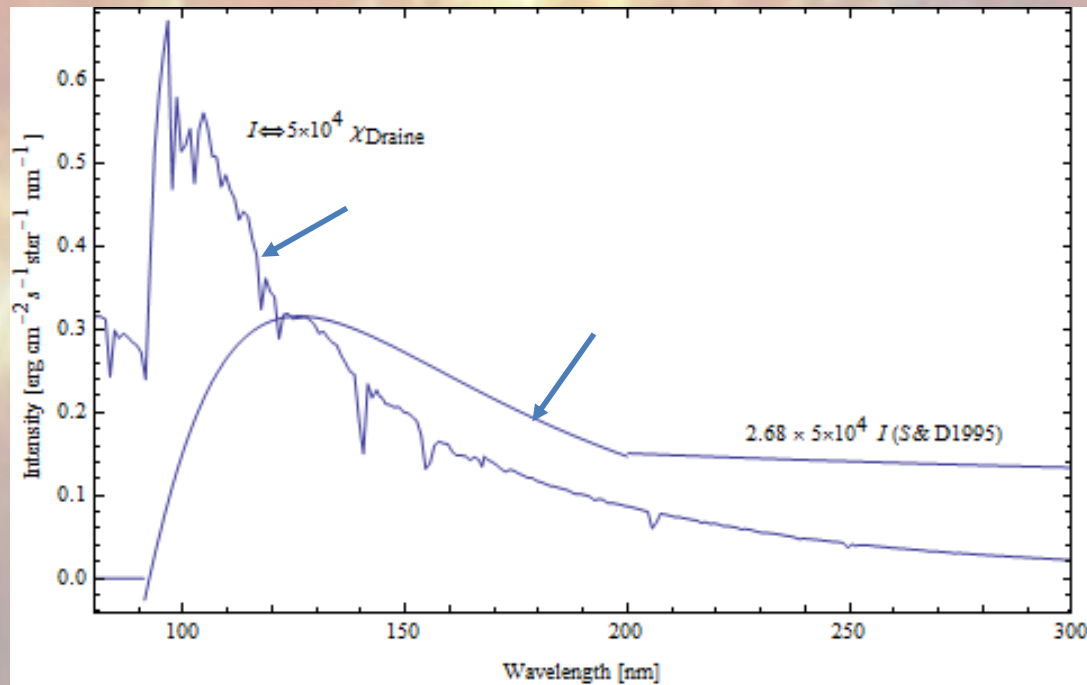
- A region where far-ultraviolet (FUV: 6-13.6 eV) photons from young, massive stars dominate the physics and the chemistry of the interstellar medium.



(young) massive stars emit a significant fraction of their energy at  $\lambda < 912 \text{\AA}$

# Introduction

- A region where far-ultraviolet (FUV: 6-13.6 eV) photons from young, massive stars dominate the physics and the chemistry of the interstellar medium.

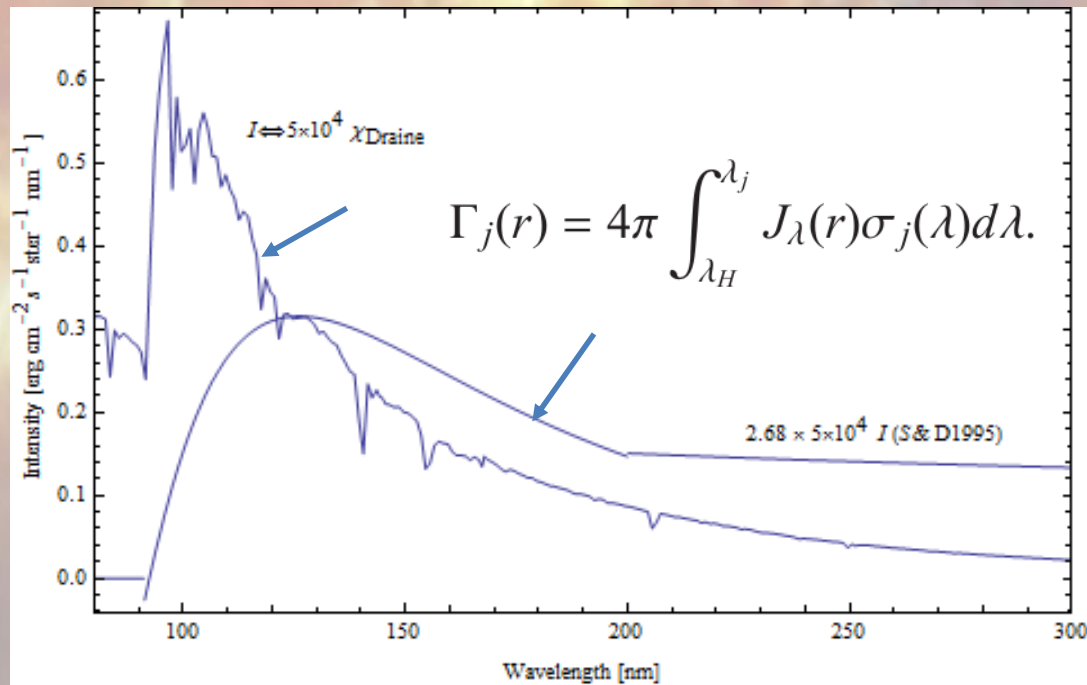


PDRs close to an OB star experience spectrally different UV radiation compared to the standard mean FUV field (Draine '78, Habing '68)

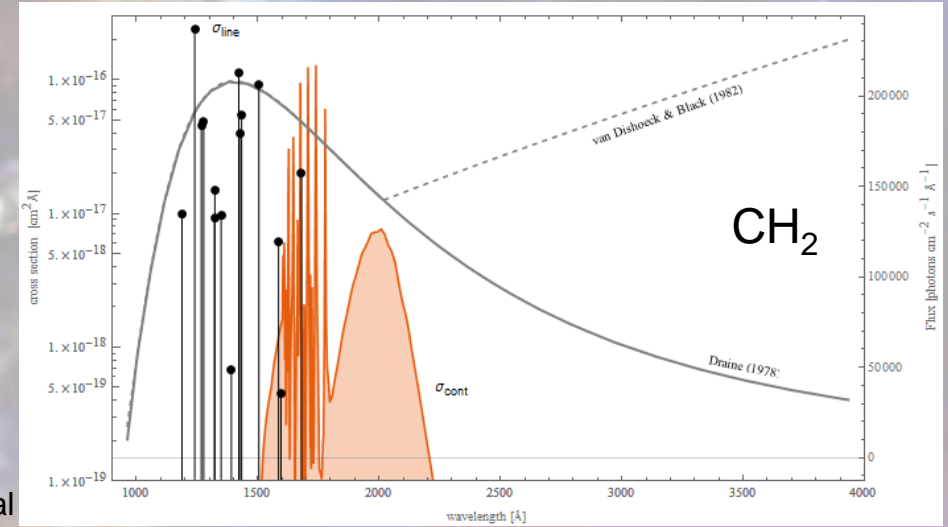
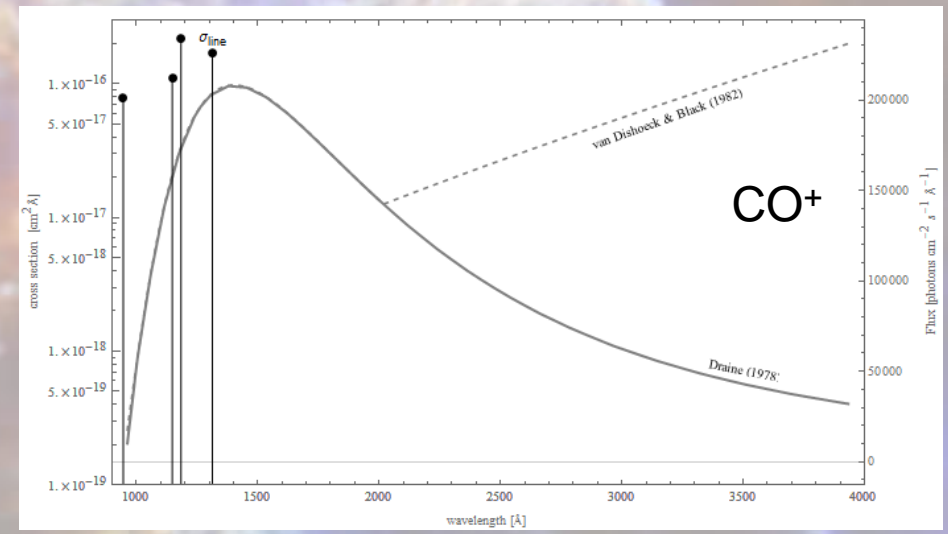


# Introduction

- The FUV spectrum affects the photo-ionisation/dissociation depending on their respective cross-sections.



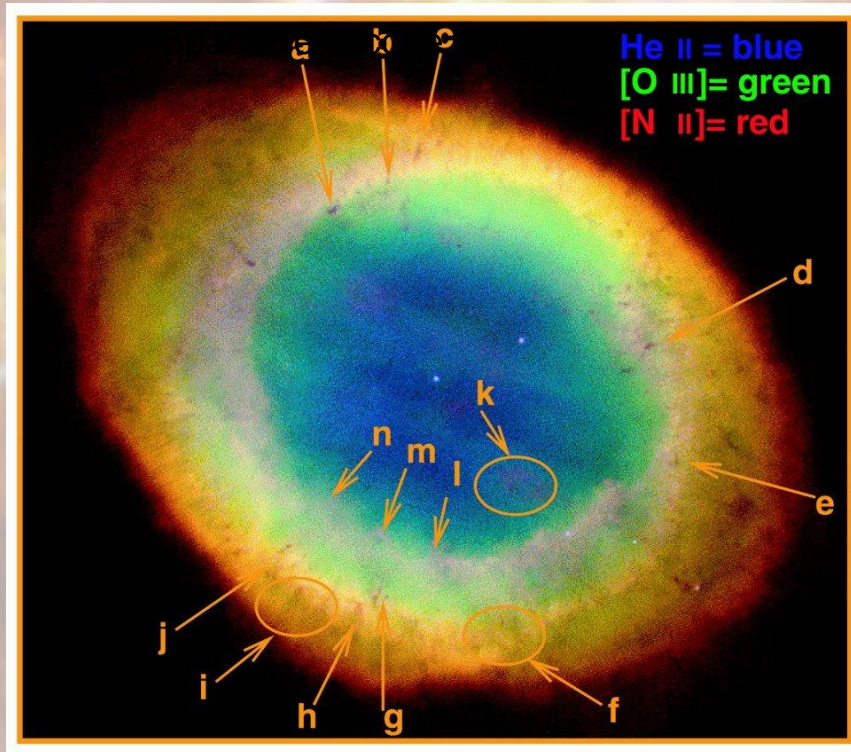
## Photodissociation cross-section



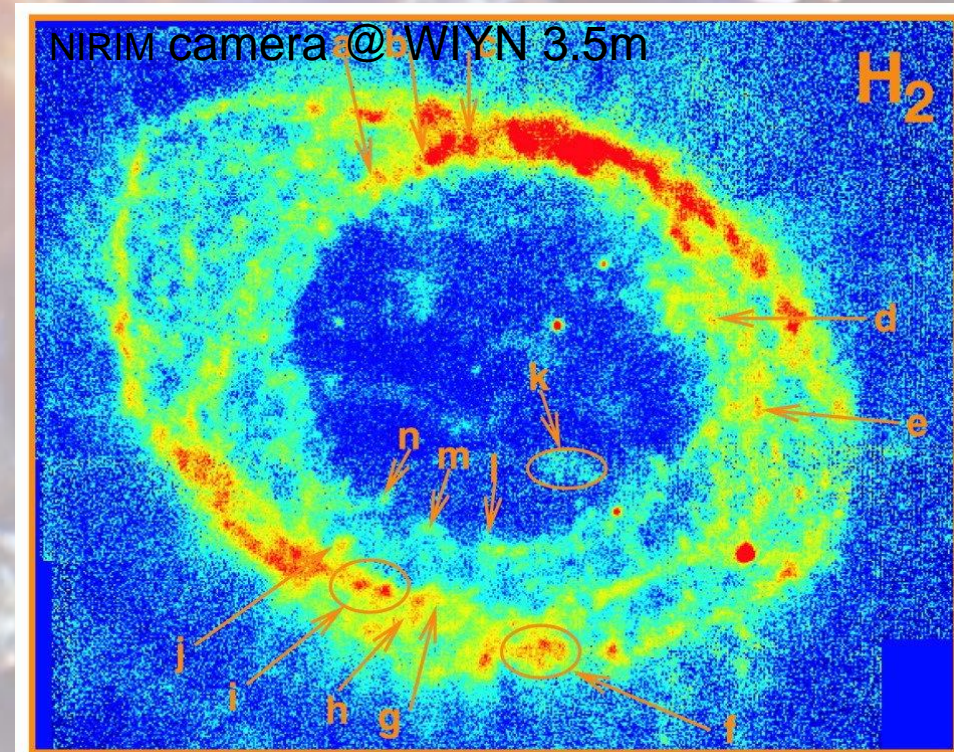


# Introduction

Ring nebula



H<sub>2</sub> 1-0 S(1) 2.122 μm



H<sub>2</sub> in dense gas clumps is shielded from the FUV

Speck et al. 2003 PASP 115, 170



# Introduction

Credit: NASA, ESA, and F. Paresce and R. O'Connell



PDRs are also observed in extragalactic source

30 Doradus in the LMC



# Introduction

Credit: ESA/Hubble & NASA



PDRs are also observed in extragalactic source

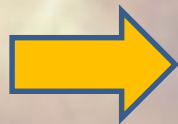
Antennae galaxies (NGC 4038/39)

# Introduction

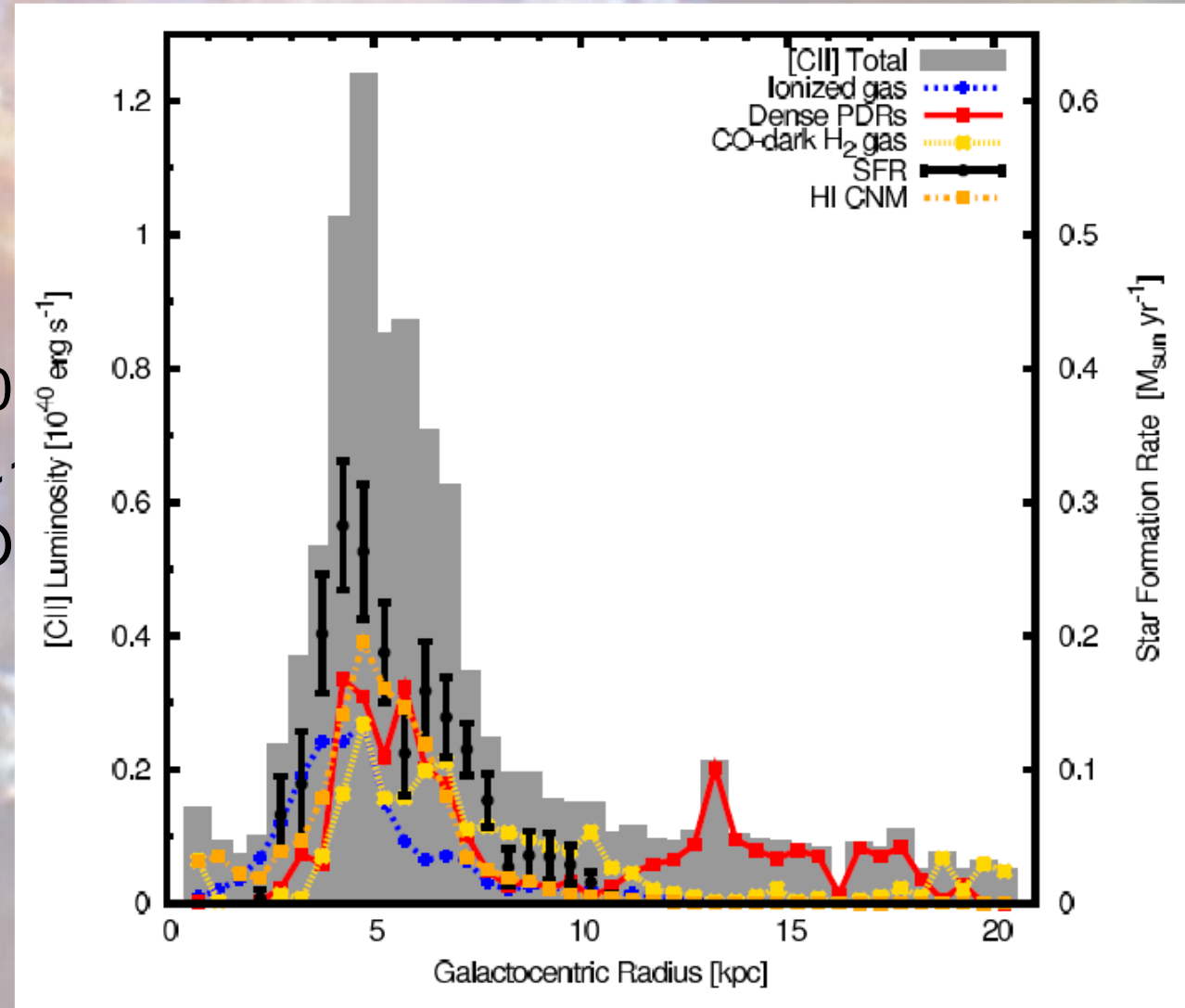
Pineda et al. 2014

Interstellar PDRs include:

- Diffuse WNM and CNM clouds.
- Translucent clouds:  $A_V < 5$ ,  $n_H < 10^4$
- Dense molecular clouds:  $A_V$  up to  $\sim 10$  including intense FUV fields near O

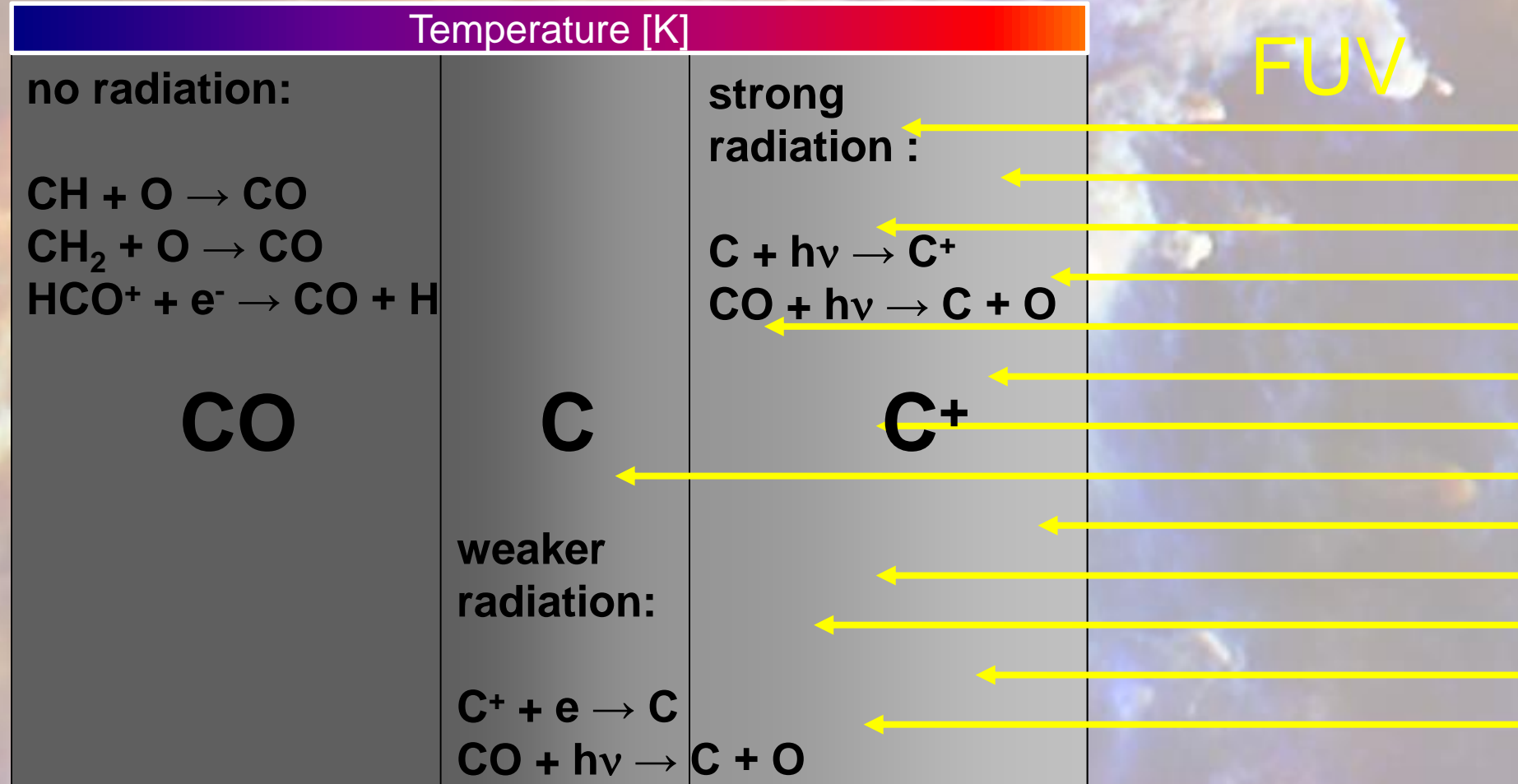


~90% of the Galactic molecular





# Introduction



Interstellar cloud surface (cross section)

young massive stars

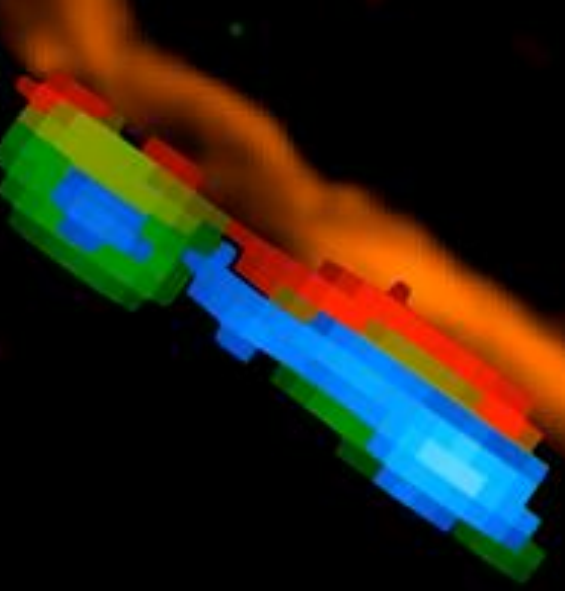


warm dust

$C_2H$

$H_2CO$

$C^{18}O$



0.1 parsec



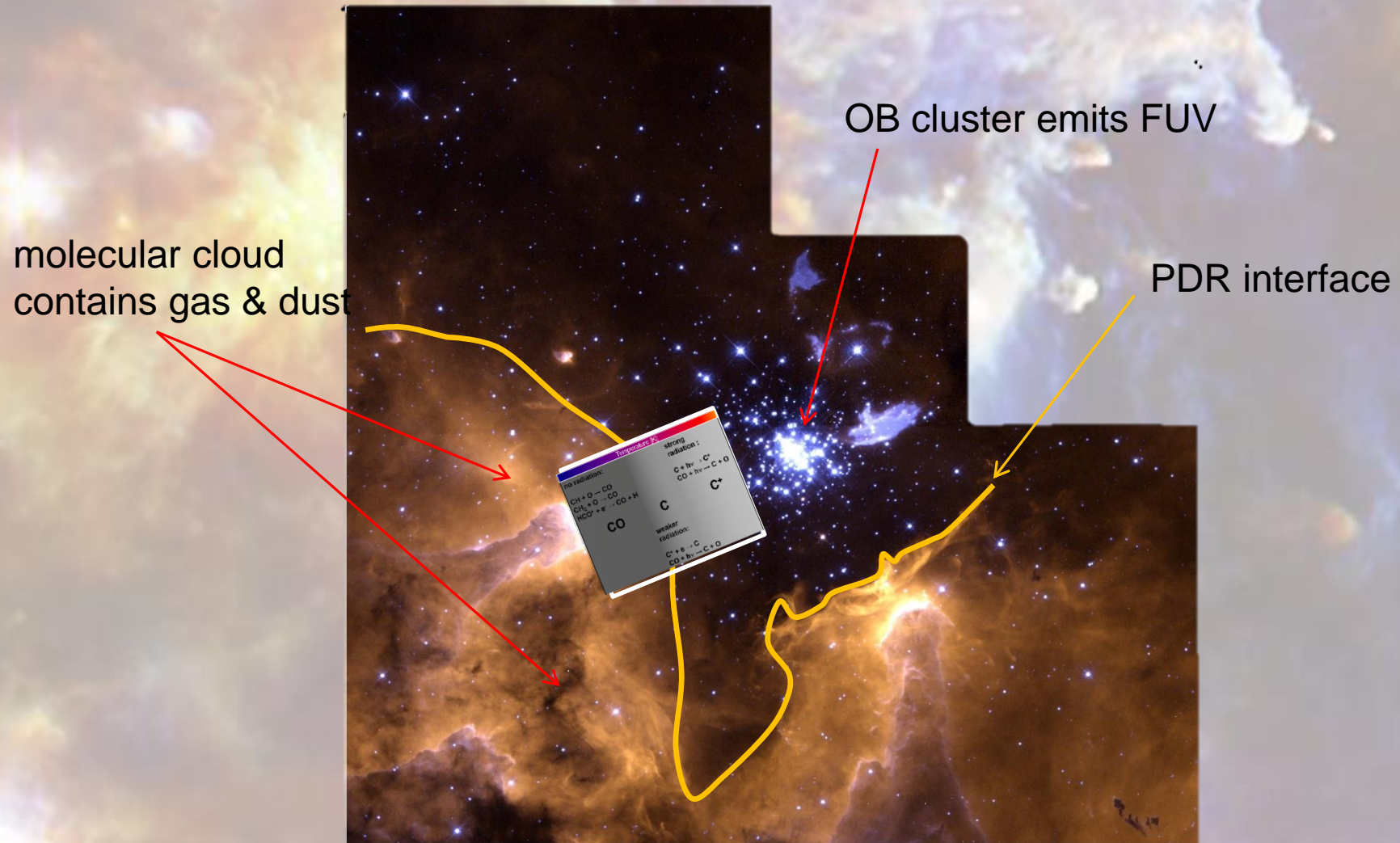
van der Wiel et al. 2009



Rosette



# Introduction



# PDR Model Complexity

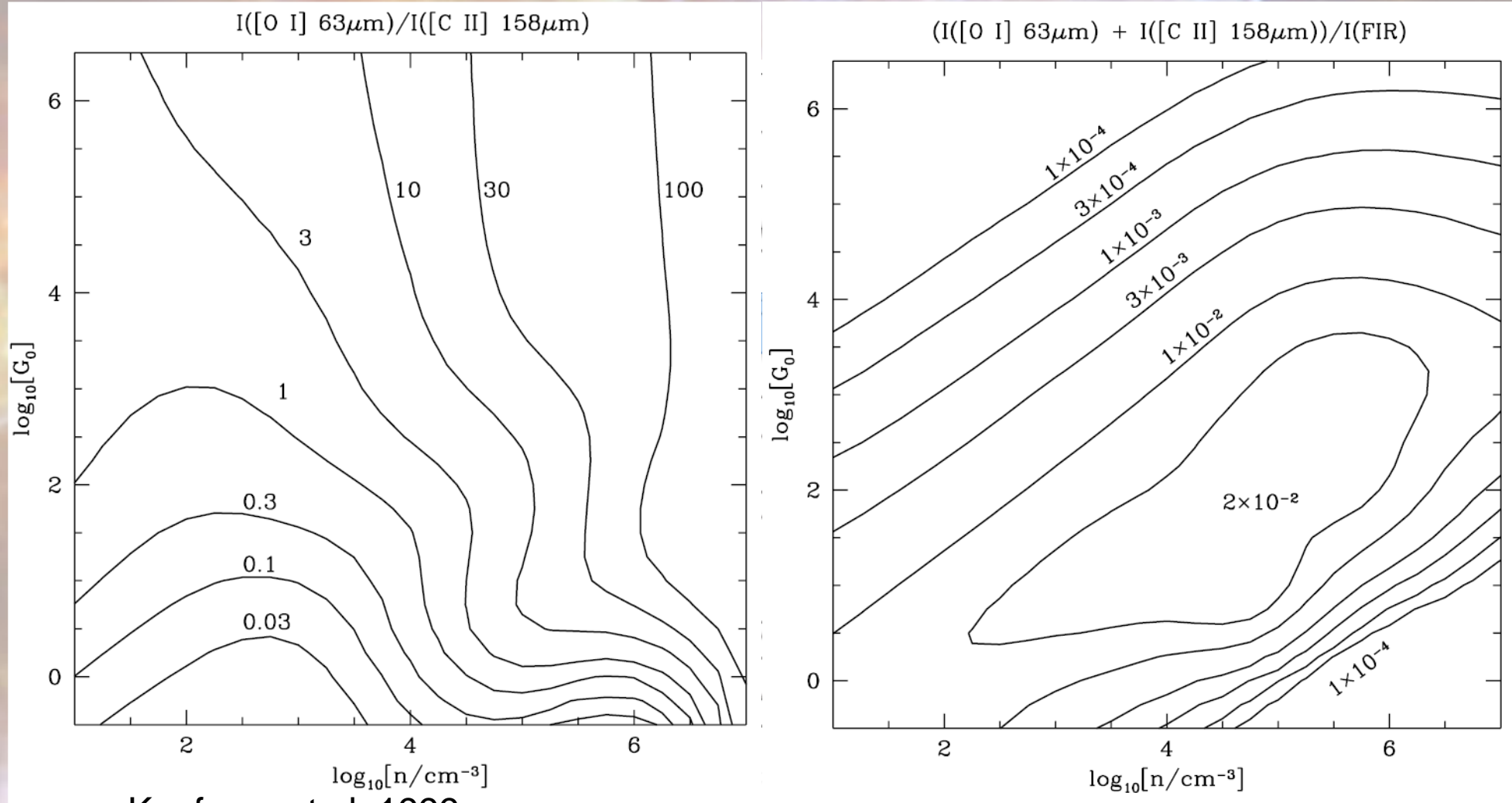
- Geometry
  - plane parallel slab
    - 1-sided / 2-sided
  - sphere (new parameter: mass)
  - circular paraboloid (outflow)
  - 3-D
  - clumpy, fractal
- Radiation field (int & ext)
  - isotropic and/or directed/inclined
  - spectral shape of FUV field
    - physics and chemistry  $\lambda$ -dependent
  - detailed photon cross-section
  - full  $\lambda$ -resolving radiative transfer
- Dust content
  - dust composition, size distribution (practically unknown)
  - very small grains, PAHs  
PE efficiency, charge exchange
  - grain surface characterization  
 $E_{\text{bind}}$  ??
- Chemistry
  - nonlinear chemical networks  
~10-20% reaction rates known
  - coupling to heating & cooling & RT
  - ice & surface & gas chemistry
  - coupling to FUV & CR & XR
  - state-to-state reaction rates



# PDR Model Complexity

- Energetics / Thermodynamics
  - heating couples to FUV RT & dust
  - cooling couples to chemistry & RT
  - full treatment of H<sub>2</sub>, HD, CO, H<sub>2</sub>O,.....
  - detailed internal RT vs. approx.
  - isobaric (p constant) vs. isochoric (n constant)
  - chemical heating & cooling
  - multi-stability solutions?
- Stationarity
  - stationary vs. time-dep solution
    - initial conditions?
- rate uncertainties more important
  - non-stationary model parameters!
    - UV field, geometry, pressure/density
- Numerics
  - non-linear coupling of geometry RT & energetics & chemistry
  - horrible scaling with problem size  
chemistry:  $N^{3.5}$
  - interpolation introduces large uncertainties
  - n-dim global root finding/minimization
  - existence of (multiple) solutions?

# Line ratio analysis

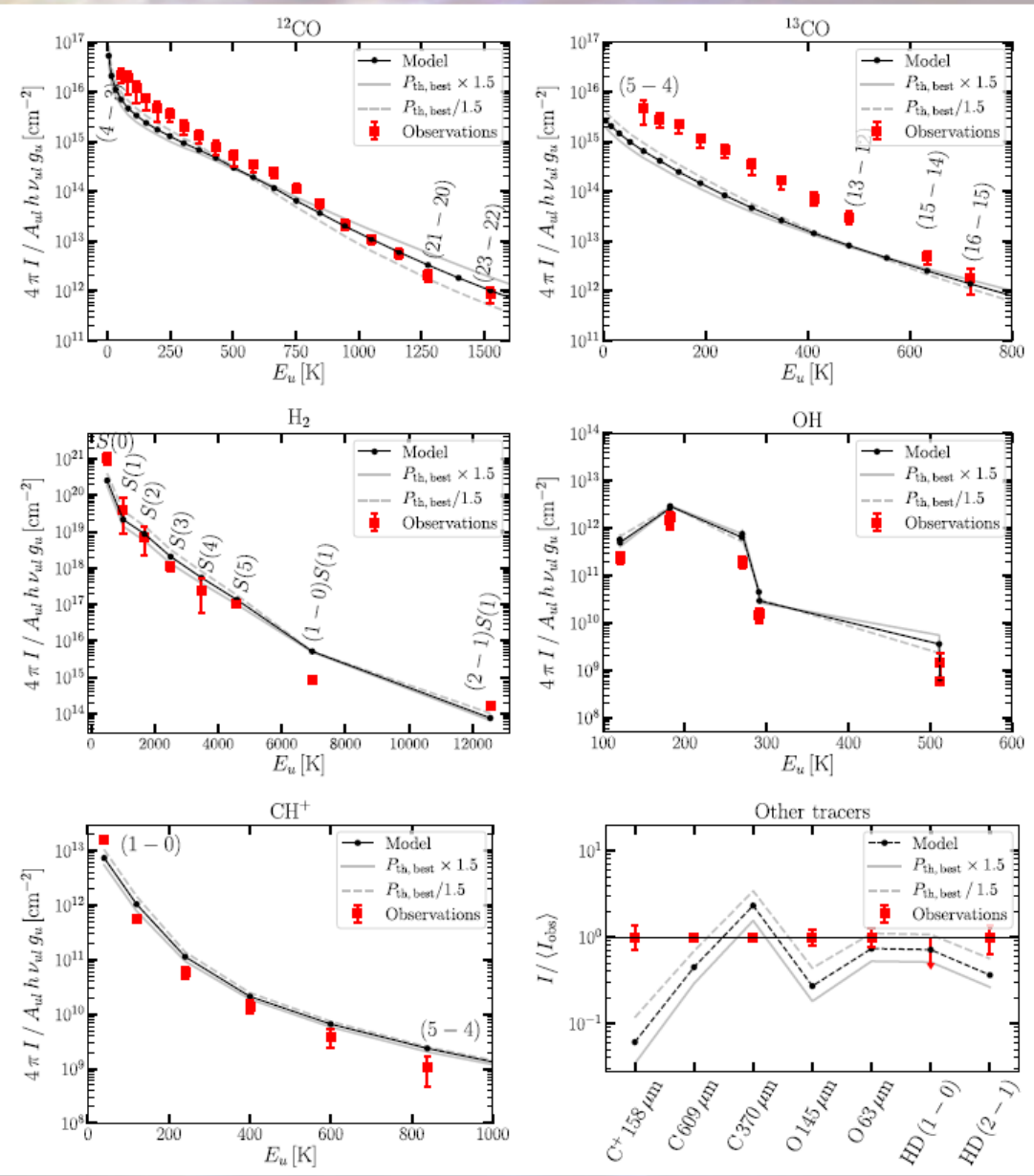
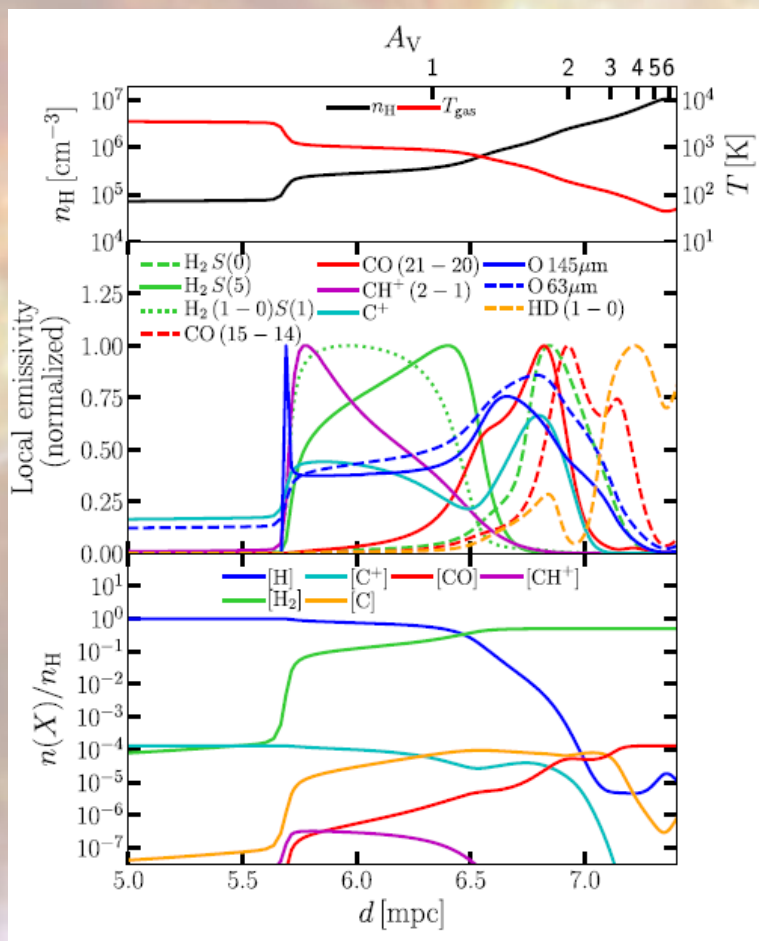


Kaufman et al. 1999



# Orion Bar Model

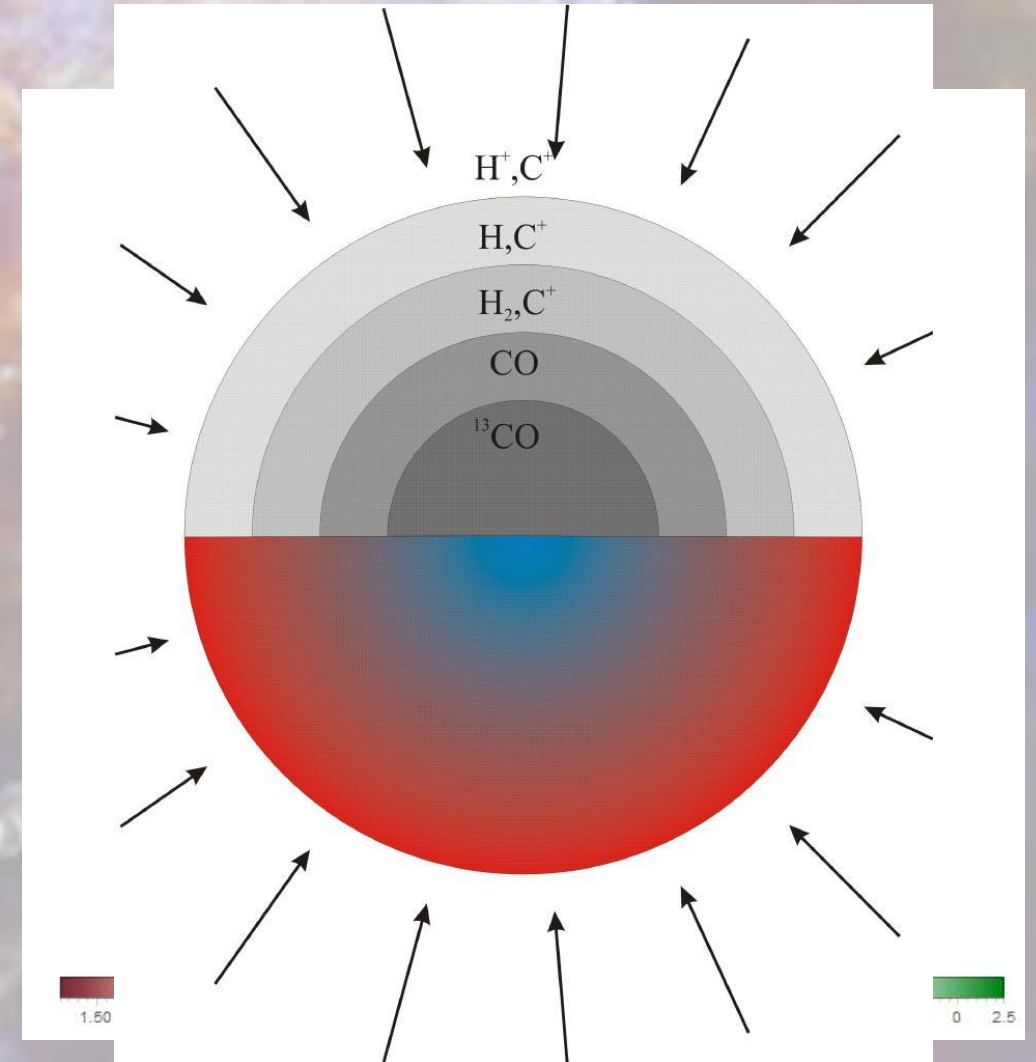
Meudon PDR Code, isobaric



Joblin et al. 2018

# The KOSMA- $\tau$ PDR Code

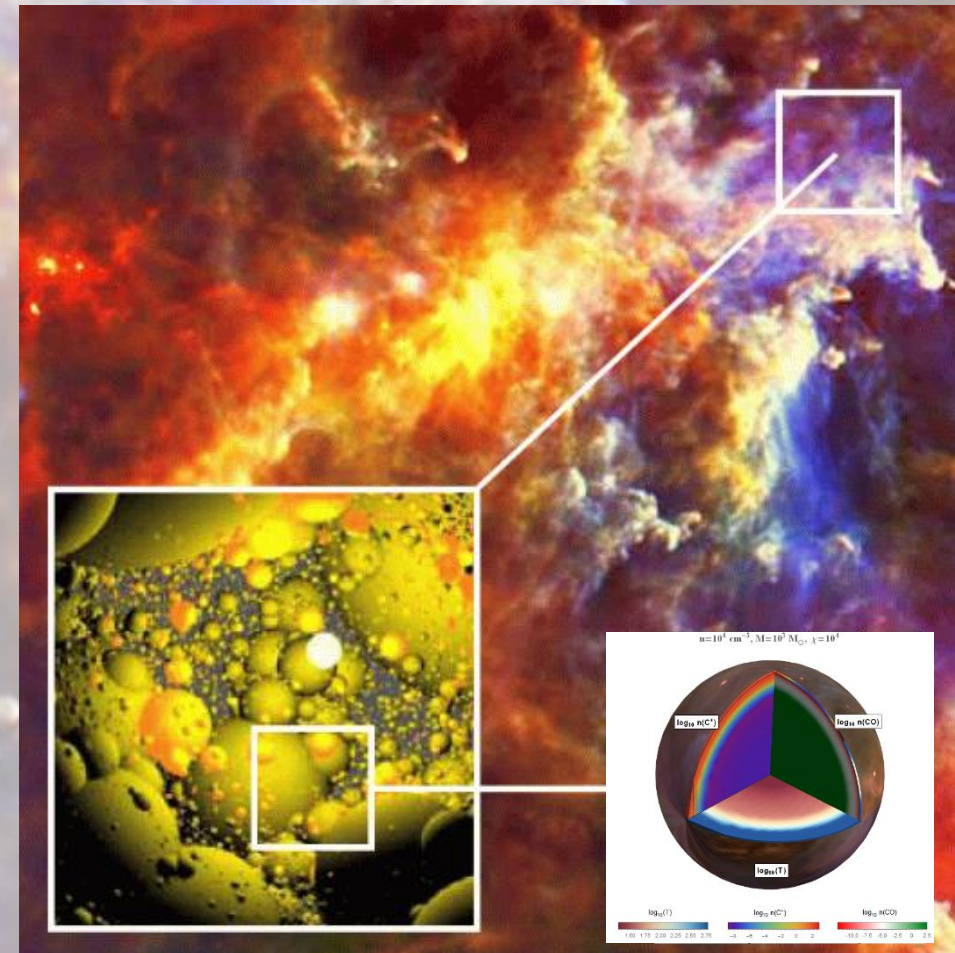
- 1-D, spherical geometry
  - power-law density profile
  - isotropic illumination
- self-consistent solution of energy- and chemical balance and radiative transfer
- self-shielding of  $H_2$ , CO (FGK, Draine & Bertoldi 1997, Visser et al. 2009)
- full dust RT and temp. computation for varying dust distribution





# The KOSMA- $\tau$ PDR Code

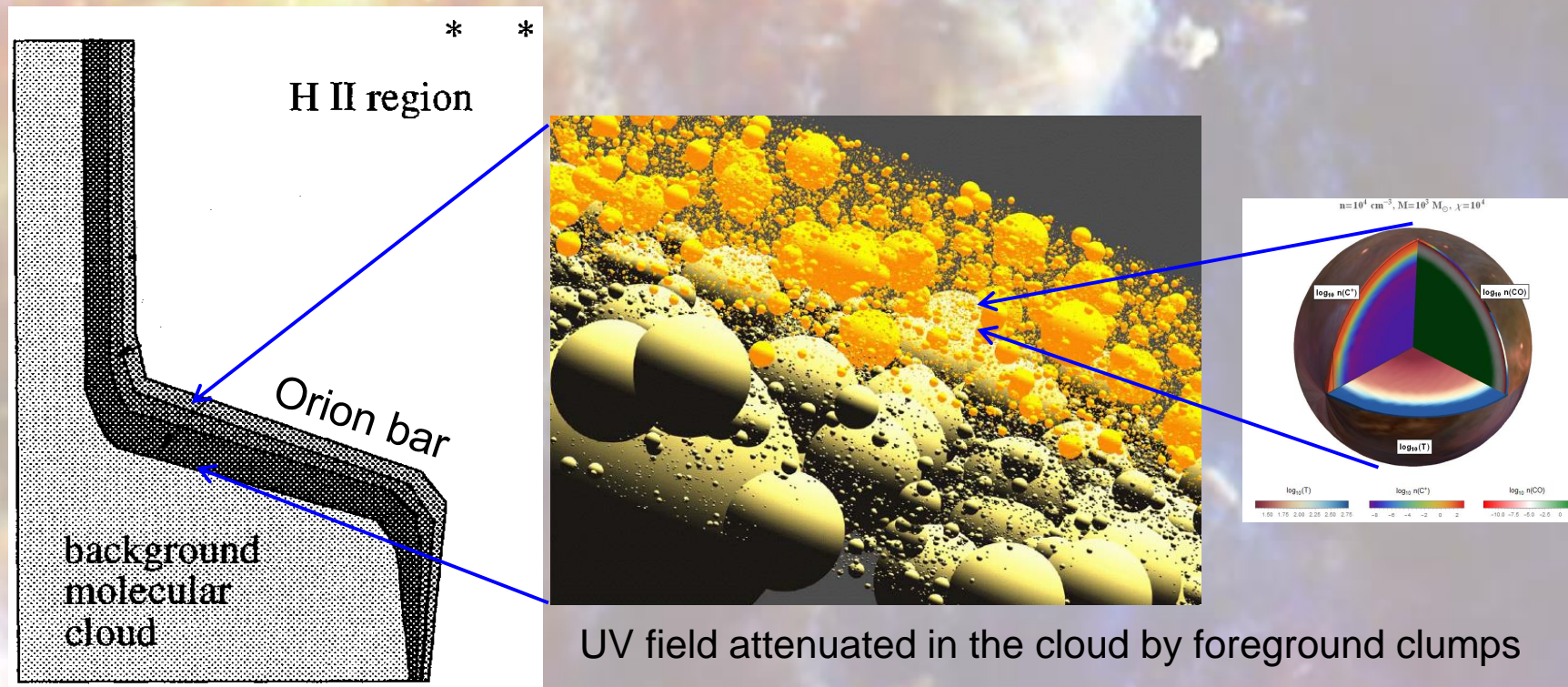
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- full dust RT and temp. computation for varying dust distribution
- clumpy cloud composition
  - stochastic clump ensemble
  - **KOSMA- $\tau$  3D** (Andree-Labsch et al. 2017)





# Applications: KOSMA- $\tau$ 3D

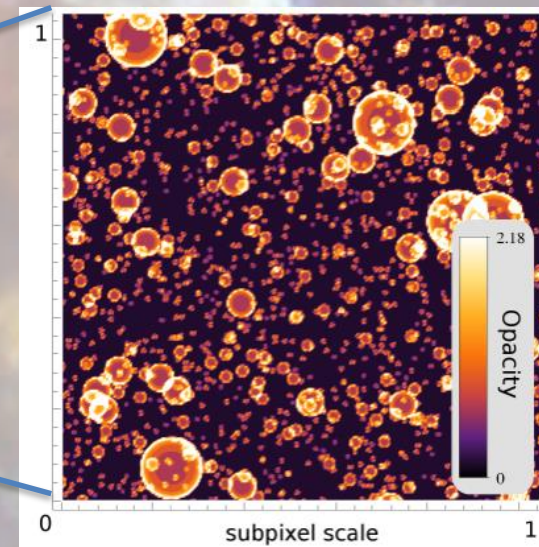
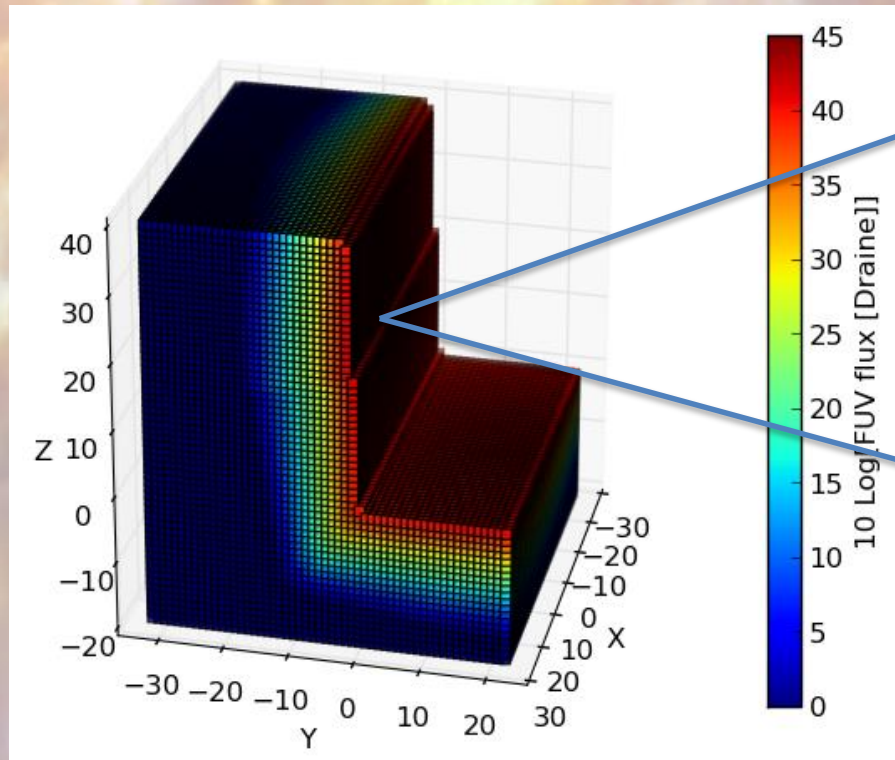
- Arbitrary 3-dim structure, each voxel populated by PDR clump ensembles with full size distribution (embedded in interclump medium)





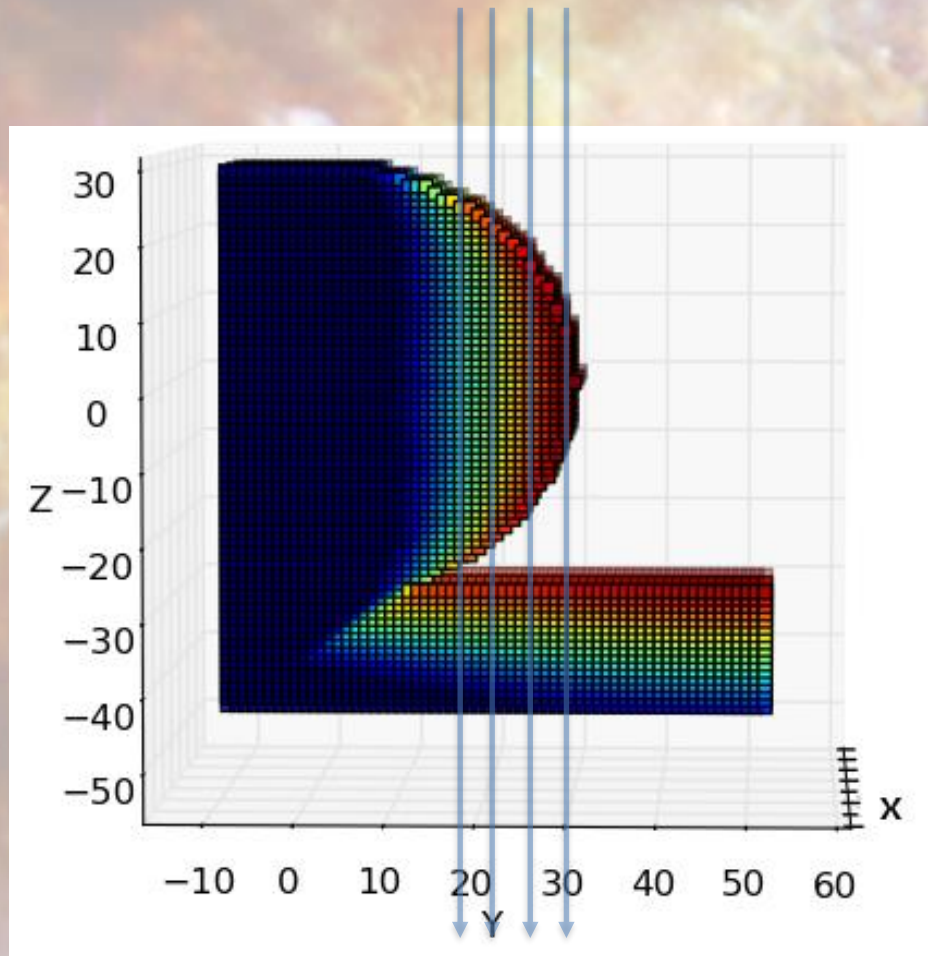
# Applications: KOSMA- $\tau$ 3D

- Radiative transfer through all voxel (including shielding) allows to simulate observations from any direction, distance, ...

