



PDR Modelling

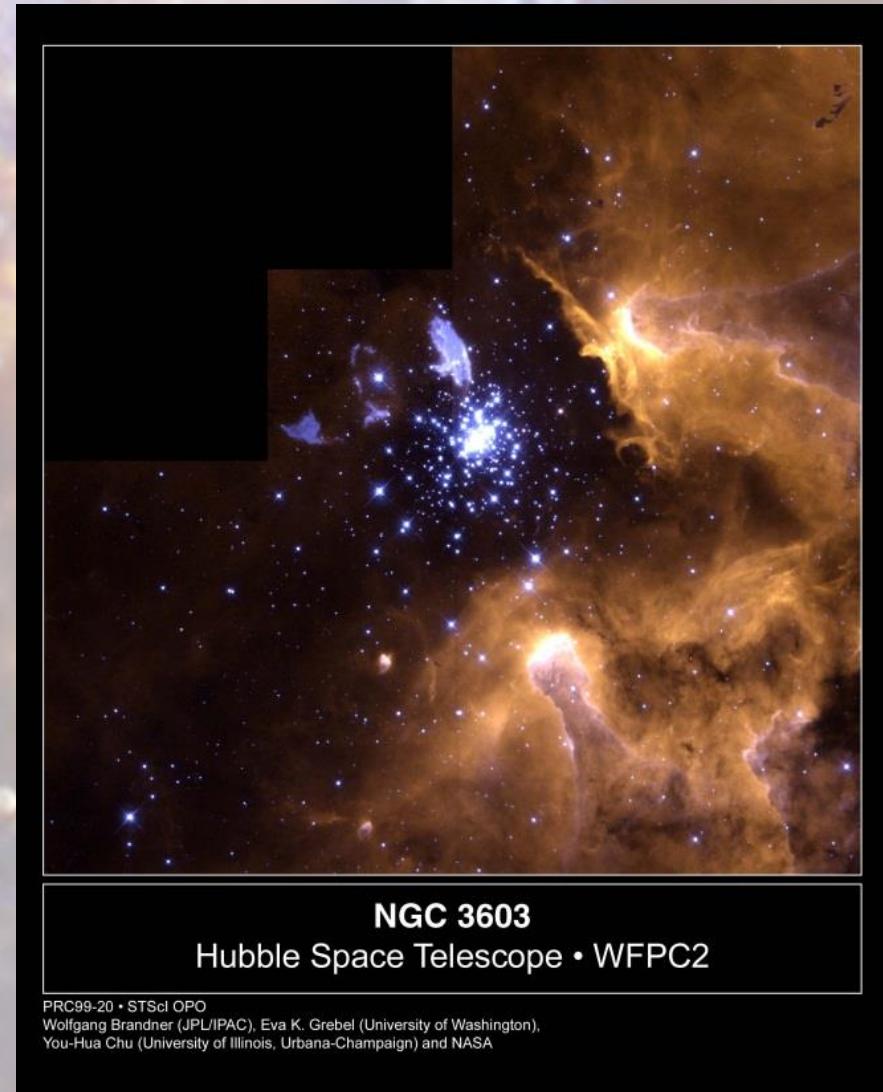
M. Röllig

I. Physikalisches Institut, Universität zu Köln



Introduction

- PDR is short for
 - Photo-Dissociation Region
 - Photon Dominated Region



NGC 3603

Hubble Space Telescope • WFPC2

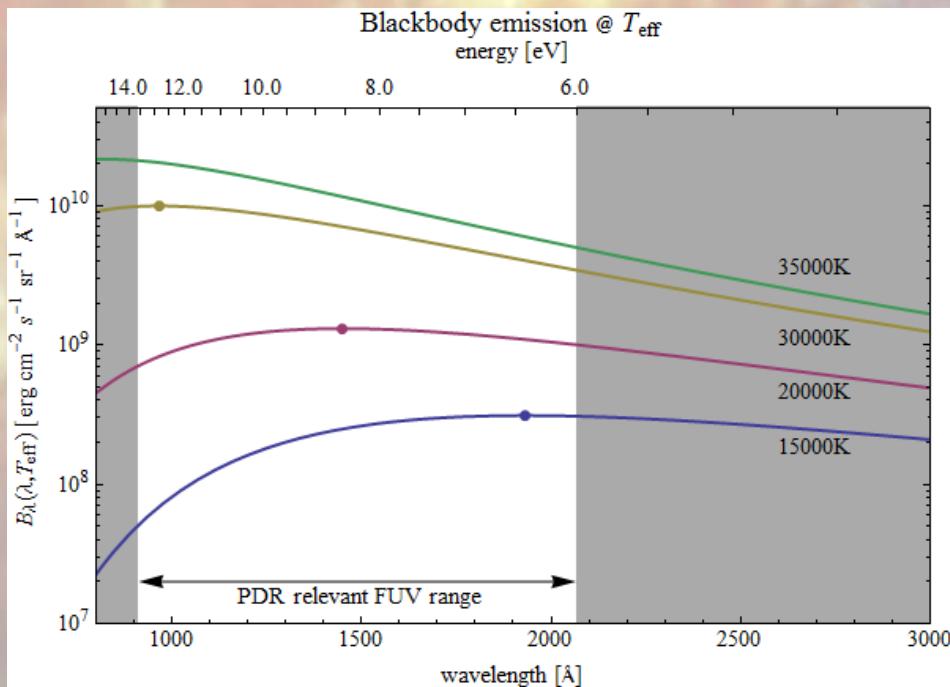
PRC99-20 • STScI OPO
Wolfgang Brandner (JPL/IPAC), Eva K. Grebel (University of Washington),
You-Hua Chu (University of Illinois, Urbana-Champaign) and NASA

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)**
11.1 eV (1117 Å)
11.3 eV (1097 Å)
 - **13.598 eV (912 Å)**
13.618 eV
14.5 eV (855 Å)
- ~ionization potential of dust/PAHs
dissociation energy of CO
ionization potential of C
ionization potential of H
ionization potential of O
ionization potential of N

Introduction

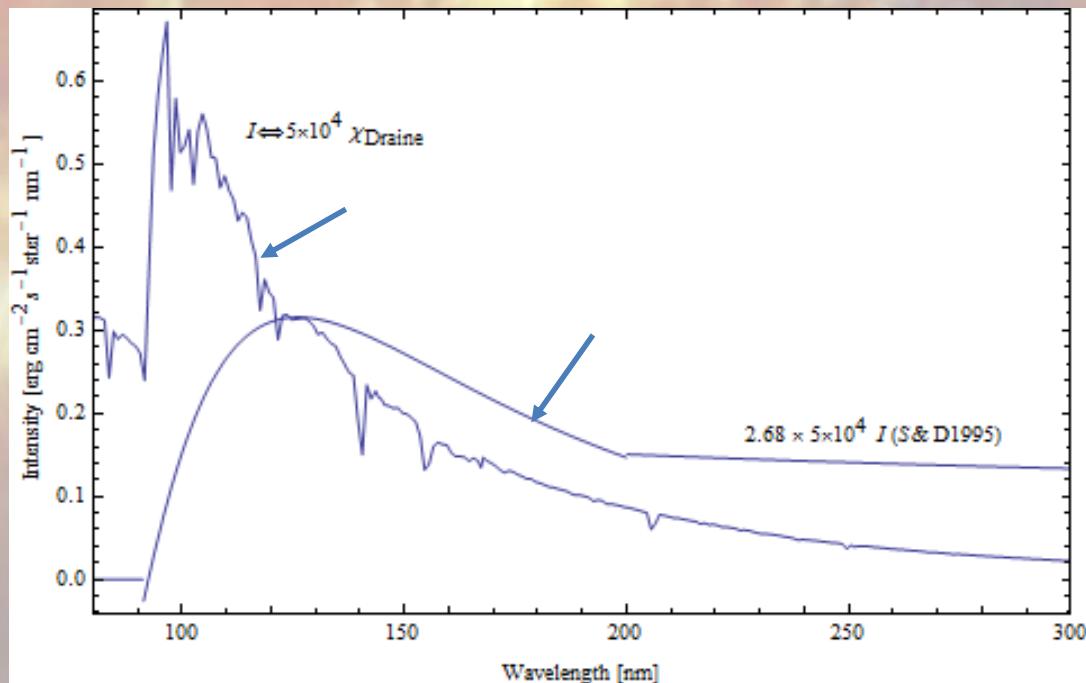
- A region where far-ultraviolet (FUV: 6-13.6 eV) photons from young, massive stars dominate the physics and the chemistry of the interstellar medium.



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

Introduction

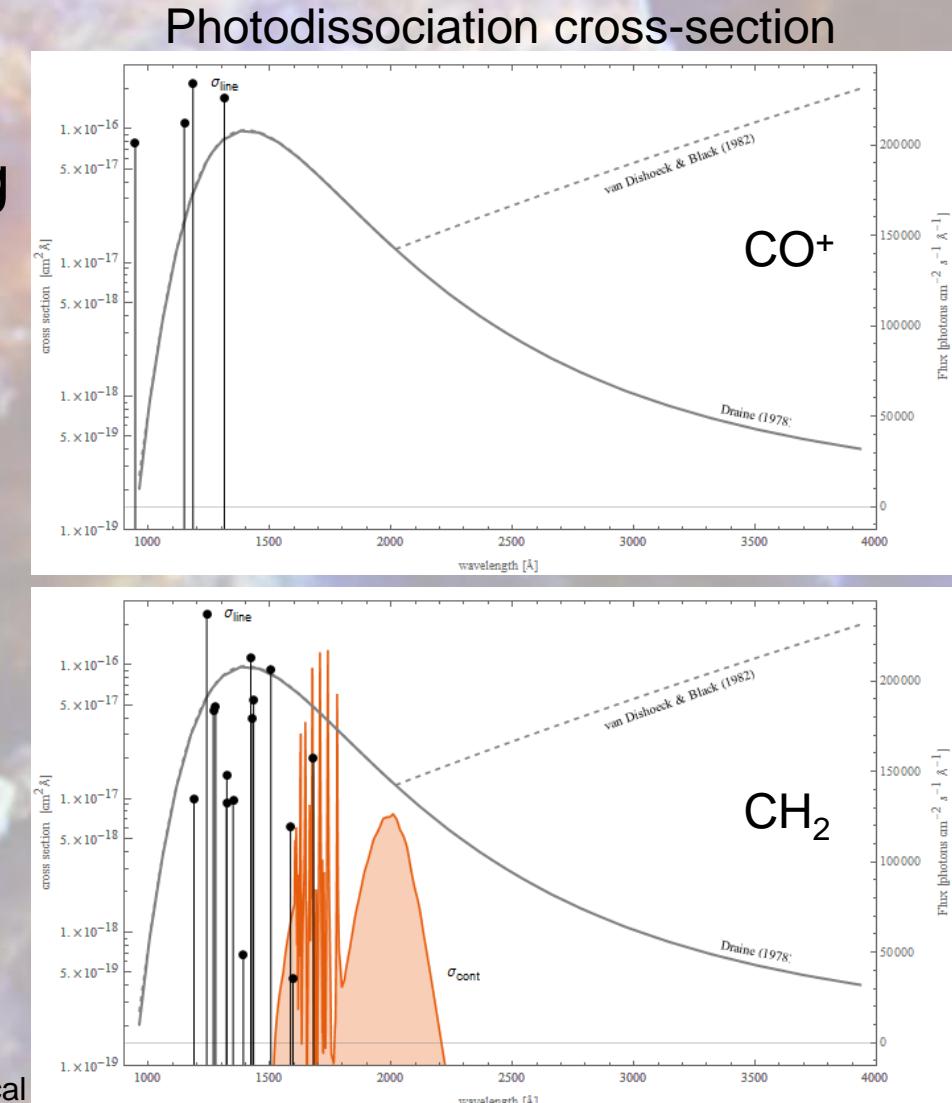
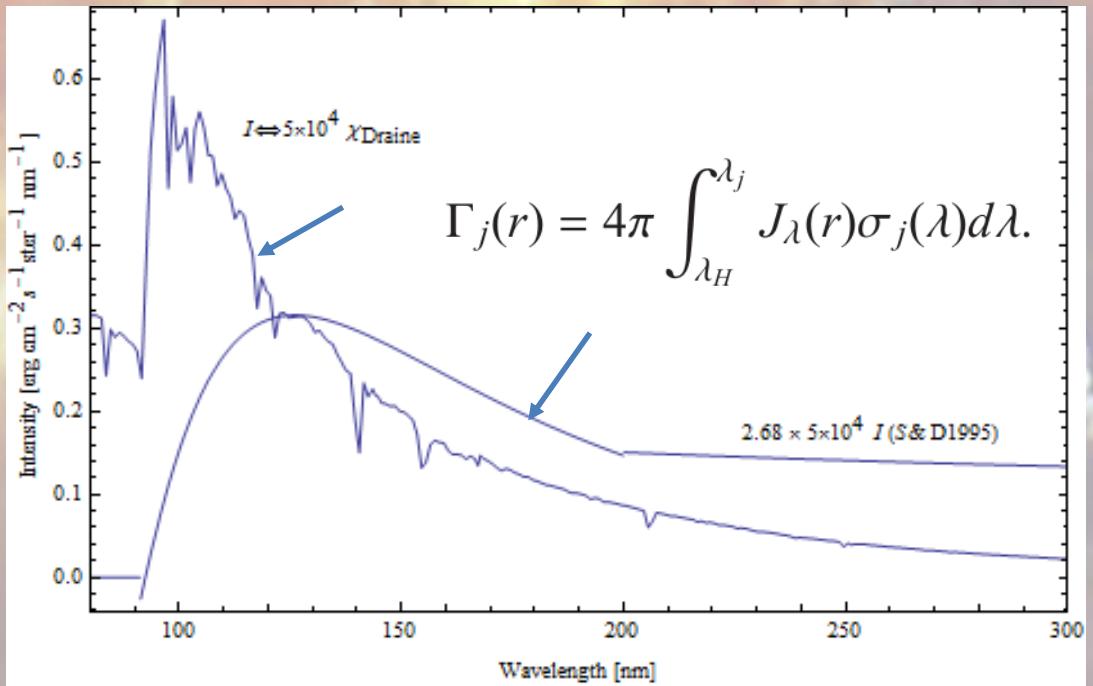
- A region where far-ultraviolet (FUV: 6-13.6 eV) photons from young, massive stars dominate the physics and the chemistry of the interstellar medium.



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

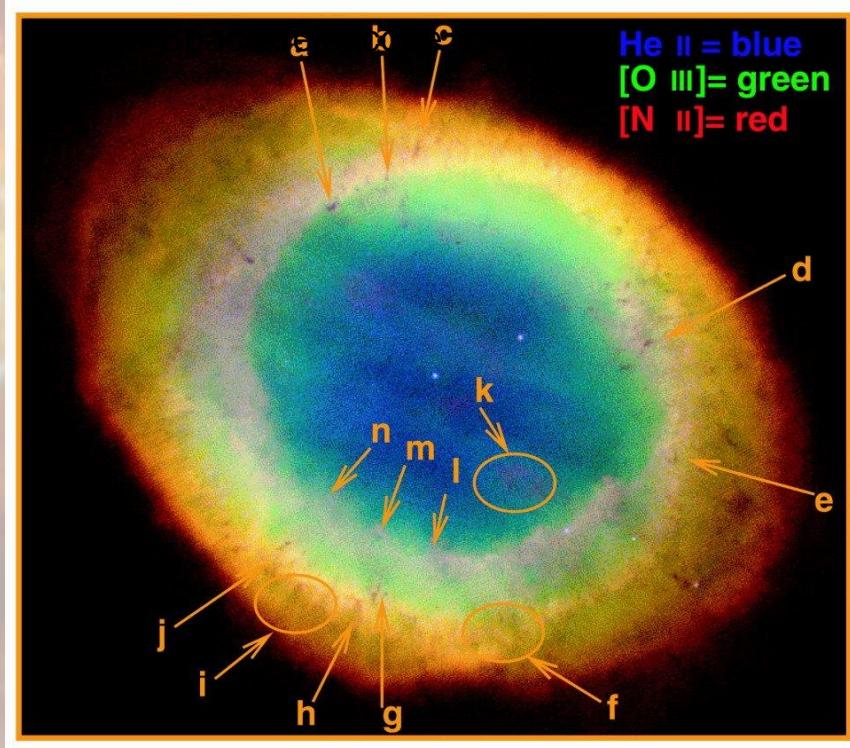
Introduction

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

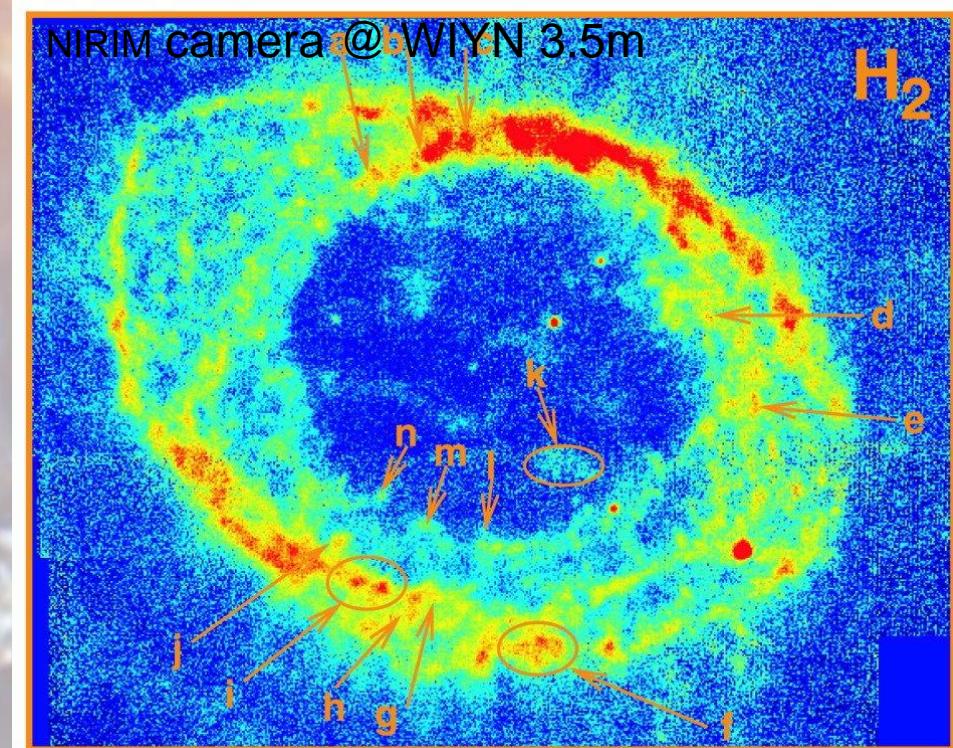


Introduction

Ring nebula



H_2 1–0 S(1) 2.122 μ m



H_2 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)

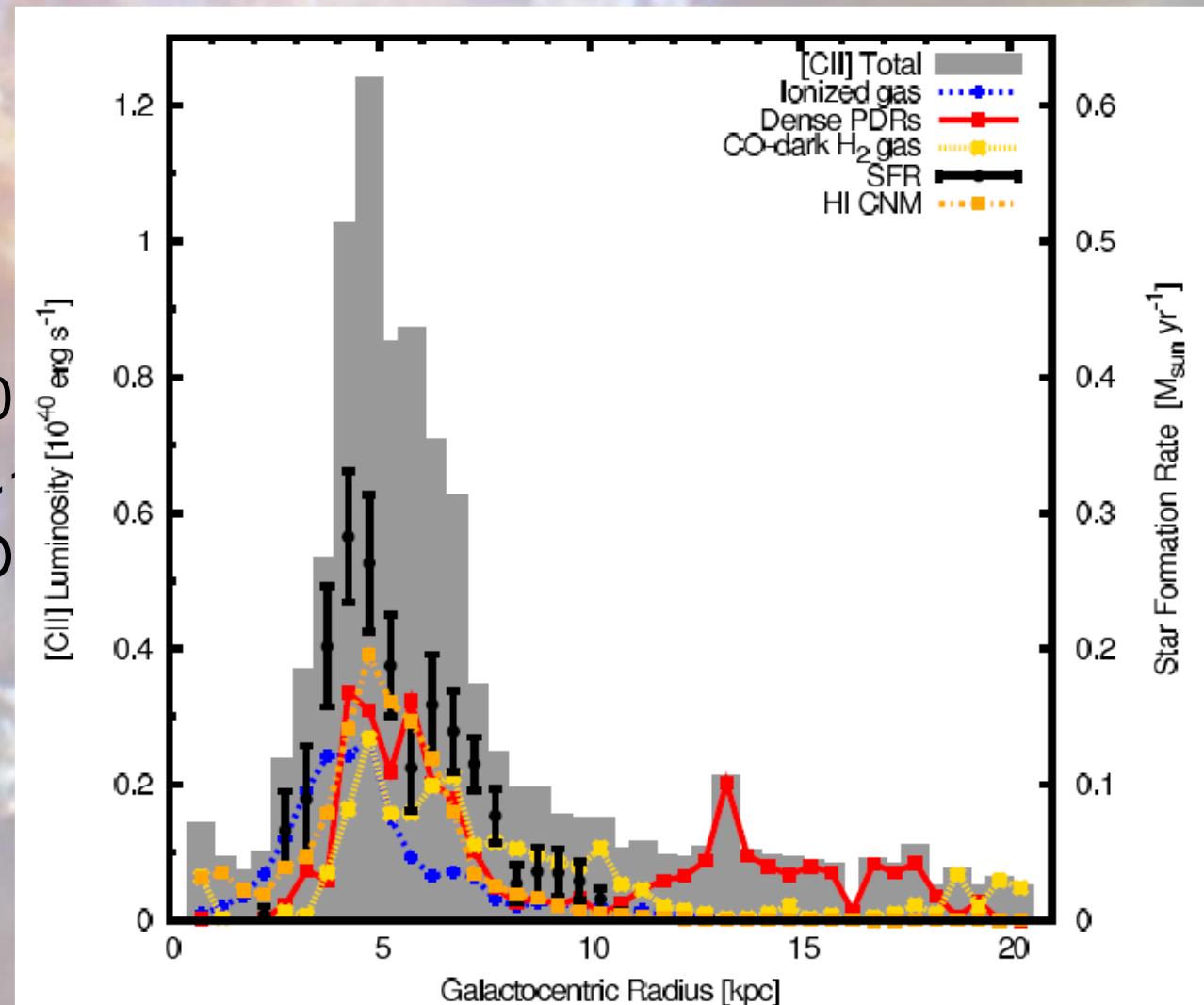
Introduction

Pineda et al. 2014

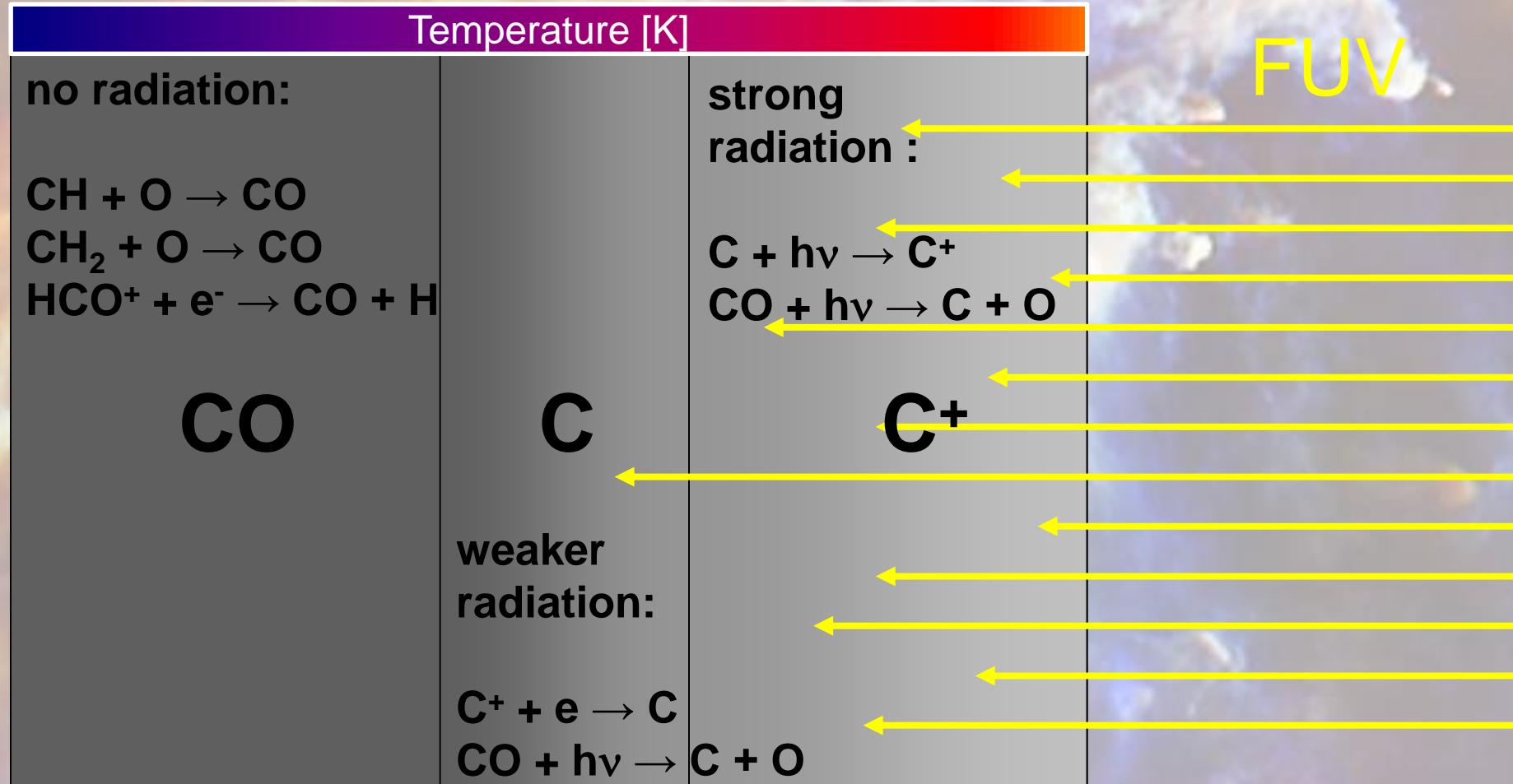
Interstellar PDRs include:

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

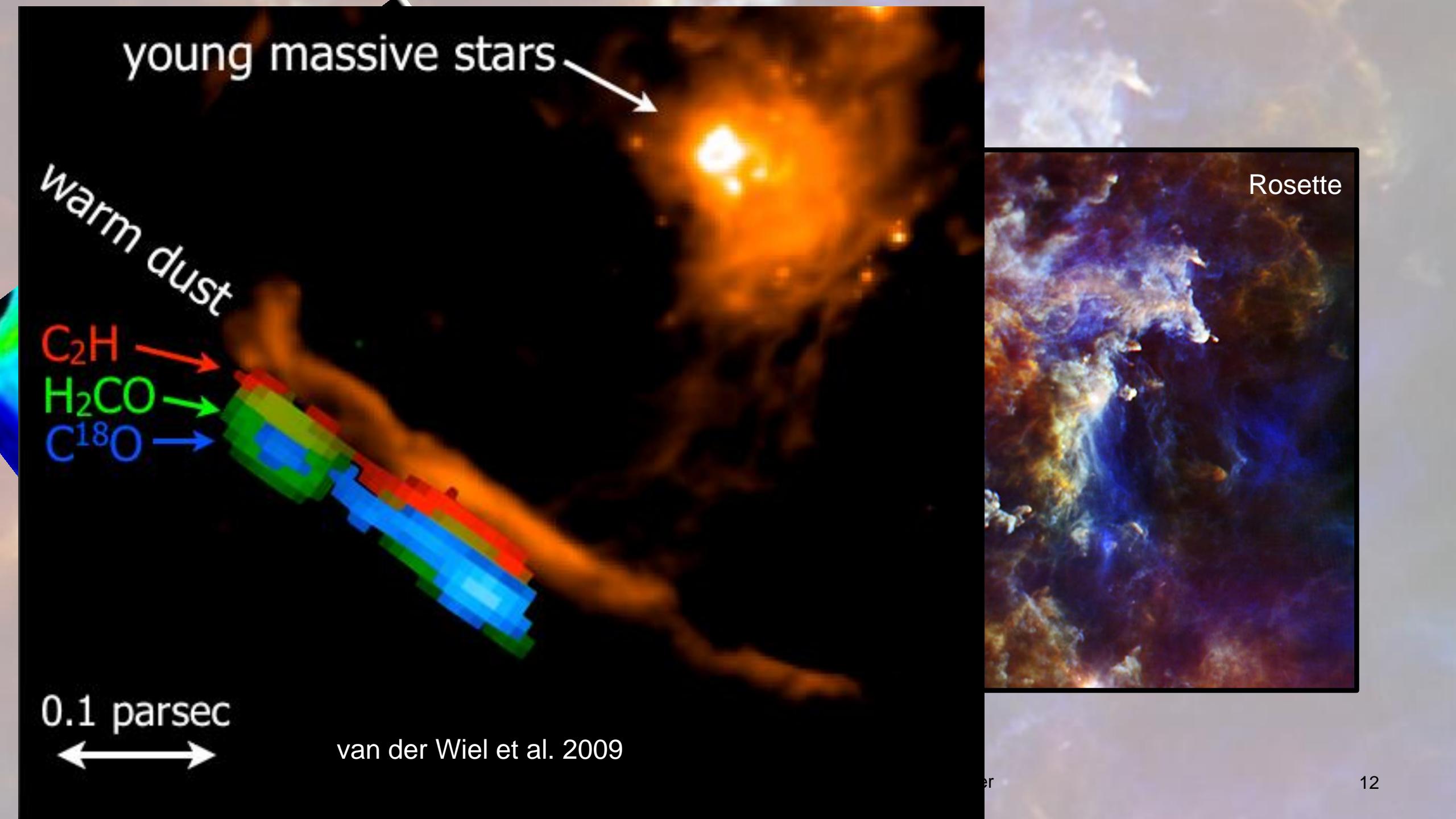
 ~90% of the Galactic molecular



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

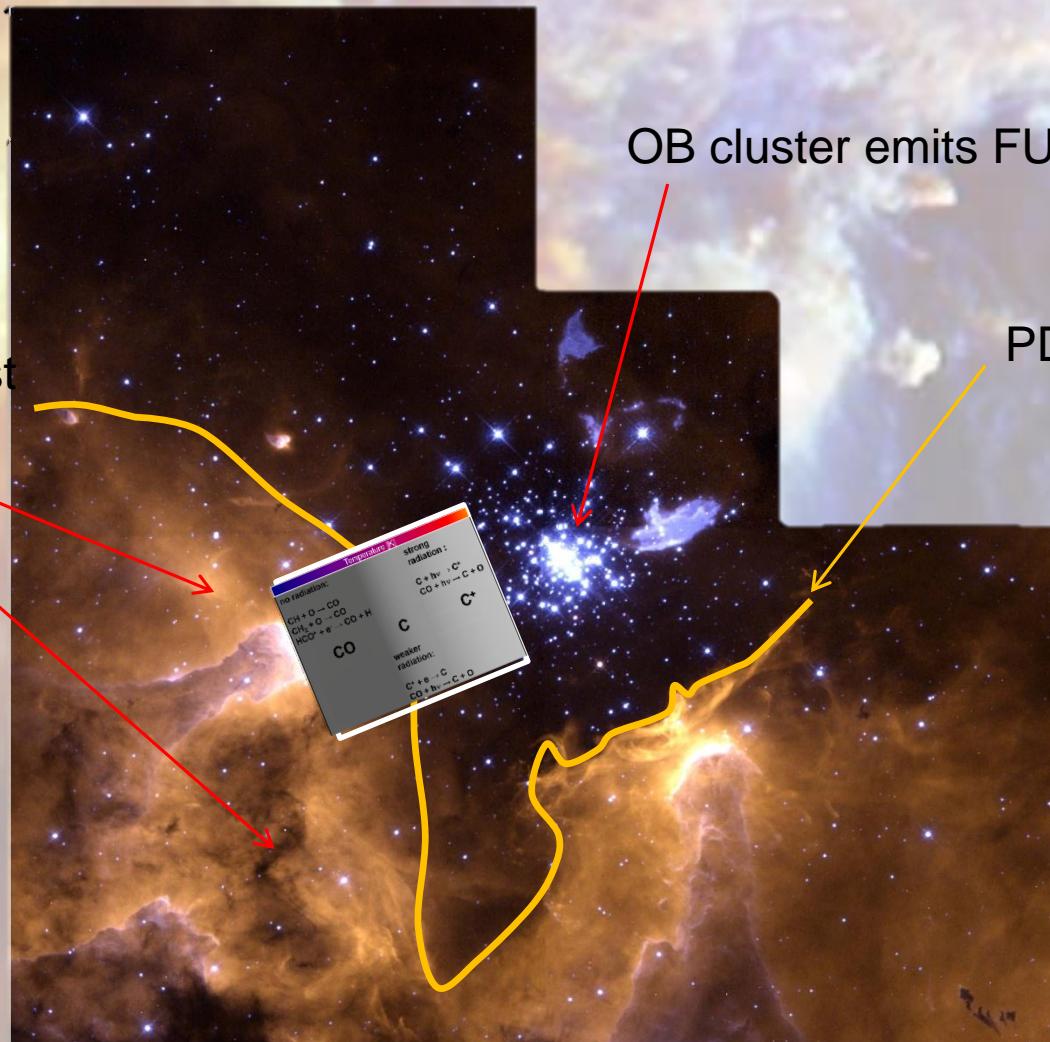
Rosette

Introduction

molecular cloud
contains gas & dust

OB cluster emits FUV

PDR interface



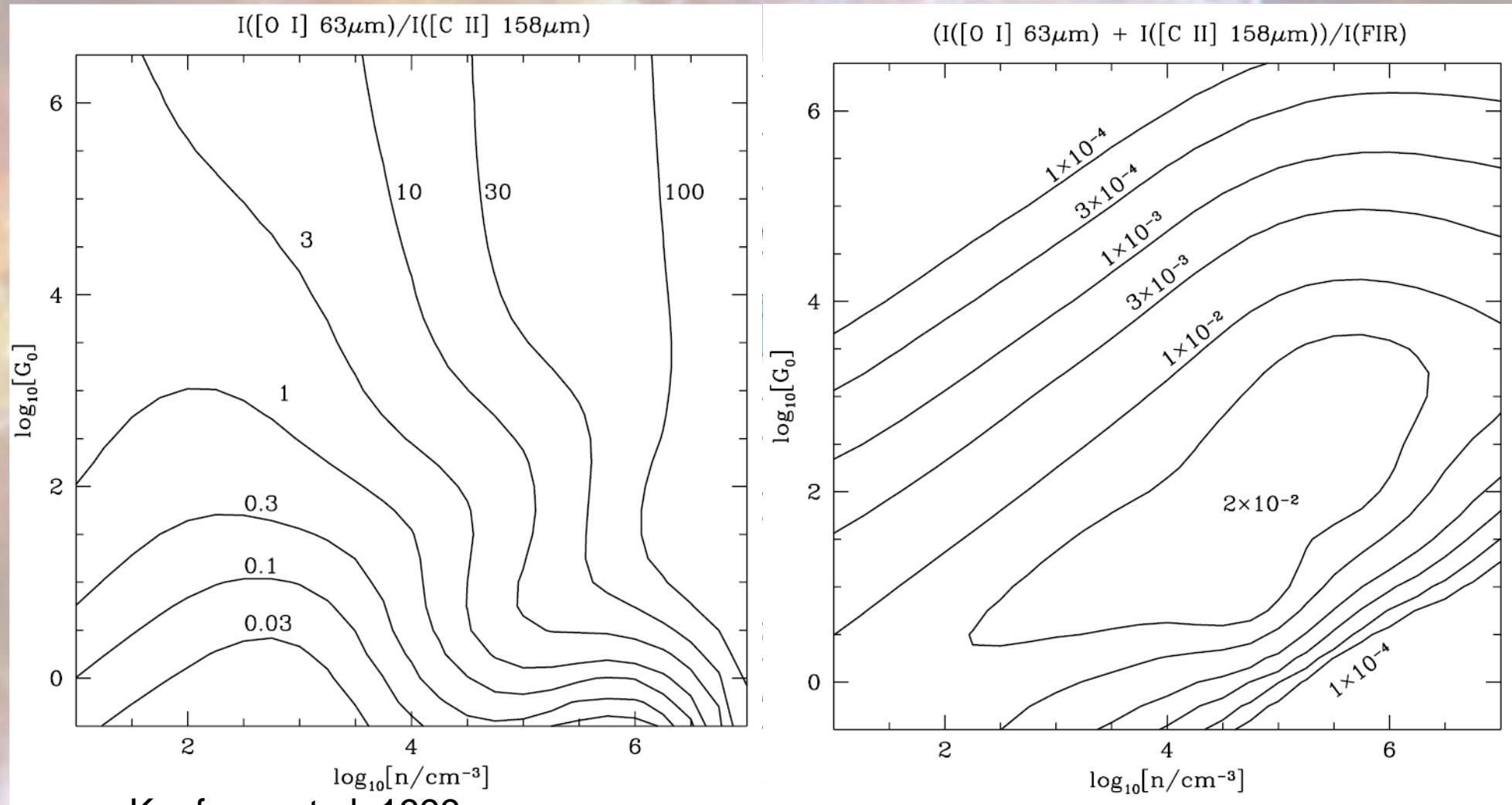
PDR Model Complexity

- 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 λ -dependent
 - detailed photon cross-section
 - full λ -resolving radiative transfer
- Dust content
 - dust composition, size distribution (practically unknown)
 - very small grains, PAHs
 - PE efficiency, charge exchange
 - grain surface characterization
 E_{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 H₂, HD, CO, H₂O,....
 - 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
 - existance of (multiple) solutions?

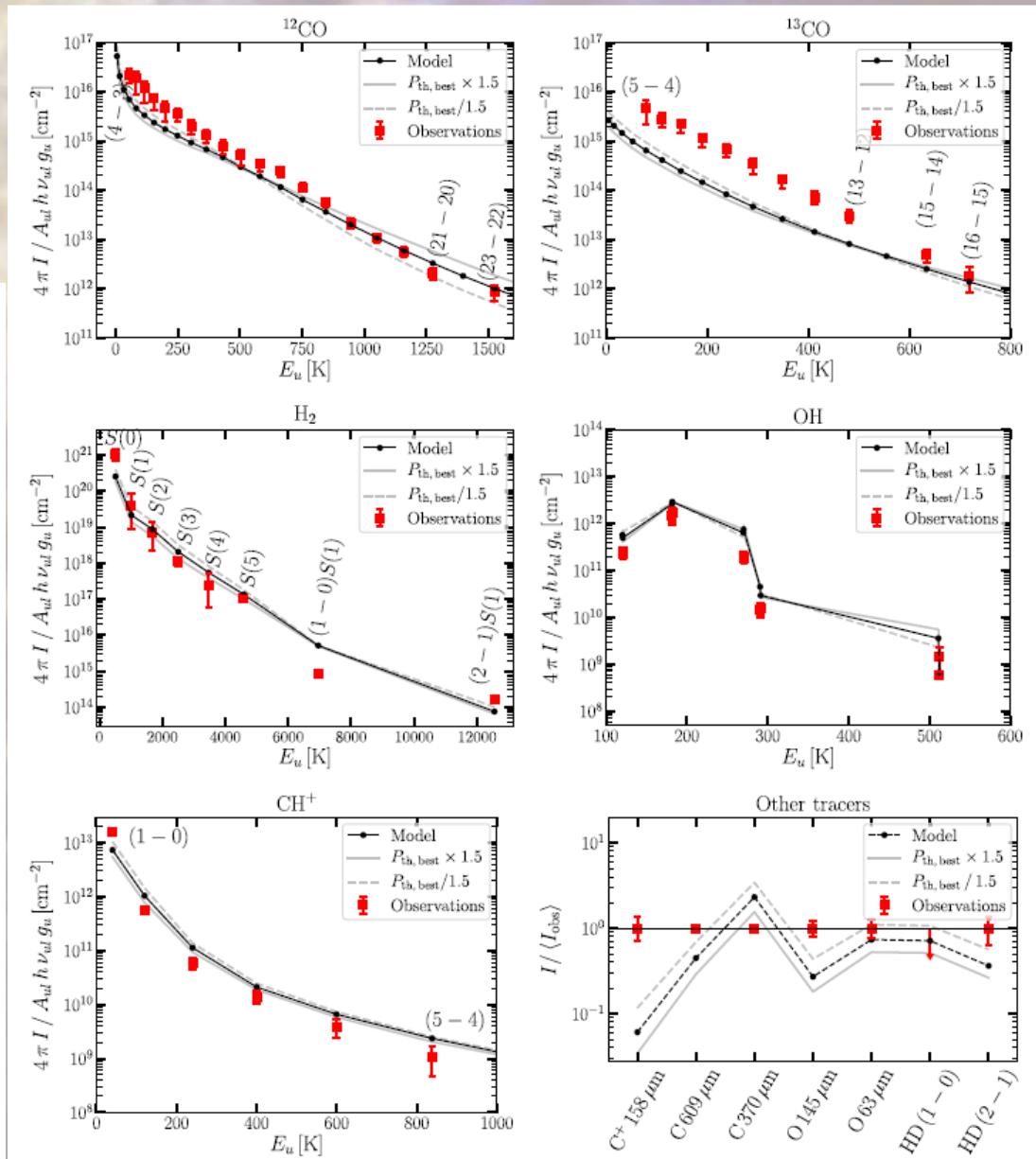
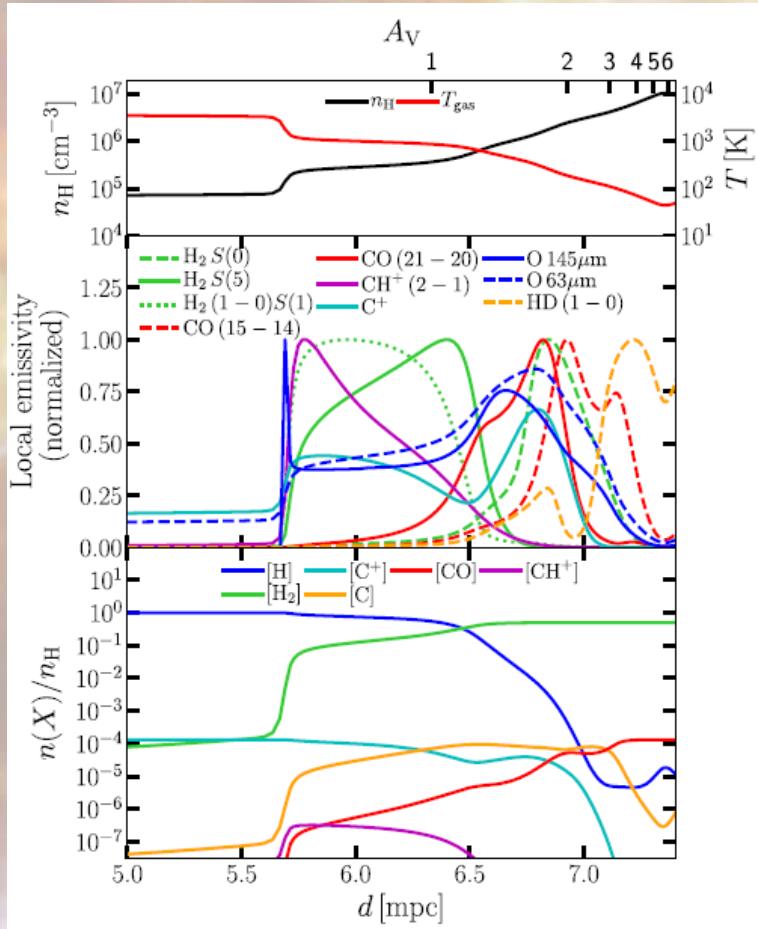
Line ratio analysis



Kaufman et al. 1999

Orion Bar Model

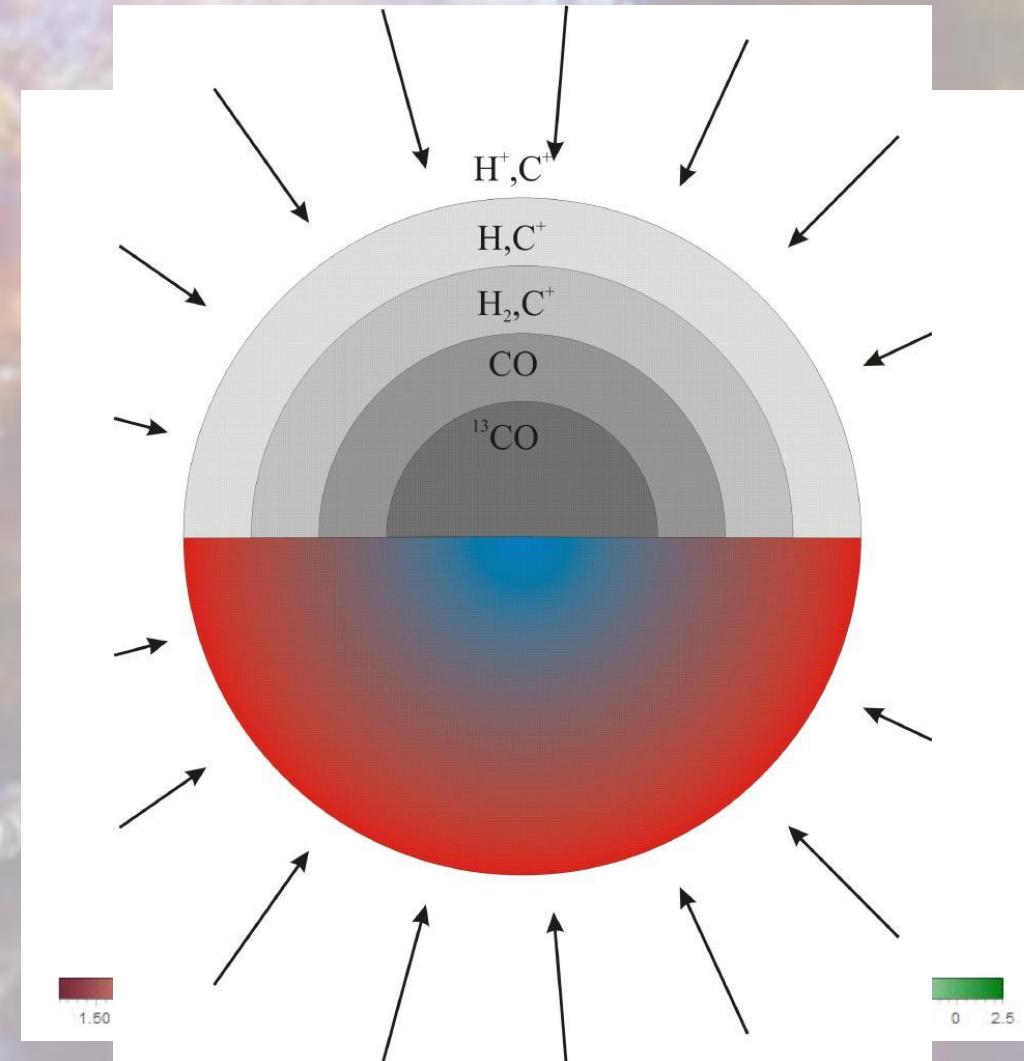
Meudon PDR Code, isobaric



Joblin et al. 2018

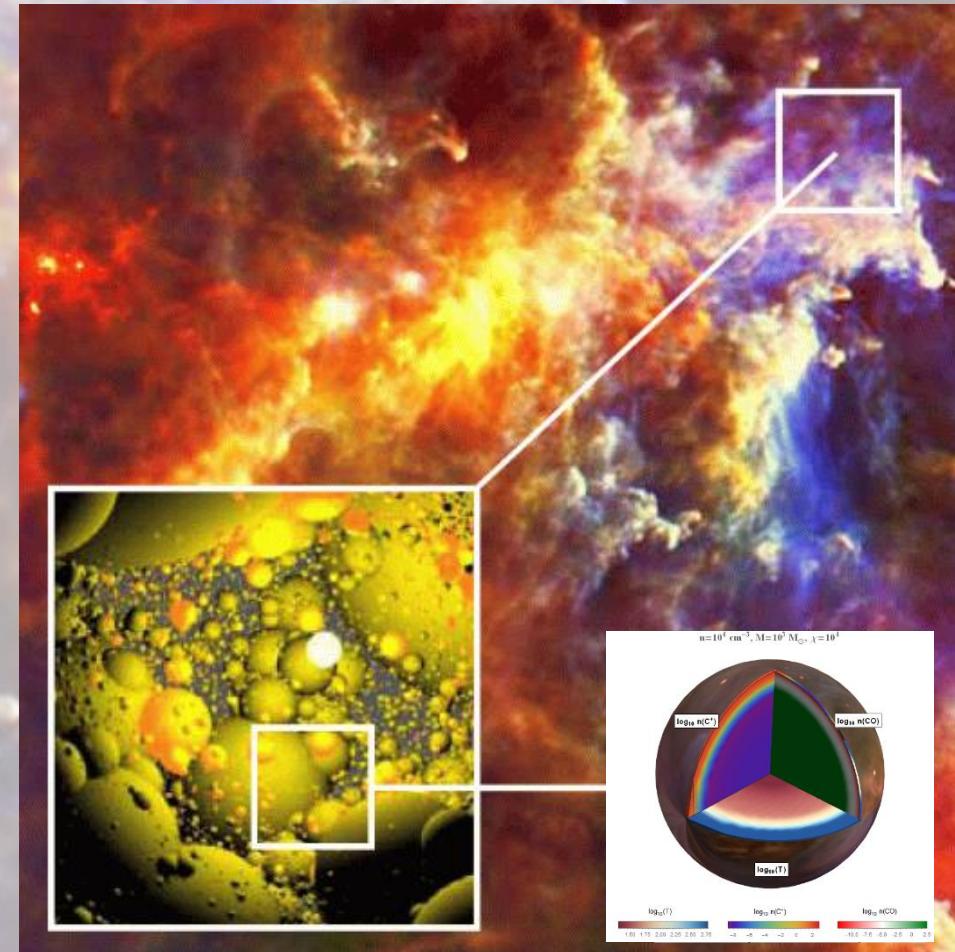
The KOSMA- τ PDR Code

- 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



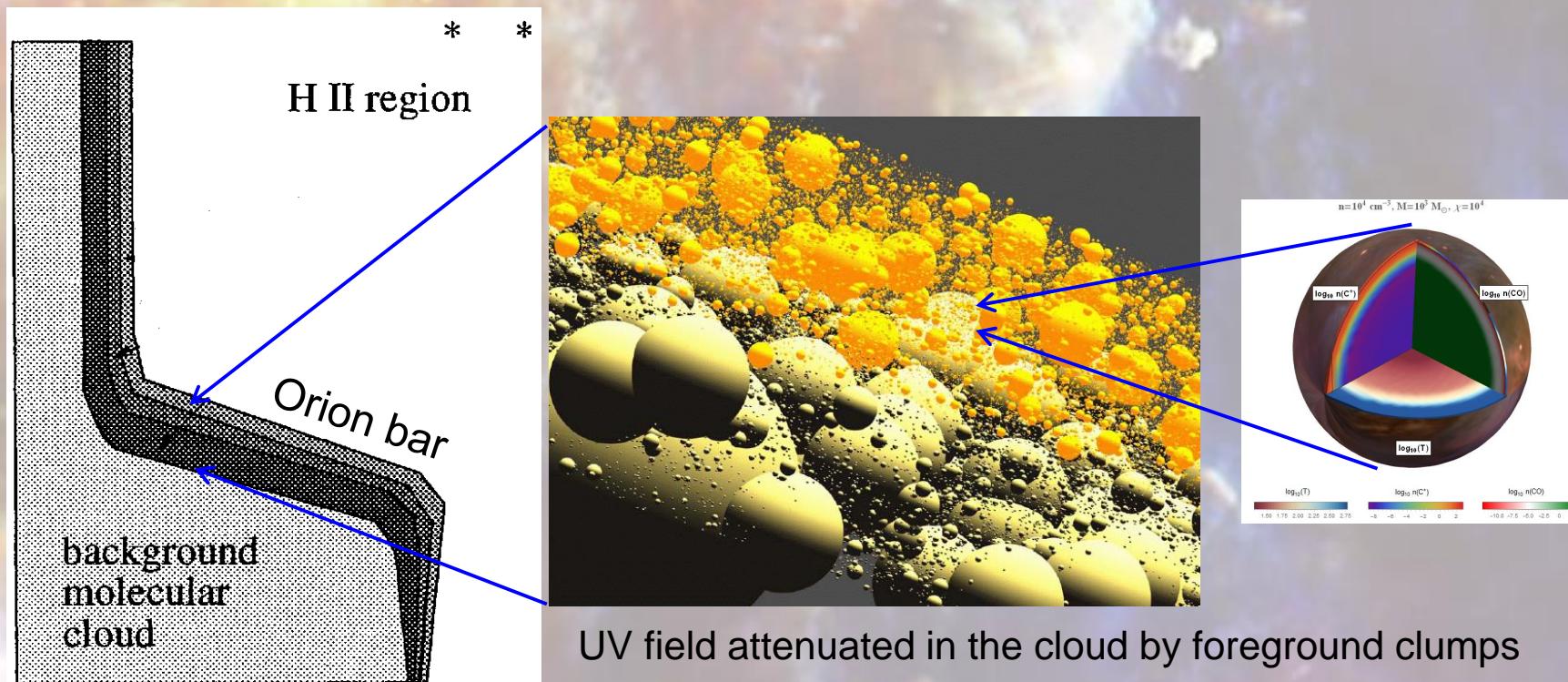
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- full dust RT and temp. computation for varying dust distribution
- clumpy cloud composition
 - stochastic clump ensemble
 - **KOSMA- τ 3D**
(Andree-Labsch et al. 2017)



