



PDR Modelling with KOSMA- τ

M. Röllig,

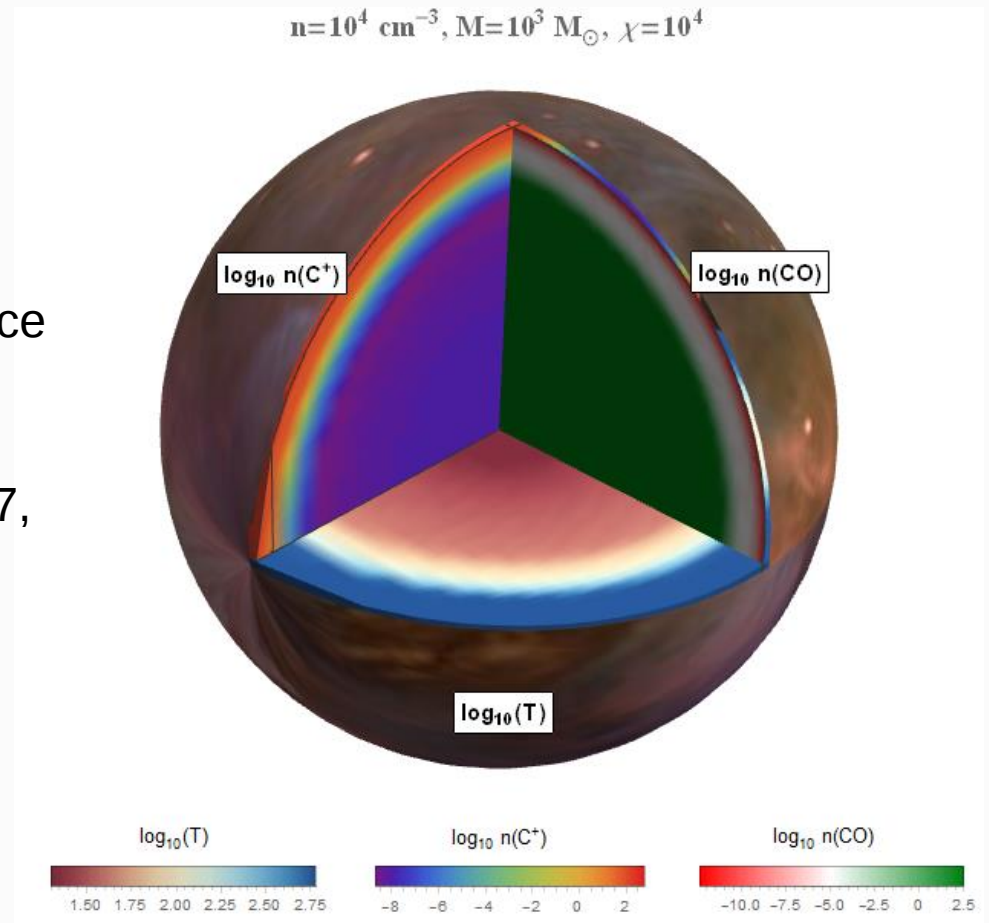
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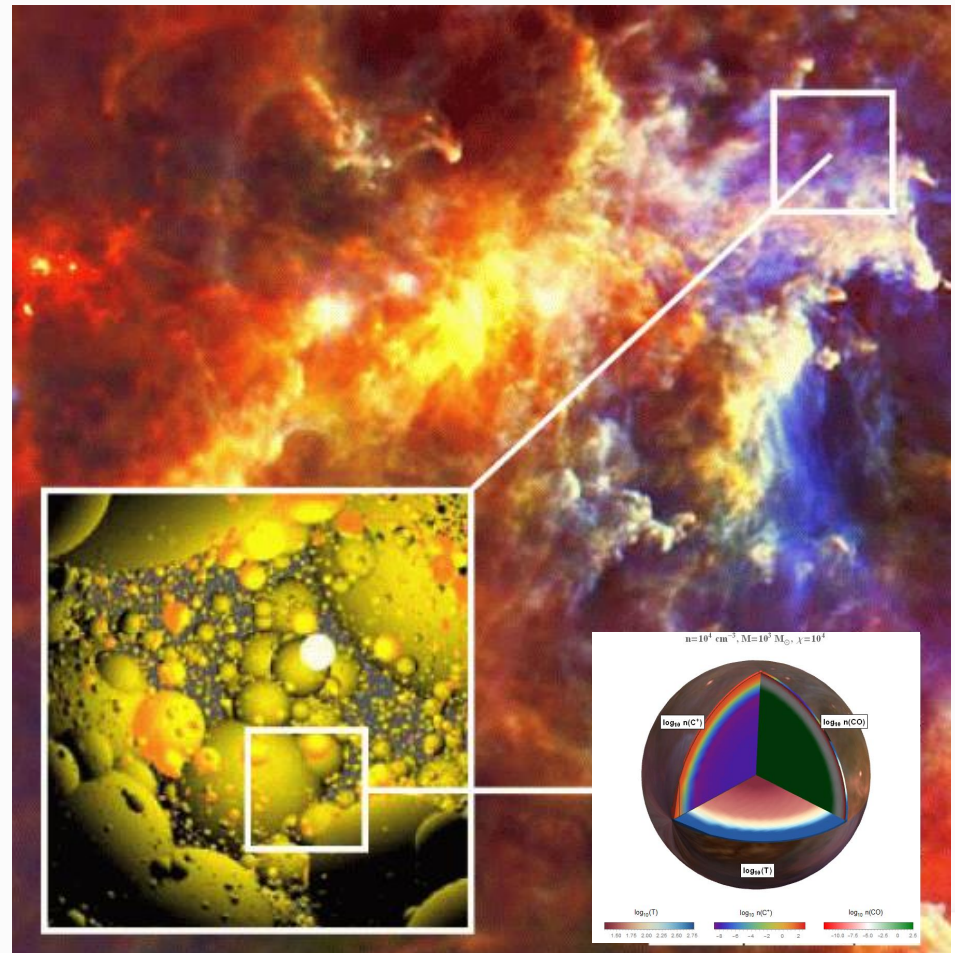
The KOSMA- τ PDR Code

- 1-D, spherical geometry
 - power-law density profile
 - isotropic illumination
- self-consistent solution of energy- and chemical balance and radiative transfer
- self-shielding of H₂, CO (FGK, Draine & Bertoldi 1997, Visser et al. 2009)
- full dust RT and temp. computation for varying dust distribution



The KOSMA- τ PDR Code

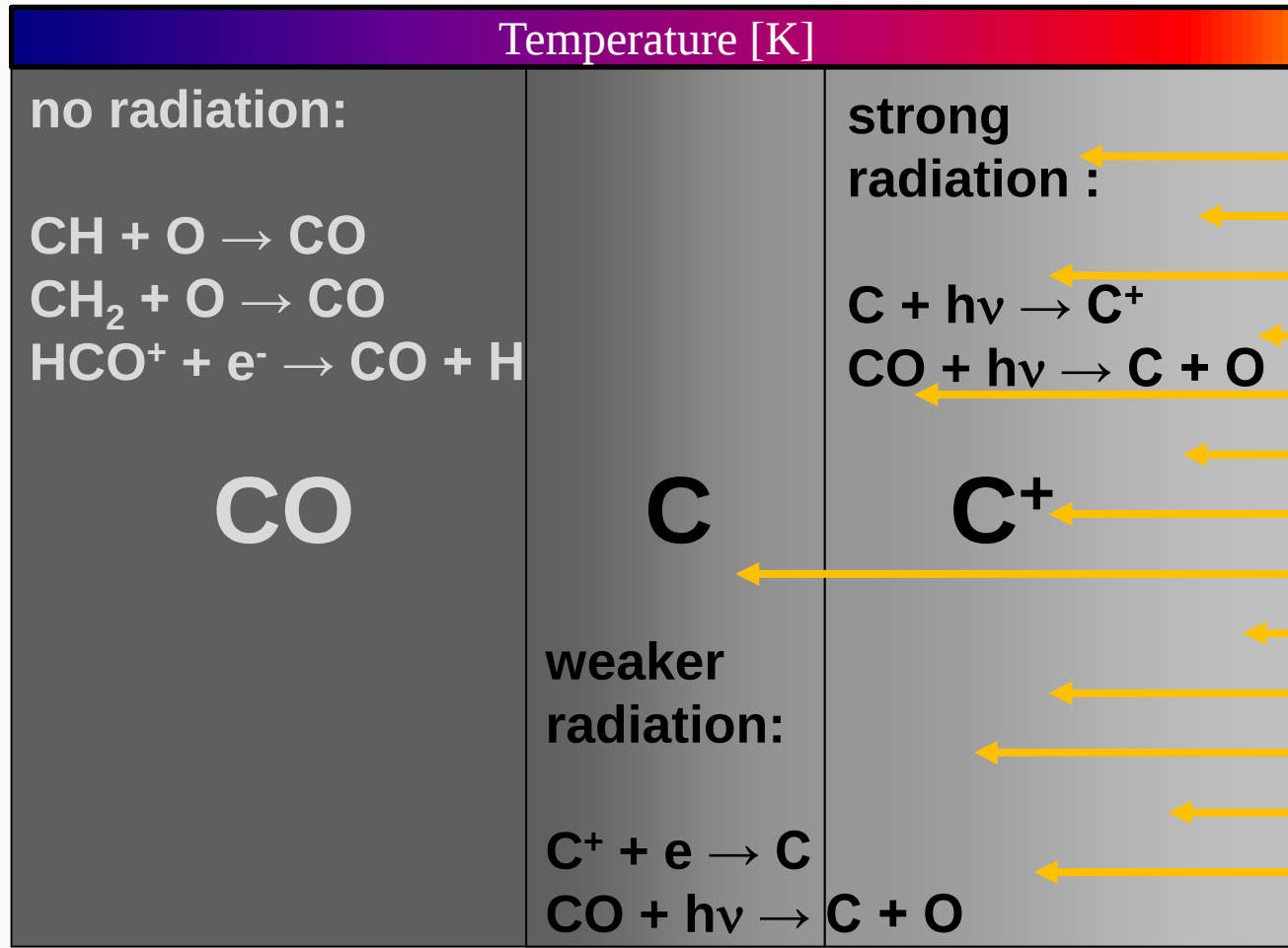
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- full dust RT and temp. computation for varying dust distribution
- clumpy cloud composition
 - stochastic clump ensemble
 - **KOSMA- τ 3D** (Andree-Labsch et al. 2017)