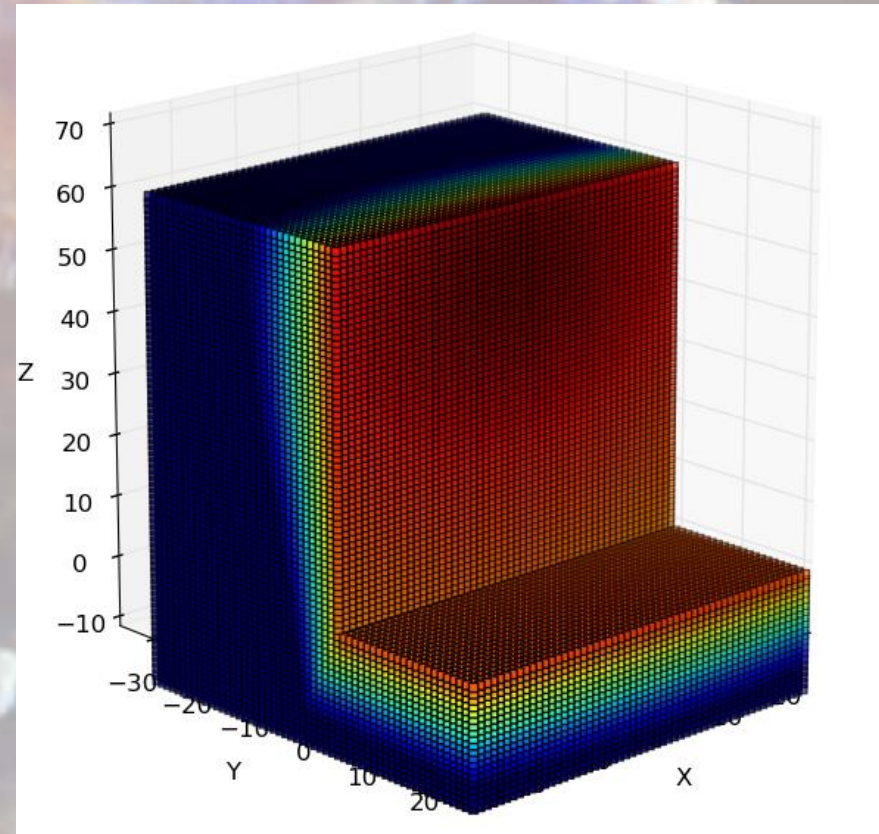


Andree-Labsch et al. 2017

# Applications: KOSMA- $\tau$ 3D



no chemical stratification

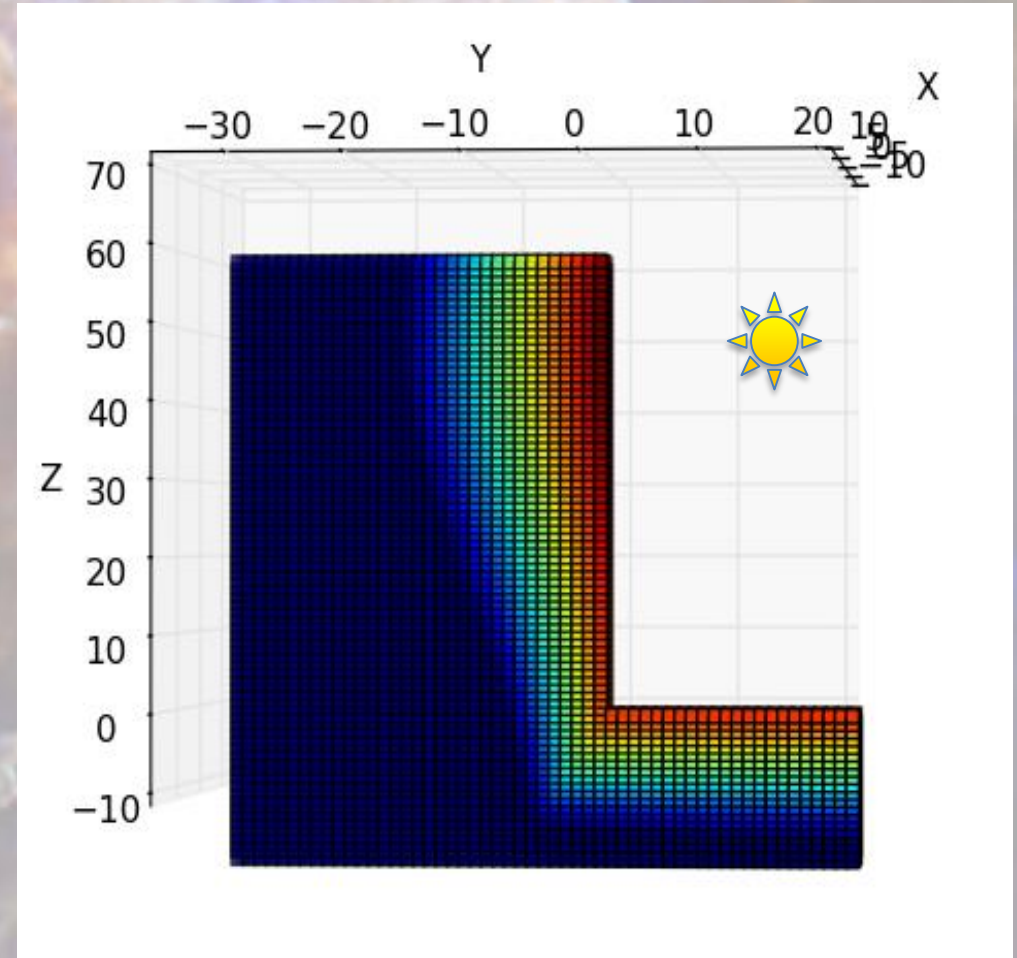
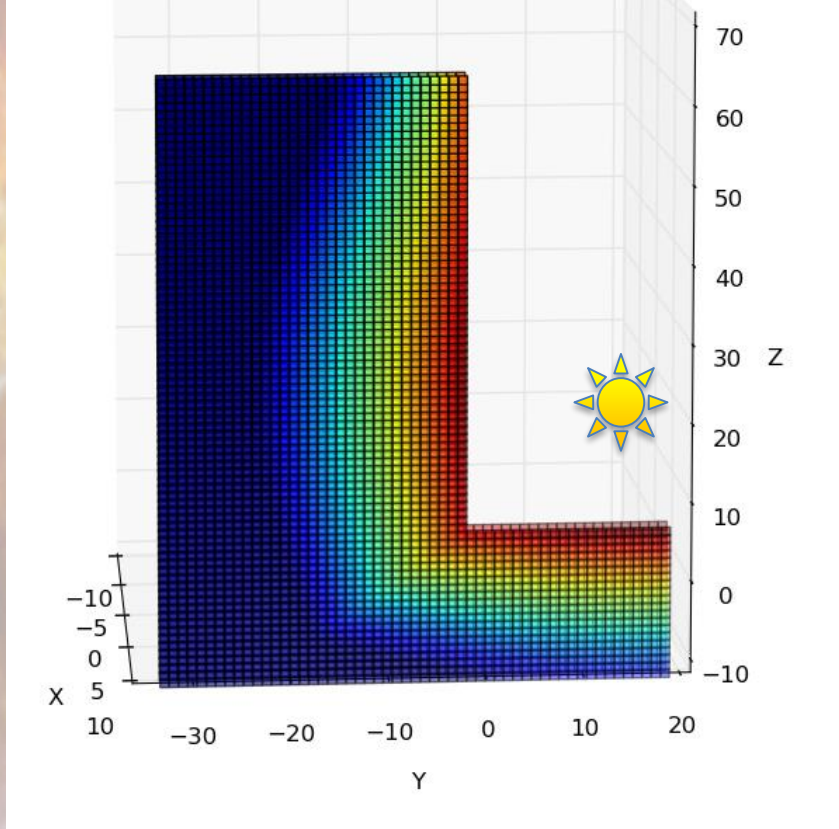


Andree-Labsch et al. 2017



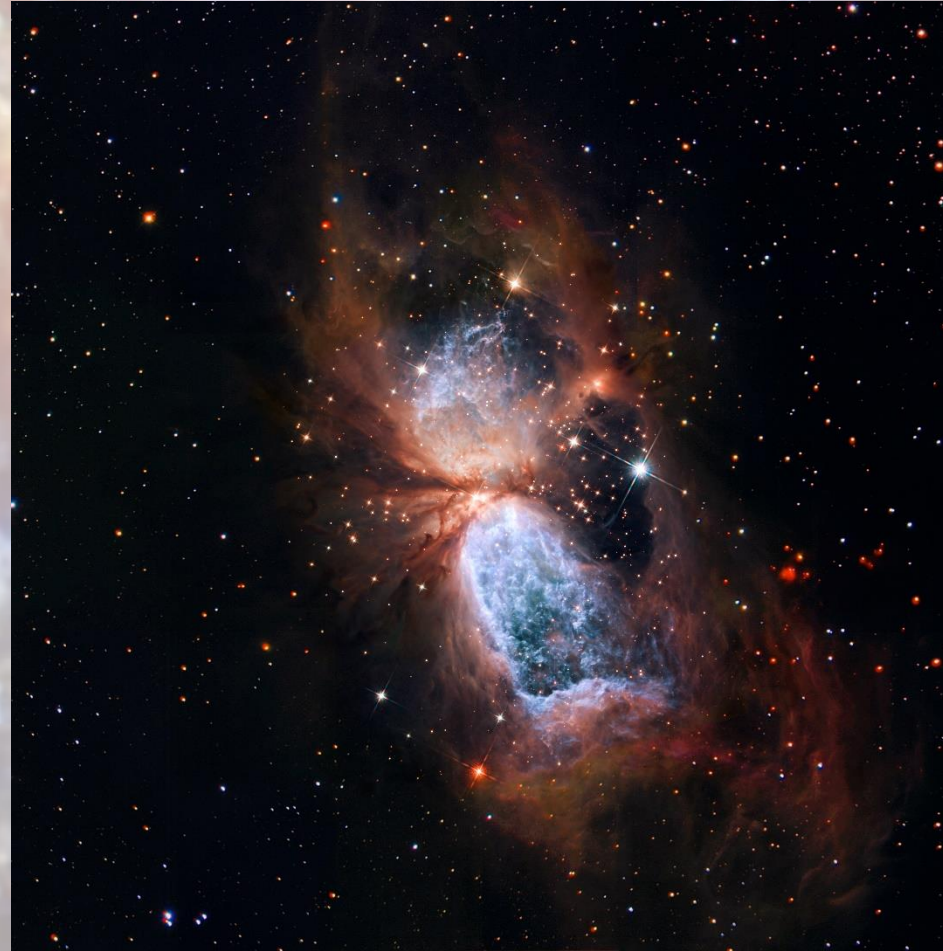
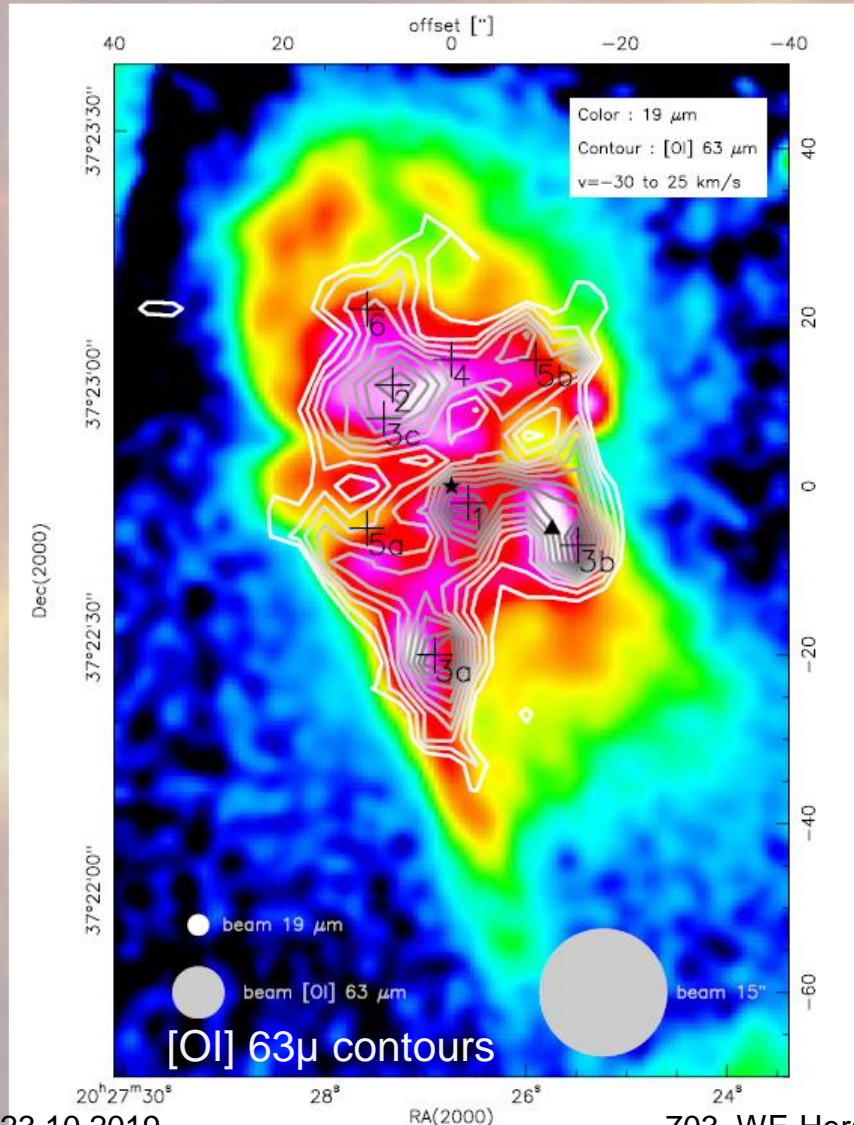
# Applications: KOSMA- $\tau$ 3D

foreground absorption  
by cool material in front of hot gas



Andree-Labsch et al. 2017

# S106

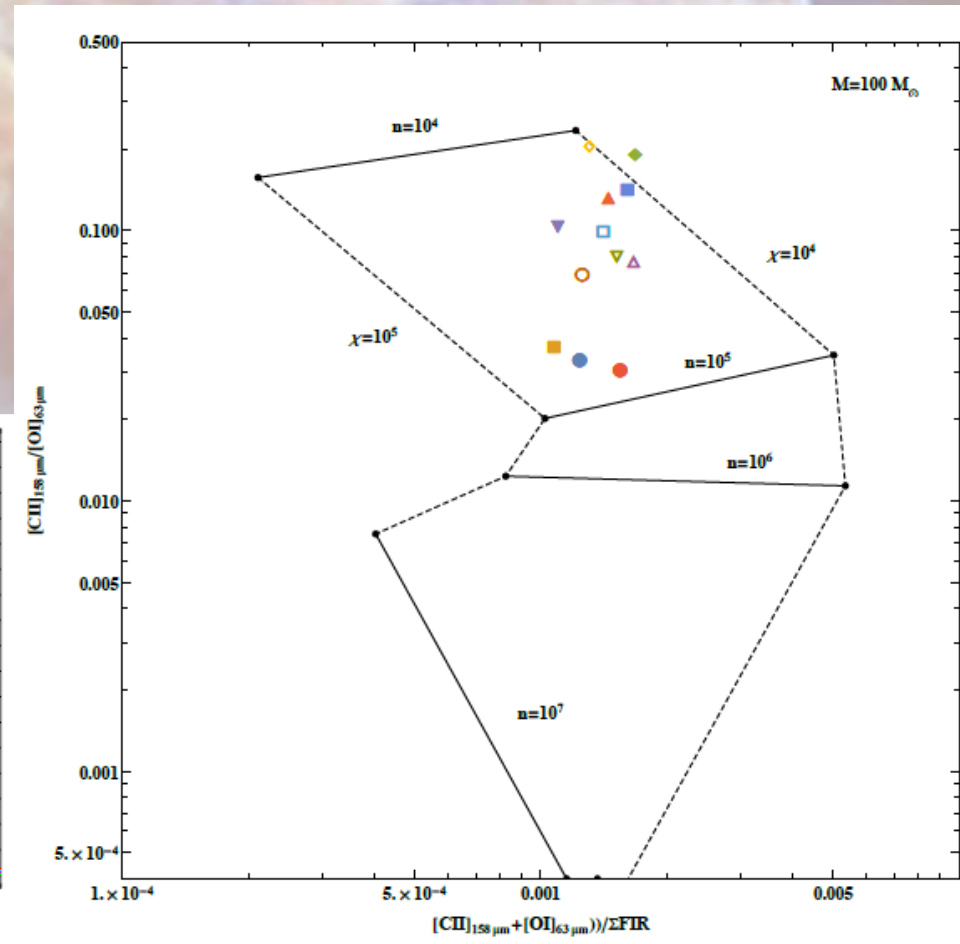
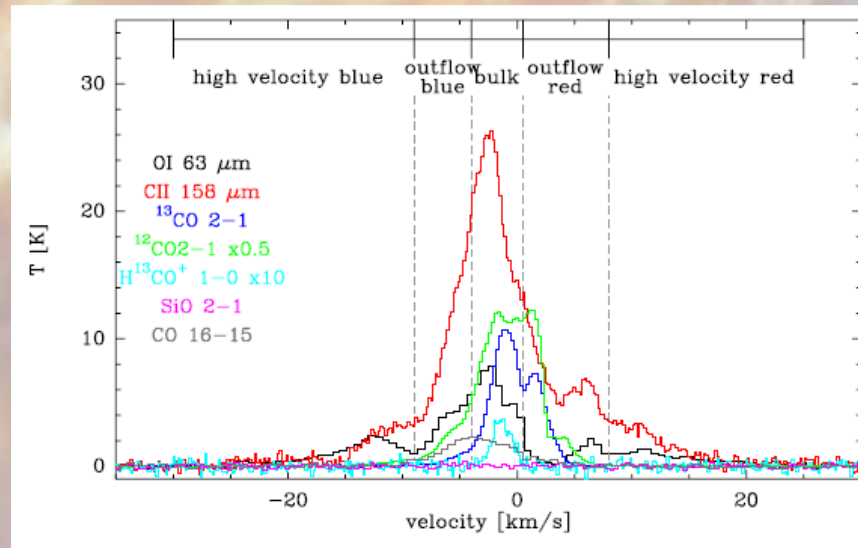




# S106

High spectral resolution of  
(up)GREAT on SOFIA allows the  
spectral identification of various  
kinematic components

Tomography of 3-D structure

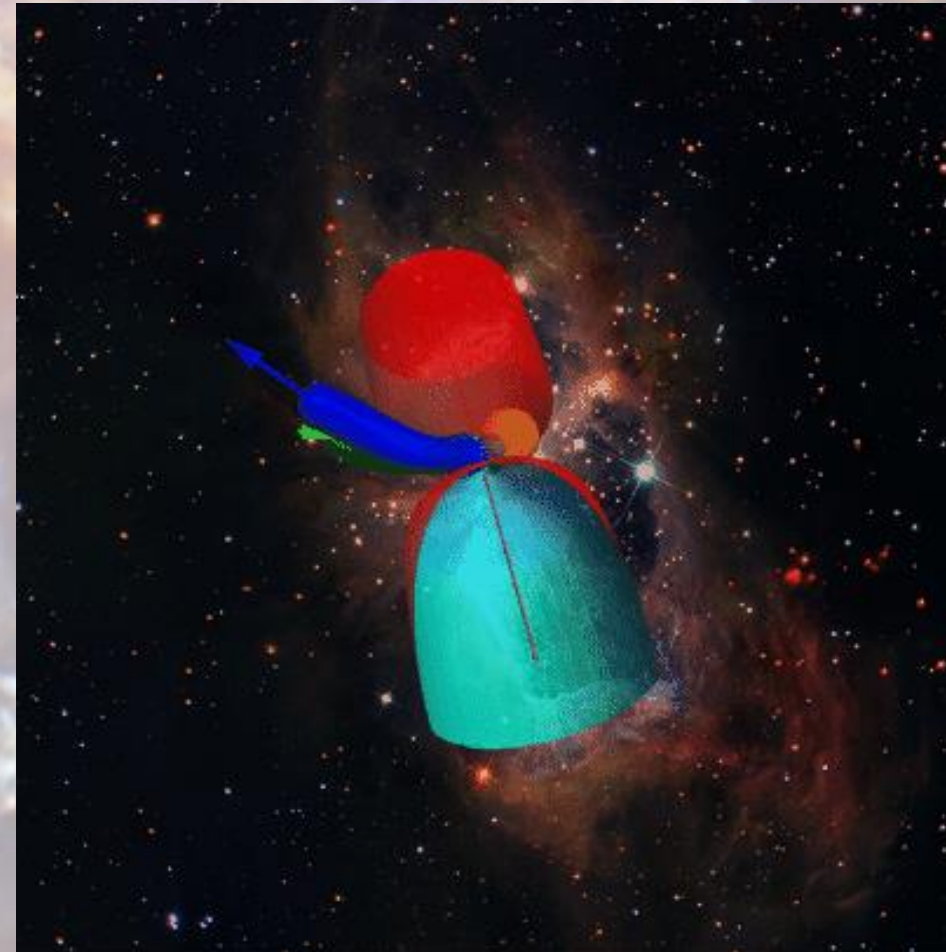
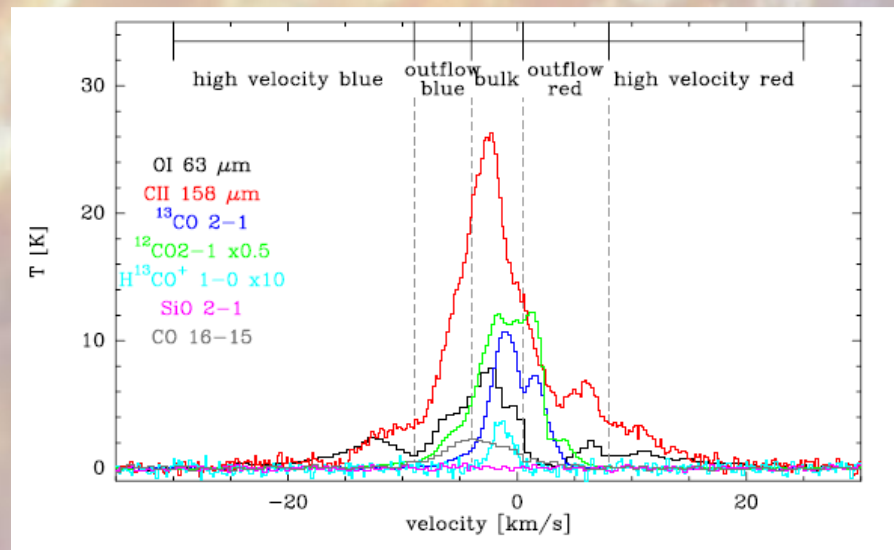


Schneider et al. 2018

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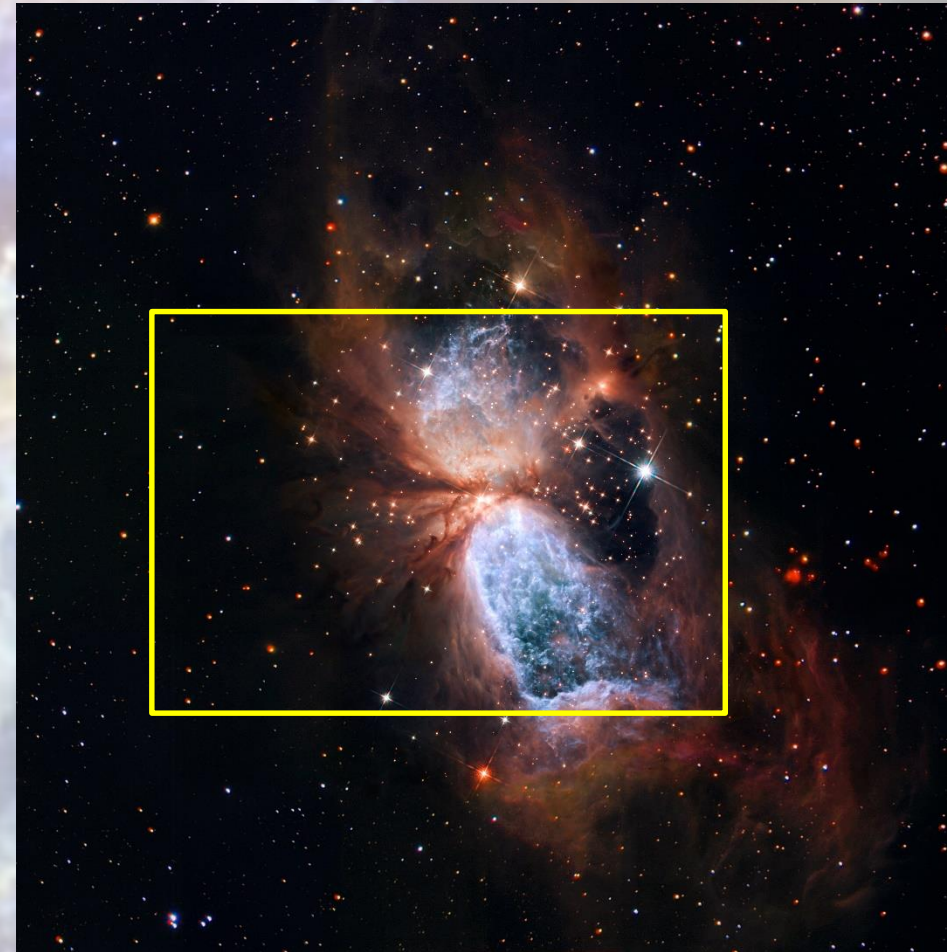
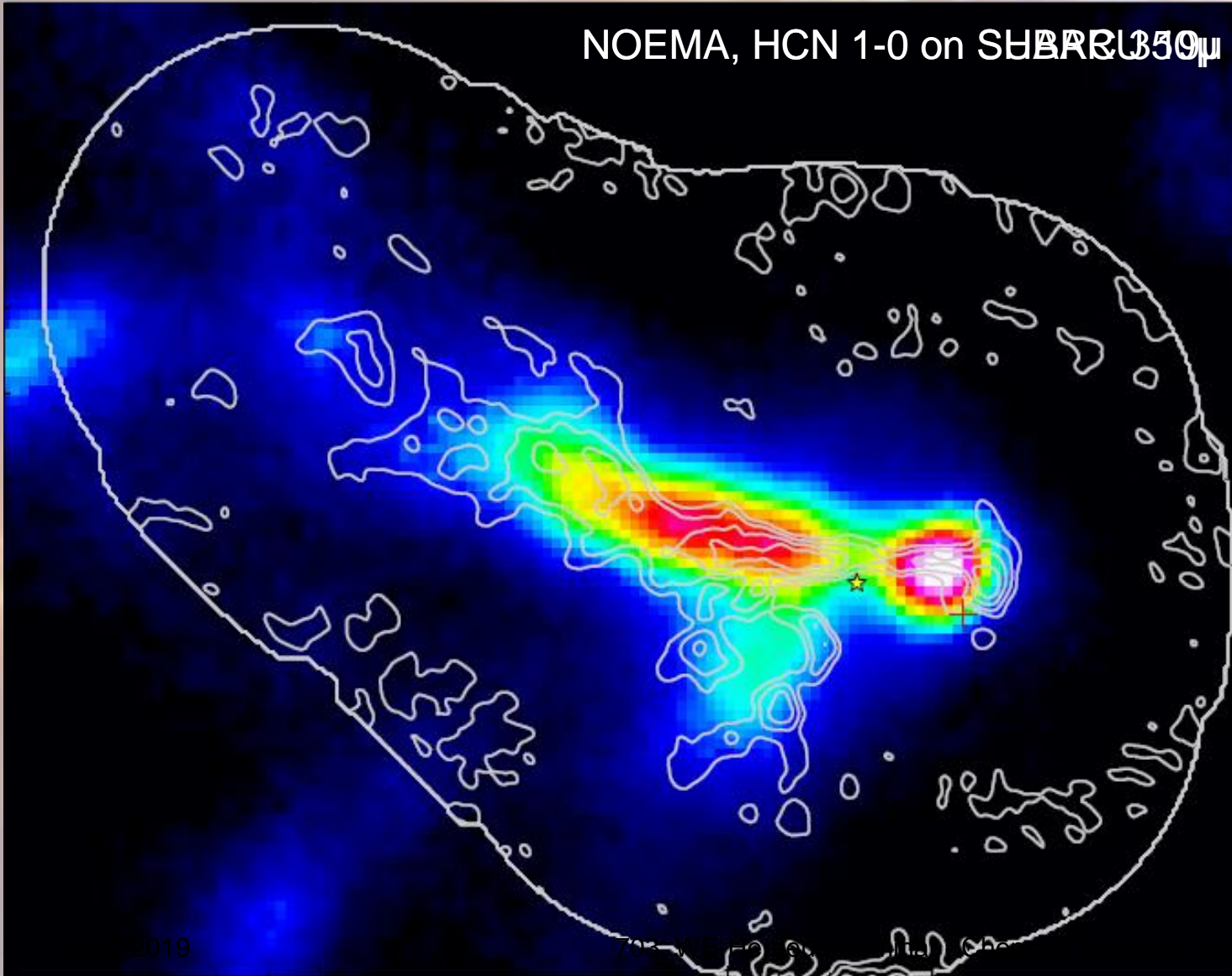


Schneider et al. 2018

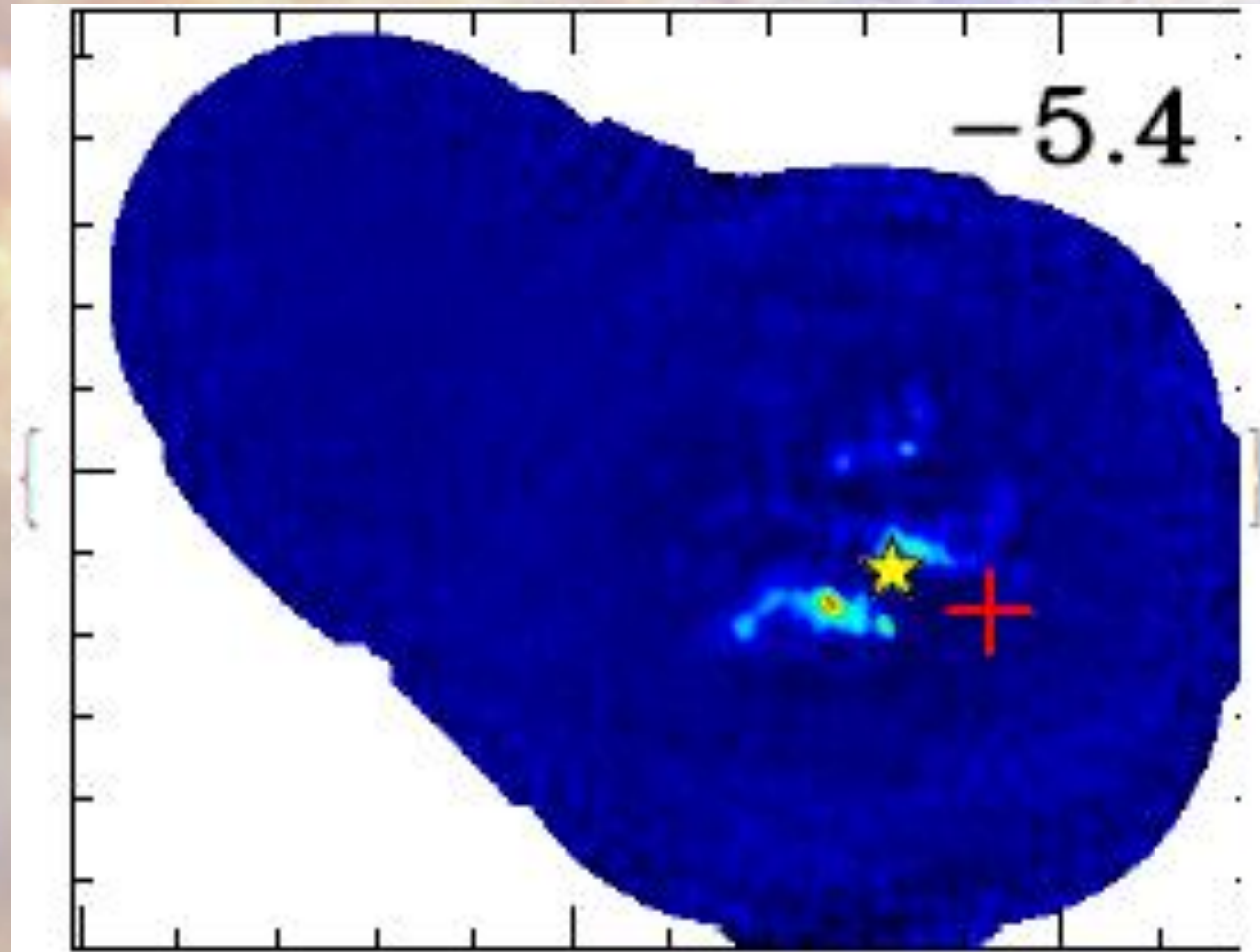


# S106

NOEMA, HCN 1-0 on SHARAD 350 $\mu$



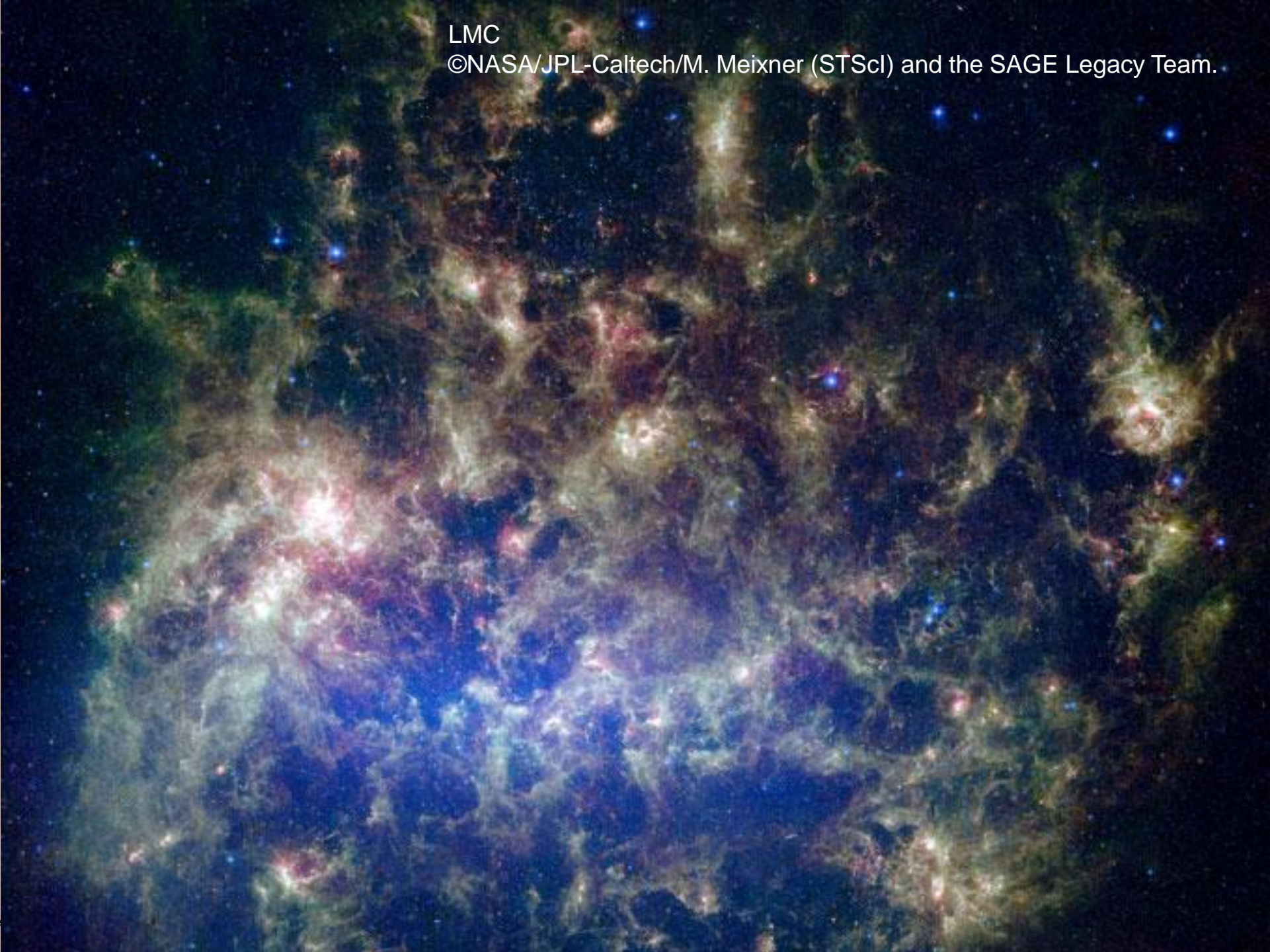
# Animation of the velocity structure





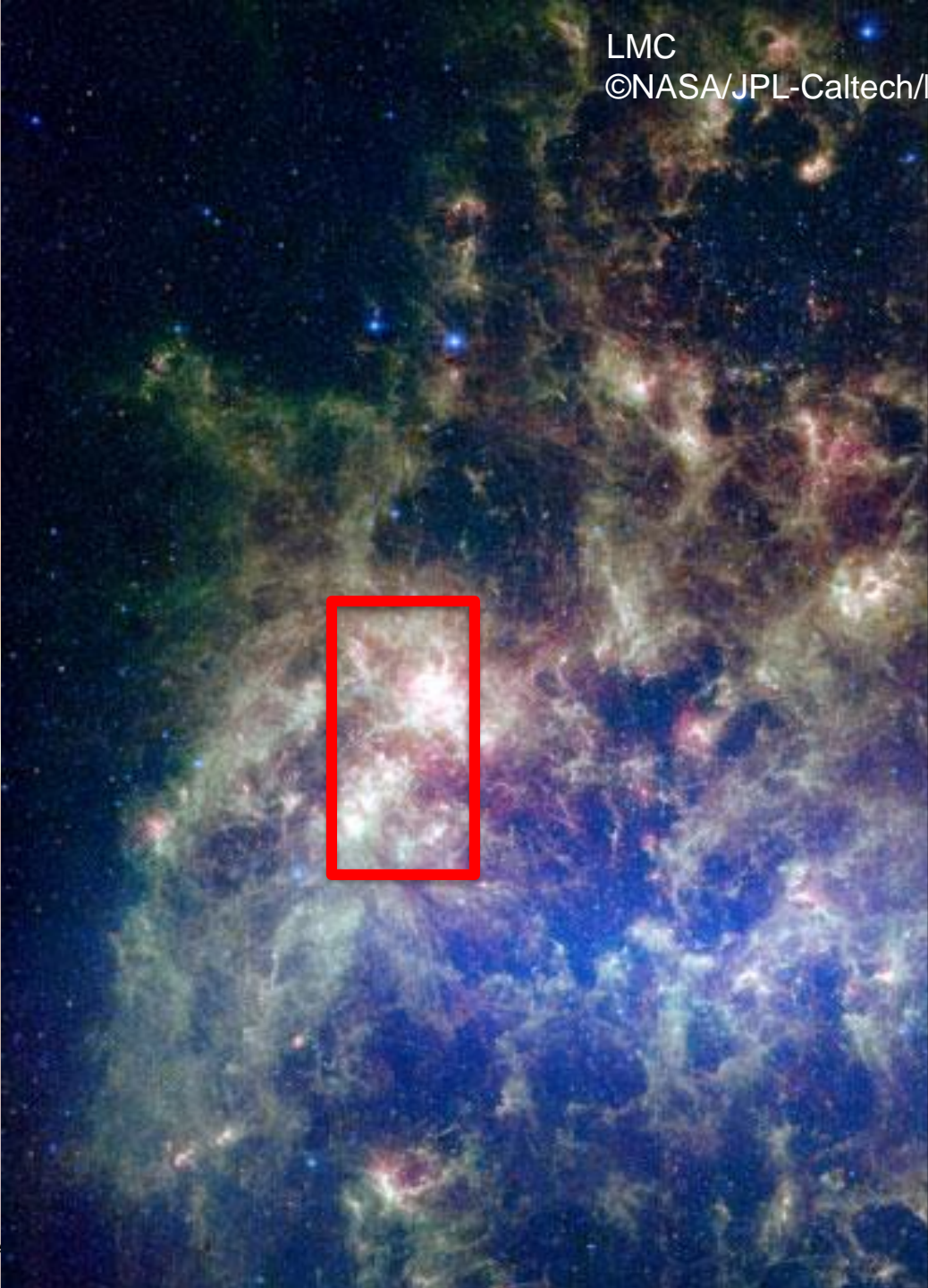
LMC

©NASA/JPL-Caltech/M. Meixner (STScI) and the SAGE Legacy Team.