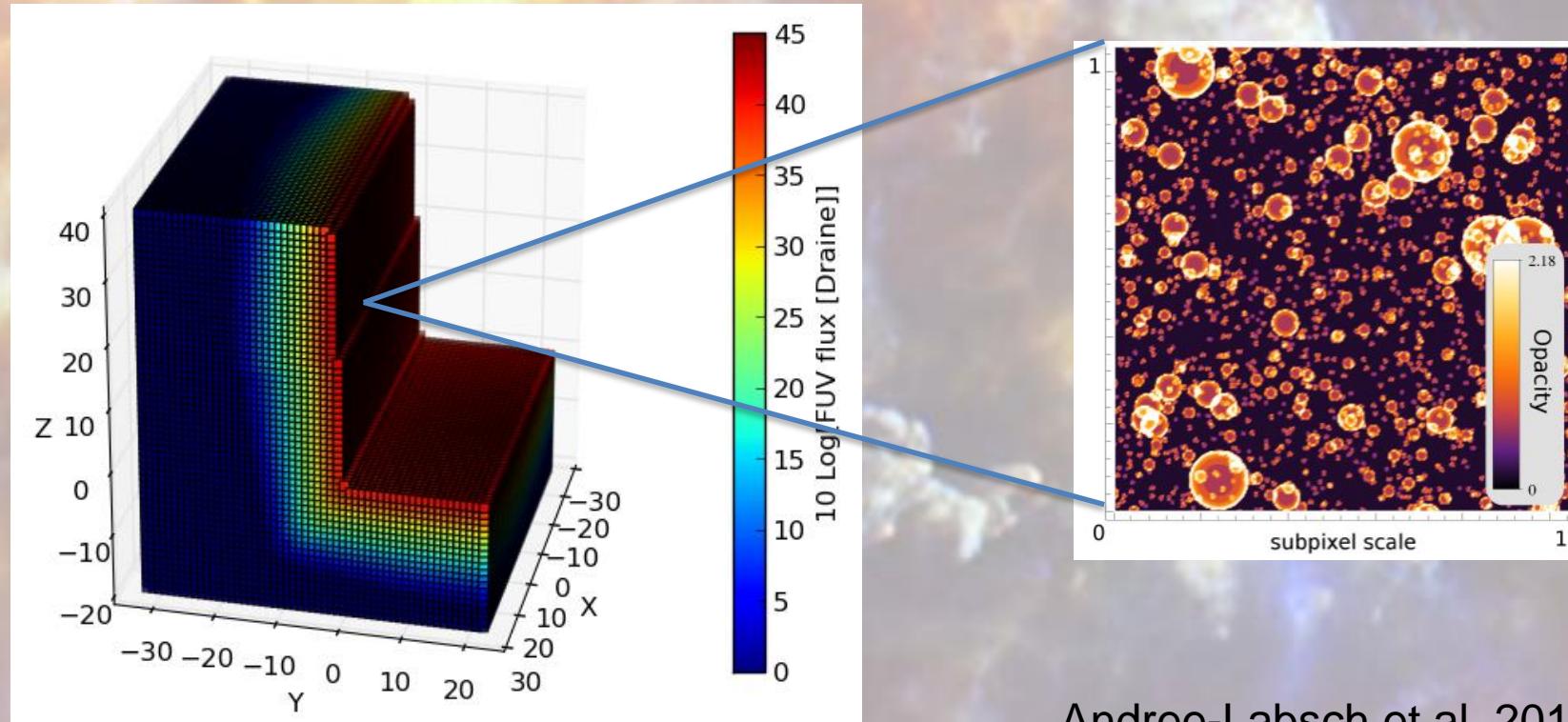
Applications: KOSMA- τ 3D

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



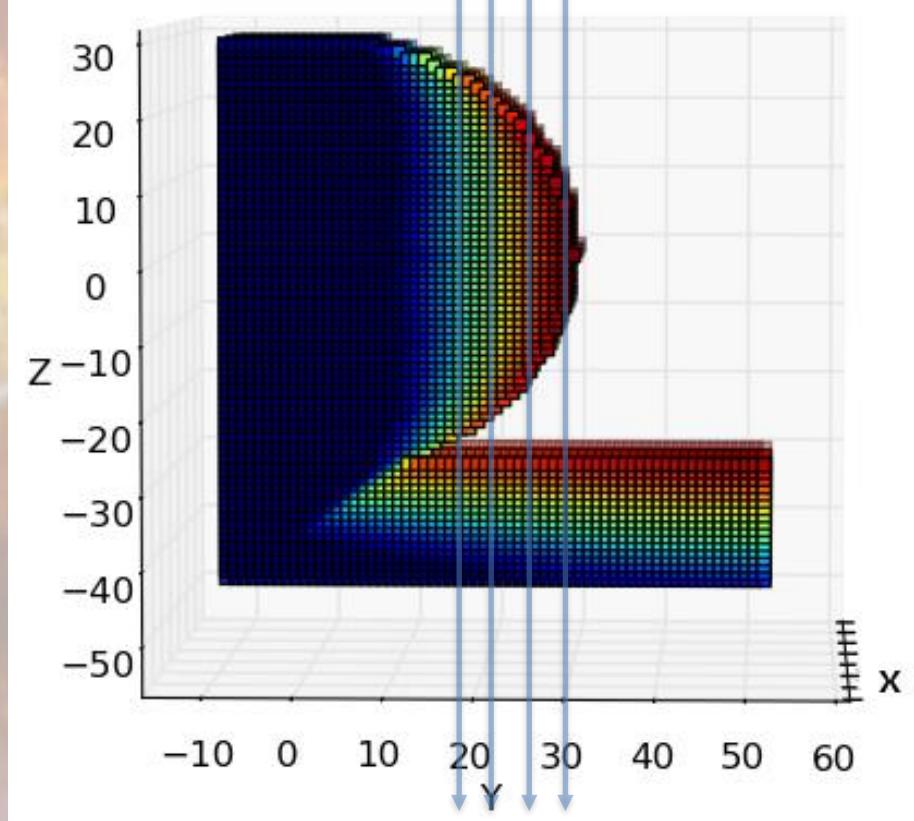
Applications: KOSMA- τ 3D

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

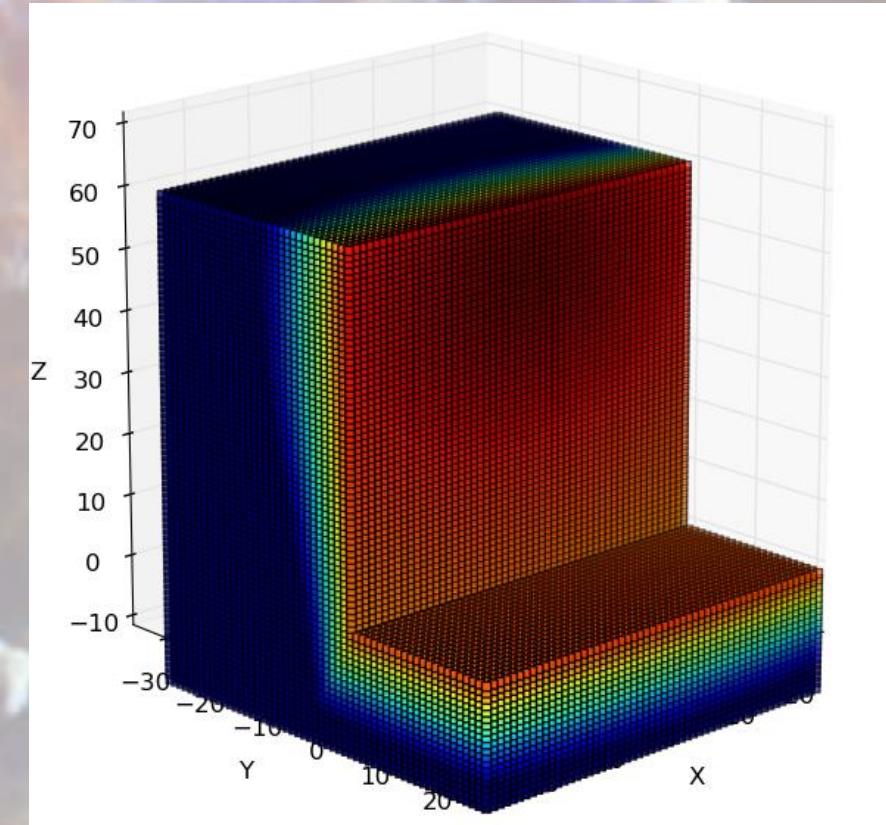


Andree-Labsch et al. 2017

Applications: KOSMA- τ 3D

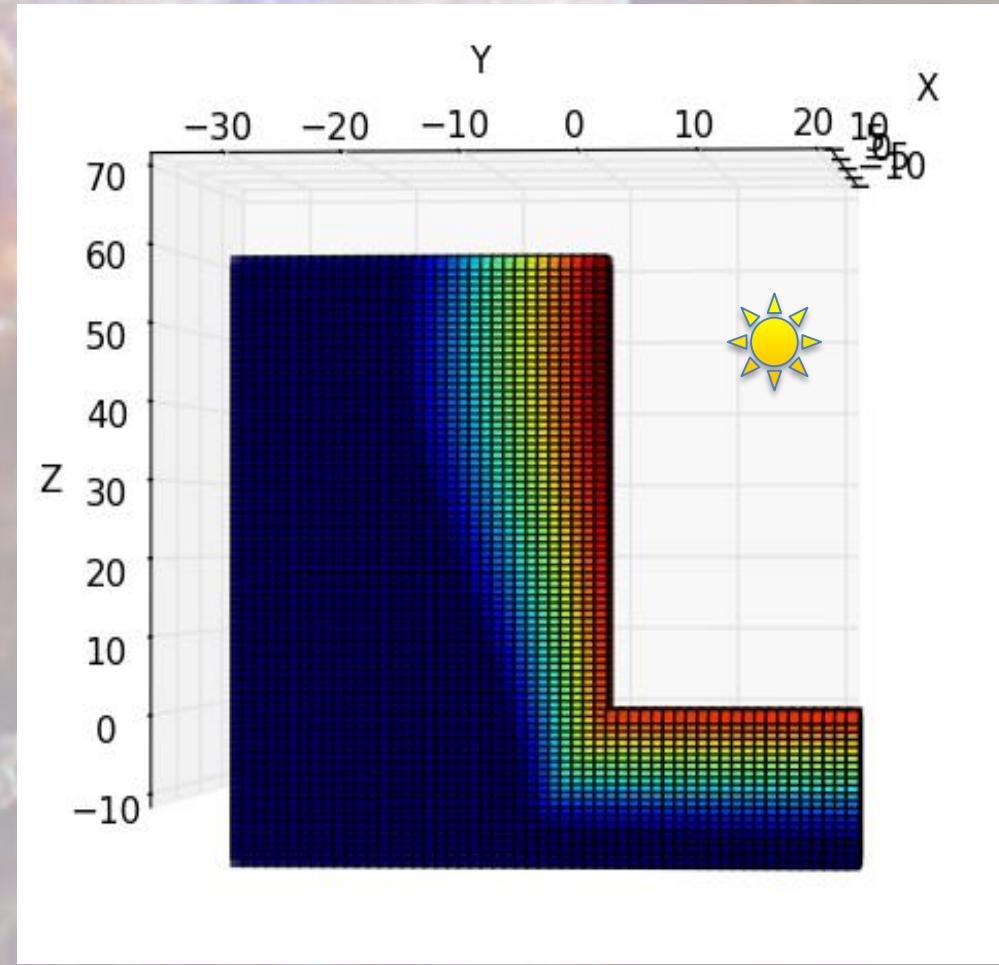
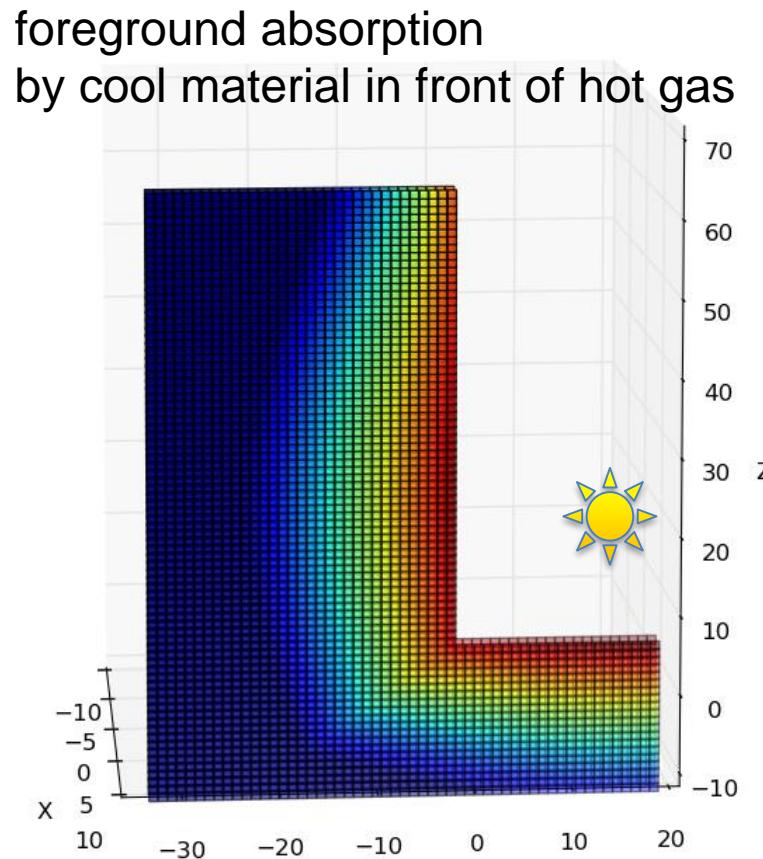


no chemical stratification



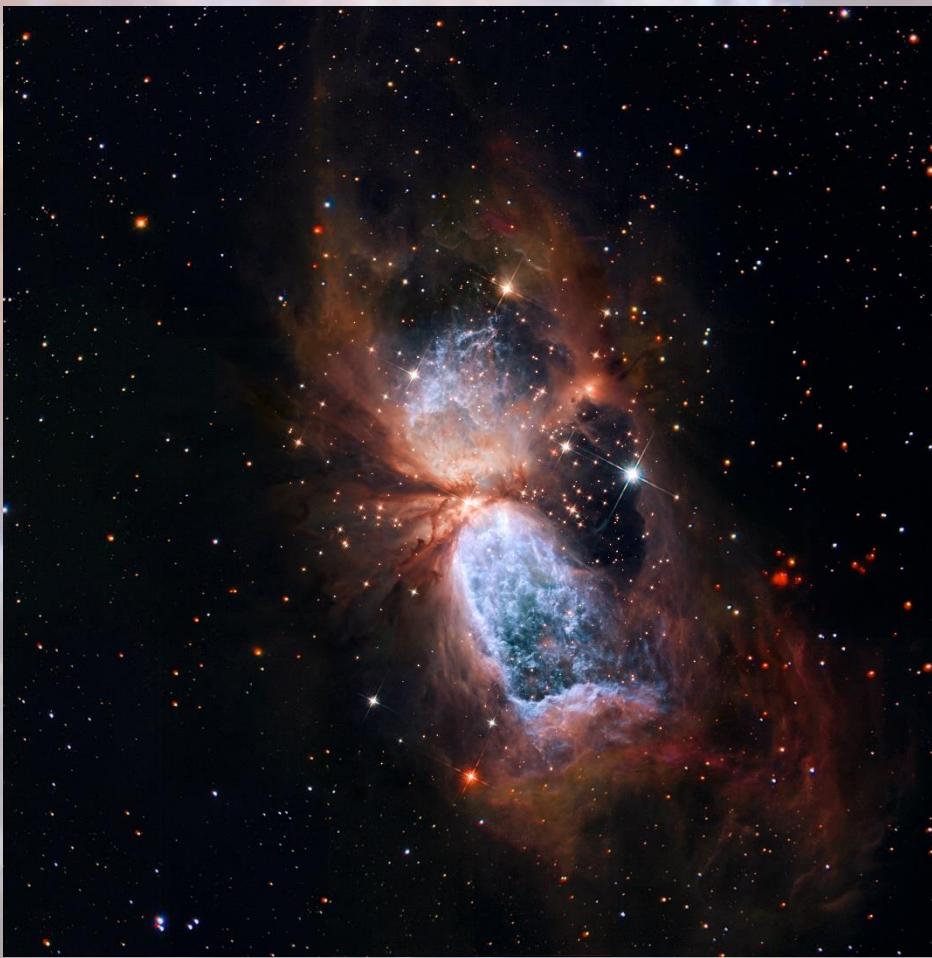
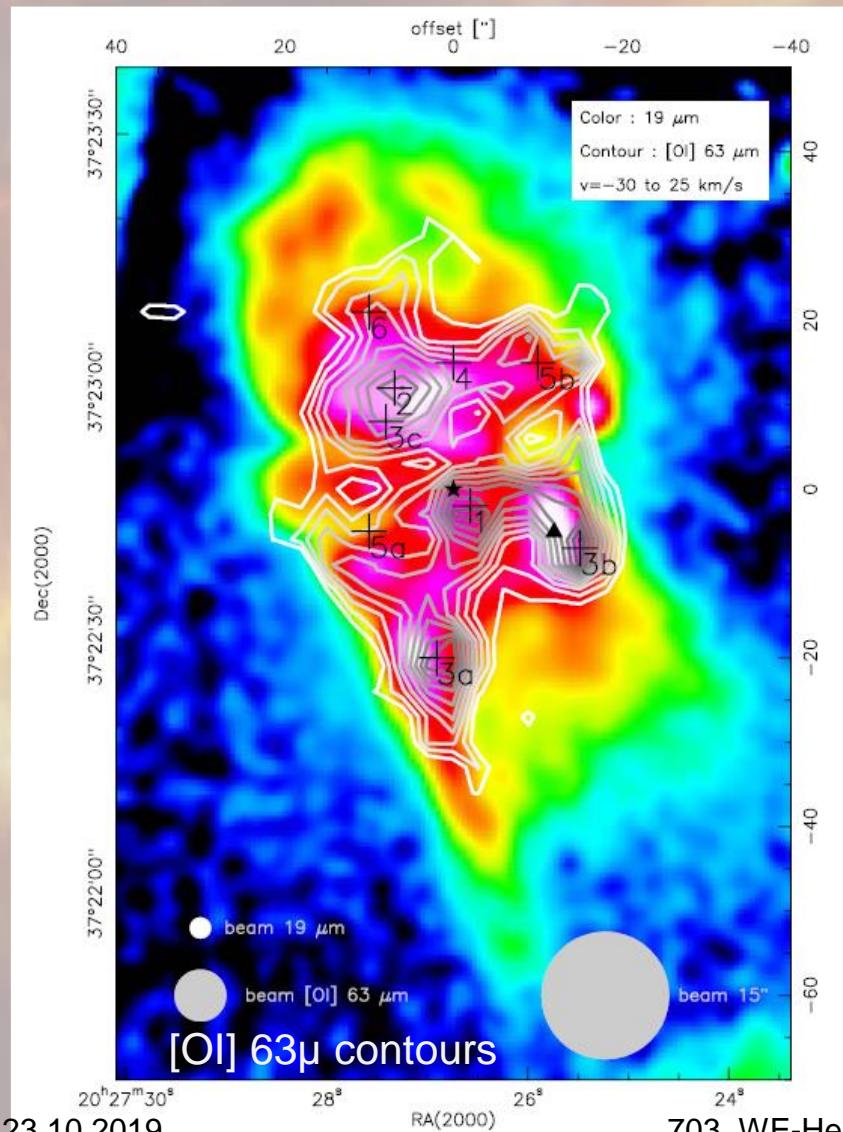
Andree-Labsch et al. 2017

Applications: KOSMA- τ 3D



Andree-Labsch et al. 2017

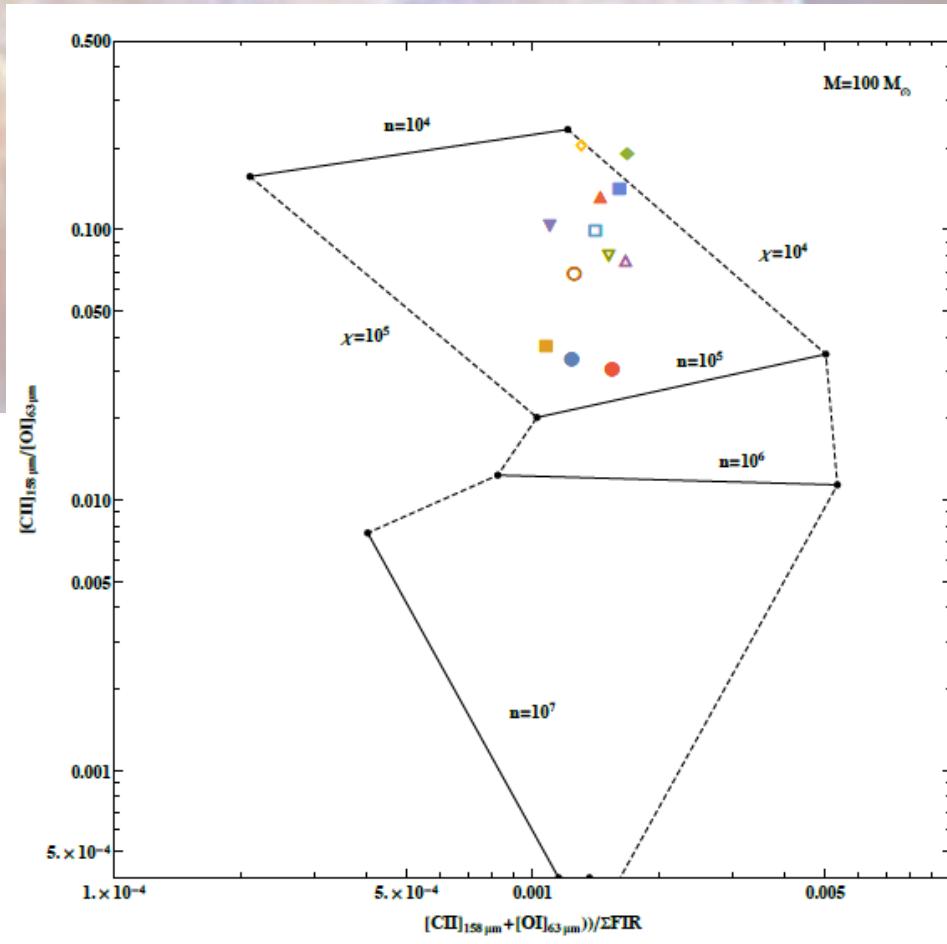
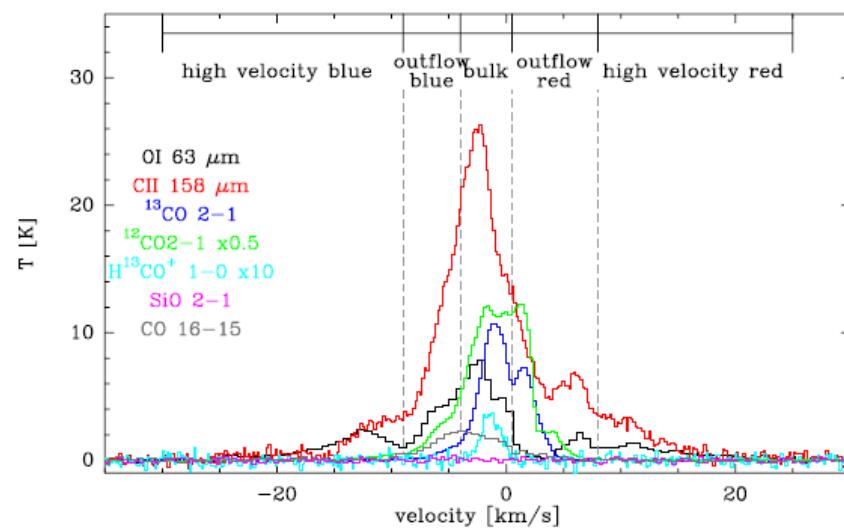
S106



S106

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

Tomography of 3-D structure

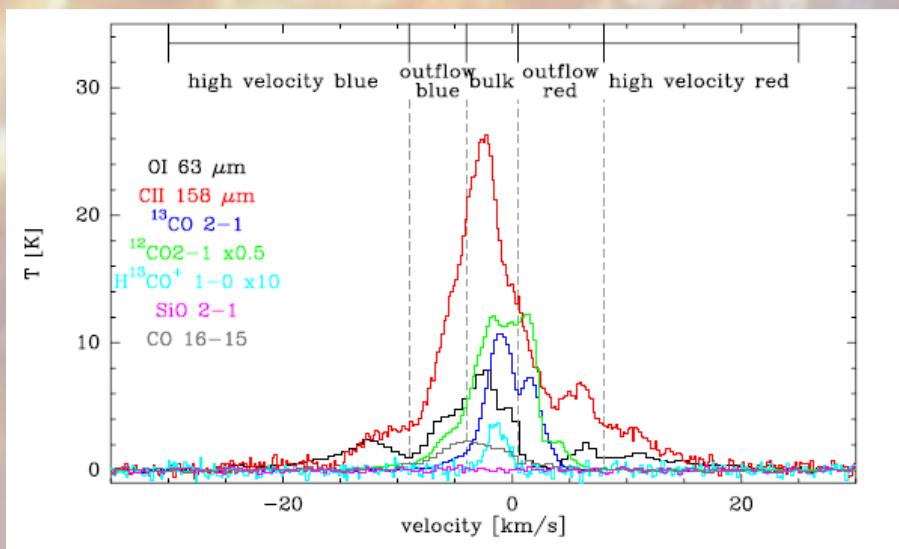


Schneider et al. 2018

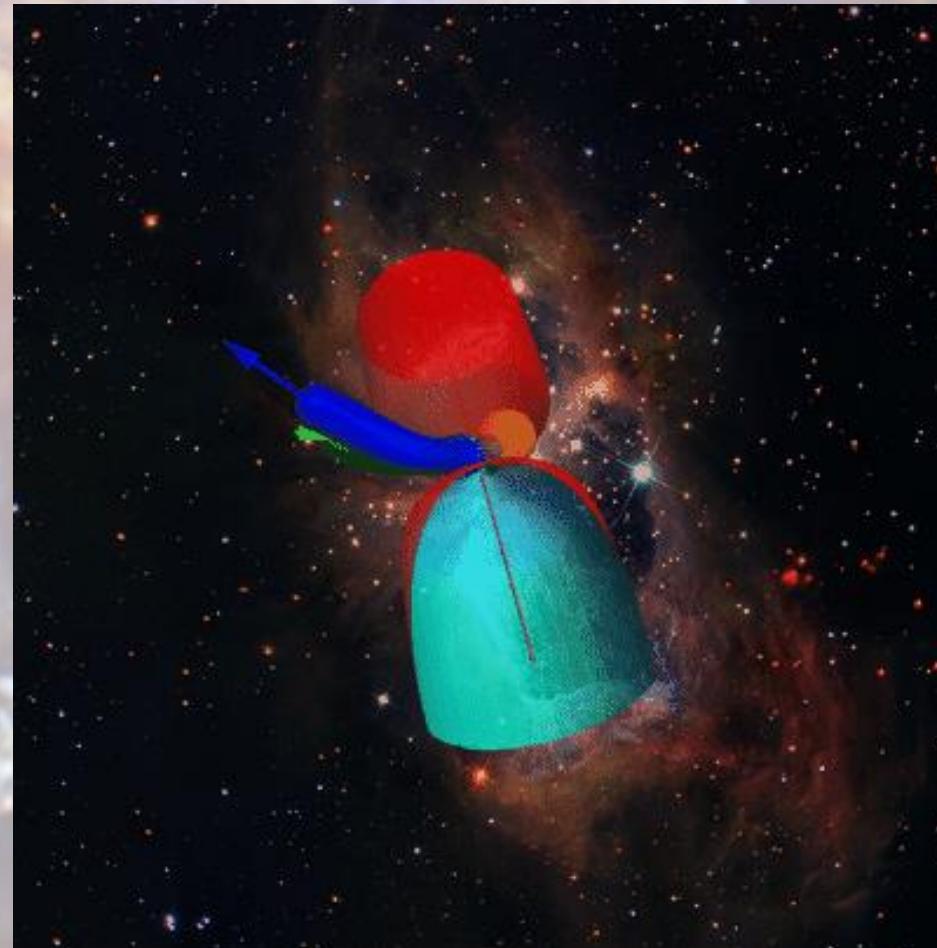
S106

High spectral resolution of upGREAT on SOFIA allows the spectral identification of various kinematic components

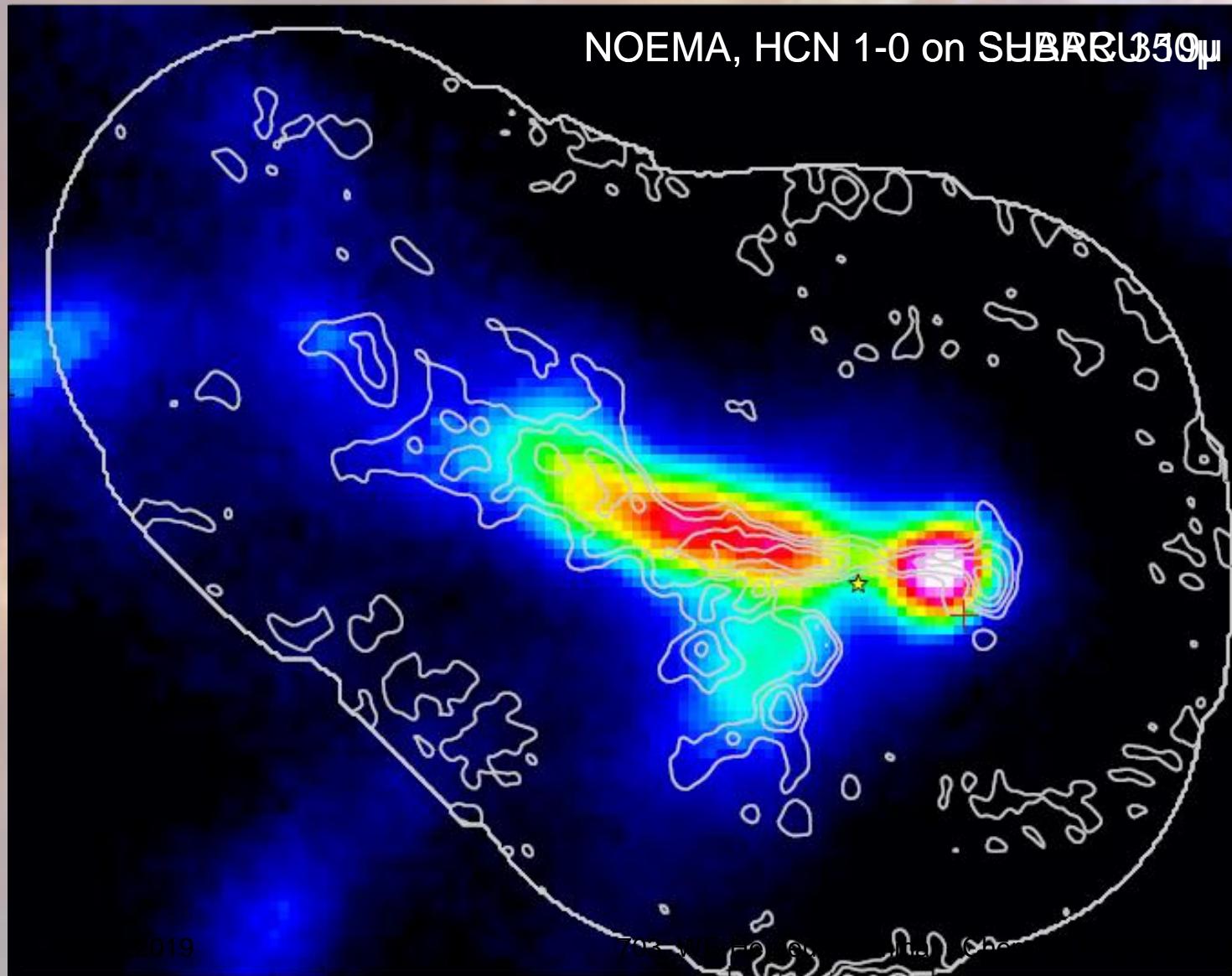
Tomography of 3-D structure



Schneider et al. 2018

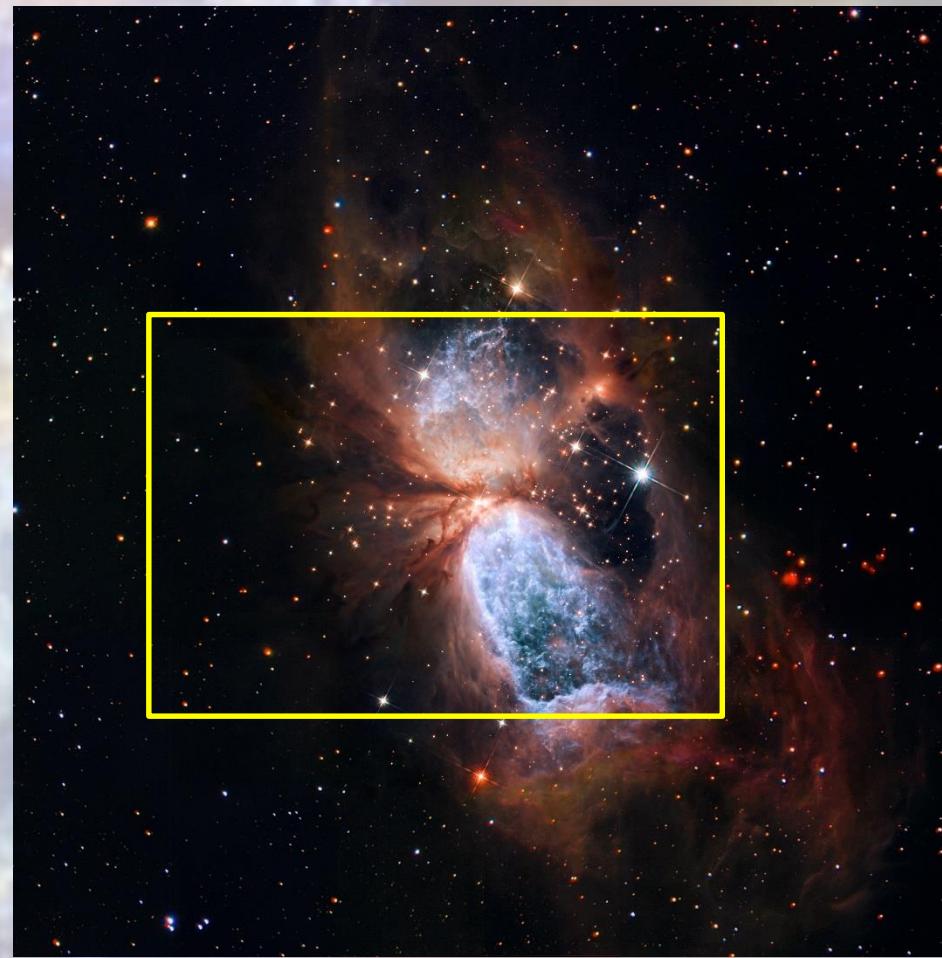


S106



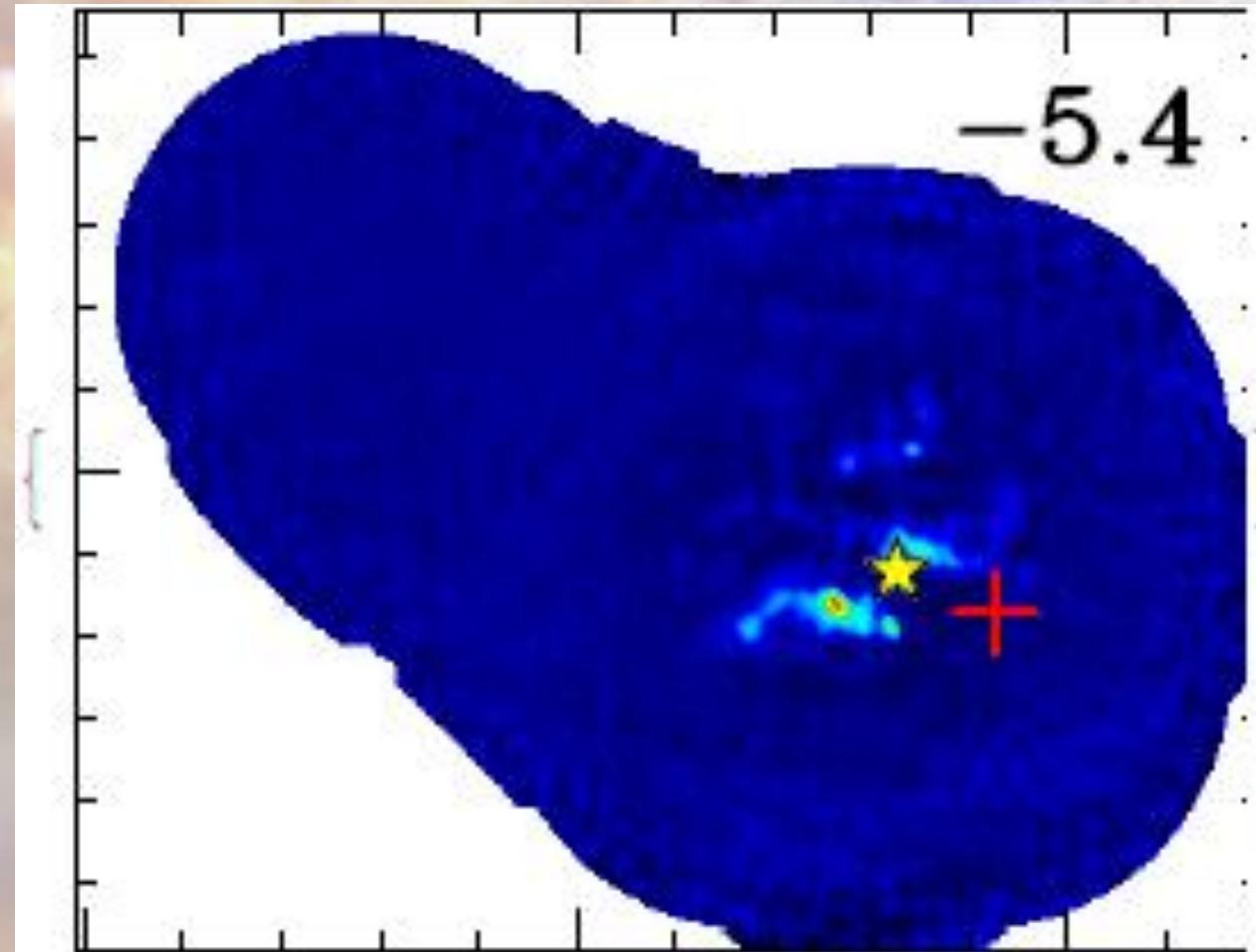
2019

Cosmic Matter

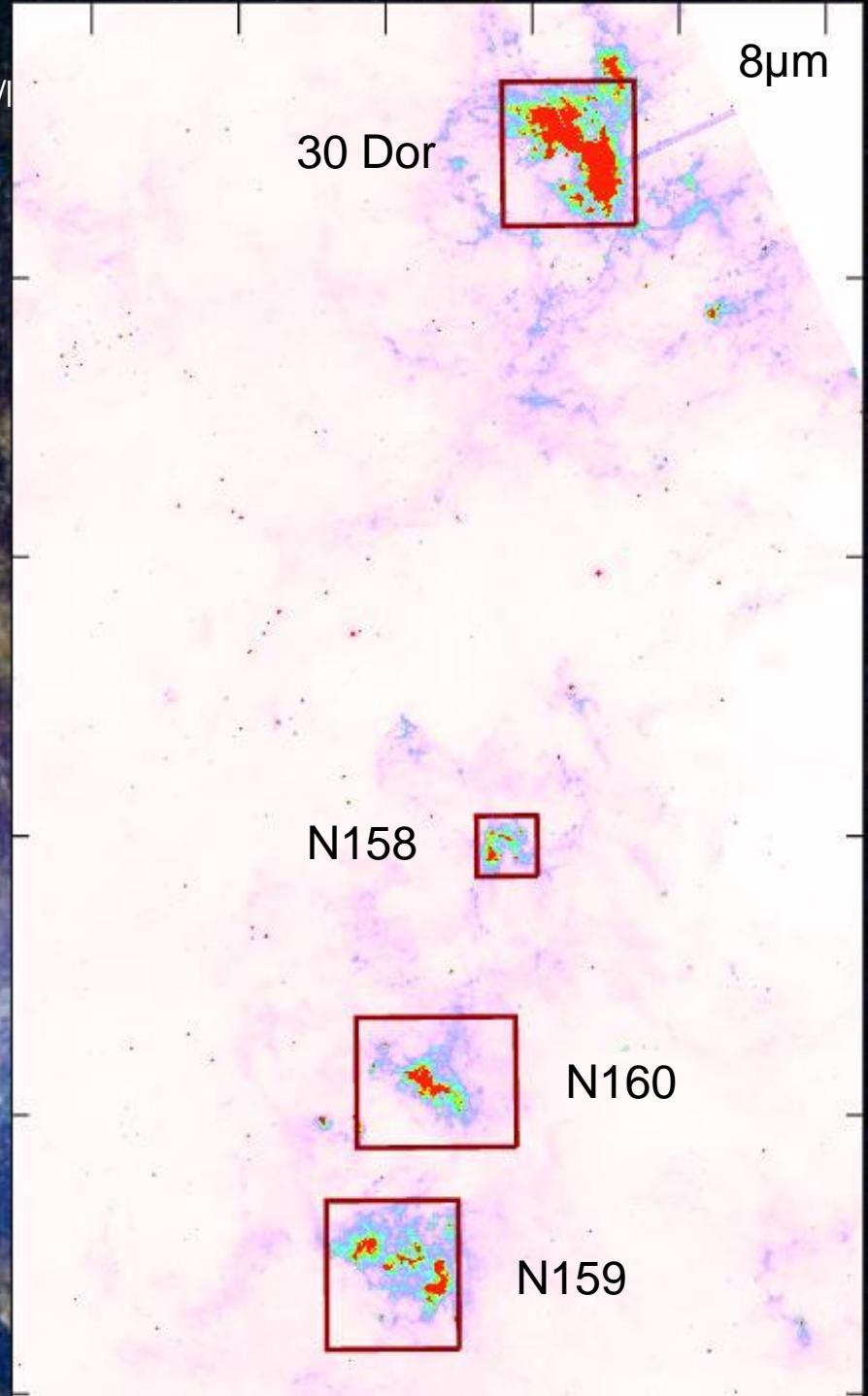
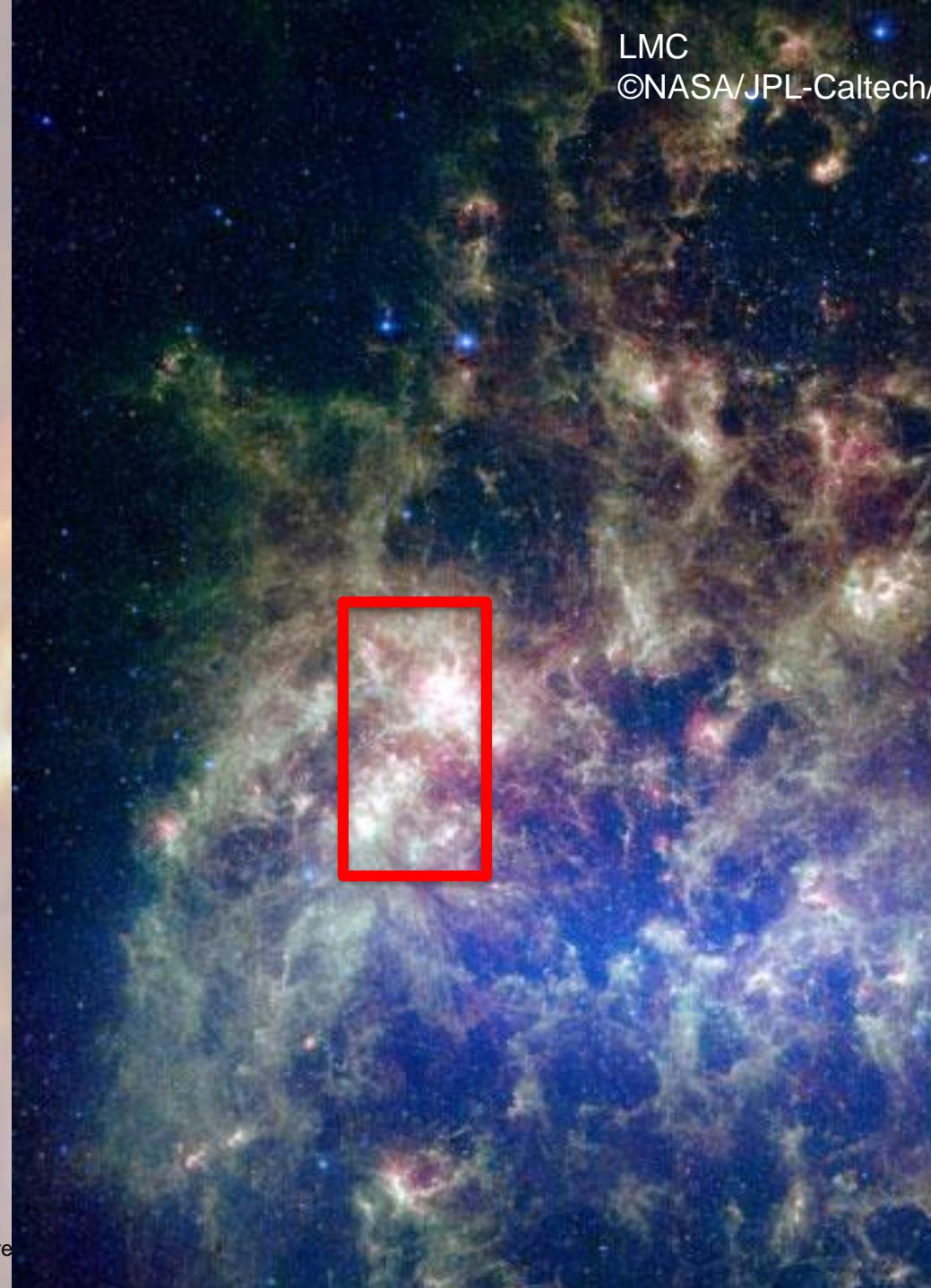