PDR - Photodissociation Region

- 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
 - **13.6 eV (912 Å)** ionization potential of H
 - 14.5 eV (855 Å) ionization potential of O
 - 14.5 eV (855 Å) ionization potential of N

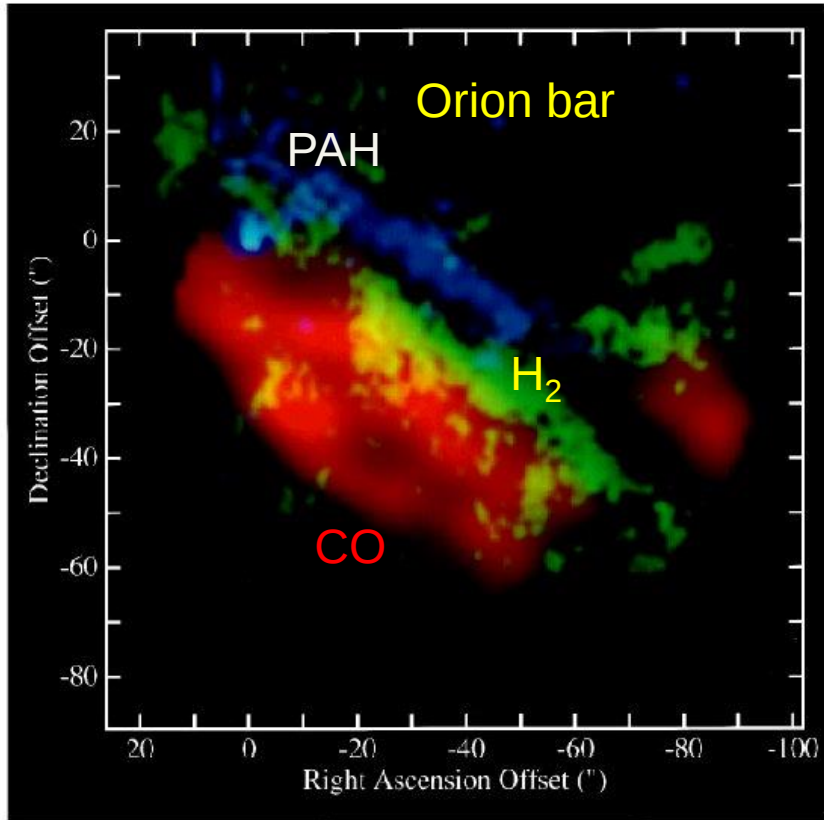
Photodissociation Region



FUV

Interstellar cloud surface (cross section)