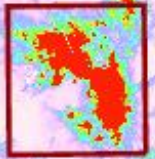


LMC  
©NASA/JPL-Caltech/



8 $\mu$ m

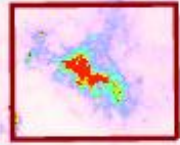
30 Dor



N158



N160

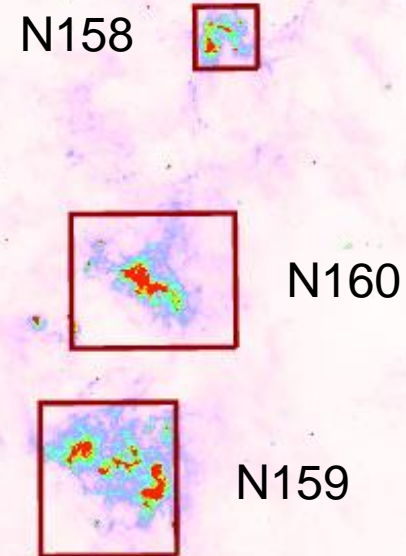
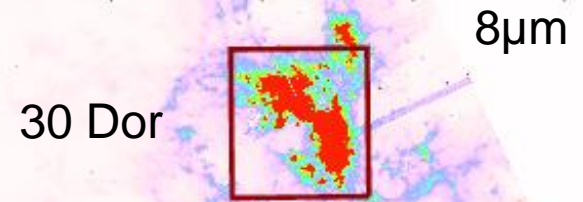
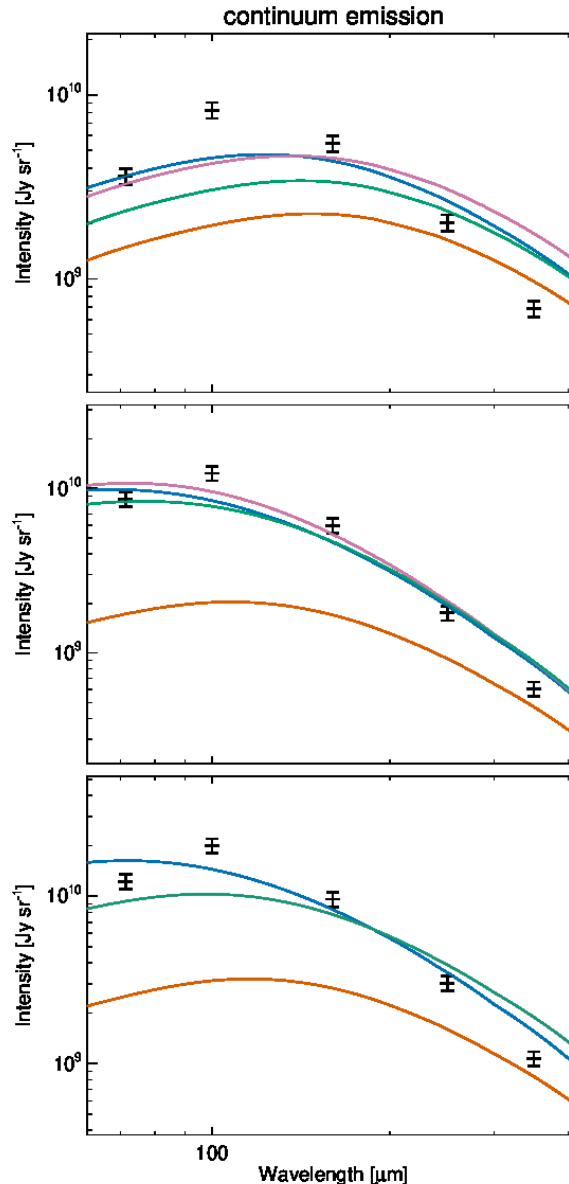
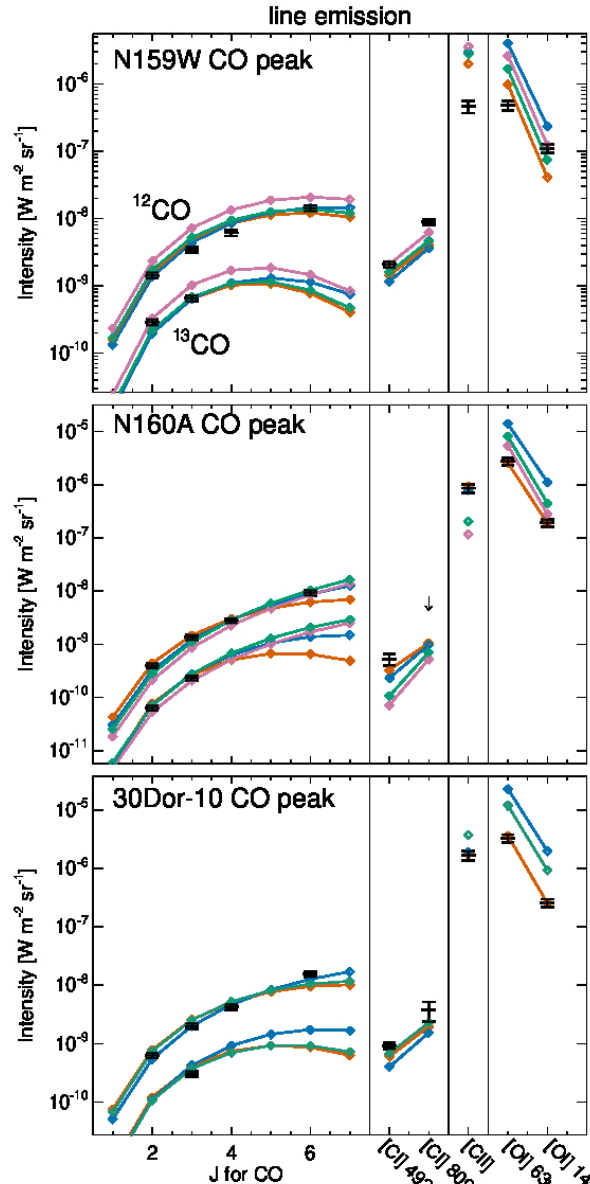


N159





# Fitting line and dust continuum emission

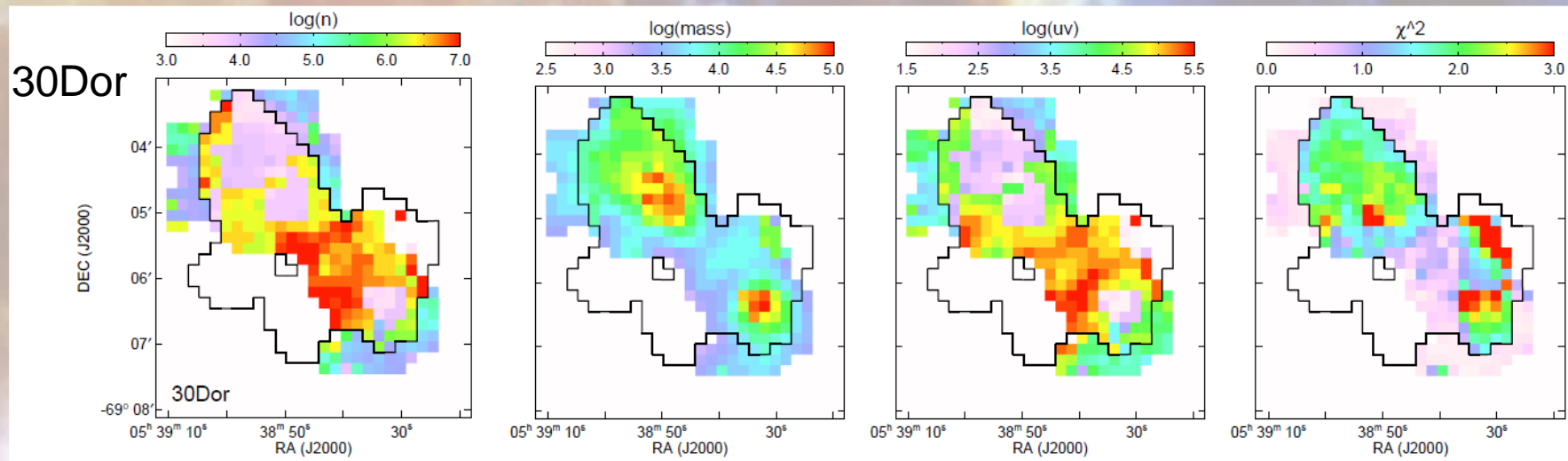
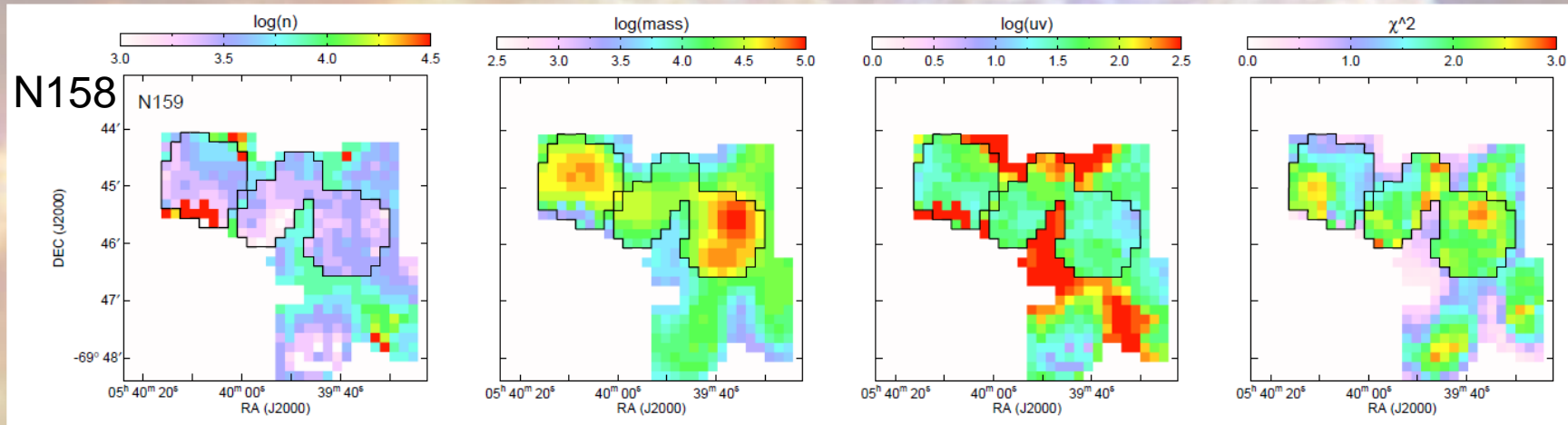


# Map-based PDR Modelling

density

mass

UV





# Current KOSMA- $\tau$ Developments

- Non-stationary PDR structure
  - t-dependent solution of chemistry (tests)
  - t-dependent parameters, e.g. FUV input
  - non-stationary particle transport , e.g. diffusion, advection, mass evaporation (PhD project A. Baby)
- KOSMA- $\tau$  3D
  - inclusion of systematic velocities
  - full line & continuum radiative transfer (PhD projects C. Bruckmann & C. Yanitski)
  - performance improvements
- Microphysics/chemistry
  - chemical heating (tests)
  - surface chemistry (done)
- full H<sub>2</sub> excitation
  - IR quadrupole emission
  - UV fluorescent line emission
  - UV continuum emission
- detailed PE heating
- non-stationary PE heating
- Misc
  - Migration to modern FORTRAN standards
  - Coupling to MHD
  - stability improvements

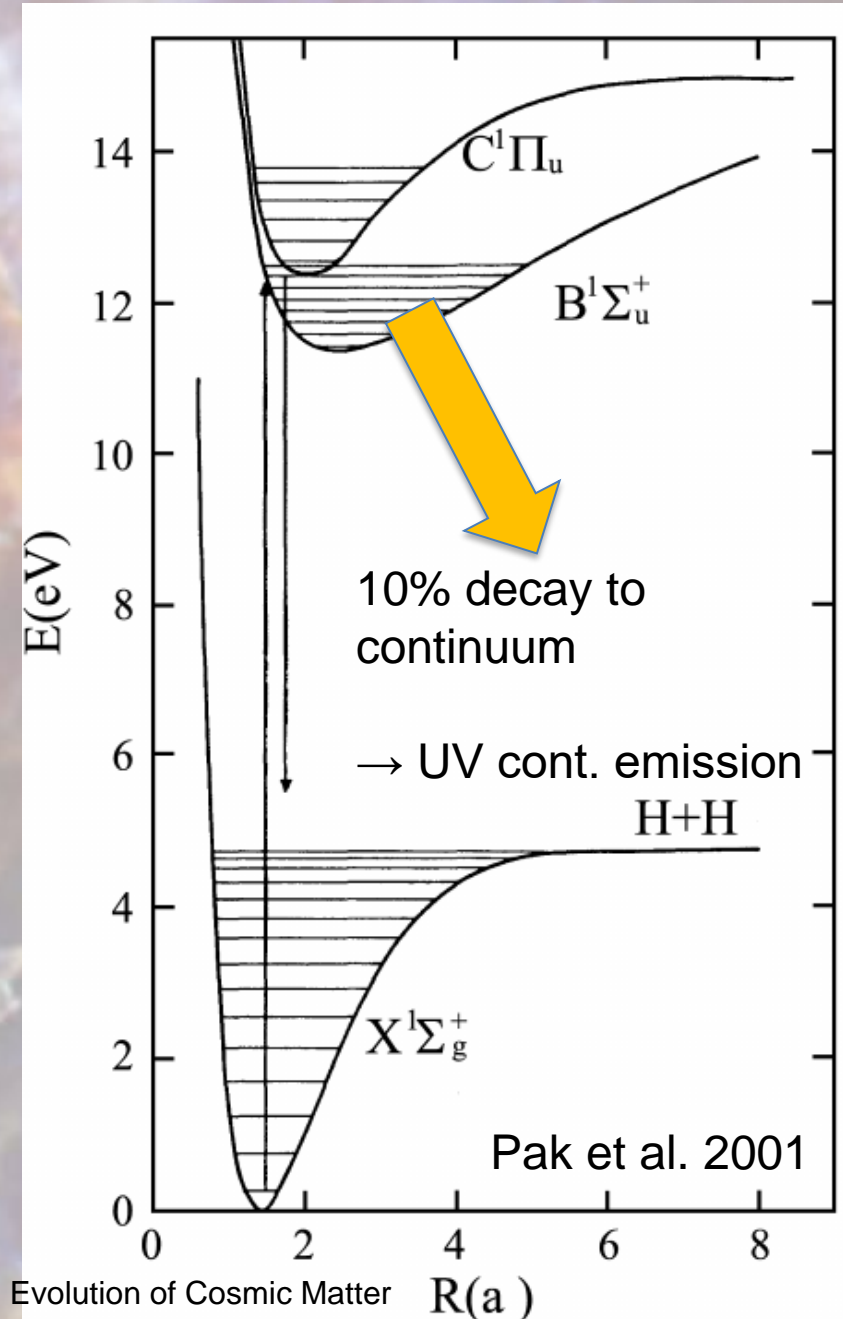
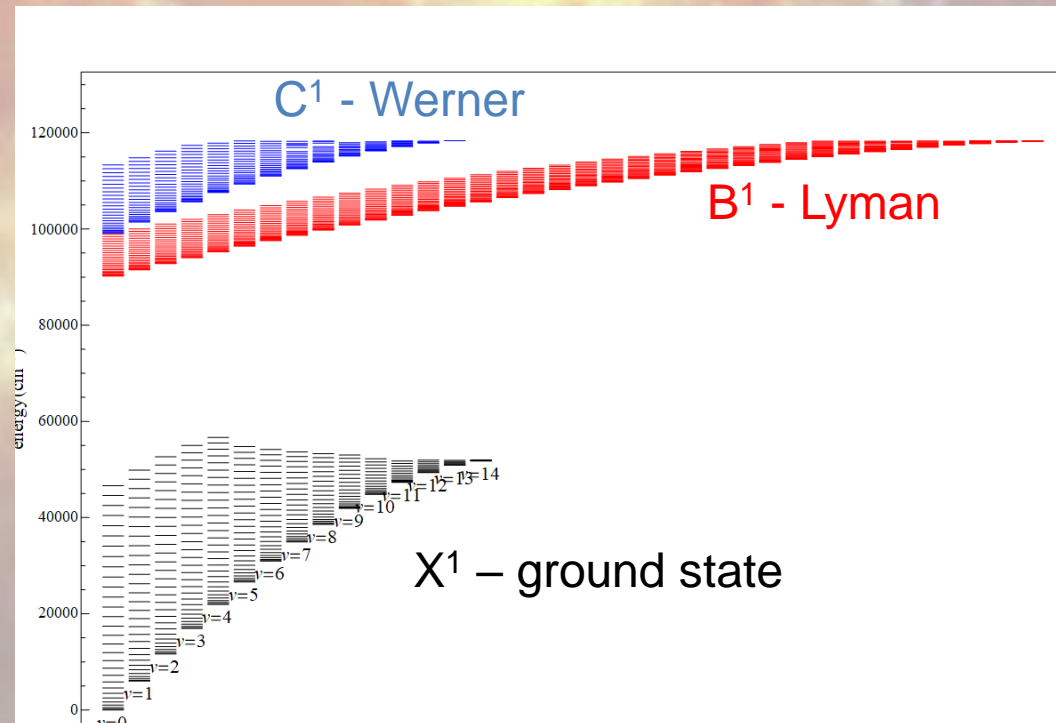
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# H<sub>2</sub> Excitation Problem

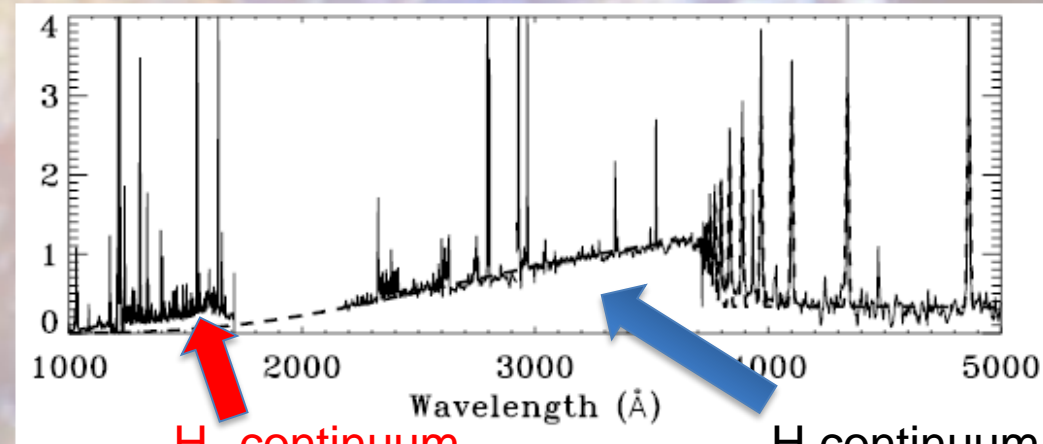
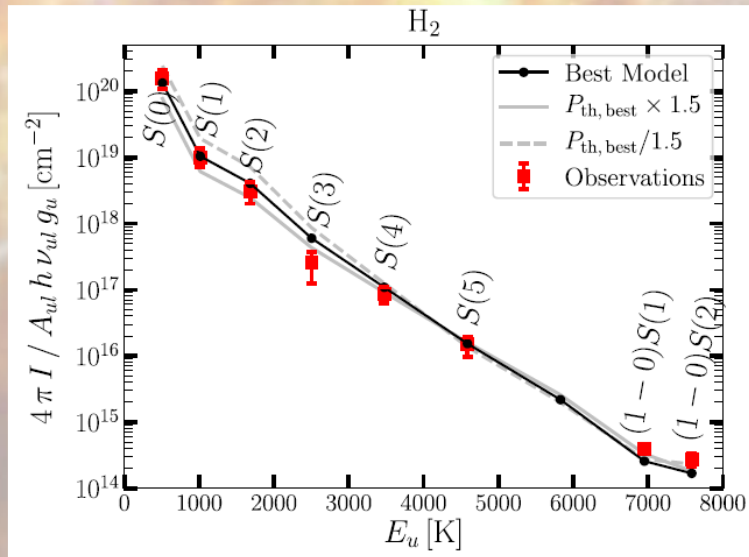
- H<sub>2</sub> dissociation via UV line absorption
- about 5000 quadrupole transitions
- about 15000 X-B and X-C dipole transitions



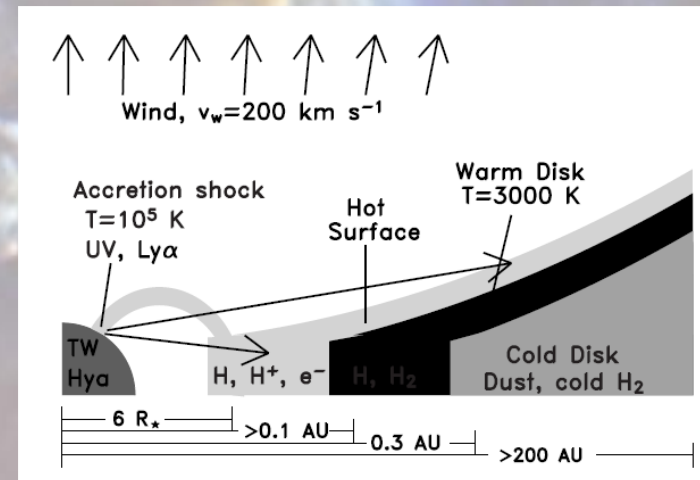
# H<sub>2</sub> excitation problem

TW Hya spectrum, Herczeg et al. 2004

H<sub>2</sub> IR emission from PDRs  
 Joblin et al. 2018,  
 Habart et al. 2011



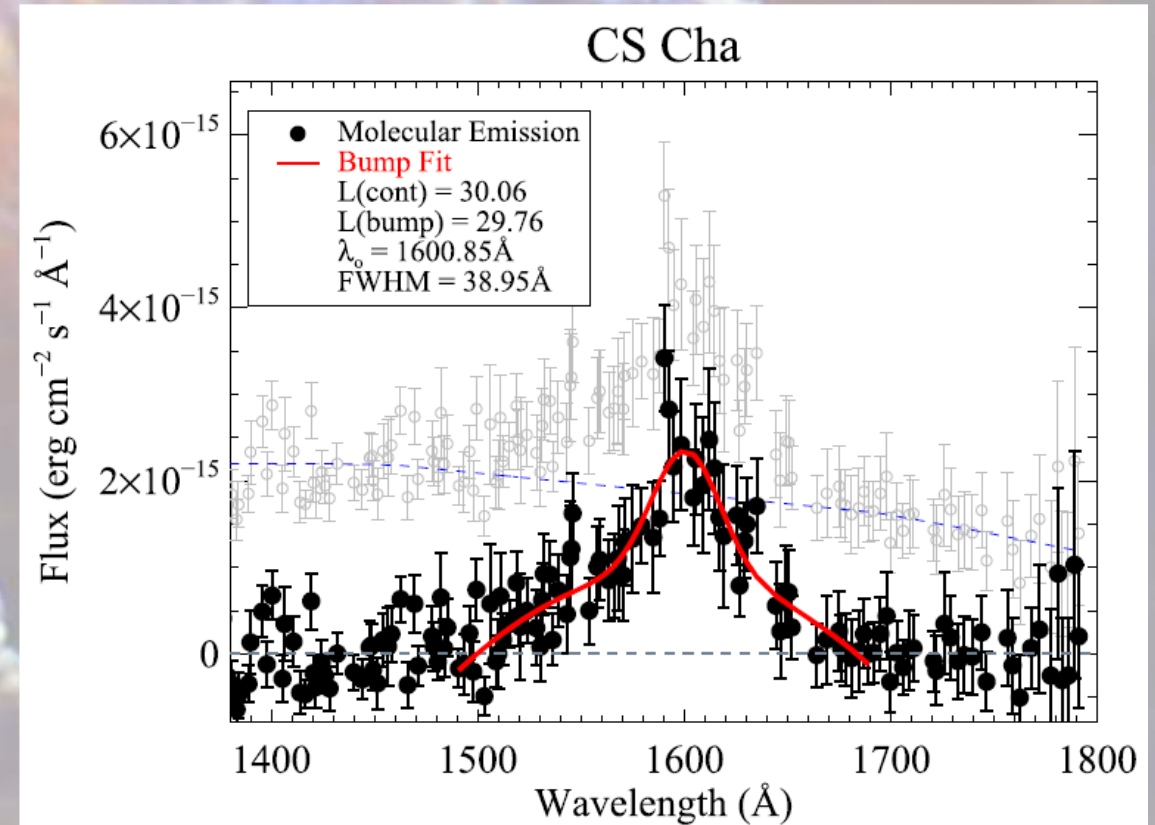
**Preparing for JWST!**





# 1600 Å bump

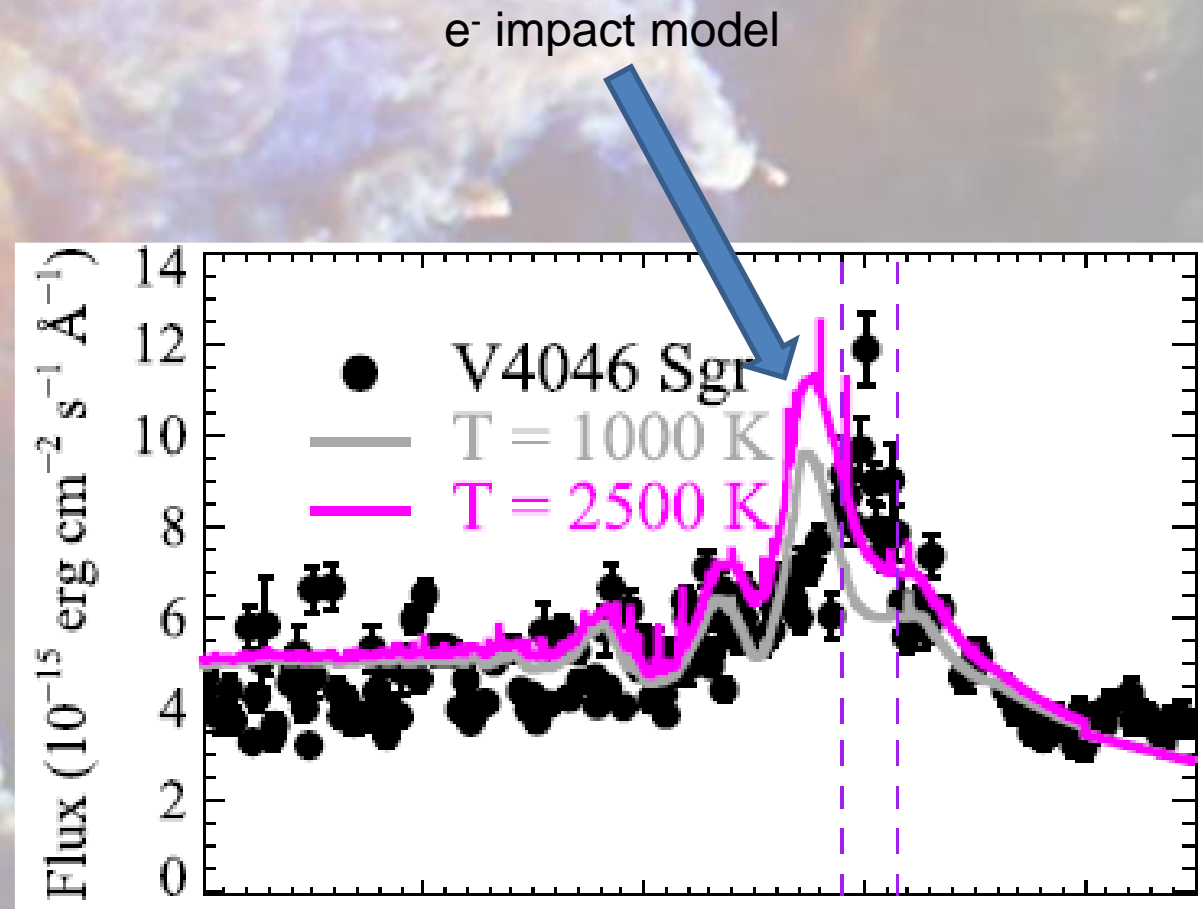
- Classical T Tauri Stars (CTTSs), show a spectral feature in the FUV continuum of some (broad emission approximately centered at 1600 Å)
- inconsistent with models of H<sub>2</sub> excited by electron-impact
- powered by Ly- $\alpha$  photons
- Ly- $\alpha$  driven dissociation of H<sub>2</sub>O



France et al. 2017

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France et al. 2017



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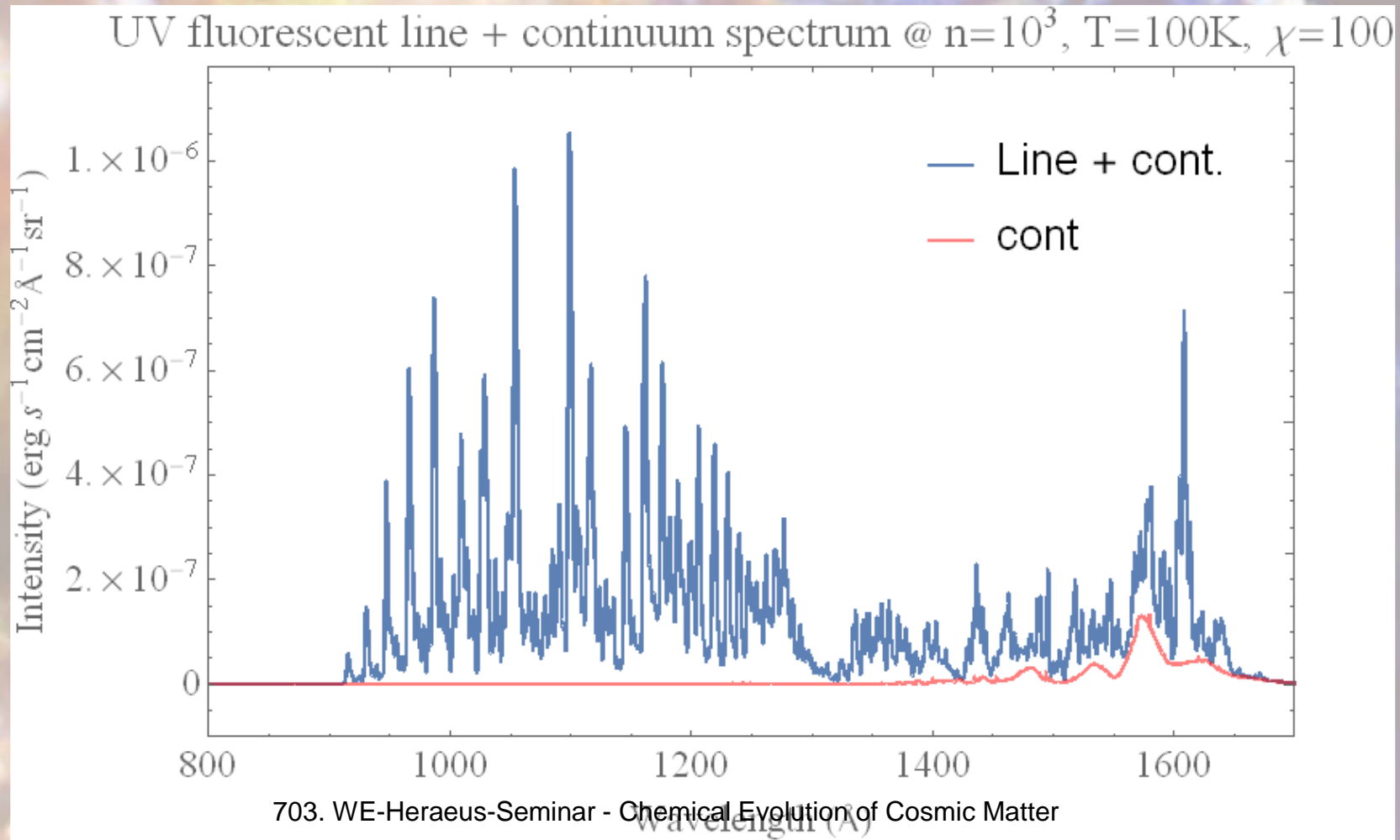
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France et al. 2017

# Fluorescent UV spectrum of H<sub>2</sub> + cont.

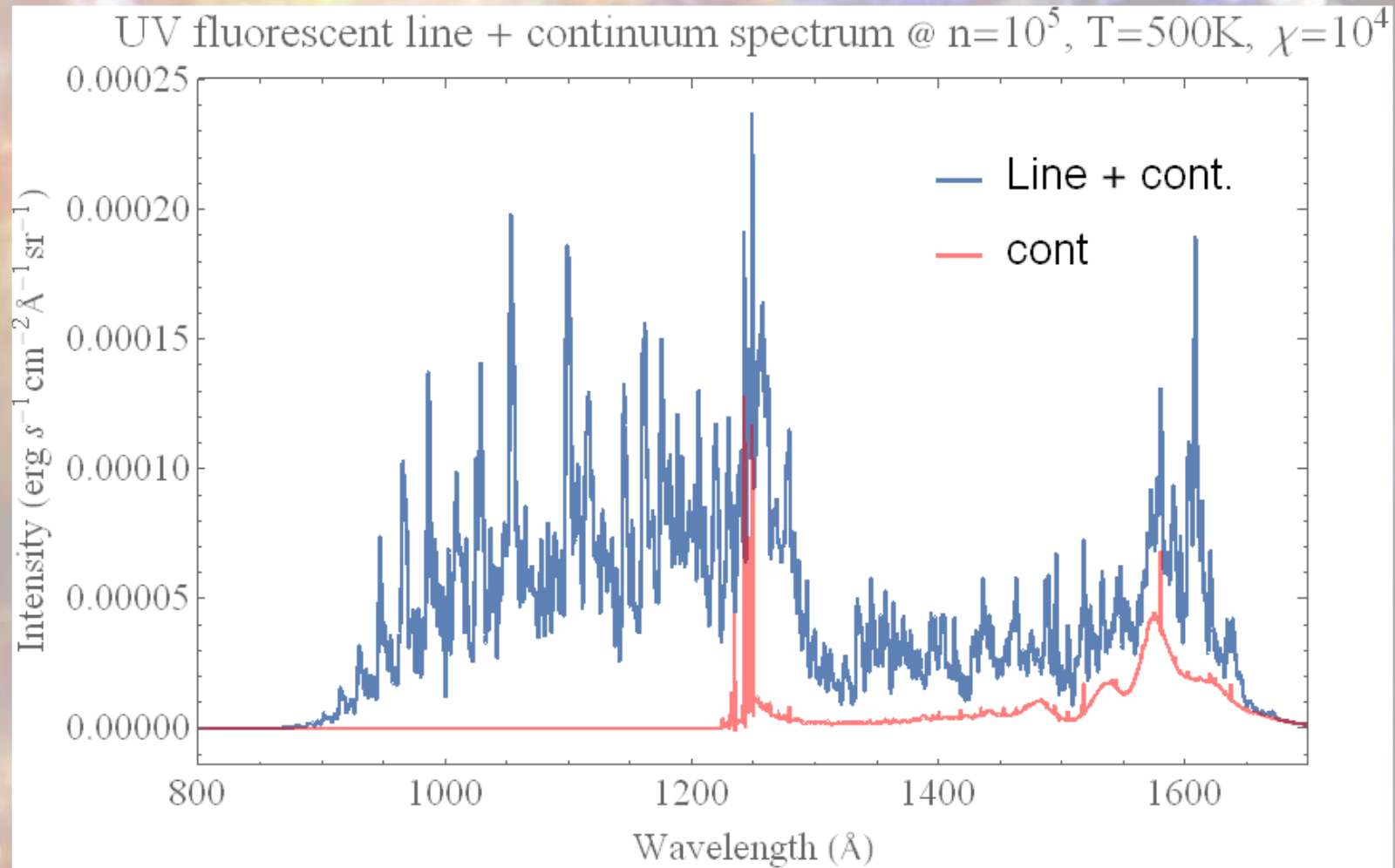
Low density, low UV, low Temp. → only ground state populated





# Fluorescent UV spectrum of H<sub>2</sub>

High density, high UV, high Temp. → higher states populated



# Chemistry





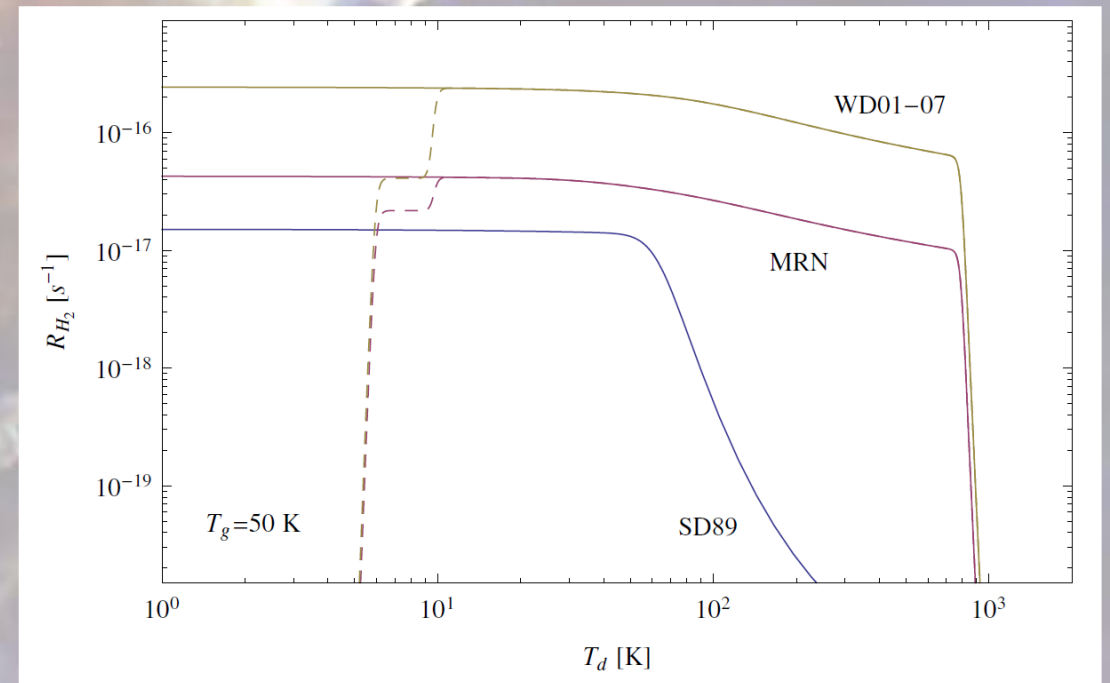
# Chemistry in KOSMA-T

- Rate equation approach
- Steady-state chemistry
  - LAPACK: DGESV, DGELSD (least squares), DGESVX (w. equilibration)
- Time-dependent chemistry (fallback for steady-state)
  - LSODE, LSODA,
- modular chemistry
  - user selects species, code selects reactions, creates conservation equations and Jacobian
- isotopologue chemistry:  $^{13}\text{C}$  and  $^{18}\text{O}$ 
  - update to the fractionation reaction from Langer et al. 84 (Mladenovic & Roueff, 2014)
  - isotopic reaction set (Röllig et al. 2013)
- Standard database: UDfA 2012 (McElroy et al. 2013)



# Chemistry in KOSMA-T

- Standard database: UDefA 2012
  - reactions with  $H_2^*$  overcome activation energy
  - $CH^+$  and  $SH^+$  formation (Agundez et al. 2010, Nagy et al. 2012)
  - cyclic and linear-isomers included (new branching ratios from Chabot et al. 2013) with all isotopologues
    - $I-C_3H_3^+$ ,  $I-C_3H_2^+$ ,  $I-C_3H_2$ ,  $I-C_3H$
  - additions
    - Fluorine chemistry (Neufeld et al. 2005)
    - Photodissociation of  $CS_2$ ,  $N_2O$  (van Dishoeck et al.)
  - $H_2$  formation
    - Chemi- & physisorption (Cazaux & Tielens 2002,04,10)



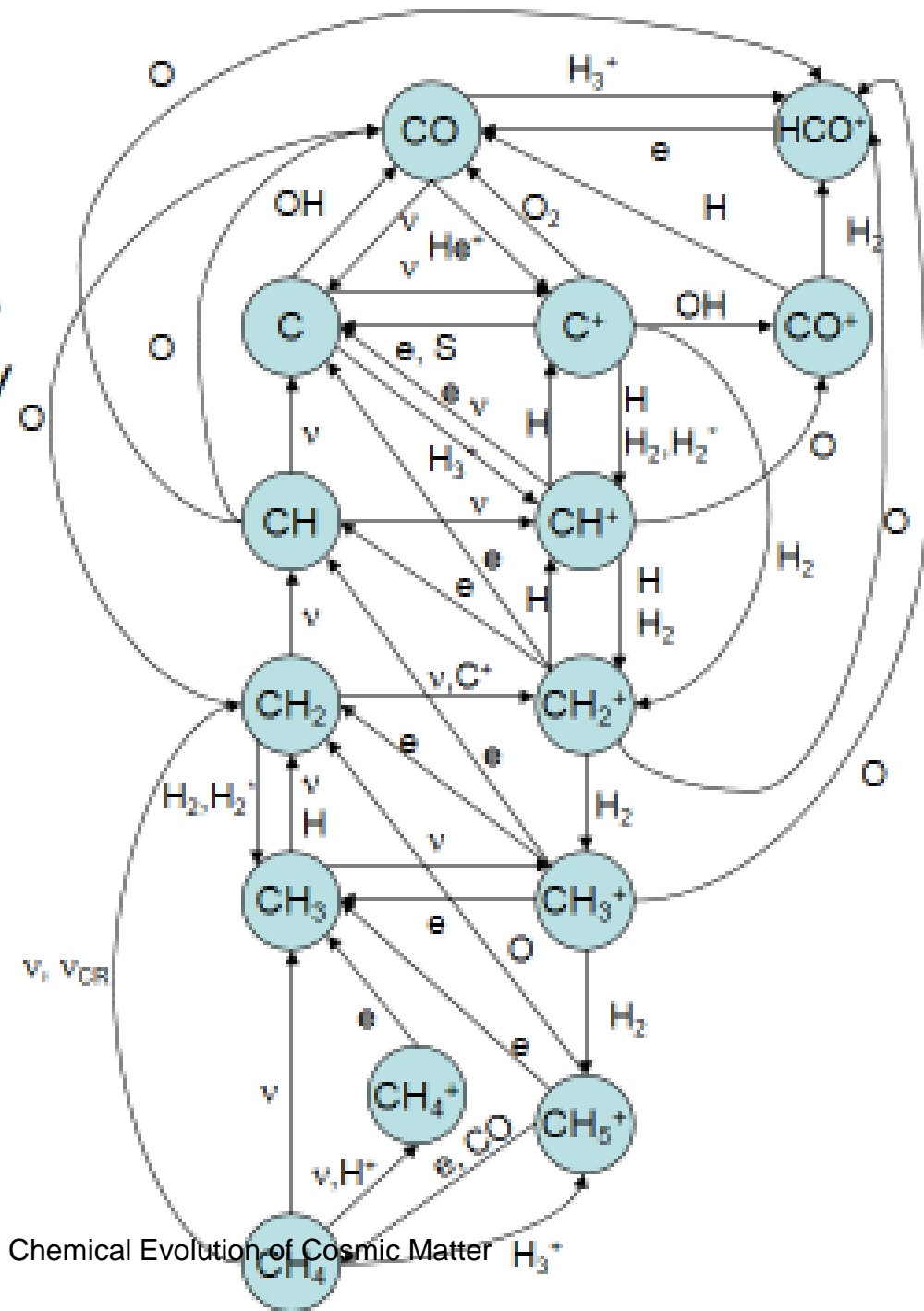


# Full Surface Chemistry Upgrade

- Coupling of gas-phase and surface chemistry
- Steady-state chemistry
- Rate equation approach (Hasegawa et al. 1992,1993)
- Processes included:
  - Adsorption (only neutrals, no sticking of H<sub>2</sub>)
  - desorption only from 2 top layers (Aikawa et al. 1996)
    - thermal desorption (binding energies from UDfA + updates)
    - photo-desorption (photo cross-section like gas-phase)
    - photo-dissociative desorption (eg. JH<sub>2</sub>O + hv → OH + H Andersson+ 08)
    - photo-dissociation on grains (equivalent to gas-phase)
    - CR induced photo-desorption/diss. (Hasegawa & Herbst 1993)
    - H<sub>2</sub>-formation induced desorption (Willacy et al. 1994, 2007)
    - chemistry induced desorption (Minissale et al. 2015, Cazaux et al. 2015)
  - surface-surface processes (Langmuir-Hinshelwood)

# The carbon roadmap

- Like any roadmap, this network describes *how to get from A to B*.
- Like on any roadmap, *some paths are quick some are slow*.
- Unlike any normal roadmap some *slow paths may become very quick* under certain conditions

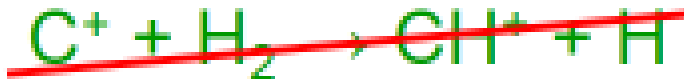




# Example: Diffuse Cloud

starting point:  $C^+$

collision with  $H_2$ :  $\Delta E = 4600K$



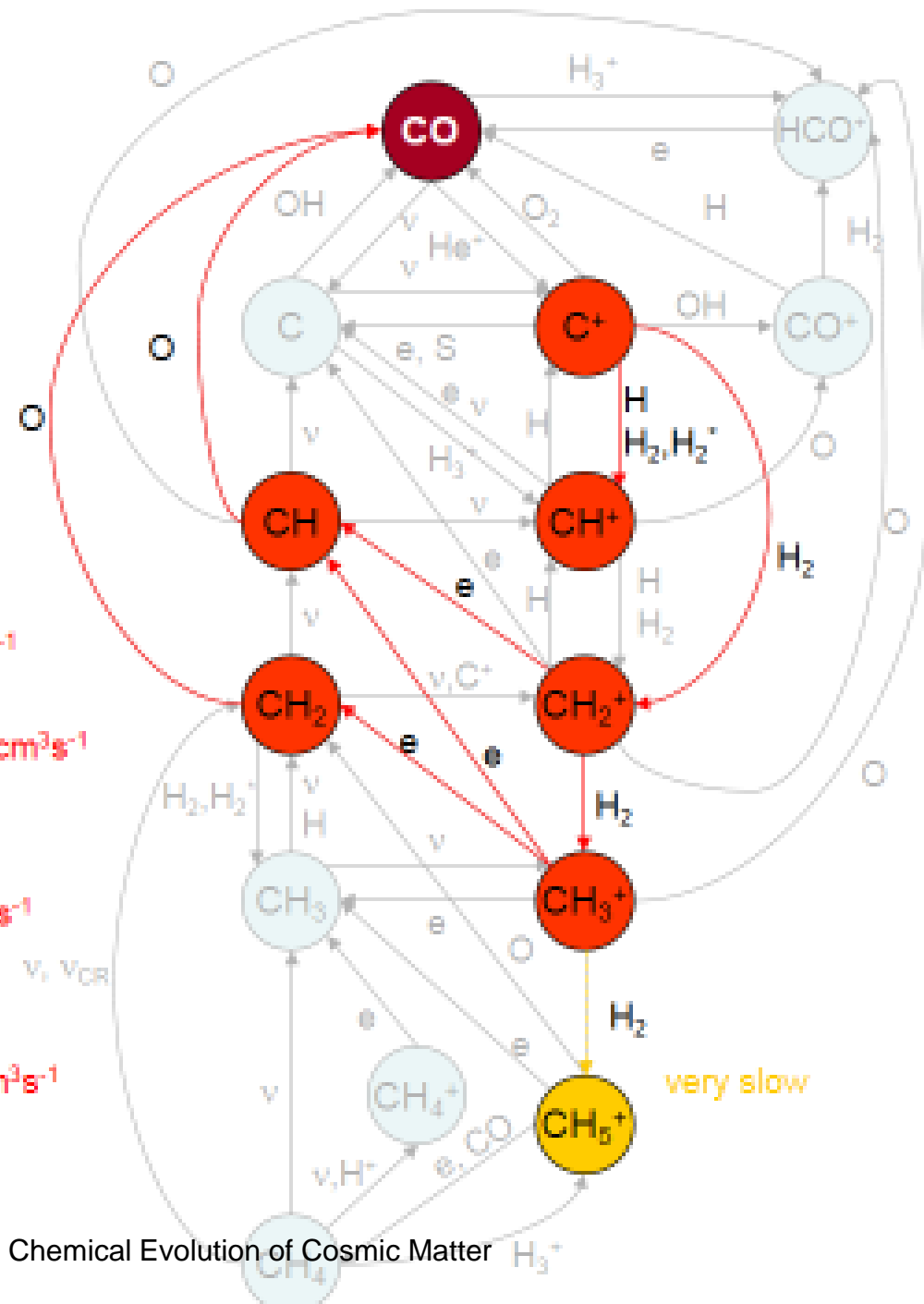
instead:



then:



and:



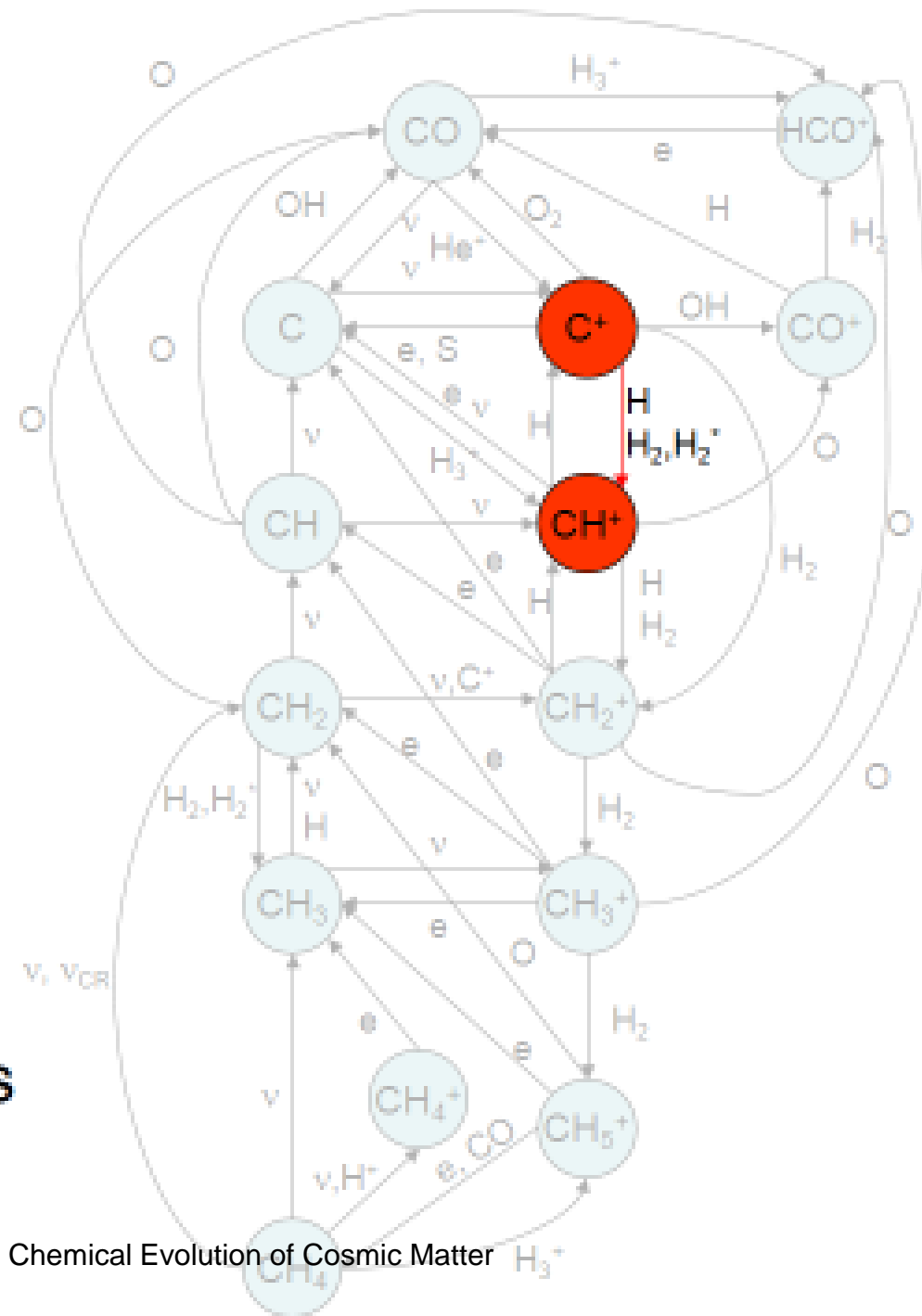
## Example: PDR

high FUV intensity heats  
the gas at the surface

→ some slow routes  
become quick



endothermic reactions  
become possible  
activation energy barriers  
become surmountable



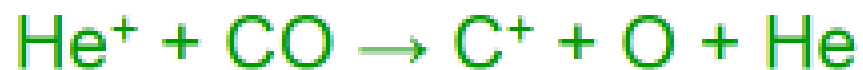


## Example: Dark Cloud

cold and dense:

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

carbon locked in CO



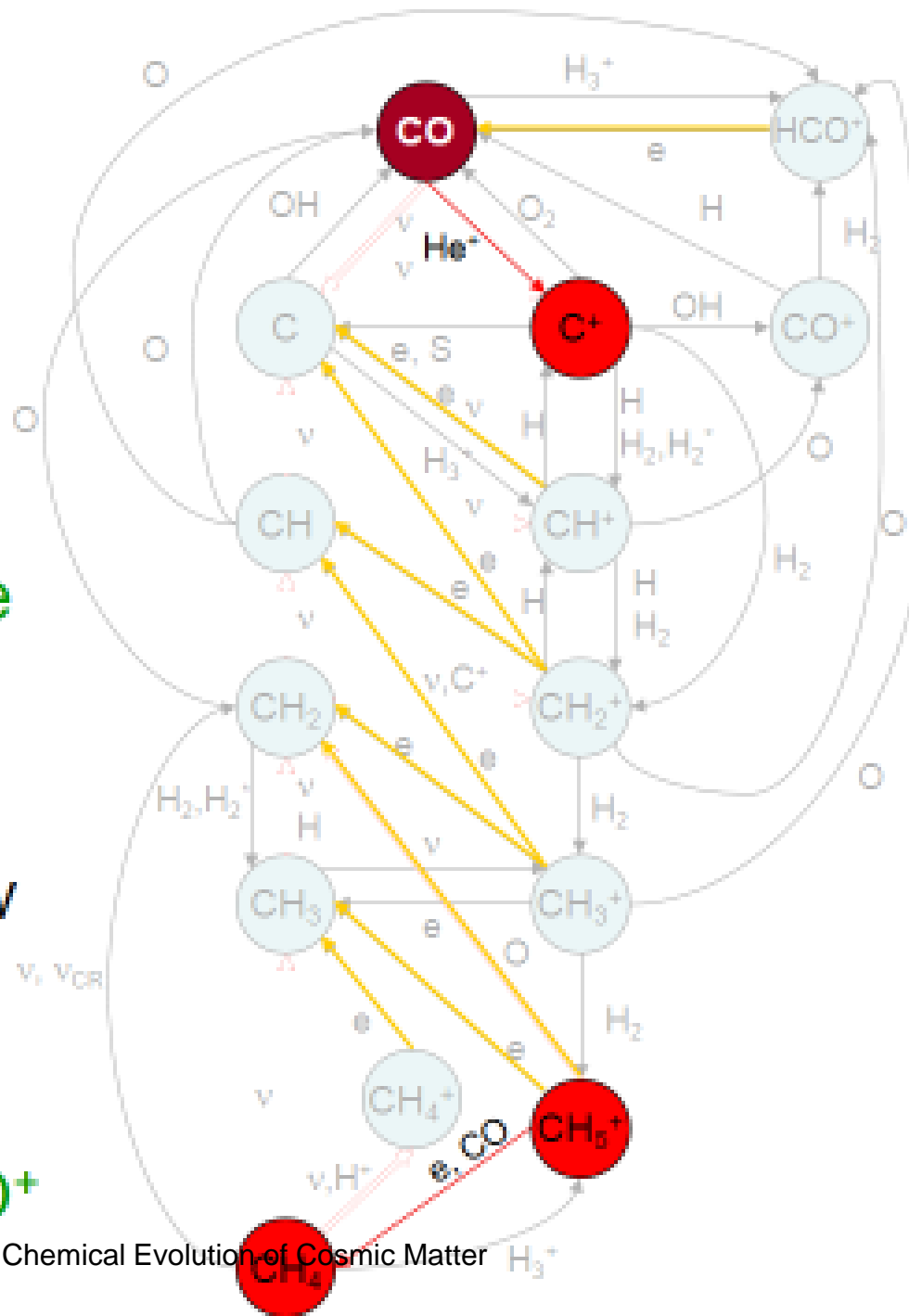
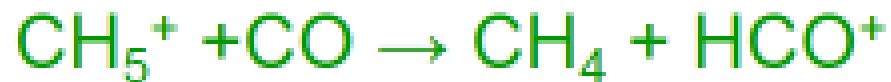
FUV fully absorbed

some roads vanish

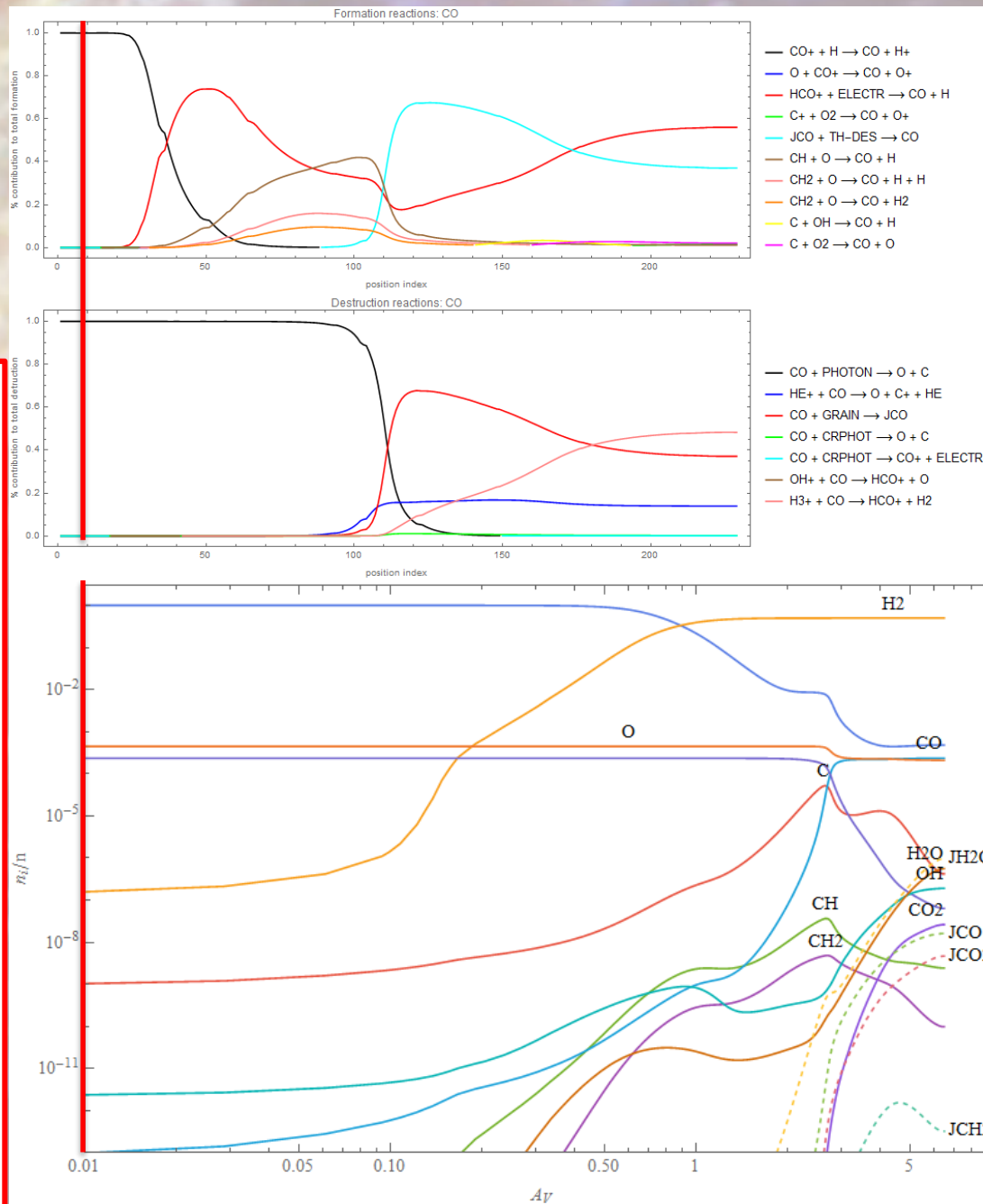
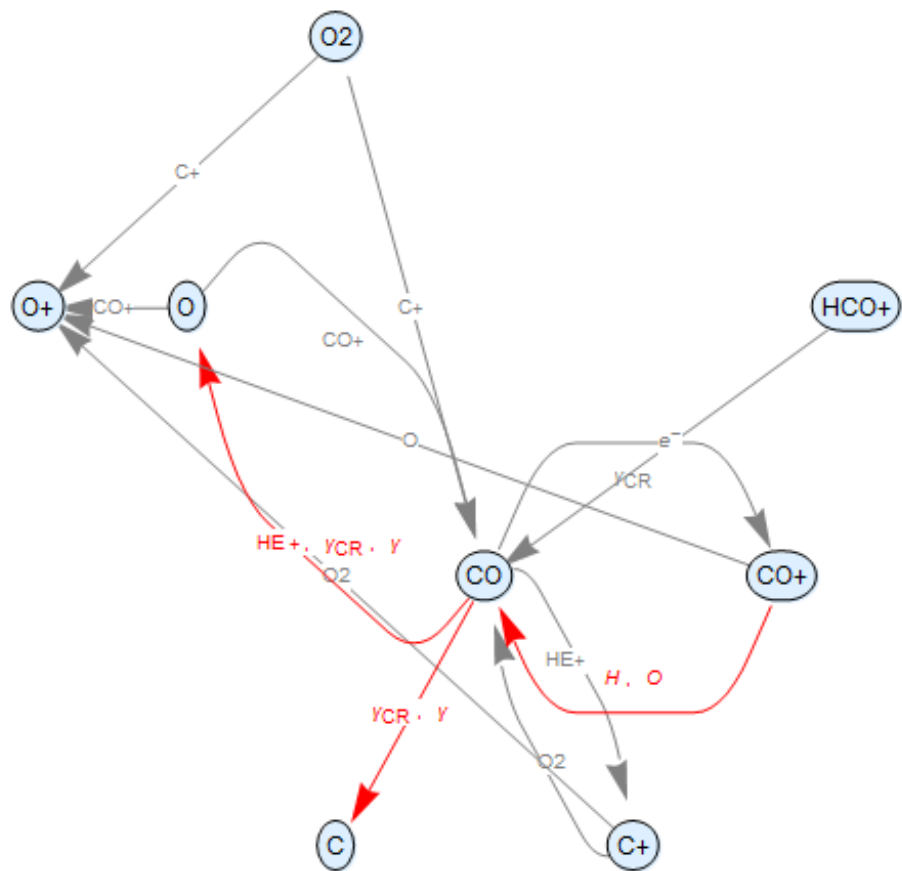
some roads become slow

e.g. reactions with  $\text{e}^-$

but:

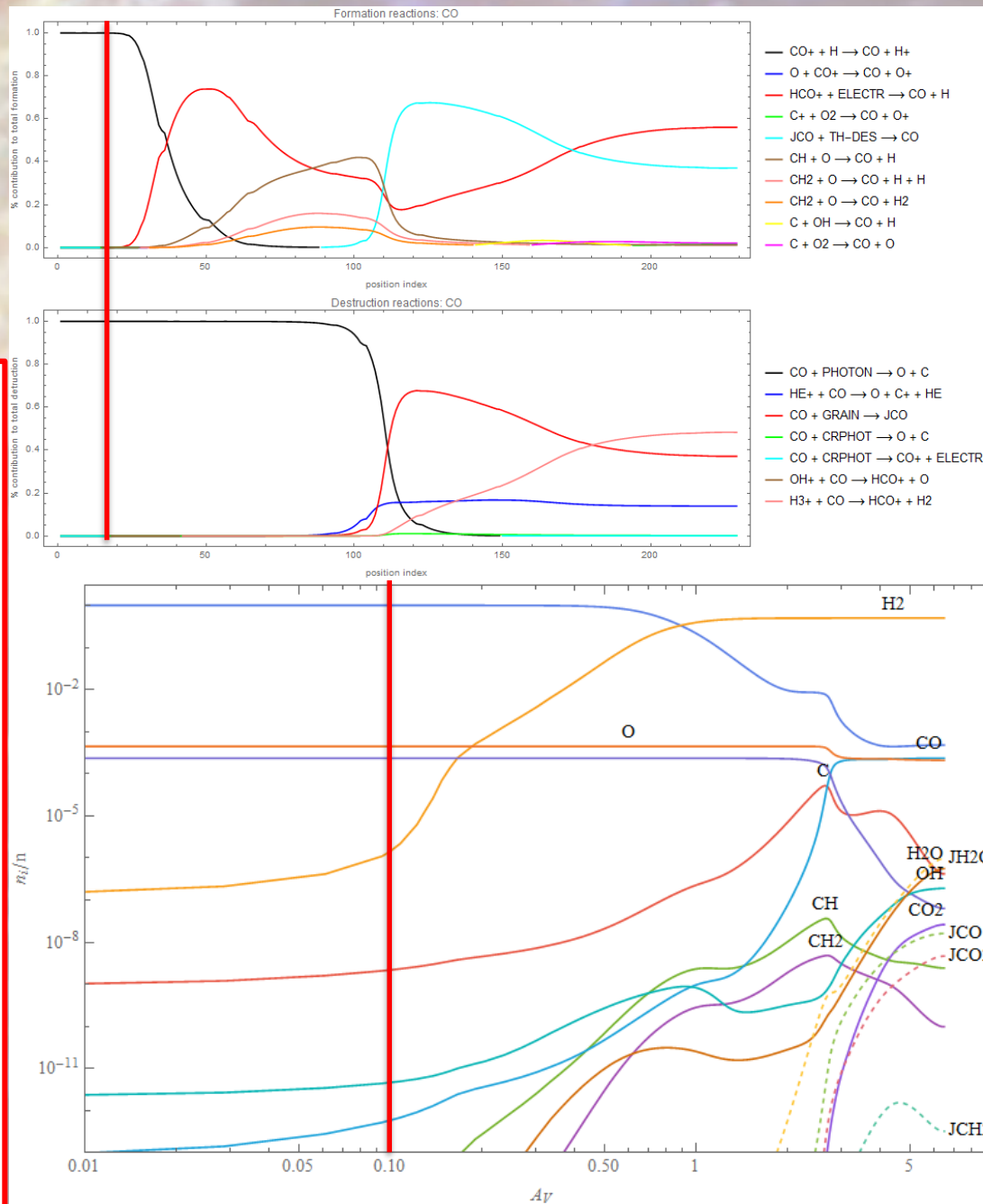
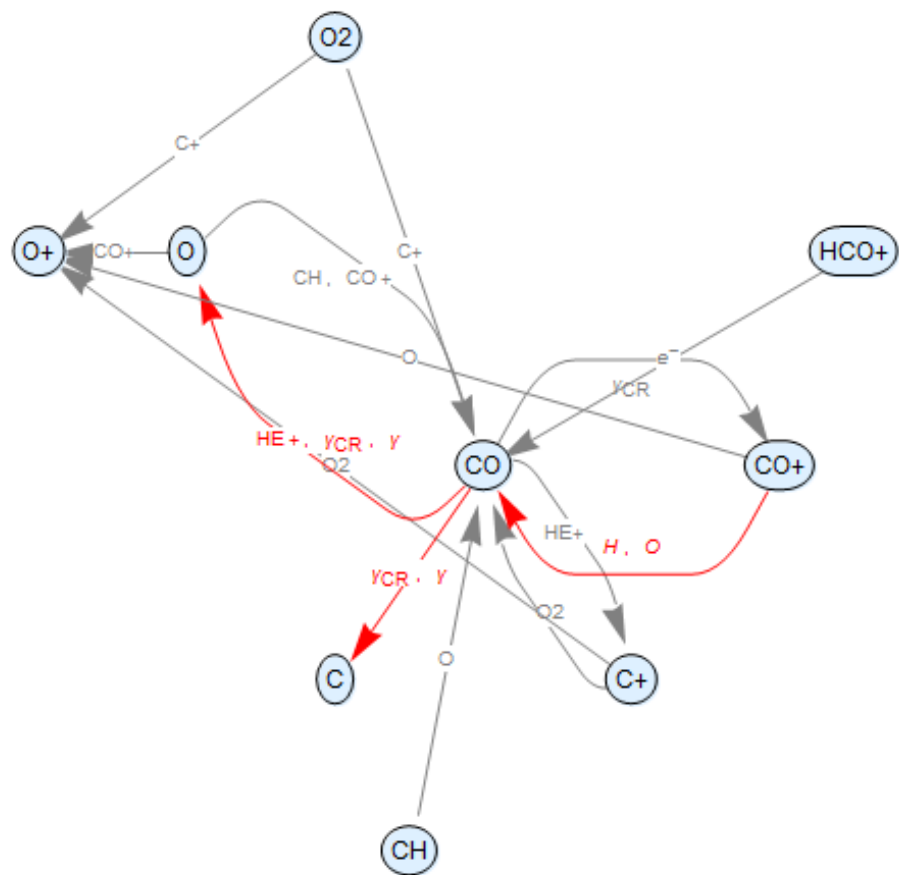


$n = 10^4 \text{ cm}^{-3}$   
 $\chi = 10^4$   
 small chemical network

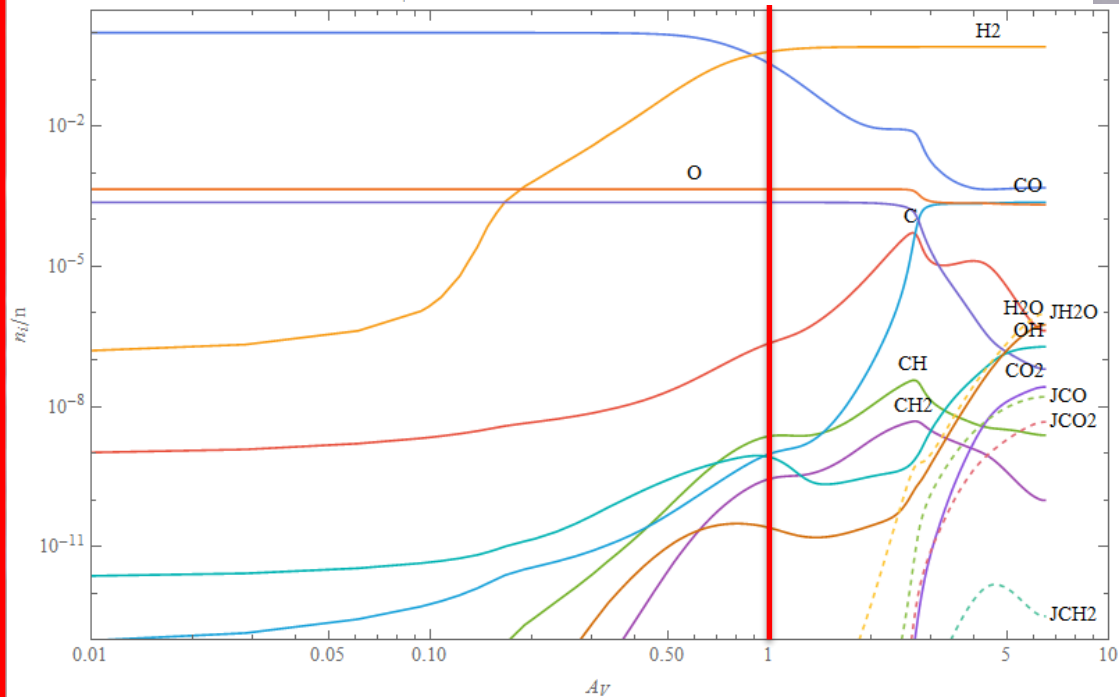
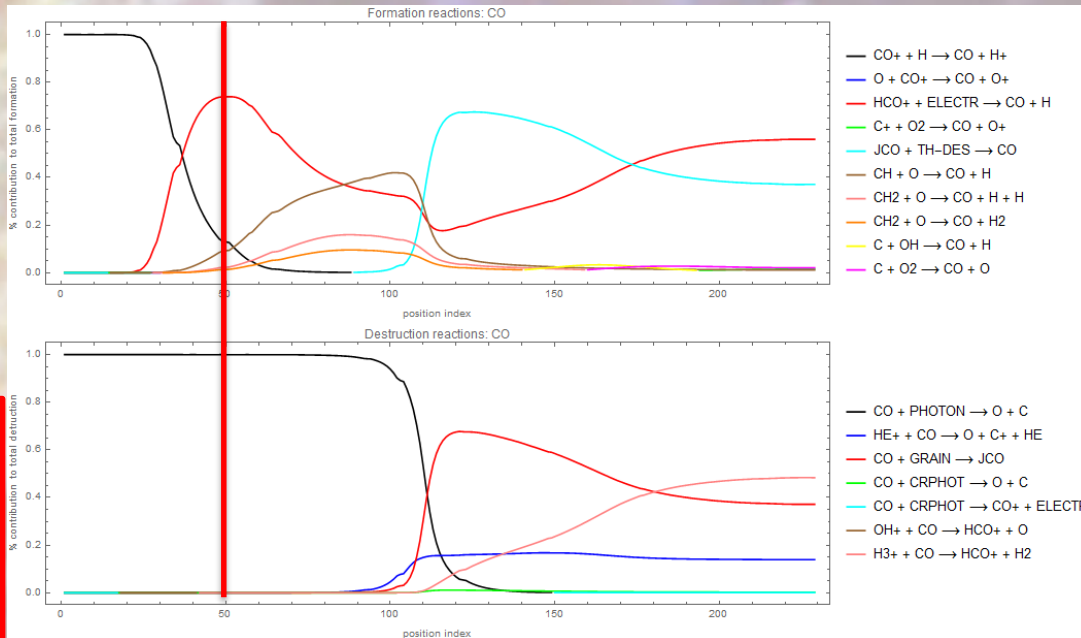
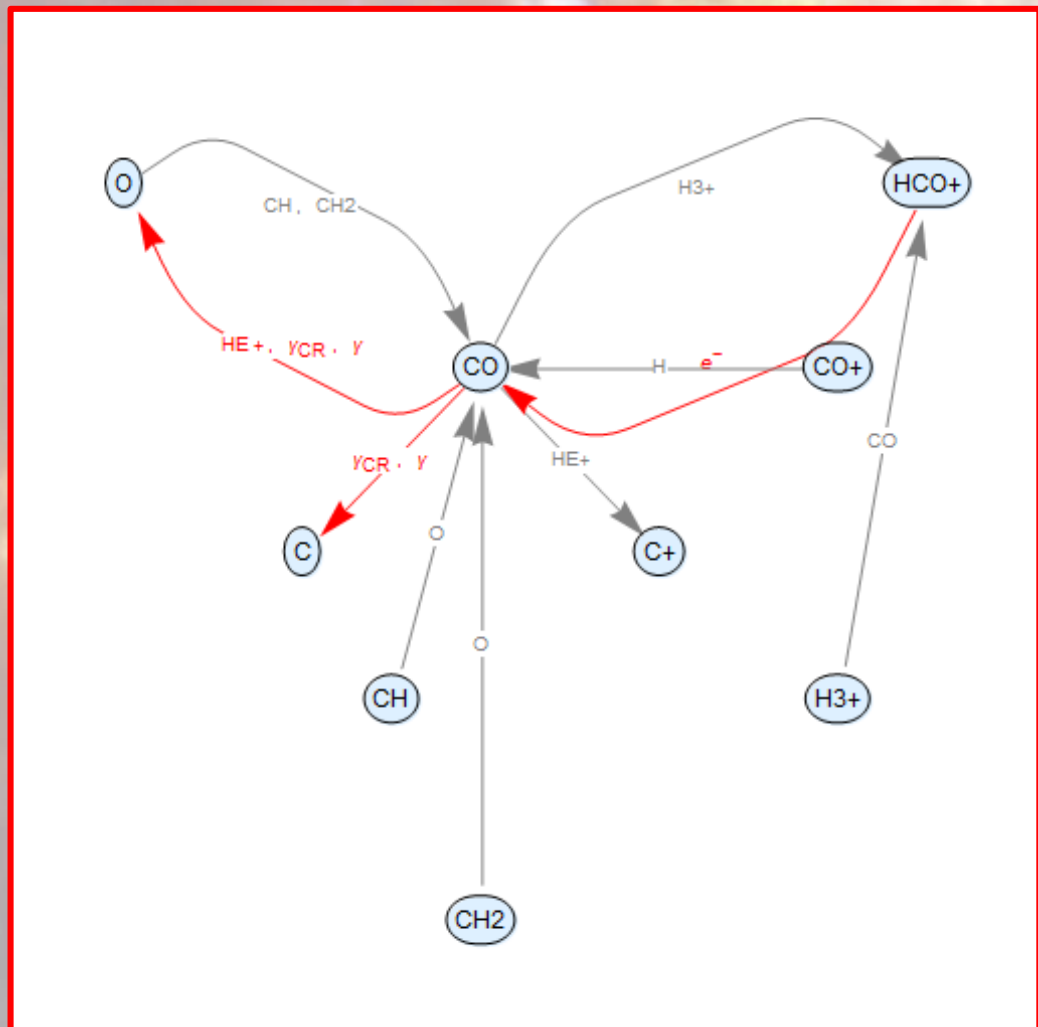




$n = 10^4 \text{ cm}^{-3}$   
 $\chi = 10^4$   
 small chemical network

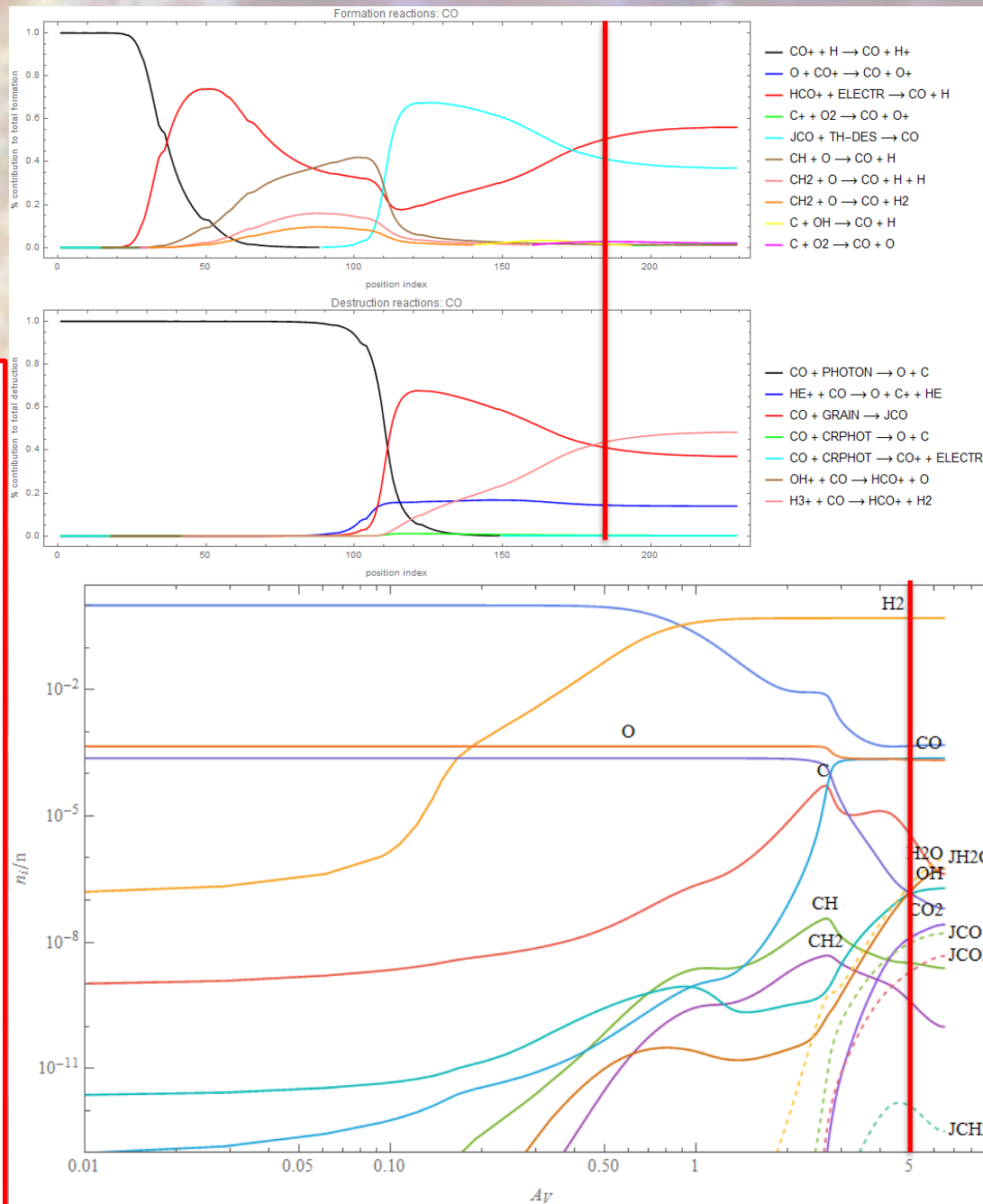
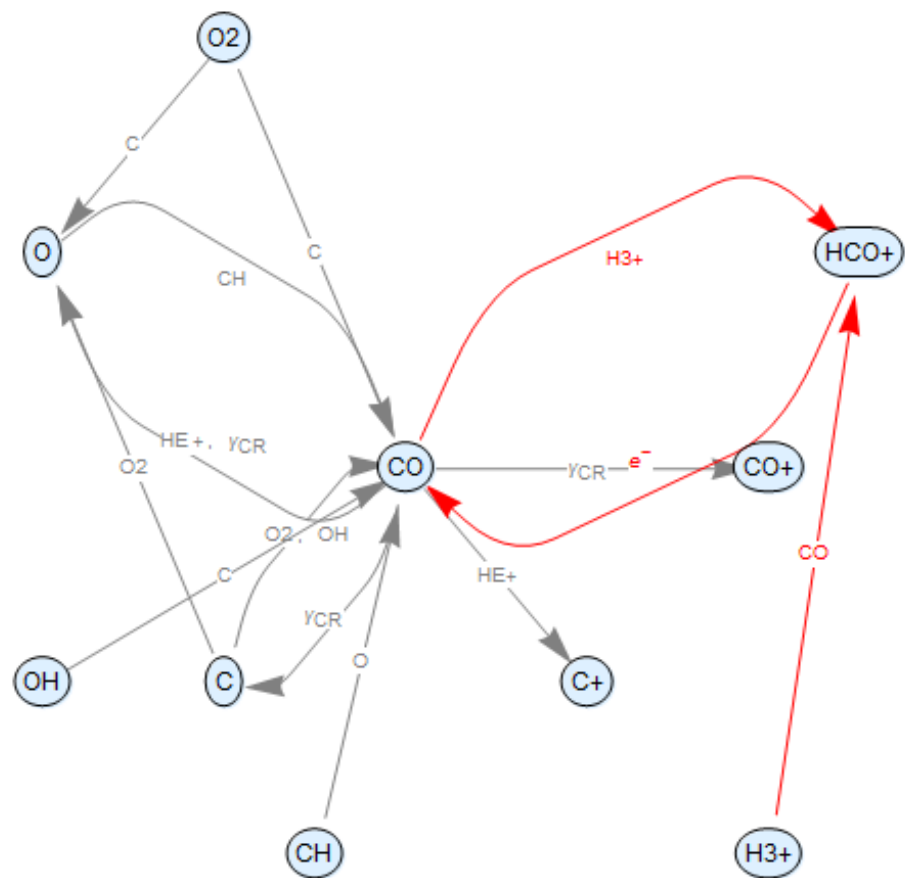


$n = 10^4 \text{ cm}^{-3}$   
 $\chi = 10^4$   
 small chemical network

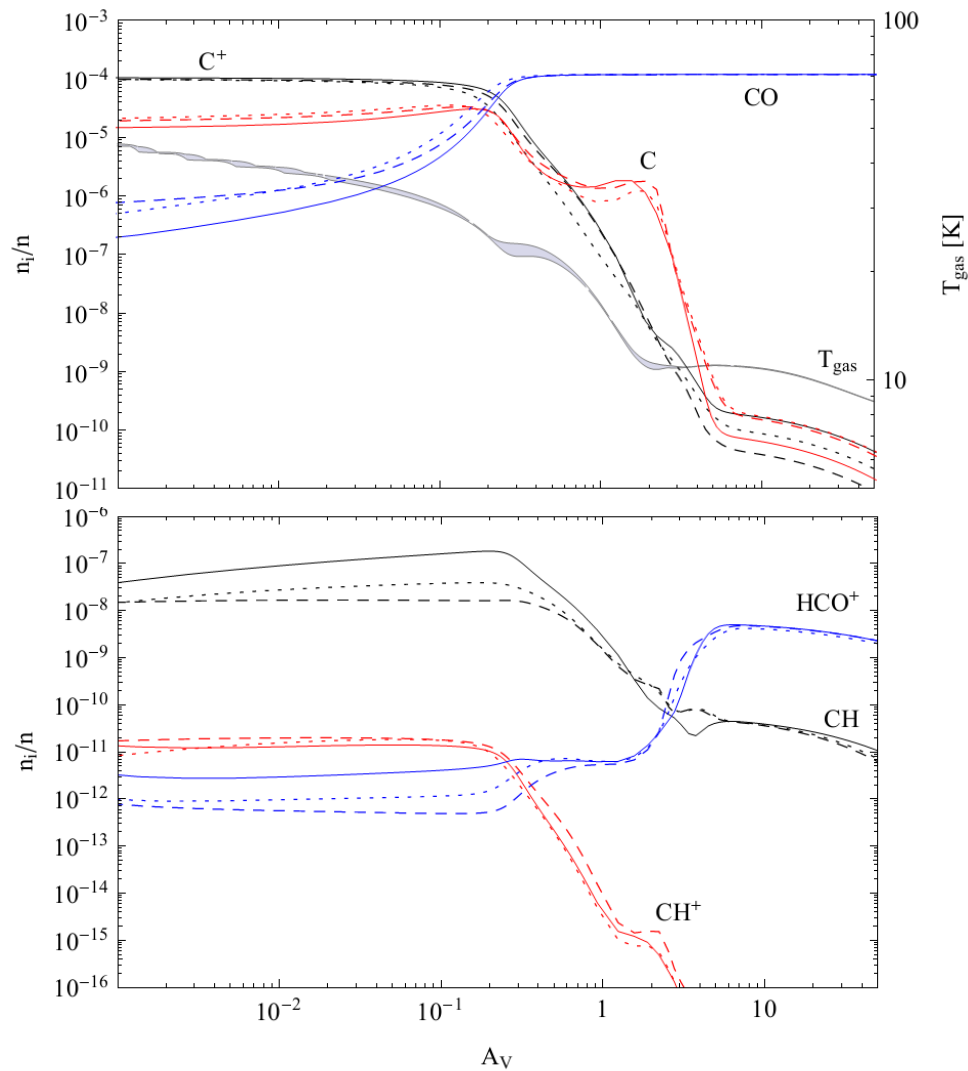




$n = 10^4 \text{ cm}^{-3}$   
 $\chi = 10^4$   
 small chemical network



# Ugly details



Model results affected by many details, e.g.:

- Influence of different chemical databases (UDfA, OSU, KIDA)

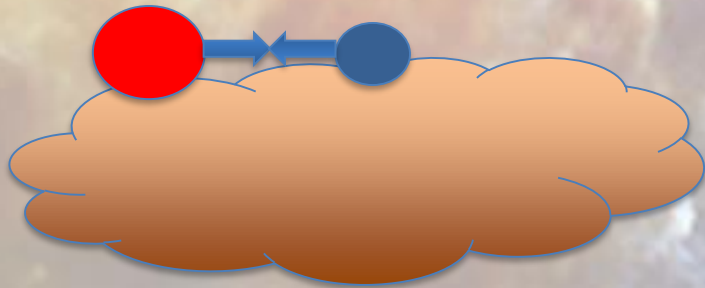
but also,

- geometry
- etc.



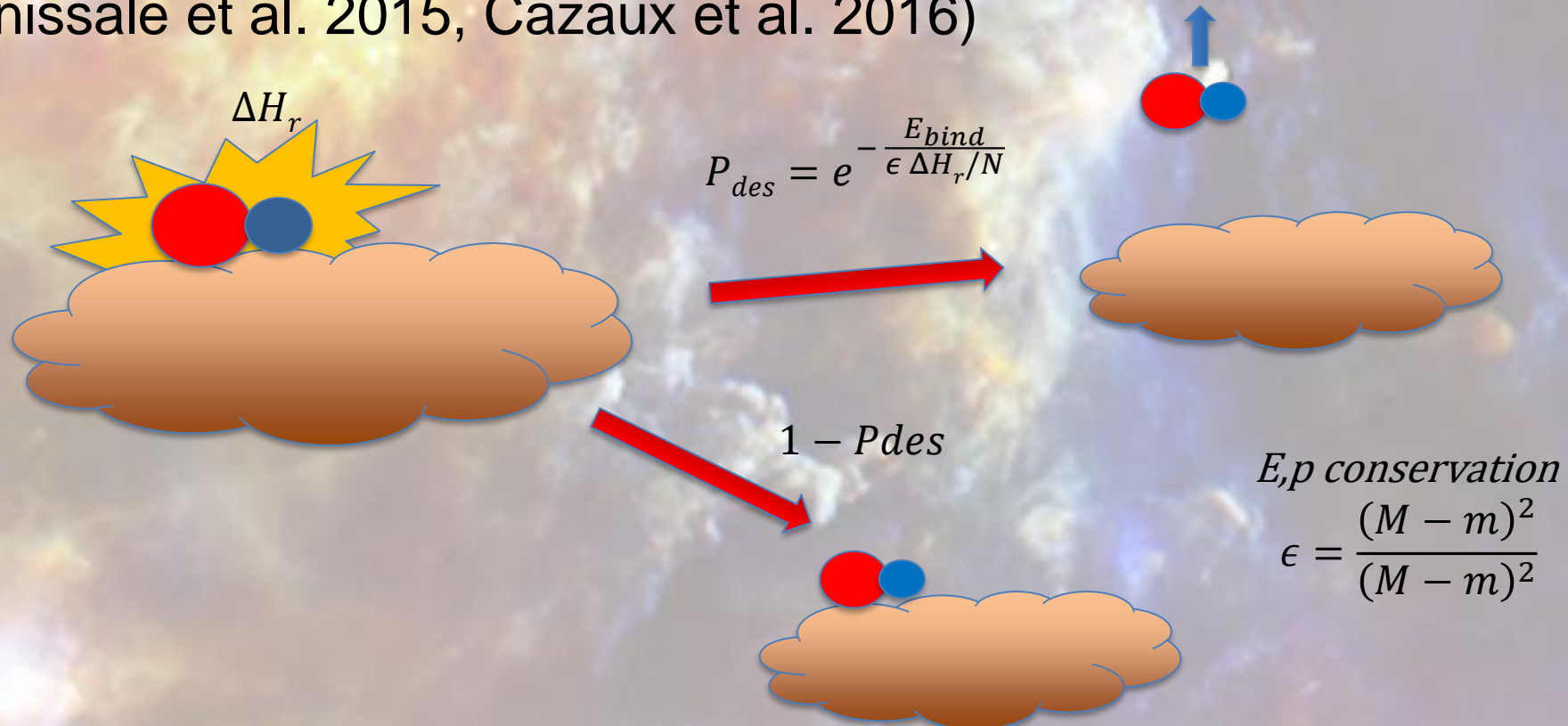
# Full Surface Chemistry Upgrade

- surface-surface processes (Langmuir-Hinshelwood)
- exoenergetic reactions may lead to desorption (Minissale et al. 2015, Cazaux et al. 2016)

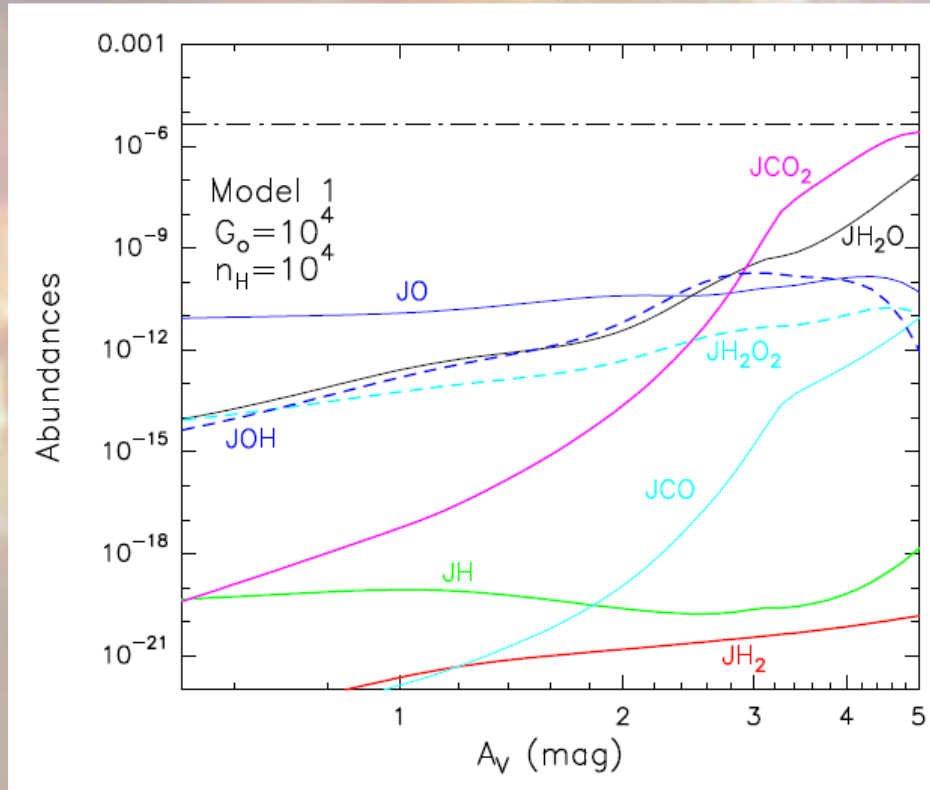


# Full Surface Chemistry Upgrade

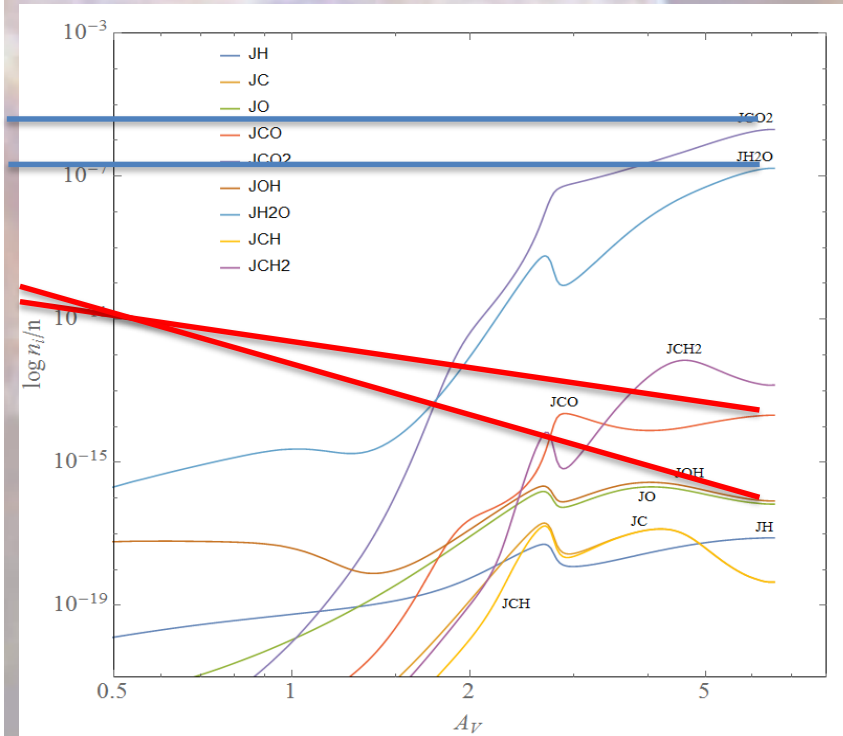
- surface-surface processes (Langmuir-Hinshelwood)
- exoenergetic reactions may lead to desorption of the product (Minissale et al. 2015, Cazaux et al. 2016)



# Chemical details with impact



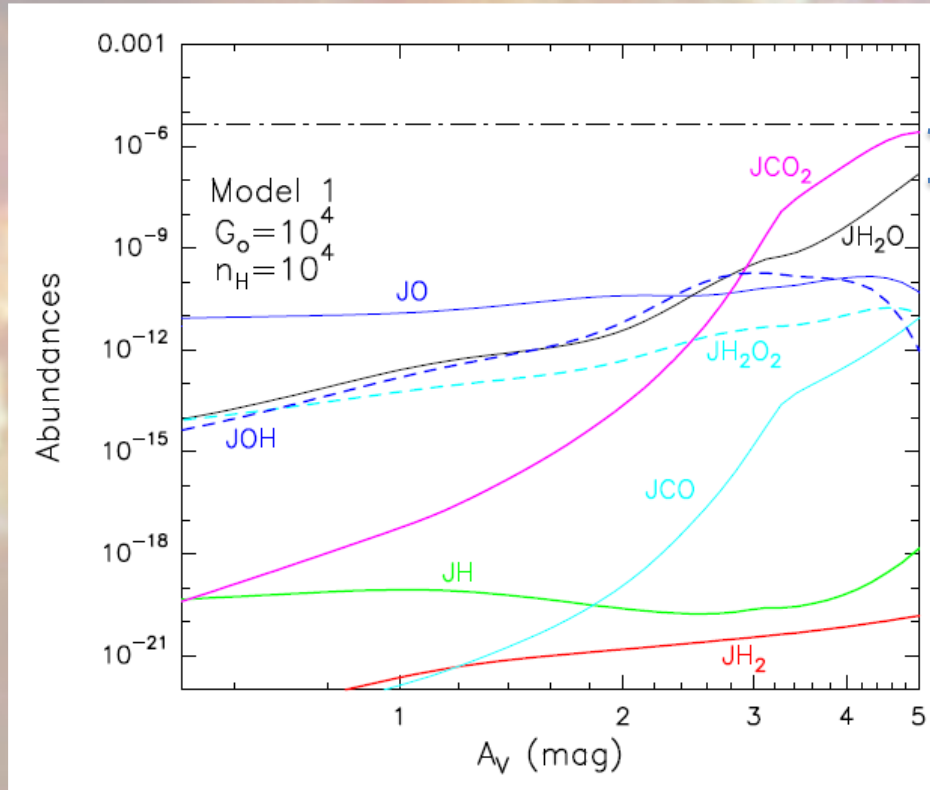
Esplugues et al. 2016



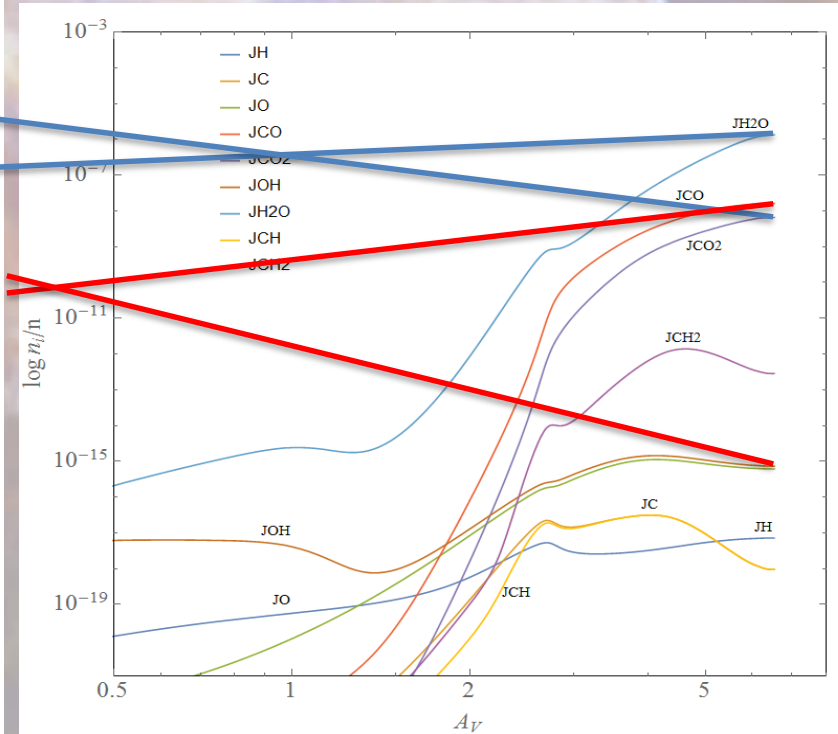
KOSMA- $\tau$  with „comparable“ setup



# Chemical details with impact



Esplugues et al. 2016



KOSMA- $\tau$  with „comparable“ setup

**plus**

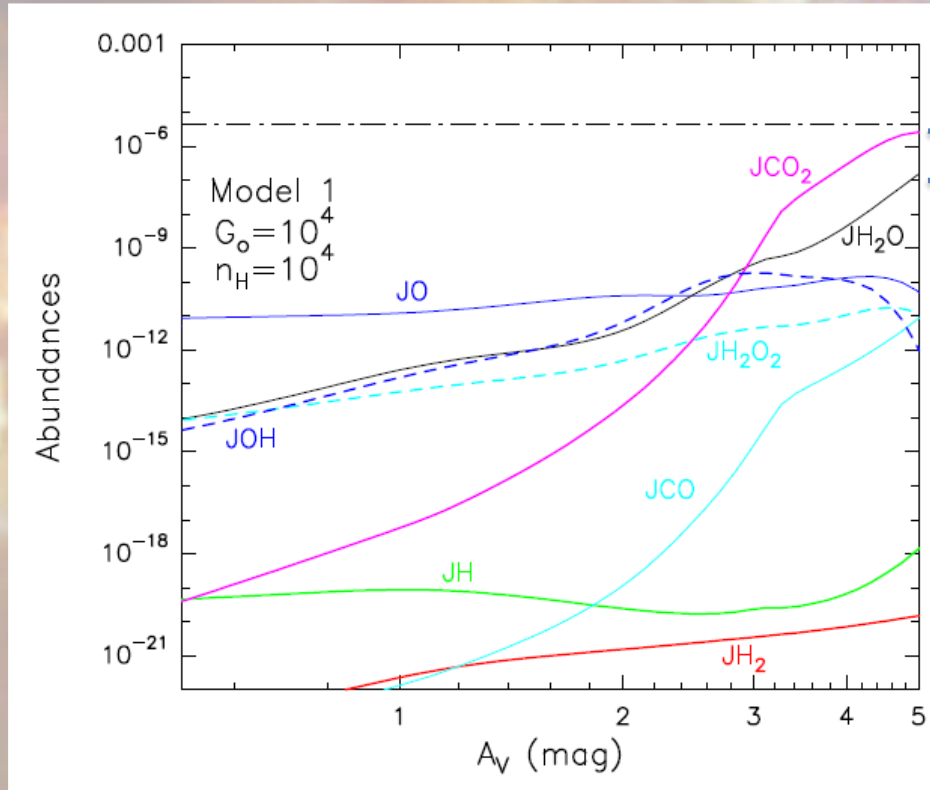
(theoretical BRs)

$JCO + JO \rightarrow CO_2$  (22%)

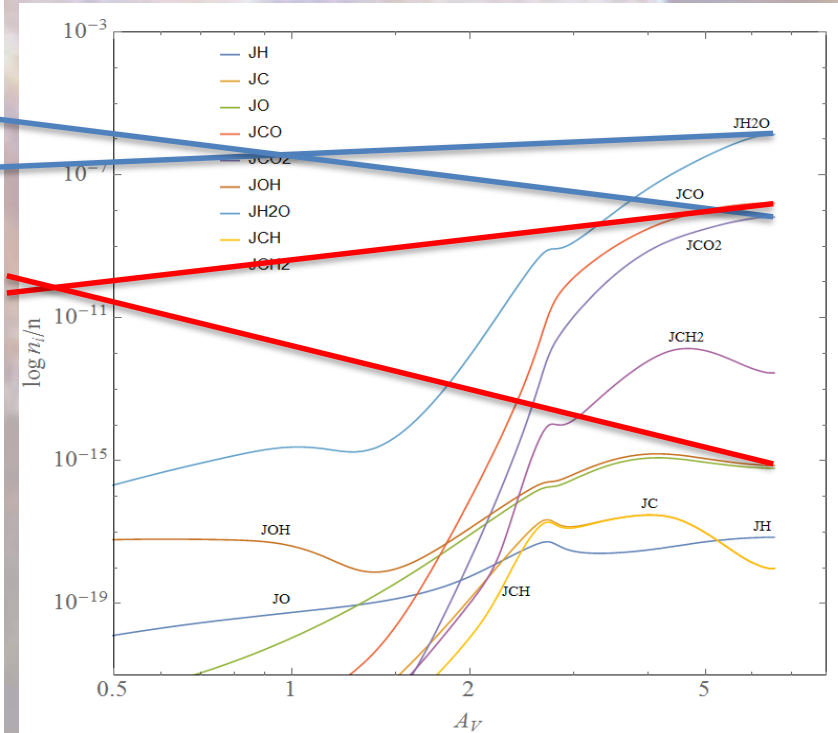
$JCO + JO \rightarrow JCO_2$  (78%)

→ significantly different ice composition

# Chemical details with impact



Esplugues et al. 2016



KOSMA- $\tau$  with „comparable“ setup

**plus**

(measured BRs)

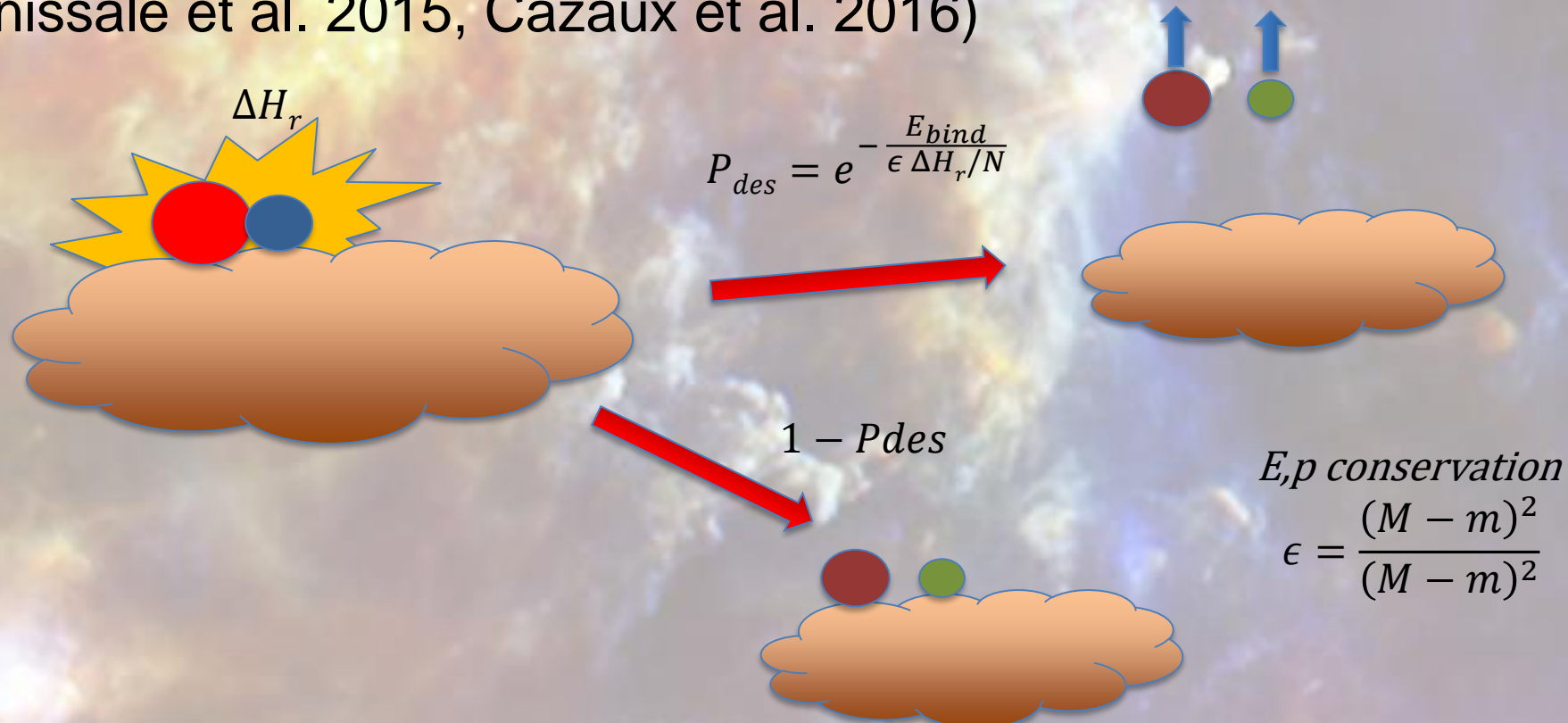
JCO + JO  $\rightarrow$  CO<sub>2</sub> (4%)

JCO + JO  $\rightarrow$  JCO<sub>2</sub> (96%)

$\rightarrow$  significantly different ice composition

# Full Surface Chemistry Upgrade

- surface-surface processes (Langmuir-Hinshelwood)
- exoenergetic reactions may lead to desorption of **both products** (Minissale et al. 2015, Cazaux et al. 2016)

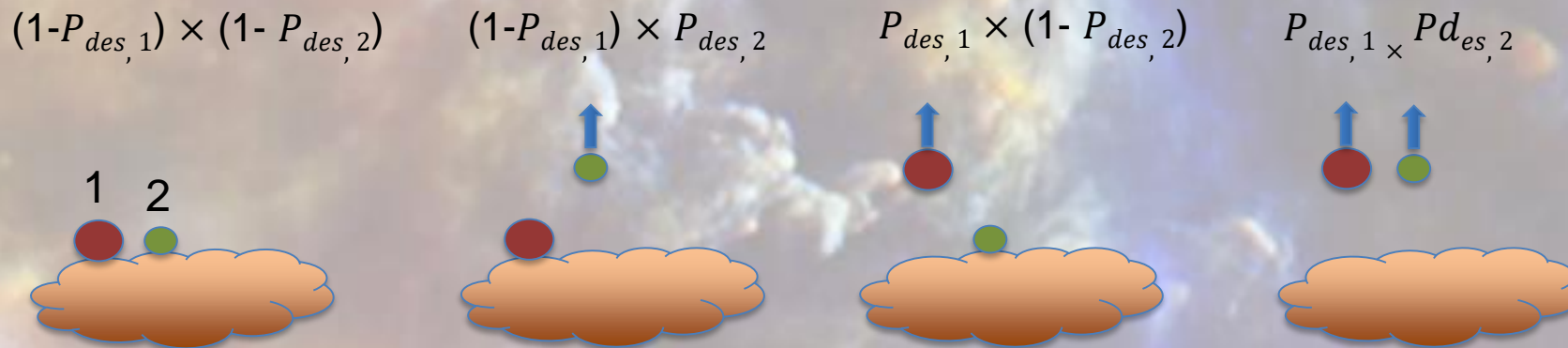




# Full Surface Chemistry Upgrade

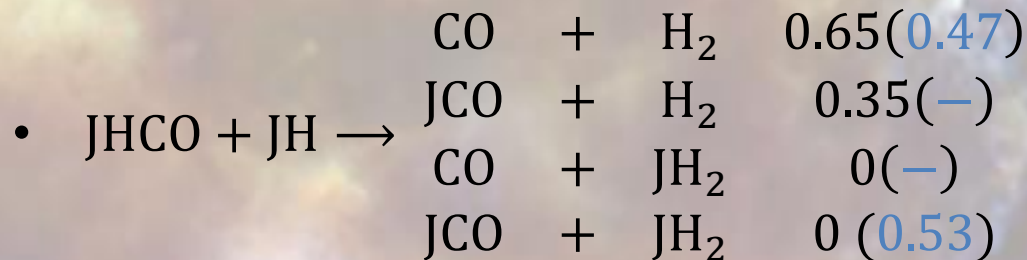
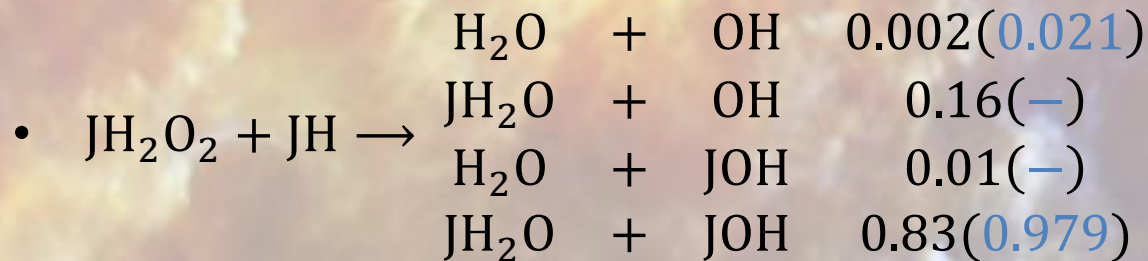
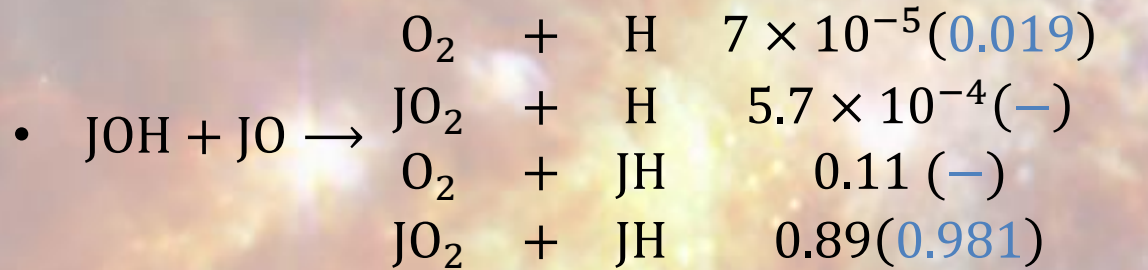
- So far assumed that all products desorb with full reaction enthalpy
- Now, we assume that formation **energy is distributed across products**

- analogue to free particle decay:  $\frac{E_1}{E_2} = \frac{m_1}{m_2}$ , :  $\frac{E_1}{E_{tot}} = \eta_1 = \frac{m_1}{m_1+m_2}$
- $P_{des,i} = e^{-\frac{E_{bind,i}}{\epsilon_i \eta_i \Delta H_r / N_i}}$ ,  $\overline{P_{des,i}} = 1 - P_{des,i}$
- H<sub>2</sub> always desorbs



Röllig et al., in prep

# Some example branching rates



BRs depend on the energy redistribution.