27

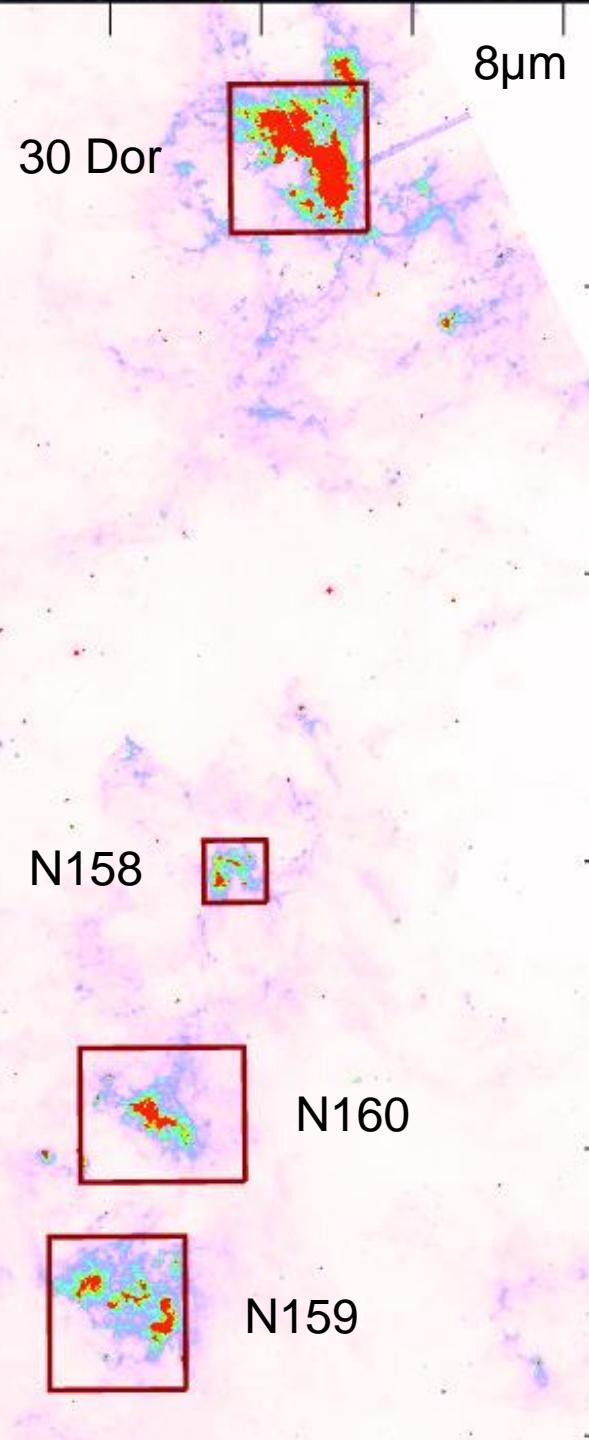
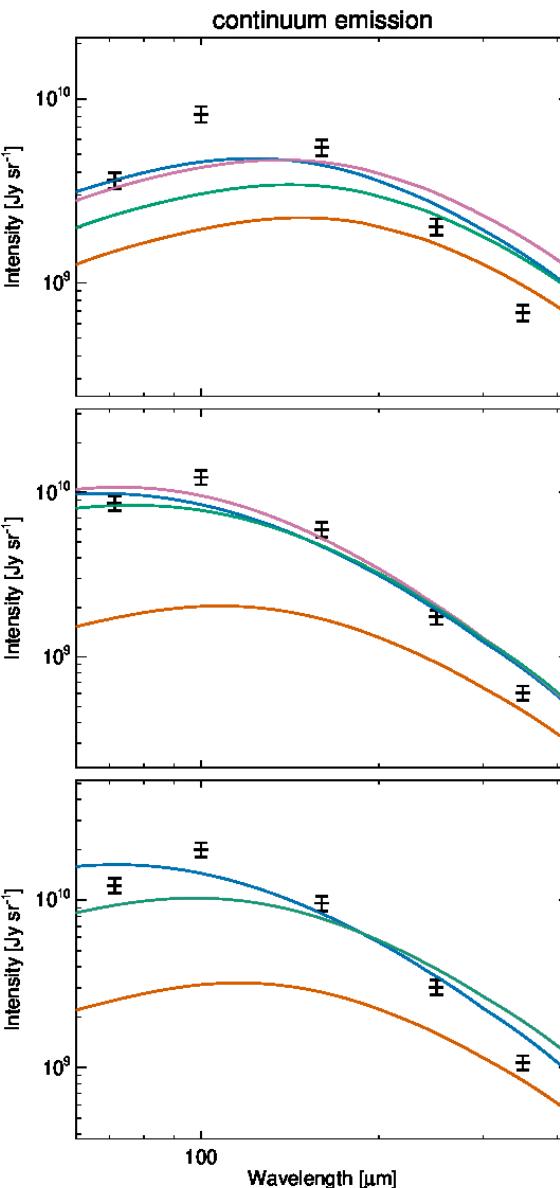
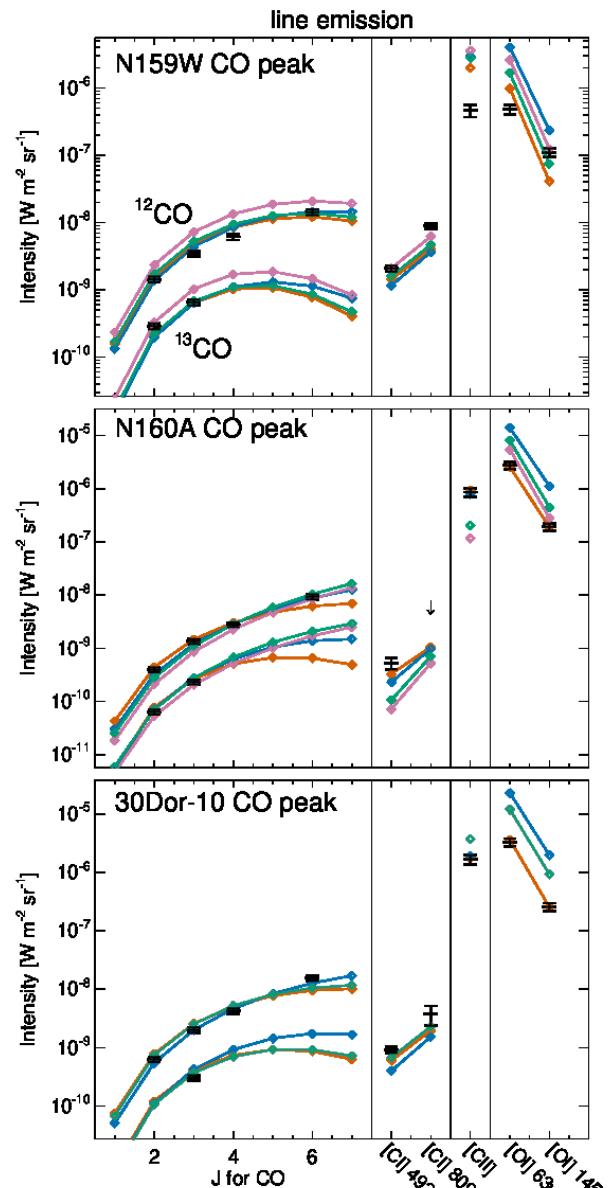
Animation of the velocity structure



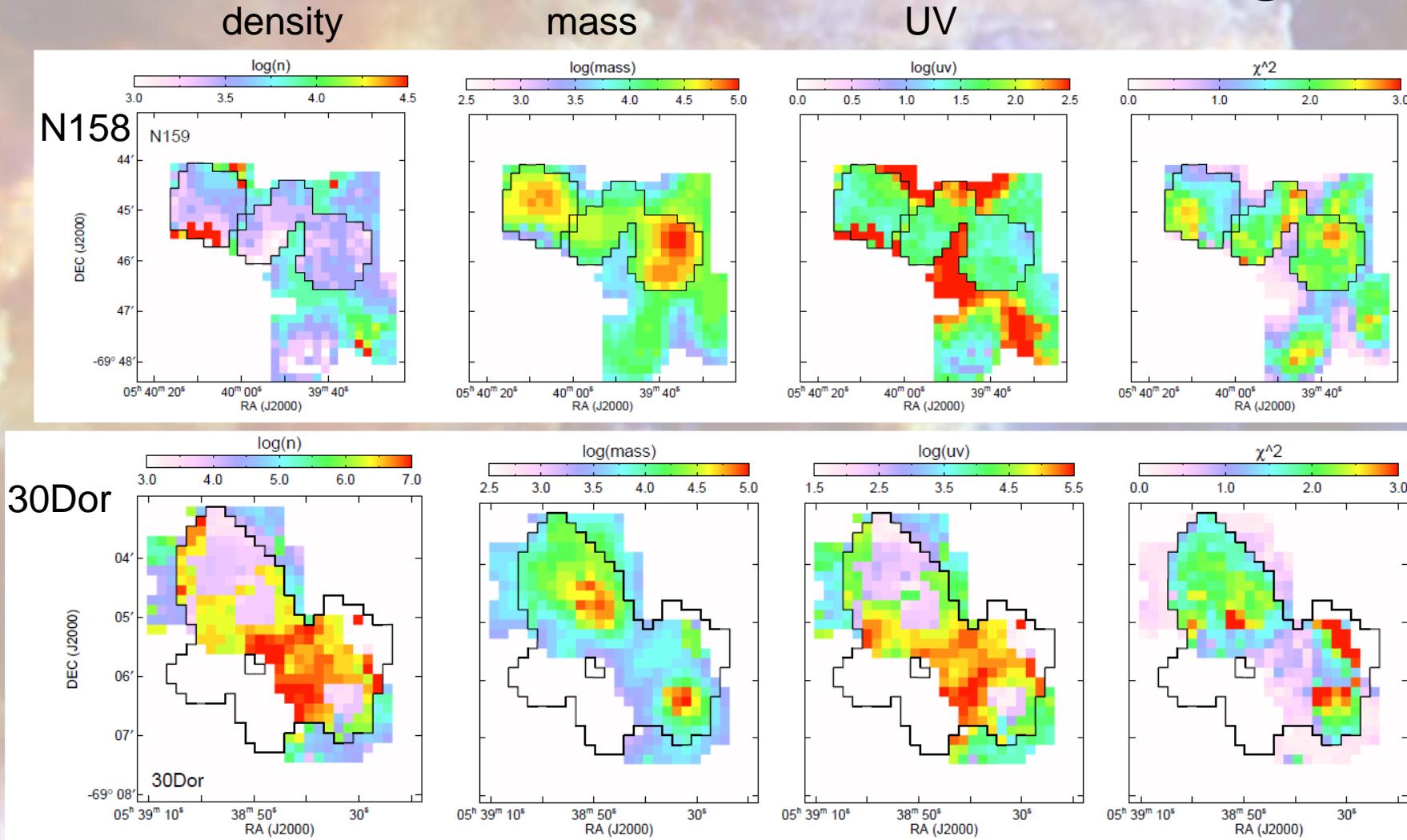
LMC
©NASA/JPL-Caltech/M. Meixner (STScI) and the SAGE Legacy Team.



Fitting line and dust continuum emission



Map-based PDR Modelling



Current KOSMA- τ Developments

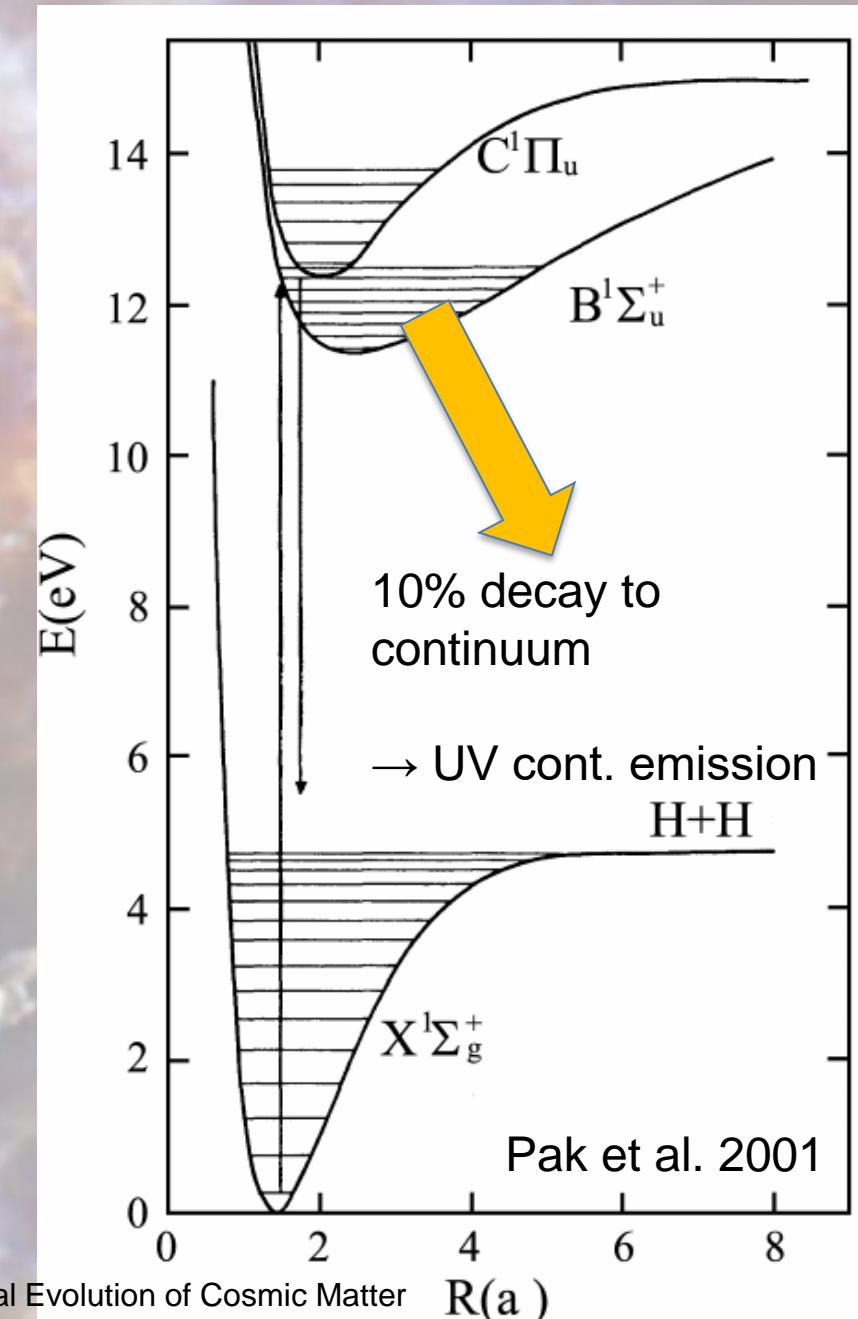
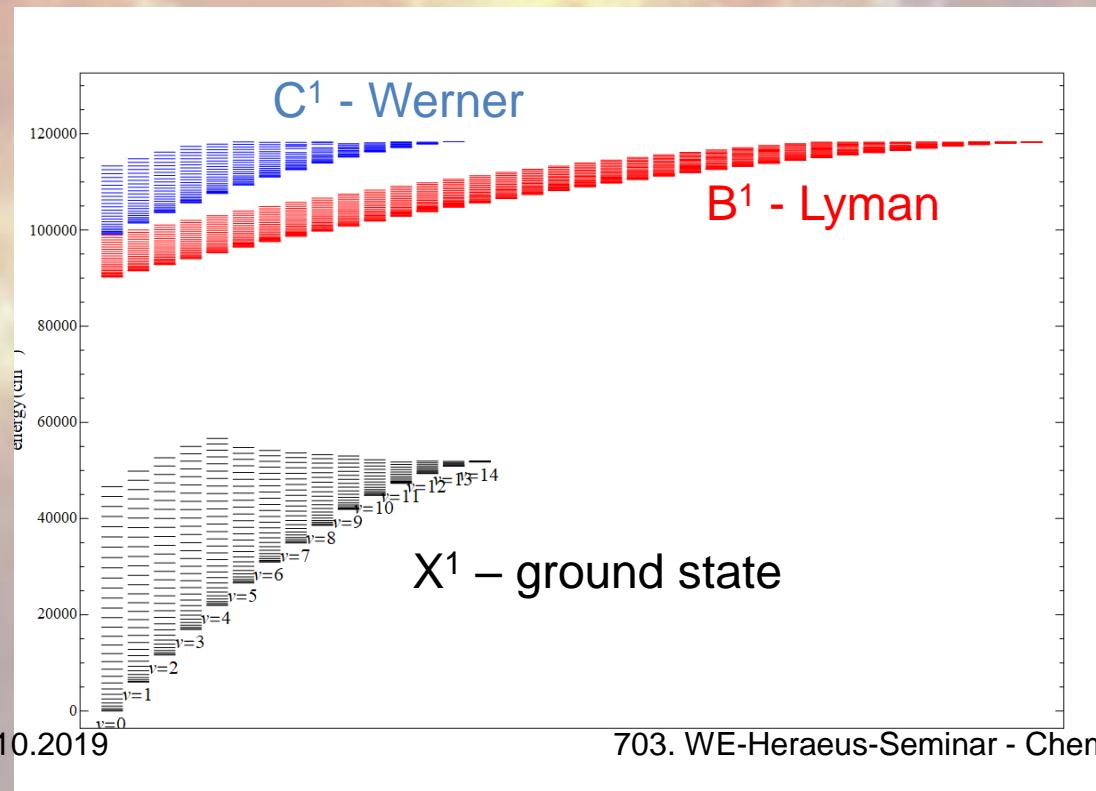
- Non-stationary PDR structure
 - t-dependent solution of chemistry (tests)
 - t-dependent parameters, e.g. FUV input
 - non-stationary particle transport , e.g. diffusion, advection, mass evaporation (PhD project A. Baby)
- KOSMA- τ 3D
 - inclusion of systematic velocities
 - full line & continuum radiative transfer (PhD projects C. Bruckmann & C. Yanitski)
 - performance improvements
- Microphysics/chemistry
 - chemical heating (tests)
 - surface chemistry (done)
- full H₂ 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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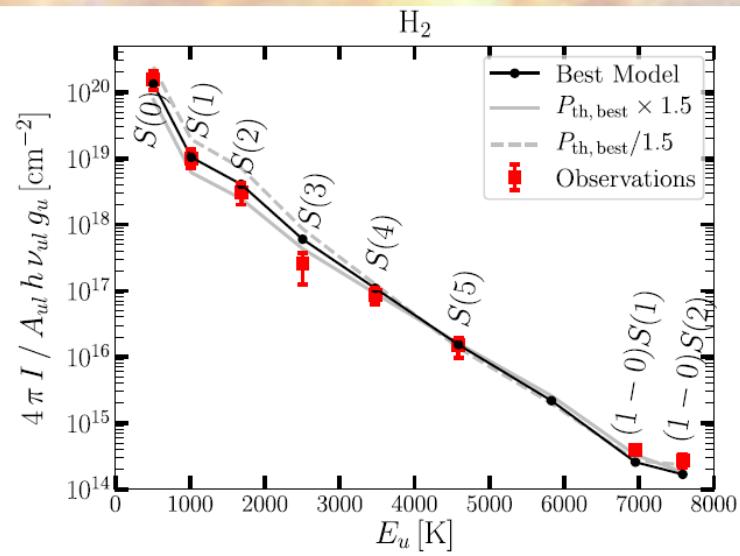
H_2 Excitation Problem

- H_2 dissociation via UV line absorption
- about 5000 quadrupole transitions
- about 15000 X-B and X-C dipole transitions



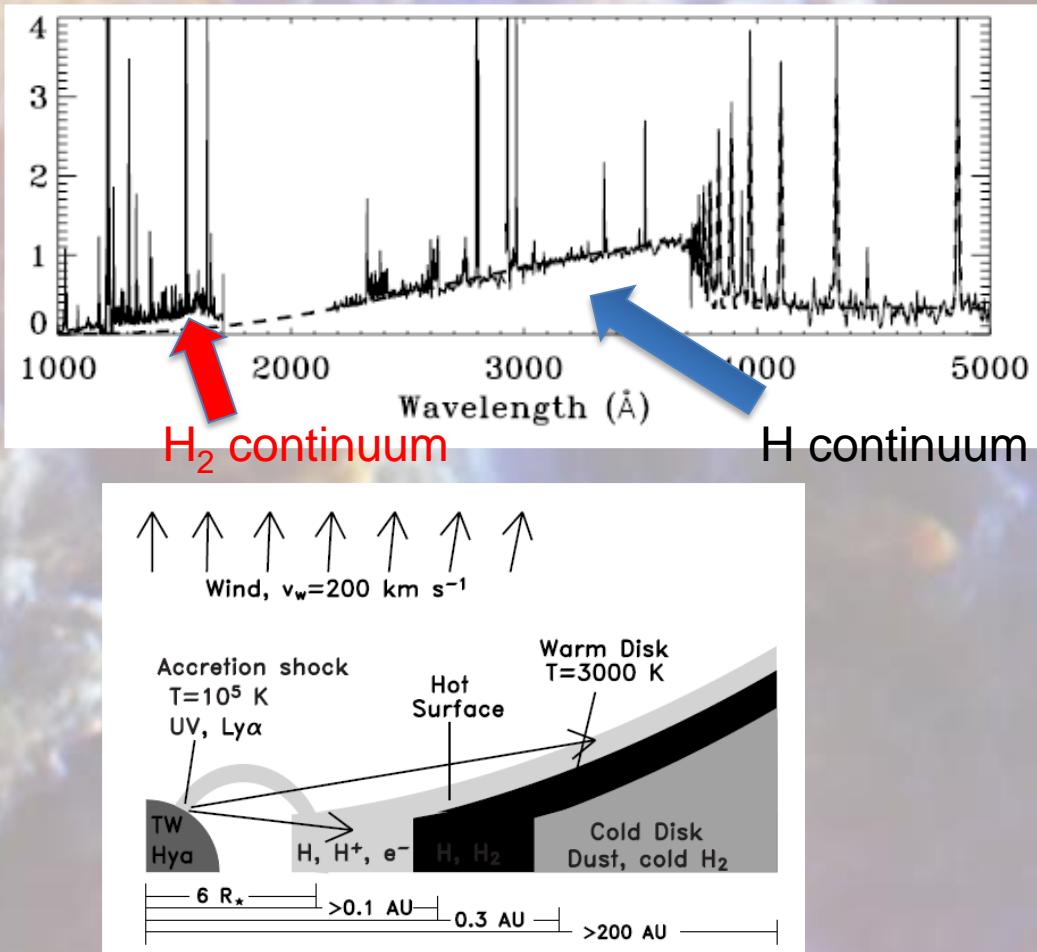
H_2 excitation problem

H_2 IR emission from PDRs
Joblin et al. 2018,
Habart et al. 2011



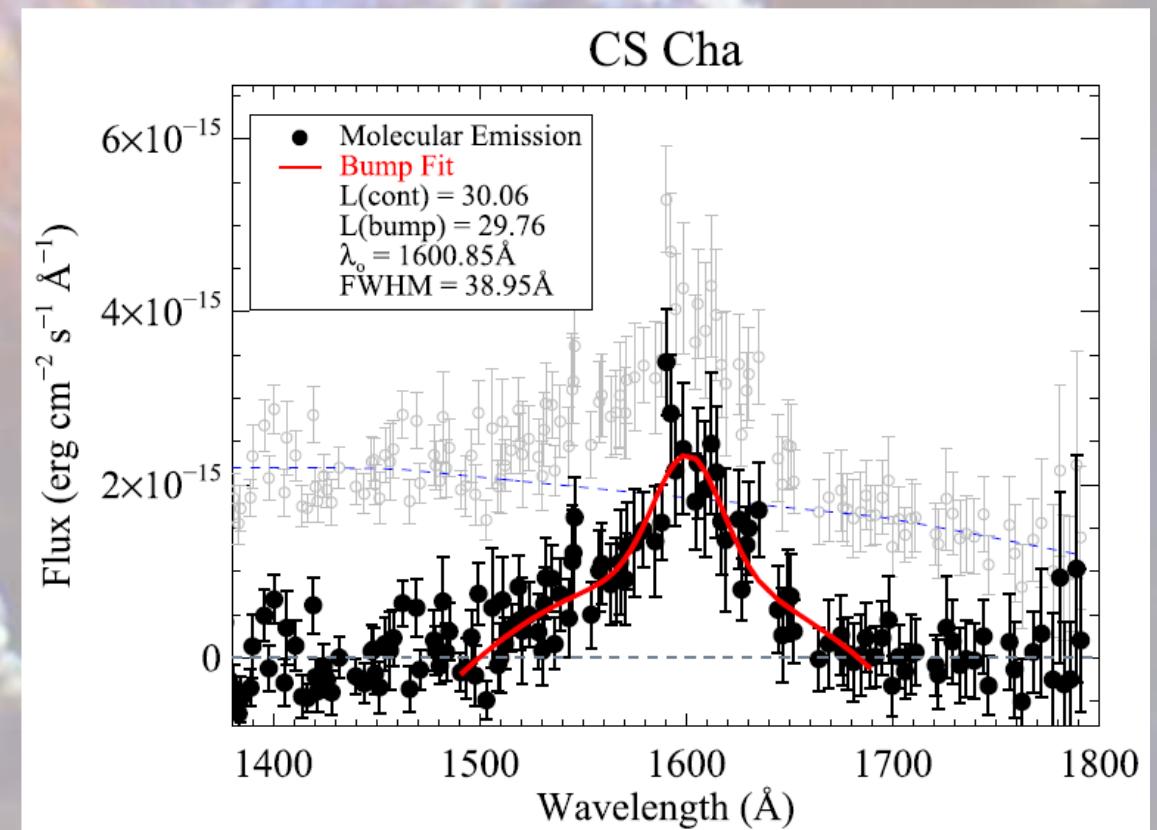
Preparing for JWST!

TW Hya spectrum, Herczeg et al. 2004



1600 Å bump

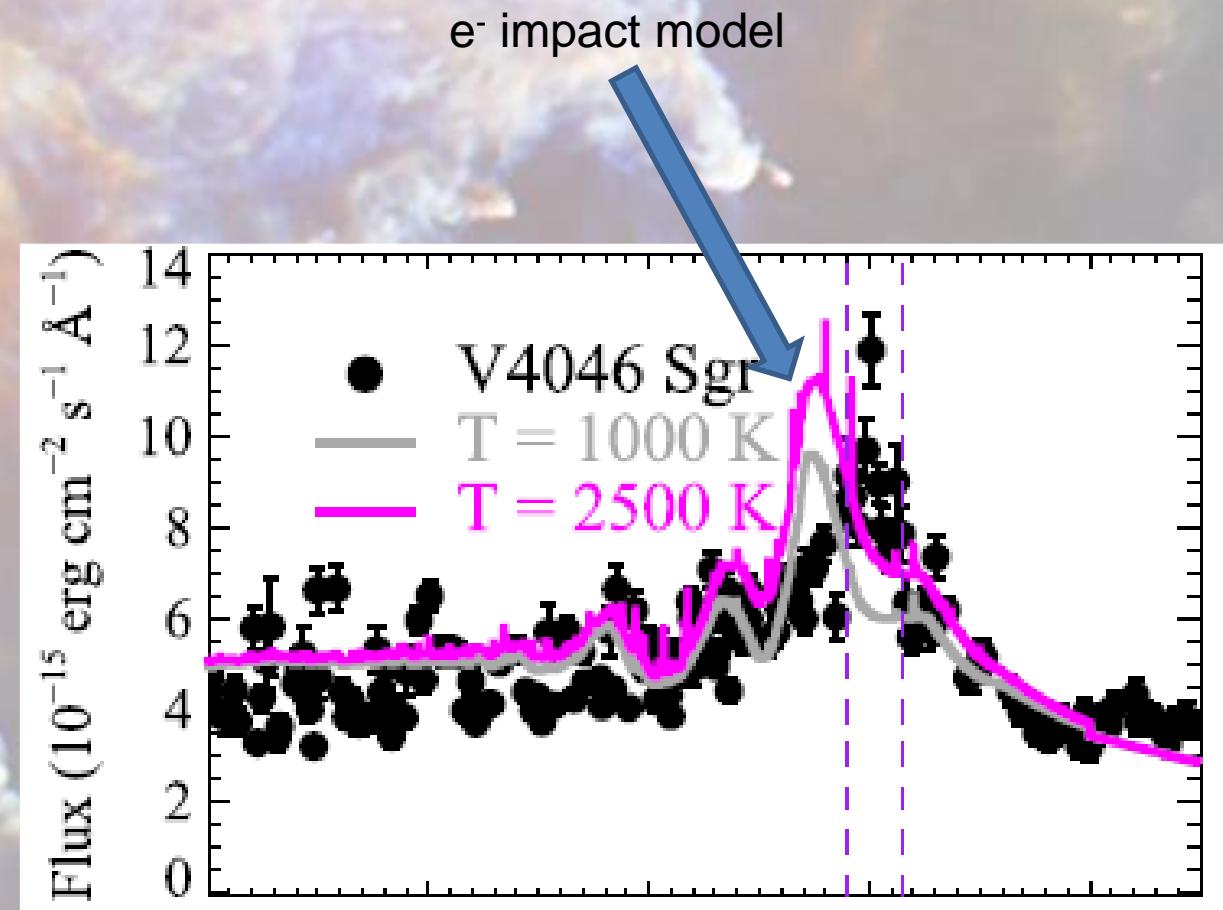
- Classical T Tauri Stars (CTTSs), show a spectral feature in the FUV continuum of some (broad emission approximately centered at 1600 Å)
- inconsistent with models of H₂ excited by electron-impact
- powered by Ly-α photons
- Ly-α driven dissociation of H₂O



France et al. 2017

1600 Å bump

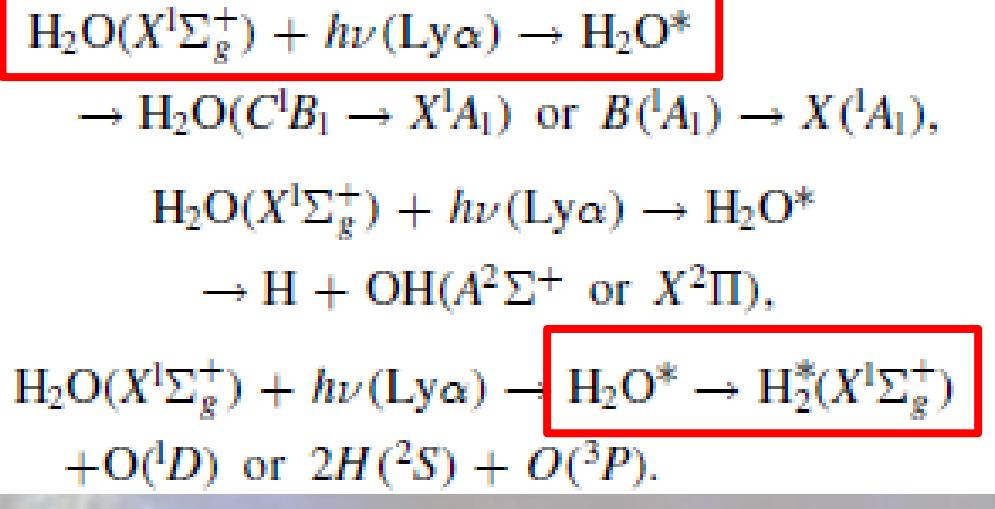
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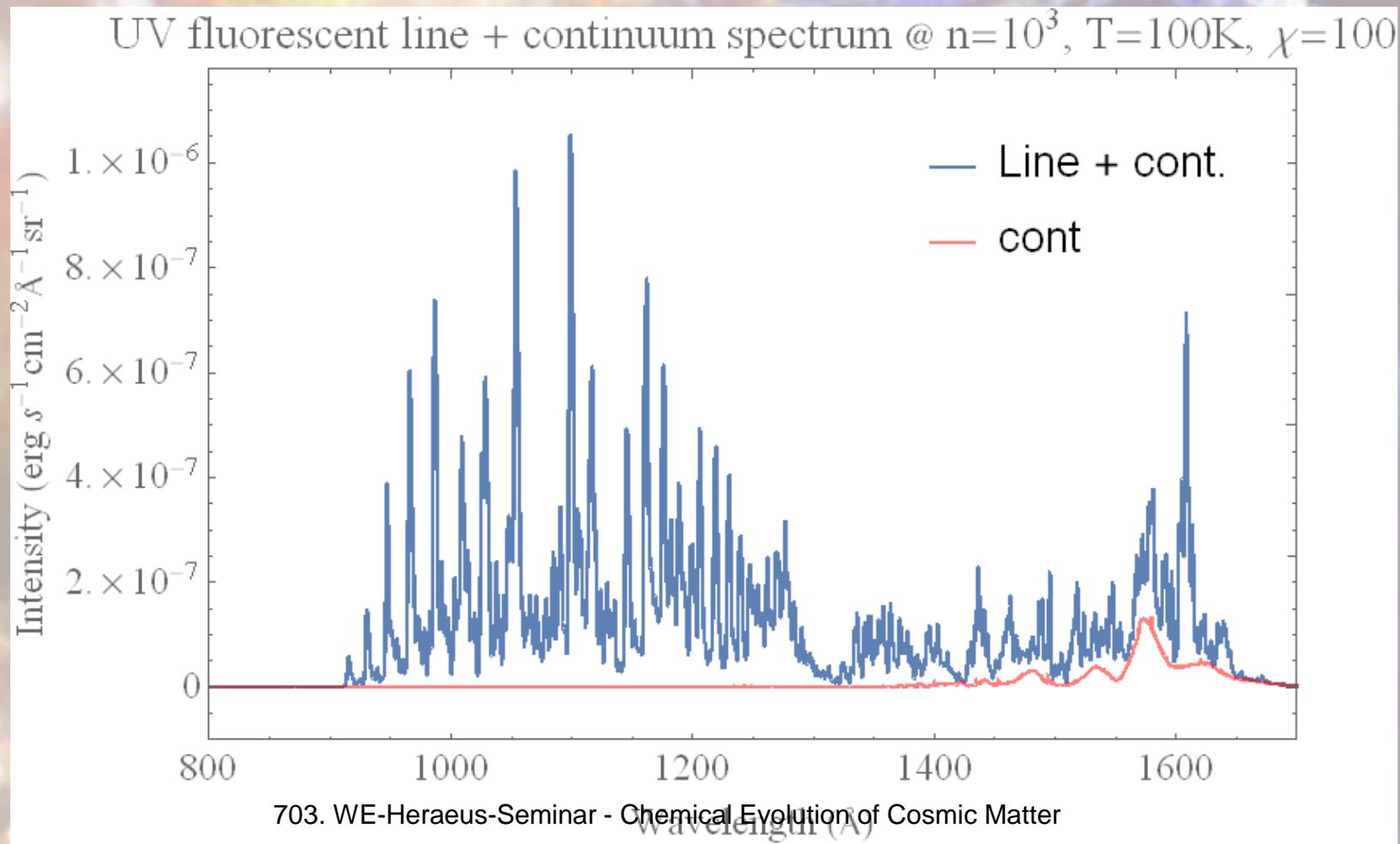
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France et al. 2017

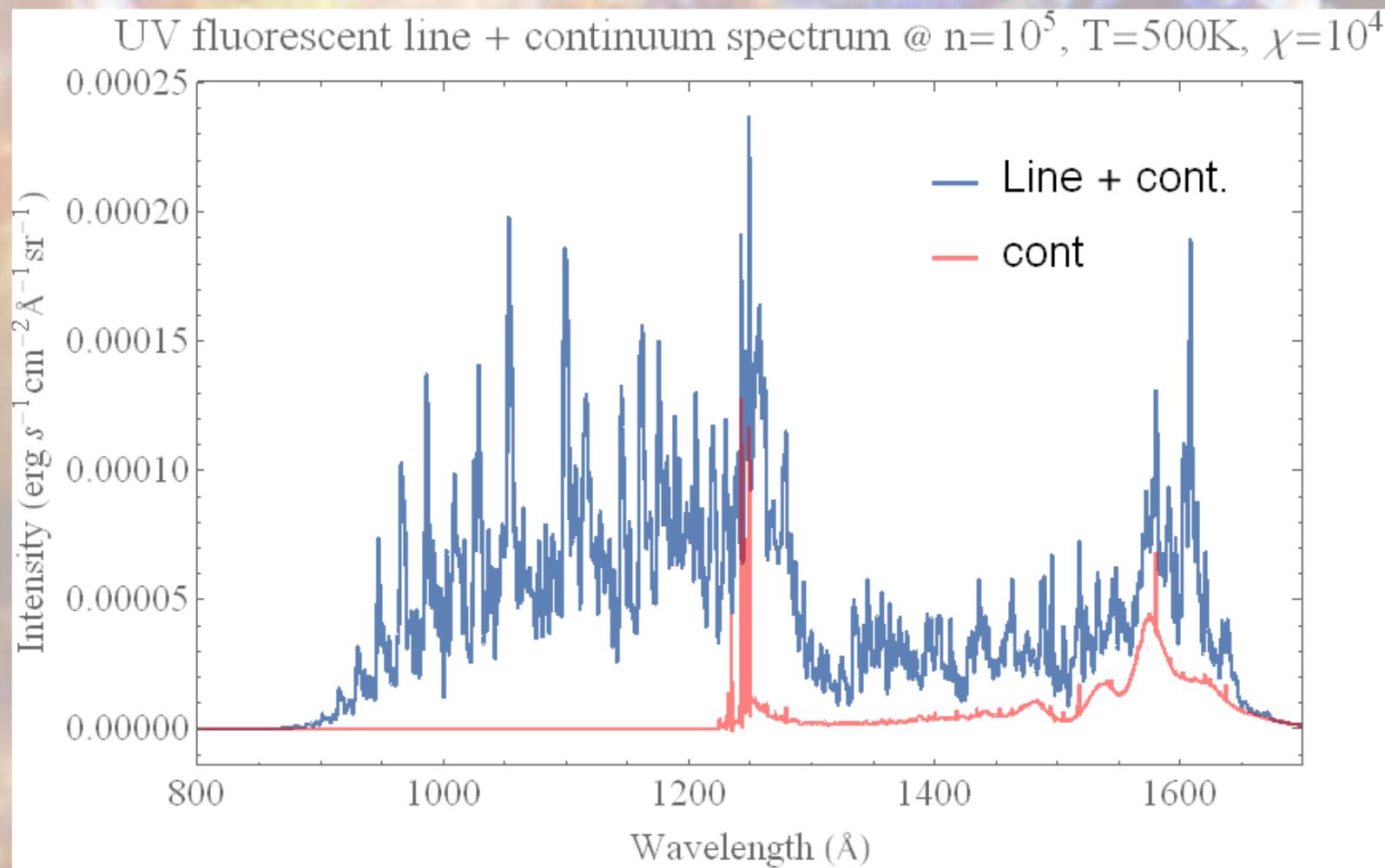
Fluorescent UV spectrum of H₂ + cont.

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



Fluorescent UV spectrum of H₂

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

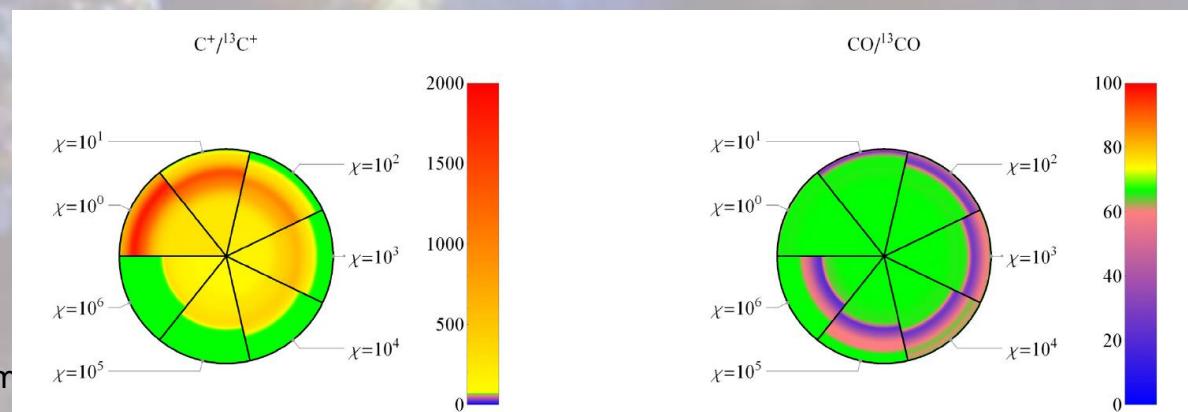


Chemistry

The background image is a composite of several astronomical observations. It features a dense, multi-colored nebula with prominent yellow and orange regions on the left, transitioning to blue and purple on the right. Interspersed throughout are numerous small, white, star-like points of varying sizes, suggesting distant galaxies or stars. A faint, dark diagonal band cuts across the center of the image.

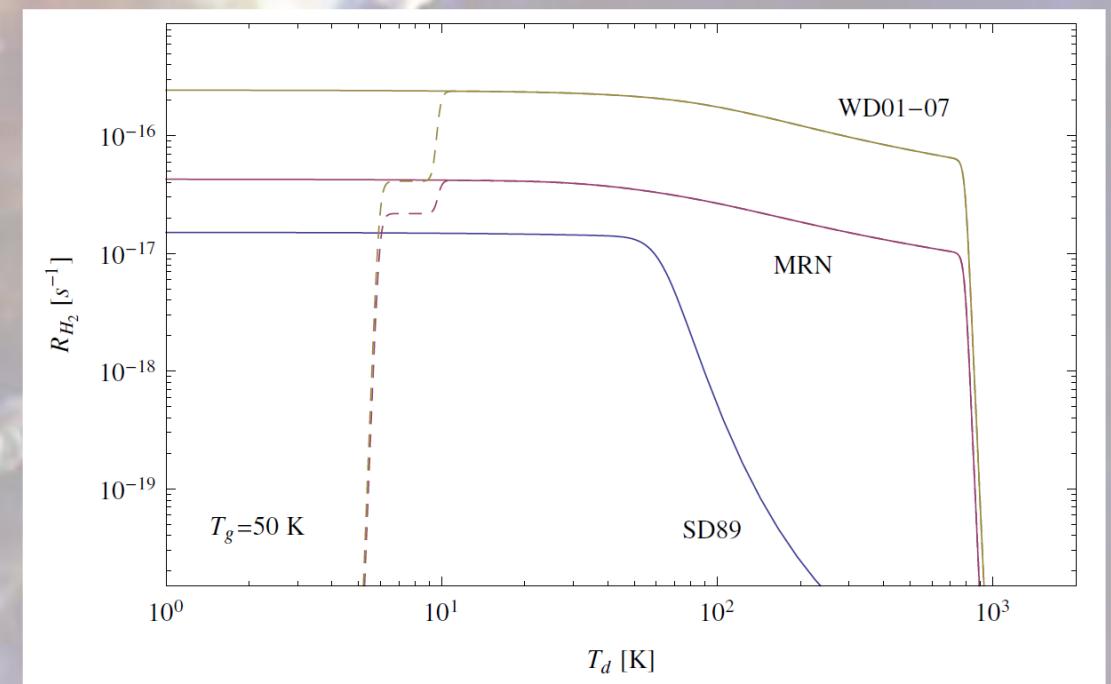
Chemistry in KOSMA-T

- 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}C and ^{18}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: UDfA 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)

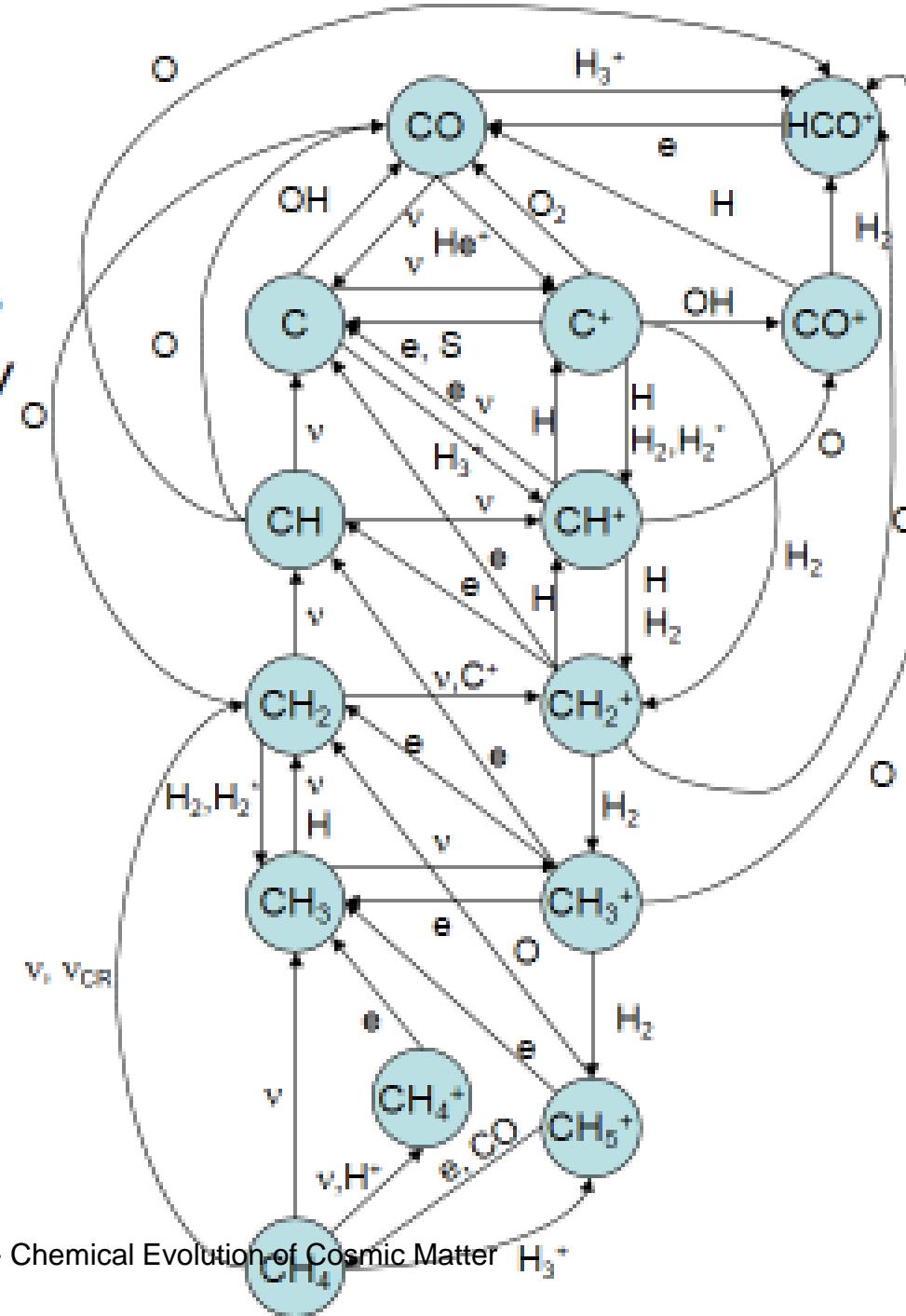


Full Surface Chemistry Upgrade

- Coupling of gas-phase and surface chemistry
 - Steady-state chemistry
 - Rate equation approach
 - Processes included:
 - Adsorption
 - desorption only from 2 top layers
 - thermal desorption
 - photo-desorption
 - photo-dissociative desorption
 - photo-dissociation on grains
 - CR induced photo-desorption/diss.
 - H₂-formation induced desorption
 - chemistry induced desorption
 - surface-surface processes
- (Hasegawa et al. 1992,1993)
- (only neutrals, no sticking of H₂)
- (Aikawa et al. 1996)
- (binding energies from UDfA + updates)
- (photo cross-section like gas-phase)
- (eg. JH₂O +hv → OH + H Andersson+ 08)
- (equivalent to gas-phase)
- (Hasegawa & Herbst 1993)
- (Willacy et al. 1994, 2007)
- (Minissale et al. 2015, Cazaux et al. 2015)
- (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 H₂:



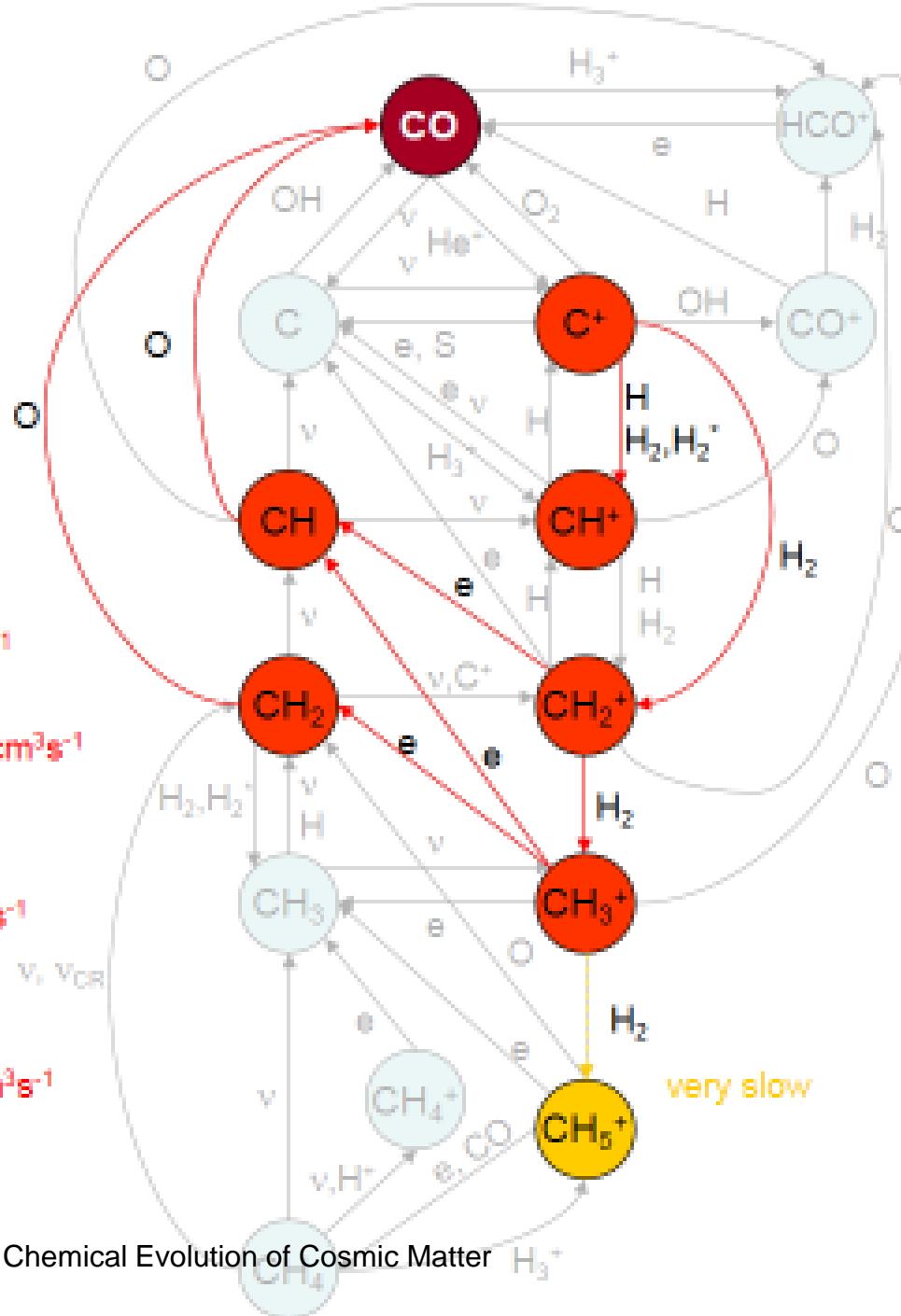
instead:



then:

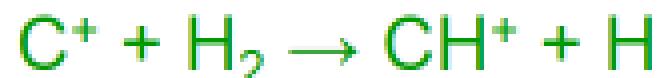


and:

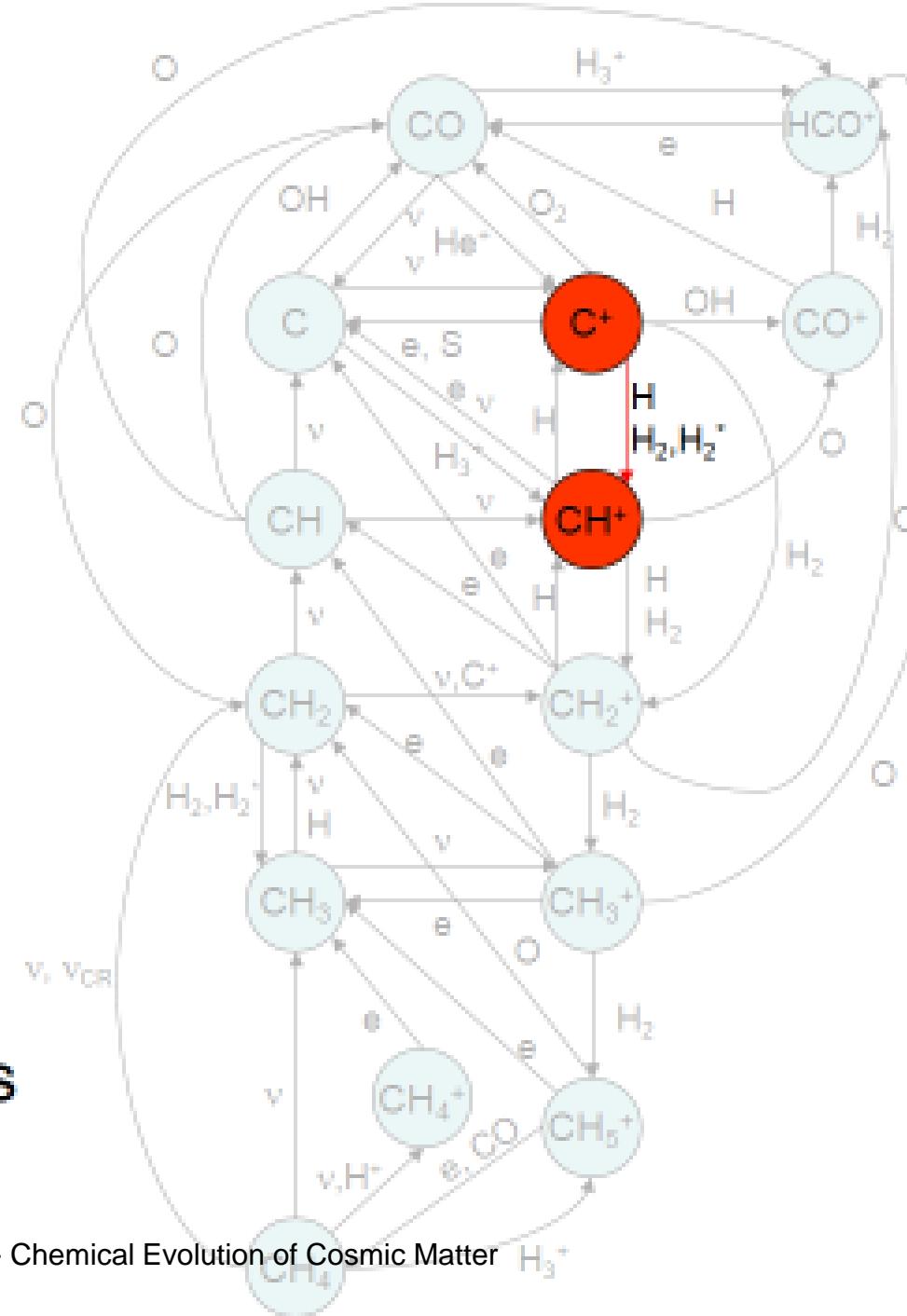


Example: PDR

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 K, n=10⁴-10⁵ cm⁻³

carbon locked in CO



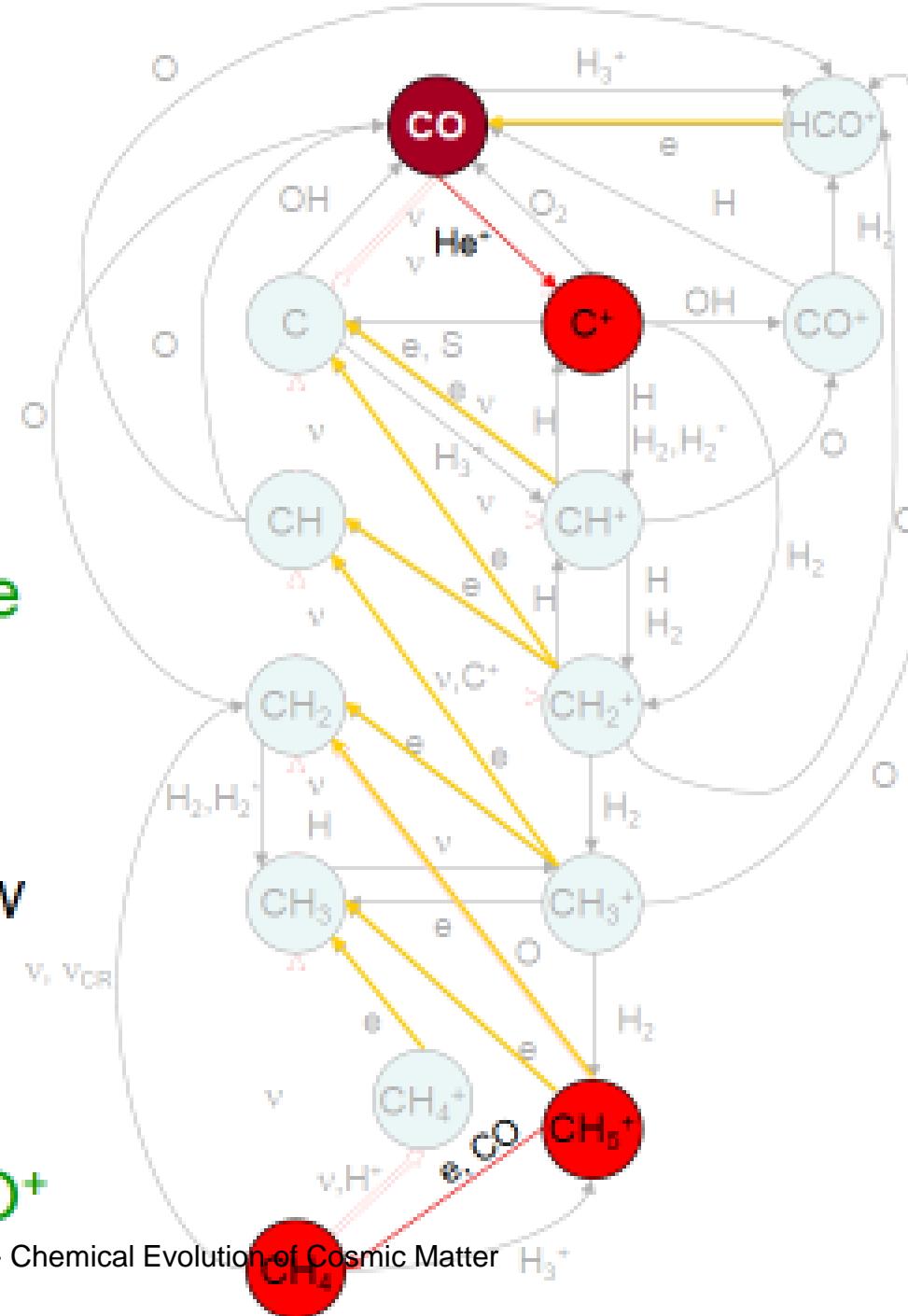
FUV fully absorbed

some roads vanish

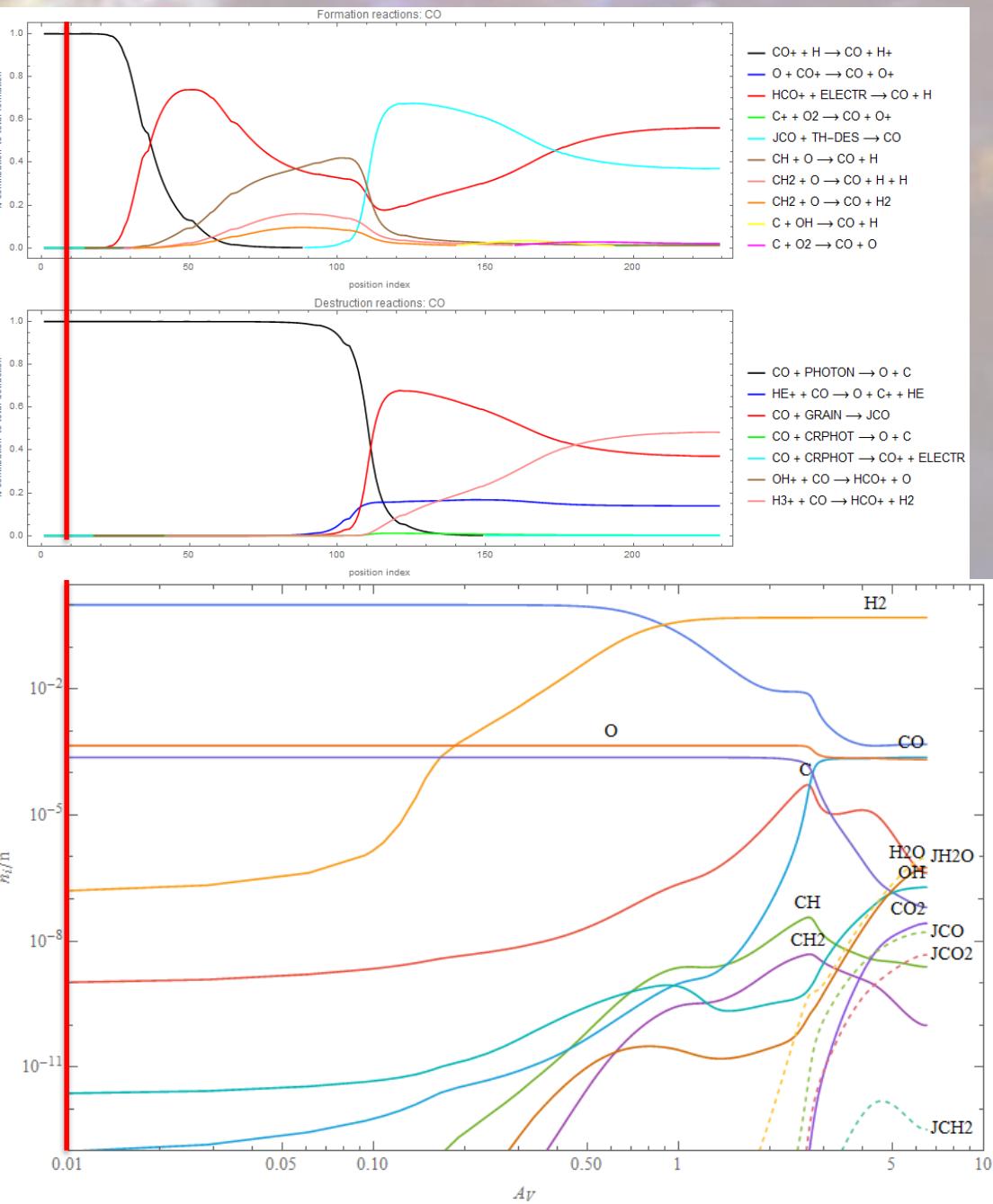
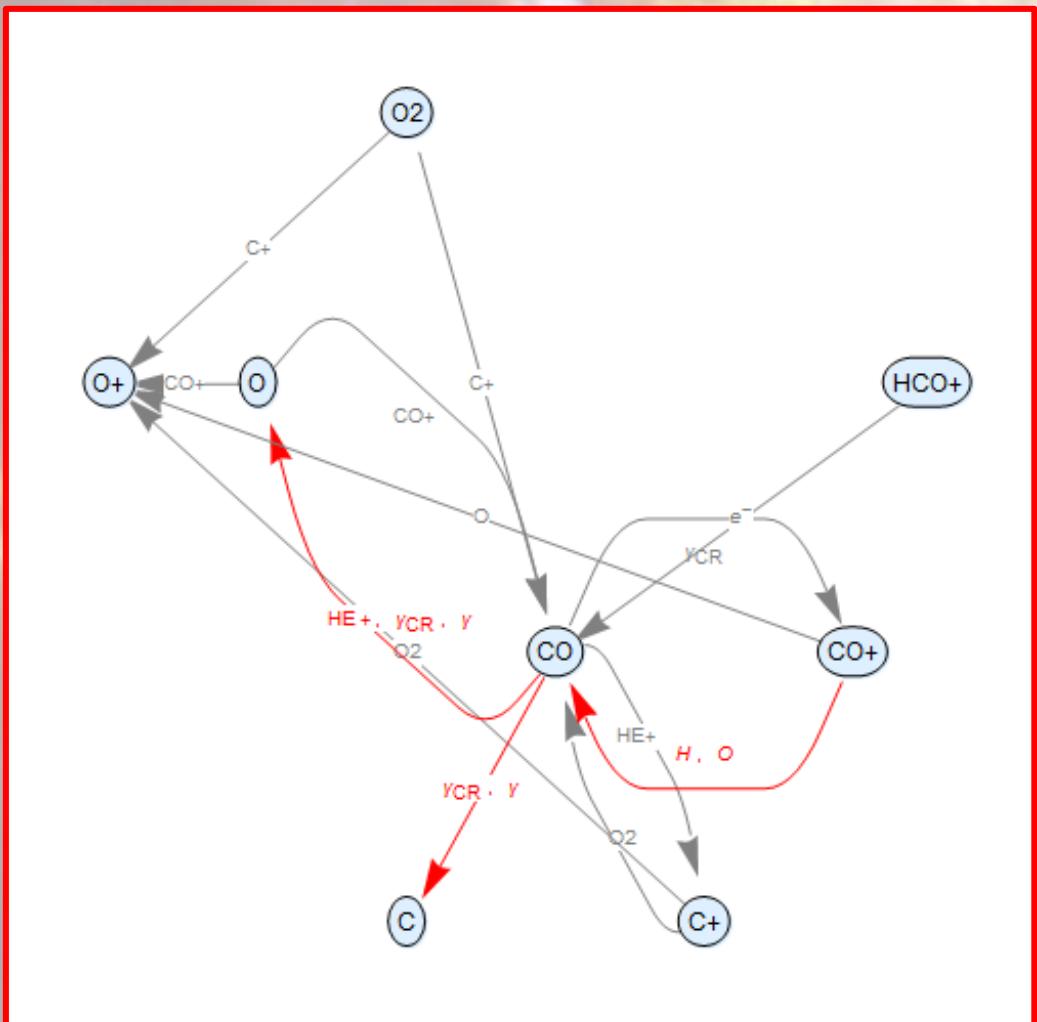
some roads become slow

e.g. reactions with e⁻

but:



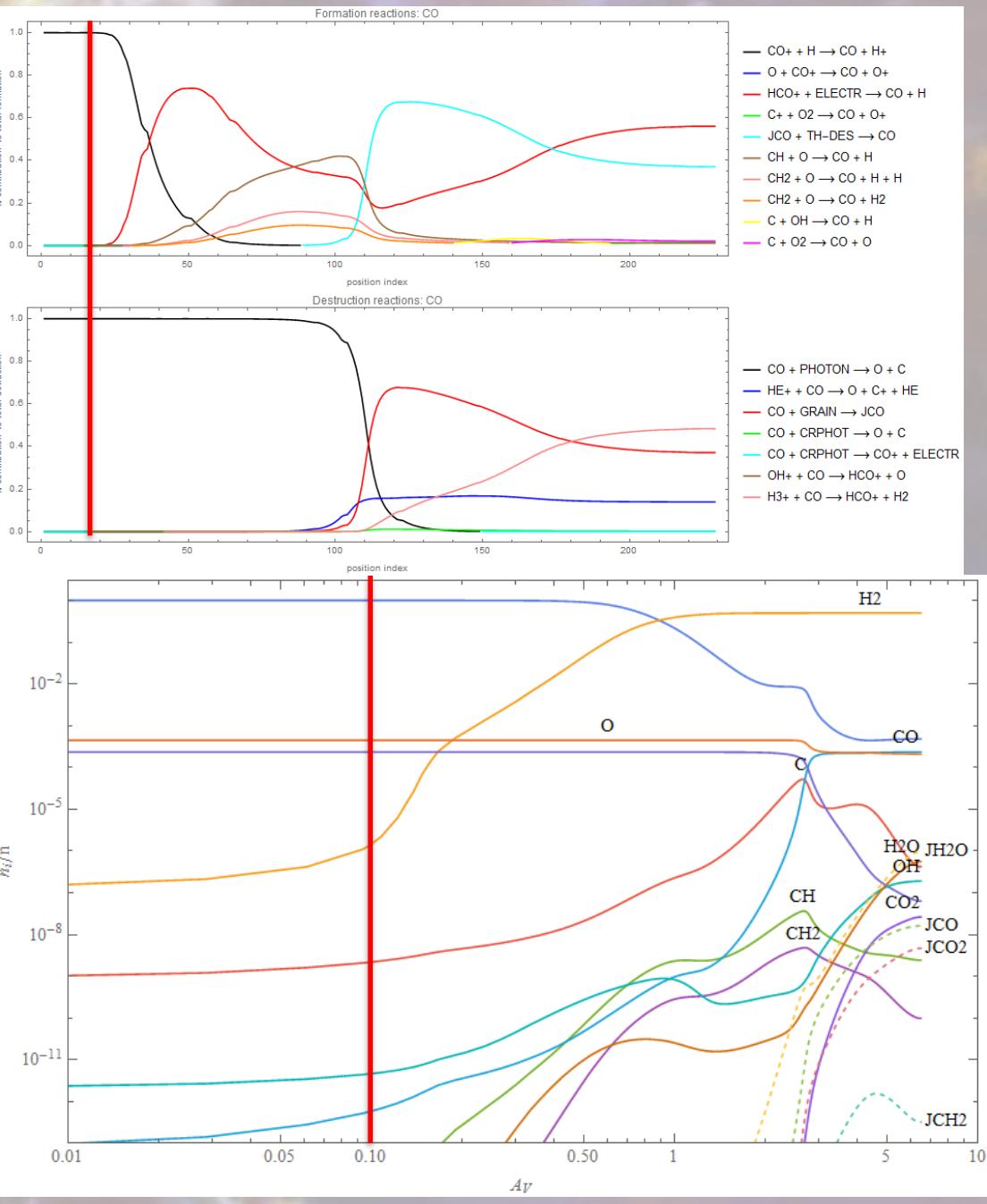
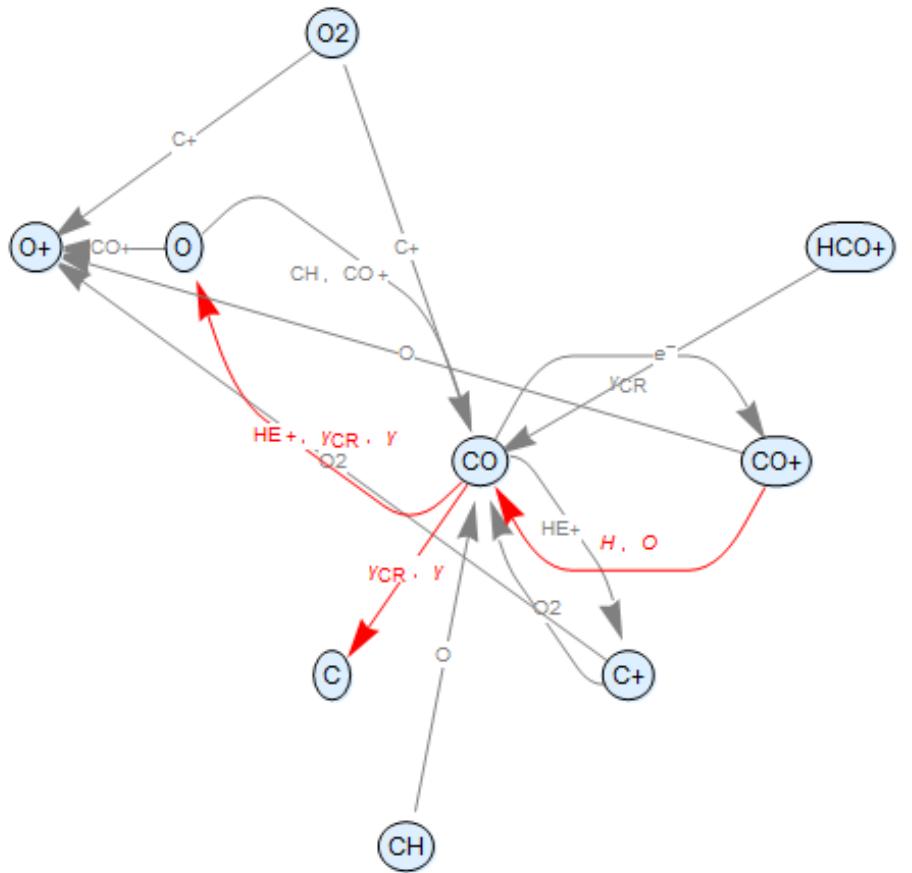
$n = 10^4 \text{ cm}^{-3}$
 $\chi = 10^4$
 small chemical network



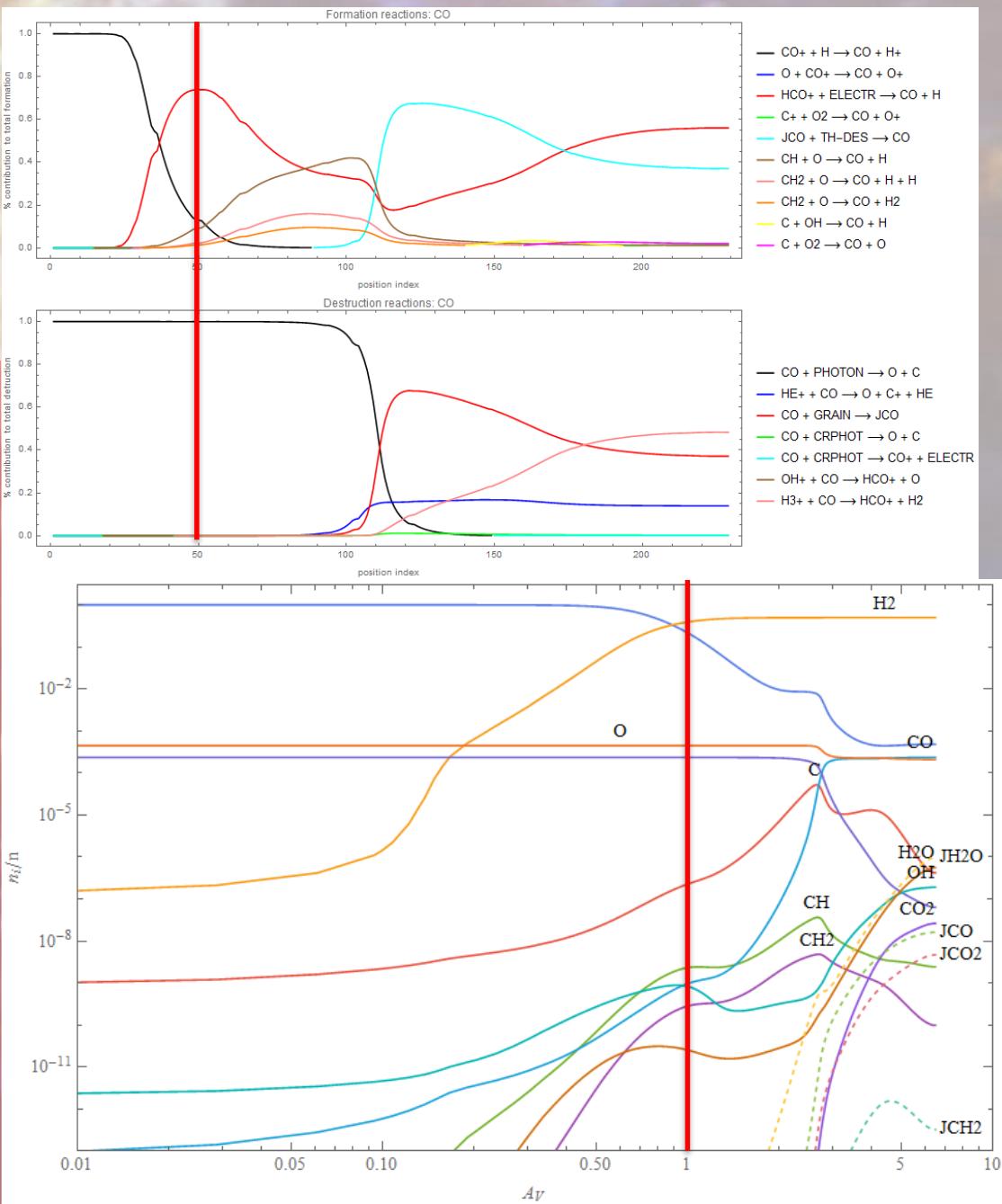
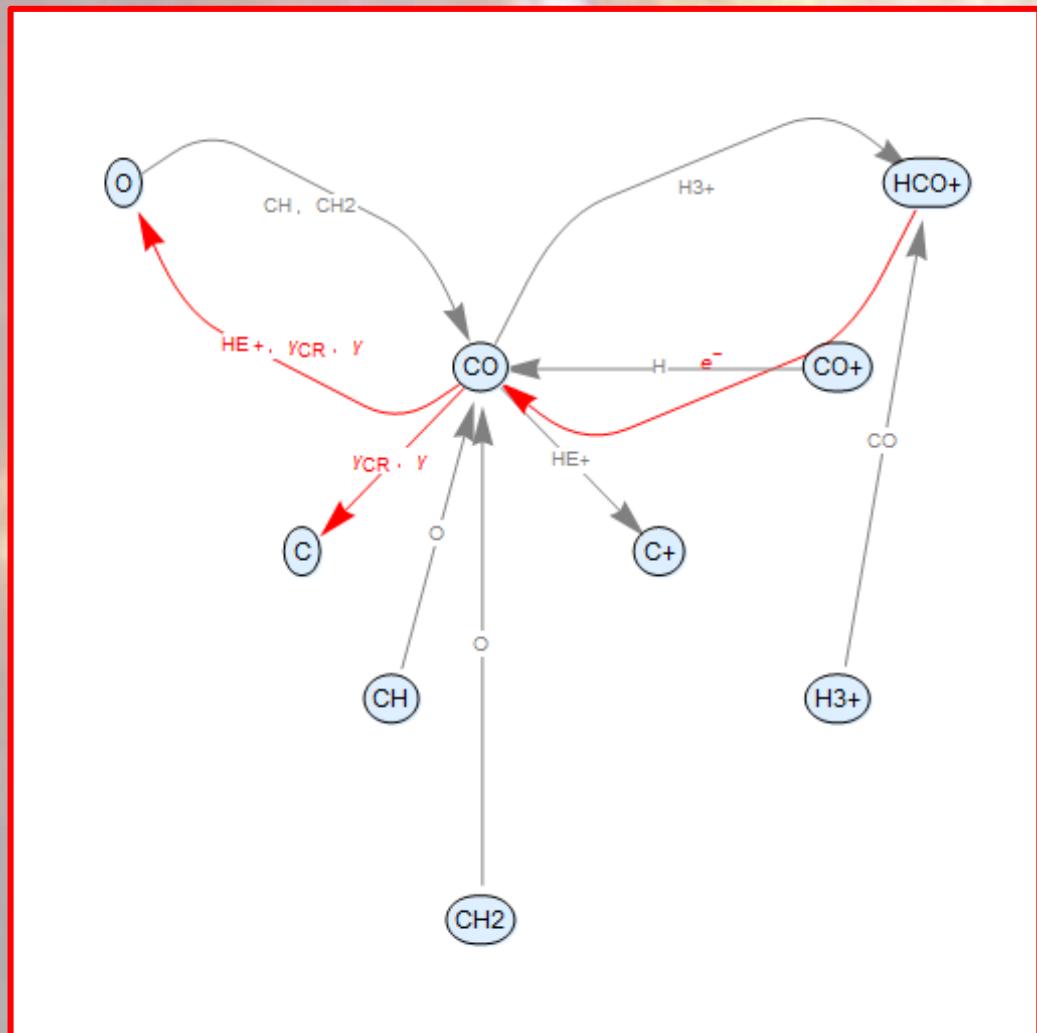
$$n = 10^4 \text{ cm}^{-3}$$

$$\chi = 10^4$$

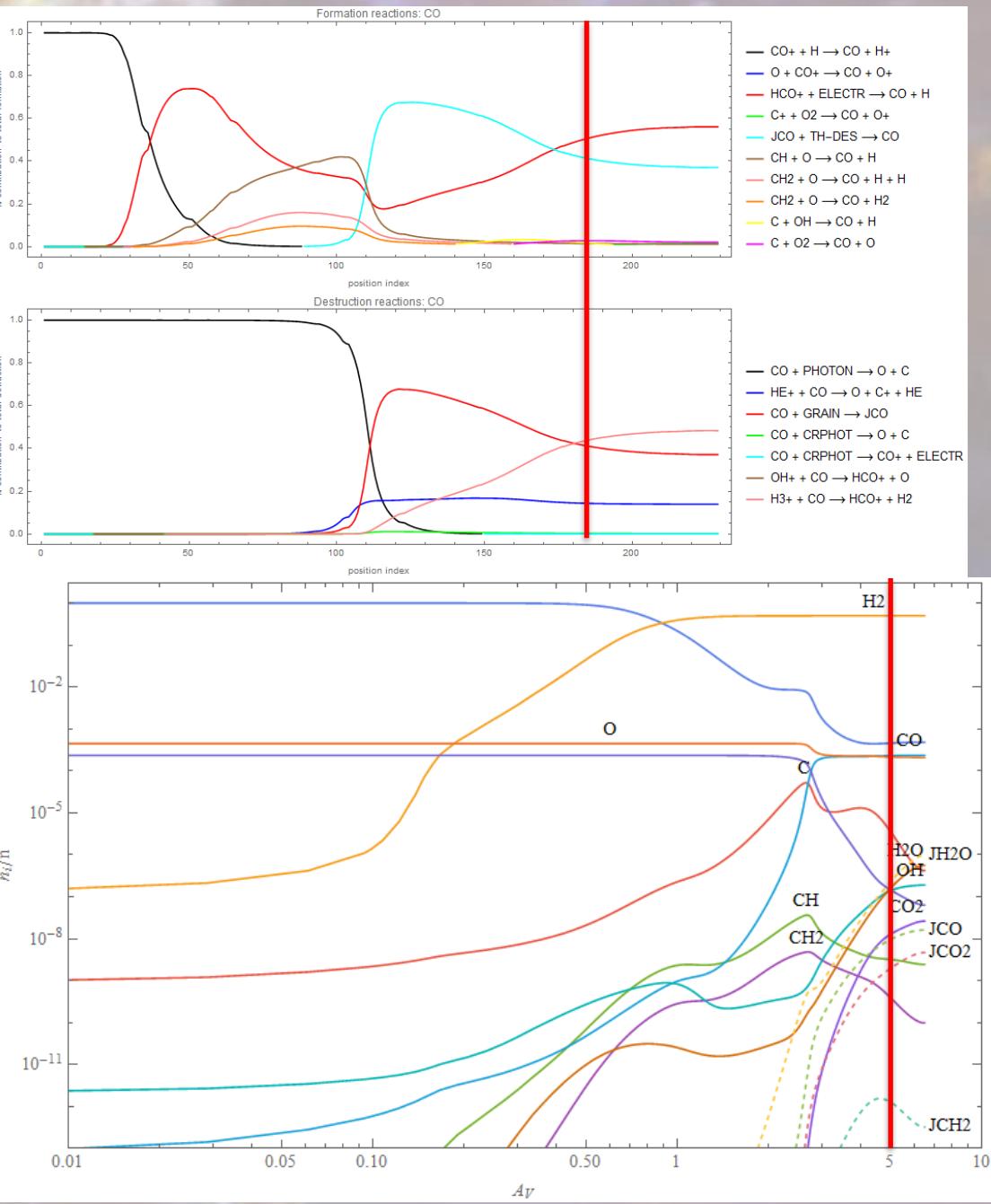
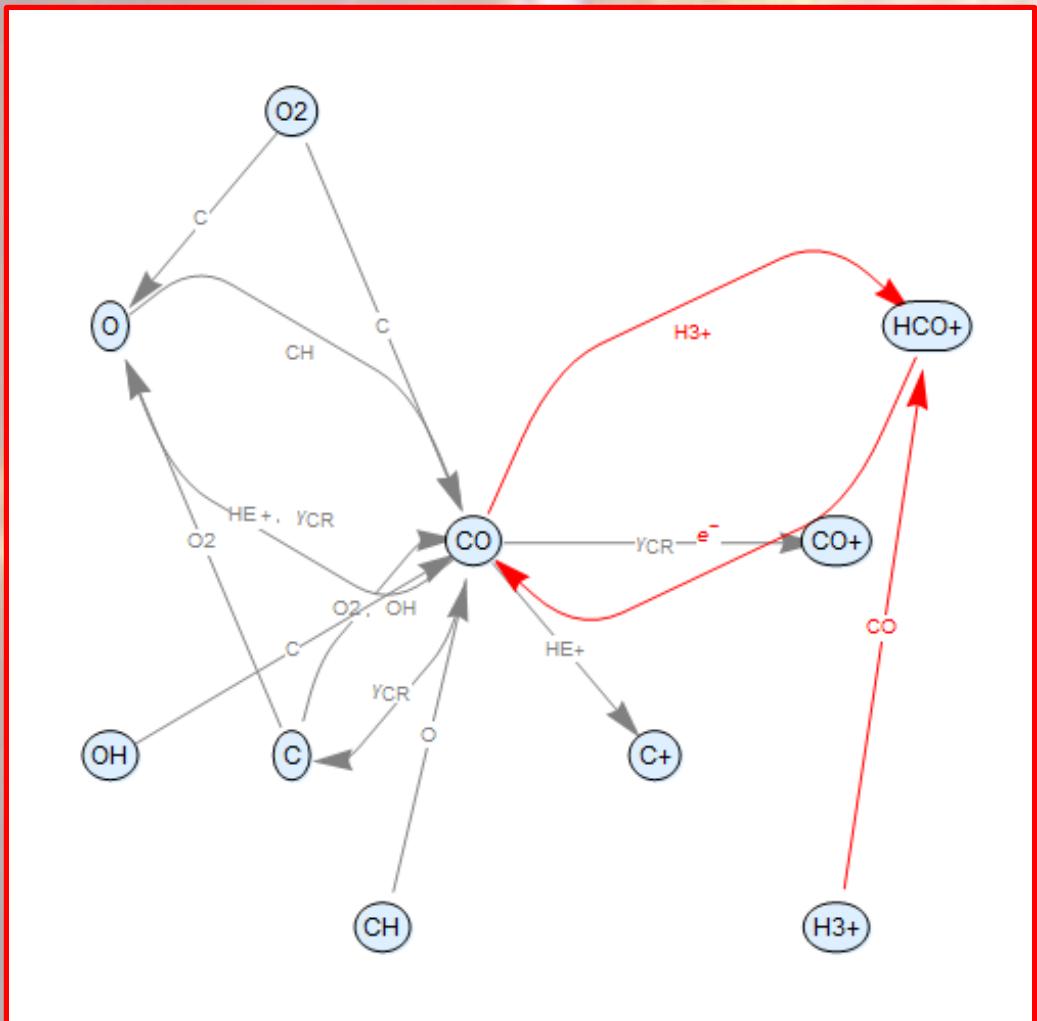
small chemical network



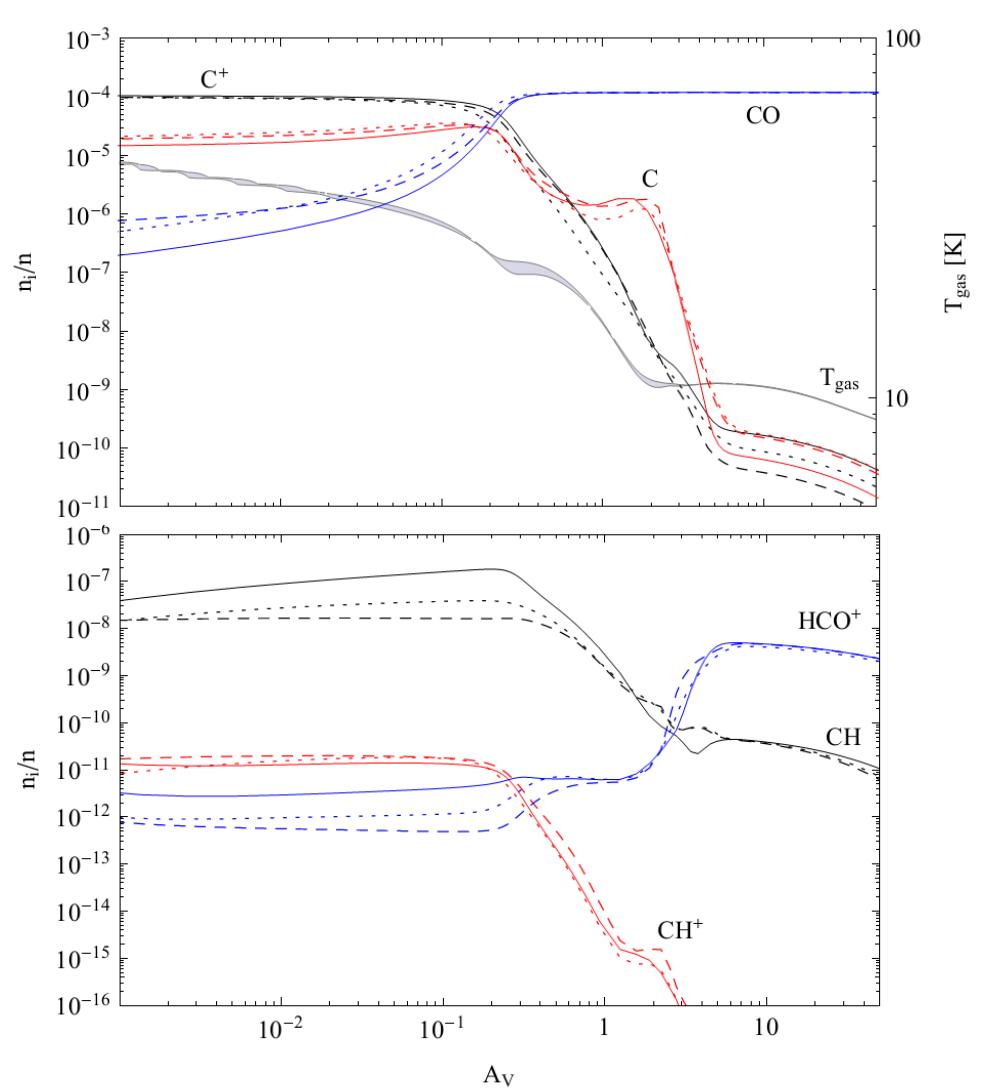
$n = 10^4 \text{ cm}^{-3}$
 $\chi = 10^4$
 small chemical network



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



Ugly details



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

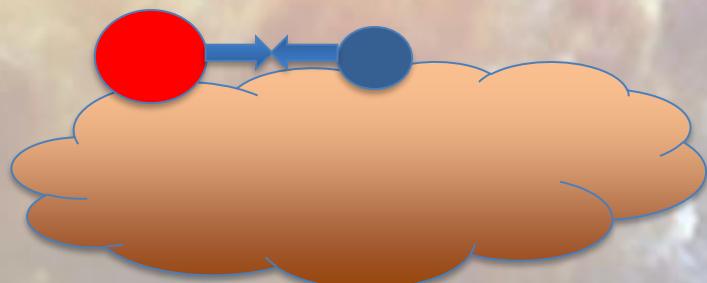
- Influence of different chemical databases
(UDfA, OSU, KIDA)

but also,

- geometry
- etc.