Photodissociation Region



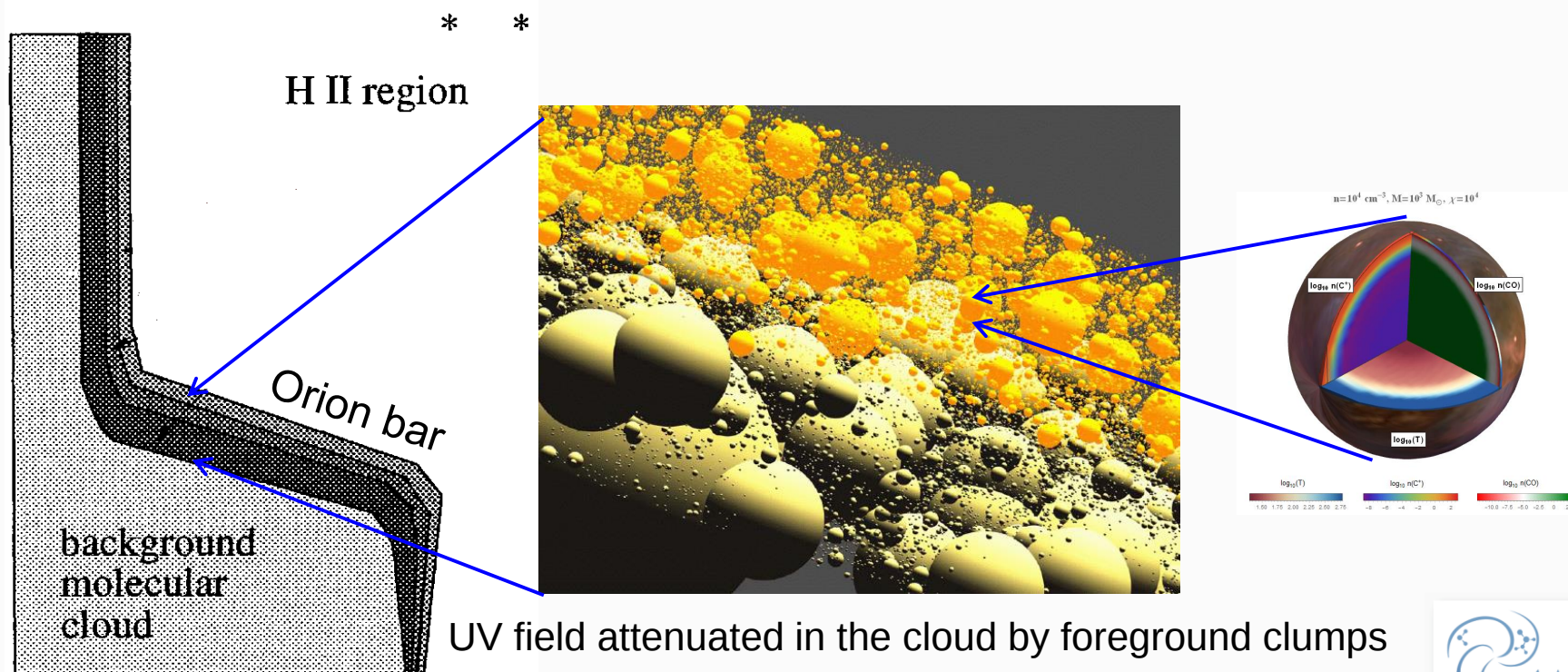
Tielens & Hollenbach 1998



Motte et al. 2010

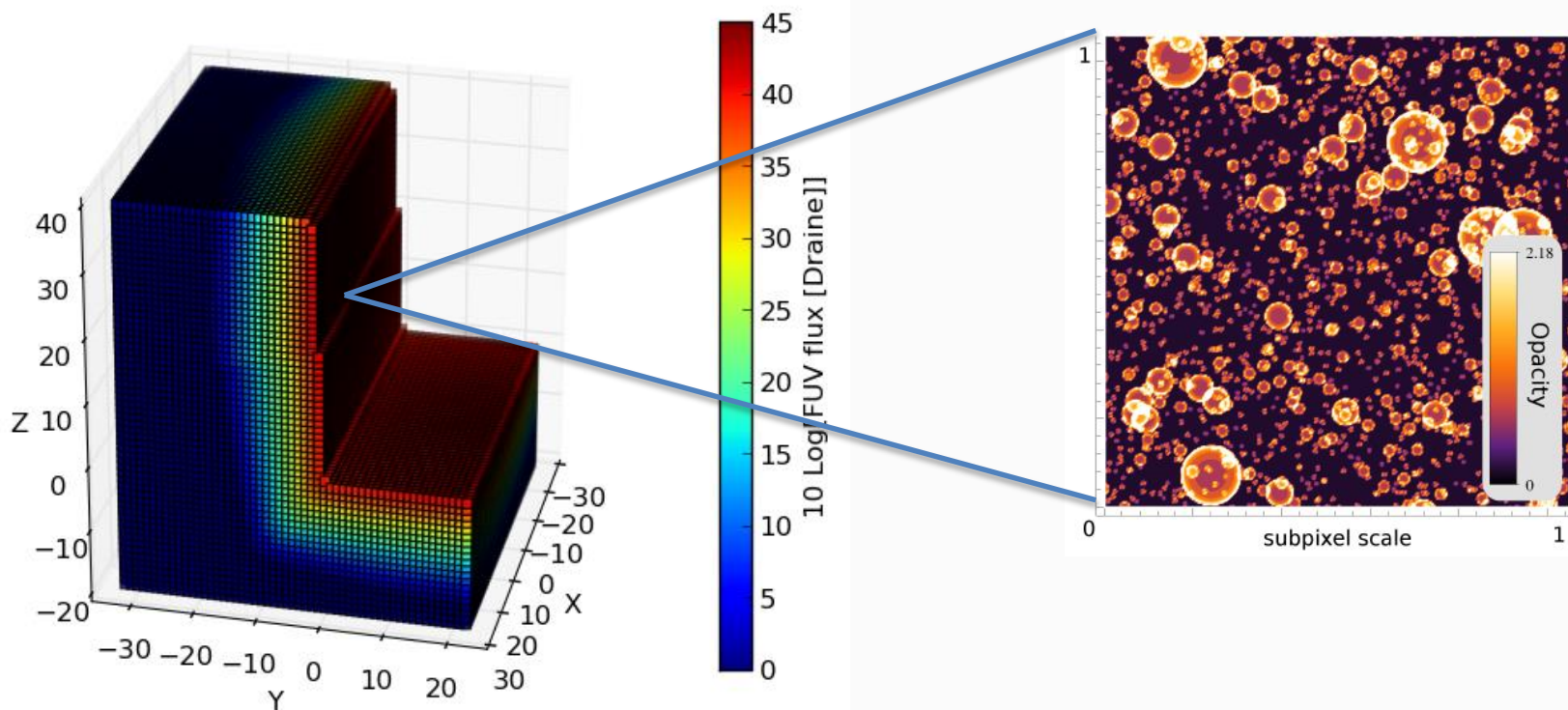
Applications: KOSMA- τ 3D

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

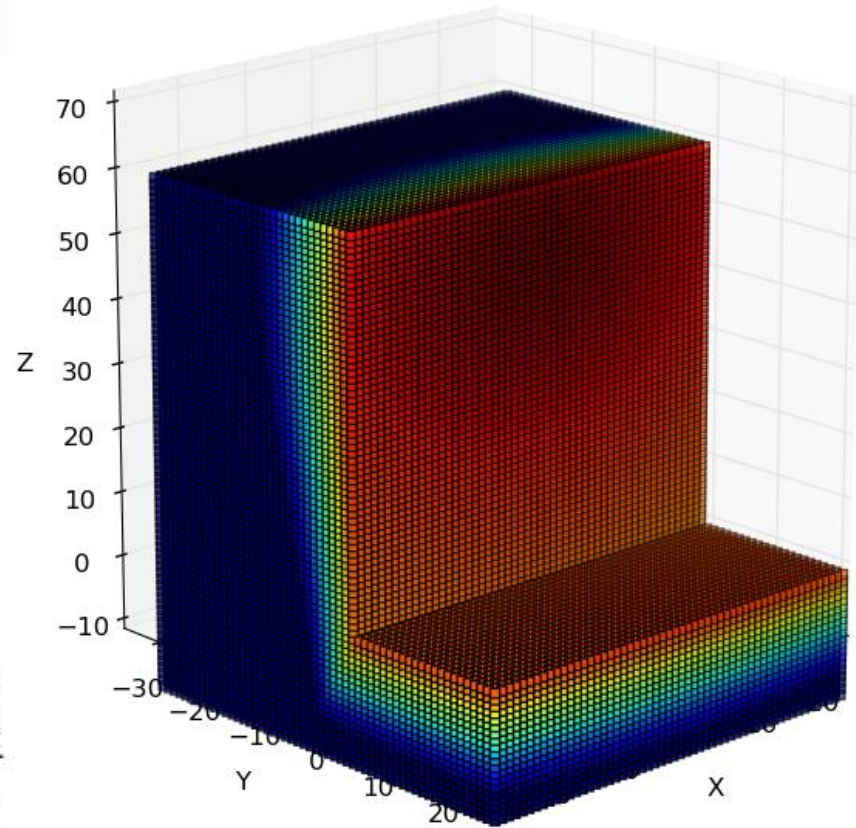
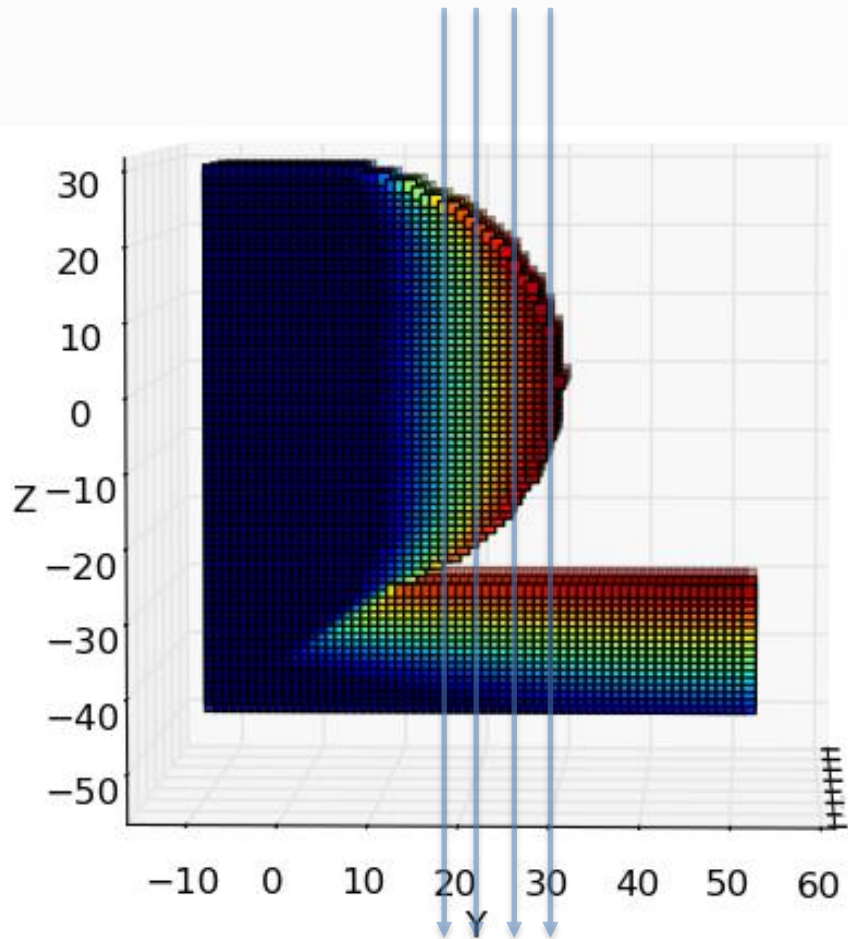


Applications: KOSMA- τ 3D

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



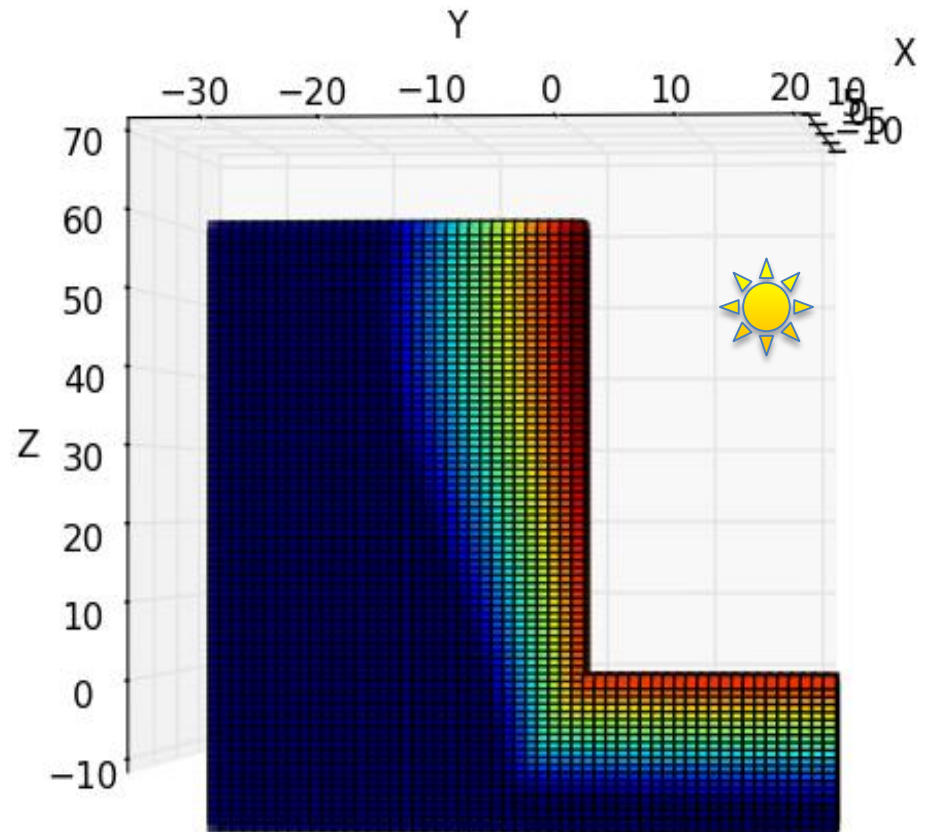
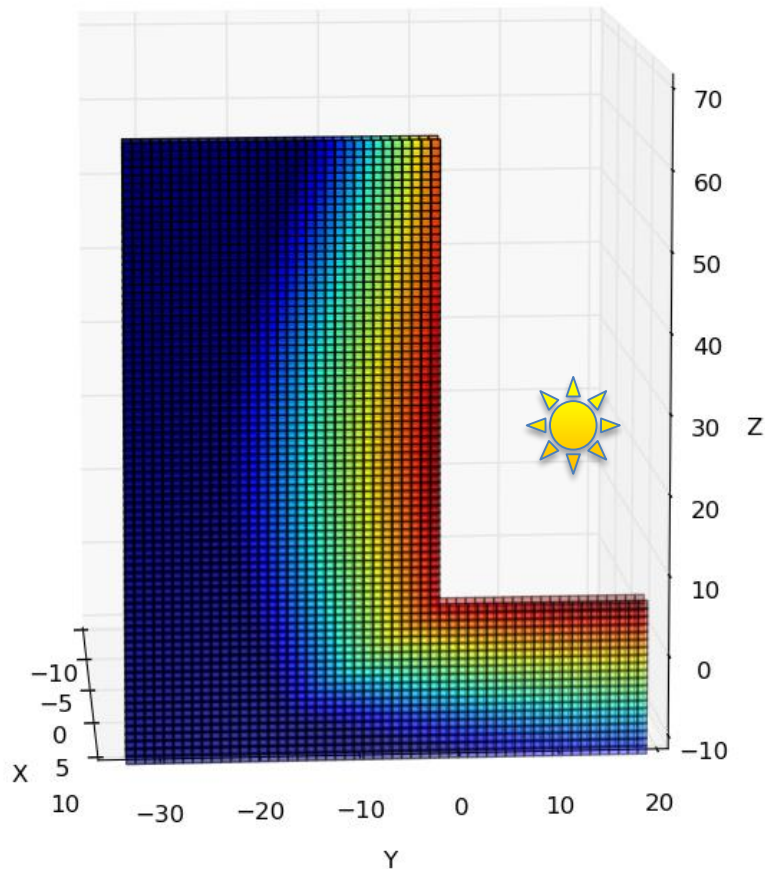
Applications: KOSMA- τ 3D



no chemical stratification

Applications: KOSMA- τ 3D

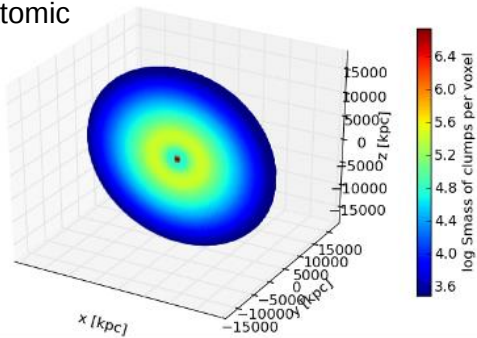
foreground absorption
by cool material in front of hot gas



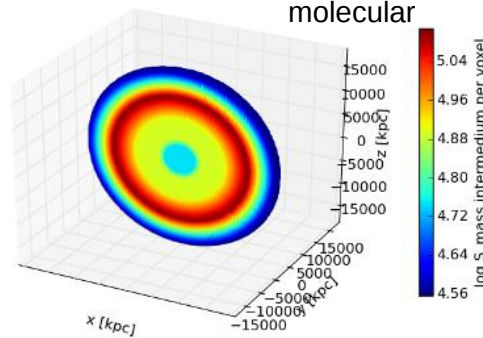
Applications: KOSMA- τ 3D

- 3-D model of Milky Way (including velocity distribution, rotation curve, UV distribution, ...)