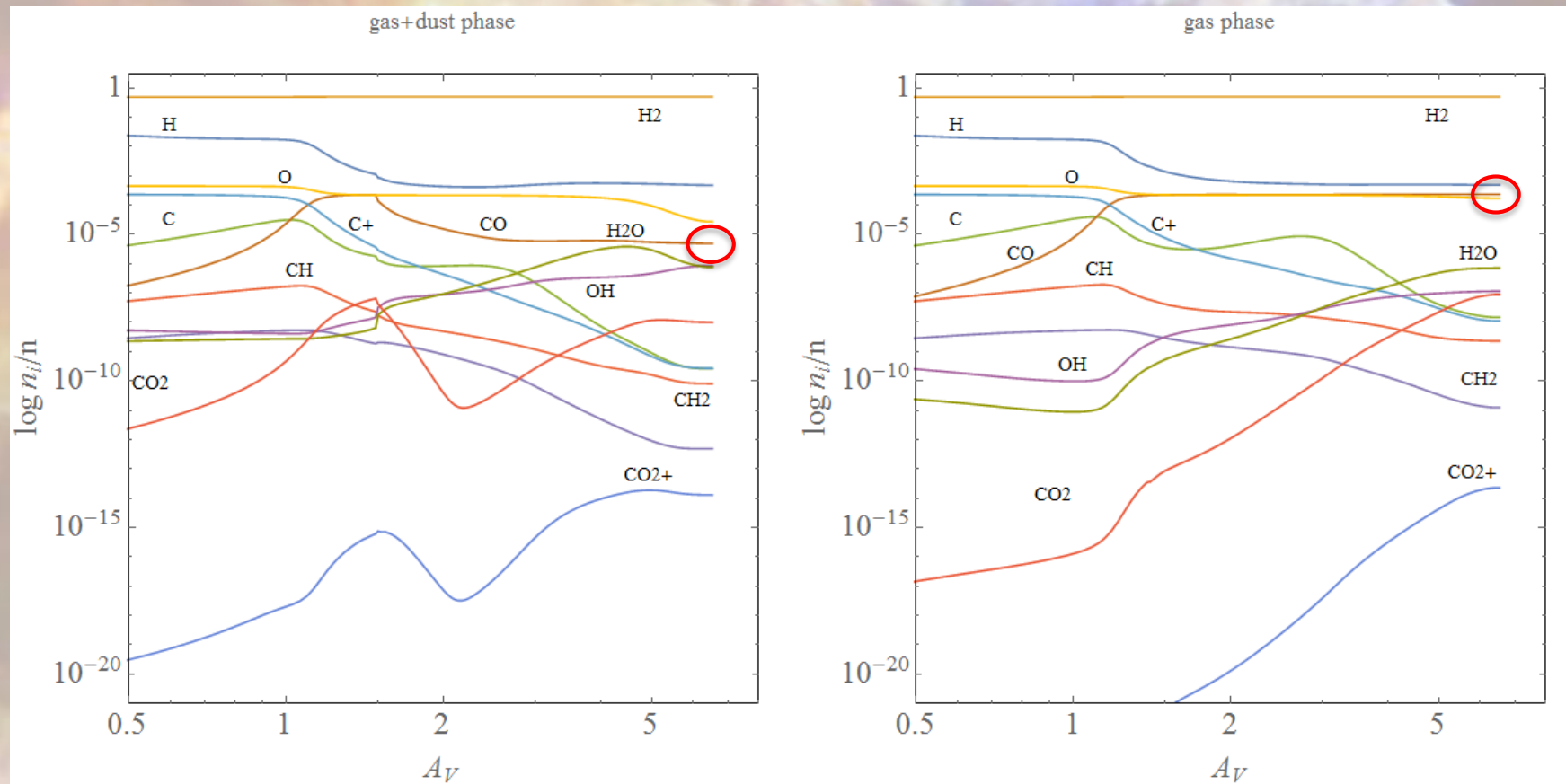
Other distribution schemes?

# Questions & Concerns

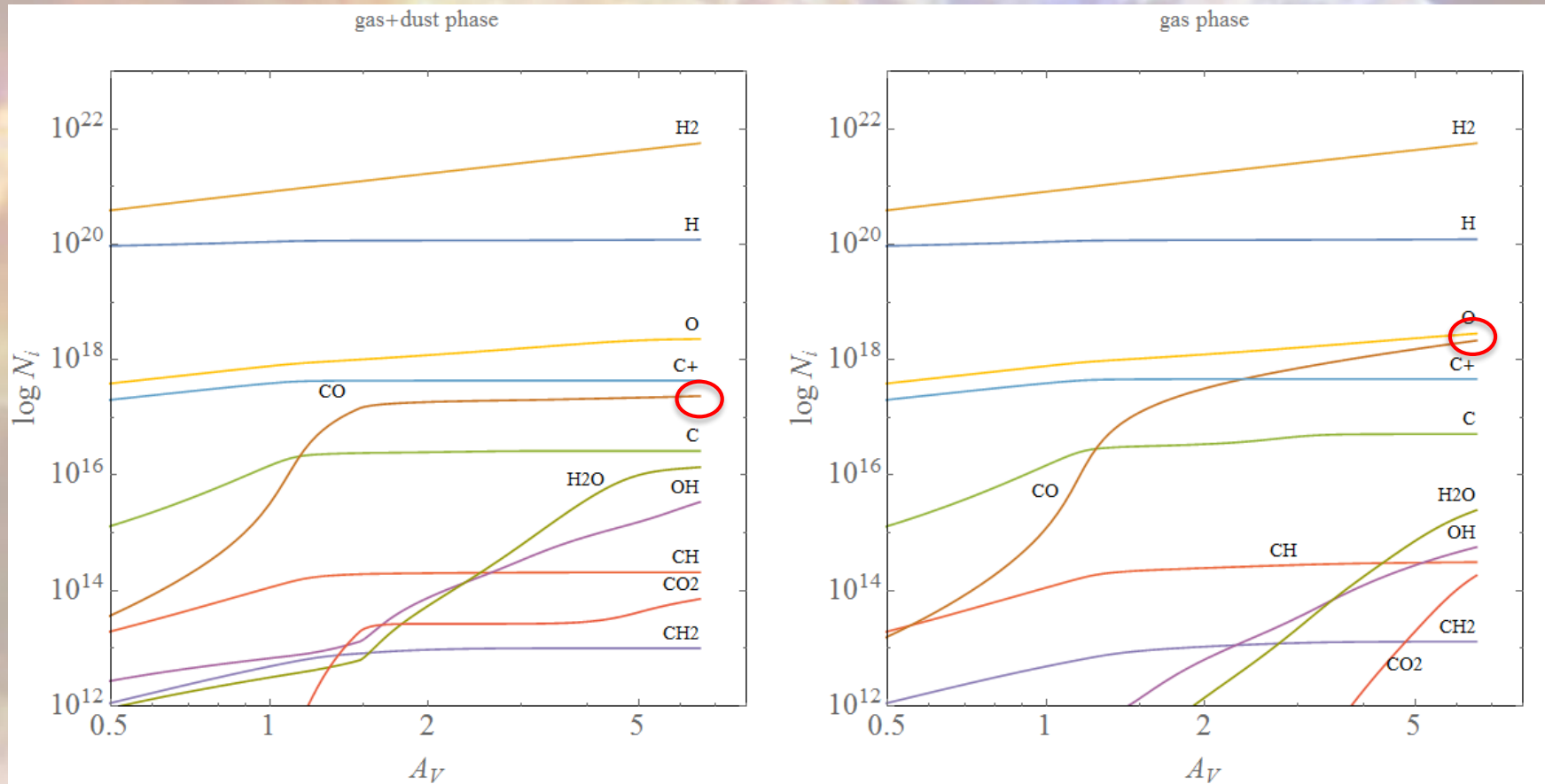
- Binding energies – Yes, but which one? (see Wakelam et al. 2017)
- How about surfaces of very small grains? PAHs?
  - Very important for H<sub>2</sub> formation
  - excitation of small hydrocarbons, H<sub>2</sub>, high-J CO
- Cross sections of surface photo-processes
  - Important for PDRs because of FUV attenuation/shielding
  - Photodesorption yields?
- Numerical stability? Convergence/steady-state ?
  - Including/excluding of
    - desorption processes
    - grain + gas phase species
    - initial abundances! PDRs are different from dark cloud models
  - Any technical/numerical comments in your papers are much appreciated.
- **(Column) density is no observable.**



# Density is no observable



# Column density is no observable



# Line intensities are observed

gas+dust phase

Line	$\int T_{mb} dv$ [K km/s]
CO J=1-0	5.8
CO J=2-1	7.3
CO J=3-2	4.3
CO J=4-3	1.4
[CII] 158 $\mu$ m	2.3
[CI] 609 $\mu$ m	8.7
[CI] 370 $\mu$ m	2.3

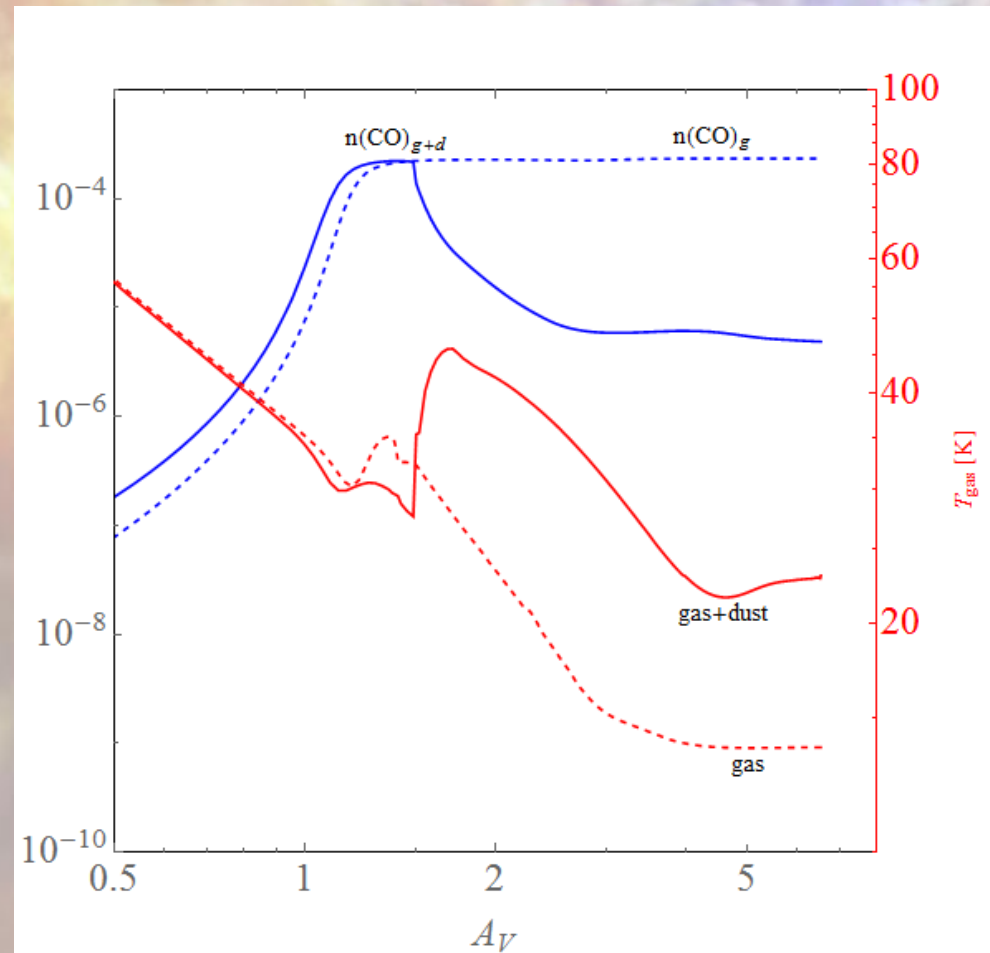
gas phase

Line	$\int T_{mb} dv$ [K km/s]
CO J=1-0	0.66
CO J=2-1	0.55
CO J=3-2	0.14
CO J=4-3	0.016
[CII] 158 $\mu$ m	2.1
[CI] 609 $\mu$ m	9.5
[CI] 370 $\mu$ m	2.6

lower column densities  
higher intensities !



# Excitation matters



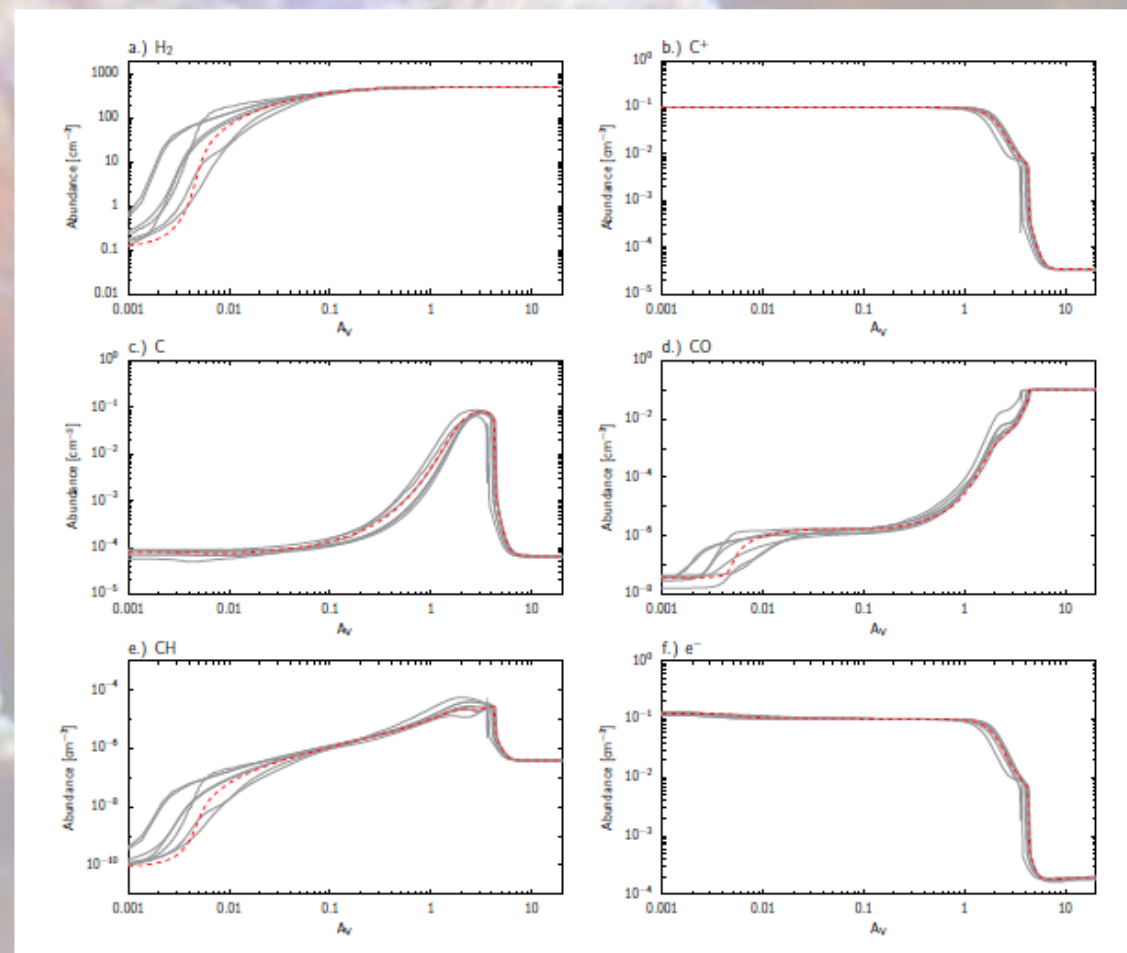
gas cooling is significantly reduced in the absence of CO

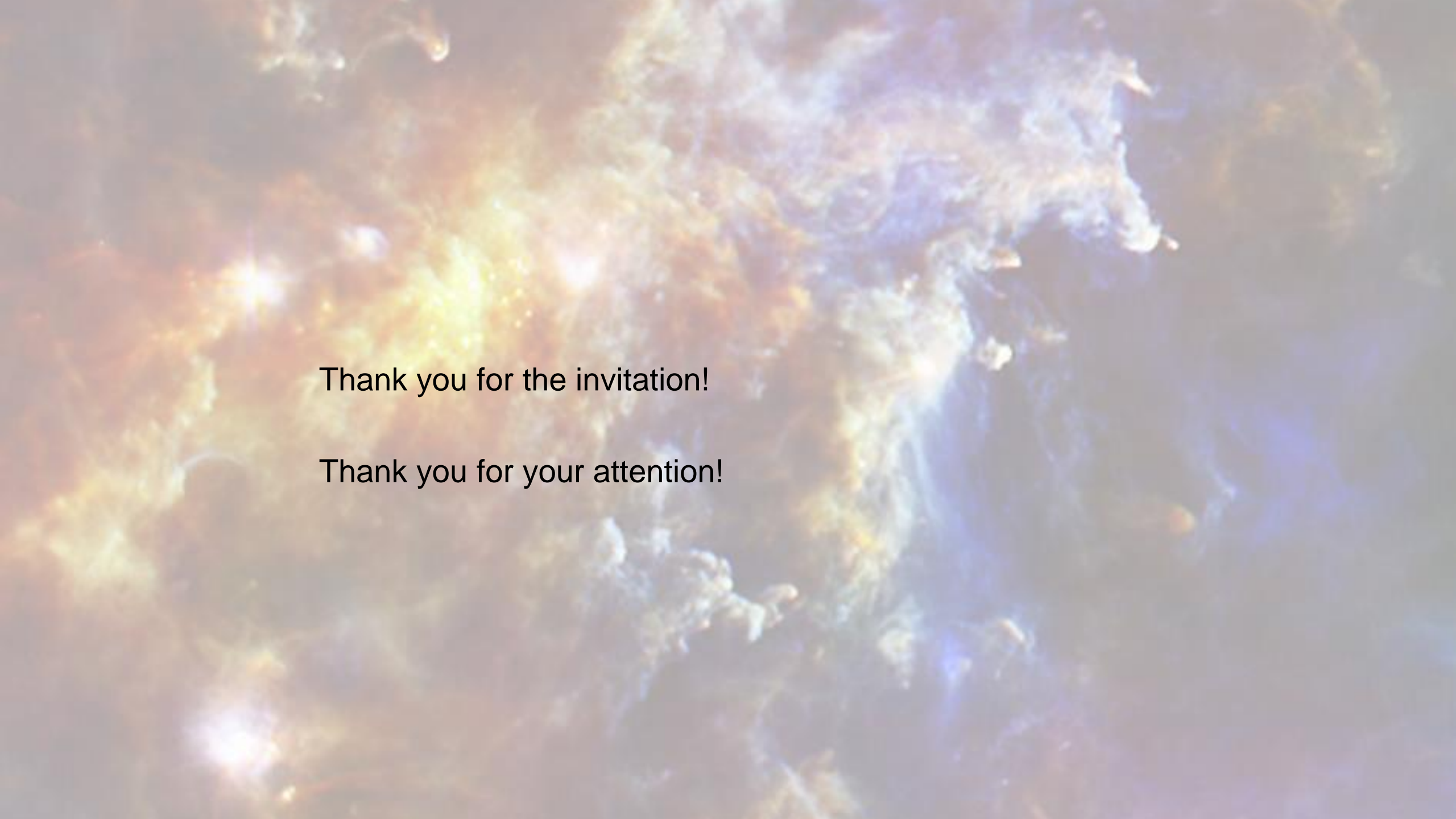
→ gas temperature increases

# PyPDR

Bruderer 2014: [http://www.mpe.mpg.de/~simonbr/research\\_pypdr/index.html](http://www.mpe.mpg.de/~simonbr/research_pypdr/index.html)

- tiny/minimal PDR code written in Python
- Plane-parallel slab (semi-infinite)
- basic chemistry with about 30 molecules, time dependent
- NLTE excitation of [OI], [CII], [CI], CO, and  $^{13}\text{CO}$  using an escape probability approach
- Major heating & cooling processes implemented





Thank you for the invitation!

Thank you for your attention!



# Benchmark Calculations

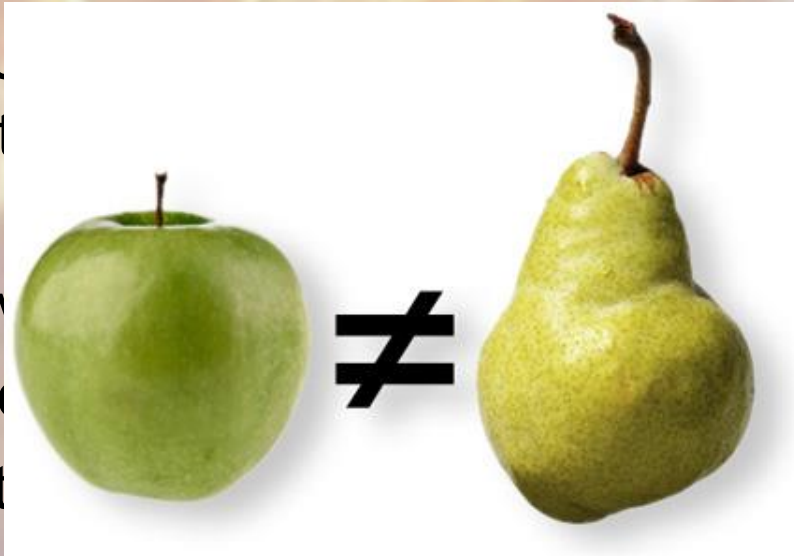
**F1** completed by all 12 groups  
F2-F4 complete by 10 groups  
F5-F8 completed by 8 groups (some with numerical 'noise')  
CLOUDY used different chemical network  
  
KOSMA/Bensch used spherical geometry  
results for Lee96mod are for  $t=10^8$  yrs

<b>F1</b> T=const $n=10^3 \text{ cm}^{-3}, \chi=10$	<b>F2</b> T=const $n=10^3 \text{ cm}^{-3}, \chi=10^5$
<b>F3</b> T=const $n=10^{5.5} \text{ cm}^{-3}, \chi=10$	<b>F4</b> T=const $n=10^{5.5} \text{ cm}^{-3}, \chi=10^5$
<b>F5</b> T=variable $n=10^3 \text{ cm}^{-3}, \chi=10$	<b>F6</b> T=variable $n=10^3 \text{ cm}^{-3}, \chi=10^5$
<b>F7</b> T=variable $n=10^{5.5} \text{ cm}^{-3}, \chi=10$	<b>F8</b> T=variable $n=10^{5.5} \text{ cm}^{-3}, \chi=10^5$

# Benchmark Calculations

**F1** completed by all 12 groups  
 F2-F4 complete by 10 groups  
 F5-F8 completed by 8 groups (some with numerical 'noise')

CLOUD  
 net  
 KOSMOS  
 geo  
 result



8 yrs

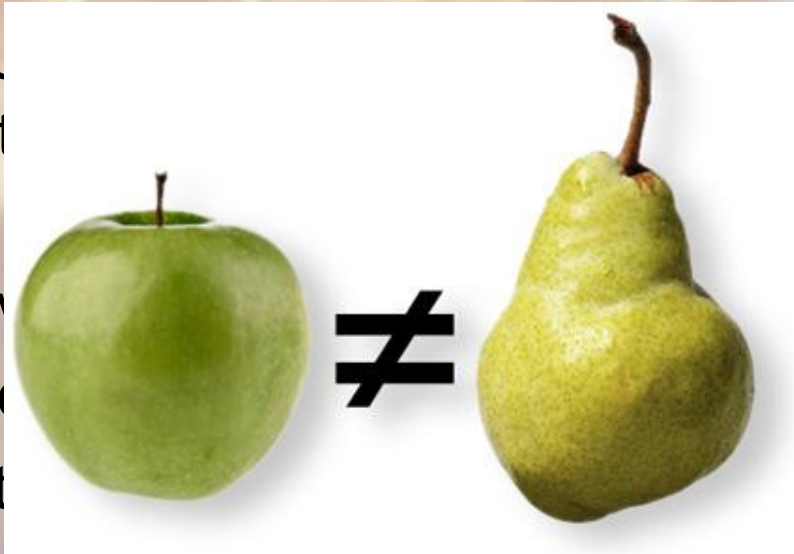
<b>F1</b> T=const $n=10^3 \text{ cm}^{-3}, \chi=10$	<b>F2</b> T=const $n=10^3 \text{ cm}^{-3}, \chi=10^5$
<b>F3</b> T=const $n=10^{5.5} \text{ cm}^{-3}, \chi=10$	<b>F4</b> T=const $n=10^{5.5} \text{ cm}^{-3}, \chi=10^5$
<b>F5</b> T=variable $n=10^3 \text{ cm}^{-3}, \chi=10$	<b>F6</b> T=variable $n=10^3 \text{ cm}^{-3}, \chi=10^5$
<b>F7</b> T=variable $n=10^{5.5} \text{ cm}^{-3}, \chi=10$	<b>F8</b> T=variable $n=10^{5.5} \text{ cm}^{-3}, \chi=10^5$

# Benchmark Calculations

- F1 completed by all 12 groups
- F2-F4 complete by 10 groups
- F5-F8 completed by 8 groups (some with numerical 'noise')

CLOU  
net

KOSM  
ge  
result



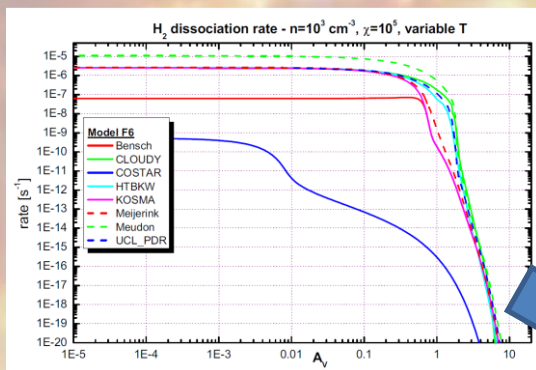
8 yrs



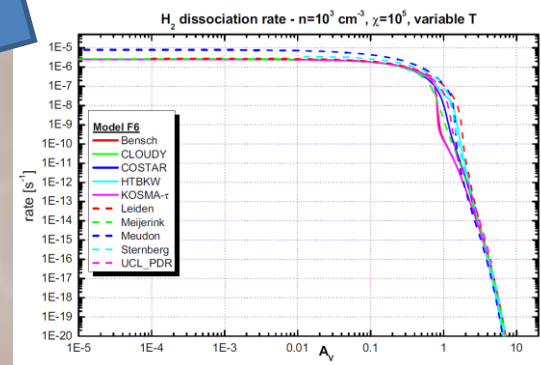


# Benchmark Data Archive

- All the results (data files, plots, documents) have been published on a website.



BEFORE



AFTER

## PDR-Comparison Benchmark

Introduction

Codes

Benchmark

Results

PRE-Benchmark

POST-Data

POST-Plots

Documents

Links

### Data Files

	F1	F2	F3	F4	V1	V2	V3	V4
<u>Bensch</u>	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T
<u>Cloudy</u>	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T
<u>COSTAR</u>	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T
<u>HTBKW</u>	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T
<u>KOSMA-tau</u>	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T
<u>Leiden</u>	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T
<u>Lee96mod</u>	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T
<u>Meijerink</u>	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T

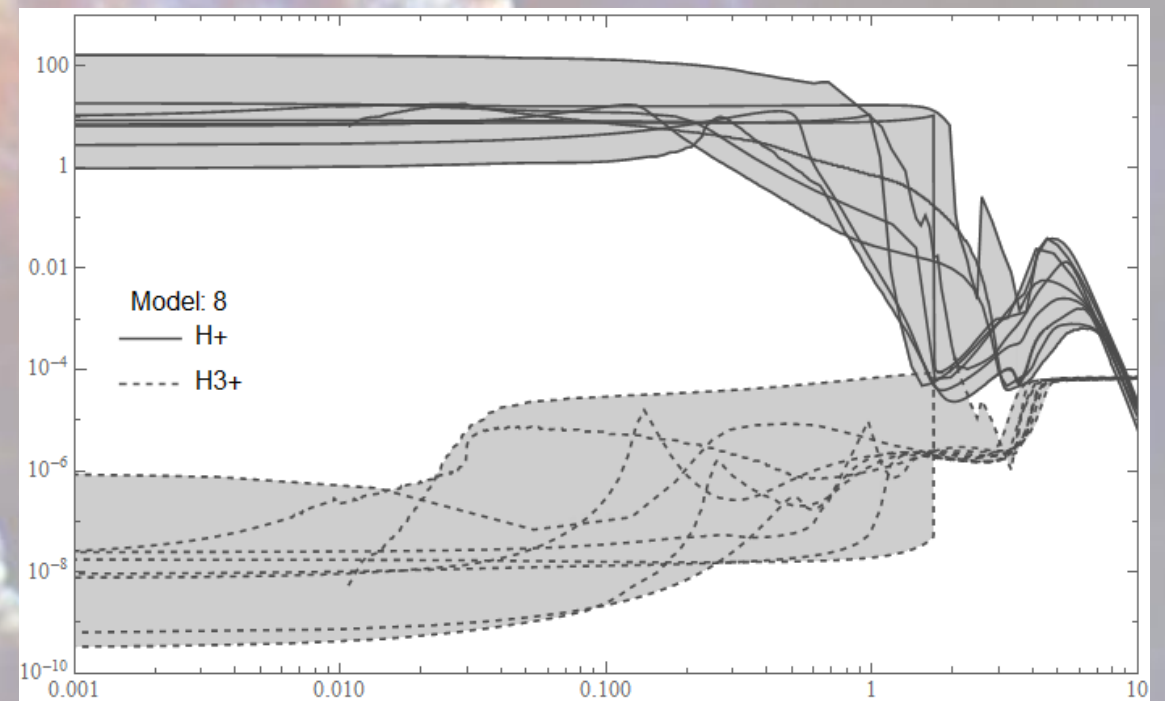
<http://www.astro.uni-koeln.de/pdr-comparison/>

# Benchmark V.2?

So much left to do:

- 2007 benchmark left many open issues

Status after the benchmark 2007



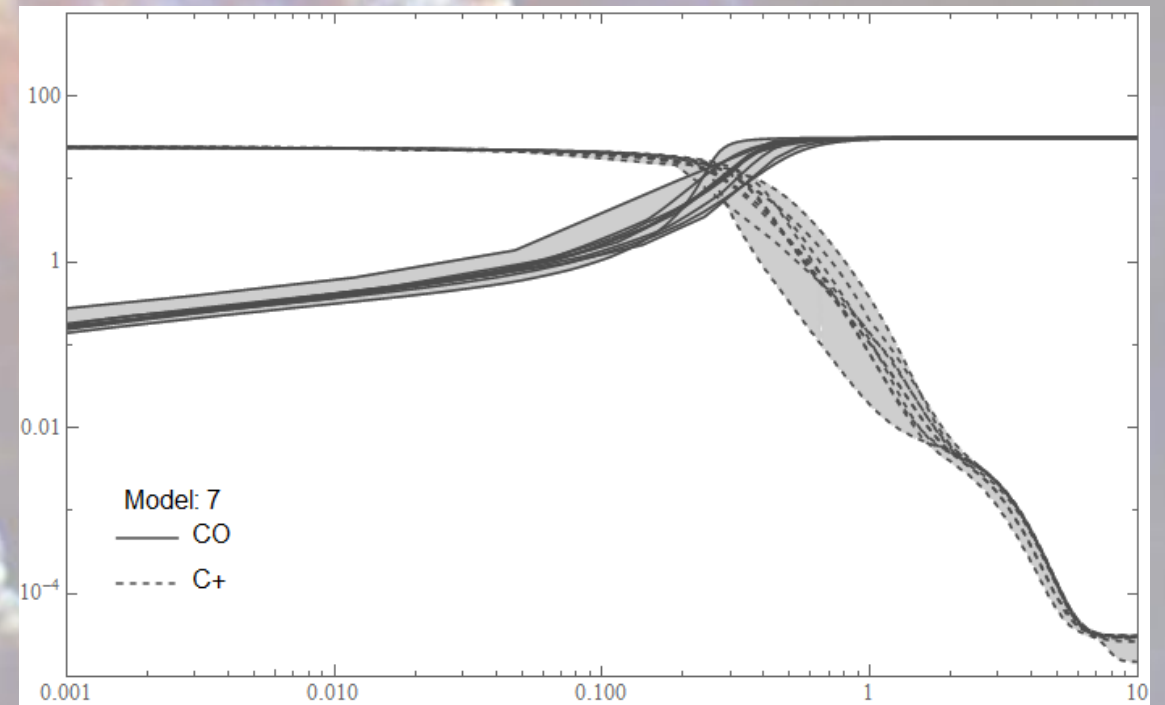
$$n=10^{5.5} \text{ cm}^{-3}, \chi=10^5$$

# Benchmark V.2?

So much left to do:

- 2007 benchmark left many open issues
- Discuss numerics

Status after the benchmark 2007



$$n=10^{5.5} \text{ cm}^{-3}, \chi=10$$

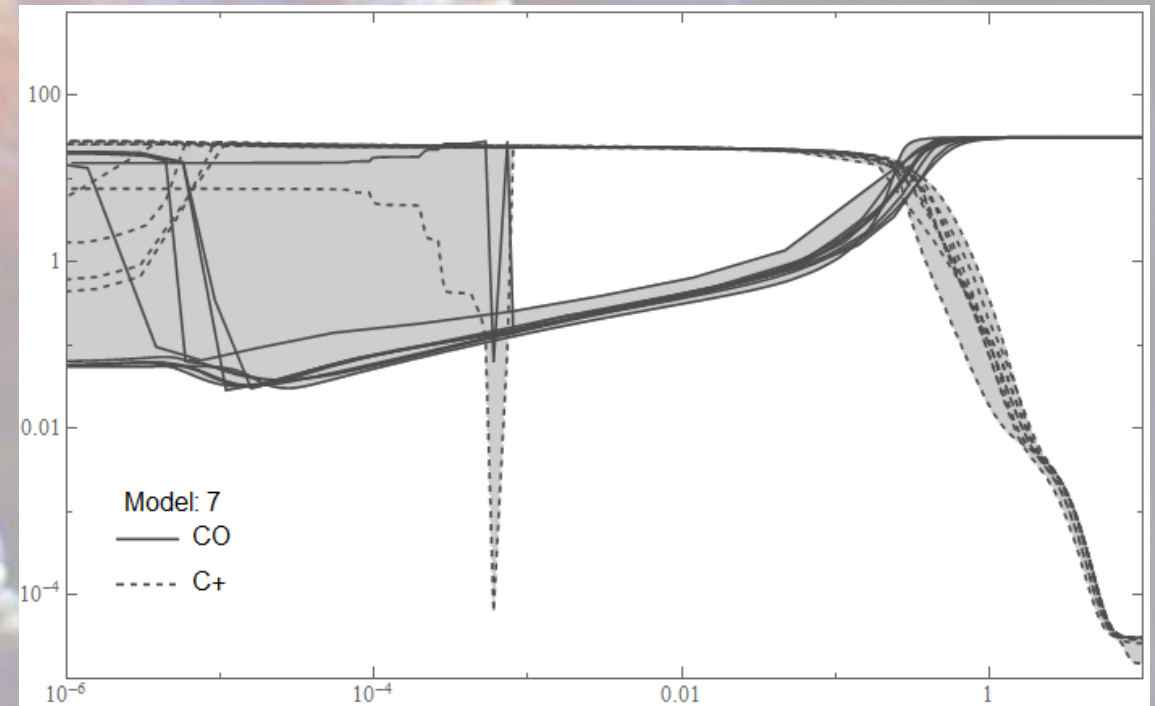


# Benchmark V.2?

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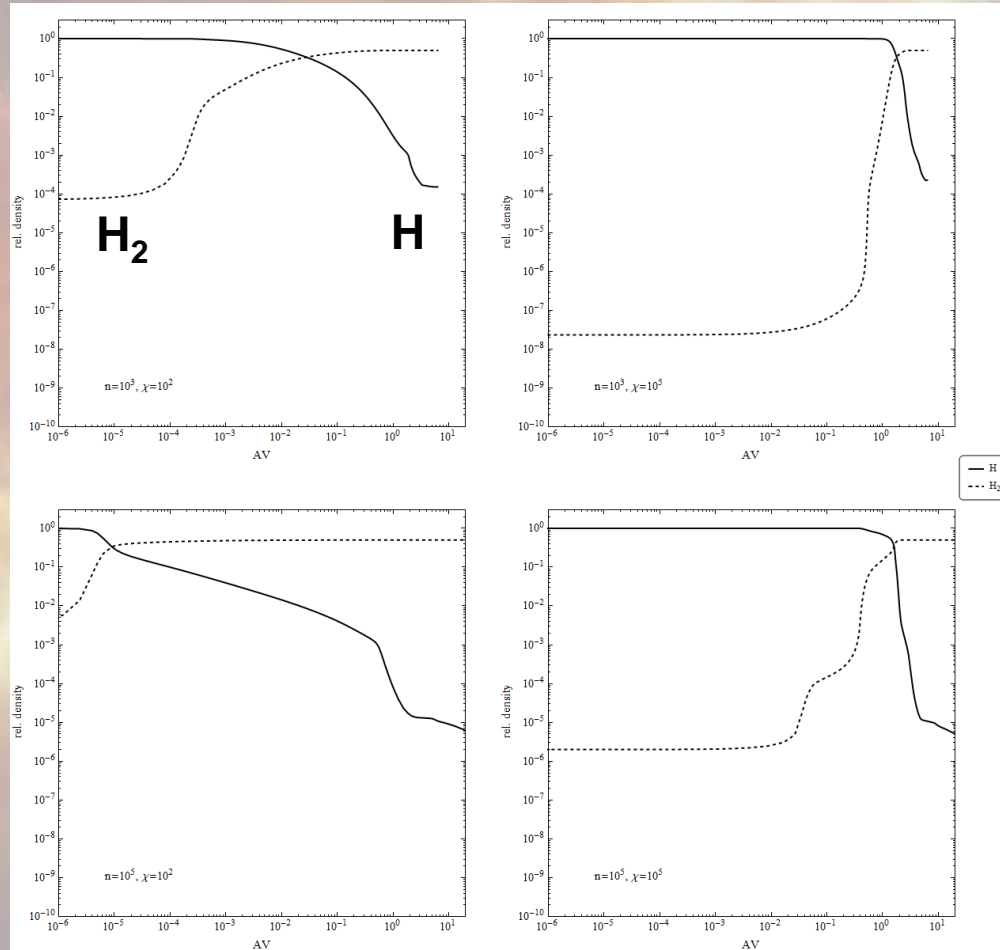
$n=10^{5.5} \text{ cm}^{-3}, \chi=10$

# PDR Model Chemistry

$\chi=100$

$\chi=10^5$

$n=10^3$



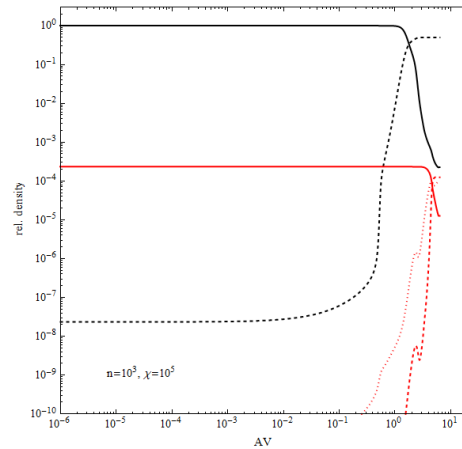
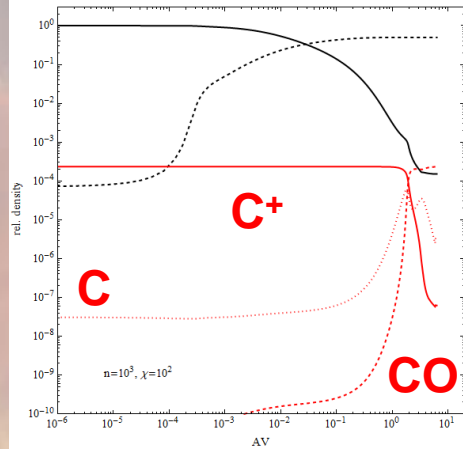
- H<sub>2</sub> photodissociation is a line absorption process. Once the absorption lines become optically thick, photodissociation becomes inefficient
- Density and UV field strength determine the depth of the H-H<sub>2</sub> transition zone

# PDR Model Chemistry

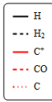
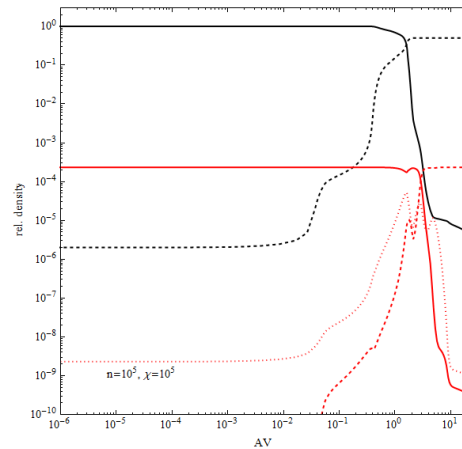
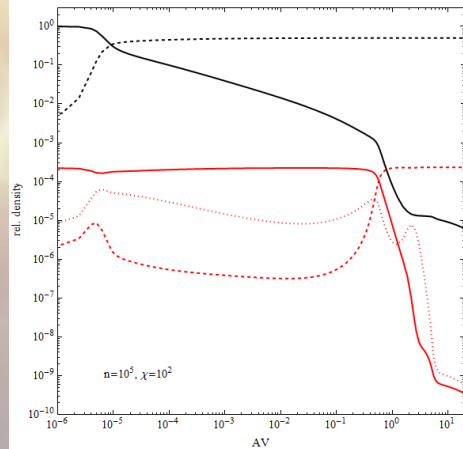
$\chi=100$

$\chi=10^5$

$n=10^3$



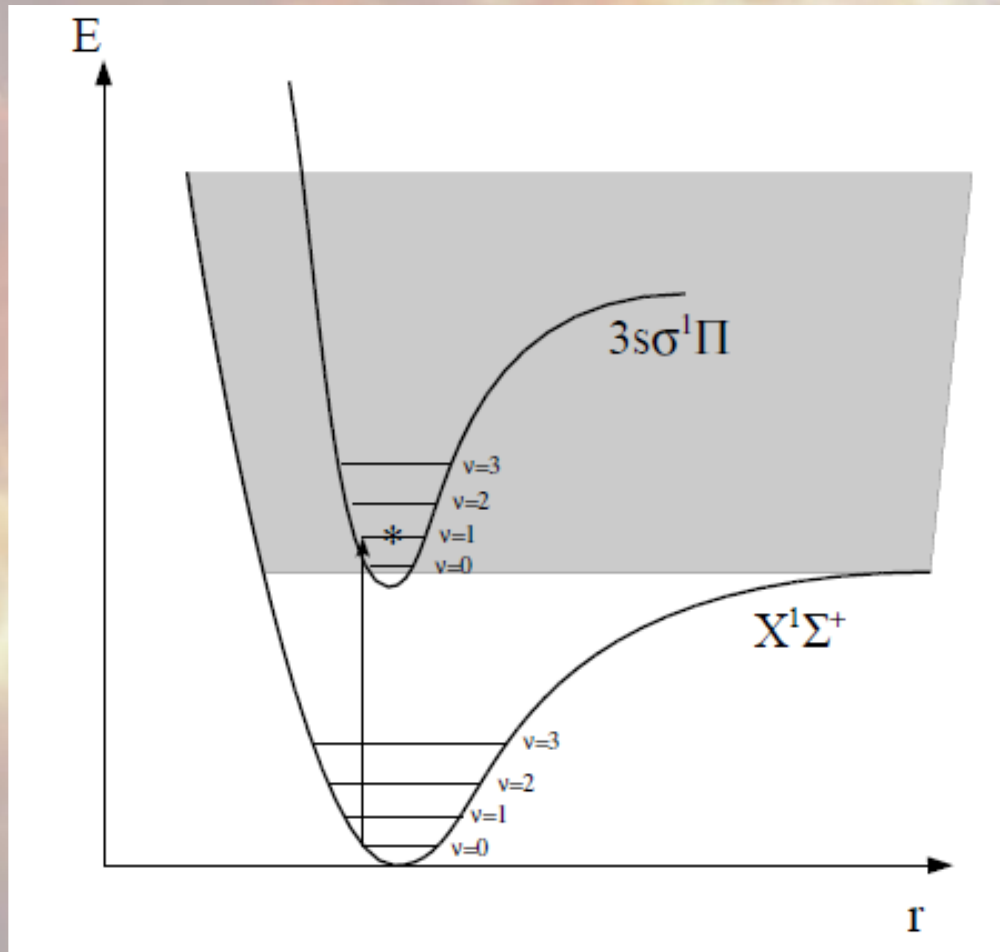
$n=10^5$



- CO photodissociation is shielded by
  - itself (self-shielding)
  - CO isotopologues (mutual shielding)
  - overlapping H<sub>2</sub> lines
  - dust attenuation
- CO photodissociation becomes inefficient for  $N_{\text{CO}} > 10^{16} \text{ cm}^{-2}$