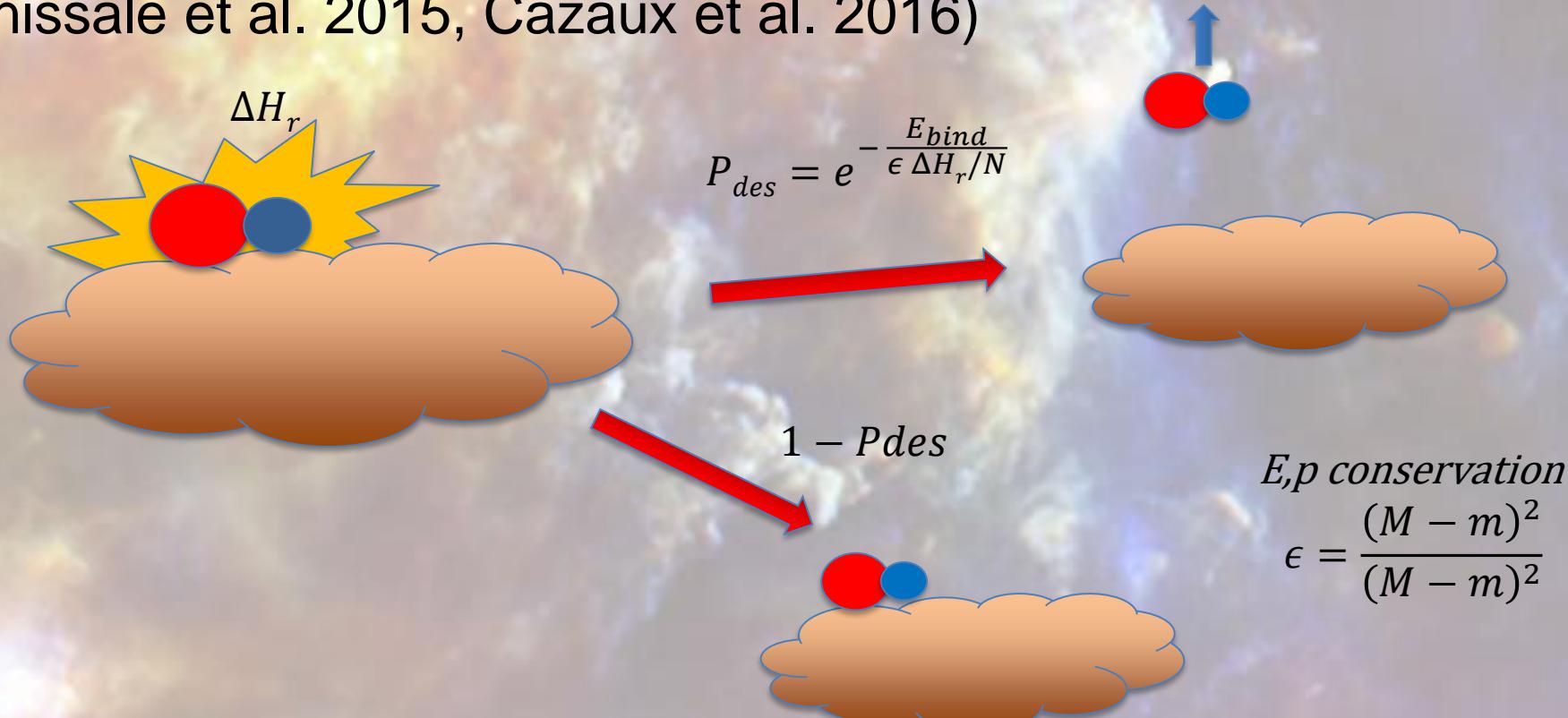
Full Surface Chemistry Upgrade

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

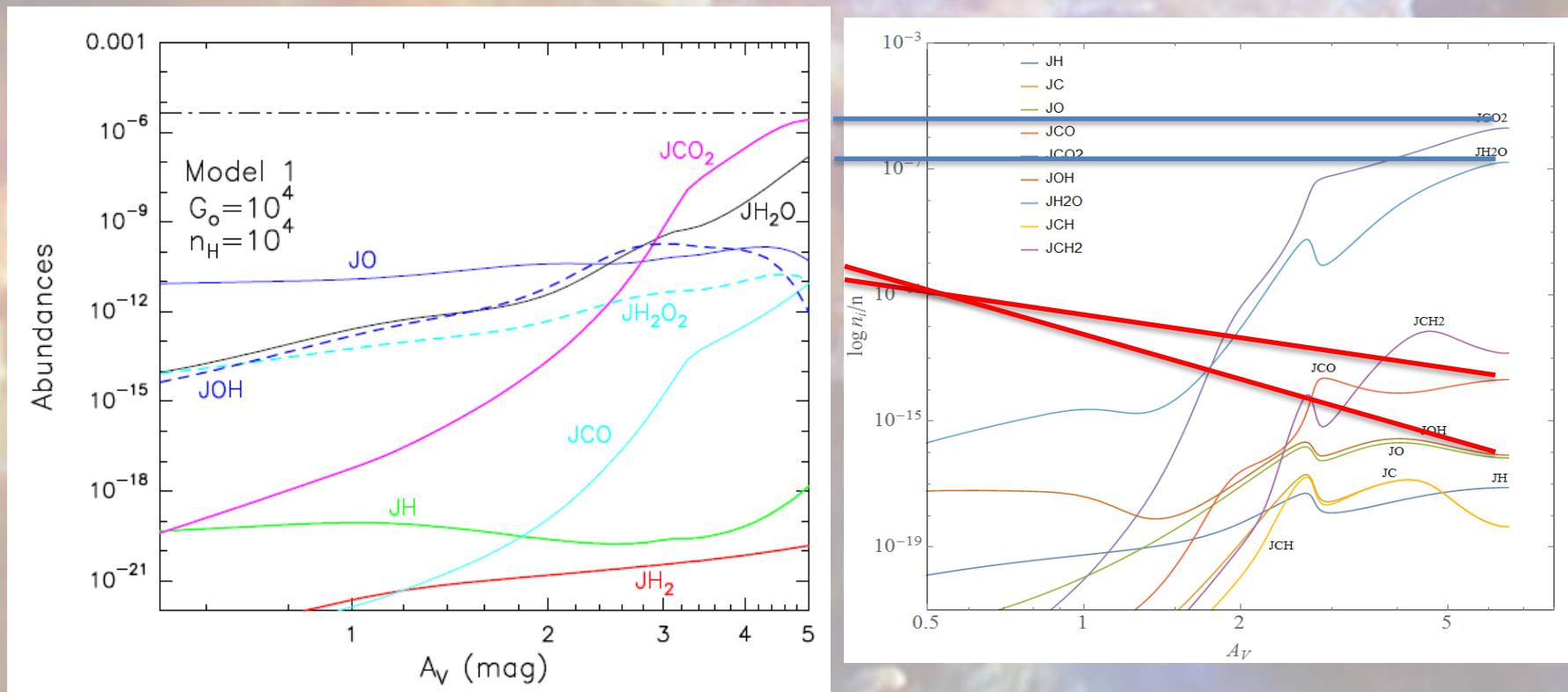


Full Surface Chemistry Upgrade

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



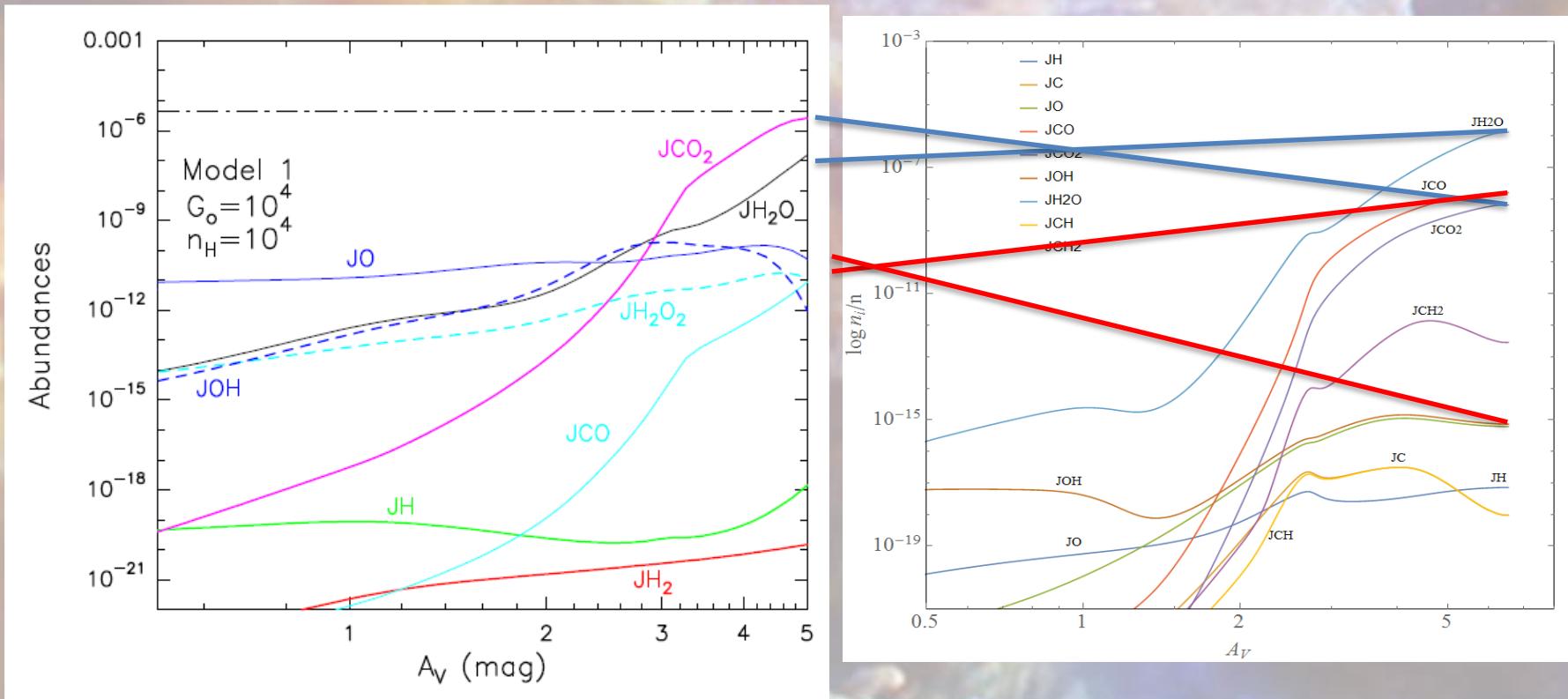
Chemical details with impact



Esplugues et al. 2016

KOSMA-τ with „comparable“ setup

Chemical details with impact



Esplugues et al. 2016

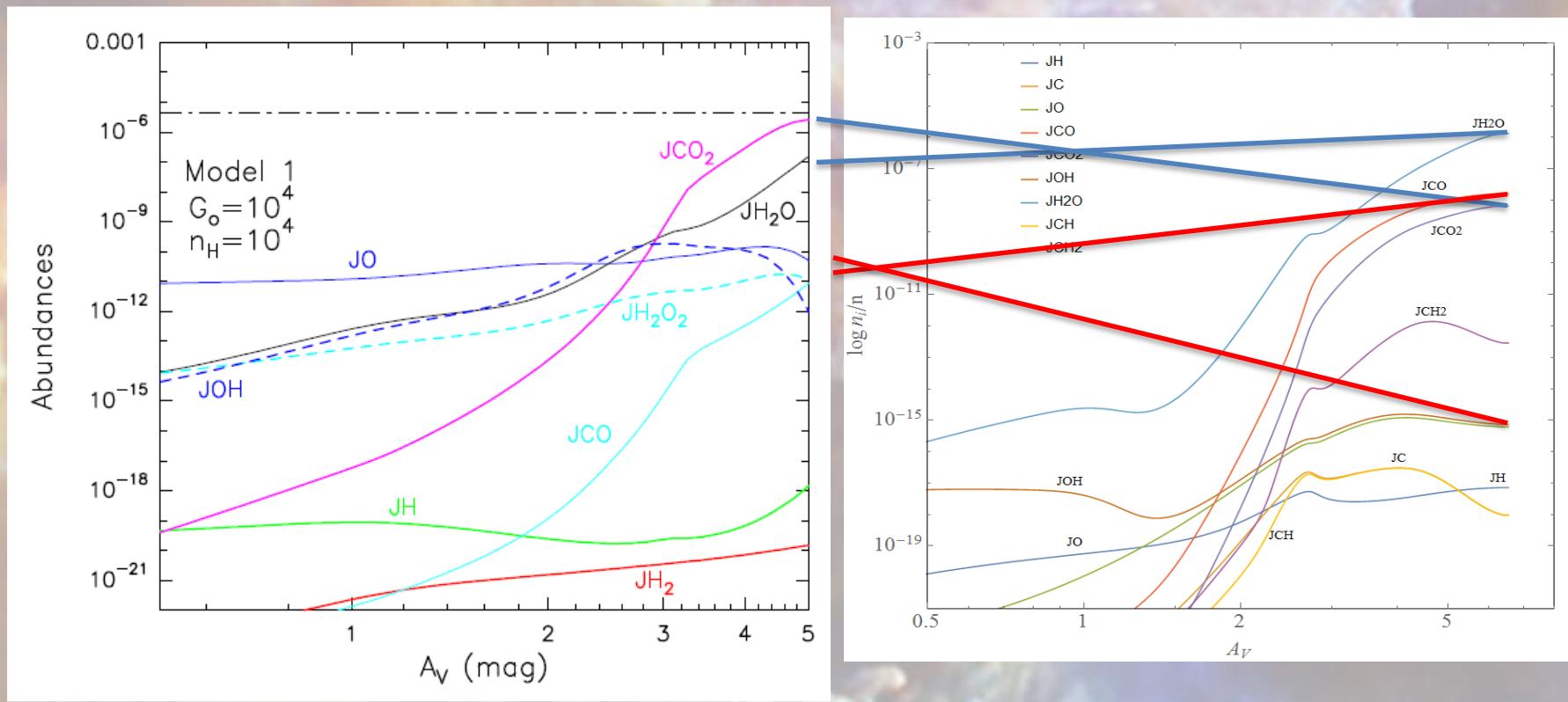
→ significantly different ice composition

KOSMA- τ with „comparable“ setup

plus

(theoretical BRs)
 $JCO + JO \rightarrow CO_2$ (22%)
 $JCO + JO \rightarrow JCO_2$ (78%)

Chemical details with impact



Esplugues et al. 2016

→ significantly different ice composition

KOSMA- τ with „comparable“ setup

plus

(measured BRs)

JCO + JO \rightarrow CO₂

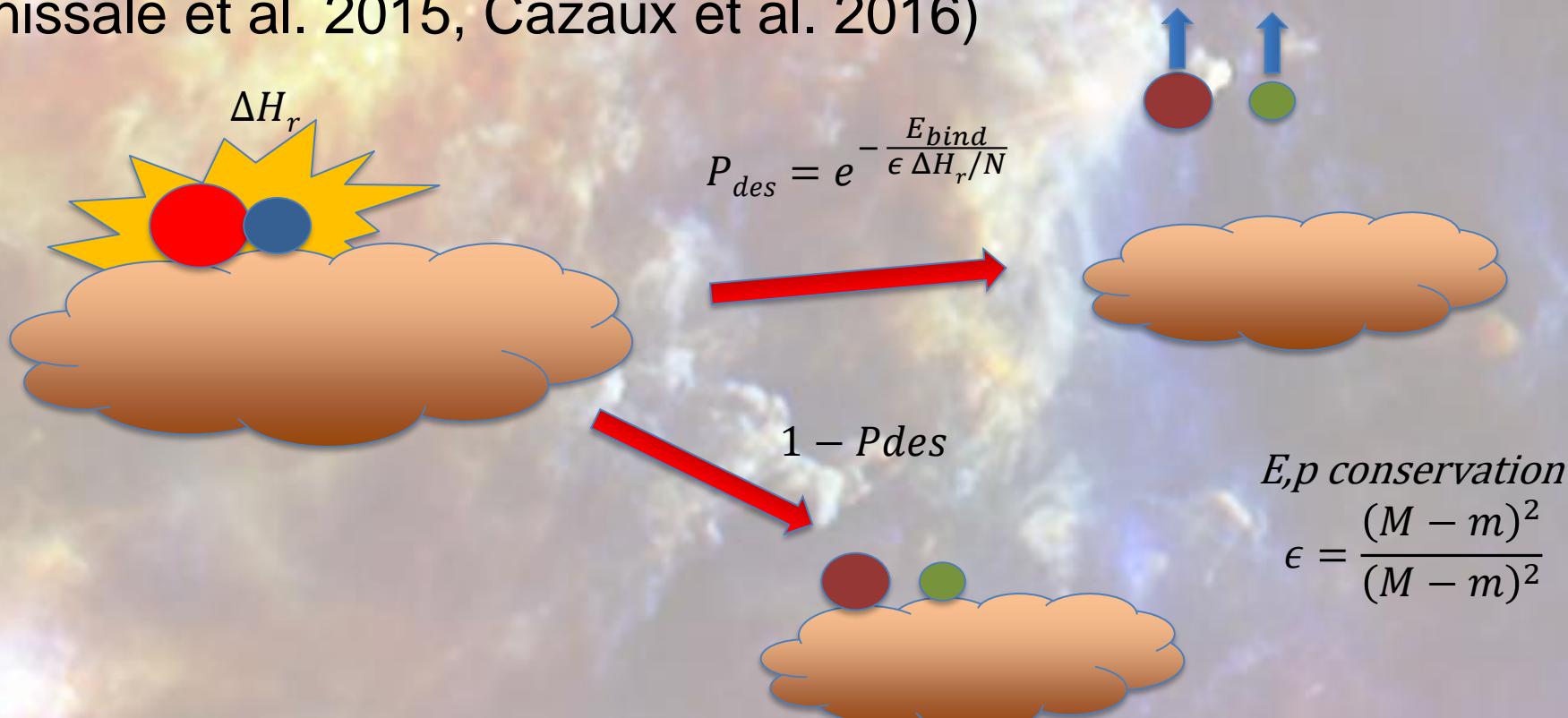
(4%)

JCO + JO \rightarrow JCO₂

(96%)

Full Surface Chemistry Upgrade

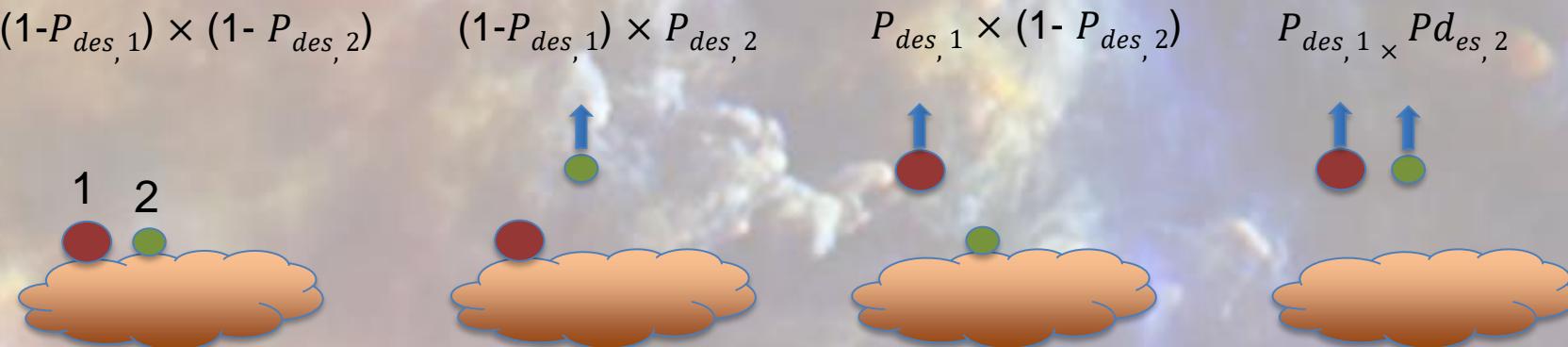
- surface-surface processes (Langmuir-Hinshelwood)
- exoenergetic reactions may lead to desorption of **both products** (Minissale et al. 2015, Cazaux et al. 2016)



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: $\frac{E_1}{E_2} = \frac{m_1}{m_2}, : \quad \frac{E_1}{E_{tot}} = \eta_1 = \frac{m_1}{m_1+m_2}$
- $P_{des,i} = e^{-\frac{E_{bind,i}}{\epsilon_i \eta_i \Delta H_r / N_i}}, \quad \overline{P_{des,i}} = 1 - P_{des,i}$
- H₂ always desorbs



Röllig et al., in prep

Some example branching rates

- $\text{JOH} + \text{JO} \rightarrow$

O_2	+	H	7×10^{-5} (0.019)
JO_2	+	H	5.7×10^{-4} (—)
O_2	+	JH	0.11(—)
JO_2	+	JH	0.89(0.981)
- $\text{JH}_2\text{O}_2 + \text{JH} \rightarrow$

H_2O	+	OH	0.002(0.021)
JH_2O	+	OH	0.16(—)
H_2O	+	JOH	0.01(—)
JH_2O	+	JOH	0.83(0.979)
- $\text{JHCO} + \text{JH} \rightarrow$

CO	+	H_2	0.65(0.47)
JCO	+	H_2	0.35(—)
CO	+	JH_2	0(—)
JCO	+	JH_2	0 (0.53)

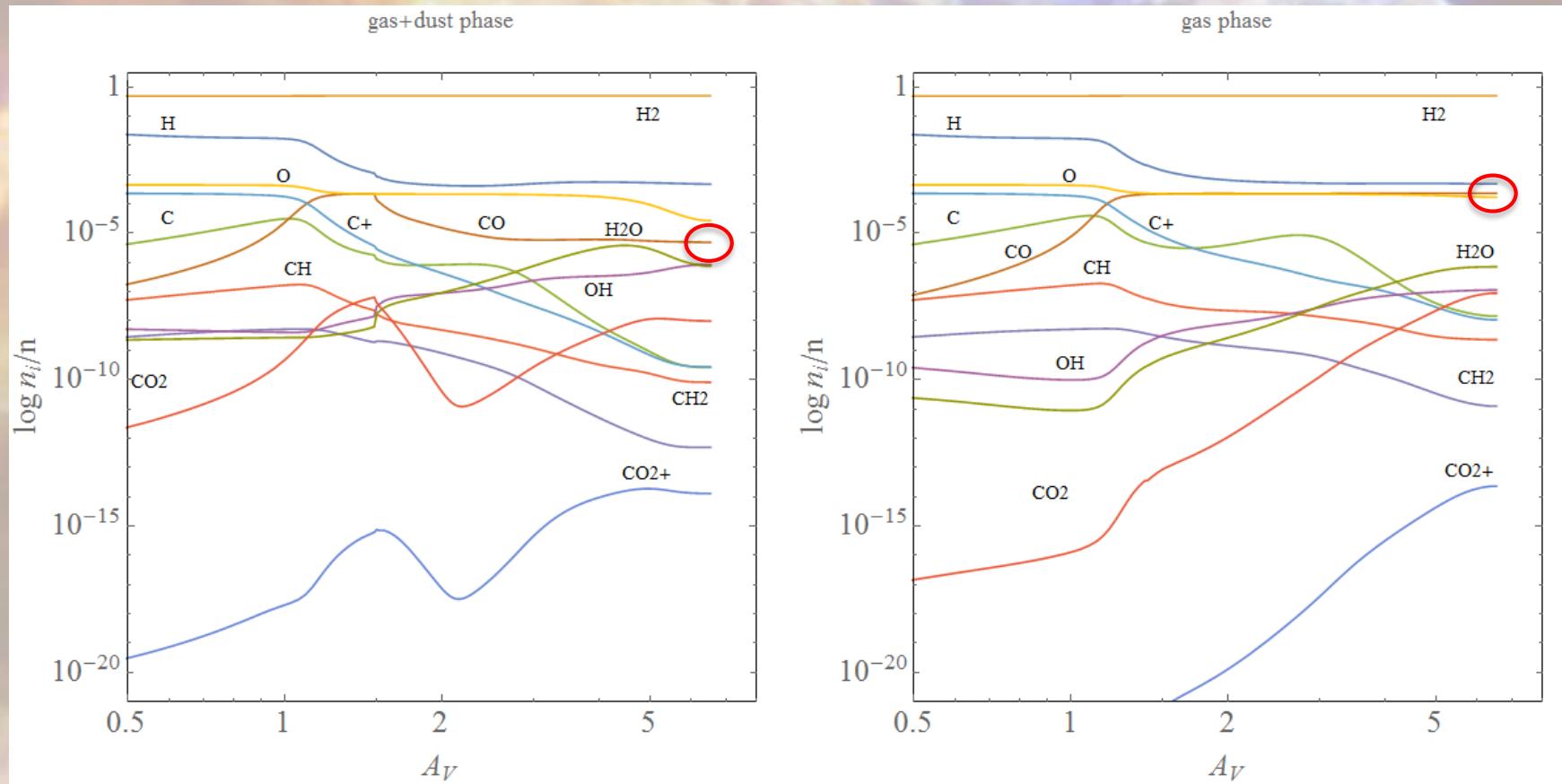
BRs depend on the energy redistribution.

Other distribution schemes?

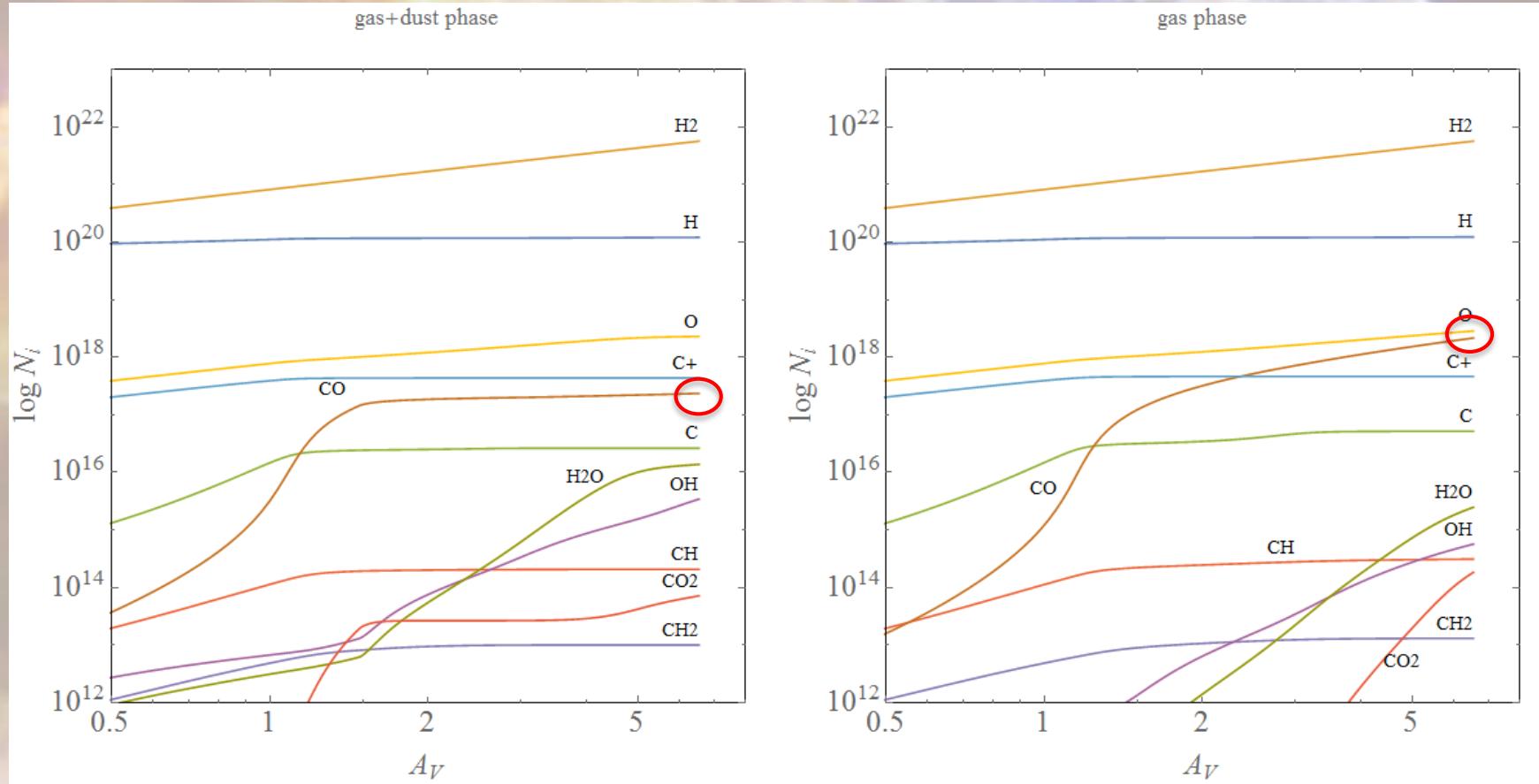
Questions & Concerns

- Binding energies – Yes, but which one? (see Wakelam et al. 2017)
- How about surfaces of very small grains? PAHs?
 - Very important for H₂ formation
 - excitation of small hydrocarbons, H₂, 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

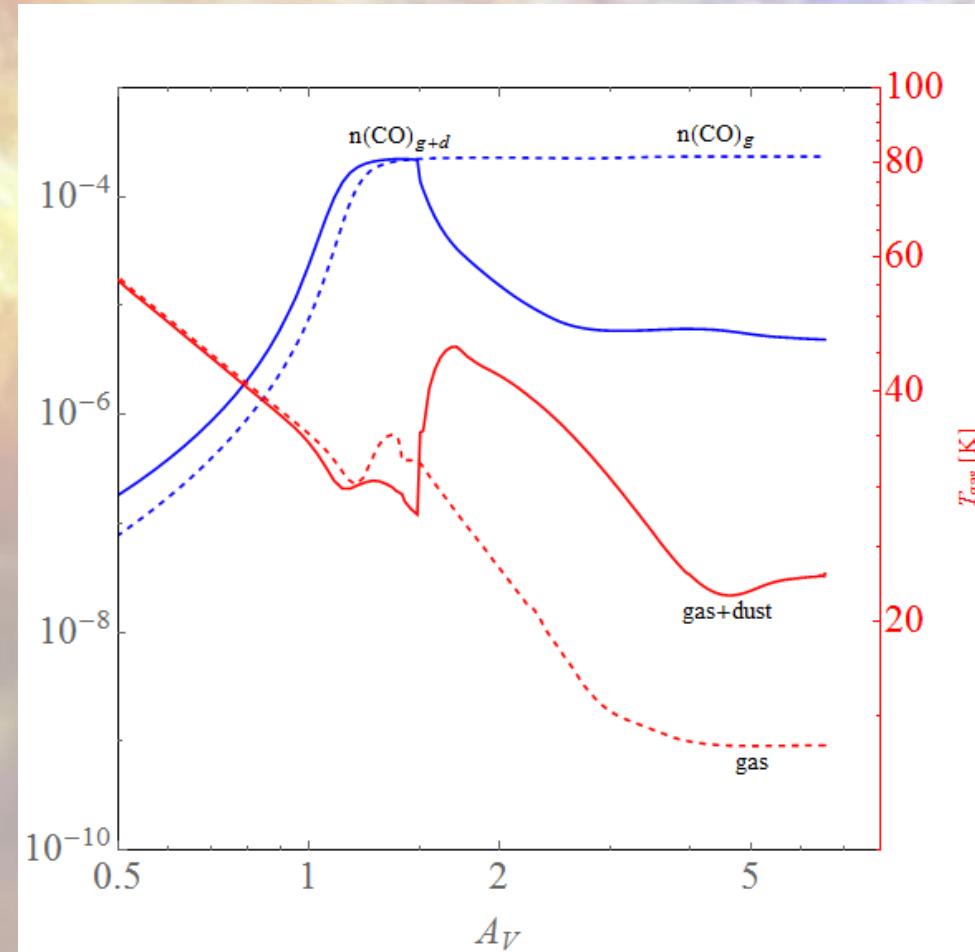
Line	$\int T_{mb} dv$ [K km/s]
CO J=1-0	5.8
CO J=2-1	7.3
CO J=3-2	4.3
CO J=4-3	1.4
[CII] 158μm	2.3
[CI] 609 μm	8.7
[CI] 370μm	2.3

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] 158μm	2.1
[CI] 609 μm	9.5
[CI] 370μm	2.6

lower column densities
higher intensities !

Excitation matters



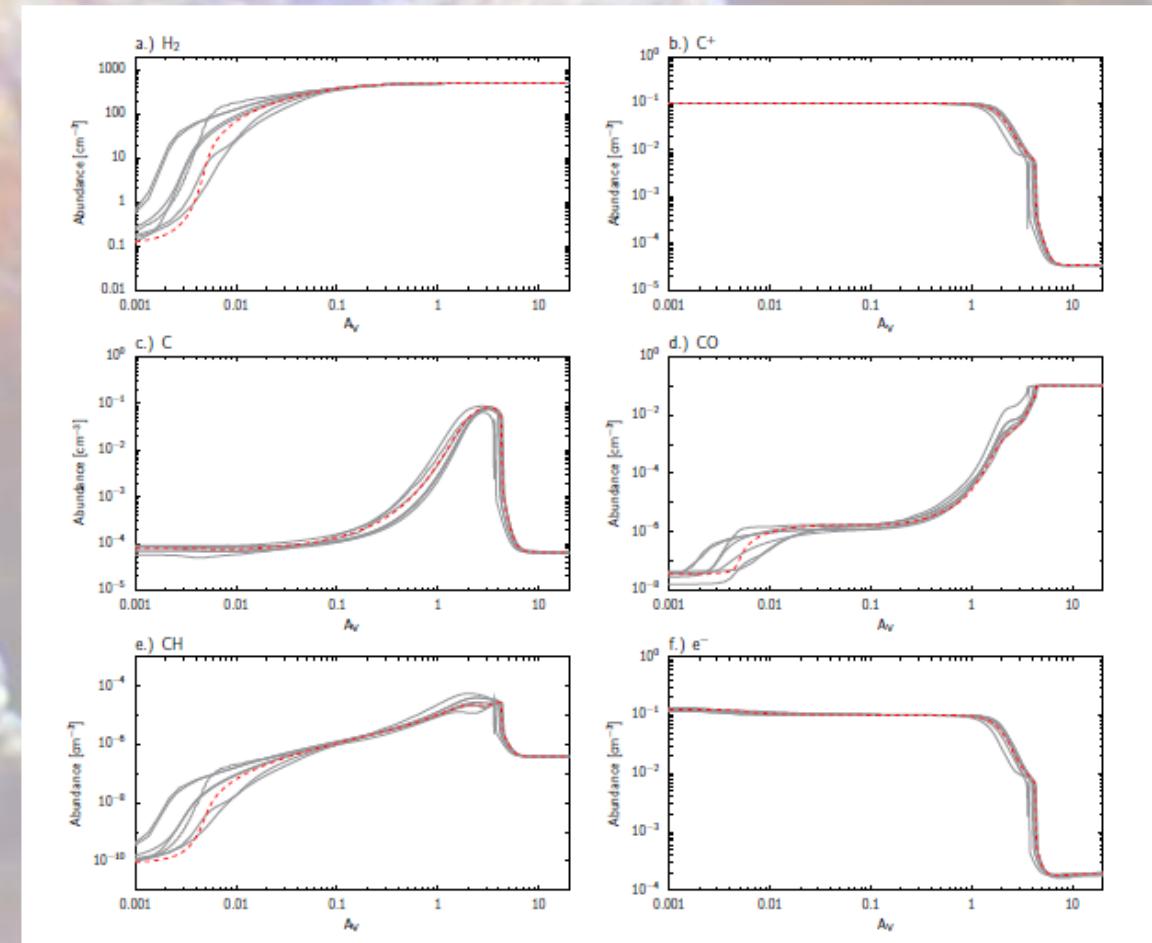
gas cooling is significantly reduced in the absence of CO

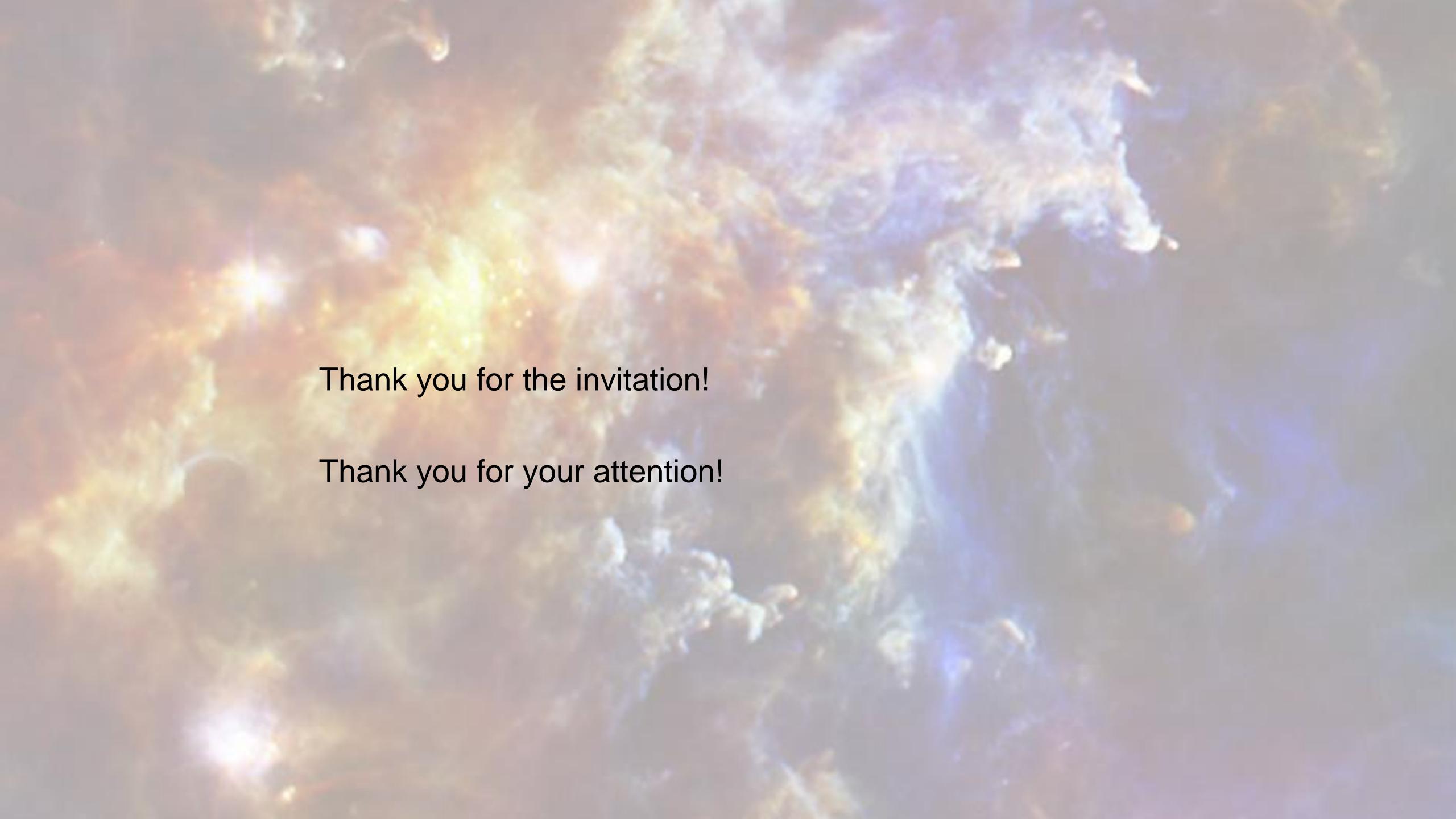
→ gas temperature increases

PyPDR

Bruderer 2014: http://www.mpe.mpg.de/~simonbr/research_pypdr/index.html

- 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}CO using an escape probability approach
- Major heating & cooling processes implemented



The background of the image is a vibrant, abstract pattern resembling a nebula or a microscopic view of organic tissue. It features a complex interplay of colors, primarily warm tones like orange and yellow on the left, transitioning into cooler tones like purple and blue on the right. The colors are not uniform; they are heavily textured with darker, more saturated hues forming intricate, winding paths and bright, glowing spots of light. Some areas appear almost black, while others are filled with intense, fiery light. The overall effect is one of dynamic movement and depth.

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

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

Benchmark Calculations

F1 completed by all 12 groups

F2-F4 complete by 10 groups

F5-F8 completed by 8 groups (some
with numerical ‘noise’)

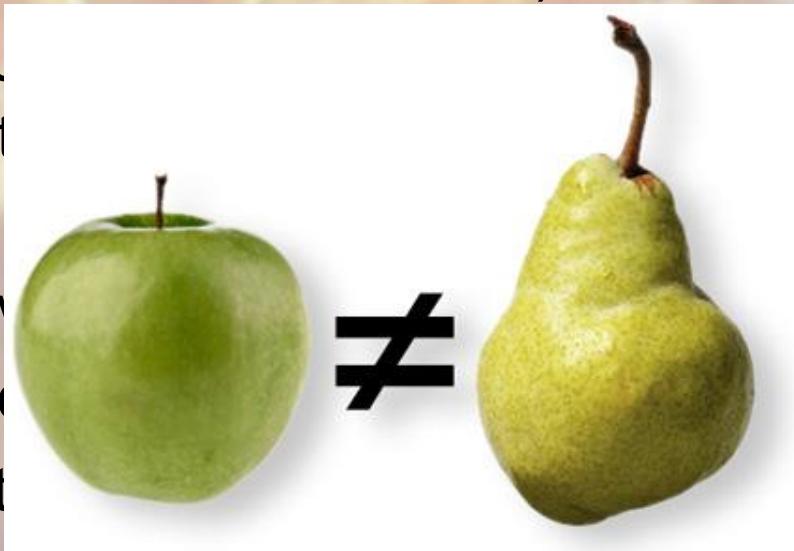
CLOUDS

net

KOSM

geo

result



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

Benchmark Calculations

F1 completed by all 12 groups

F2-F4 complete by 10 groups

F5-F8 completed by 8 groups (some
with numerical ‘noise’)

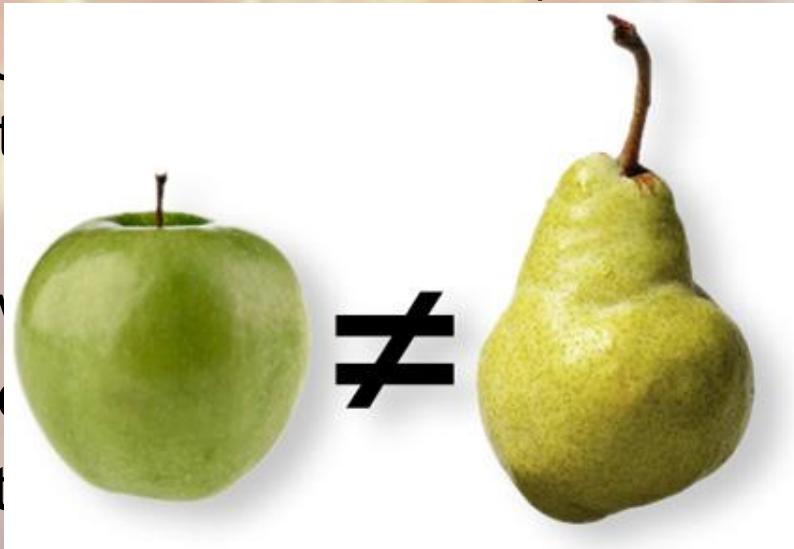
CLOUD

net

KOSM

geo

result

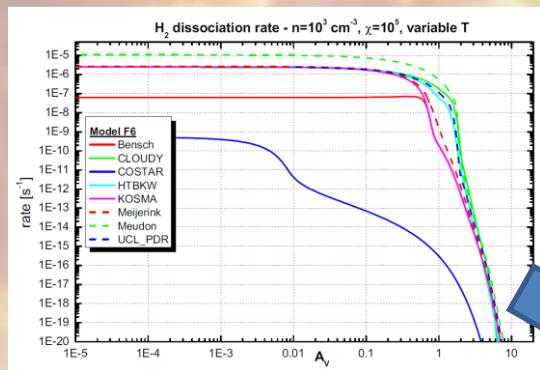


8 yrs

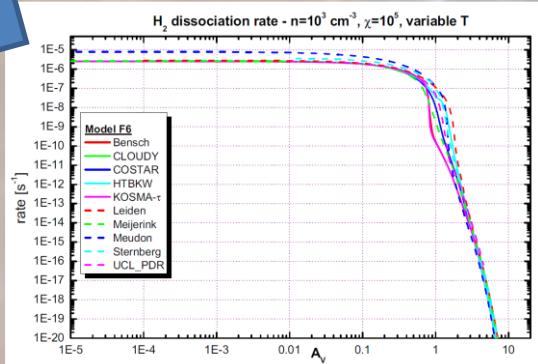


Benchmark Data Archive

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



BEFORE



AFTER

The screenshot shows a dark background with a colorful nebula image. The title "PDR-Comparison Benchmark" is displayed in large, golden-yellow letters. Below the title is a navigation menu with links to "Introduction", "Codes", "Benchmark", "Results", "PRE-Benchmark", "POST-Data", "POST-Plots", "Documents", and "Links". To the right is a table titled "Data Files" showing file names for various models across different categories (F1, F2, F3, F4, V1, V2, V3, V4).

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

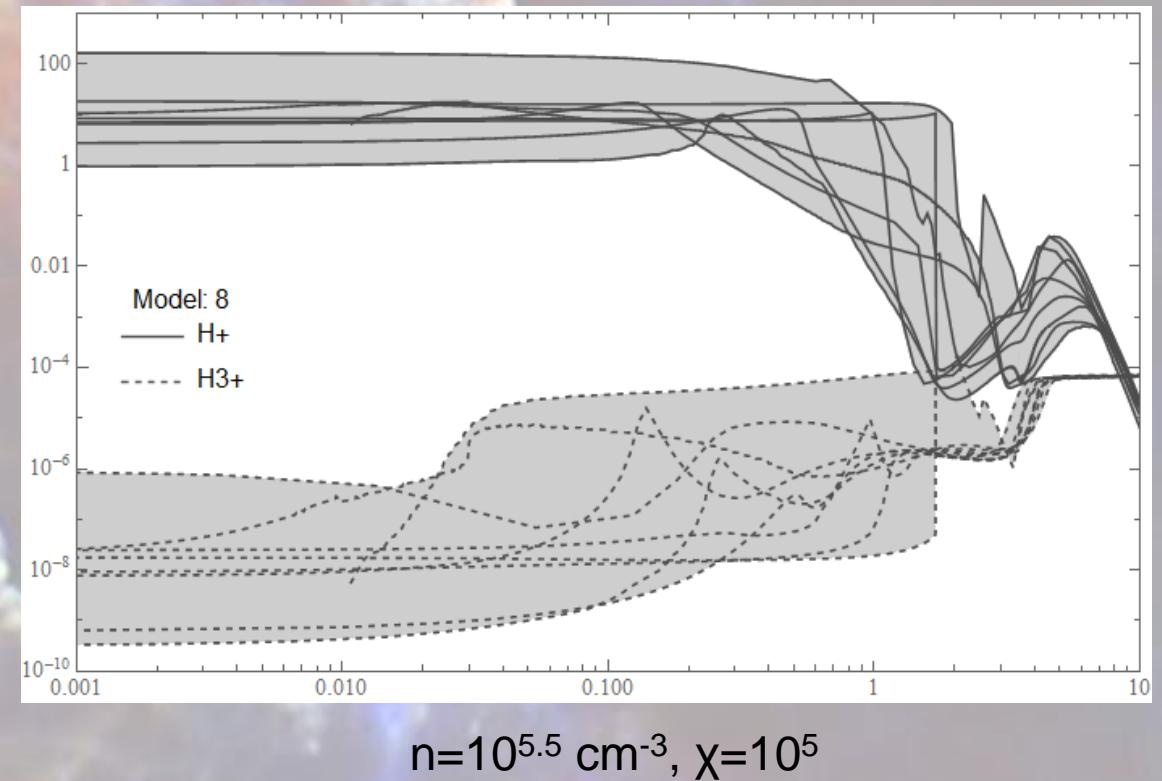
<http://www.astro.uni-koeln.de/pdr-comparison/>

Benchmark V.2?

So much left to do:

- 2007 benchmark left many open issues

Status after the benchmark 2007



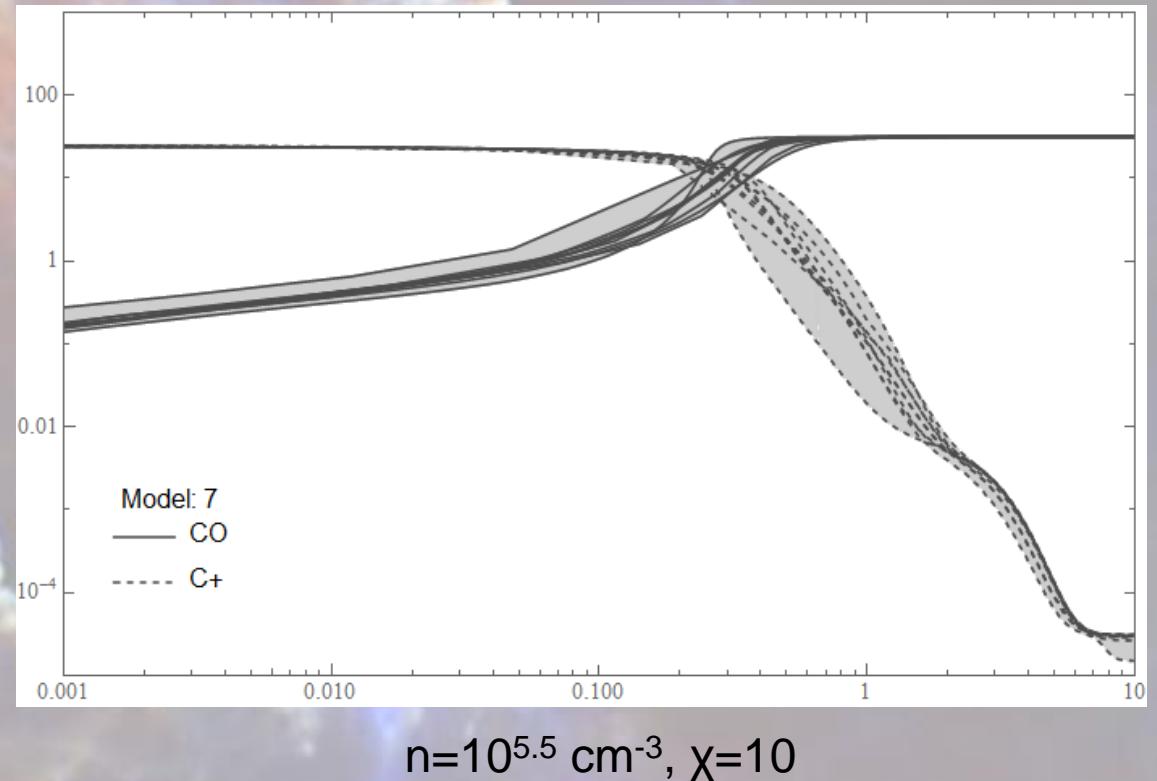
Benchmark V.2?

So much left to do:

- 2007 benchmark left many open issues
- Discuss numerics

• Improve atomic models
• New up-to-date atomic data
• More models
• Benchmark against real world problems
• Exchange of experience; include the new models
• PDR modelling roadmap

Status after the benchmark 2007

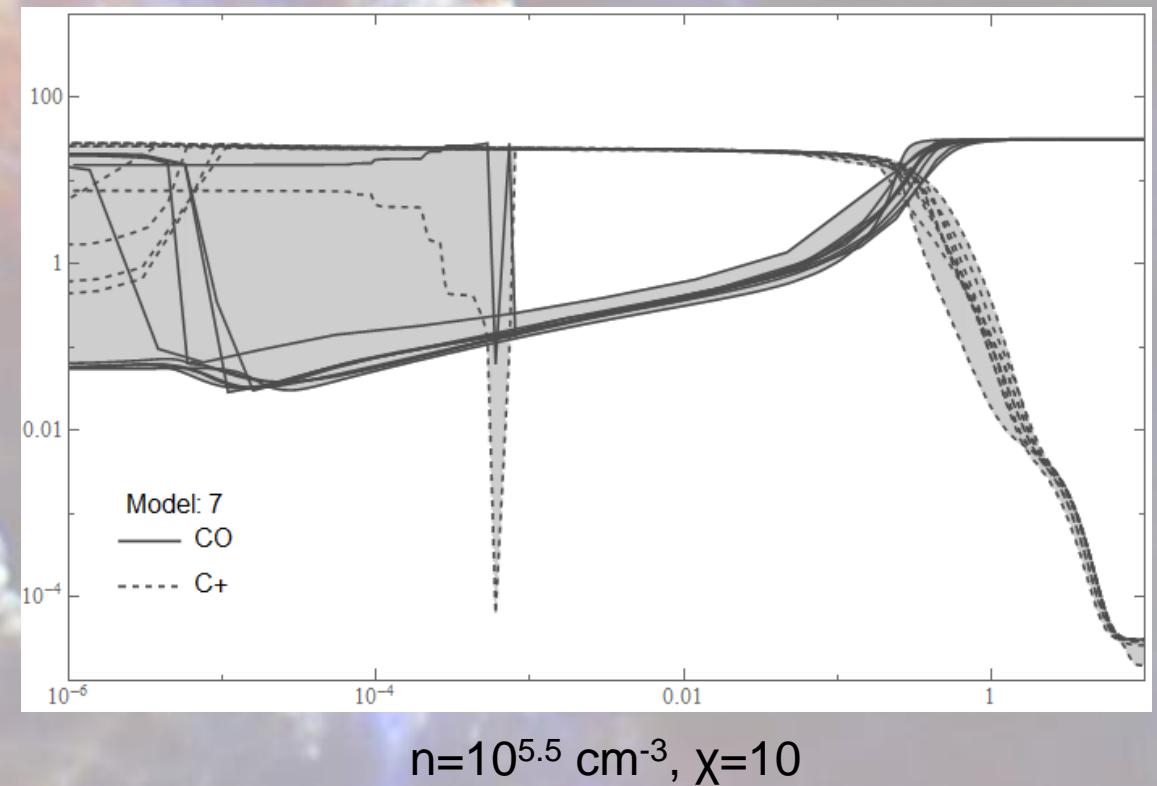


Benchmark V.2?