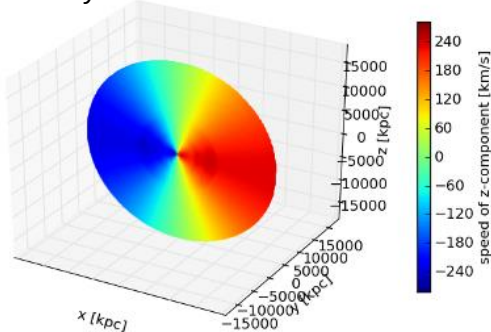
atomic



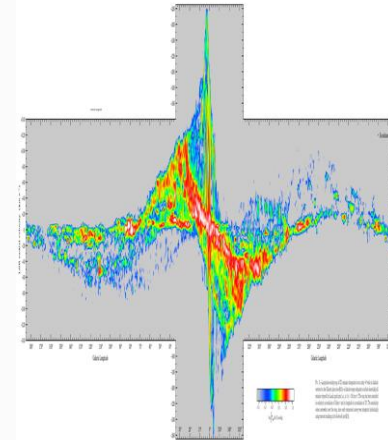
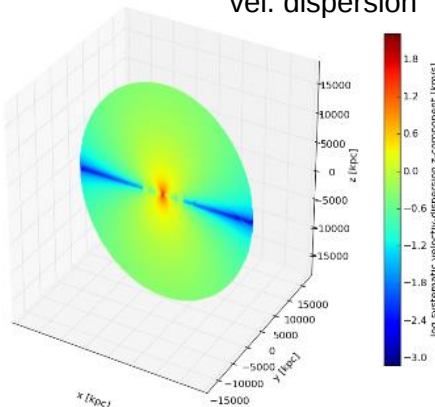
molecular



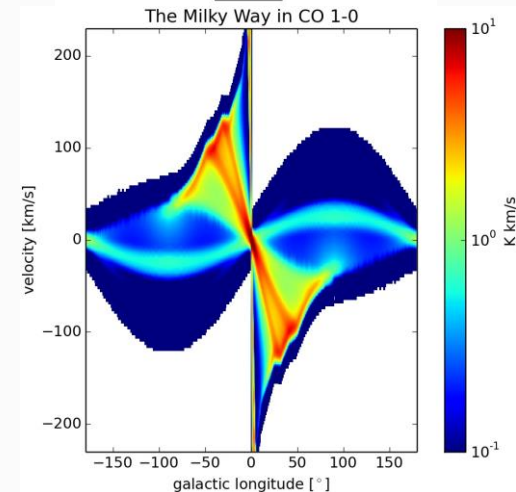
velocity distribution



vel. dispersion

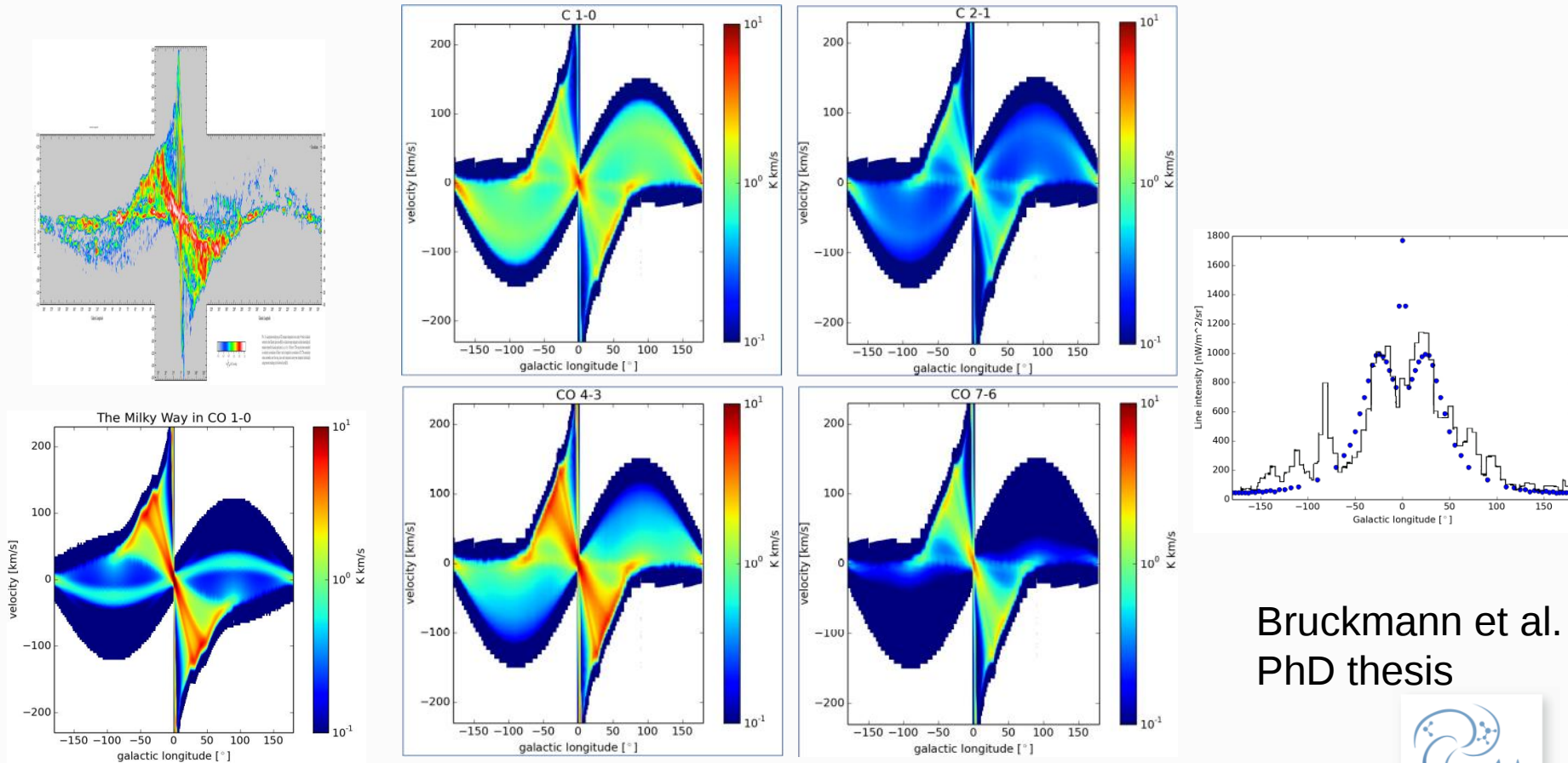


CO 1-0



Applications: KOSMA- τ 3D

- 3-D model of Milky Way (including velocity distribution, rotation curve, UV distribution, ...)

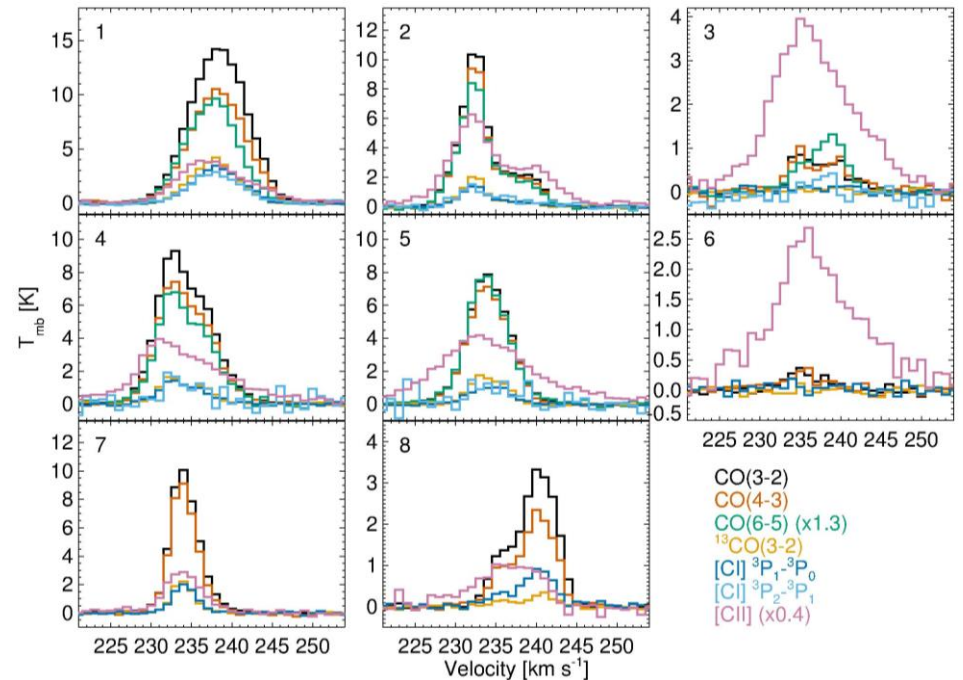
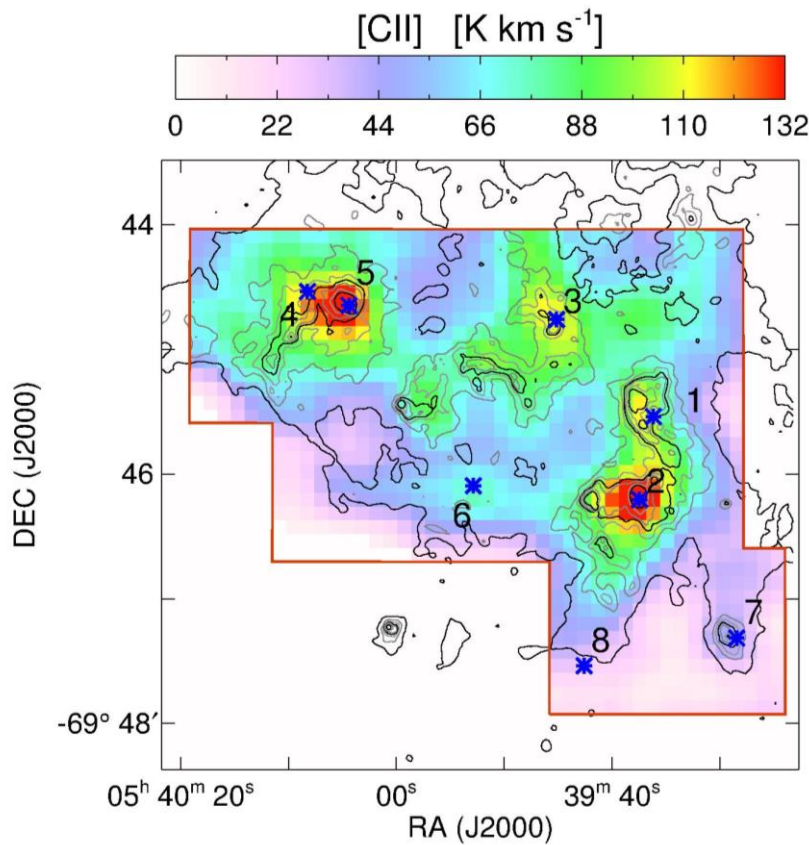