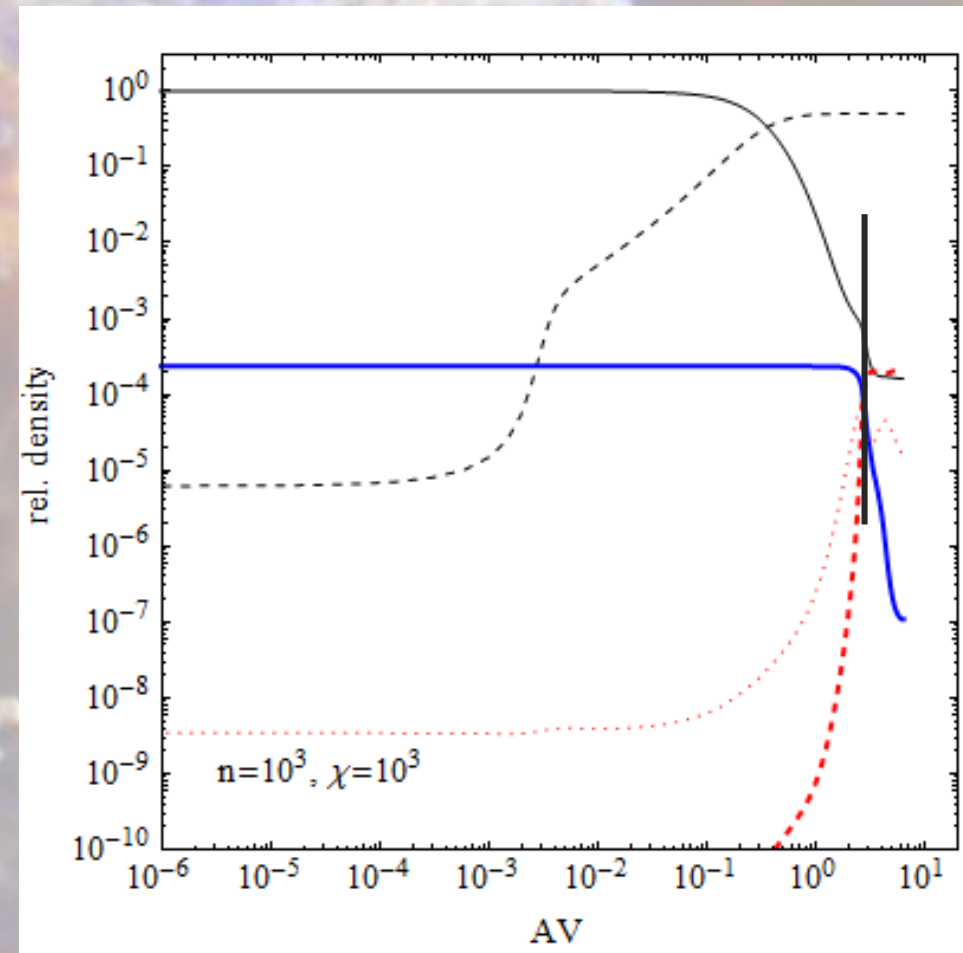
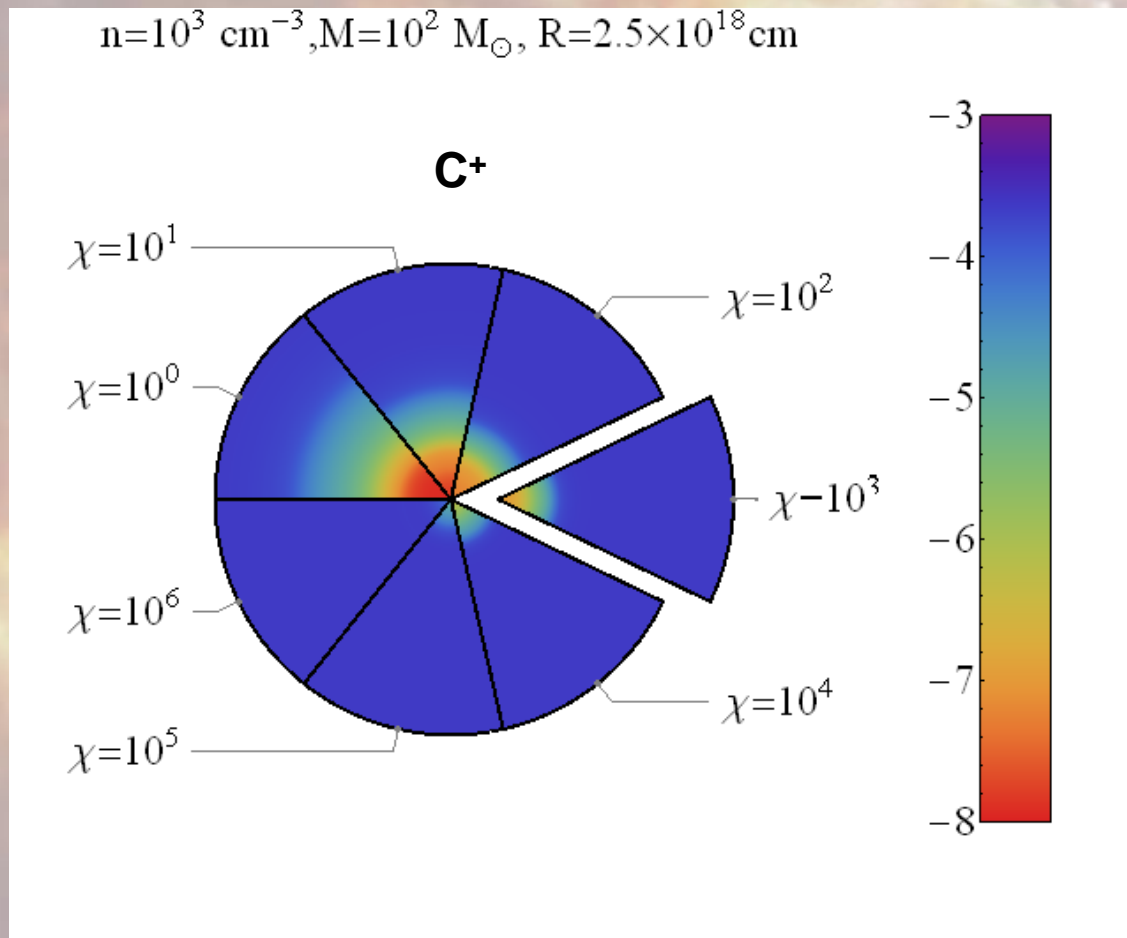
# CO Dissociation



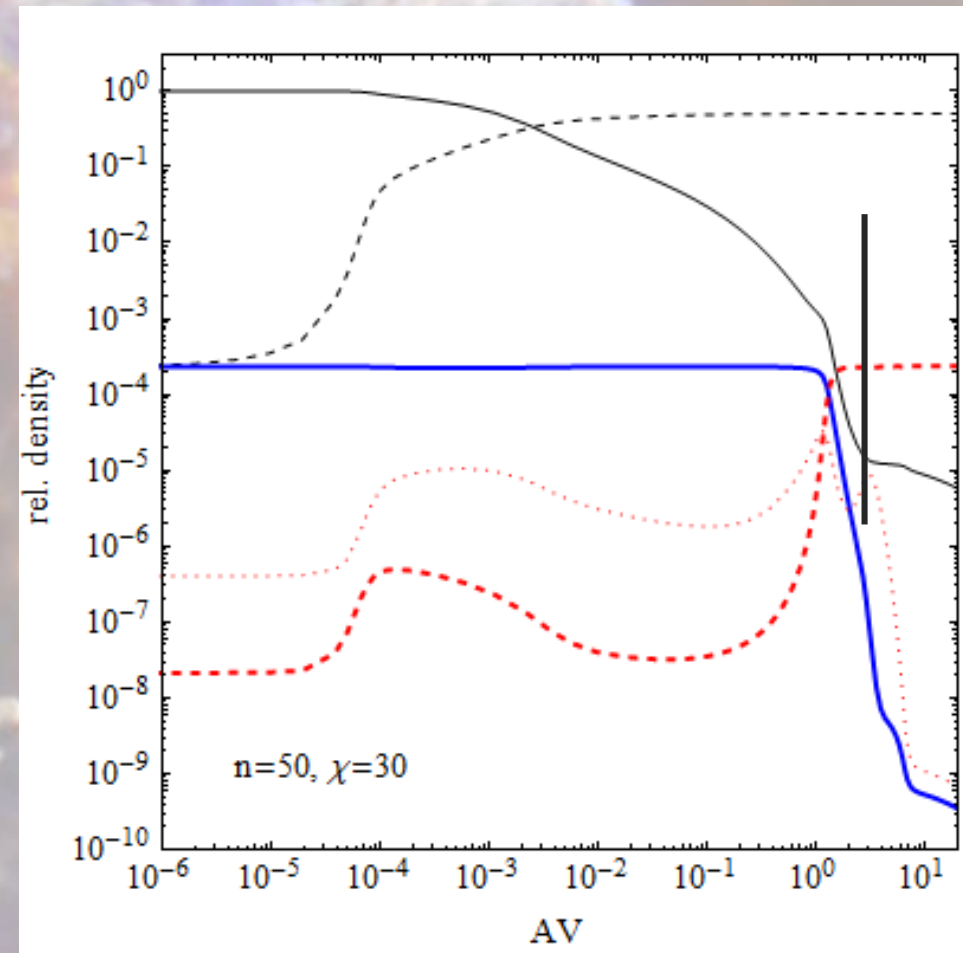
- CO dissociation occurs via line absorption!
- Absorbed photons excite *predissociated* electronic states that can decay into unbound continuum of the ground elect. state radiationless.
- More than 30 absorption bands in the range  $913 \text{ \AA} \leq \lambda \leq 1077 \text{ \AA}$
- Line absorption leads to optical thickness effects (self-shielding)

Warin et al. 1996

# $A_V$ is not a spatial coordinate

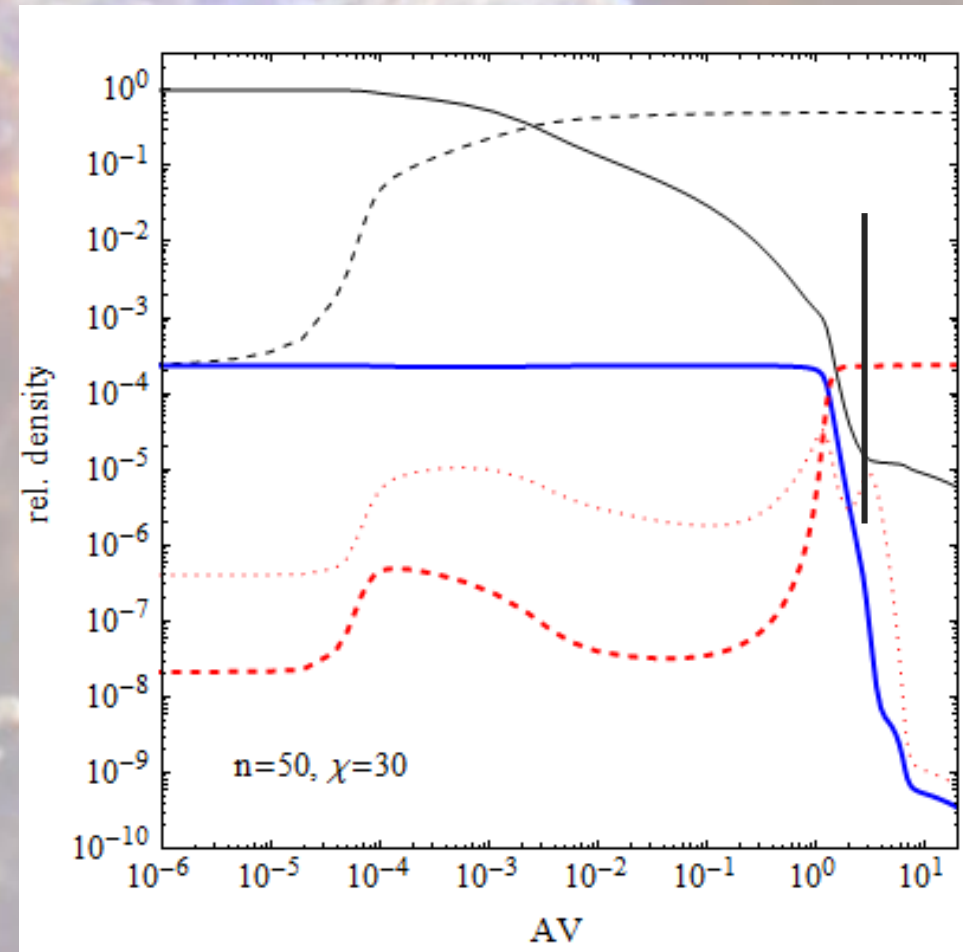
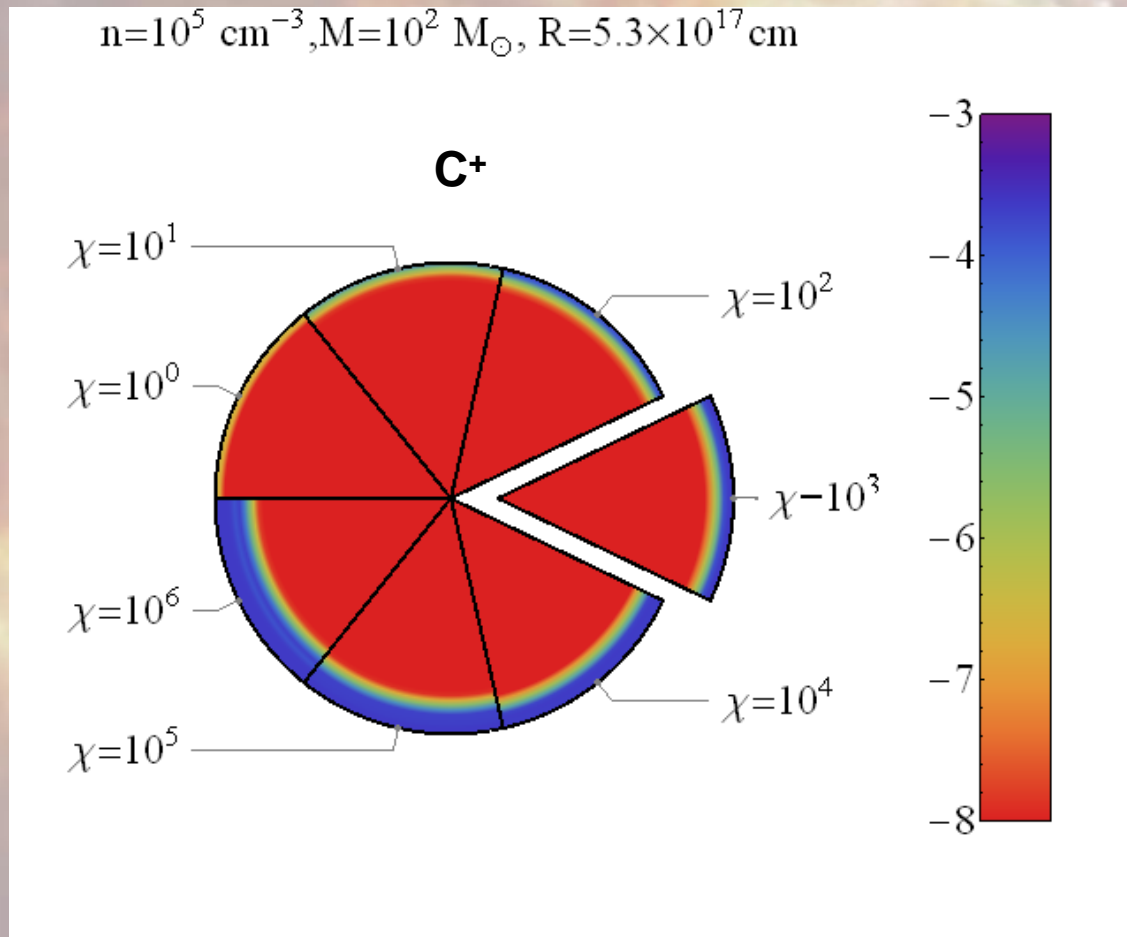


# $A_V$ is not a spatial coordinate





# $A_V$ is not a spatial coordinate

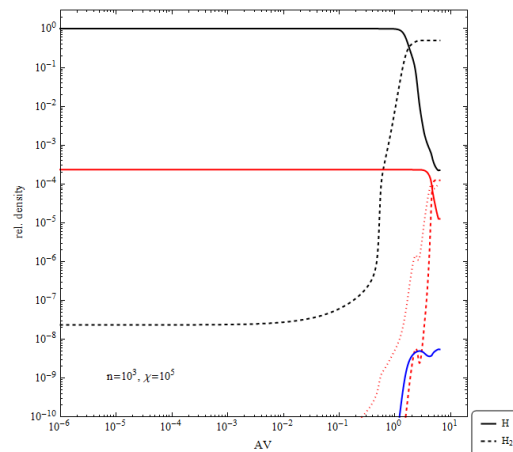
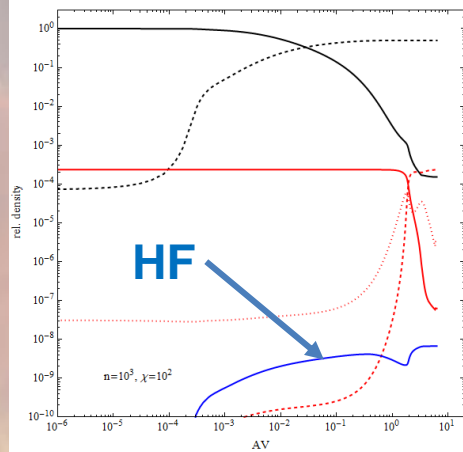


# PDR Model Chemistry

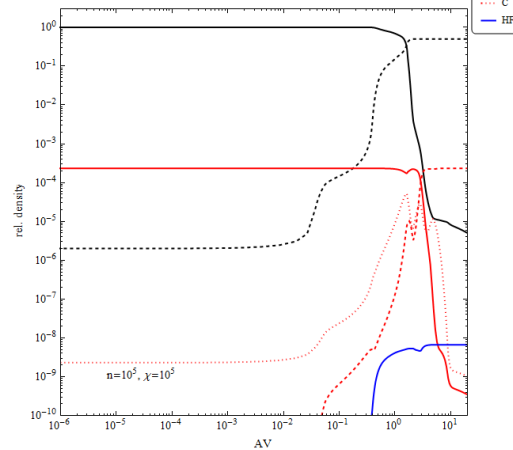
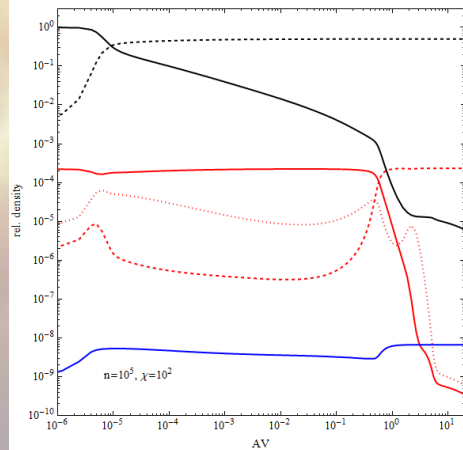
$\chi=100$

$\chi=10^5$

$n=10^3$



$n=10^5$



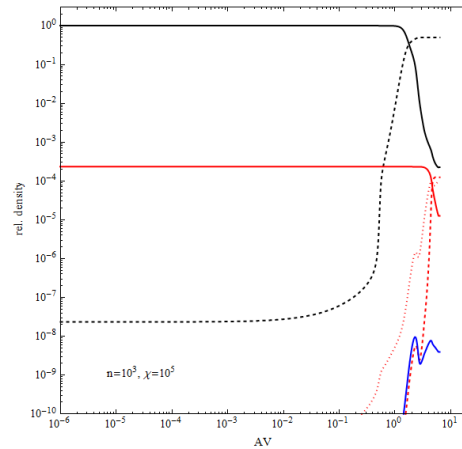
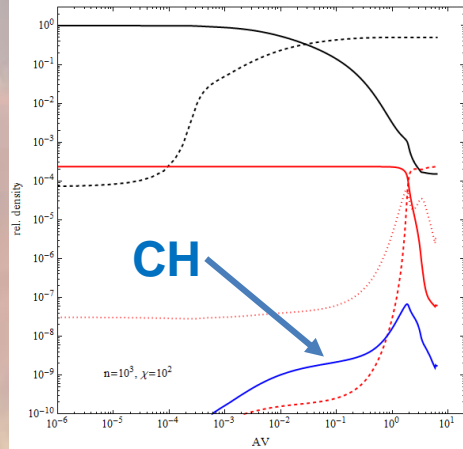
- „Standard“ models show a good H<sub>2</sub>-HF correlation (in agreement with empirical findings)

# PDR Model Chemistry

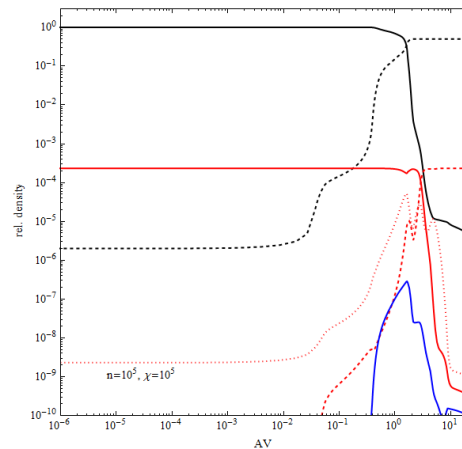
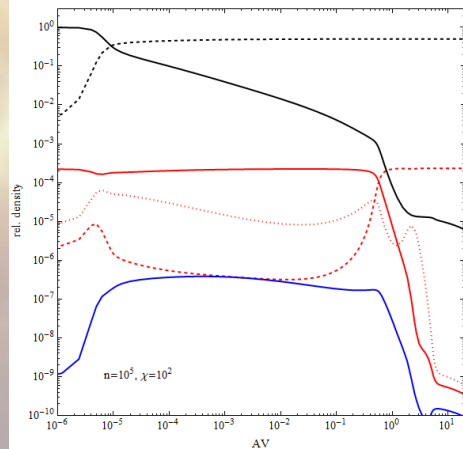
$\chi=100$

$\chi=10^5$

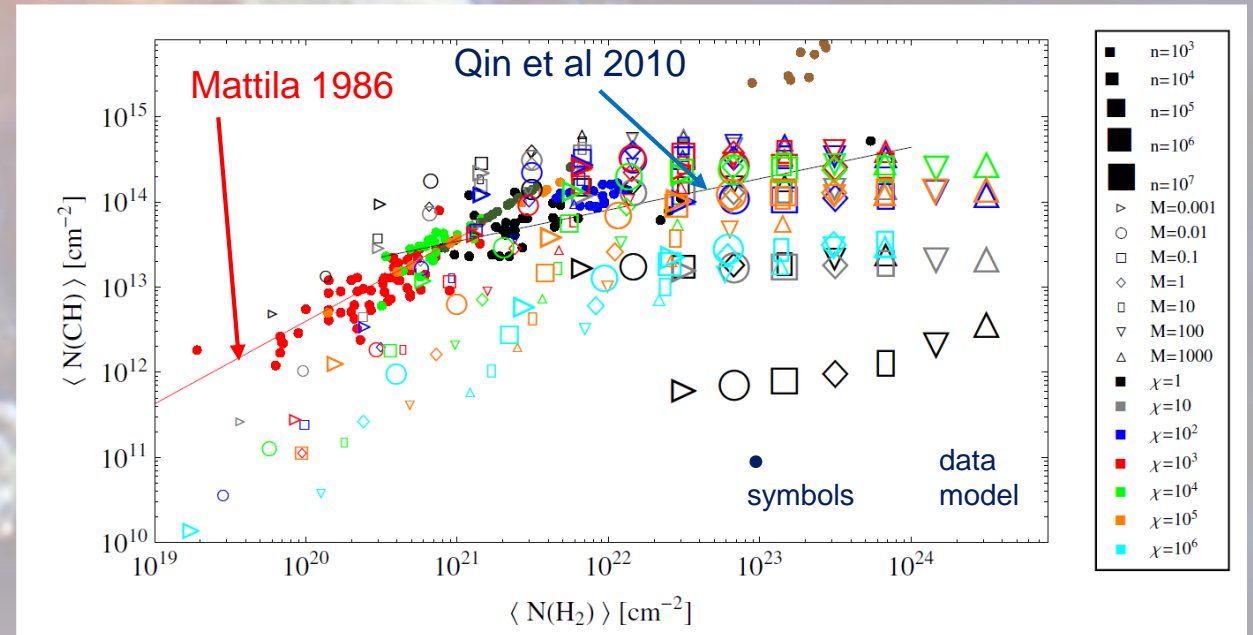
$n=10^3$



$n=10^5$



- $H_2$ -CH correlation changes from diffuse to denser clouds



Röllig & Ossenkopf 2013, A&A 550, A56

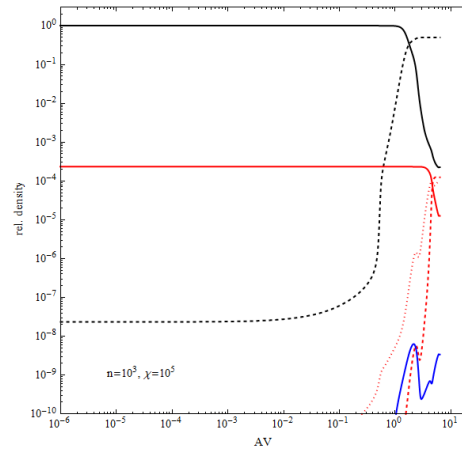
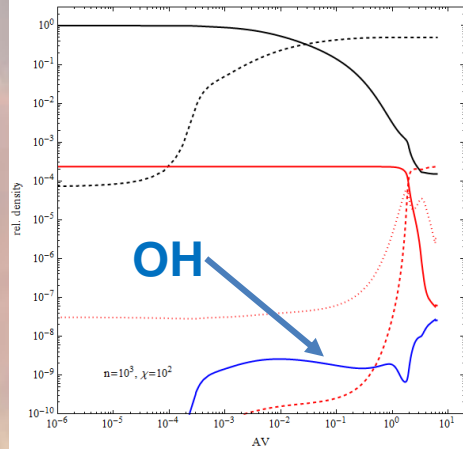


# PDR Model Chemistry

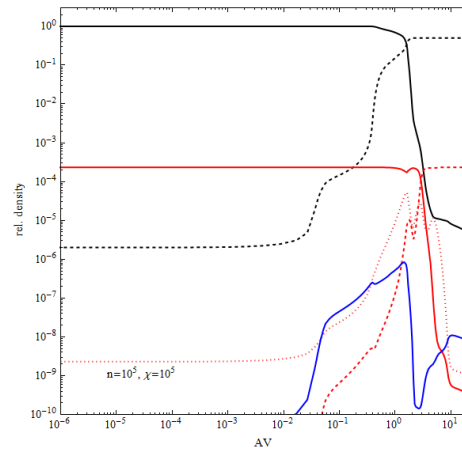
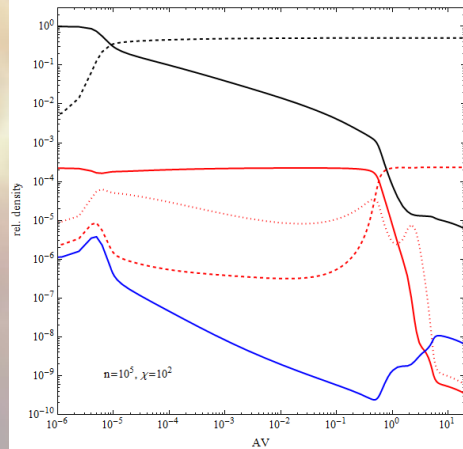
$\chi=100$

$\chi=10^5$

$n=10^3$

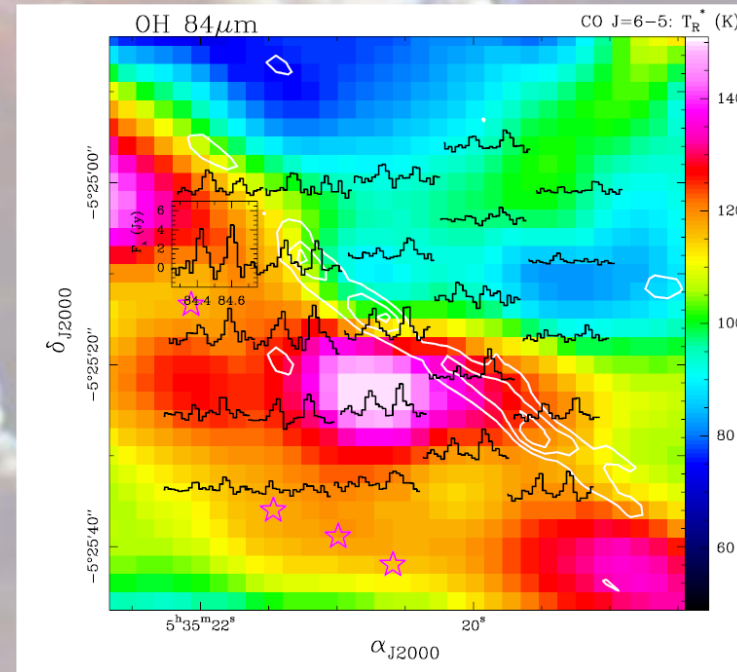


$n=10^5$



— H  
- - - H<sub>2</sub>  
... C<sup>-</sup>  
- - - CO  
... C  
— OH

- OH appears to be a reasonable PDR interface tracer
- column densities not well modelled

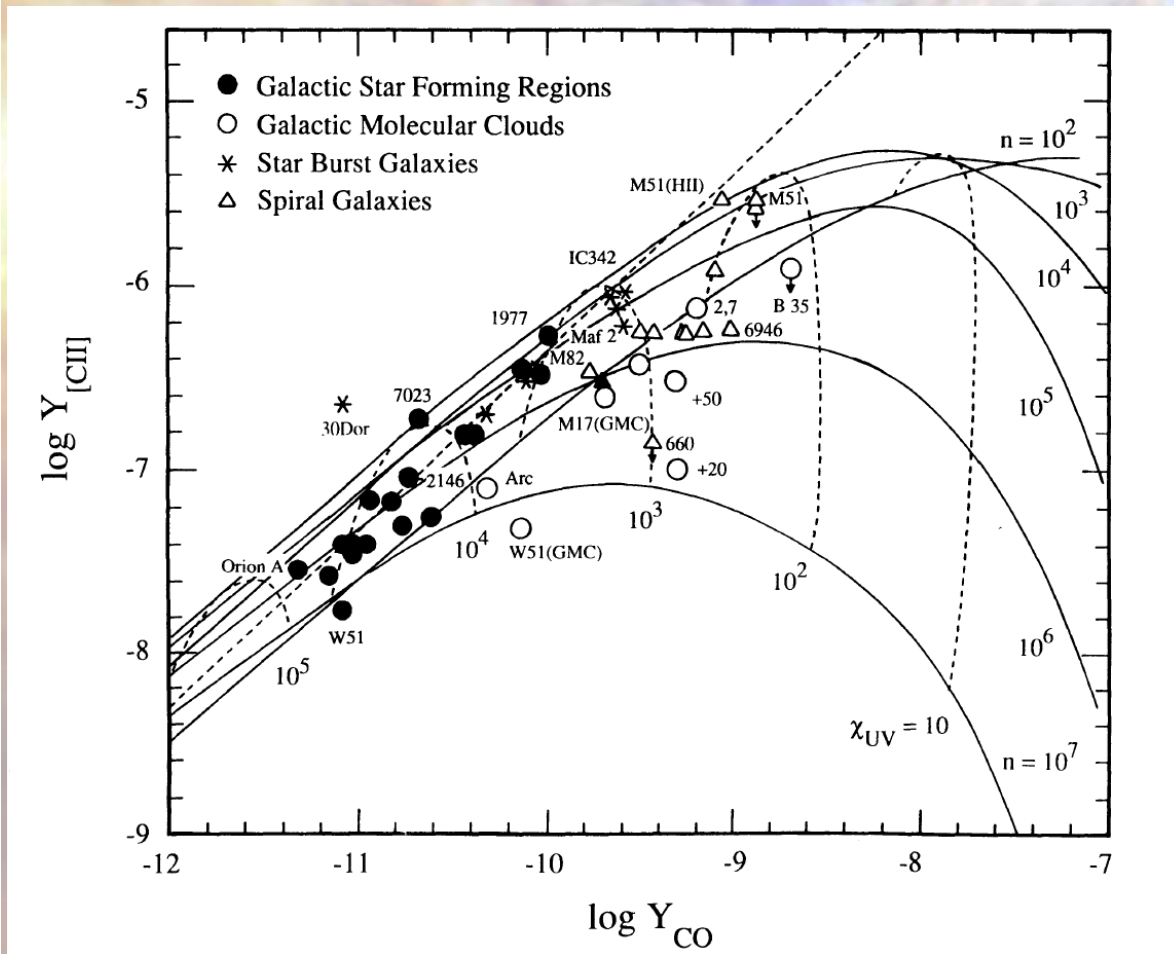
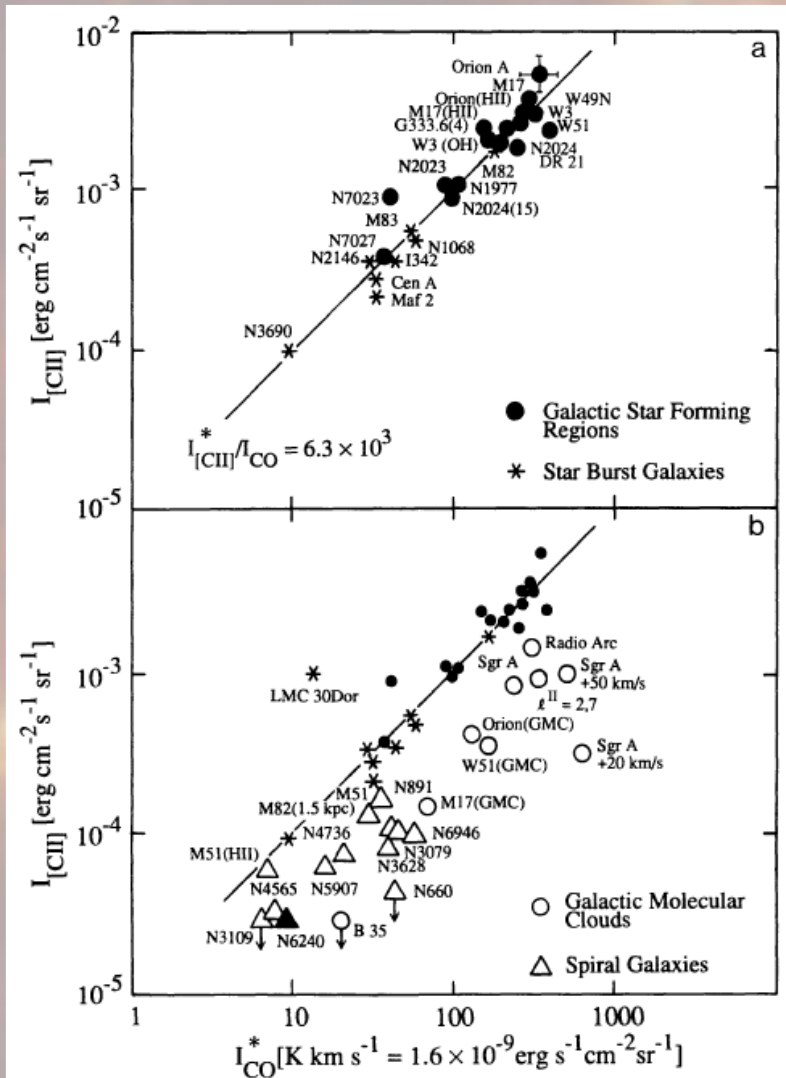


Orion bar

contours: OH 84  $\mu\text{m}$   
( $E_{\text{J}}/k = 291 \text{ K}$ )  
colors: CO (6-5)

Goicoechea et al. 2011

# PDR Diagnostics



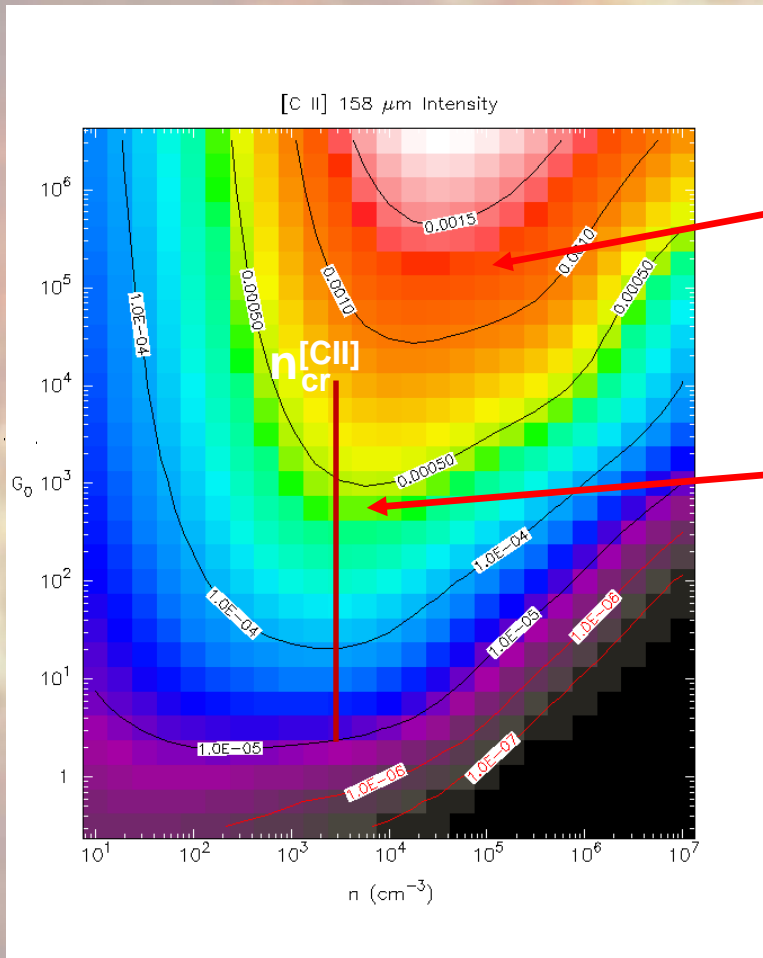
$$Y_{\text{CII}} = I_{\text{CII}} / I_{\text{FIR}}$$

$$Y_{\text{CO}} = I_{\text{CO}} / I_{\text{FIR}}$$

Stacey et al. 1991

# PDR Diagnostics

Model calculations

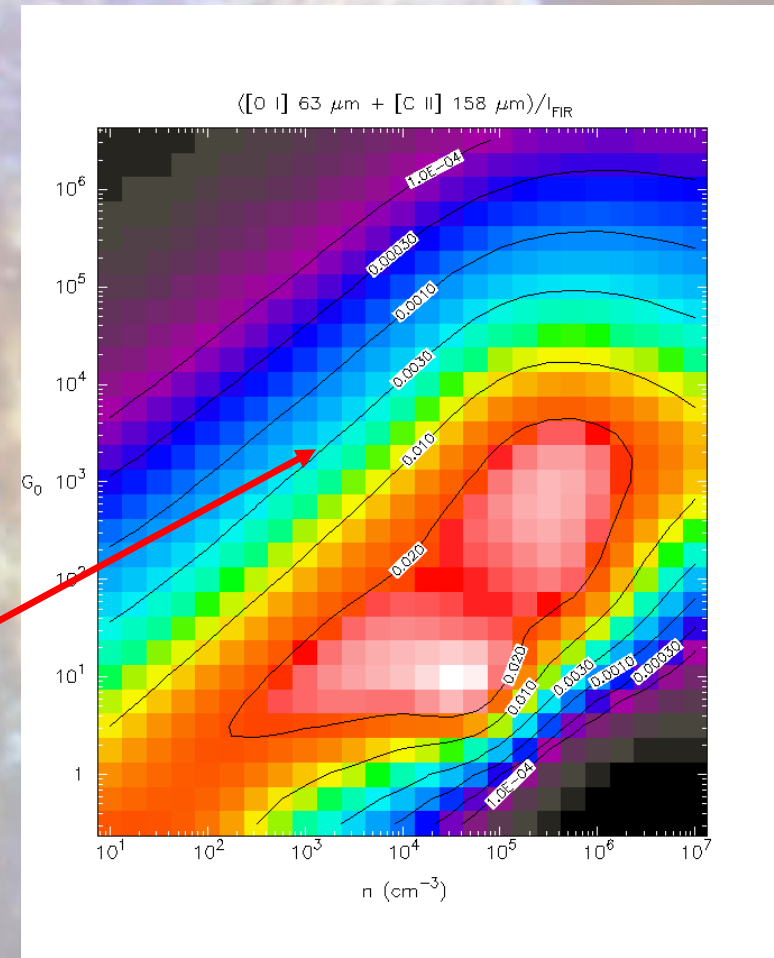


Orion PDR

Classic PDRs

$G_0/n = \text{const}$

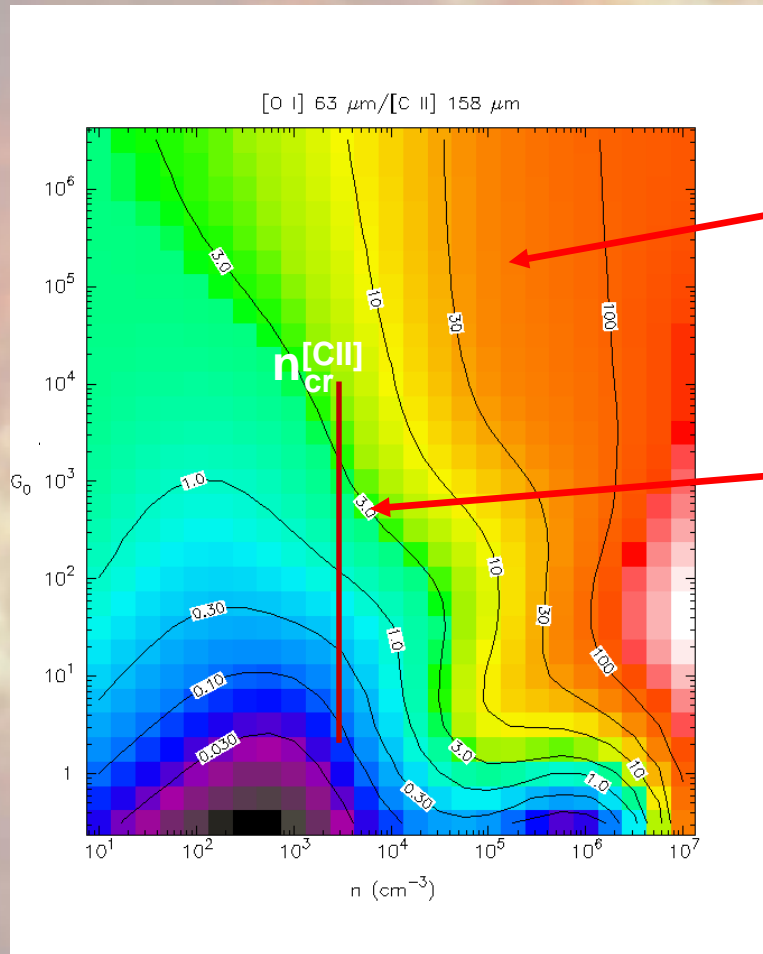
Kaufman et al. 1999





# PDR Diagnostics

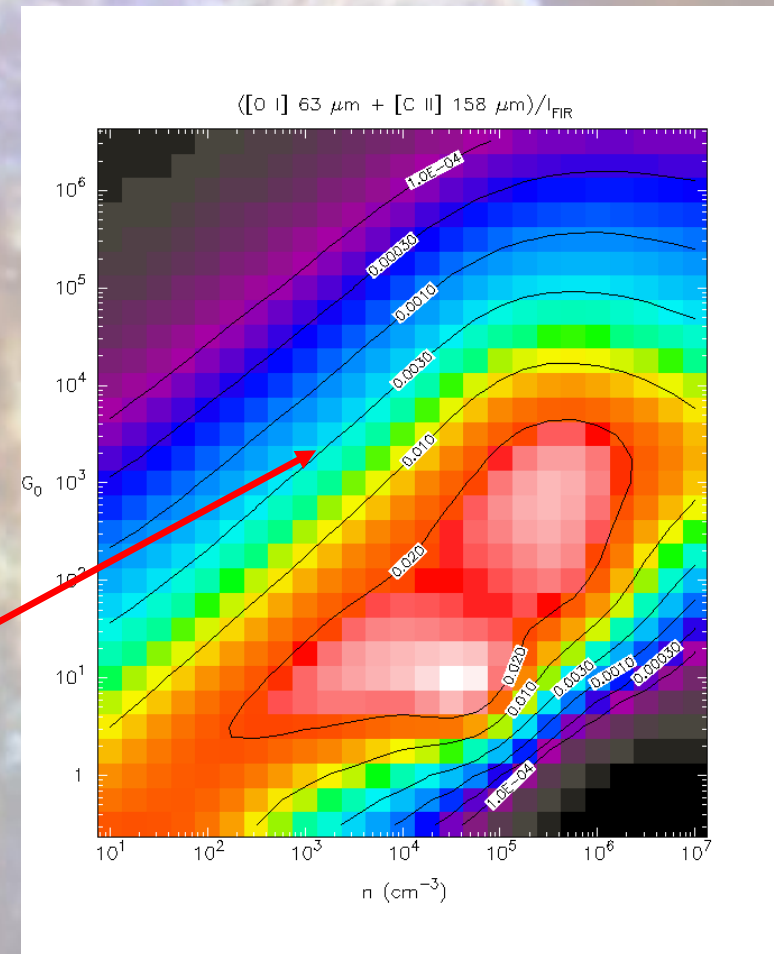
Model calculations



Orion PDR

Classic PDRs

$G_0/n = \text{const}$



Kaufman et al. 1999

Credit: Slide by A. Fuente, M. Wolfire

23.10.2019

703. WE-Heraeus-Seminar - Chemical Evolution of Cosmic Matter

88

# PDR diagnostic model diagrams

PDR diagnostic diagrams are useful to derive global properties. If the main heating mechanism is the photoelectric effect, heating efficiency depends on the grain charge which is itself governed by the parameter  $G_0 T^{1/2} / n_e$ .

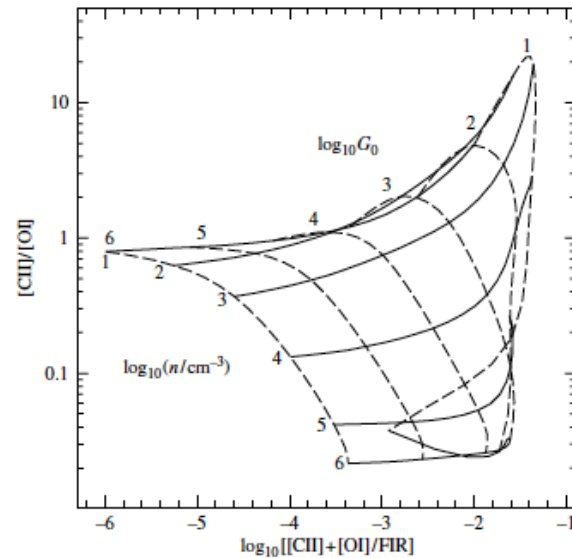


Figure 9.9 A diagnostic diagram for PDRs based on the observed intensity ratio of the [CII] 158  $\mu\text{m}$  and [OI] 63  $\mu\text{m}$  lines and the overall cooling efficiency. The lines present the results of detailed model calculations for different densities and incident FUV fields. Figure kindly provided by M.J. Kaufman; derived from the models described in M. J. Kaufman, M. G. Wolfire, D. Hollenbach, and M.L. Luhman, 1999, *Ap. J.*, 527, p. 795.

$$\frac{F_{\text{OI}} + F_{\text{CII}}}{2F_{\text{IR}}}$$

Gas heating efficiency

Since the [CII] 158  $\mu\text{m}$  and [OI] 63  $\mu\text{m}$  lines have different critical densities, their intensity ratio is a good measure of the density.

# PDR Online Extraction Tool

<http://hera.ph1.uni-koeln.de/~pdr/>

**Spherical Photon Dominated Region Model**

Home Model Help **Extract**

This page provides an interface to view the model calculations of the [KOSMA- \$\tau\$  Spherical Photon Dominated Region \(PDR\) Model](#) developed at the University of Cologne. This interface can be used to extract the intensity ratios of the spectral lines of many important molecular and atomic species. Although effort has been given to make sure the tools extract the correct data from the database, we encourage the user to contact J. Stutzki or M. Röllig for scientific use of the results.

**Update 24. June 2005:** We added the possibility to download the output from the web-interface in a number of additional formats, including FITS.

Report problems to: M.Röllig; Email: [roellig@ph1.uni-koeln.de](mailto:roellig@ph1.uni-koeln.de)



# PDR Online Extraction Tool

<http://hera.ph1.uni-koeln.de/~pdr/>

**Spherical Photon Dominated Region Model**

Home Model Help Extract

- Enable Javascript in your browser to use this form.
- Two of the four possible model parameters should be fixed before submitting the form.