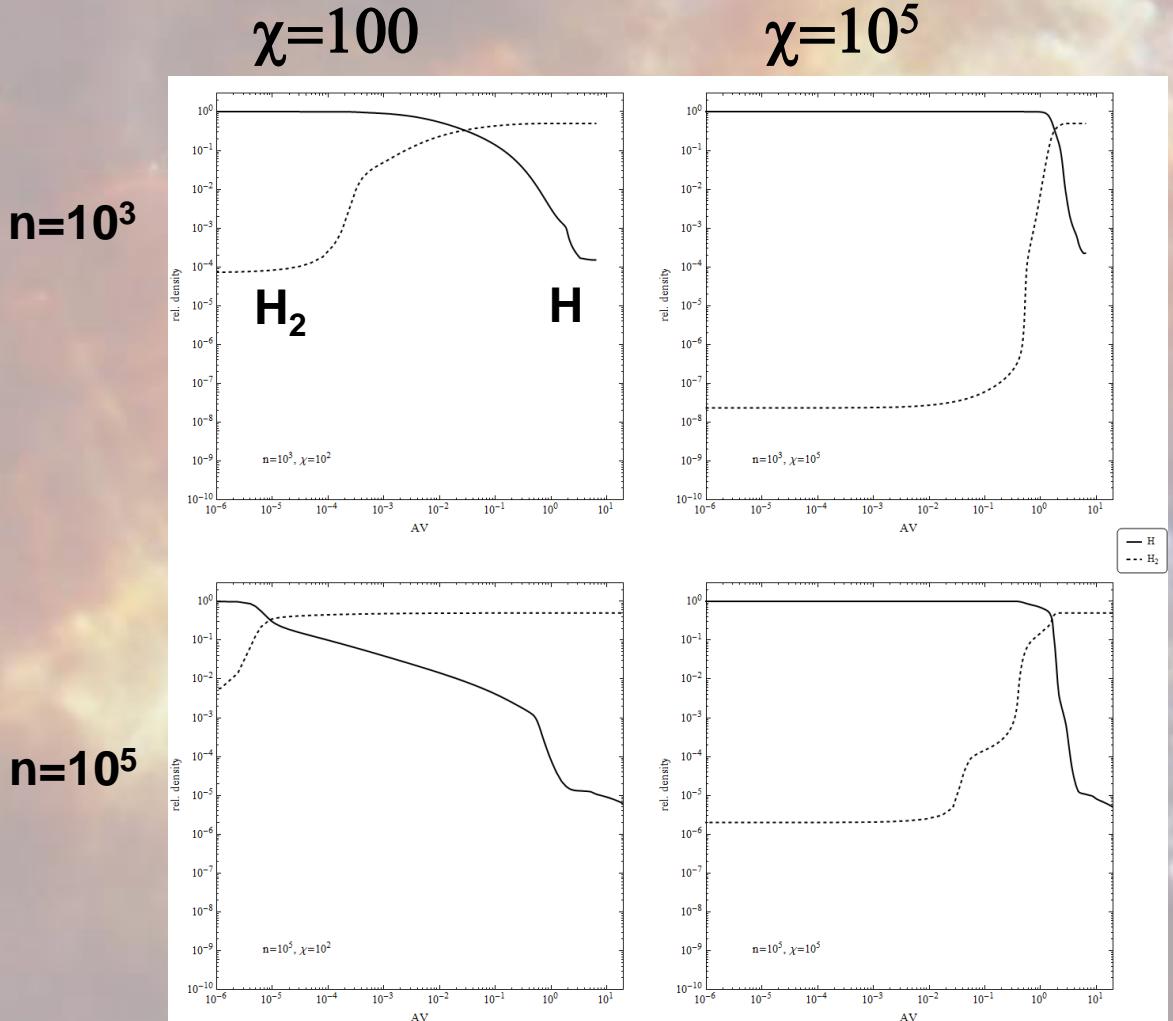
So much left to do:

- 2007 benchmark left many open issues
- Discuss numerics

Status after the benchmark 2007



PDR Model Chemistry

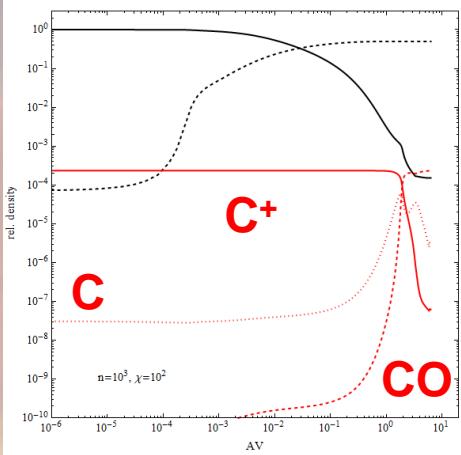


- H_2 photodissociation is a line absorption process. Once the absorption lines become optically thick, photodissociation becomes inefficient
- Density and UV field strength determine the depth of the $H-H_2$ transition zone

PDR Model Chemistry

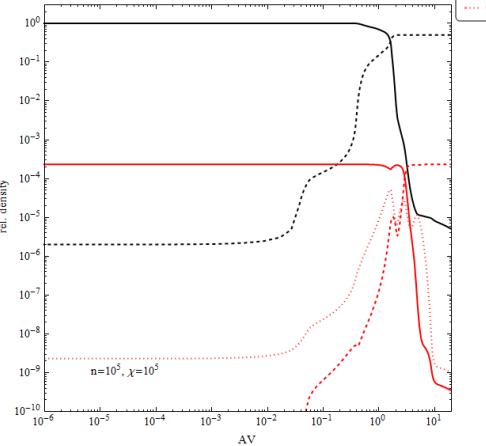
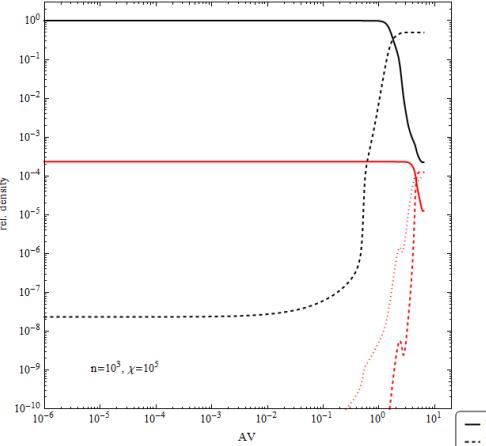
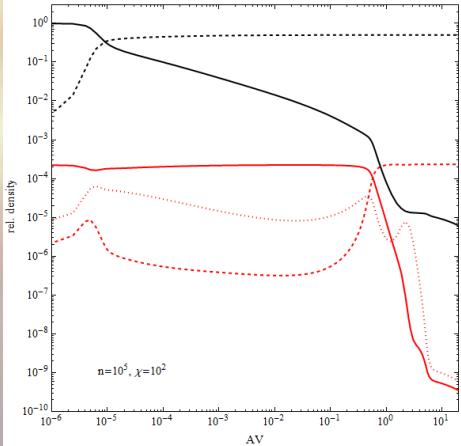
$\chi=100$

$n=10^3$



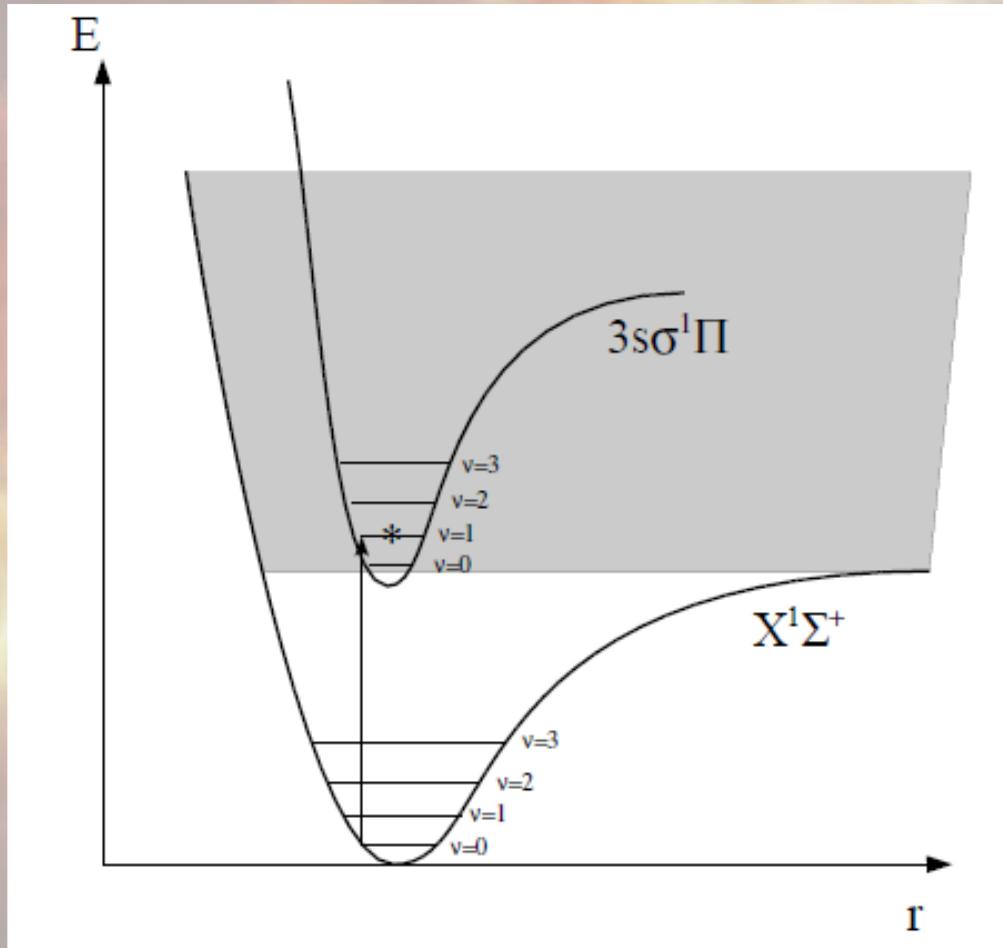
$\chi=10^5$

$n=10^5$



- CO photodissociation is shielded by
 - itself (self-shielding)
 - CO isotopologues (mutual shielding)
 - overlapping H₂ lines
 - dust attenuation
- CO photodissociation becomes inefficient for $N_{CO} > 10^{16} \text{ cm}^{-2}$

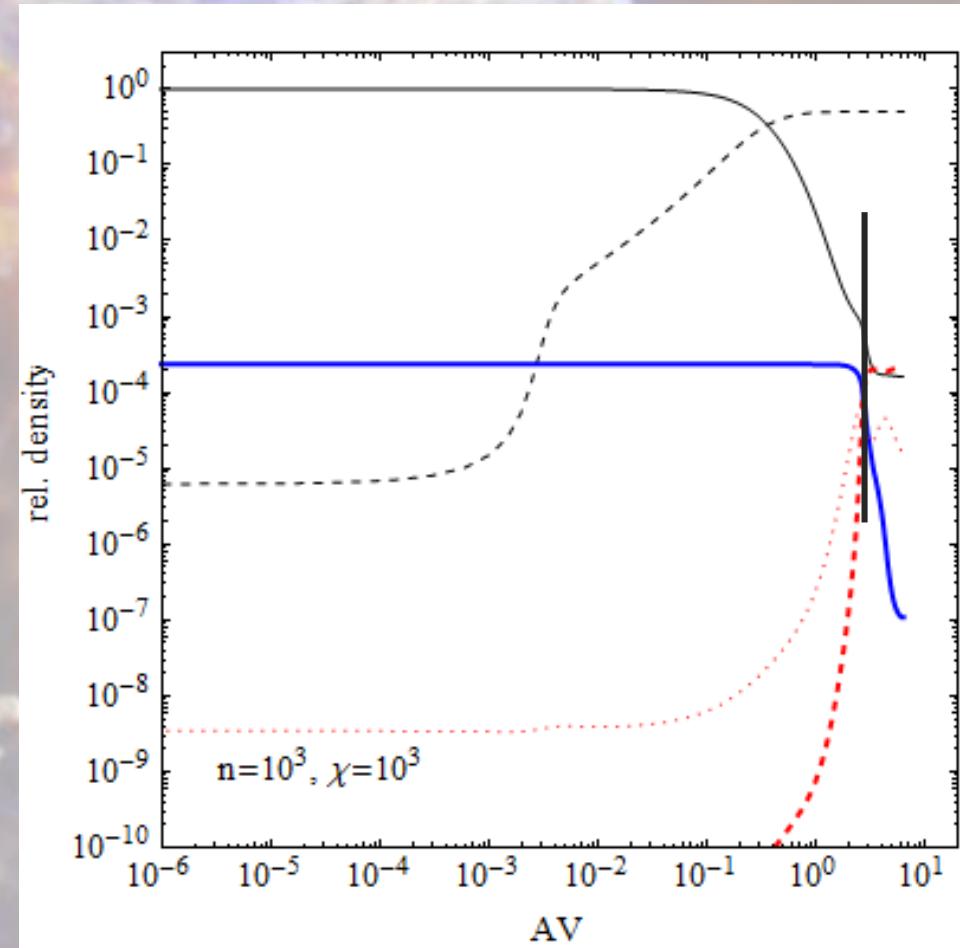
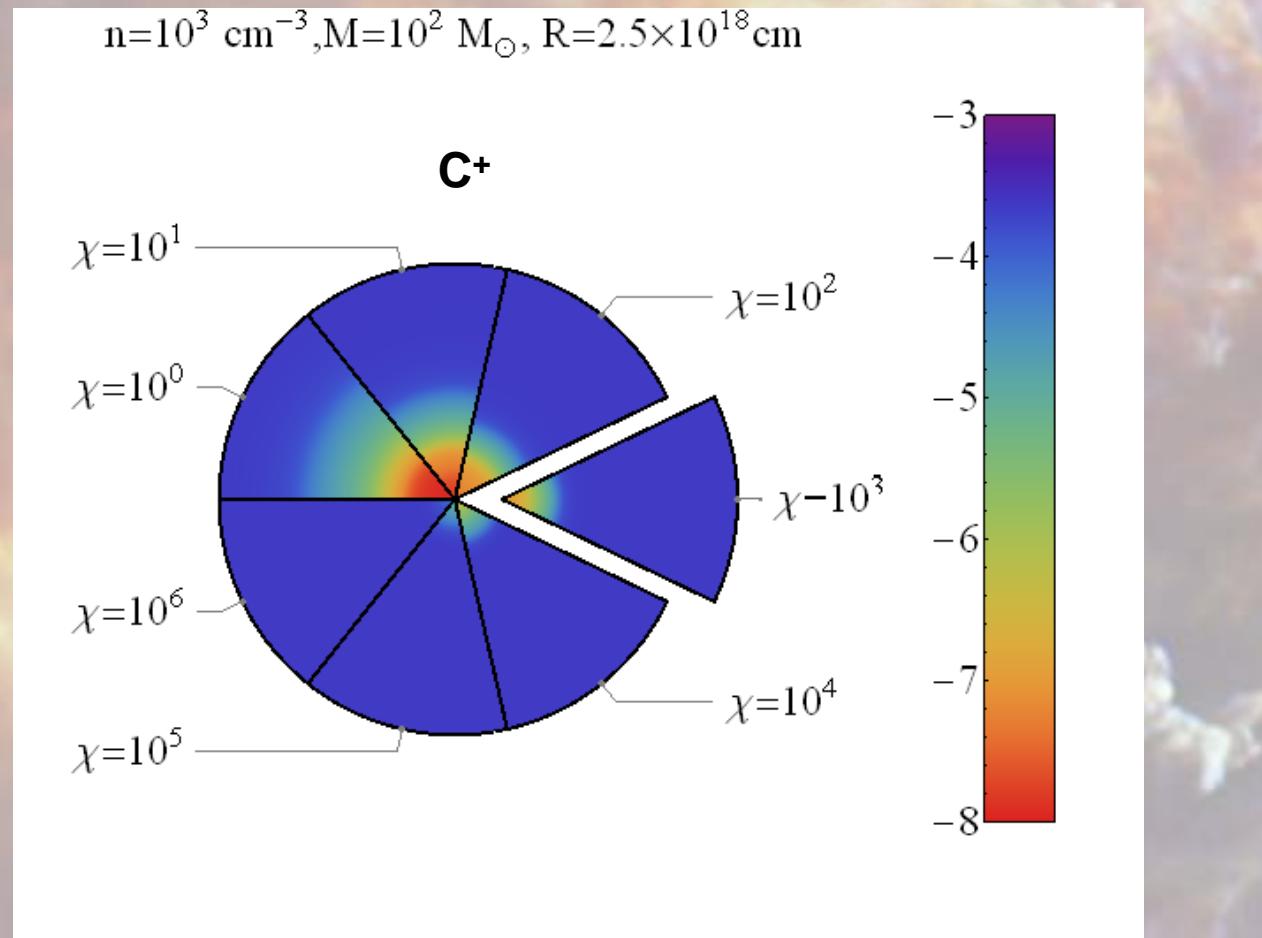
CO Dissociation



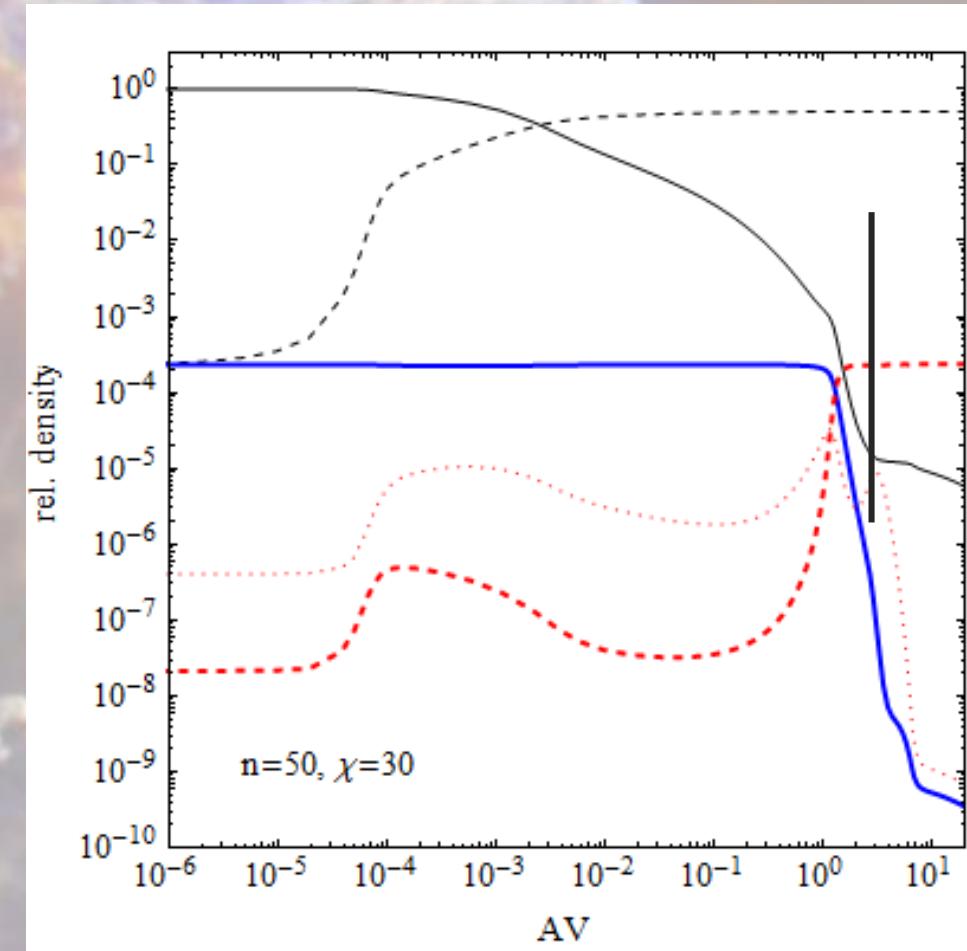
- CO dissociation occurs via line absorption!
- Absorbed photons excite *predissociated* electronic states that can decay into unbound continuum of the ground elect. state radiationless.
- More than 30 absorption bands in the range $913 \text{ \AA} \leq \lambda \leq 1077 \text{ \AA}$
- Line absorption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

Warin et al. 1996

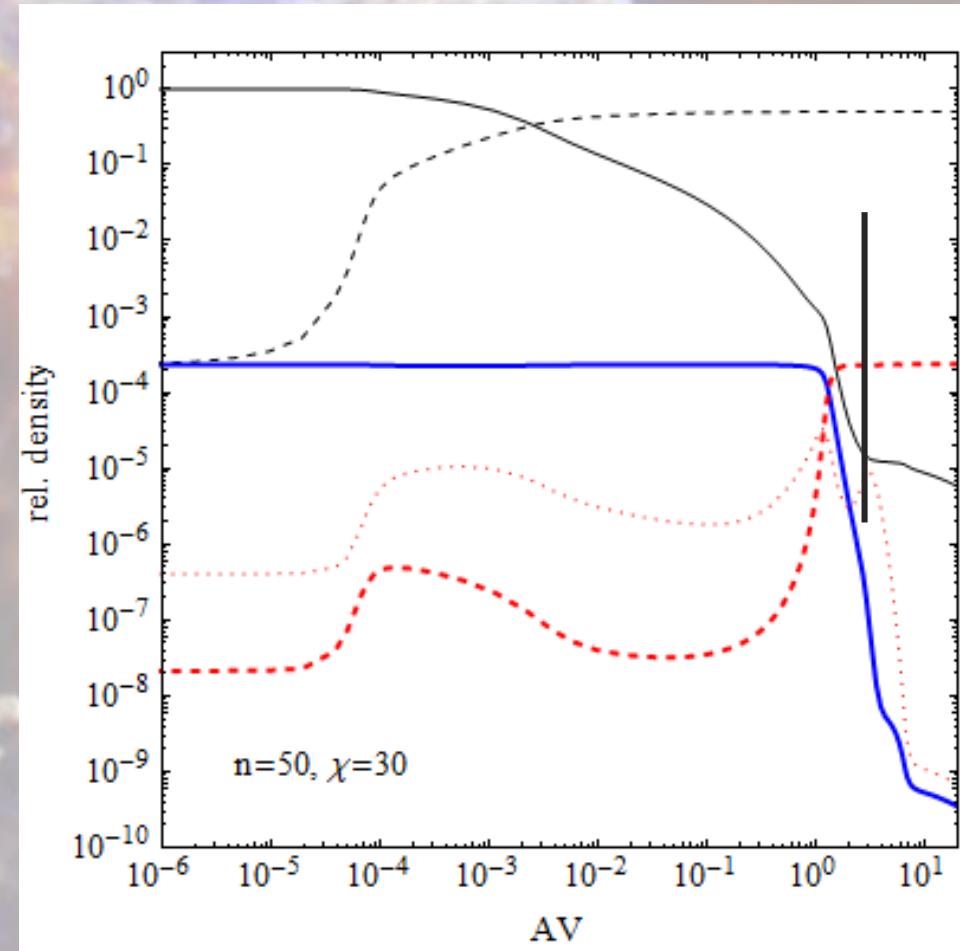
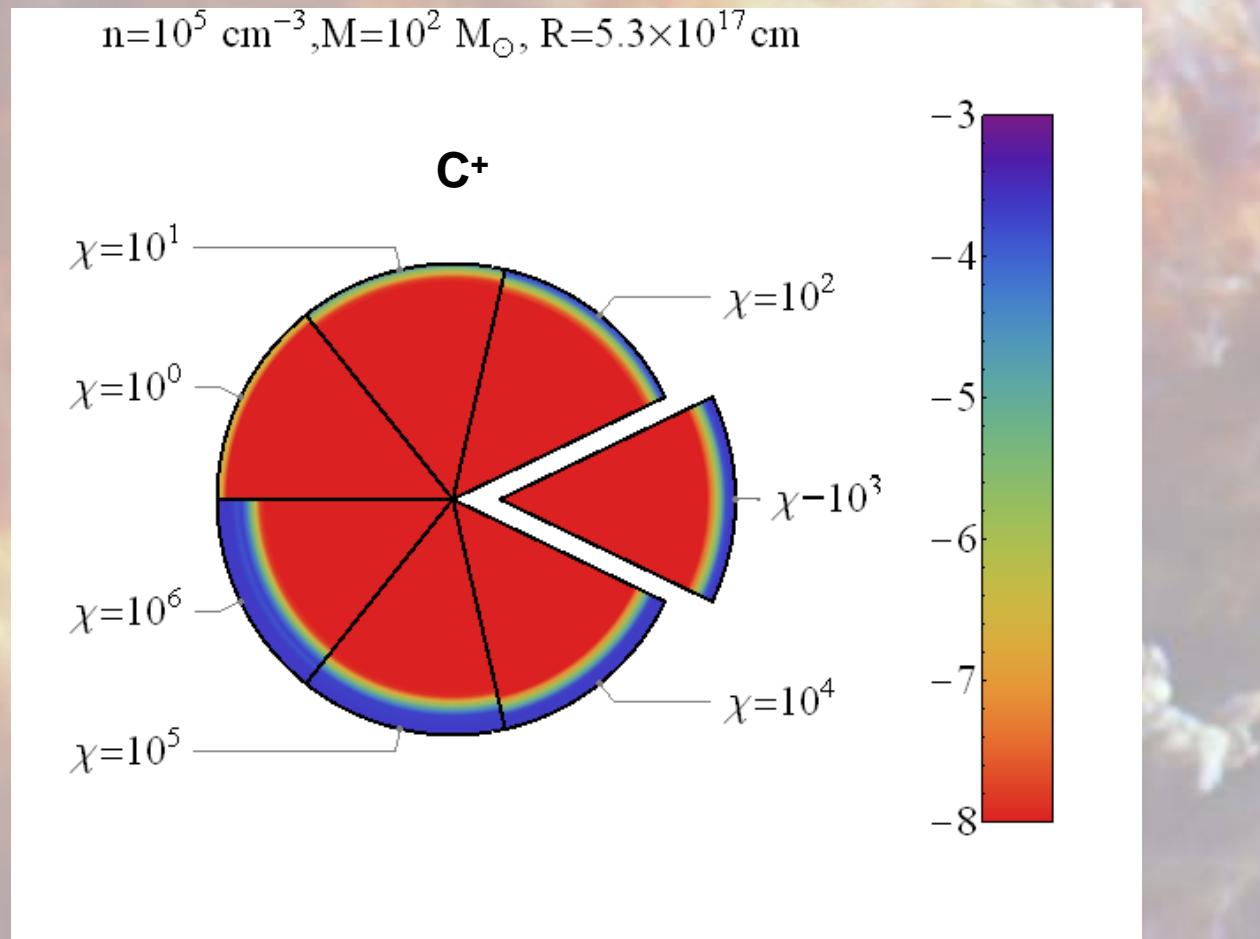
A_V is not a spatial coordinate



A_V is not a spatial coordinate



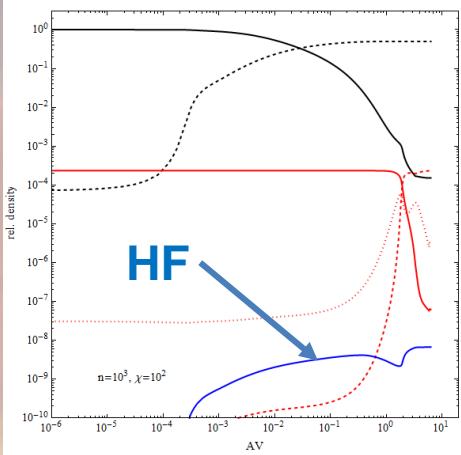
A_V is not a spatial coordinate



PDR Model Chemistry

$\chi=100$

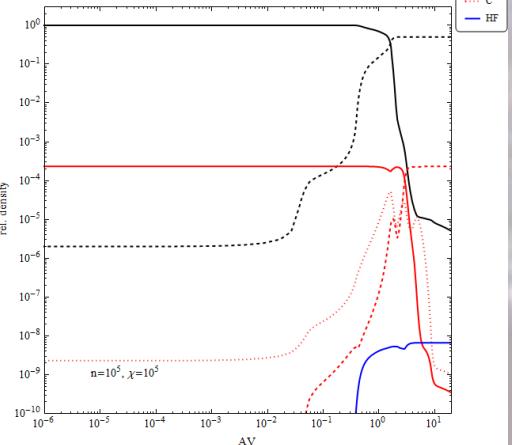
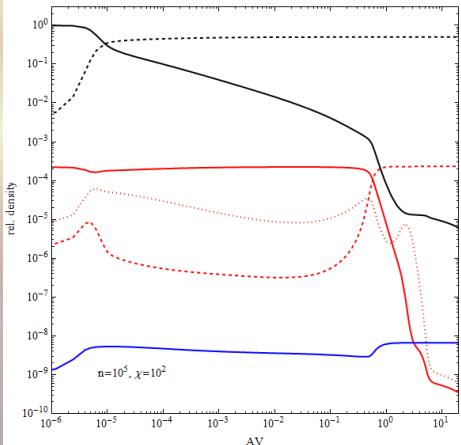
$n=10^3$



$\chi=10^5$

- „Standard“ models show a good H₂-HF correlation (in agreement with empirical findings)

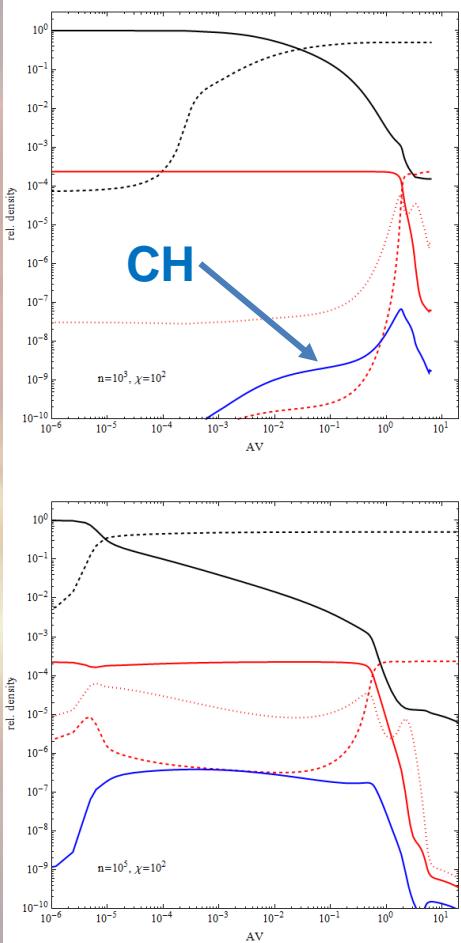
$n=10^5$



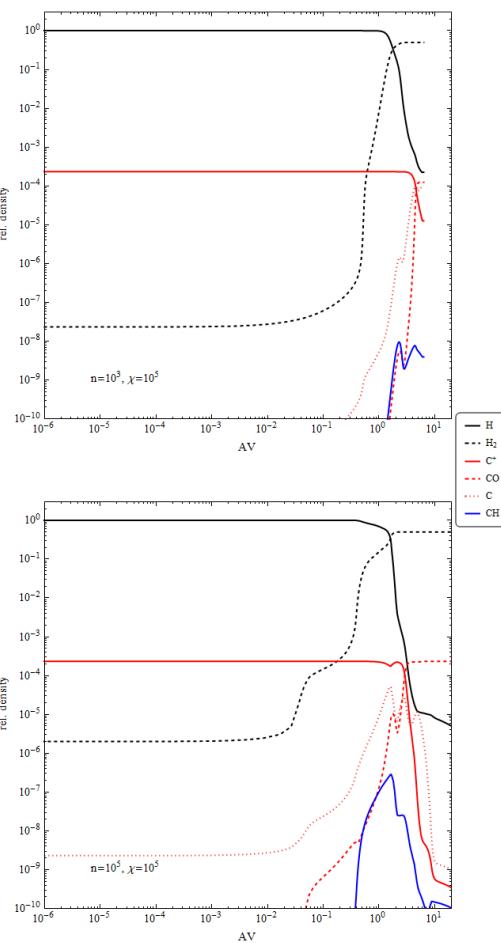
PDR Model Chemistry

$\chi=100$

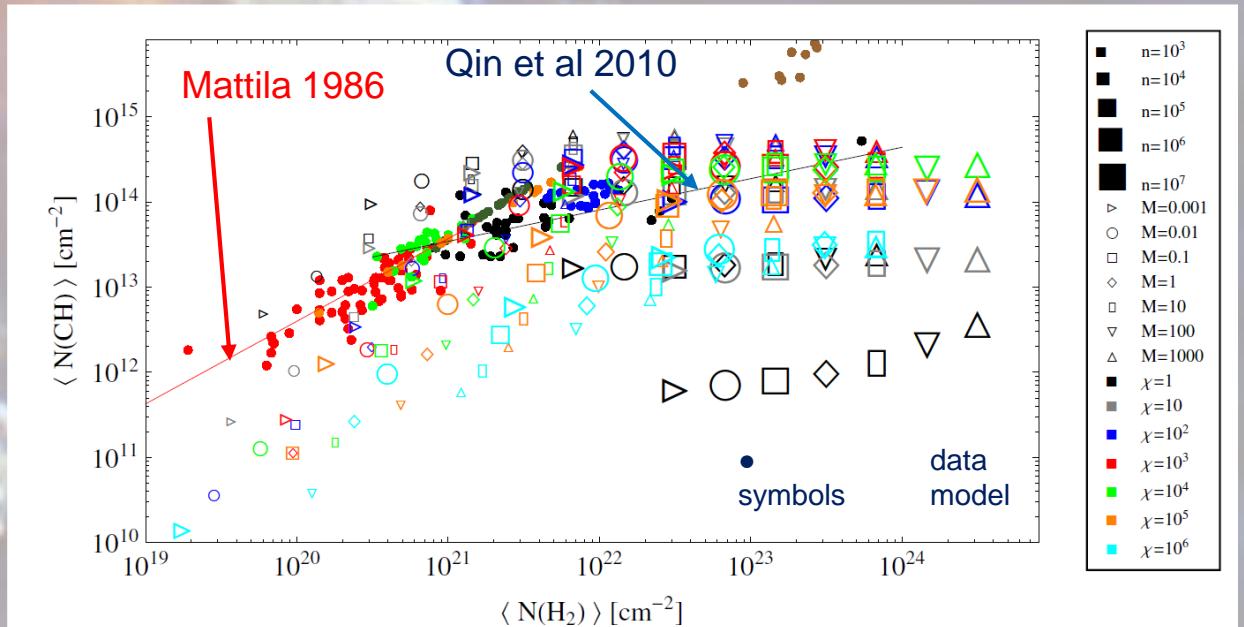
$n=10^3$



$\chi=10^5$

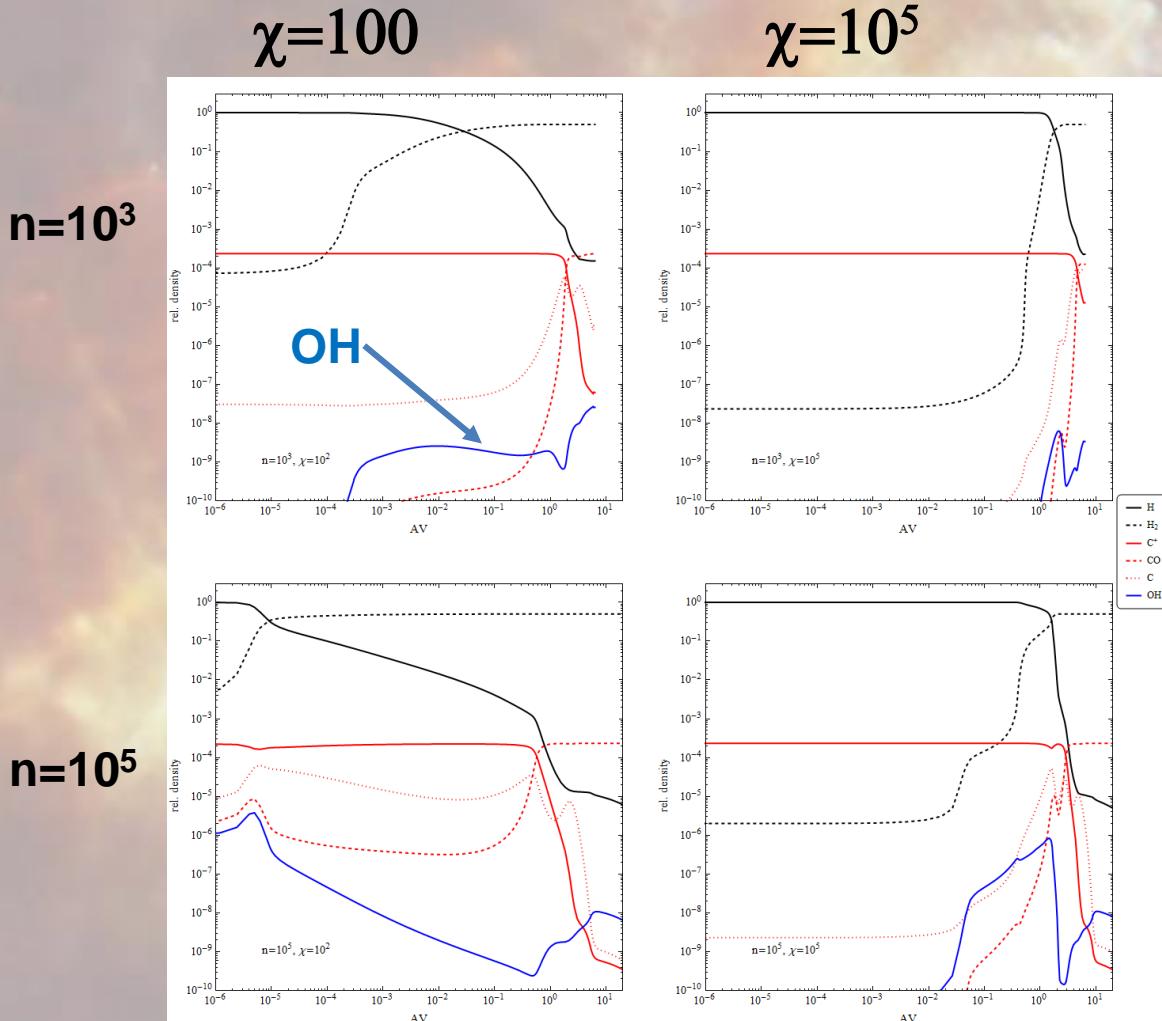


- H₂-CH correlation changes from diffuse to denser clouds

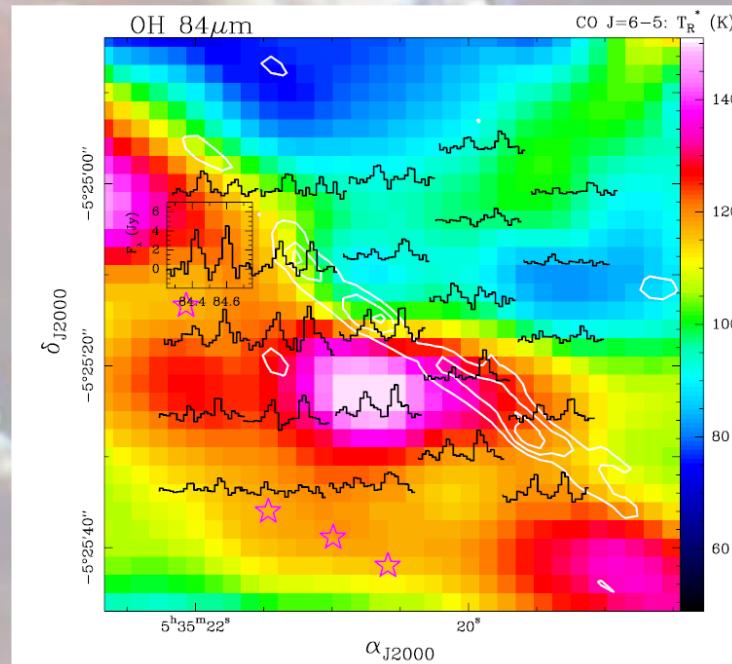


Röllig & Ossenkopf 2013, A&A 550, A56

PDR Model Chemistry

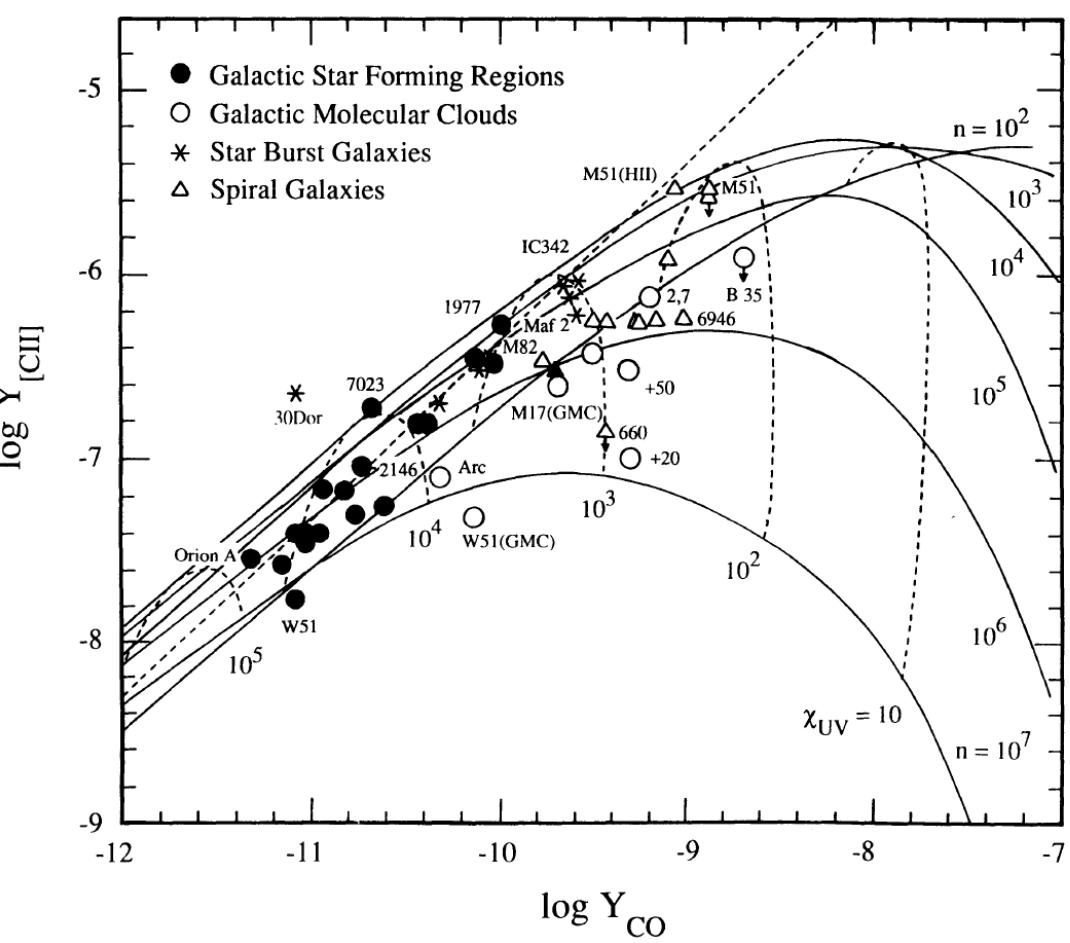
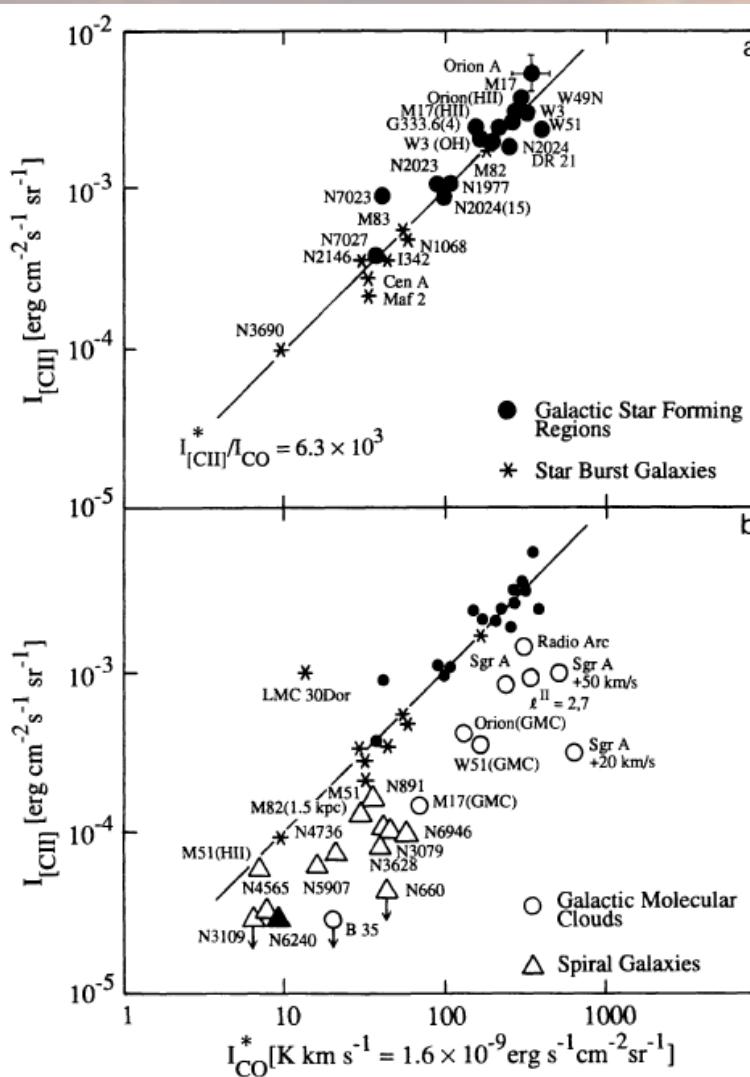


- OH appears to be a reasonable PDR interface tracer
- column densities not well modelled



Goicoechea et al. 2011

PDR Diagnostics



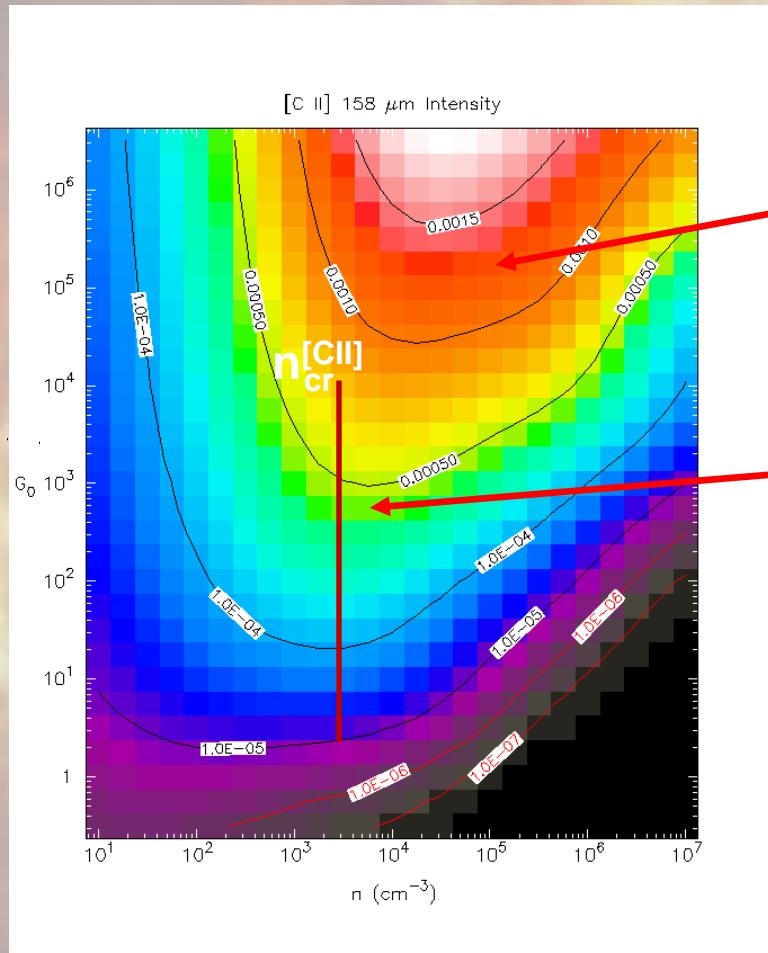
$$Y_{[CII]} = I_{[CII]}/I_{\text{FIR}}$$

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

Stacey et al. 1991

PDR Diagnostics

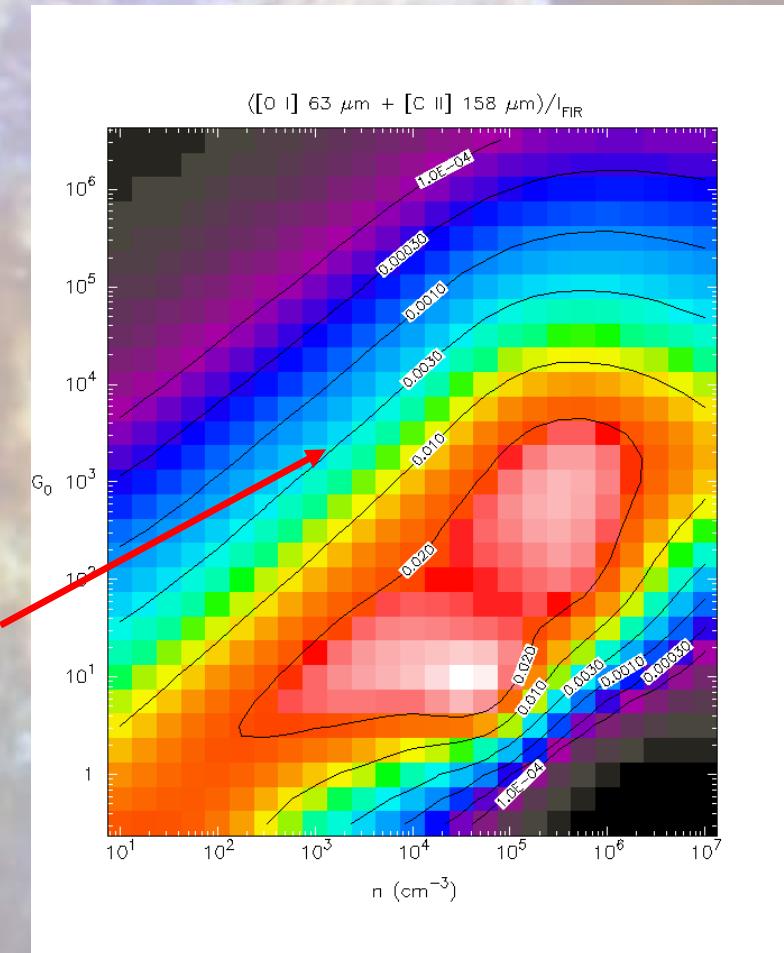
Model calculations



Orion PDR

Classic PDRs

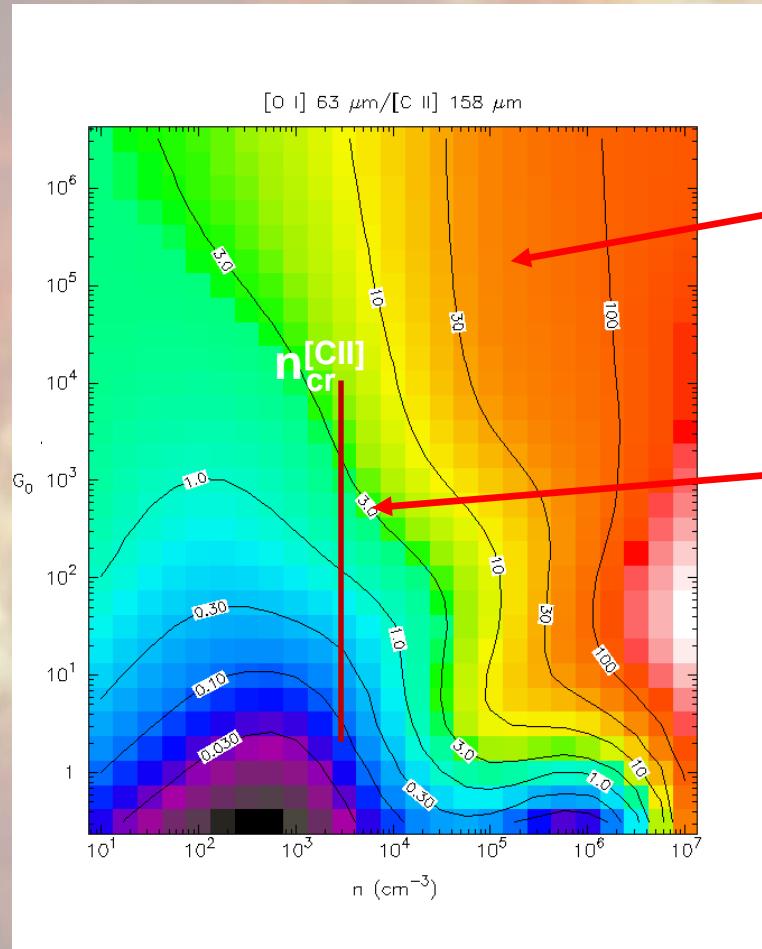
$G_0/n = \text{const}$



Kaufman et al. 1999

PDR Diagnostics

Model calculations

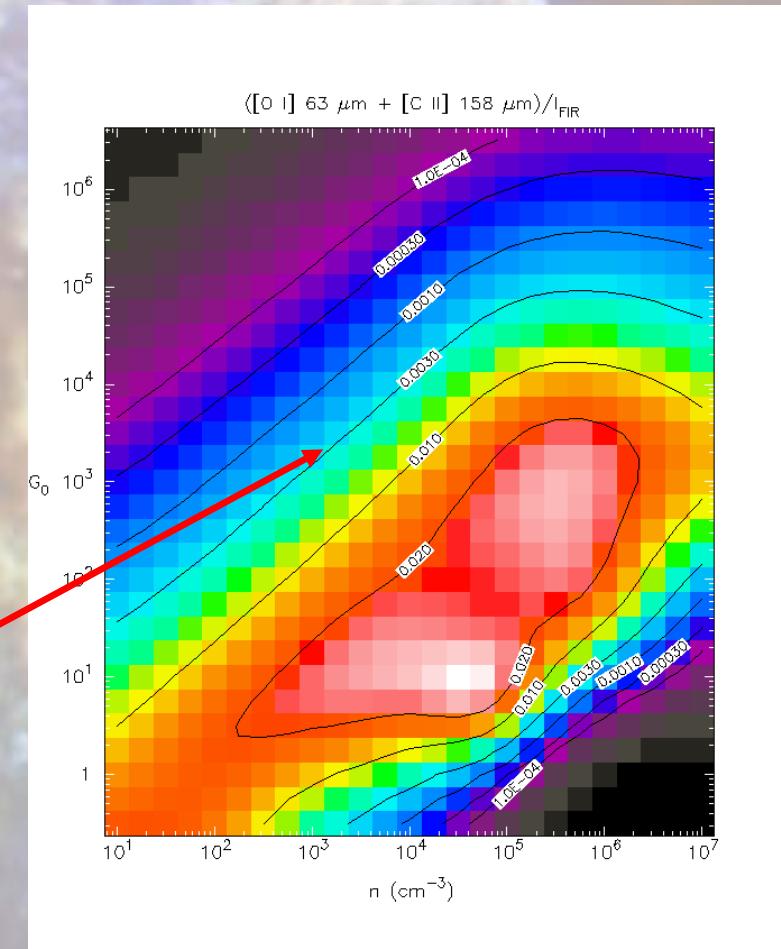


Orion PDR

Classic PDRs

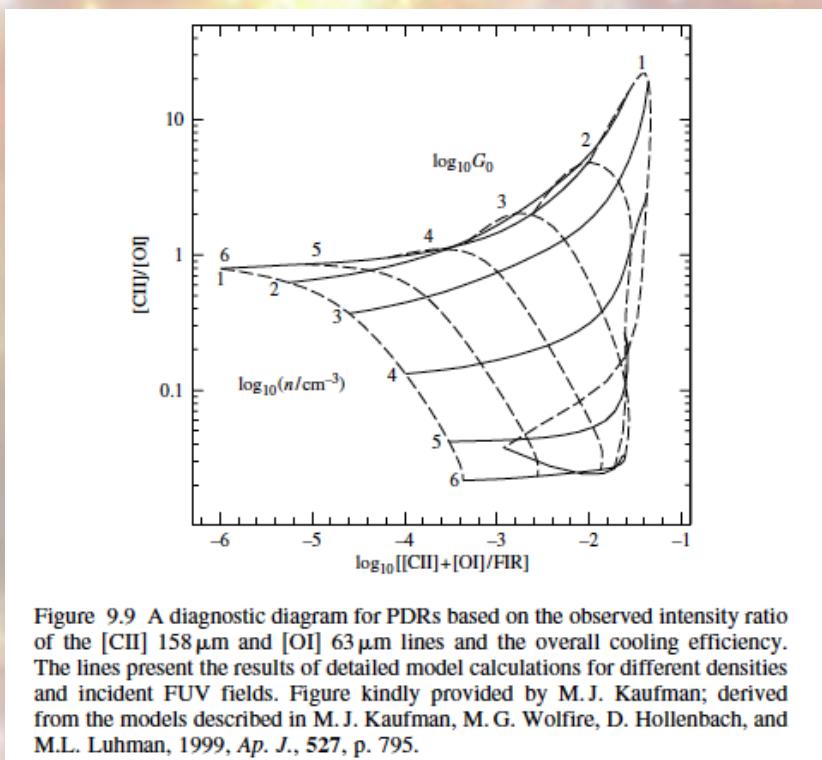
$G_0/n = \text{const}$

Kaufman et al. 1999



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 $G_0 T^{1/2} / n_e$.



$$\frac{F_{\text{OI}} + F_{\text{CII}}}{2F_{\text{IR}}} \quad \text{Gas heating efficiency}$$

Since the [CII] 158 μm and [OI] 63 μm 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/>

The screenshot shows a web browser window with the URL <http://hera.ph1.uni-koeln.de/~pdr/> in the address bar. The page title is "Spherical Photon Dominated Region Model". A red oval highlights the "Extract" button in the top navigation bar. Below the title is a diagram of a spherical region with concentric layers. The innermost layer is purple and labeled "UV". Surrounding it are three pink layers labeled "H₂", "C_t", and "C_e". Wavy lines radiate from the outer edges of the pink layers, representing emission or absorption features. The text below the diagram reads: "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." A note at the bottom states: "Update 24. June 2005: We added the possibility to download the output from the web-interface in a number of additional formats, including FITS." At the very bottom, there is a link: "Report problems to: M.Röllig; Email: roellig@ph1.uni-koeln.de".