Bruckmann et al.
PhD thesis



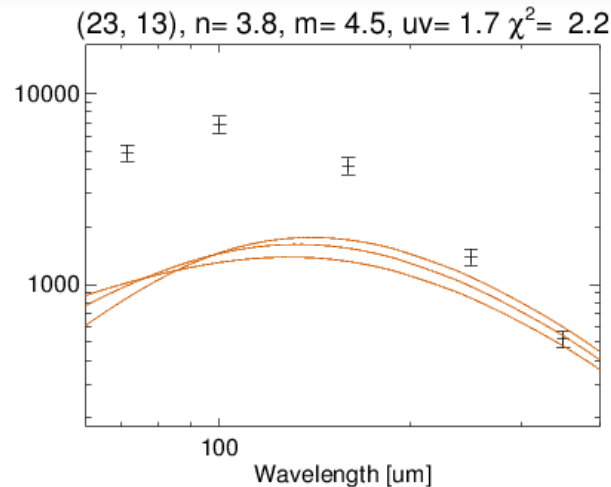
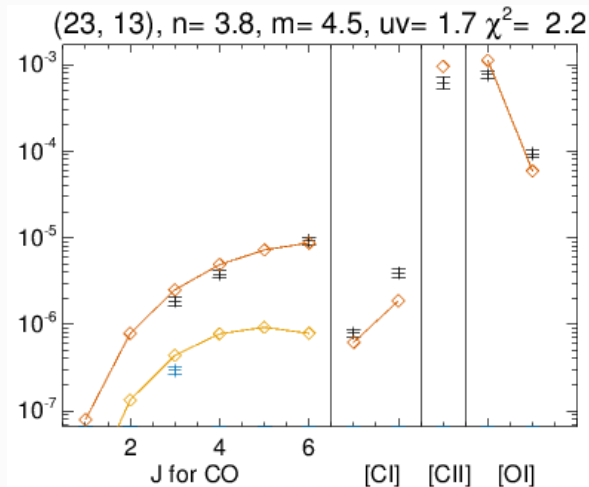
Low Metallicity PDR Modelling

Star forming region N159 in LMC, observed with GREAT/SOFIA

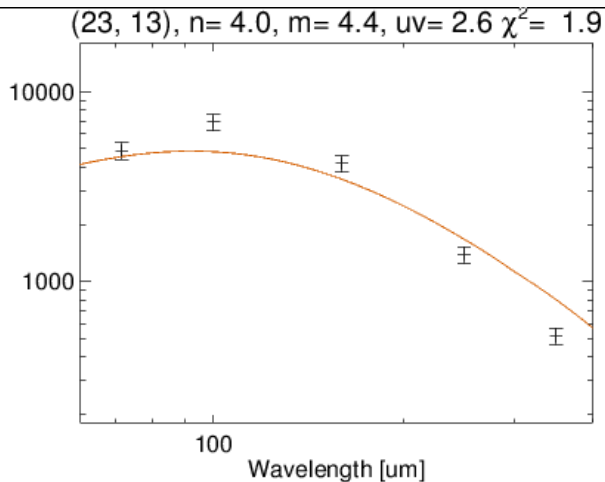
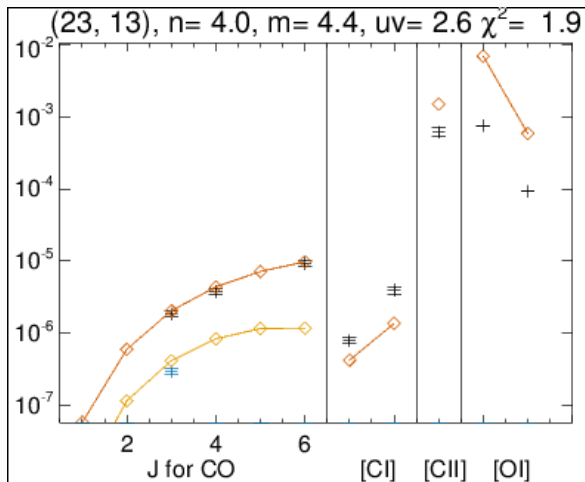


Low Metallicity PDR Modelling

LMC dust distribution from Weingartner & Draine 2001



model fit w/o continuum



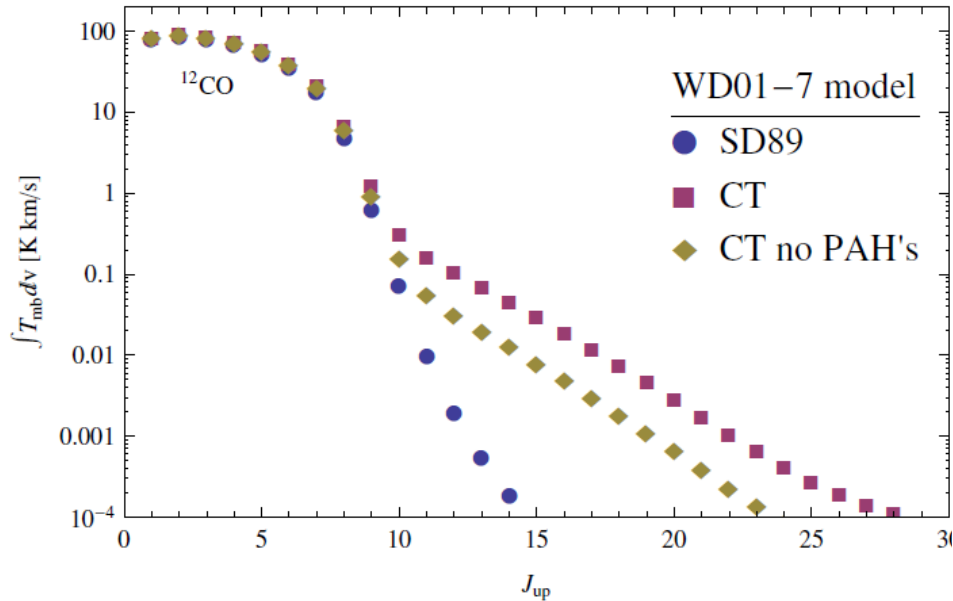
model fit with continuum

Dust in KOSMA- τ

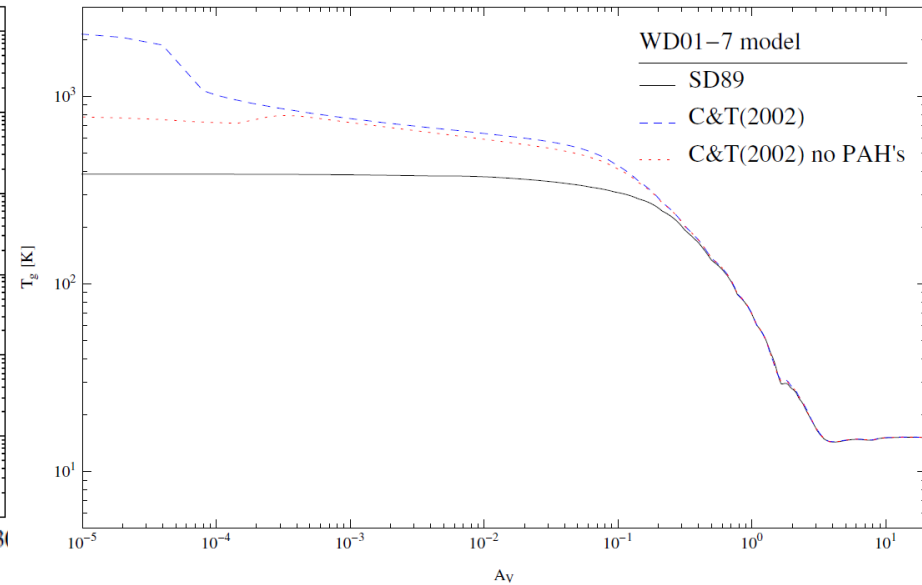
- Implementation of Weingartner & Draine 2001 dust model
 - multiple dust components (carbonaceous, olivine, PAHs⁰, PAH⁺)
 - dust grain size distribution
 - detailed UV continuum radiative transfer
 - self consistent computation of dust temperature
 - self-consistent photo-electric heating and recombination cooling
 - low-metallicity (LMC, SMC, linearly scaled) included
(Röllig et al., in prep., Okada et al. in prep.)
- detailed information on how much available surface at which temperature