**Model Parameters**

Metallicity 1.0  log(Density) All  log(Mass) 0  log(UV) All

**Line Info**

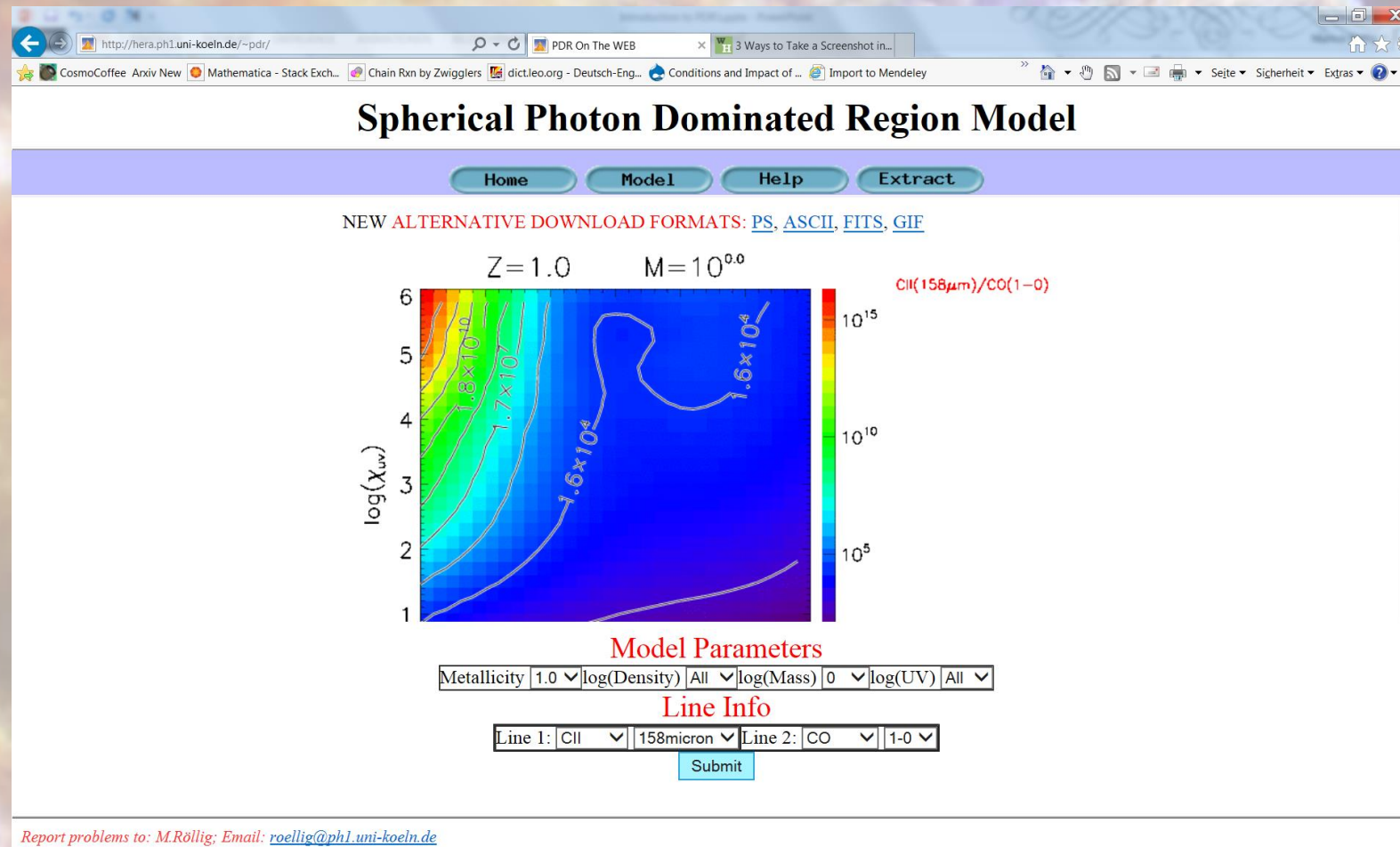
Line 1: CII  158micron  Line 2: CII  158micron

Submit

Report problems to: M.Röllig; Email: [roellig@ph1.uni-koeln.de](mailto:roellig@ph1.uni-koeln.de)

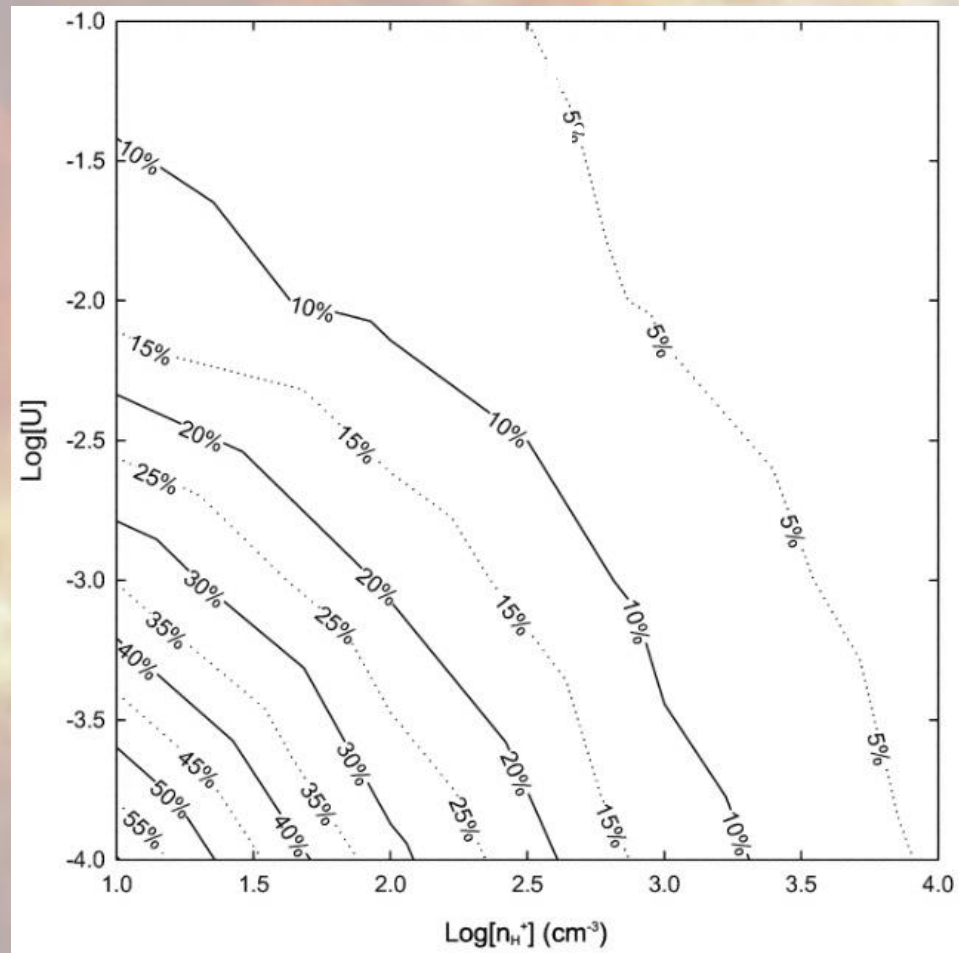
# PDR Online Extraction Tool

<http://hera.ph1.uni-koeln.de/~pdr/>



# [CII] contribution from HII regions

$T_{\text{eff}} = 42000 \text{ K}$



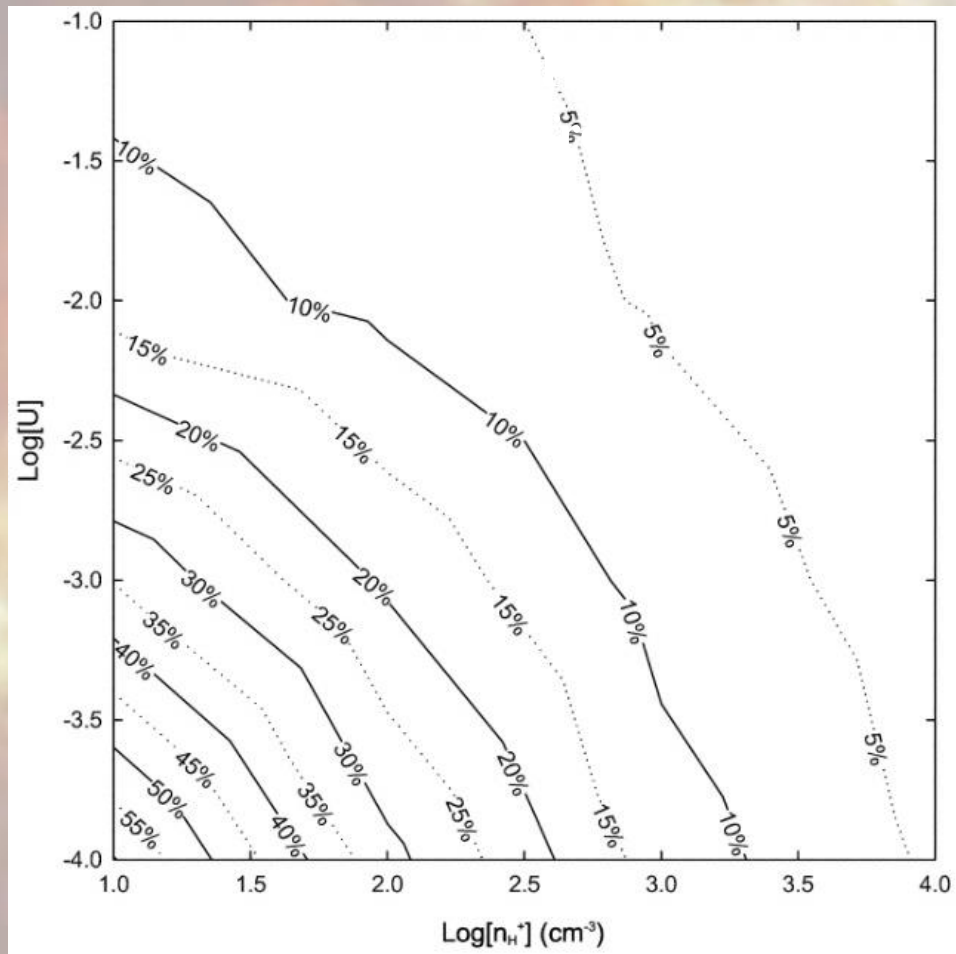
Abel et al 2005

- $\text{C}^+$  is also present in the ionized gas
- When observing a PDR you always observe the neighbouring HII region
- [CII] emission is partly produced in the HII region. ( $\sim 10\text{-}30\%$ )

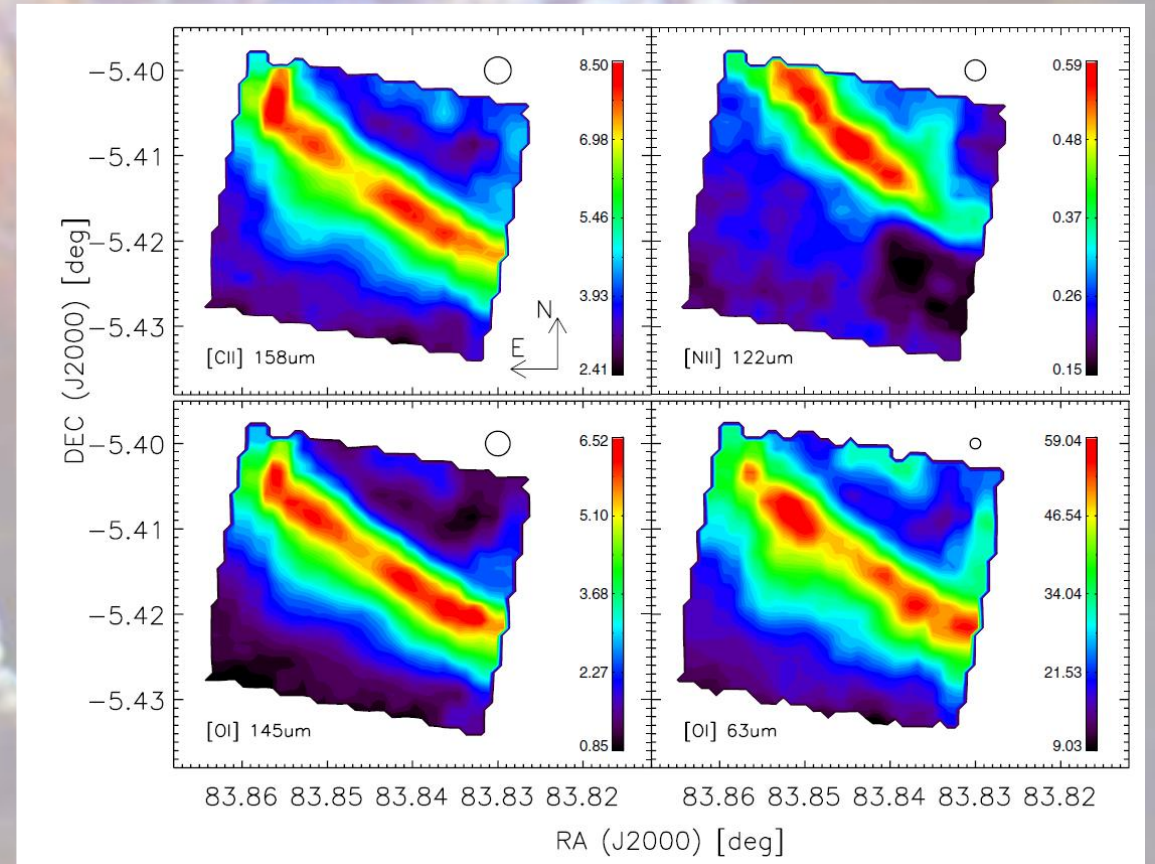


# [CII] contribution from HII regions

$T_{\text{eff}} = 42000 \text{ K}$

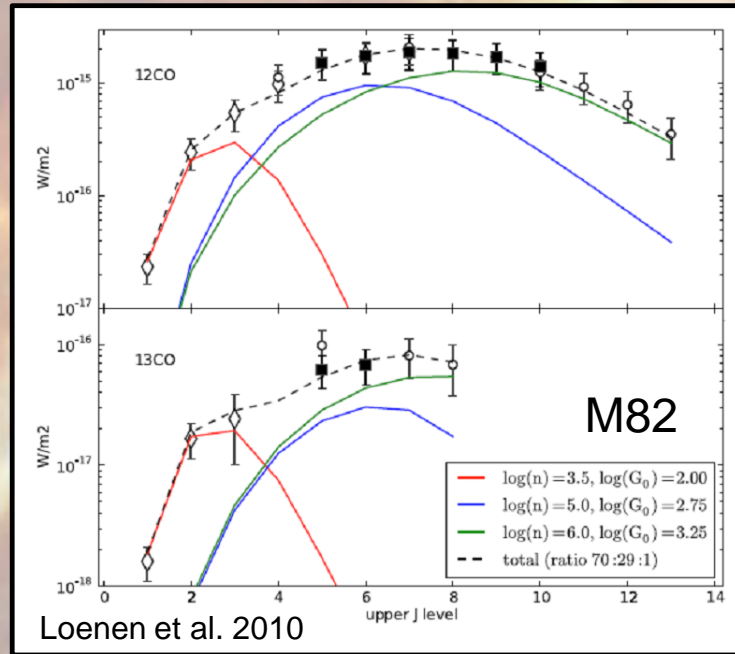


Abel et al 2005

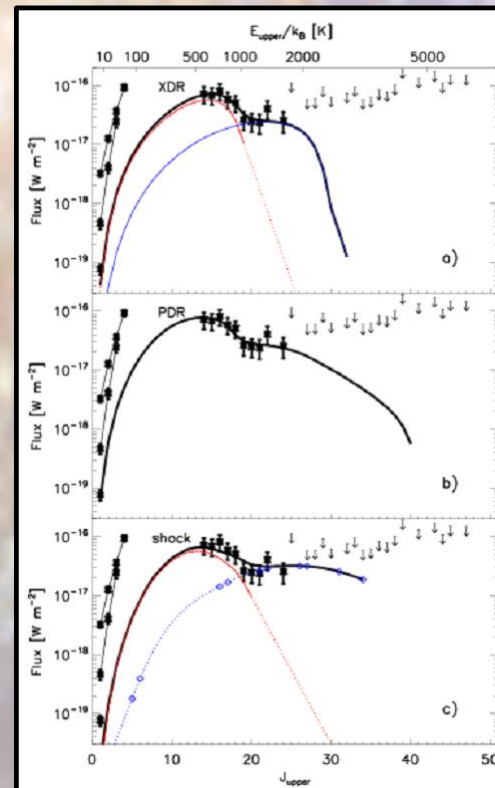


Bernard-Salas et al. 2012

# CO in PDRs, Shocks, XDRs ???

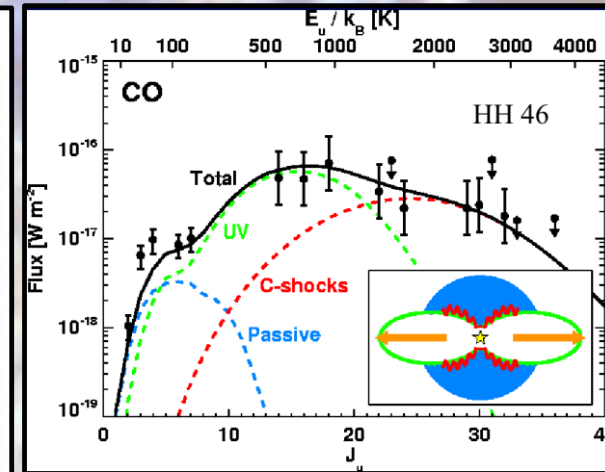


Loenen et al. 2010



Hailey-Dunsheath et al. 2012

NGC 1068



Visser et al. 2012, van Kempen et al. 2010

High-J CO lines reveal  
new insights into the  
local physics!

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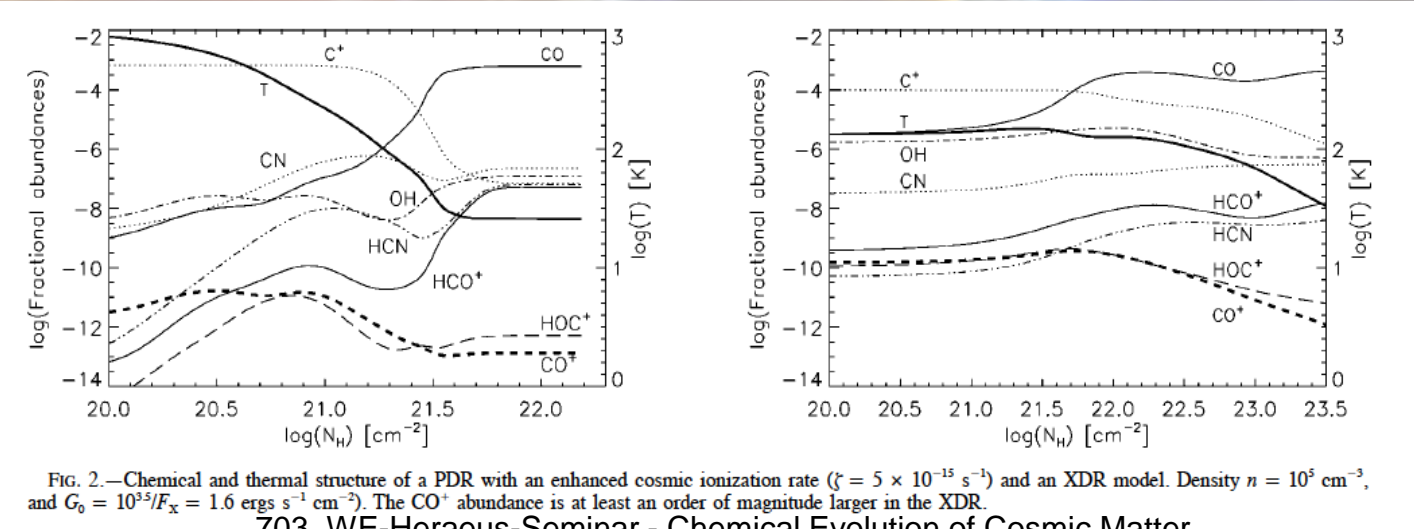


# XDR or PDR?

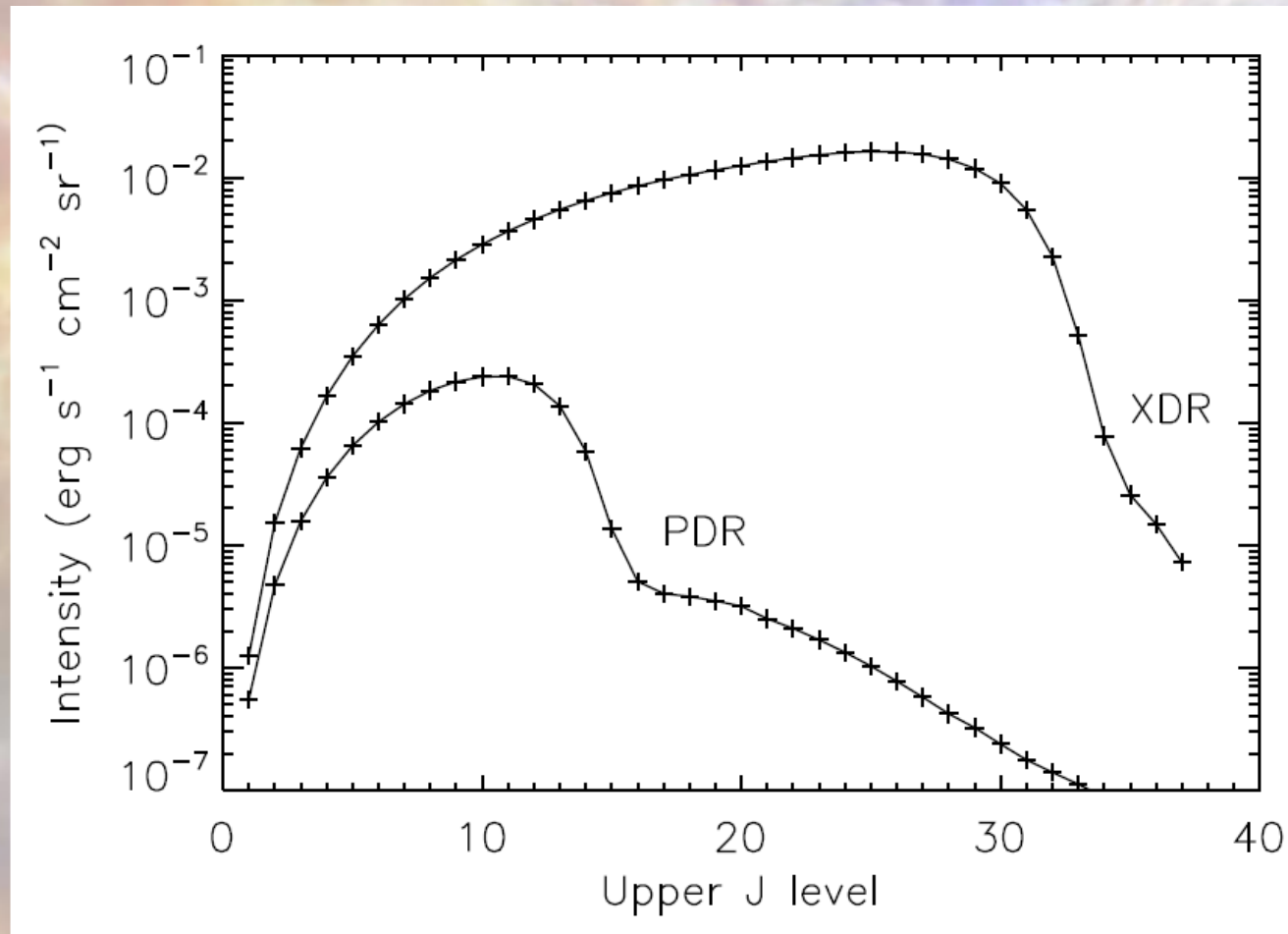
(Spaans & Meijerink 2007, ApJ 664, L23)

TABLE 1  
COLUMN DENSITIES AND COLUMN DENSITY RATIOS

$N_{\text{H}}$	$N(\text{CO}^+)$	$N(\text{HOC}^+)$	$N(\text{HCO}^+)$	$N(\text{CN})$	$N(\text{HCN})$	$\text{CO}^+/\text{HCO}^+$	$\text{HCO}^+/\text{HOC}^+$	$\text{CN}/\text{HCN}$
XDR: $n = 10^5 \text{ cm}^{-3}$ and $F_{\text{X}} = 5.1 \text{ ergs s}^{-1} \text{ cm}^{-2}$								
1.0E22 .....	3.0E12	3.3E12	4.3E13	1.1E15	6.0E12	0.07	13.2	181
2.0E22 .....	4.8E12	5.0E12	1.6E14	2.7E15	2.8E13	0.03	31.5	95.4
3.0E22 .....	5.7E12	5.9E12	2.7E14	4.7E15	5.9E13	0.02	46.4	78.9
XDR: $n = 10^{3.5} \text{ cm}^{-3}$ and $F_{\text{X}} = 1.6 \text{ ergs s}^{-1} \text{ cm}^{-2}$								
3.0E22 .....	1.2E12	5.7E11	1.5E12	5.2E13	3.2E10	0.8	2.6	1.6E3
6.0E22 .....	8.3E12	6.9E12	3.7E13	5.1E14	9.4E11	0.2	5.4	543
9.1E22 .....	1.8E13	1.5E13	1.3E14	1.5E15	3.8E12	0.14	8.5	400
PDR: $n = 10^5 \text{ cm}^{-3}$ , $G_0 = 10^{3.5}$ , and $\zeta = 5 \times 10^{15} \text{ s}^{-1}$								
1.0E22 .....	1.6E10	1.0E10	2.8E14	2.3E15	3.5E14	5.6E-5	2.8E4	6.6
2.0E22 .....	1.7E10	1.5E10	7.8E14	4.5E15	9.5E14	2.2E-5	5.2E4	4.7
3.0E22 .....	1.9E10	2.0E10	1.3E15	6.7E15	1.6E15	1.4E-5	6.5E4	4.3



# XDR vs. PDR



Spaans & Meijerink 2008

FINE-STRUCTURE ATOMIC COOLING PARAMETERS

Species (0, 1, 2) <sup>a</sup>	$\frac{E_{ji}}{k}$ (K) <sup>b</sup>	$\lambda_a^c$	$n_{cr}^e$ (cm <sup>-3</sup> ) <sup>d</sup>	$n_{cr}^H$ (cm <sup>-3</sup> ) <sup>d</sup>	$A_{ij}$ (s <sup>-1</sup> ) <sup>e</sup>	$\gamma_{ij}^e$ (cm <sup>-3</sup> s <sup>-1</sup> ) <sup>f</sup>	$\gamma_{ij}^H$ (cm <sup>3</sup> s <sup>-1</sup> ) <sup>f</sup>	$N_{\tau}$ (cm <sup>-2</sup> ) <sup>g</sup>
C I ( <sup>3</sup> P <sub>0</sub> , <sup>3</sup> P <sub>1</sub> , <sup>3</sup> P <sub>2</sub> ) .....	2.4(1)	609.2	3.9(0)T <sub>2</sub> <sup>-0.13</sup>	1.6(2)T <sub>2</sub> <sup>-0.34</sup>	7.9(-8)	3.0(-9)	1.6(-10)T <sub>2</sub> <sup>0.14</sup>	2.3(20)
	6.3(1)	229.9	1.3(1)	7.0(2)T <sub>2</sub> <sup>-0.26</sup>	2.0(-14)	5.0(-9)	9.2(-11)T <sub>2</sub> <sup>0.26</sup>	9.8(27)
	3.9(1)	369.0	...	...	2.7(-7)	1.5(-8)	2.9(-10)T <sub>2</sub> <sup>0.26</sup>	5.3(20)
C II ( <sup>2</sup> P <sub>1/2</sub> , <sup>2</sup> P <sub>3/2</sub> ) .....	9.2(1)	157.7	8.7(0)T <sub>2</sub> <sup>0.50</sup>	3.0(2)T <sub>2</sub> <sup>-0.07</sup>	2.4(-6)	2.8(-7)T <sub>2</sub> <sup>-0.5</sup>	8.0(-10)T <sub>2</sub> <sup>0.07</sup>	6.5(20)
Cl I ( <sup>2</sup> P <sub>3/2</sub> , <sup>2</sup> P <sub>1/2</sub> ) .....	1.3(3)	11.4	2.6(5)	1.4(7)T <sub>2</sub> <sup>-0.17</sup>	1.2(-2)	4.7(-8)	8.3(-10)T <sub>2</sub> <sup>0.17</sup>	1.1(24)
Cl II ( <sup>3</sup> P <sub>2</sub> , <sup>3</sup> P <sub>1</sub> , <sup>3</sup> P <sub>0</sub> ) .....	1.0(3)	14.4	1.4(4)T <sub>2</sub> <sup>0.45</sup>	5.4(6)	7.5(-3)	5.3(-7)T <sub>2</sub> <sup>-0.5</sup>	1.4(-9)	7.5(23)
	1.4(3)	10.0	1.6(3)T <sub>2</sub> <sup>0.50</sup>	8.1(5)	4.8(-7)	5.3(-7)T <sub>2</sub> <sup>-0.5</sup>	1.1(-9)	1.0(29)
	4.3(2)	33.4	...	...	1.4(-3)	3.2(-7)T <sub>2</sub> <sup>-0.5</sup>	6.3(-10)	5.7(23)
Fe I ( <sup>5</sup> D <sub>4</sub> , <sup>5</sup> D <sub>3</sub> , <sup>5</sup> D <sub>2</sub> ) .....	6.0(2)	24.0	2.1(4)T <sub>2</sub> <sup>-0.13</sup>	3.1(6)T <sub>2</sub> <sup>-0.28</sup>	2.5(-3)	1.2(-7)	8.0(-10)T <sub>2</sub> <sup>0.17</sup>	6.6(21)
	1.0(3)	14.2	7.5(3)	1.3(6)T <sub>2</sub> <sup>-0.17</sup>	1.0(-9)	1.2(-7)	6.9(-10)T <sub>2</sub> <sup>0.17</sup>	9.3(26)
	4.2(2)	34.2	...	...	1.6(3)	9.3(-8)	5.3(-10)T <sub>2</sub> <sup>0.17</sup>	3.7(21)
Fe II ( <sup>6</sup> D <sub>9/2</sub> , <sup>6</sup> D <sub>7/2</sub> , <sup>6</sup> D <sub>5/2</sub> ) ..	5.6(2)	26.0	1.2(3)T <sub>2</sub> <sup>0.41</sup>	2.2(6)T <sub>2</sub> <sup>-0.09</sup>	2.1(-3)	1.8(-6)T <sub>2</sub> <sup>-0.5</sup>	9.5(-10)	6.0(21)
	9.6(2)	15.0	6.0(2)T <sub>2</sub> <sup>0.50</sup>	1.5(6)	1.5(-9)	1.8(-6)T <sub>2</sub> <sup>-0.5</sup>	5.7(-10)	5.9(28)
	4.1(2)	35.4	...	...	1.6(-3)	8.7(-7)T <sub>2</sub> <sup>-0.5</sup>	4.7(-10)	3.3(21)
Ne II ( <sup>2</sup> P <sub>3/2</sub> , <sup>2</sup> P <sub>1/2</sub> ) .....	1.1(3)	12.8	5.4(4)T <sub>2</sub> <sup>0.50</sup>	6.6(6)	8.6(-3)	1.6(-7)T <sub>2</sub> <sup>-0.5</sup>	1.3(-9)	1.9(22)
Ni I ( <sup>3</sup> F <sub>4</sub> , <sup>3</sup> F <sub>3</sub> , <sup>3</sup> F <sub>2</sub> ) .....	1.9(3)	7.5	5.2(5)T <sub>2</sub> <sup>-0.06</sup>	7.8(7)T <sub>2</sub> <sup>-0.22</sup>	6.2(-2)	1.2(-7)	8.0(-10)T <sub>2</sub> <sup>0.17</sup>	1.1(23)
	3.2(3)	4.5	1.2(5)	2.0(7)T <sub>2</sub> <sup>0.17</sup>	3.6(-9)	1.2(-7)	6.9(-10)T <sub>2</sub> <sup>0.17</sup>	1.3(31)
	1.3(3)	11.3	...	...	2.5(-2)	9.3(-8)	5.3(-10)T <sub>2</sub> <sup>0.17</sup>	8.9(22)
Ni II ( <sup>2</sup> D <sub>5/2</sub> , <sup>2</sup> D <sub>3/2</sub> ) .....	2.2(3)	6.6	5.0(4)T <sub>2</sub> <sup>0.50</sup>	5.0(7)	5.5(-2)	1.1(-6)T <sub>2</sub> <sup>-0.5</sup>	1.1(-9)	2.2(23)
O I ( <sup>3</sup> P <sub>2</sub> , <sup>3</sup> P <sub>1</sub> , <sup>3</sup> P <sub>0</sub> ) .....	2.3(2)	63.1	6.3(3)T <sub>2</sub> <sup>-0.03</sup>	8.5(5)T <sub>2</sub> <sup>-0.69</sup>	9.0(-5)	1.4(-8)	9.2(-11)T <sub>2</sub> <sup>0.67</sup>	4.9(20)
	3.3(2)	44.2	8.9(2)	1.1(5)T <sub>2</sub> <sup>-0.57</sup>	1.0(-10)	1.4(-8)	4.3(-11)T <sub>2</sub> <sup>0.80</sup>	3.8(27)
	9.8(1)	145.6	...	...	1.7(-5)	5.0(-9)	1.1(-10)T <sub>2</sub> <sup>0.44</sup>	3.7(20)
Si I ( <sup>3</sup> P <sub>2</sub> , <sup>3</sup> P <sub>1</sub> , <sup>3</sup> P <sub>0</sub> ) .....	5.7(2)	25.2	4.2(4)T <sub>2</sub> <sup>-0.03</sup>	1.8(6)T <sub>2</sub> <sup>-0.22</sup>	1.4(-3)	3.3(-8)	7.5(-10)T <sub>2</sub> <sup>0.17</sup>	2.0(22)
	8.2(2)	17.4	6.7(3)	2.7(5)T <sub>2</sub> <sup>-0.17</sup>	7.1(-8)	3.3(-8)	7.1(-10)T <sub>2</sub> <sup>0.17</sup>	3.7(27)
	2.5(2)	56.6	...	...	3.0(-4)	1.2(-8)	4.2(-10)T <sub>2</sub> <sup>0.17</sup>	1.5(22)
Si II ( <sup>3</sup> P <sub>0</sub> , <sup>3</sup> P <sub>1</sub> , <sup>3</sup> P <sub>2</sub> ) .....	1.1(2)	129.6	7.2(2)T <sub>2</sub> <sup>-0.50</sup>	1.9(4)T <sub>2</sub> <sup>-0.47</sup>	8.4(-6)	7.2(-9)	3.5(-10)T <sub>2</sub> <sup>-0.03</sup>	2.3(21)
	3.2(2)	44.8	1.4(3)	6.3(4)T <sub>2</sub> <sup>-0.17</sup>	2.4(-10)	7.2(-9)	1.7(-10)T <sub>2</sub> <sup>0.17</sup>	2.0(27)
	2.1(2)	68.4	...	...	4.2(-5)	2.2(-8)	5.0(-10)T <sub>2</sub> <sup>0.17</sup>	5.6(21)
Si II ( <sup>2</sup> P <sub>1/2</sub> , <sup>2</sup> P <sub>3/2</sub> ) .....	4.1(2)	34.8	1.2(2)T <sub>2</sub> <sup>0.50</sup>	3.2(5)	2.1(-4)	1.7(-6)T <sub>2</sub> <sup>-0.5</sup>	8.0(-10)T <sub>2</sub> <sup>-0.07</sup>	7.1(21)

<sup>a</sup> The levels are arranged as follows: 0 = ground state, 1 = first excited state, and 2 = second excited state.

<sup>b</sup> For three-level systems, the energies listed are  $E_{10}$ ,  $E_{20}$ , and  $E_{21}$ , respectively.

<sup>c</sup> The wavelength in microns; note that the 2→0 transition is generally forbidden.

<sup>d</sup> The critical densities (see text) are listed to achieve LTE in levels 1 and 2, respectively,  $T_2 = T/100$  K. The power law fits for the three level systems are accurate to 30% in the temperature range  $30 \text{ K} < T < 3000 \text{ K}$ .

<sup>e</sup> The spontaneous transition rates listed in order  $A_{10}$ ,  $A_{20}$ , and  $A_{21}$ . These are taken from Aller (1984), Garstang 1958, 1962, 1964, 1968; Grevesse, Nussbaumer, and Swings 1971; and Wiese et al. 1966, 1969.

<sup>f</sup> The rate coefficients for collisional deexcitation are listed in the same order. They are calculated from formulae given by Bahcall and Wolf 1968 with the exceptions C I and O I (Launay and Roueff 1977a), C II (Launay and Roueff 1977b), Fe II (Aannestad 1973), Ne II (Osterbrock 1974). Proton rates are substituted for electron rates for neutral target atoms.

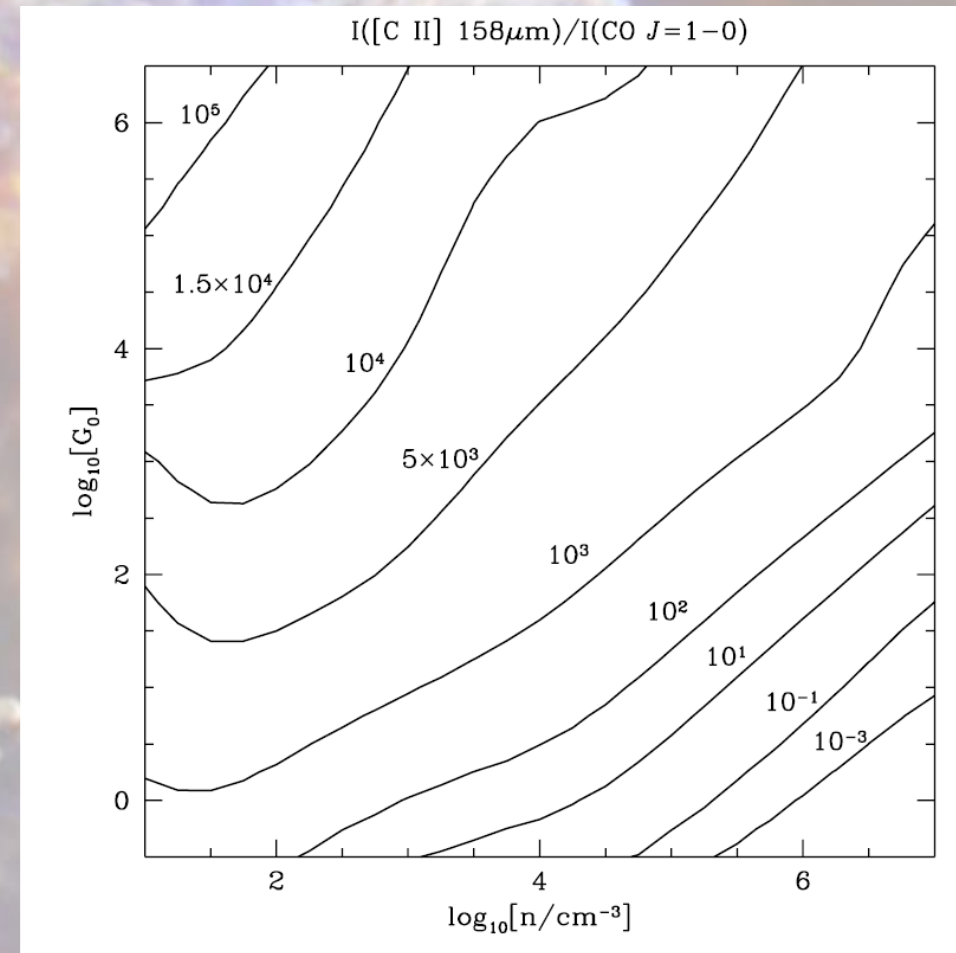
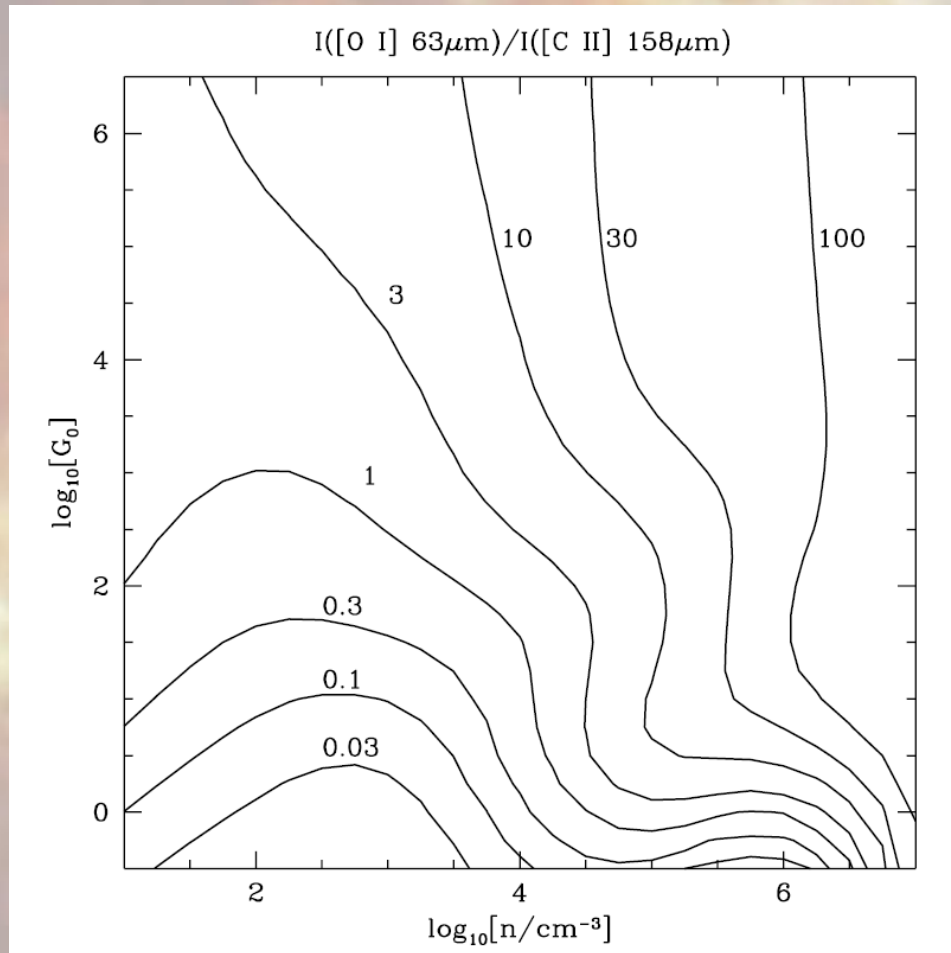
<sup>g</sup>  $N_{\tau}$  is the column density of hydrogen nuclei which provide unit optical depth at line center, assuming solar abundances of the species in the lower state of the transition.

Hollenbach & Mckee, 1989, ApJ 342, 306



# PDR Diagnostics

Kaufmann et al. 1999



# PDR Diagnostics

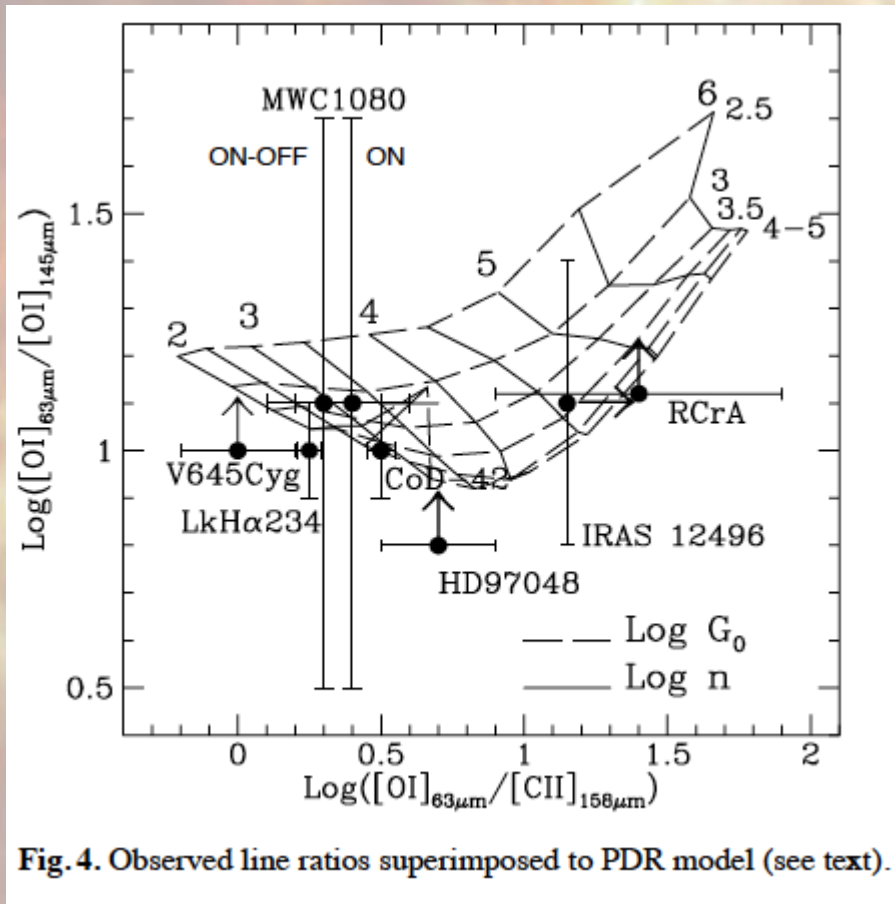
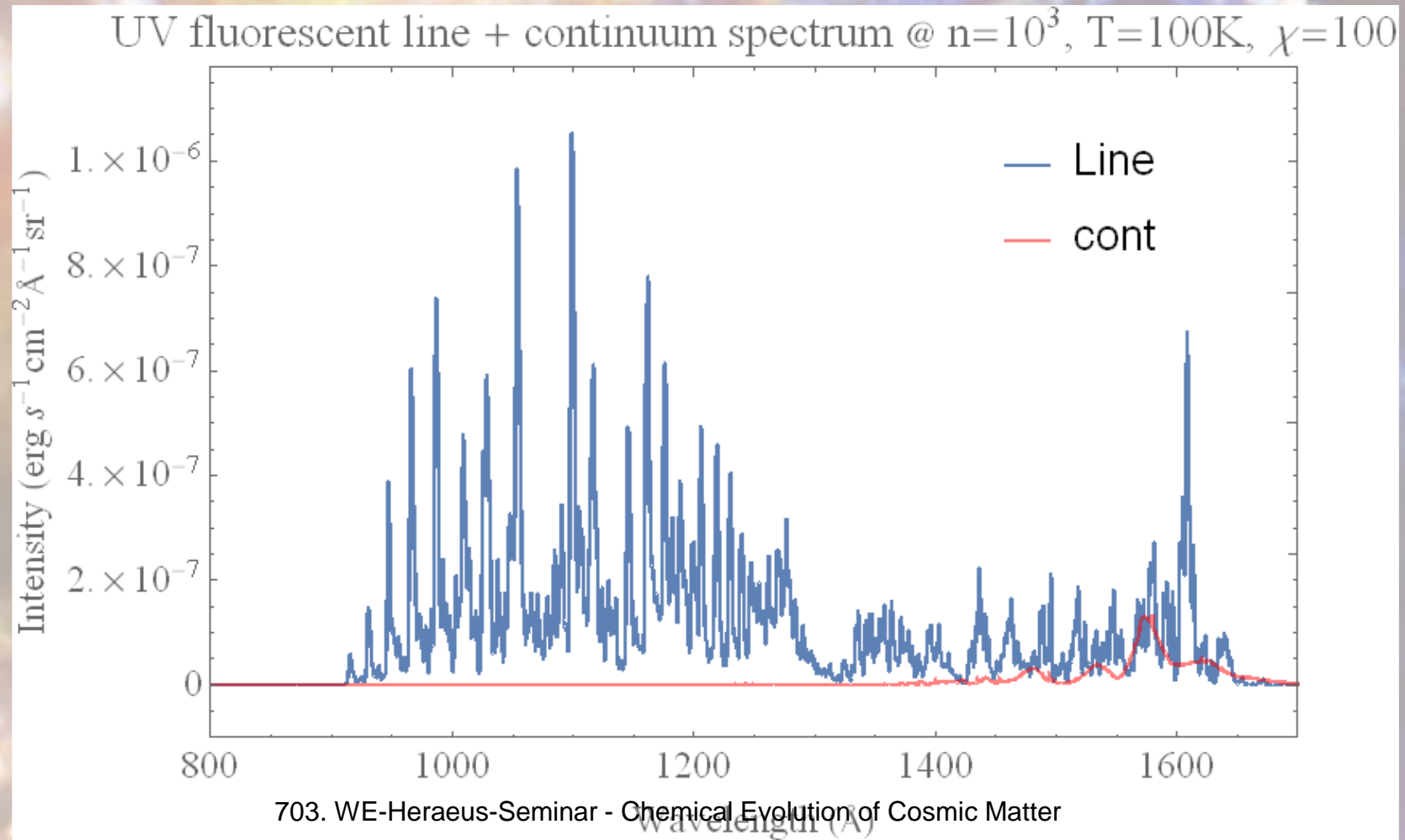


Fig. 4. Observed line ratios superimposed to PDR model (see text).

- Absolute intensities always involve an (unknown) filling factor
- Lorenzetti et al (1999) used the  $[\text{OI}]_{63\mu\text{m}}/[\text{CII}]_{157\mu\text{m}}$  and  $[\text{OI}]_{63\mu\text{m}}/[\text{OI}]_{145\mu\text{m}}$  intensity ratios to derive the physical conditions of the PDRs associated with Herbig Ae/Be stars based on ISO data.