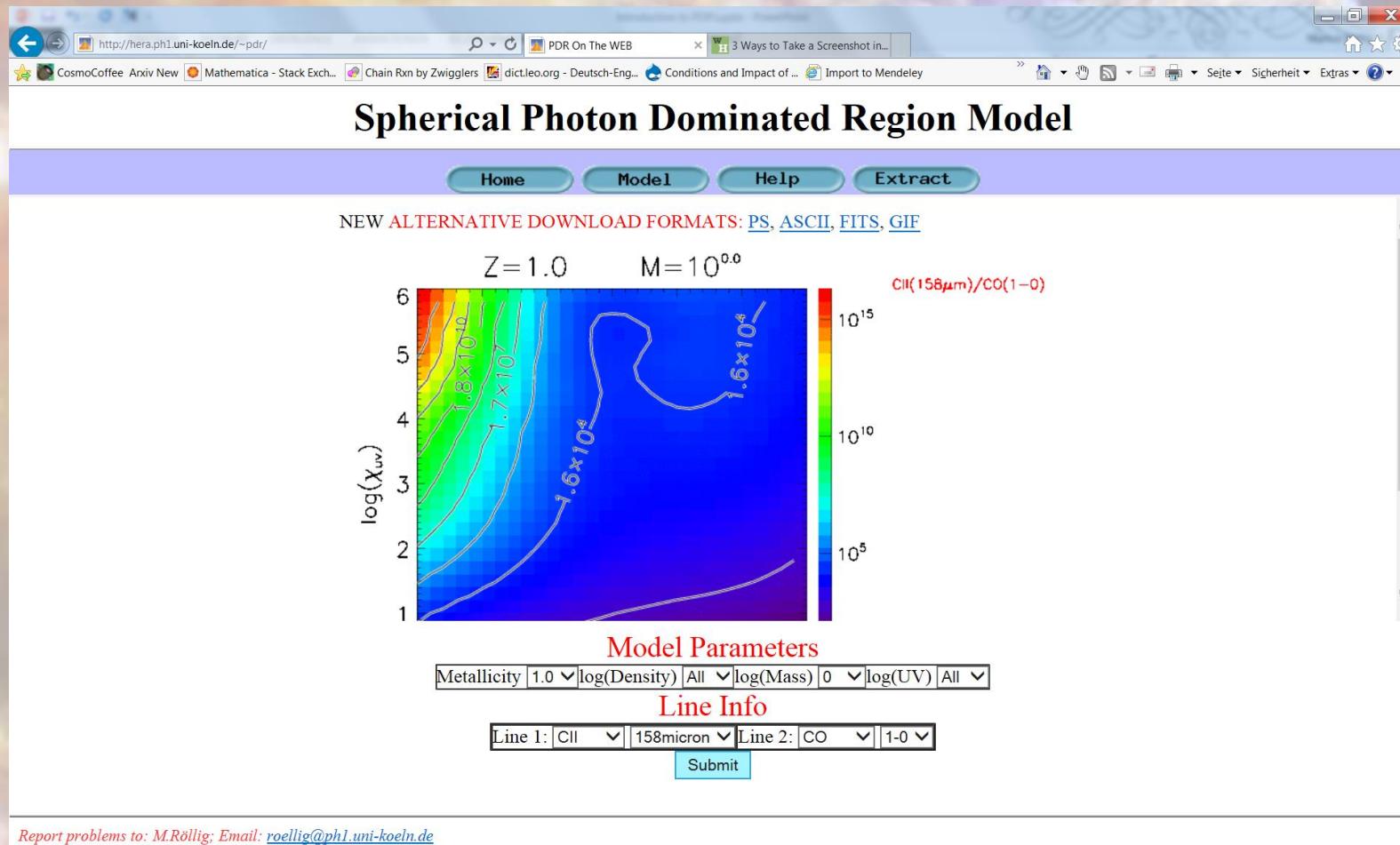
PDR Online Extraction Tool

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

The screenshot shows a web browser window with the URL <http://hera.ph1.uni-koeln.de/~pdr/> in the address bar. The title of the page is "Spherical Photon Dominated Region Model". Below the title is a navigation menu with four buttons: "Home", "Model", "Help", and "Extract". A note at the top of the main content area says: "Enable Javascript in your browser to use this form. Two of the four possible model parameters should be fixed before submitting the form." Below this note is a red-bordered box containing the "Model Parameters" and "Line Info" sections. The "Model Parameters" section includes dropdown menus for Metallicity (1.0), log(Density) (All), log(Mass) (0), and log(UV) (All). The "Line Info" section contains two dropdown menus for Line 1 and Line 2, both set to CII 158micron. A "Submit" button is located at the bottom of this red-bordered box. At the very bottom of the page, there is a footer with the text: "Report problems to: M.Röllig; Email: roellig@ph1.uni-koeln.de".

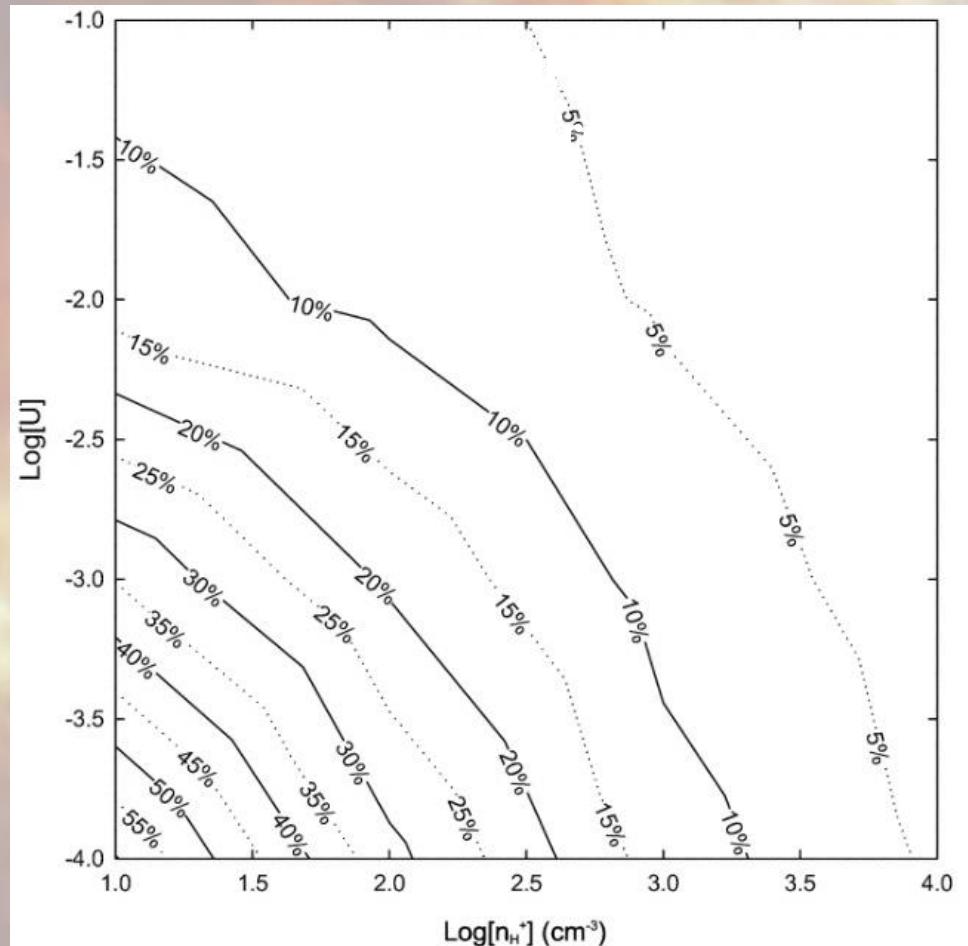
PDR Online Extraction Tool

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



[CII] contribution from HII regions

Teff= 42000 K

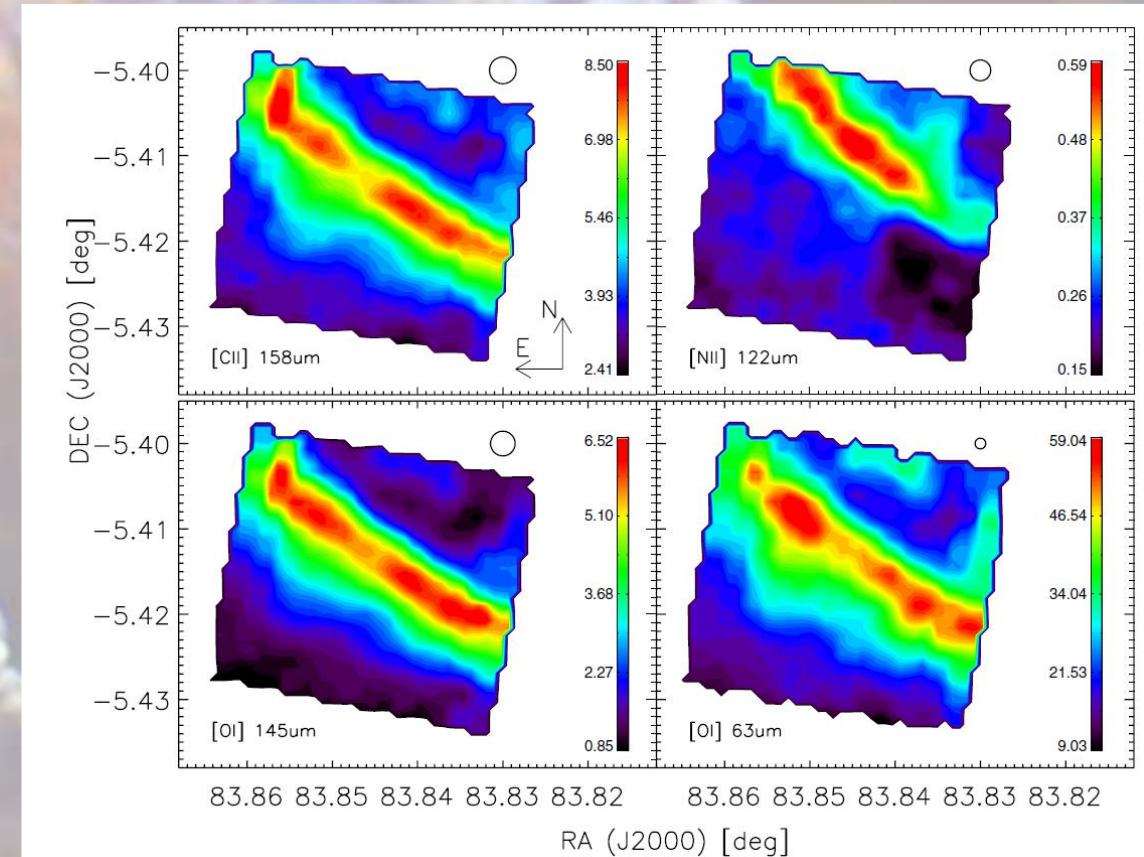
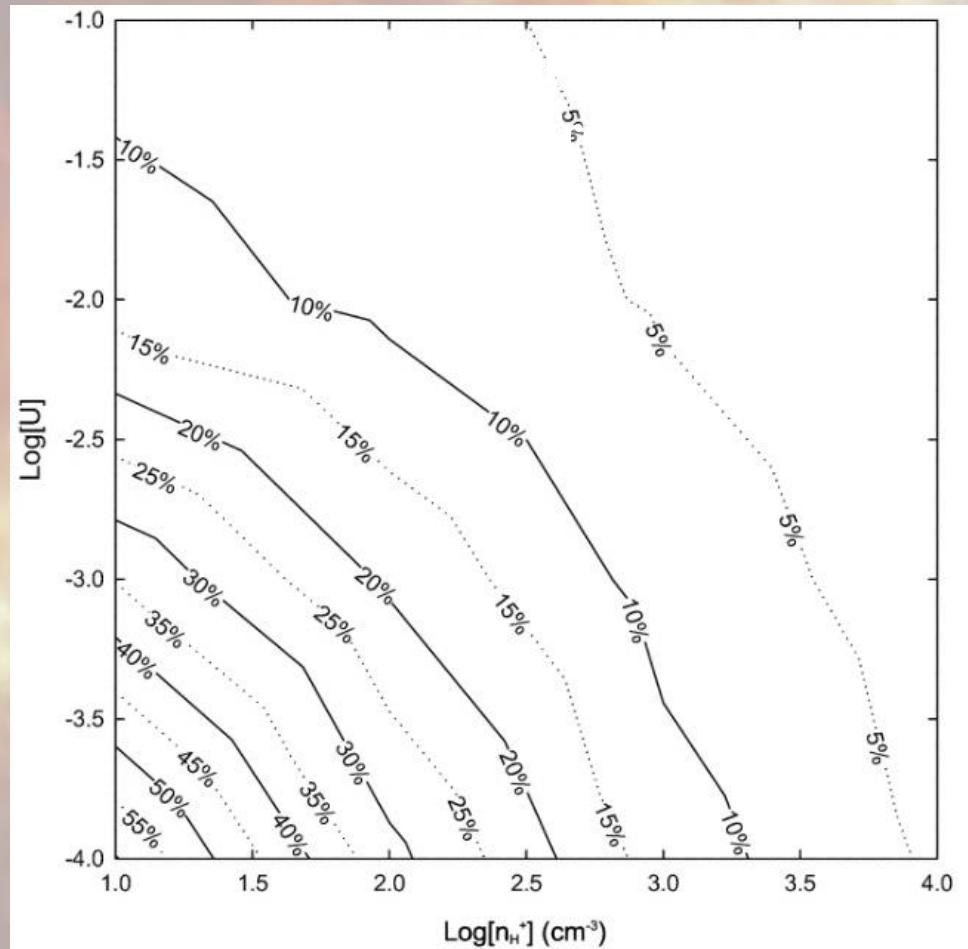


Abel et al 2005

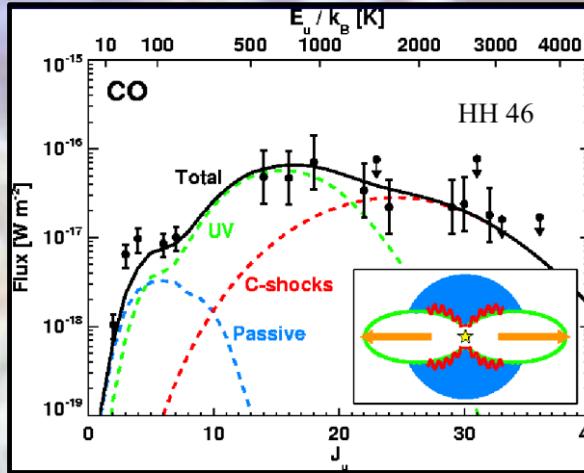
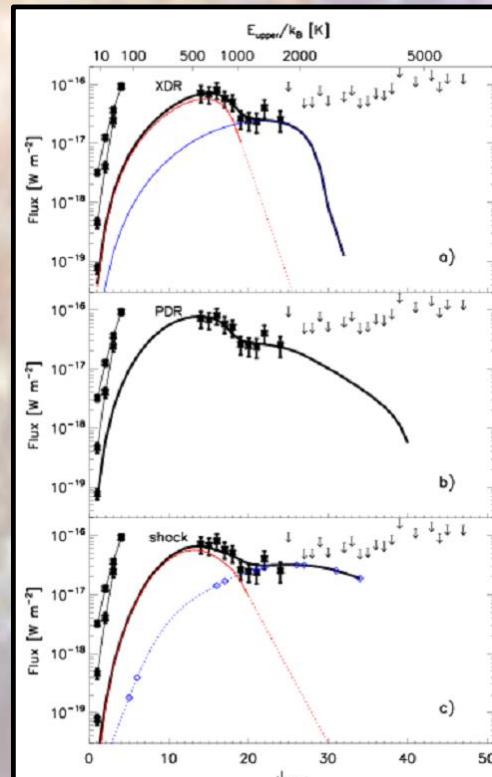
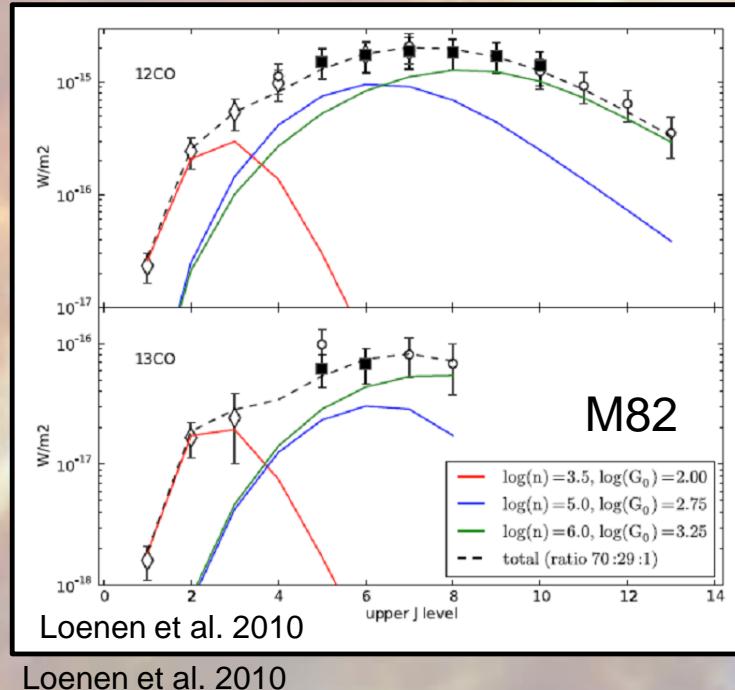
- C⁺ is also present in the ionized gas
- When observing a PDR you always observe the neighbouring HII region
- [CII] emission is partly produced in the HII region. (~10-30%)

[CII] contribution from HII regions

Teff= 42000 K



CO in PDRs, Shocks, XDRs ???



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

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

Hailey-Dunsheath et al. 2012

NGC 1068

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XDR or PDR?

(Spaans & Meijerink 2007, ApJ 664, L23)

TABLE 1

COLUMN DENSITIES AND COLUMN DENSITY RATIOS

N_{H}	$N(\text{CO}^+)$	$N(\text{HOC}^+)$	$N(\text{HCO}^+)$	$N(\text{CN})$	$N(\text{HCN})$	CO^+/HCO^+	$\text{HCO}^+/\text{HOC}^+$	CN/HCN
XDR: $n = 10^5 \text{ cm}^{-3}$ and $F_x = 5.1 \text{ ergs s}^{-1} \text{ cm}^{-2}$								
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 $F_x = 1.6 \text{ ergs s}^{-1} \text{ cm}^{-2}$								
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

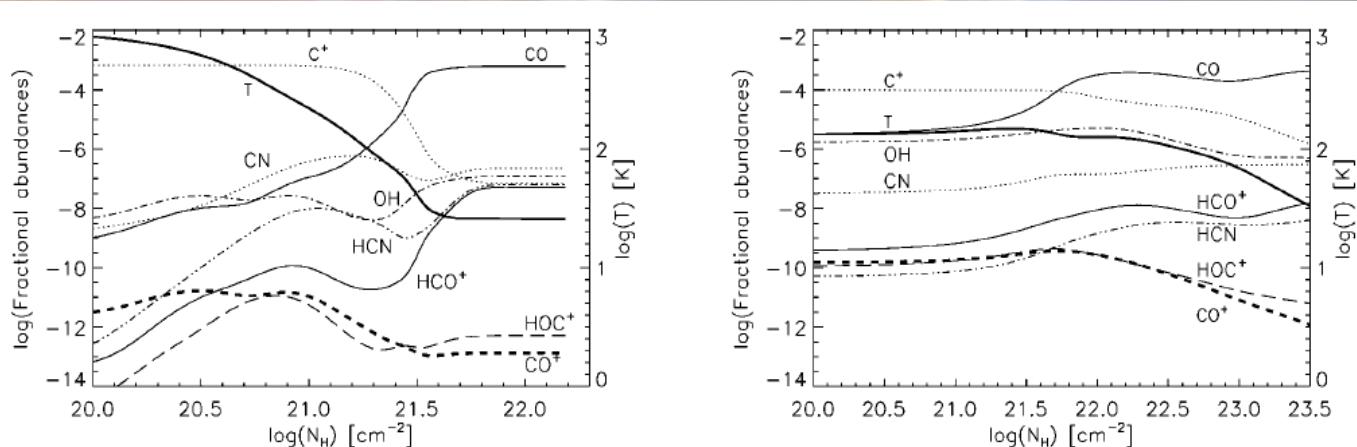
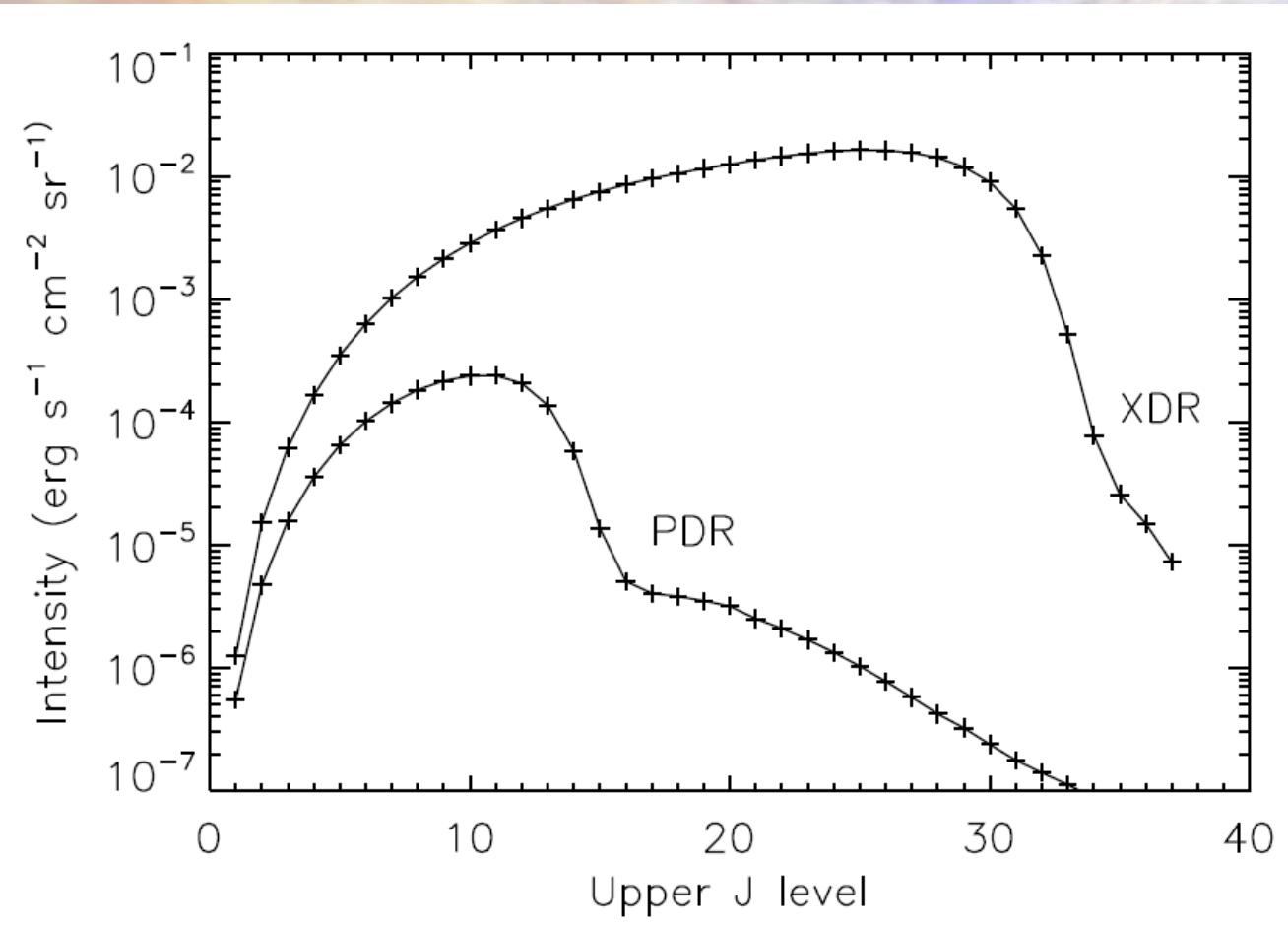


FIG. 2.—Chemical and thermal structure of a PDR with an enhanced cosmic ionization rate ($\zeta = 5 \times 10^{-15} \text{ s}^{-1}$) and an XDR model. Density $n = 10^5 \text{ cm}^{-3}$, and $G_0 = 10^{3.5}/F_x = 1.6 \text{ ergs s}^{-1} \text{ cm}^{-2}$). The CO^+ abundance is at least an order of magnitude larger in the XDR.

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

XDR vs. PDR



Spaans & Meijerink 2008

FINE-STRUCTURE ATOMIC COOLING PARAMETERS

Species (0, 1, 2) ^a	$\frac{E_{ij}}{k}$ (K) ^b	λ_{μ} ^c	n_{cr}^e (cm ⁻³) ^d	n_{cr}^H (cm ⁻³) ^d	A_{ij} (s ⁻¹) ^e	γ_{ij}^e (cm ⁻³ s ⁻¹) ^f	γ_{ij}^H (cm ³ s ⁻¹) ^f	N_r (cm ⁻²) ^g
C I (³ P ₀ , ³ P ₁ , ³ P ₂)	2.4(1)	609.2	3.9(0) $T_2^{-0.13}$	1.6(2) $T_2^{-0.34}$	7.9(-8)	3.0(-9)	1.6(-10) $T_2^{0.14}$	2.3(20)
	6.3(1)	229.9	1.3(1)	7.0(2) $T_2^{-0.26}$	2.0(-14)	5.0(-9)	9.2(-11) $T_2^{0.26}$	9.8(27)
	3.9(1)	369.0	...		2.7(-7)	1.5(-8)	2.9(-10) $T_2^{0.26}$	5.3(20)
C II (² P _{1/2} , ² P _{3/2})	9.2(1)	157.7	8.7(0) $T_2^{0.50}$	3.0(2) $T_2^{-0.07}$	2.4(-6)	2.8(-7) $T_2^{-0.5}$	8.0(-10) $T_2^{0.07}$	6.5(20)
Cl I (² P _{3/2} , ² P _{1/2})	1.3(3)	11.4	2.6(5)	1.4(7) $T_2^{-0.17}$	1.2(-2)	4.7(-8)	8.3(-10) $T_2^{0.17}$	1.1(24)
Cl II (³ P ₂ , ³ P ₁ , ³ P ₀)	1.0(3)	14.4	1.4(4) $T_2^{0.45}$	5.4(6)	7.5(-3)	5.3(-7) $T_2^{-0.5}$	1.4(-9)	7.5(23)
	1.4(3)	10.0	1.6(3) $T_2^{0.50}$	8.1(5)	4.8(-7)	5.3(-7) $T_2^{-0.5}$	1.1(-9)	1.0(29)
	4.3(2)	33.4	1.4(-3)	3.2(-7) $T_2^{-0.5}$	6.3(-10)	5.7(23)
Fe I (⁵ D ₄ , ⁵ D ₃ , ⁵ D ₂)	6.0(2)	24.0	2.1(4) $T_2^{-0.13}$	3.1(6) $T_2^{-0.28}$	2.5(-3)	1.2(-7)	8.0(-10) $T_2^{0.17}$	6.6(21)
	1.0(3)	14.2	7.5(3)	1.3(6) $T_2^{-0.17}$	1.0(-9)	1.2(-7)	6.9(-10) $T_2^{0.17}$	9.3(26)
	4.2(2)	34.2	1.6(3)	9.3(-8)	5.3(-10) $T_2^{0.17}$	3.7(21)
Fe II (⁶ D _{9/2} , ⁶ D _{7/2} , ⁶ D _{5/2}) ..	5.6(2)	26.0	1.2(3) $T_2^{0.41}$	2.2(6) $T_2^{-0.09}$	2.1(-3)	1.8(-6) $T_2^{-0.5}$	9.5(-10)	6.0(21)
	9.6(2)	15.0	6.0(2) $T_2^{0.50}$	1.5(6)	1.5(-9)	1.8(-6) $T_2^{-0.5}$	5.7(-10)	5.9(28)
	4.1(2)	35.4	1.6(-3)	8.7(-7) $T_2^{-0.5}$	4.7(-10)	3.3(21)
Ne II (² P _{3/2} , ² P _{1/2})	1.1(3)	12.8	5.4(4) $T_2^{0.50}$	6.6(6)	8.6(-3)	1.6(-7) $T_2^{-0.5}$	1.3(-9)	1.9(22)
Ni I (³ F ₄ , ³ F ₃ , ³ F ₂)	1.9(3)	7.5	5.2(5) $T_2^{-0.06}$	7.8(7) $T_2^{-0.22}$	6.2(-2)	1.2(-7)	8.0(-10) $T_2^{0.17}$	1.1(23)
	3.2(3)	4.5	1.2(5)	2.0(7) $T_2^{0.17}$	3.6(-9)	1.2(-7)	6.9(-10) $T_2^{0.17}$	1.3(31)
	1.3(3)	11.3	2.5(-2)	9.3(-8)	5.3(-10) $T_2^{0.17}$	8.9(22)
Ni II (² D _{5/2} , ² D _{3/2})	2.2(3)	6.6	5.0(4) $T_2^{0.50}$	5.0(7)	5.5(-2)	1.1(-6) $T_2^{-0.5}$	1.1(-9)	2.2(23)
O I (³ P ₂ , ³ P ₁ , ³ P ₀)	2.3(2)	63.1	6.3(3) $T_2^{-0.03}$	8.5(5) $T_2^{-0.69}$	9.0(-5)	1.4(-8)	9.2(-11) $T_2^{0.67}$	4.9(20)
	3.3(2)	44.2	8.9(2)	1.1(5) $T_2^{-0.57}$	1.0(-10)	1.4(-8)	4.3(-11) $T_2^{0.80}$	3.8(27)
	9.8(1)	145.6	1.7(-5)	5.0(-9)	1.1(-10) $T_2^{0.44}$	3.7(20)
S I (³ P ₂ , ³ P ₁ , ³ P ₀)	5.7(2)	25.2	4.2(4) $T_2^{-0.03}$	1.8(6) $T_2^{-0.22}$	1.4(-3)	3.3(-8)	7.5(-10) $T_2^{0.17}$	2.0(22)
	8.2(2)	17.4	6.7(3)	2.7(5) $T_2^{0.17}$	7.1(-8)	3.3(-8)	7.1(-10) $T_2^{0.17}$	3.7(27)
	2.5(2)	56.6	3.0(-4)	1.2(-8)	4.2(-10) $T_2^{0.17}$	1.5(22)
Si I (³ P ₀ , ³ P ₁ , ³ P ₂)	1.1(2)	129.6	7.2(2) $T_2^{0.50}$	1.9(4) $T_2^{-0.47}$	8.4(-6)	7.2(-9)	3.5(-10) $T_2^{-0.03}$	2.3(21)
	3.2(2)	44.8	1.4(3)	6.3(4) $T_2^{-0.17}$	2.4(-10)	7.2(-9)	1.7(-10) $T_2^{0.17}$	2.0(27)
	2.1(2)	68.4	4.2(-5)	2.2(-8)	5.0(-10) $T_2^{0.17}$	5.6(21)
Si II (² P _{1/2} , ² P _{3/2})	4.1(2)	34.8	1.2(2) $T_2^{0.50}$	3.2(5)	2.1(-4)	1.7(-6) $T_2^{-0.5}$	8.0(-10) $T_2^{-0.07}$	7.1(21)

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

^b For three-level systems, the energies listed are E_{10} , E_{20} , and E_{31} , respectively.

^c The wavelength in microns; note that the 2→0 transition is generally forbidden.

^d 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 $30 \text{ K} < T < 3000 \text{ K}$.

^e The spontaneous transition rates listed in order A_{10} , A_{20} , and A_{31} . These are taken from Aller (1984), Garstang 1958, 1962, 1964, 1968; Grevesse, Nussbaumer, and Swings 1971; and Wiese *et al.* 1966, 1969.

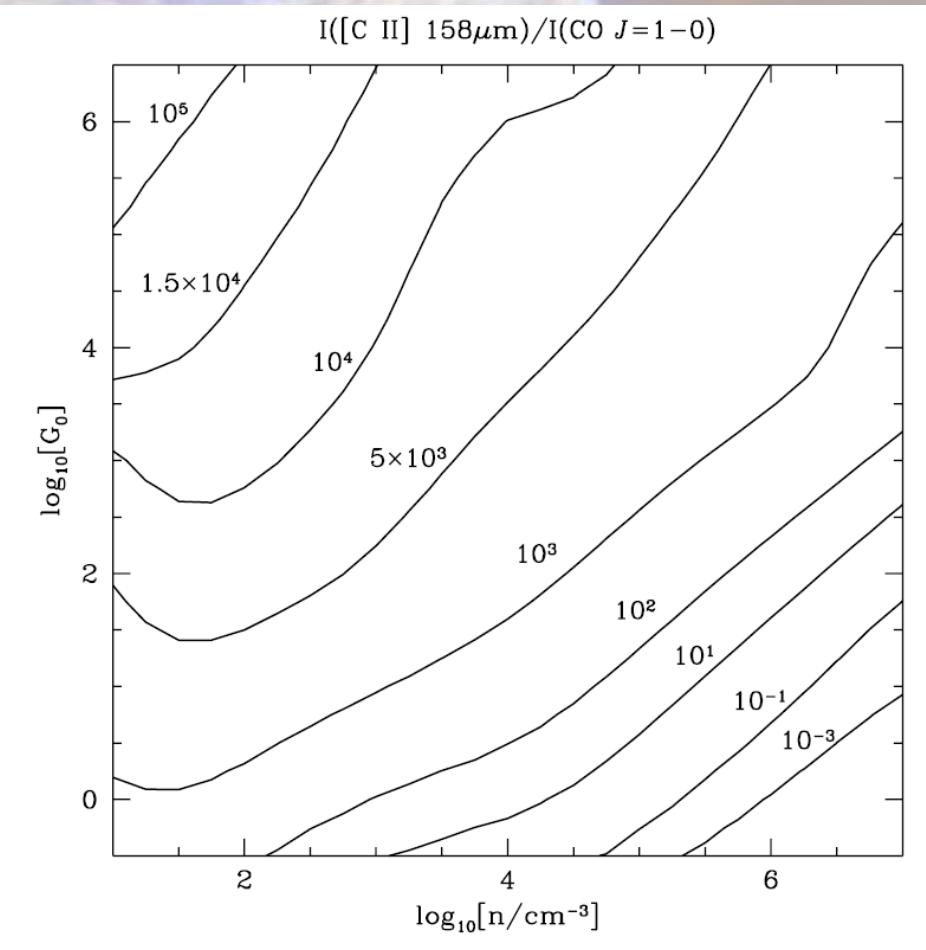
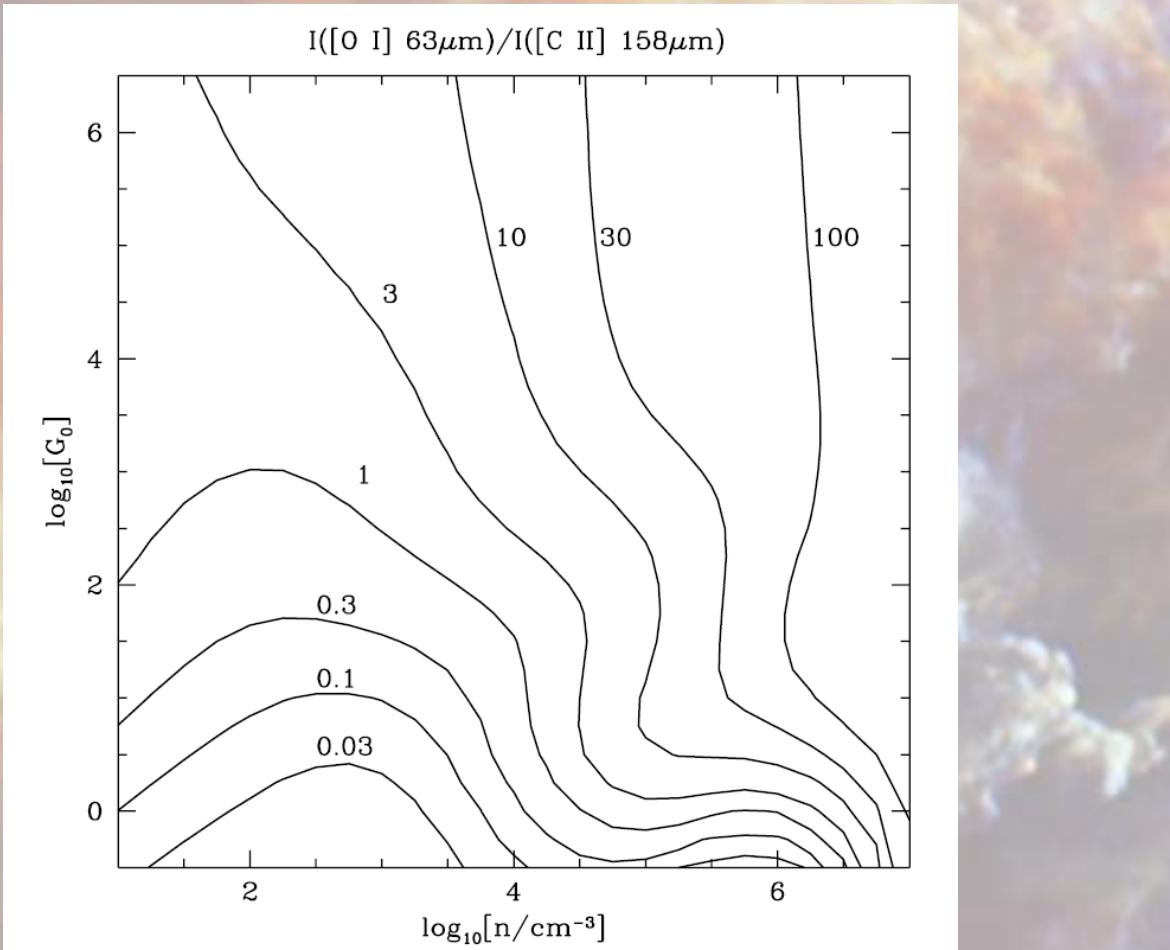
^f The rate coefficients for collisional deexcitation are listed in the same order. They are calculated from formulae given by Bahcall and Wolf 1968 with the exceptions C I and O I (Launay and Roueff 1977a), C II (Launay and Roueff 1977b), Fe II (Aannestad 1973), Ne II (Osterbrock 1974). Proton rates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

^g N_r 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

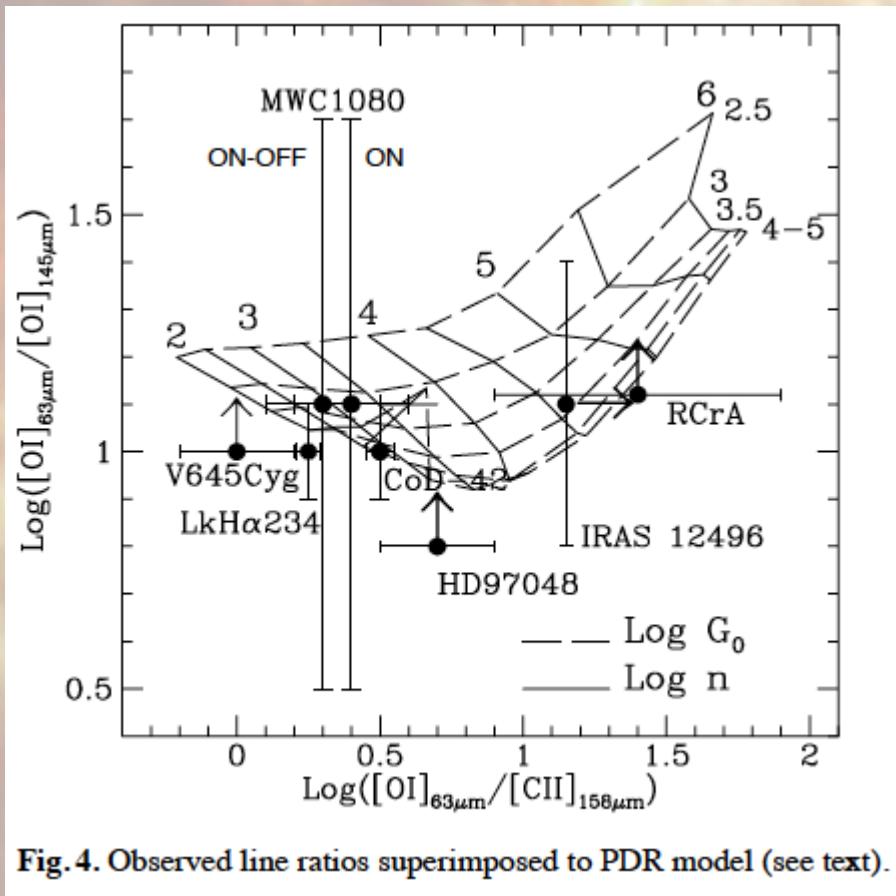
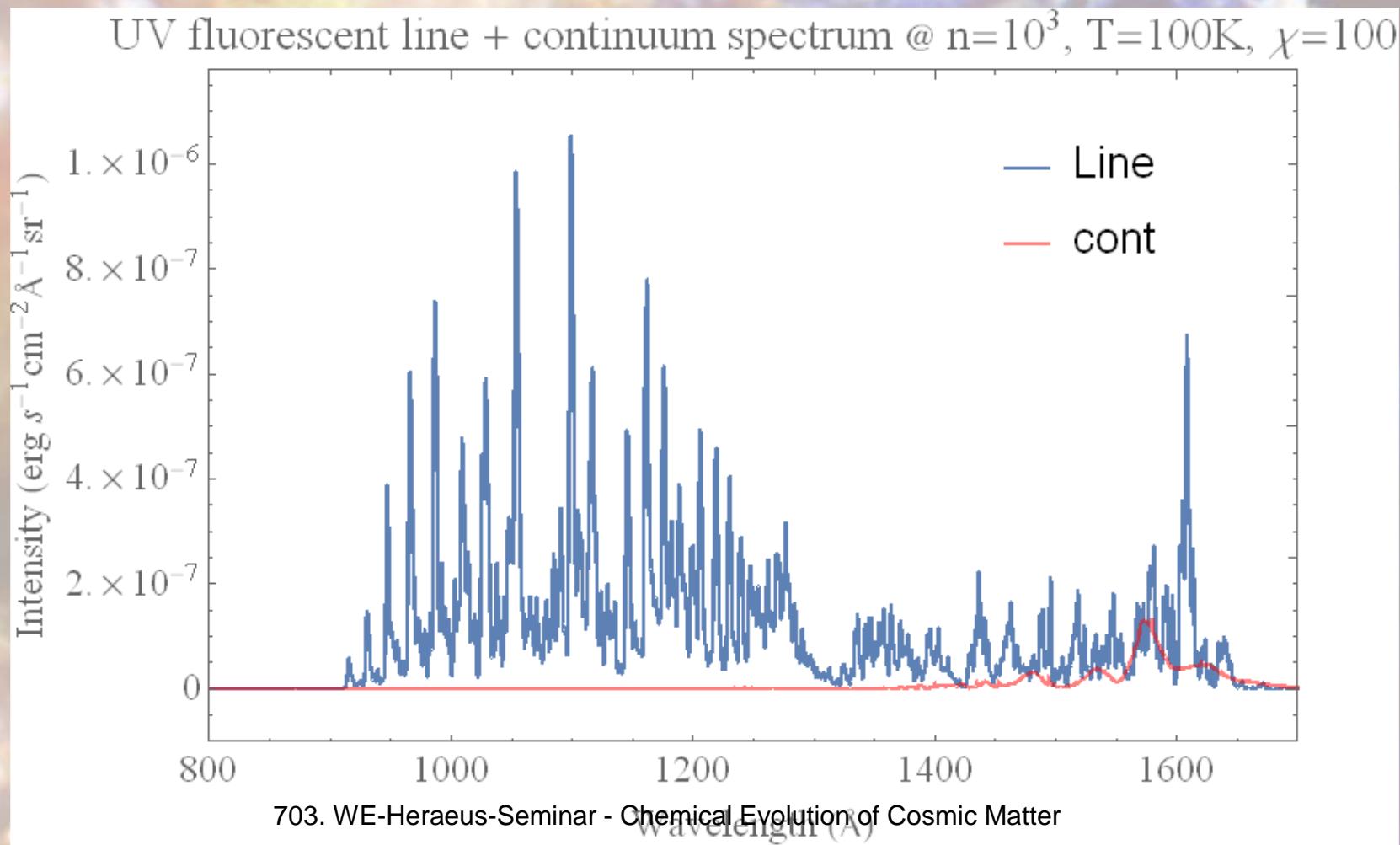


Fig. 4. Observed line ratios superimposed to PDR model (see text).