H₂ formation heating

CO line emission



gas temperature

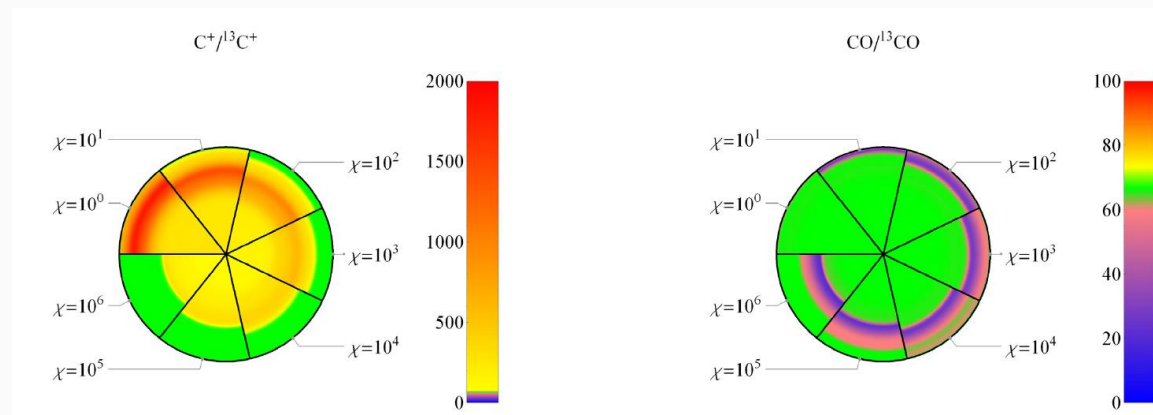


Röllig et al. 2013

Dust content & physics influence high-J CO emission

Chemistry in KOSMA- τ

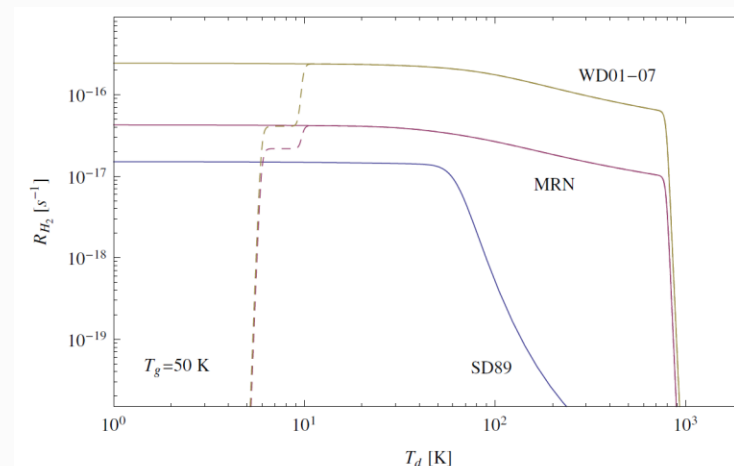
- Rate equation approach
- Steady-state chemistry
 - LAPACK: DGESV, DGELSD (least squares), DGESVX (w. equilibration)
- modular chemistry
 - user selects species, code selects reactions, creates conservation equations and computes Jacobian
- isotopologue chemistry: ^{13}C and ^{18}O
 - update to the 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- τ

- 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
 - $\text{I-C}_3\text{H}_3^+$, $\text{I-C}_3\text{H}_2^+$, $\text{I-C}_3\text{H}_2$, $\text{I-C}_3\text{H}$
 - 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)

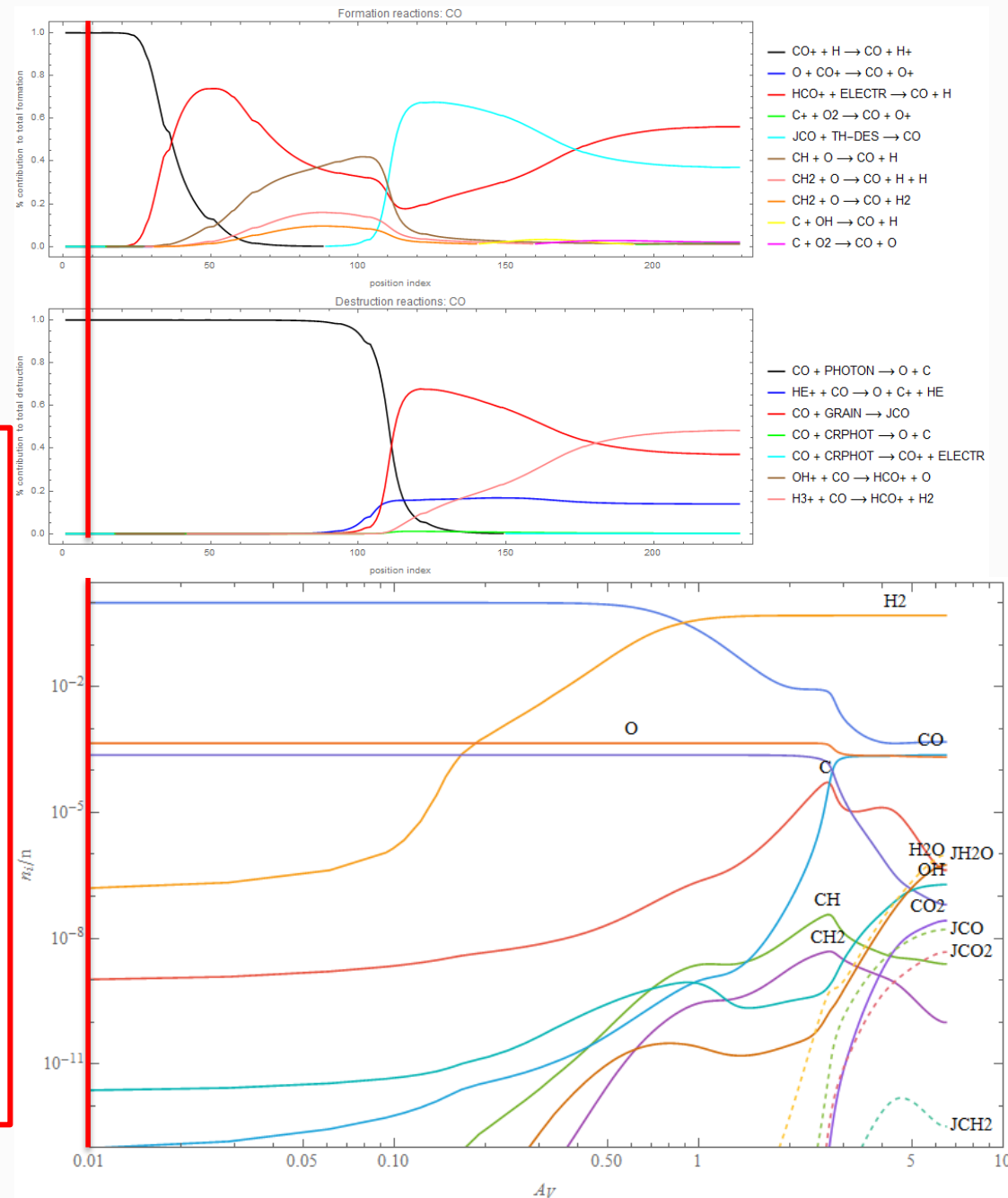
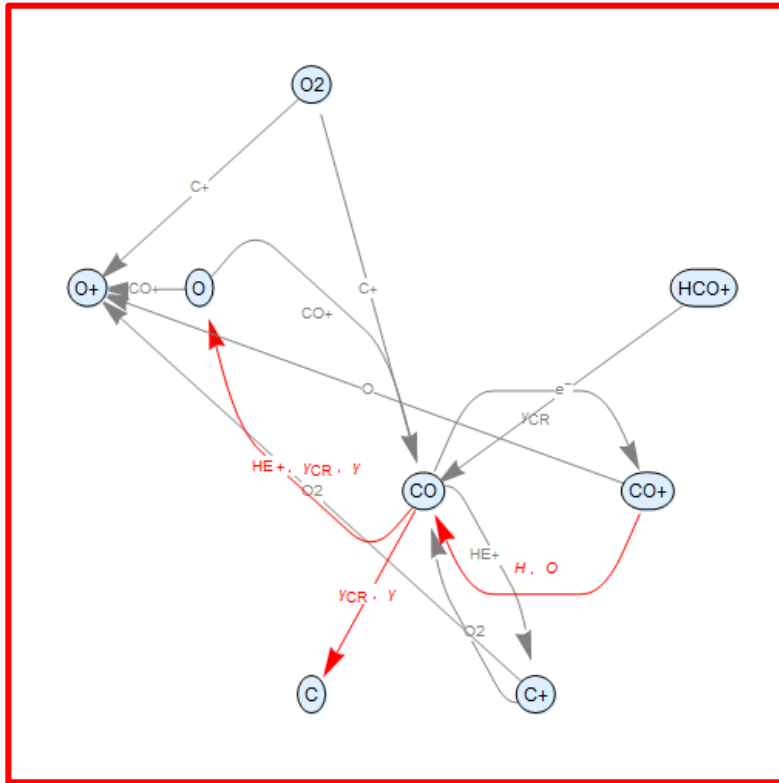
Röllig et al. 2013