# Fluorescent UV spectrum of H<sub>2</sub> + cont.

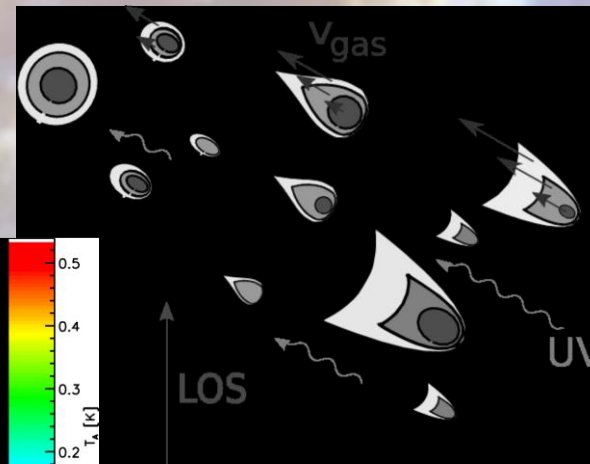
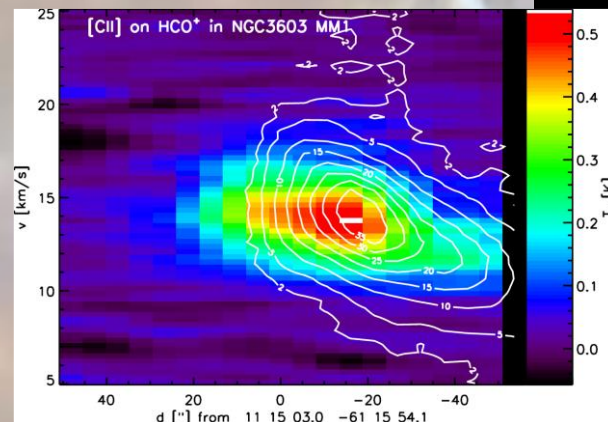
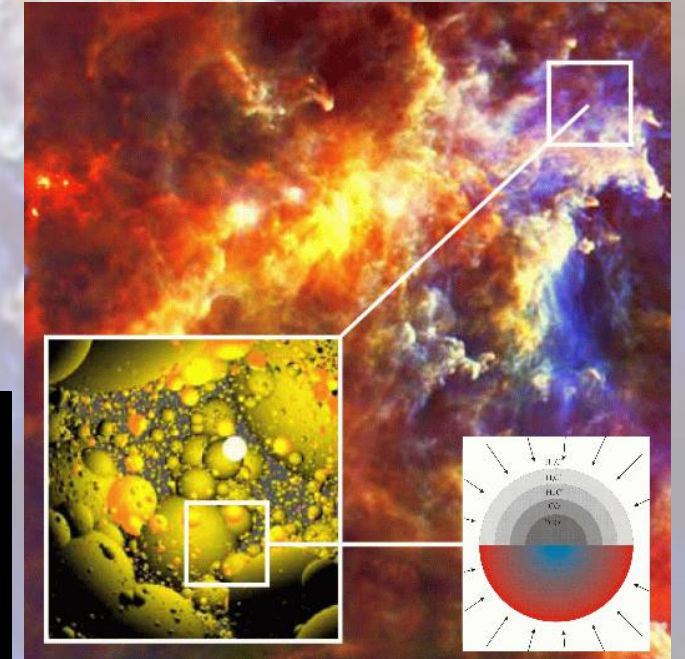
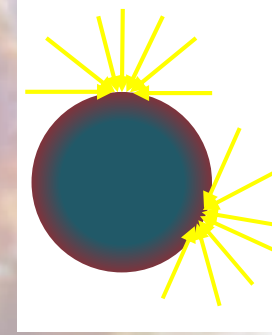
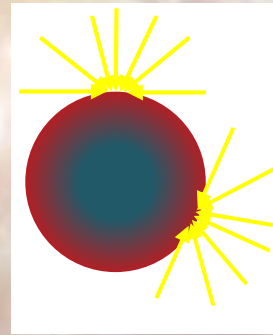
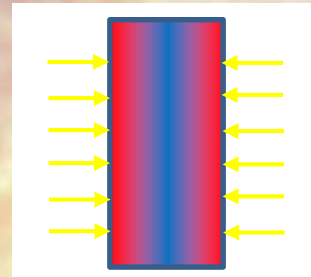
Low density, low UV, low Temp. → only ground state populated





# Physical structure

- Temperature
  - heating
  - cooling
- Density
- Geometry
- Dynamics

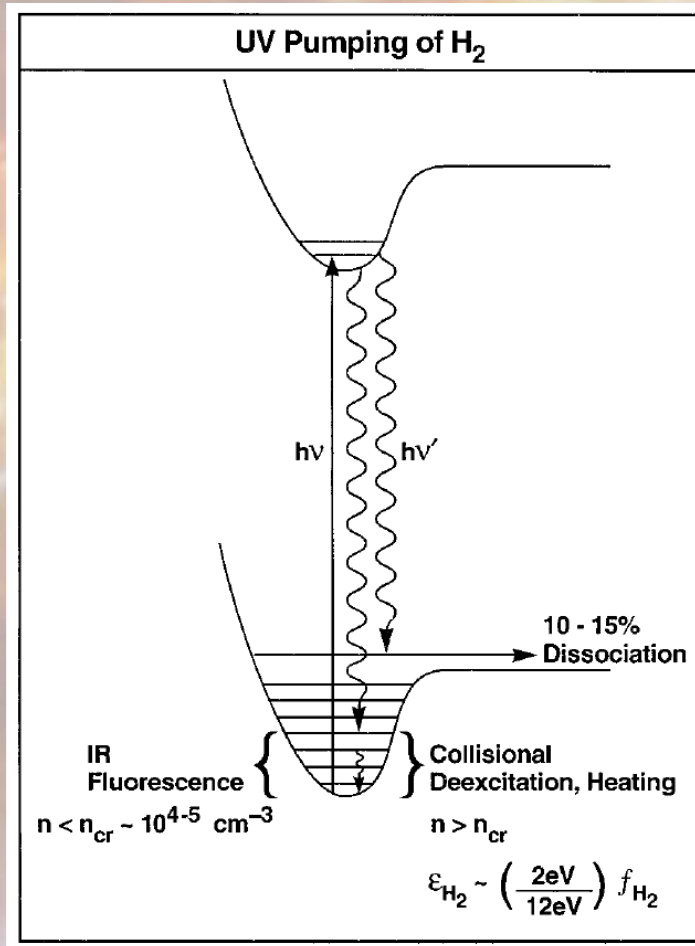


# Gas heating

1. FUV photons
  1. Photoelectric heating
  2. vibrational deexcitation of electronically pumped  $\text{H}_2$
  3.  $\text{H}_2$  formation heating
  4. gas-grain collisions
  5. photodissociation of  $\text{H}_2$
  6. ionization of atomic carbon
2. Cosmic rays/X-rays
3. Shocks
4. Turbulence



# H<sub>2</sub> pumping



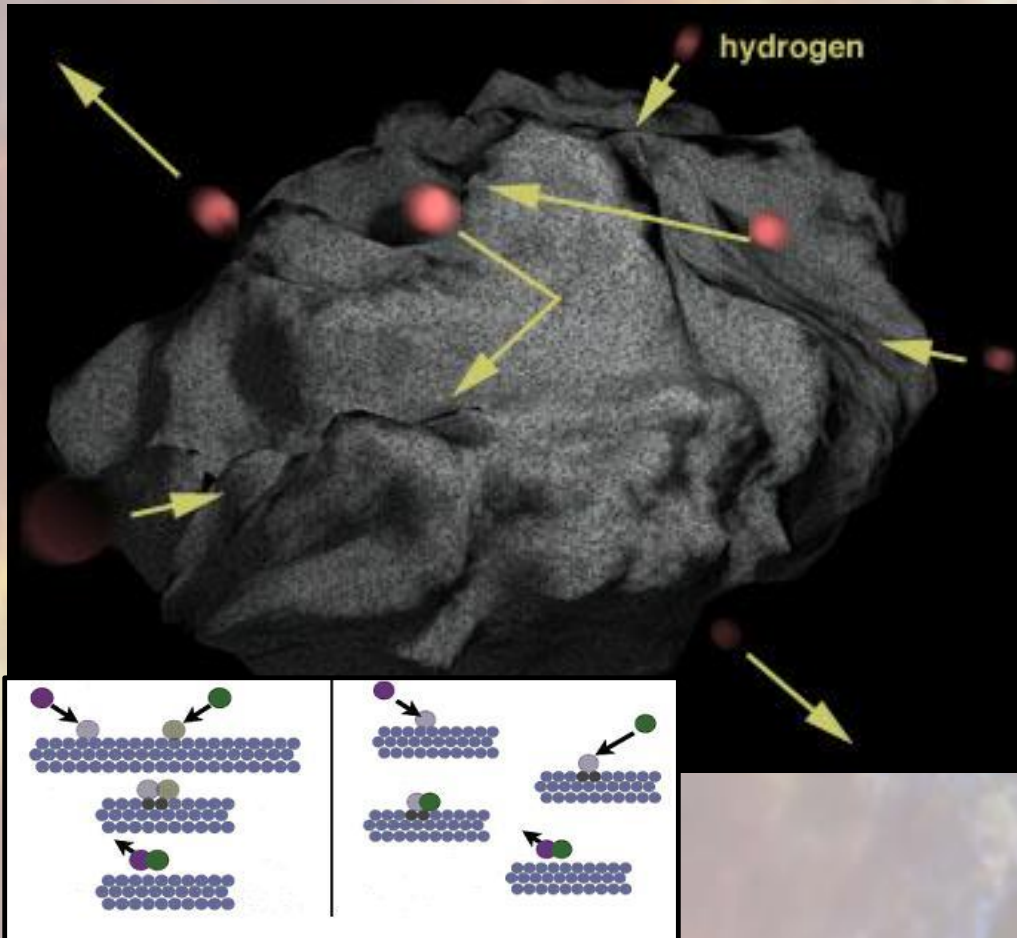
Tielens & Hollenbach 1999

- line absorption of FUV photons pumps electronically excited state (Lyman, Werner bands)
  - 10-15 % fluoresce back to vib. continuum of the ground el. state → photo-dissociation
  - 85-90 % fall back to bound vib. states of the el. ground state  
→  $E_{\text{vib}} \sim 2 \text{ eV}$  available for heating
- efficient at high densities

$$n\Gamma_{H_2} \simeq 2.9 \times 10^{-11} n n_H k_d \left[ 1 + \left( \frac{n_{cr}}{n} \right) + \frac{4.4 \times 10^2 G_0}{n T^{1/2} \exp[-1000/T]} \right]^{-1} \text{ erg cm}^{-3} \text{ s}^{-1}$$



# H<sub>2</sub> formation heating



- H<sub>2</sub> forms on dust surfaces
- binding energy of H<sub>2</sub> ~ 4.5 eV
- newly formed H<sub>2</sub> molecules are released into the gas-phase and carry away part of the binding energy as kinetic and internal energy  
→ heating via collisions

$$\Gamma_{\text{H}_2 \text{ form}} = 2.4 \times 10^{-12} R_{\text{H}_2 \text{ form}} n_{\text{H}} \text{ erg cm}^{-3} \text{ s}^{-1}$$

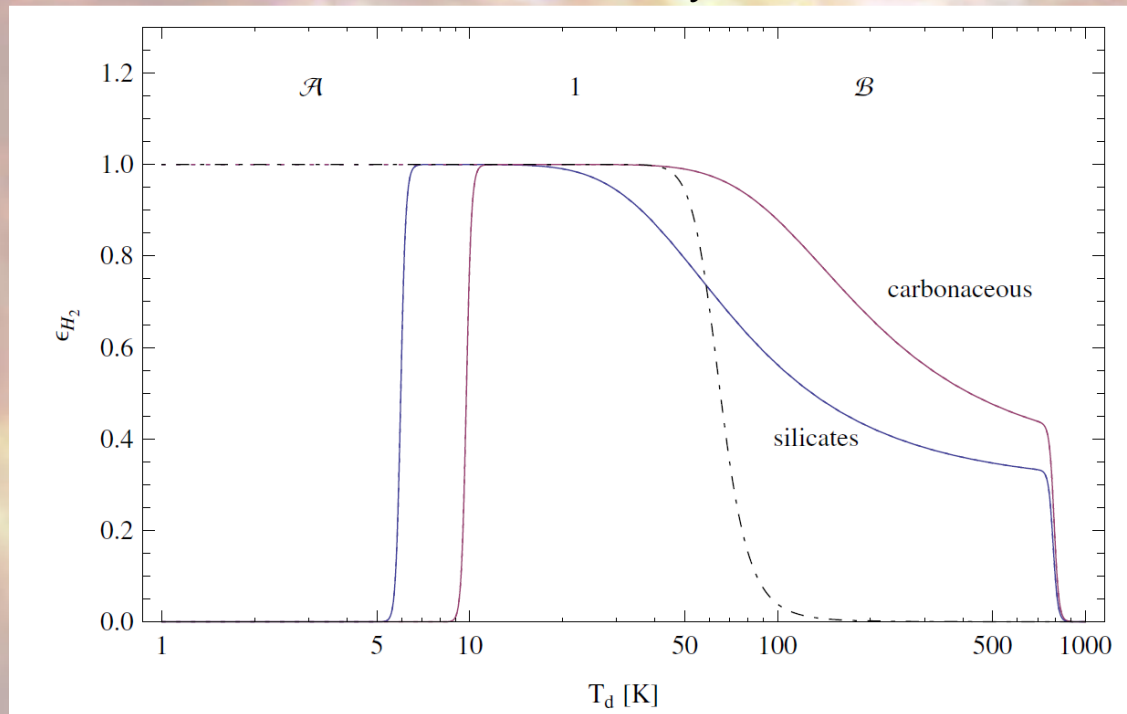
$R_{\text{H}_2 \text{ form}}$ : H<sub>2</sub> formation rate

Langmuir-Hinshelwood

Eley-Rideal

# H<sub>2</sub> formation heating

formation efficiency



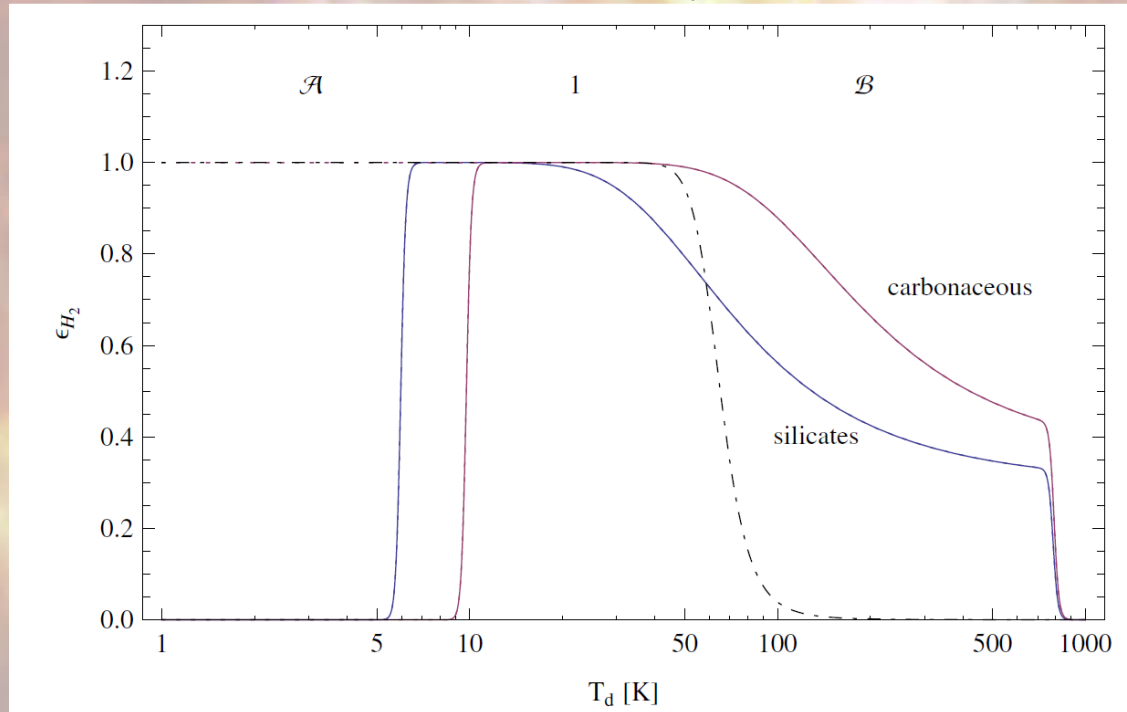
Cazaux & Tielens (2002, 2010)

Chemisorption leads to efficient H<sub>2</sub> formation at high temperatures

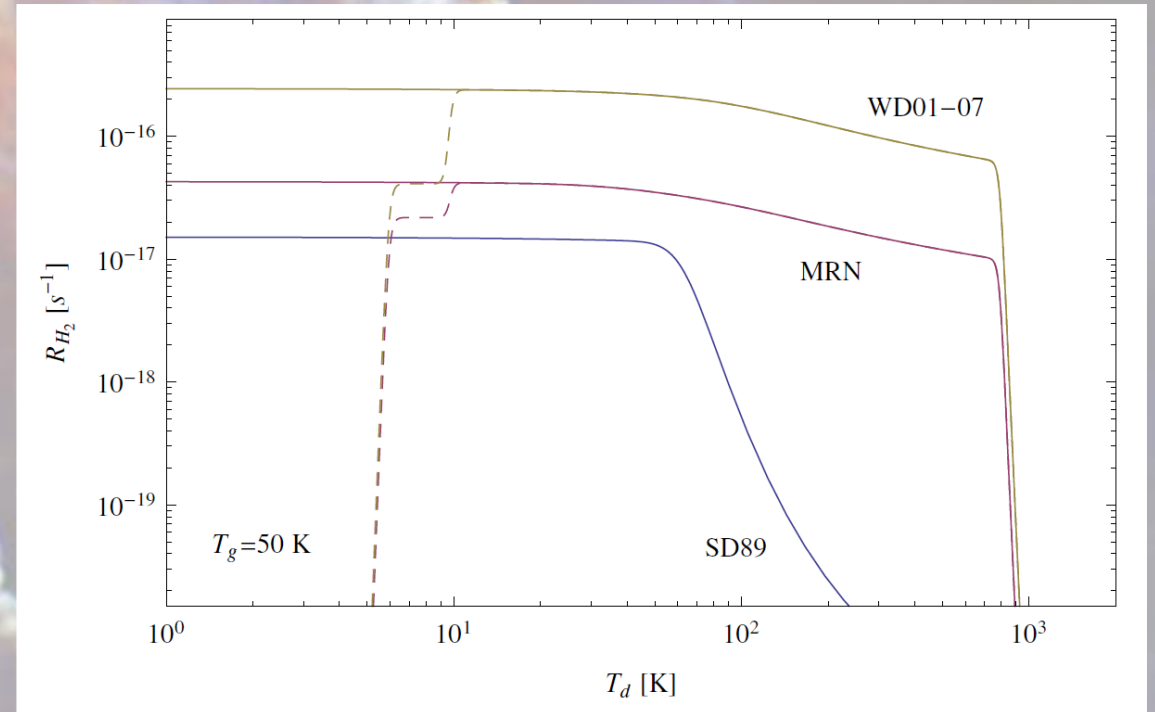
- H-binding to the grain surface determines its mobility and resistance against thermal desorption
  - weak binding (physisorption),  $T < 50\text{-}80\text{K}$
  - strong binding (chemisorption),  $T < \sim 500\text{-}800\text{K}$

# H<sub>2</sub> formation heating

formation efficiency



formation rate



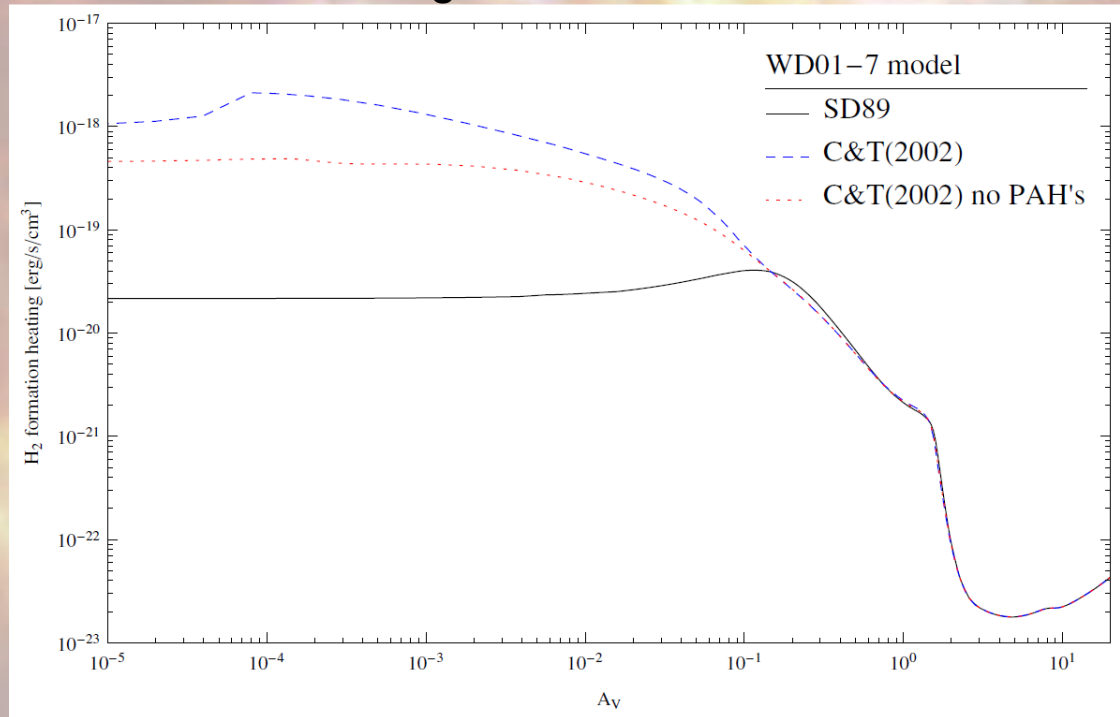
Cazaux & Tielens (2002,2010)

Chemisorption leads to efficient H<sub>2</sub> formation at high temperatures

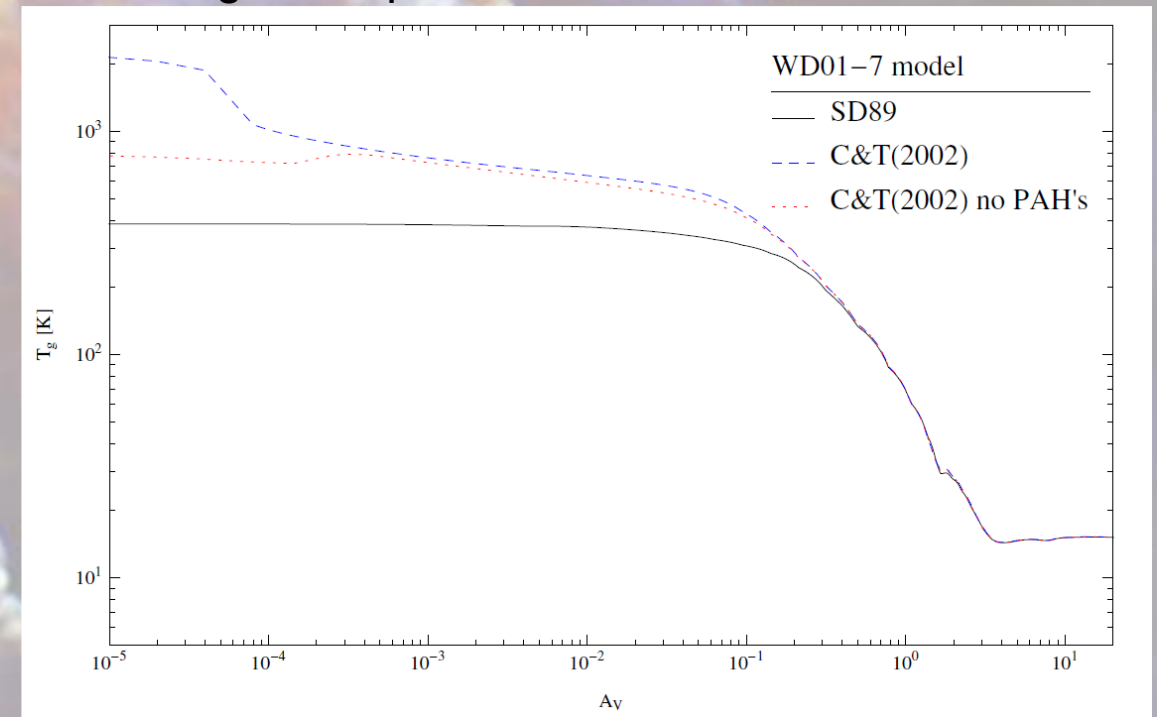


# H<sub>2</sub> formation heating

heating rate



gas temperature

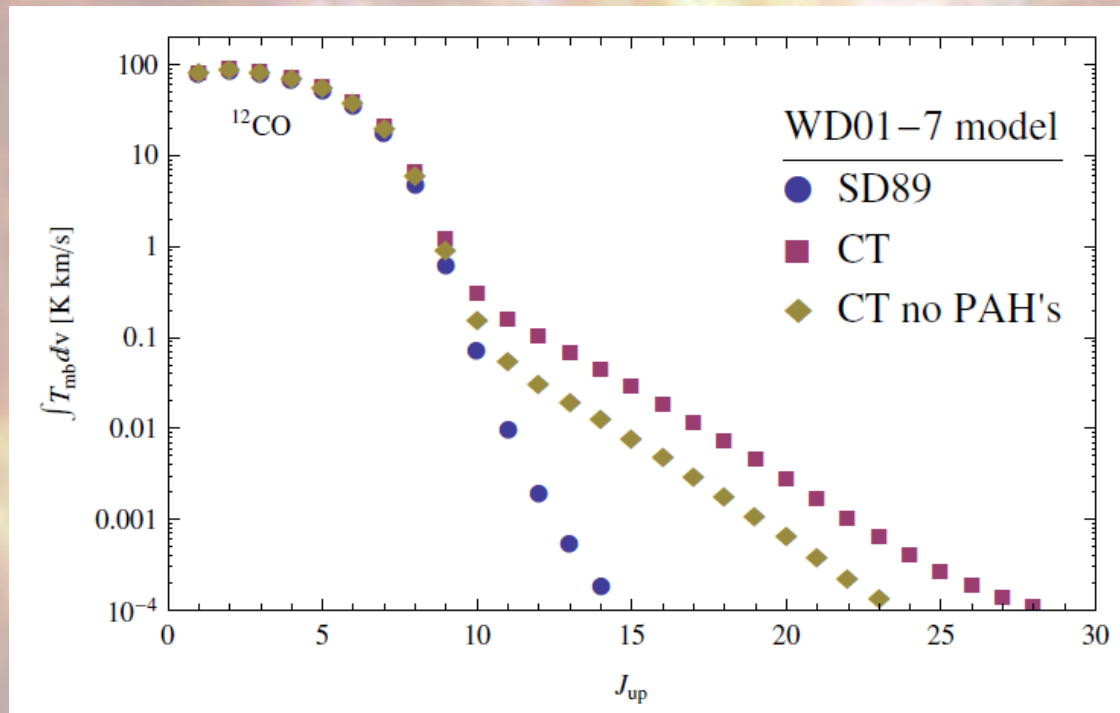


More efficient H<sub>2</sub> formation leads to stronger gas heating.

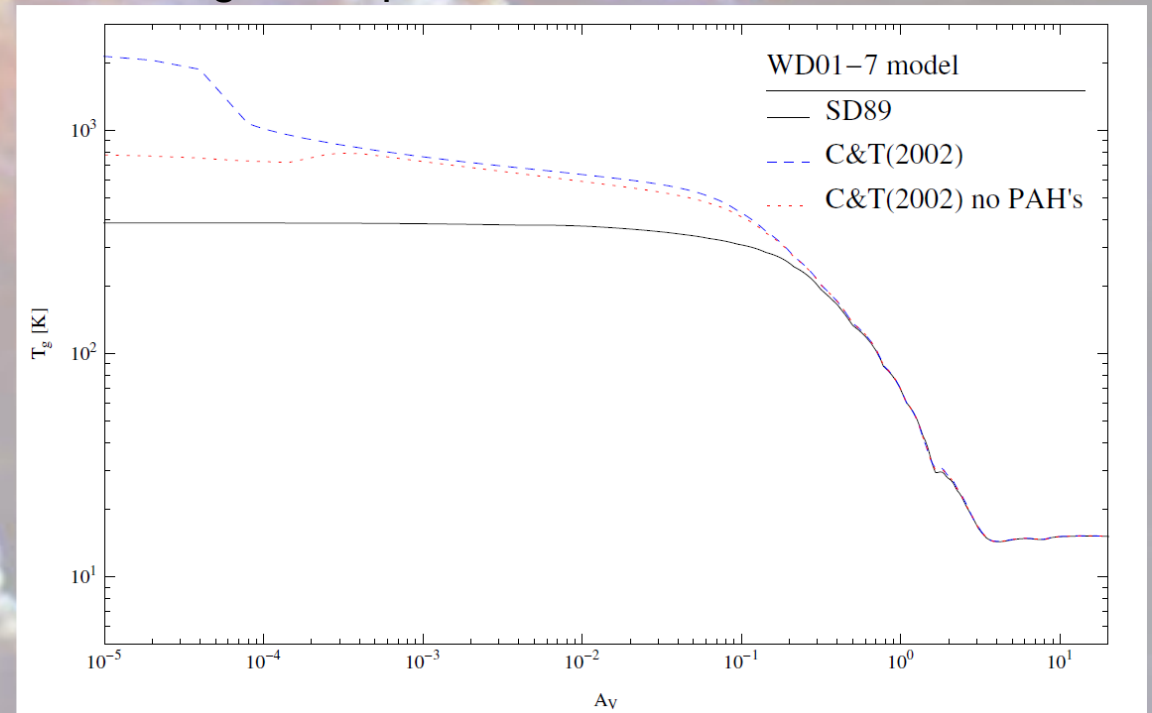
Röllig et al. 2013

# H<sub>2</sub> formation heating

CO line emission



gas temperature



Dust content & physics influences high-J CO emission

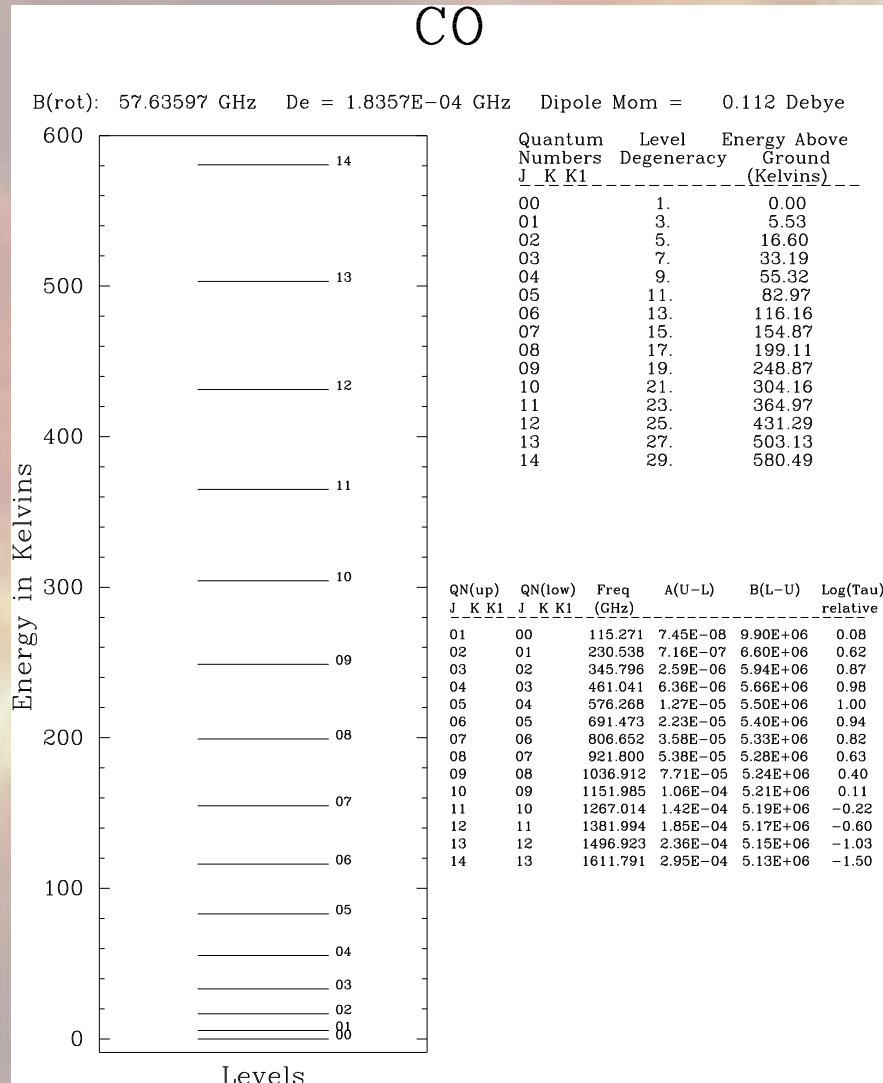
Röllig et al. 2013

# Radiative line cooling

- When a transition of a species is excited collisionally and decays radiatively, the transition energy is carried away by photons and the gas is cooled.
- Coolant conditions:
  - abundant
  - collisionally excitable energy levels given ISM conditions
  - rapid decay times (large  $A_{ij}$ )
- Good coolants:  
C<sup>+</sup>, O, C, CO, H<sub>2</sub>O



# Radiative line cooling



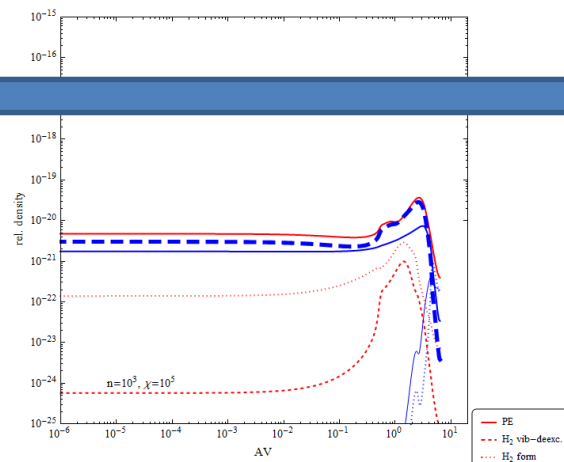
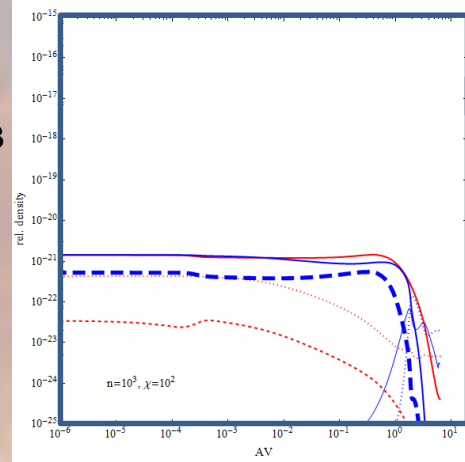
- When a transition of a species is excited collisionally and decays radiatively, the transition energy is carried away by photons and the gas is cooled.
- Coolant conditions:
  - abundant
  - collisionally excitable energy levels given ISM conditions
  - rapid decay times (large  $A_{ij}$ )
- Good coolants:  $C^+$ , O, C, CO,  $H_2O$

# PDR heating/cooling

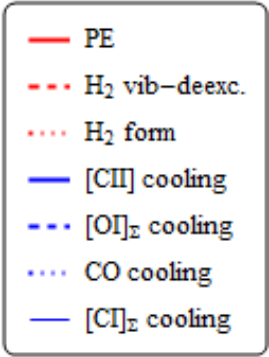
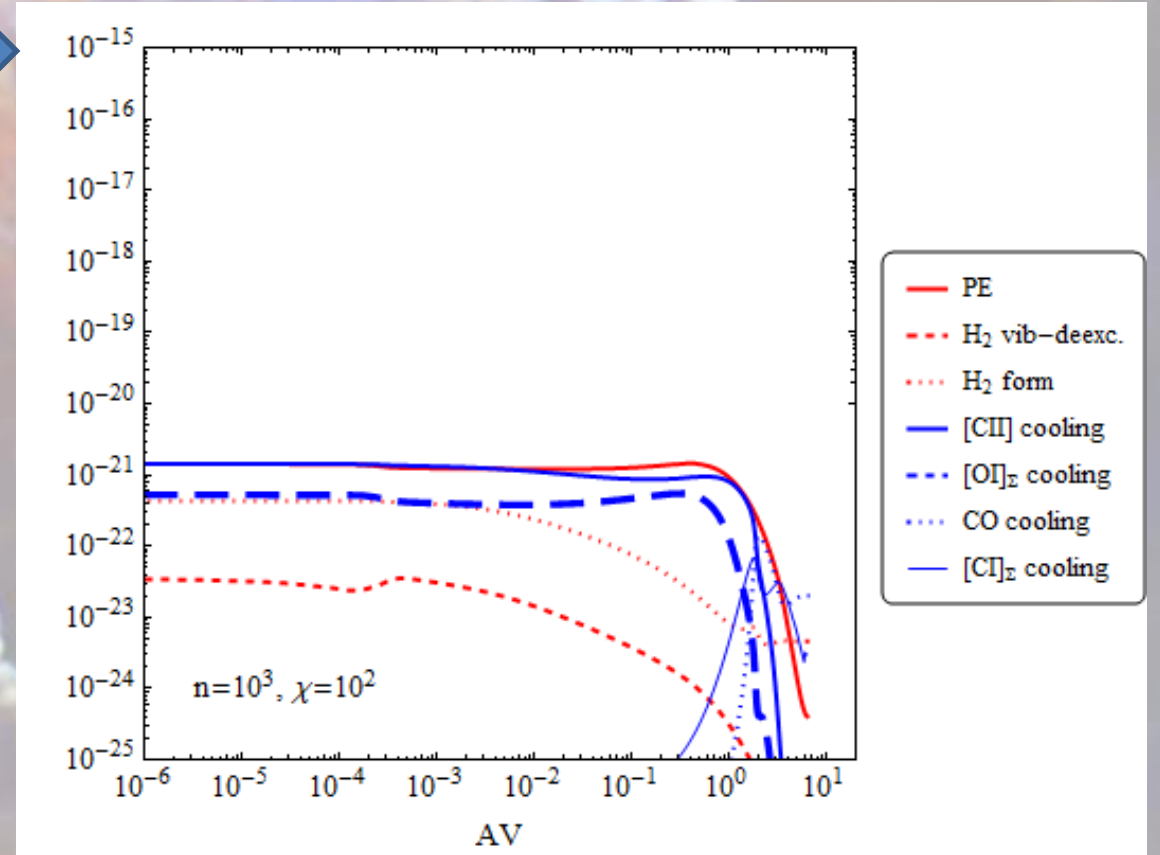
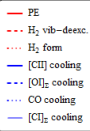
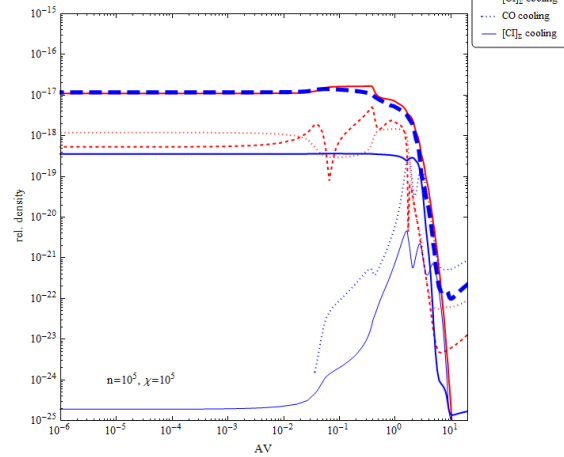
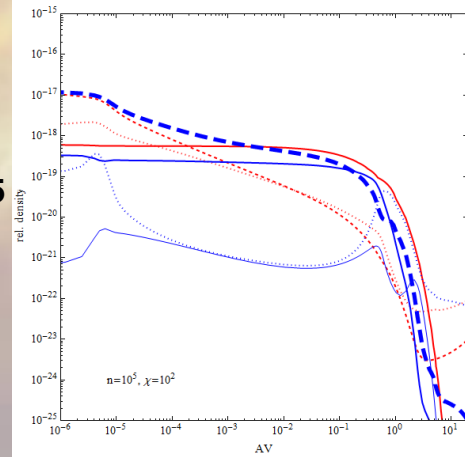
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$\chi=10^5$

$n=10^3$



$n=10^5$

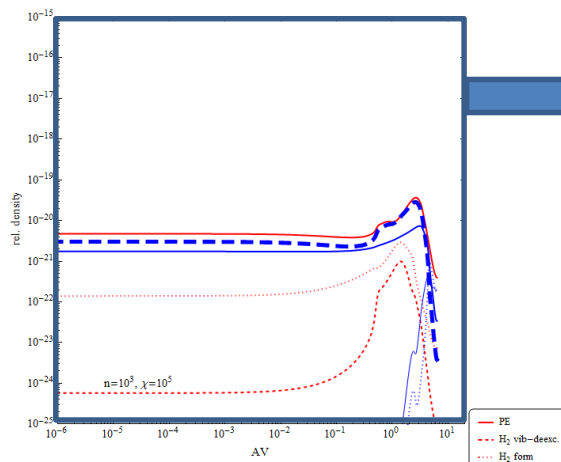
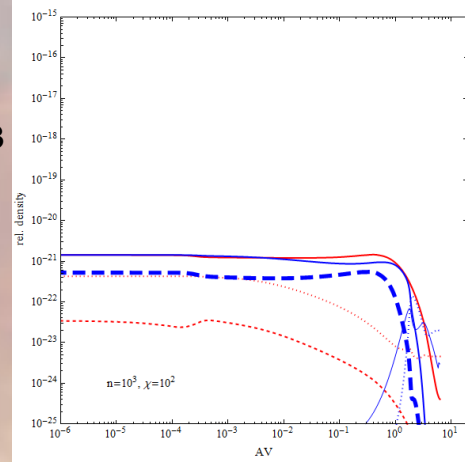


# PDR heating/cooling

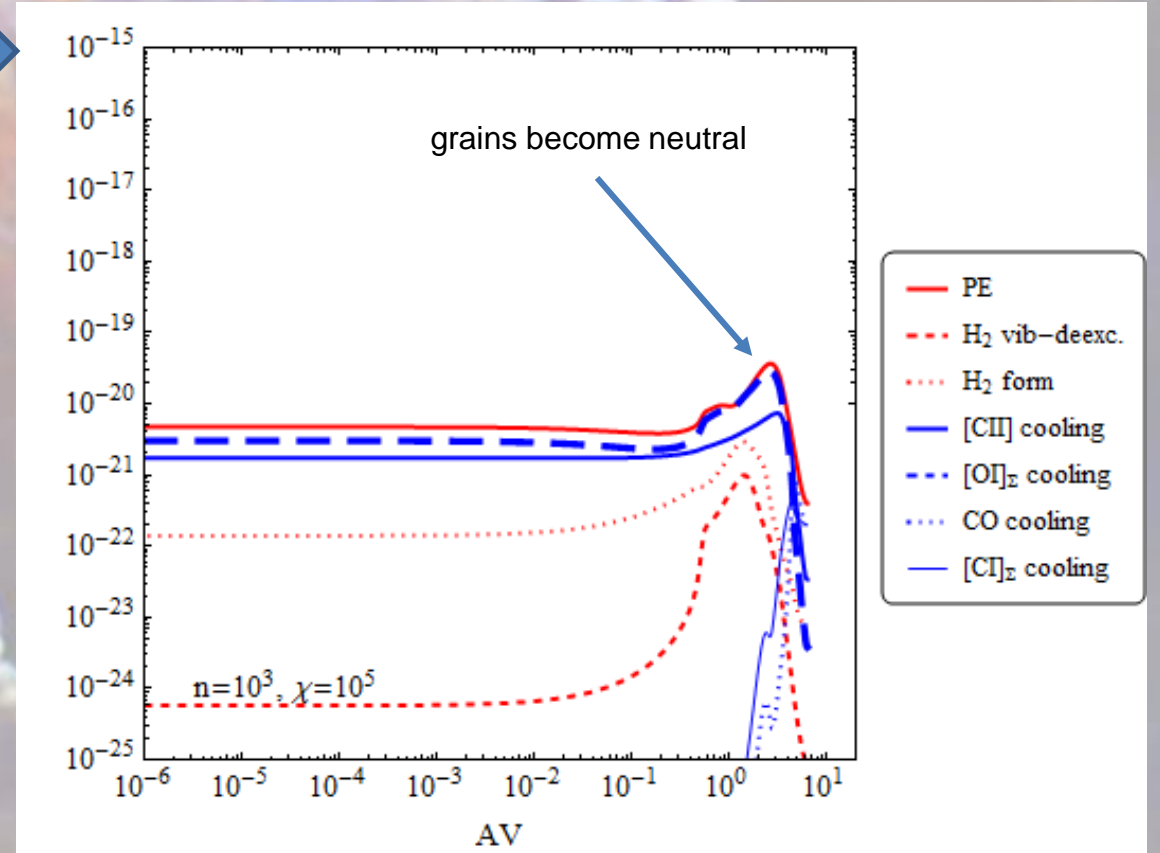
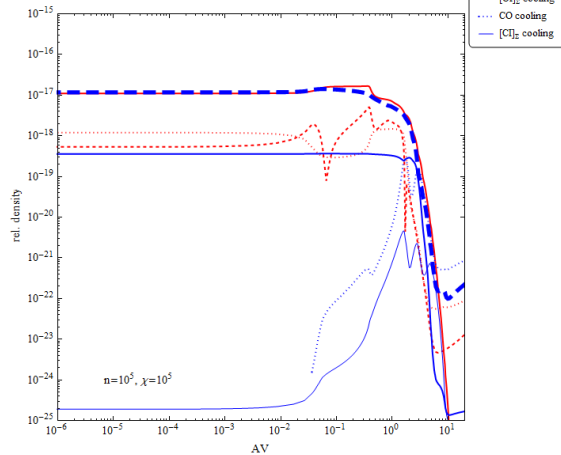
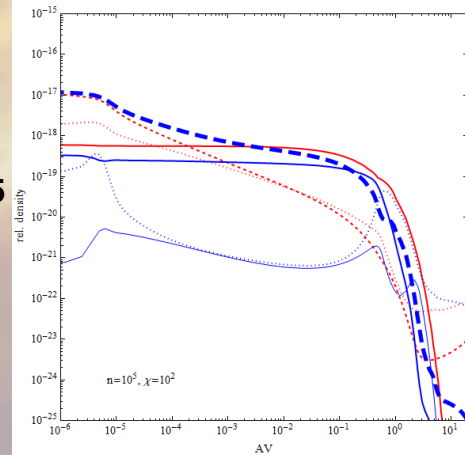
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$\chi=10^5$

$n=10^3$



$n=10^5$



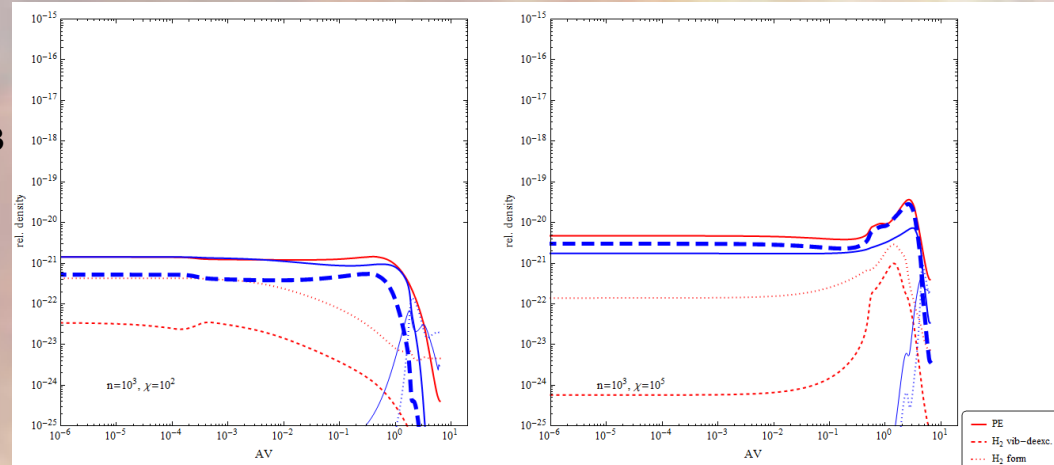


# PDR heating/cooling

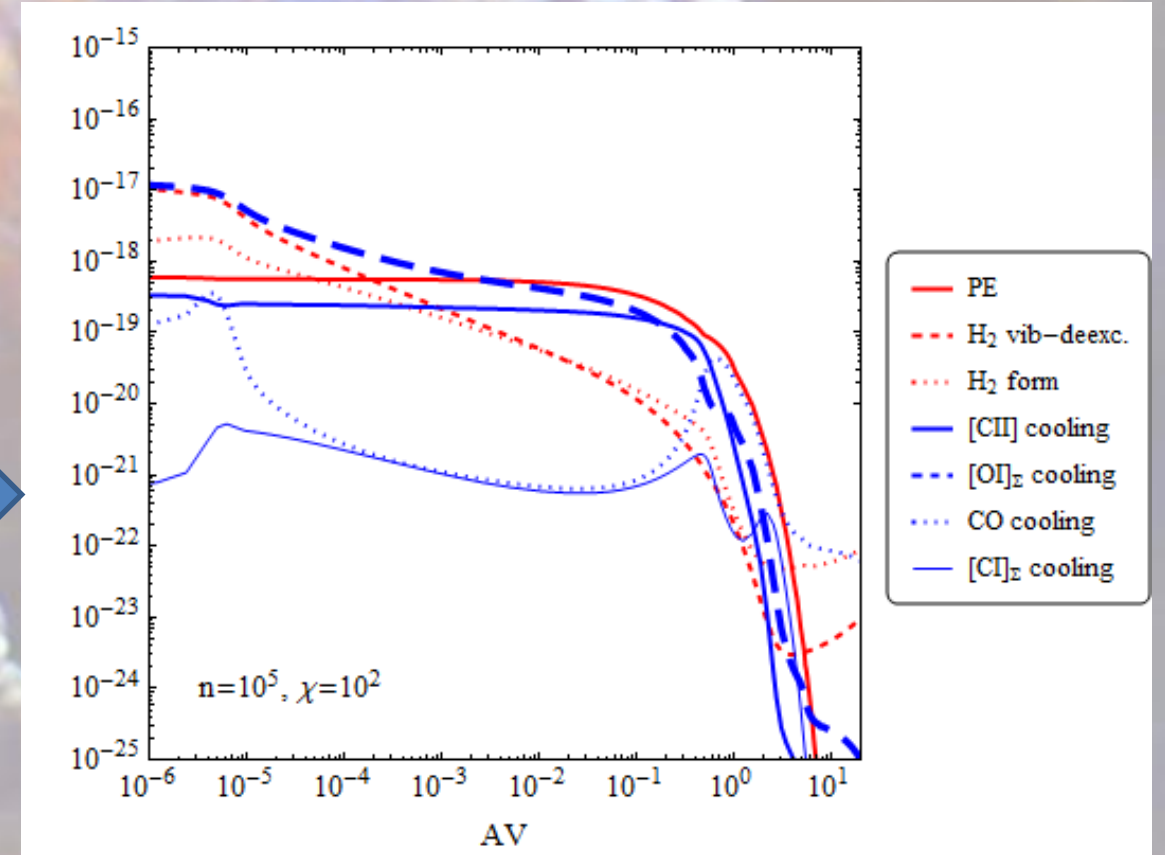
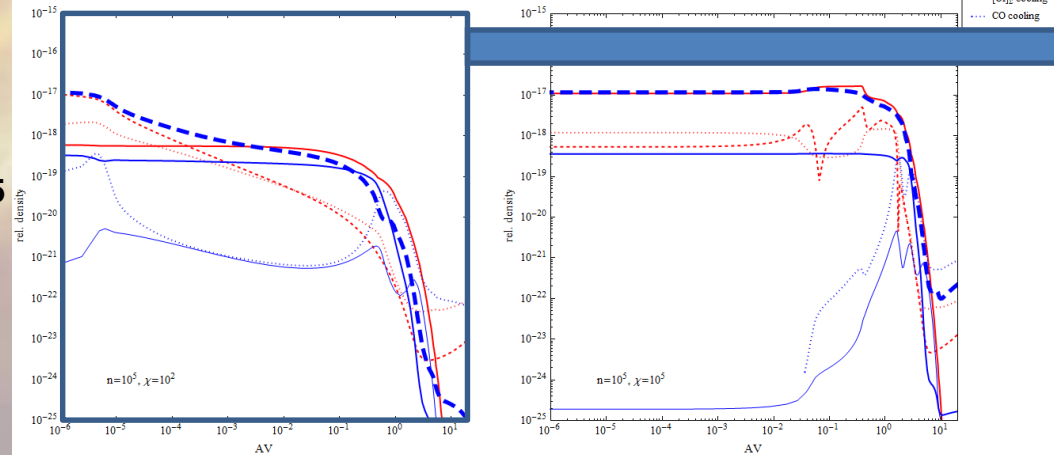
$\chi=100$

$\chi=10^5$

$n=10^3$



$n=10^5$

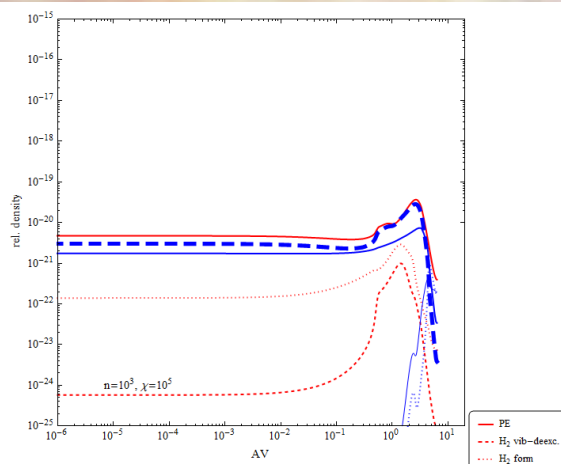
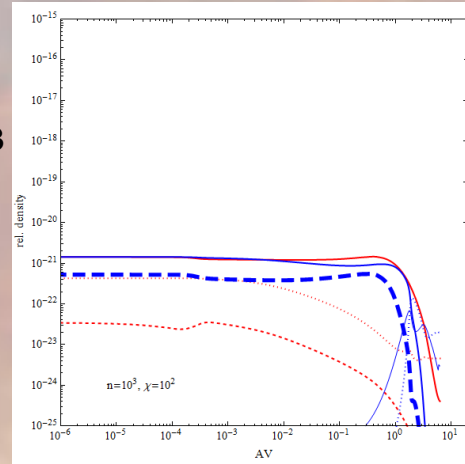


# PDR heating/cooling

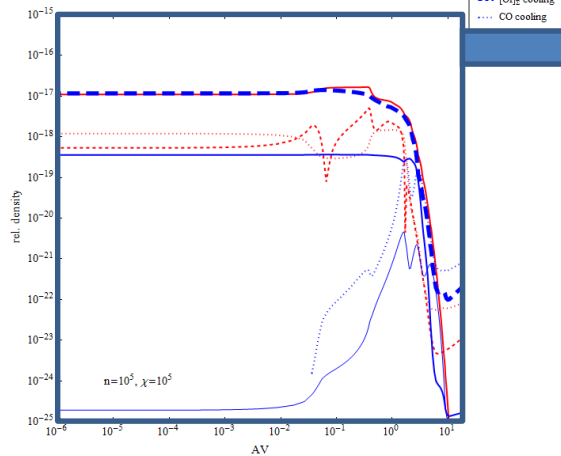
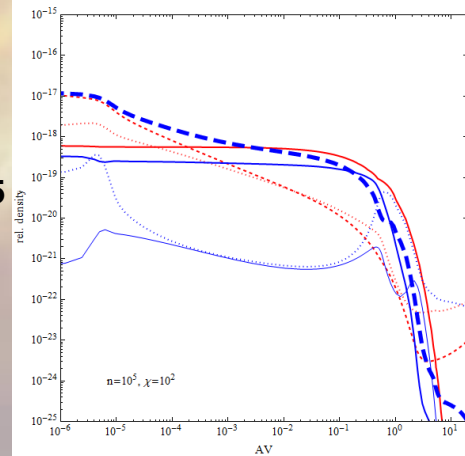
$\chi=100$

$\chi=10^5$

$n=10^3$



$n=10^5$



- PE
- - - H<sub>2</sub> vib-deexc.
- ... H<sub>2</sub> form
- [CII] cooling
- - - [OI]<sub>2</sub> cooling
- ... CO cooling