- 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.

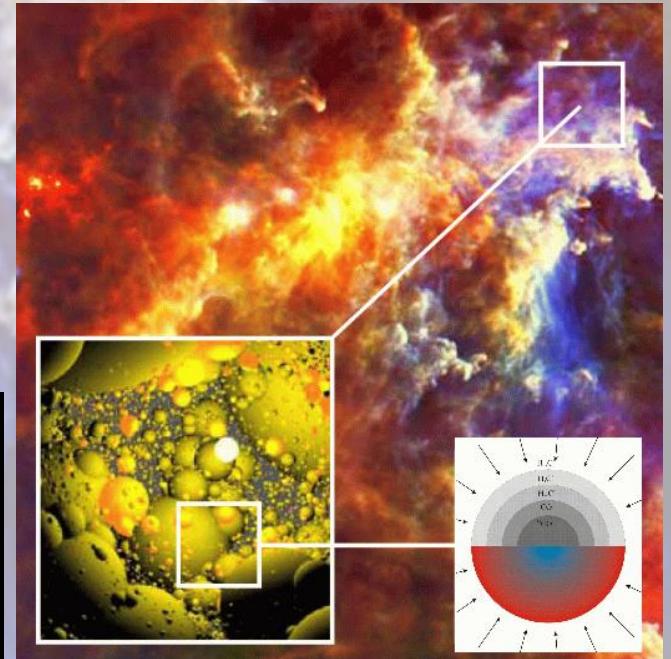
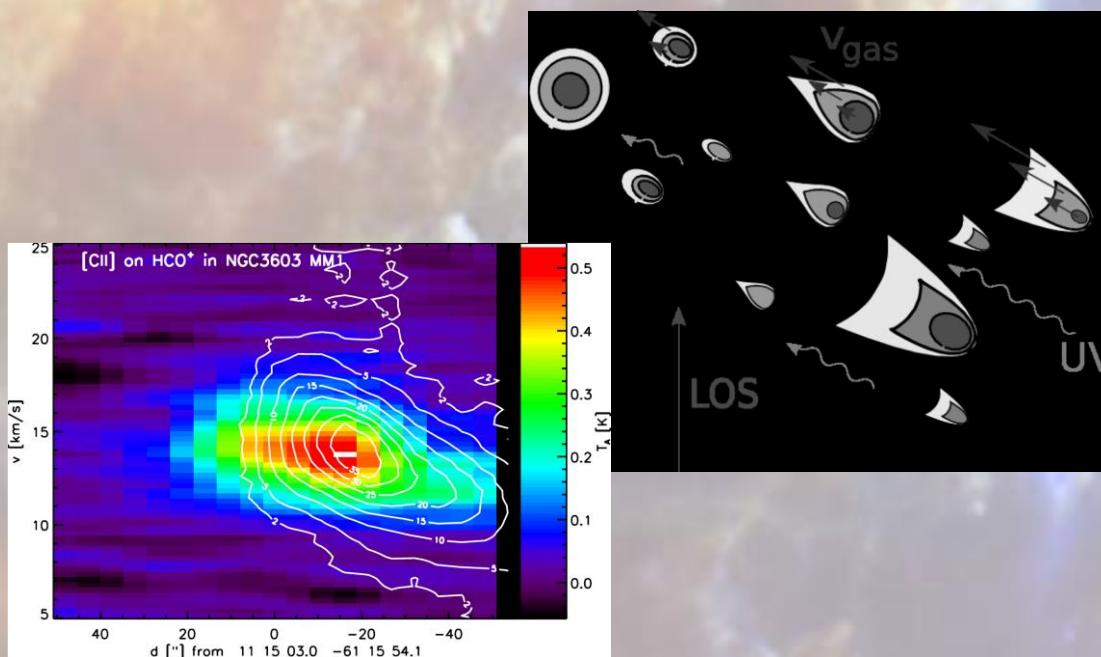
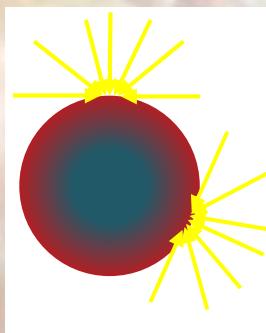
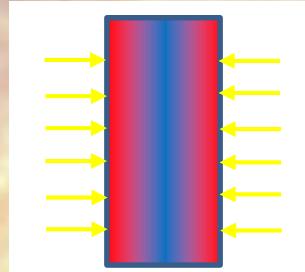
Fluorescent UV spectrum of H₂ + cont.

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



Physical structure

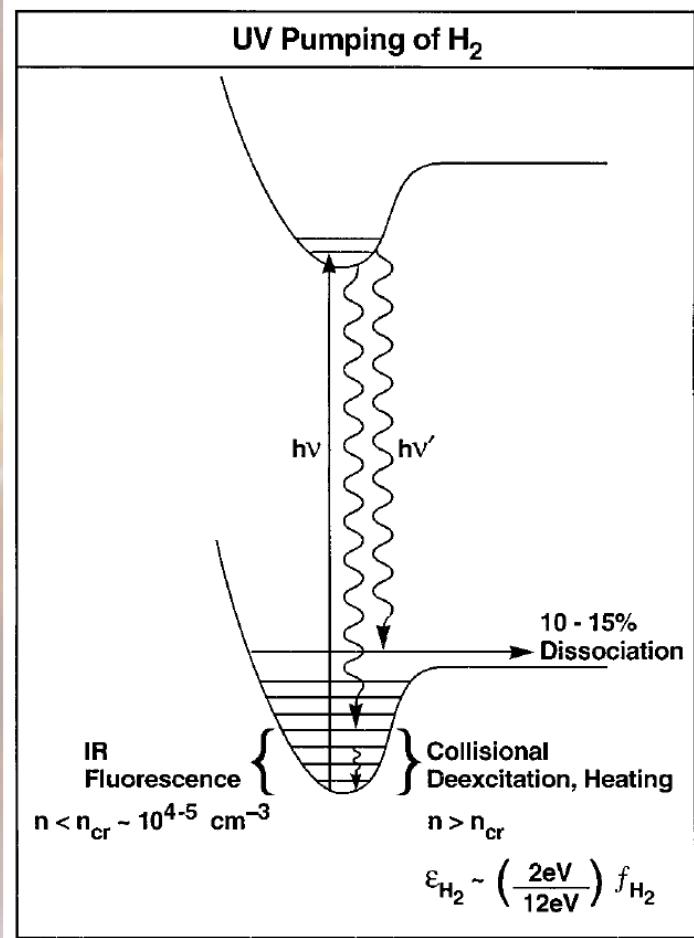
- Temperature
 - heating
 - cooling
- Density
- Geometry
- Dynamics



Gas heating

1. FUV photons
 1. Photoelectric heating
 2. vibrational deexcitation of electronically pumped H₂
 3. H₂ formation heating
 4. gas-grain collisions
 5. photodissociation of H₂
 6. ionization of atomic carbon
2. Cosmic rays/X-rays
3. Shocks
4. Turbulence

H₂ pumping

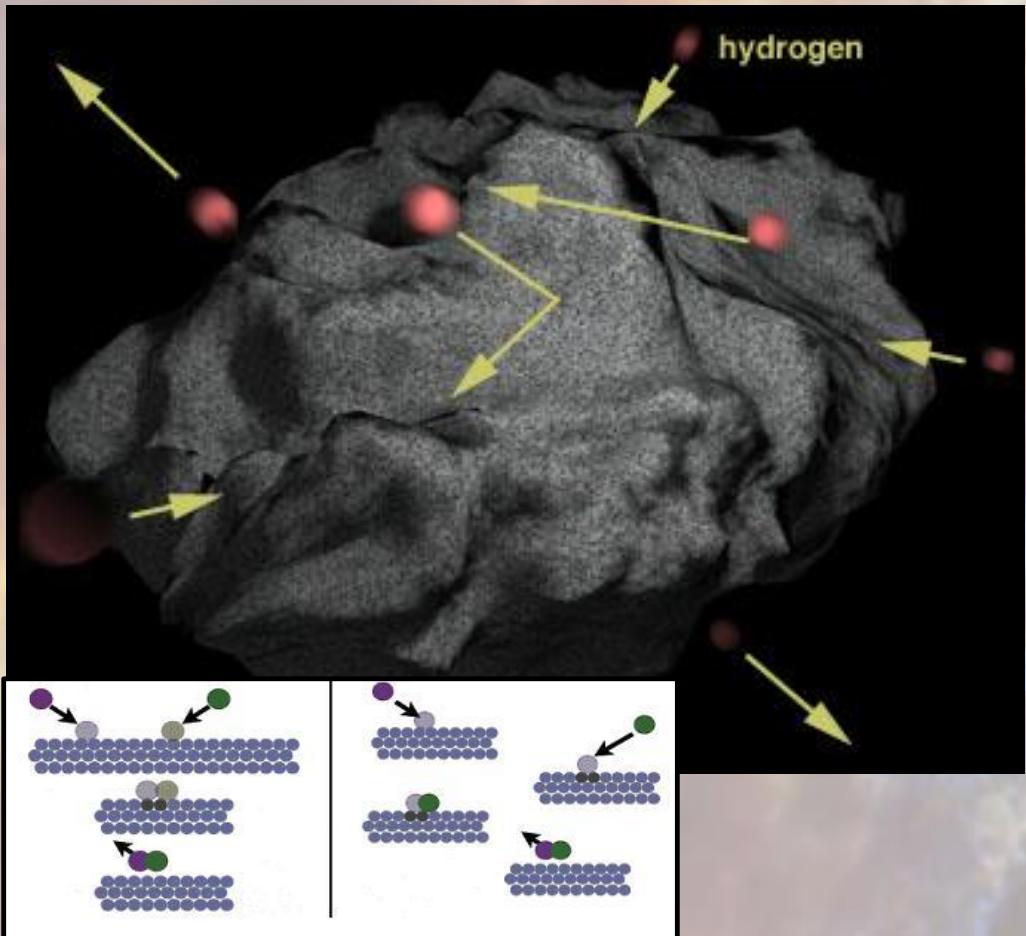


Tielens & Hollenbach 1999

- 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
→ $E_{vib} \sim 2 \text{ eV}$ available for heating
- efficient at high densities

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

H₂ formation heating

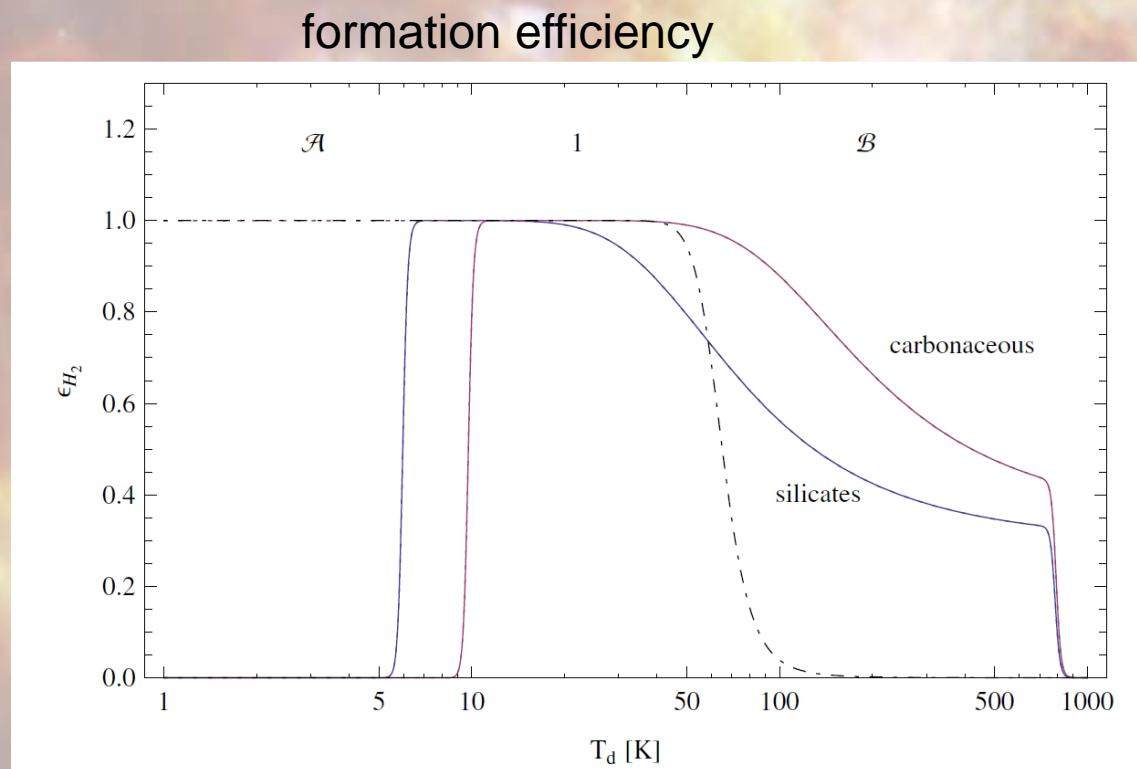


- H₂ forms on dust surfaces
- binding energy of H₂ ~ 4.5 eV
- newly formed H₂ molecules are released into the gas-phase and carry away part of the binding energy as kinetic and internal energy
→ heating via collisions

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

R_{H2form}: H₂ formation rate

H_2 formation heating



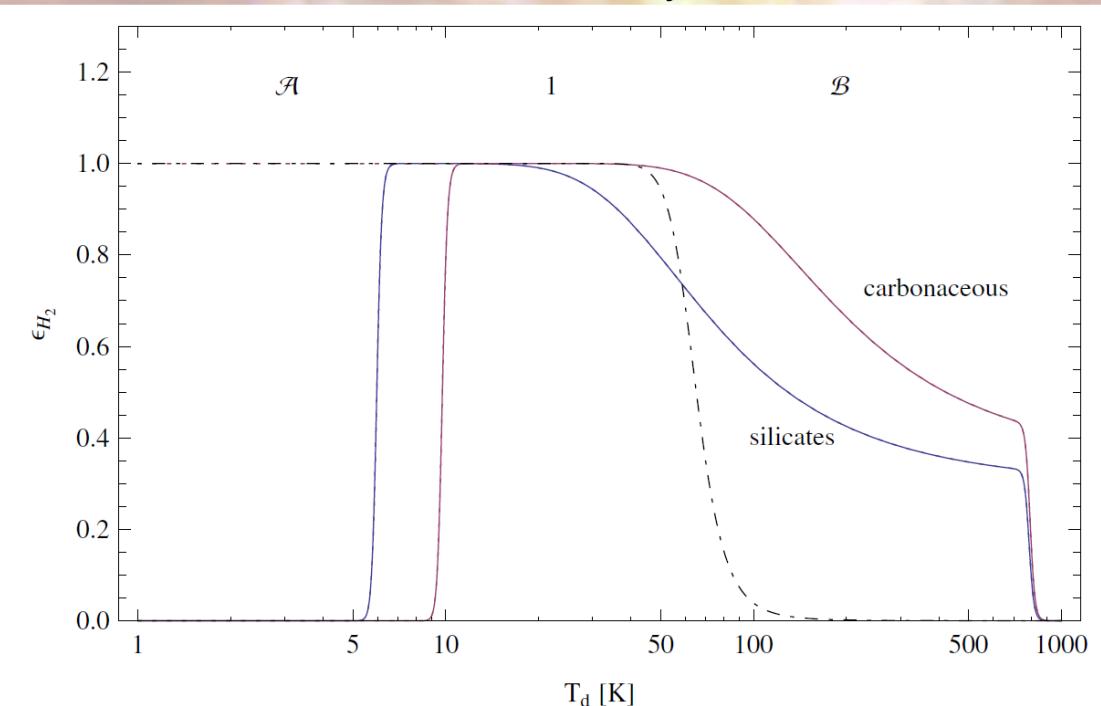
Cazaux & Tielens (2002, 2010)

Chemisorption leads to efficient H_2 formation at high temperatures

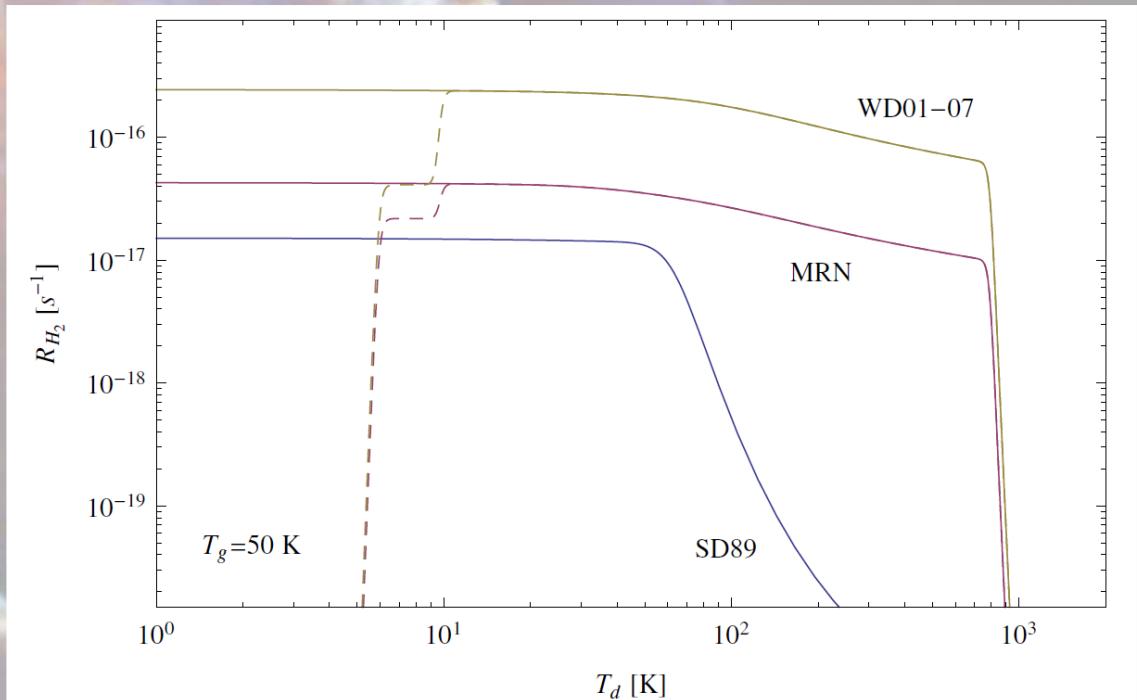
- H-binding to the grain surface determines its mobility and resistance against thermal desorption
 - weak binding (physisorption), $T < 50-80\text{K}$
 - strong binding (chemisorption), $T < \sim 500-800\text{ K}$

H_2 formation heating

formation efficiency



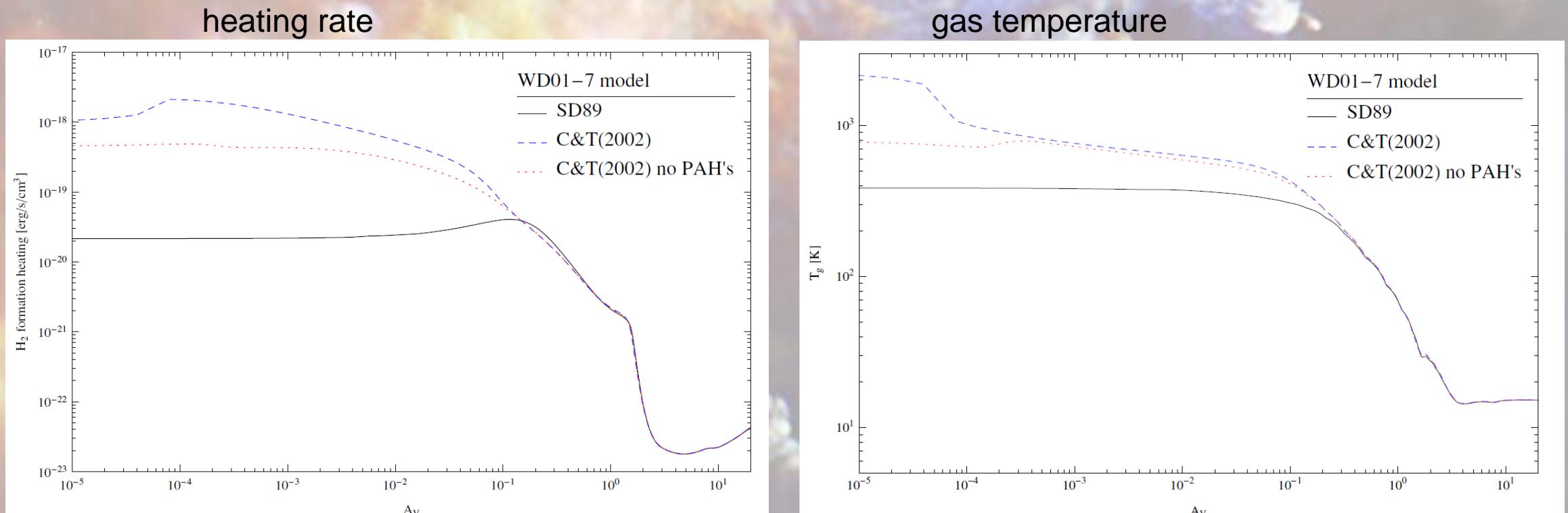
formation rate



Cazaux & Tielens (2002,2010)

Chemisorption leads to efficient H_2 formation at high temperatures

H_2 formation heating

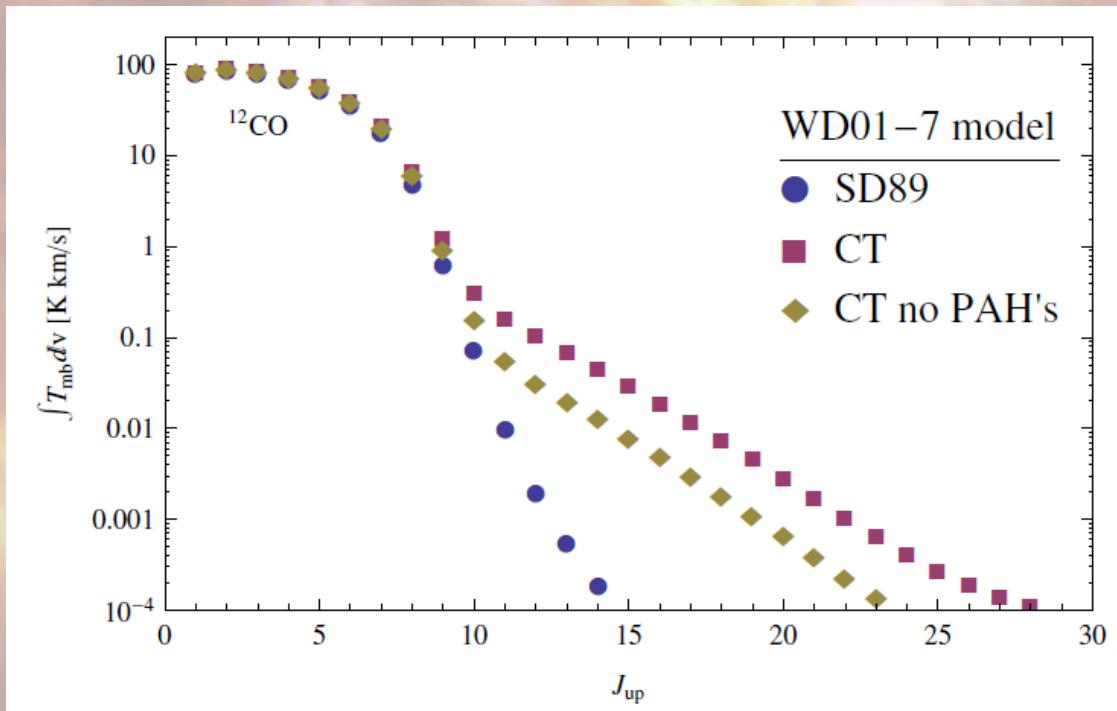


More efficient H_2 formation leads to stronger gas heating.

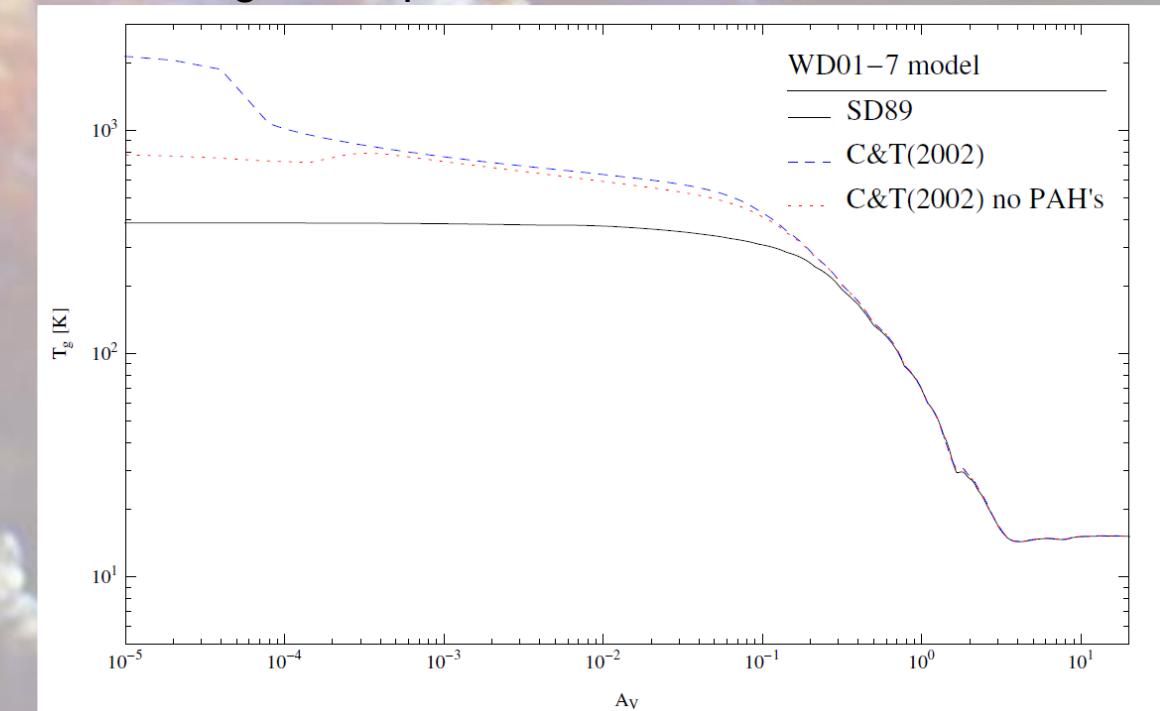
Röllig et al. 2013

H₂ formation heating

CO line emission



gas temperature



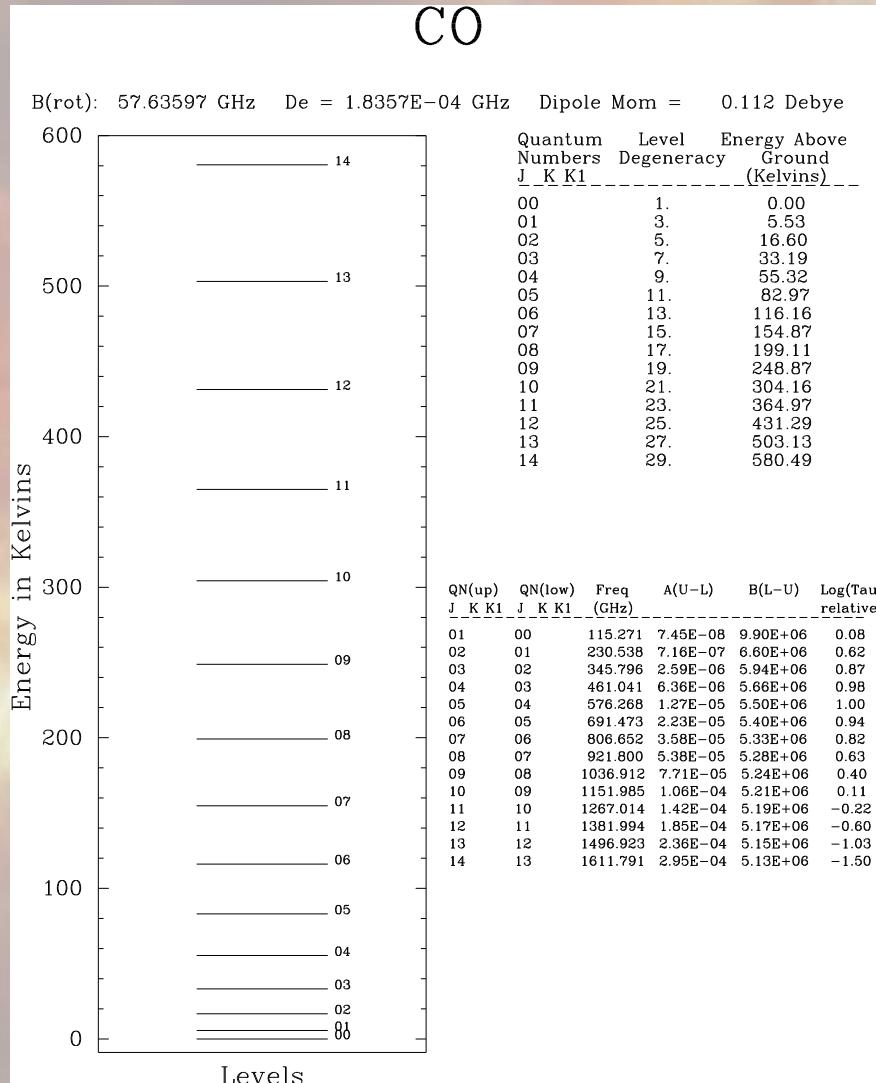
Dust content & physics influences high-J CO emission

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^+ , O, C, CO, H_2O

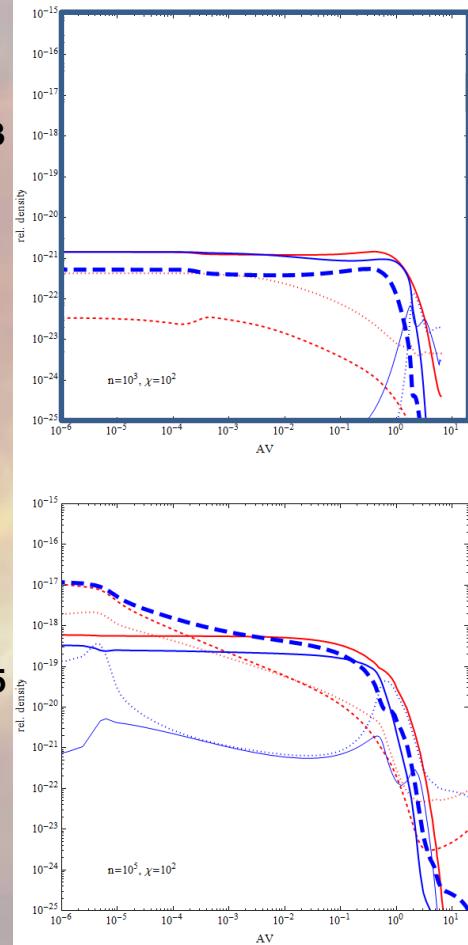
Radiative line cooling



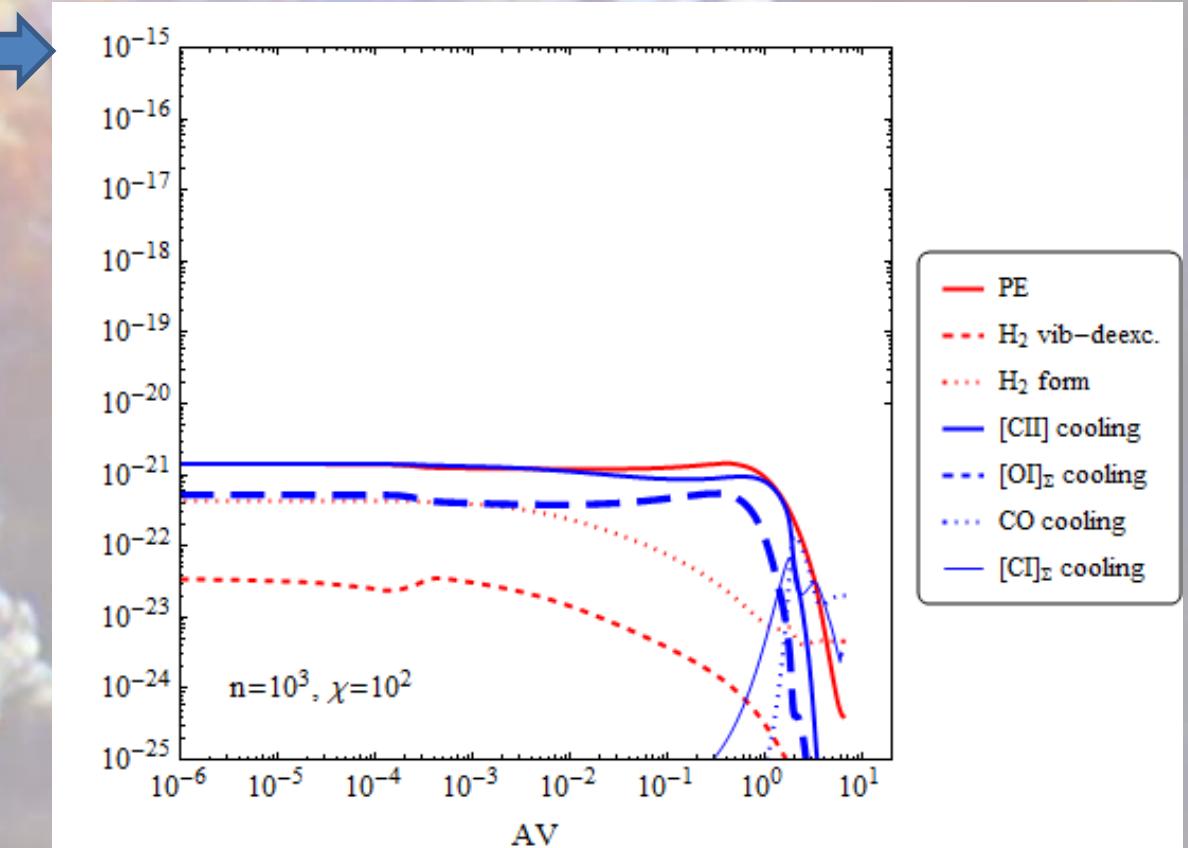
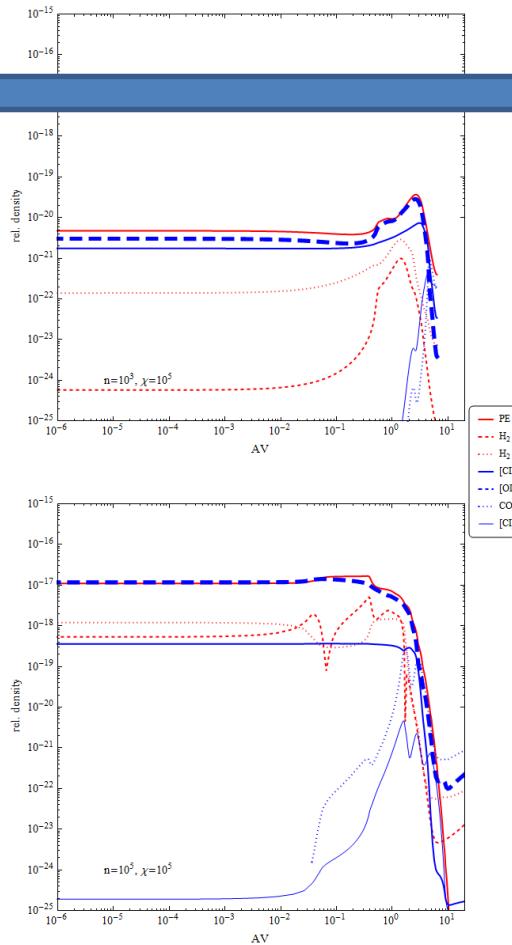
- When a transition of a species is excited collisionally and decays radiatively, the transition energy is carried away by photons and the gas is cooled.
- Coolant conditions:
 - abundant
 - collisionally excitable energy levels given ISM conditions
 - rapid decay times (large A_{ij})
- Good coolants: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

PDR heating/cooling

$\chi=100$

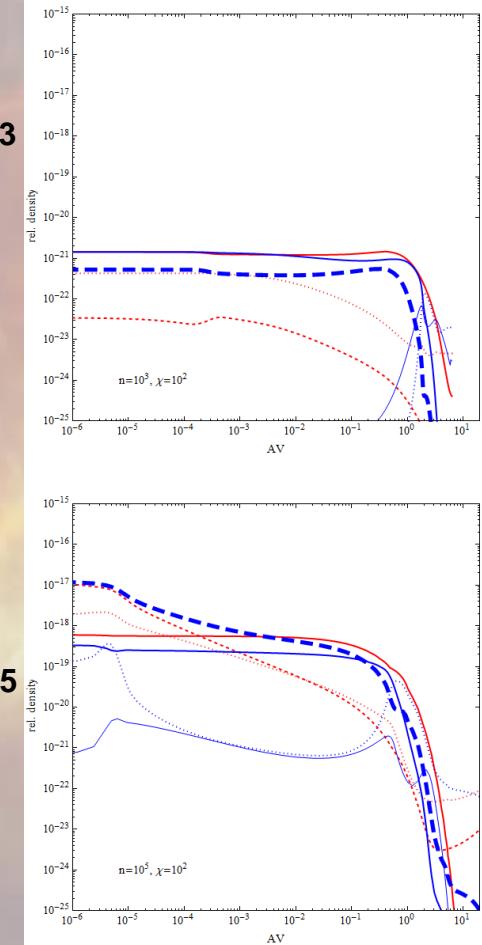


$\chi=10^5$

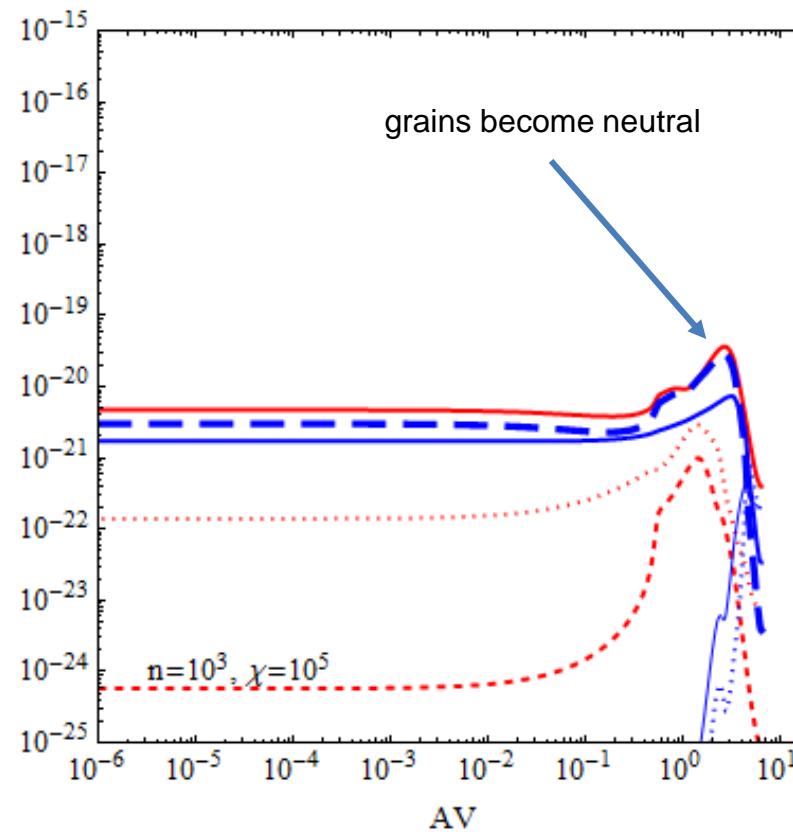
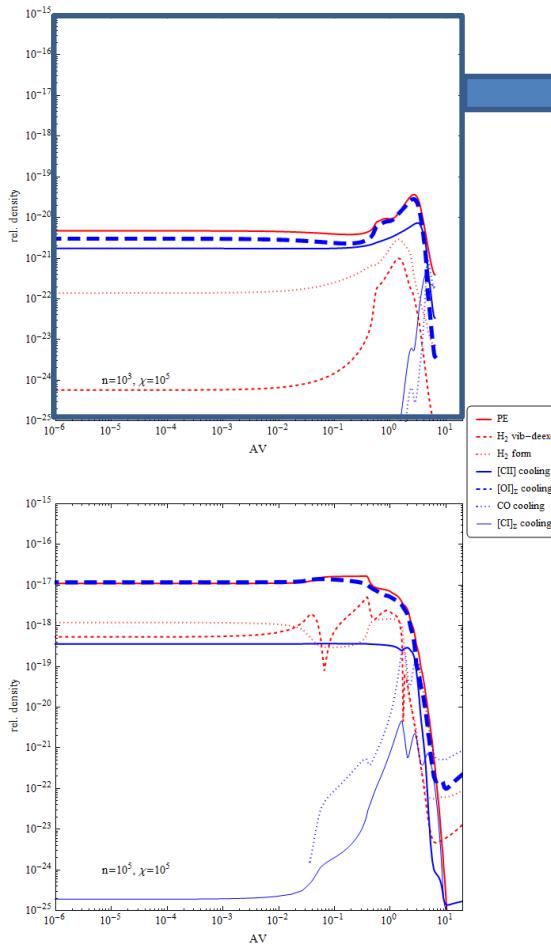


PDR heating/cooling

$\chi=100$



$\chi=10^5$

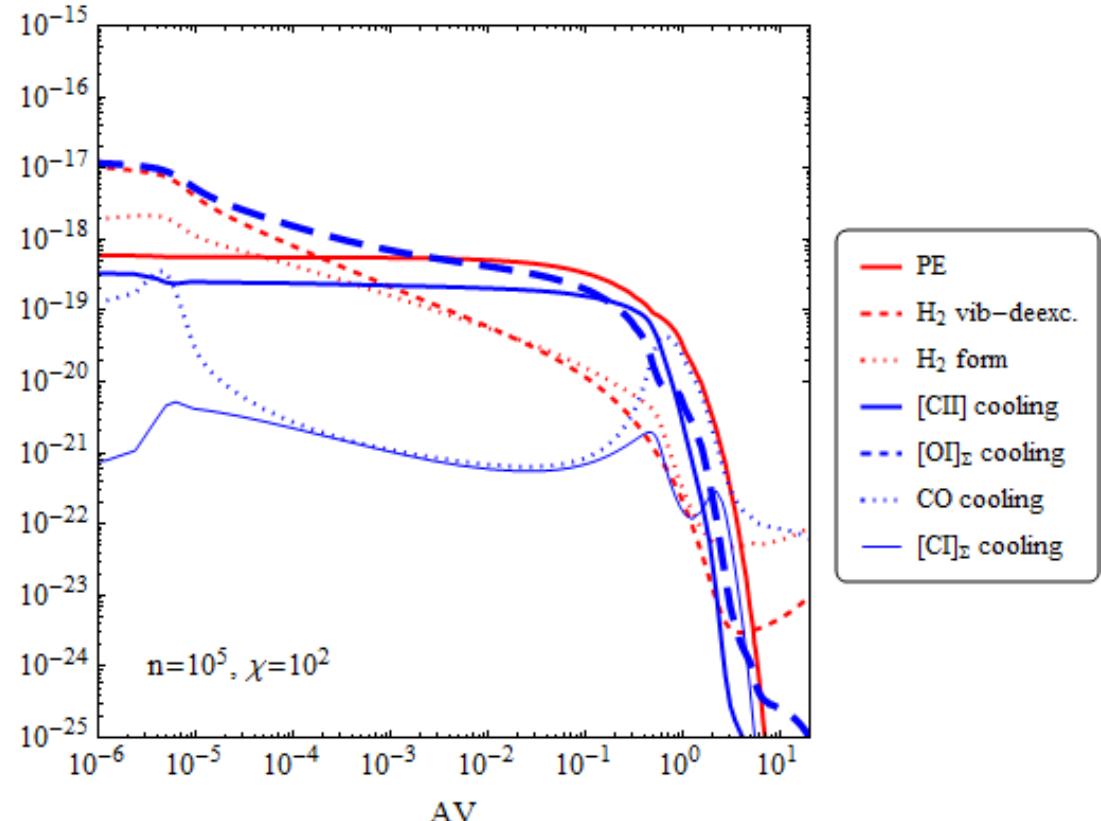
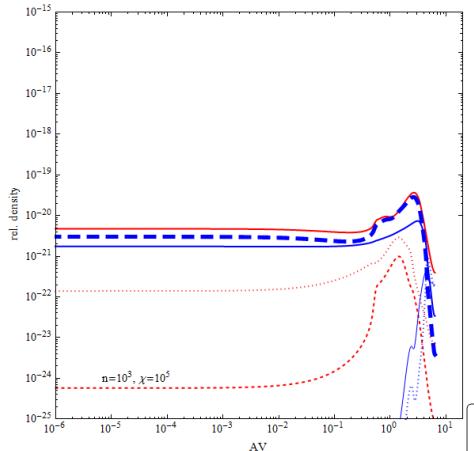
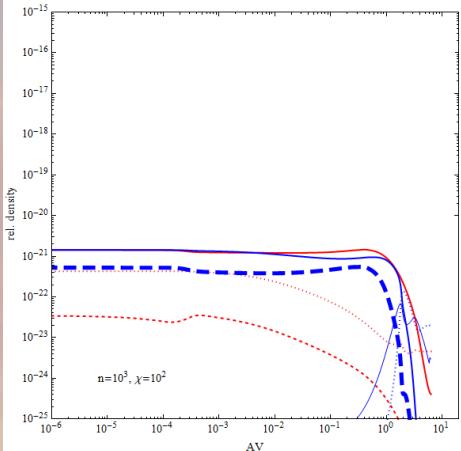


PDR heating/cooling

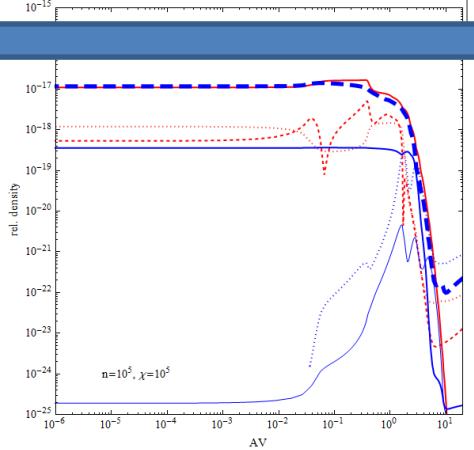
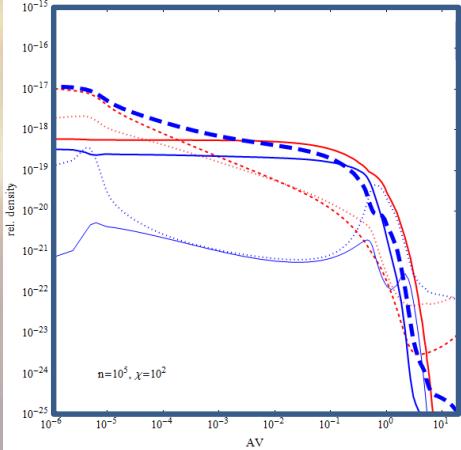
$\chi=100$

$\chi=10^5$

$n=10^3$



$n=10^5$

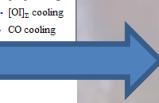
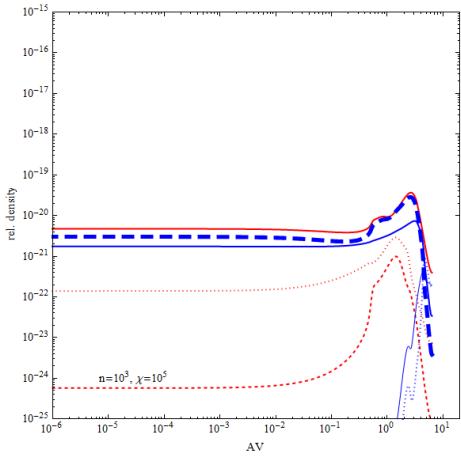
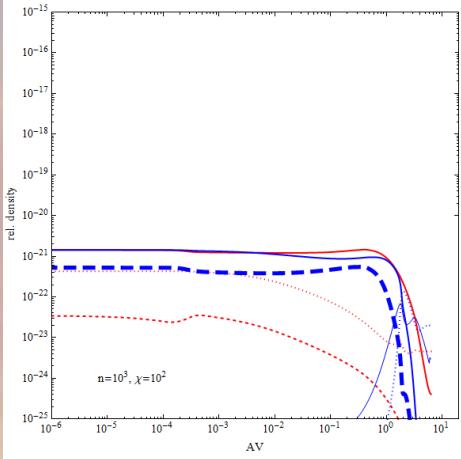


PDR heating/cooling

$\chi=100$

$\chi=10^5$

$n=10^3$



$n=10^5$