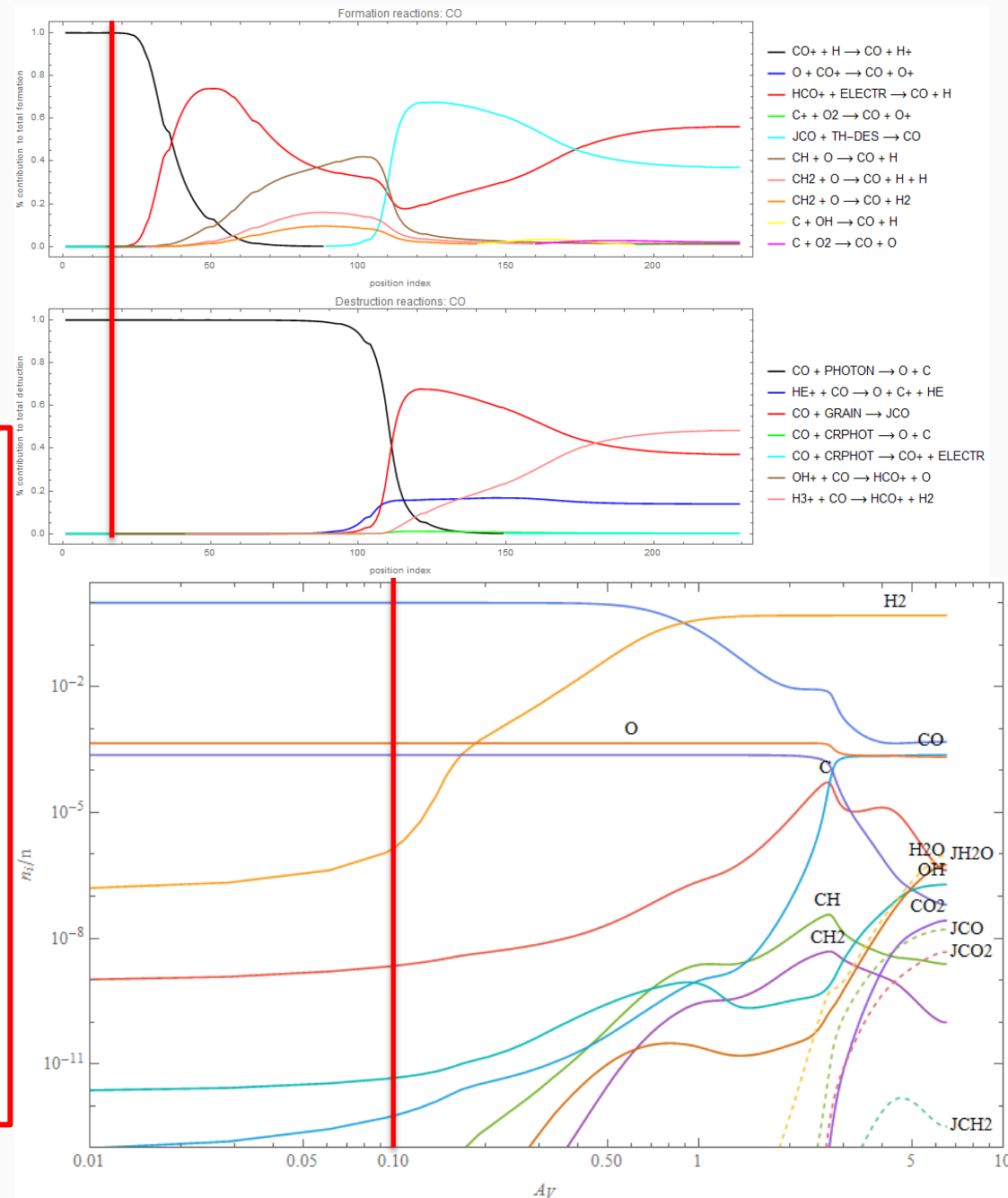
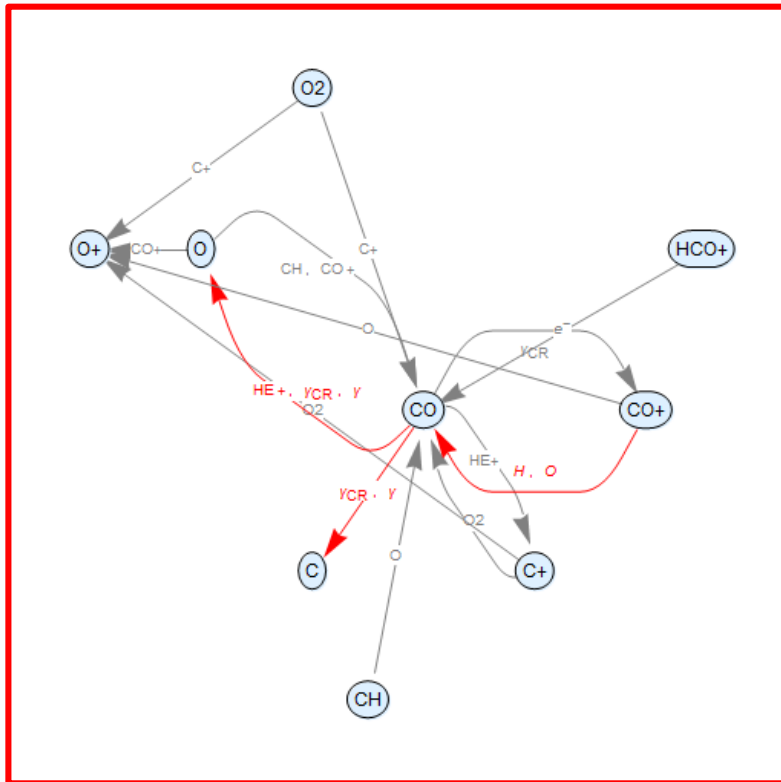
Full Surface Chemistry Upgrade

- 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 H₂)
 - 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. $\text{JH}_2\text{O} + h\nu \rightarrow \text{OH} + \text{H}$ Andersson+ 08)
 - photo-dissociation on grains (equivalent to gas-phase)
 - CR induced photo-desorption/diss. (Hasegawa & Herbst 1993)
 - H₂-formation induced desorption (Willacy et al. 1994, 2007)
 - chemistry induced desorption (Minissale et al. 2015, Cazaux et al. 2015)
 - surface-surface processes (Langmuir-Hinshelwood)

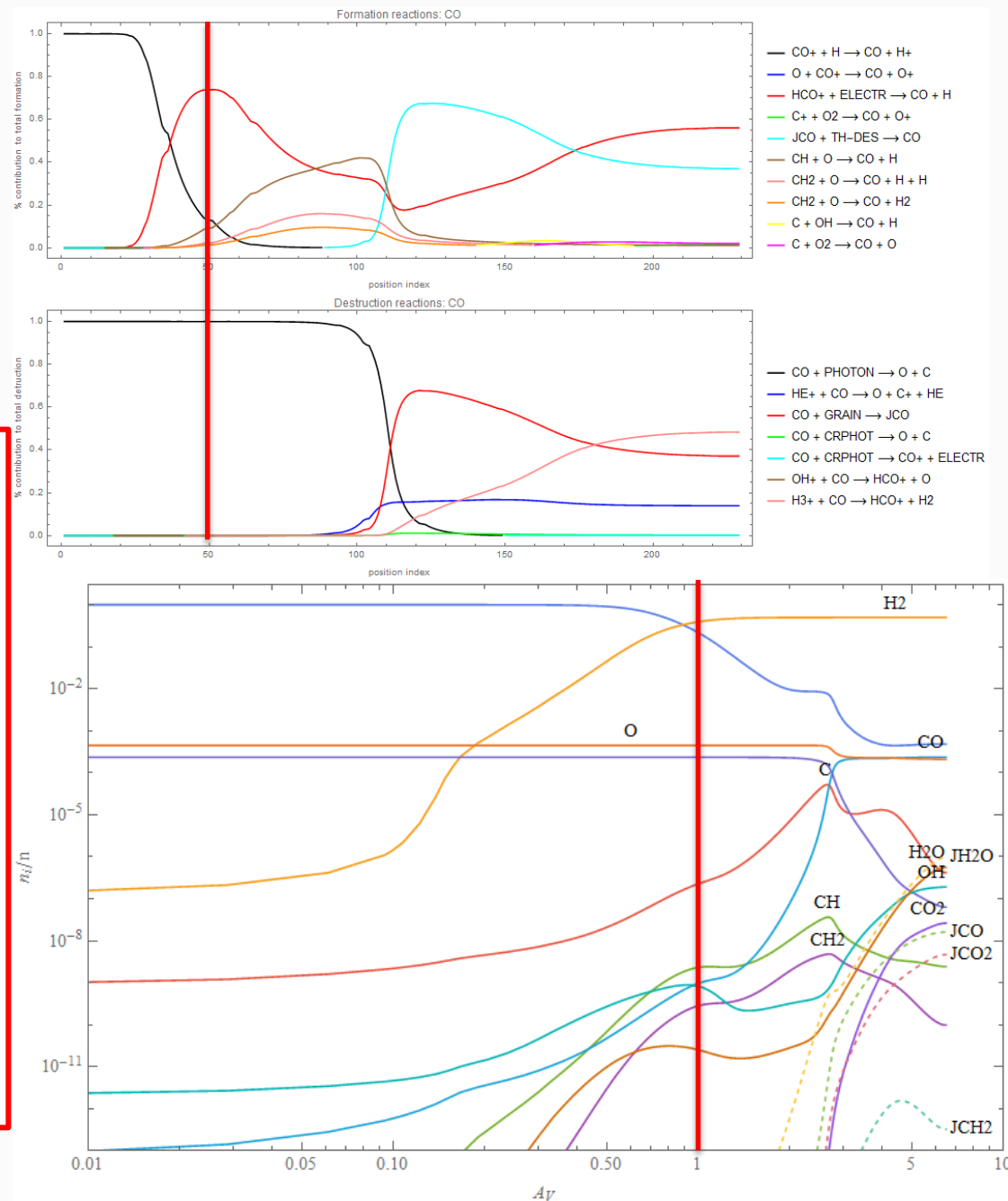
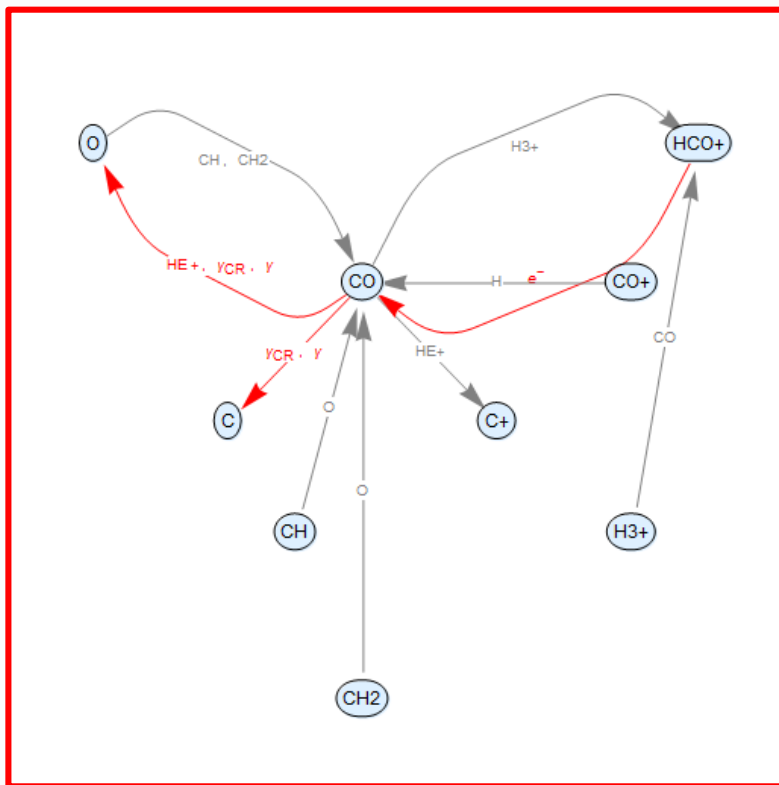
$n = 10^4 \text{ cm}^{-3}$
 $\chi = 10^4$
 small chemical network



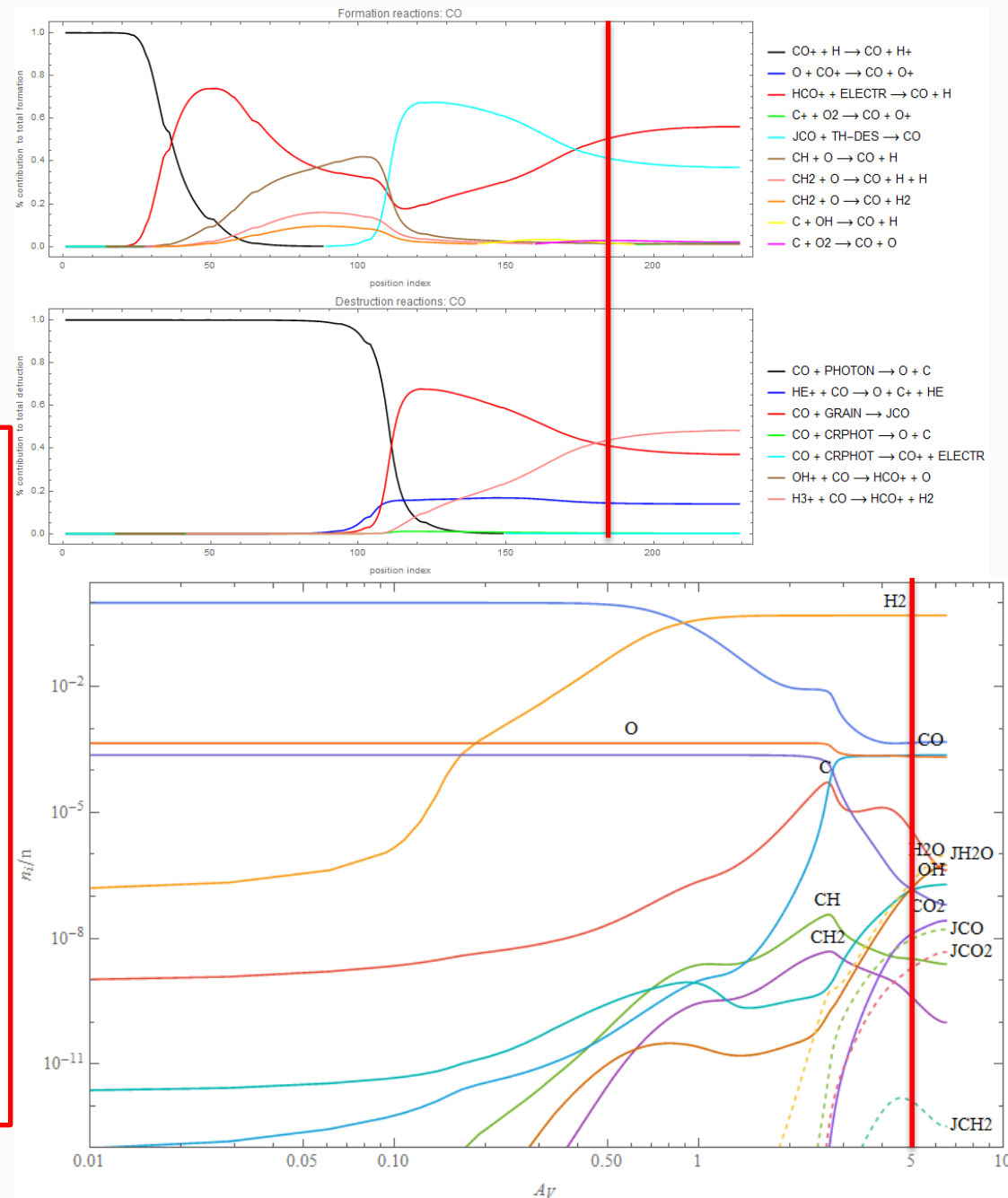
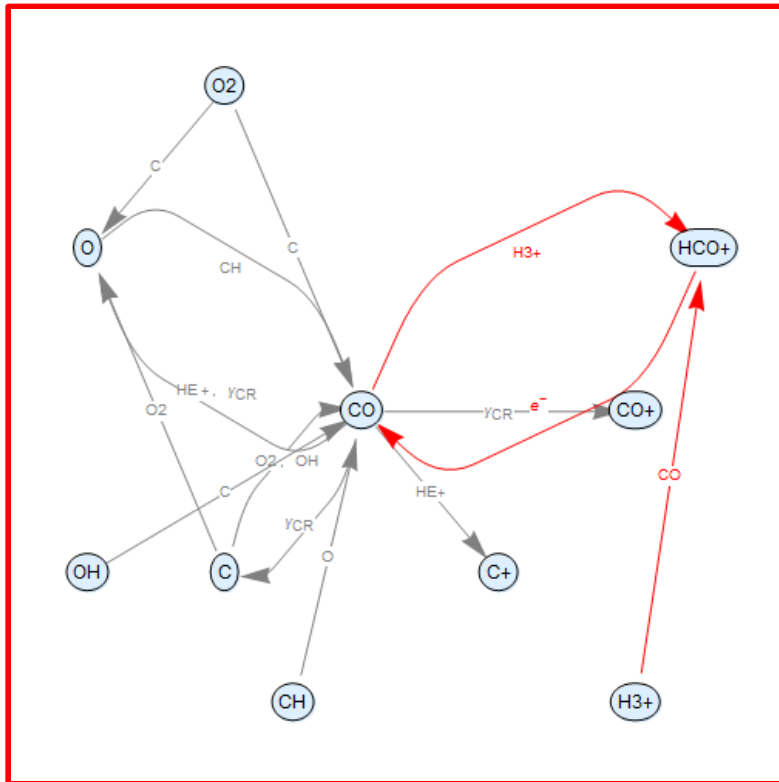
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small chemical network

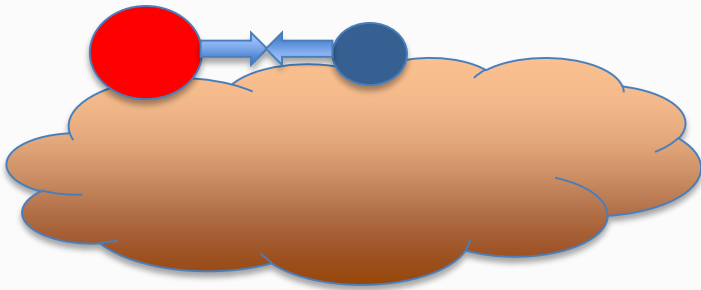


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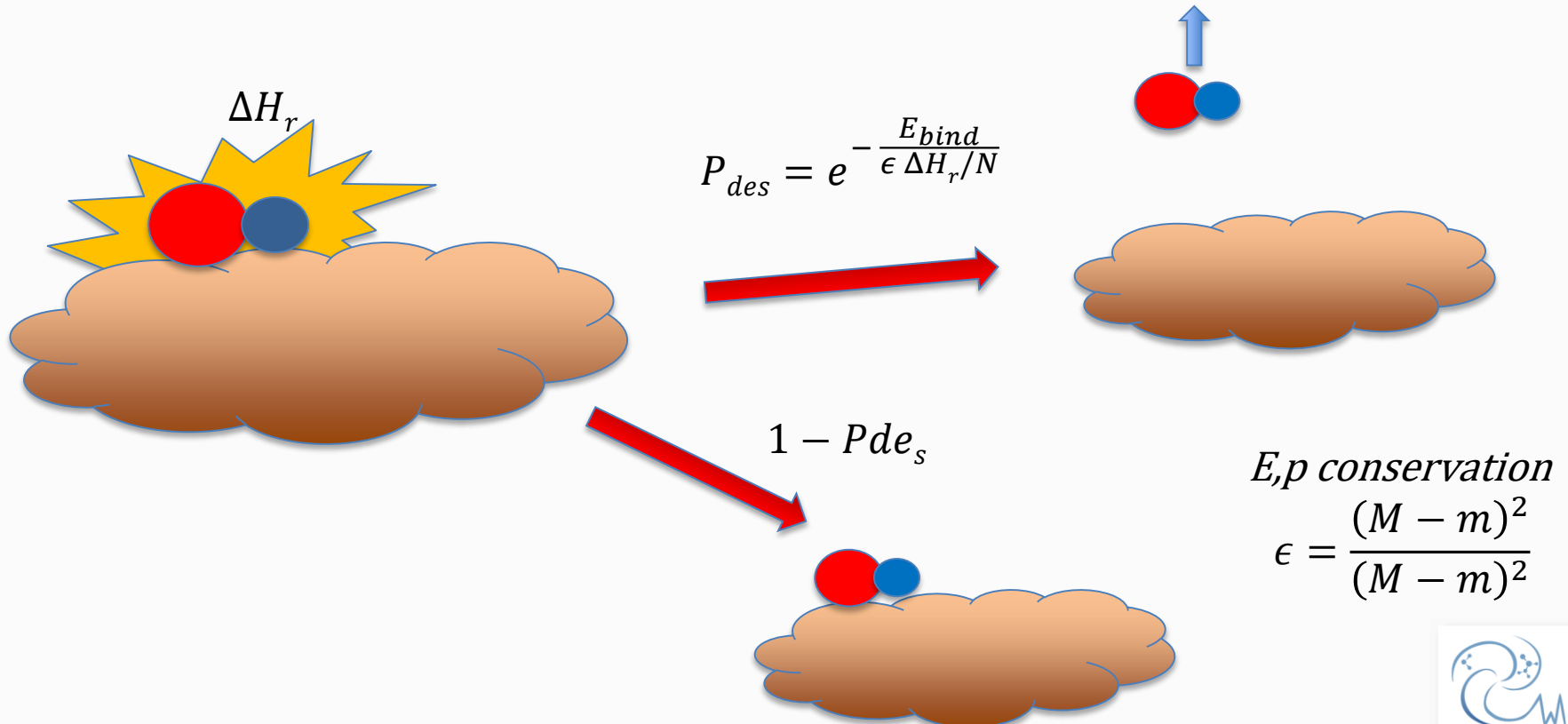
Full Surface Chemistry Upgrade

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

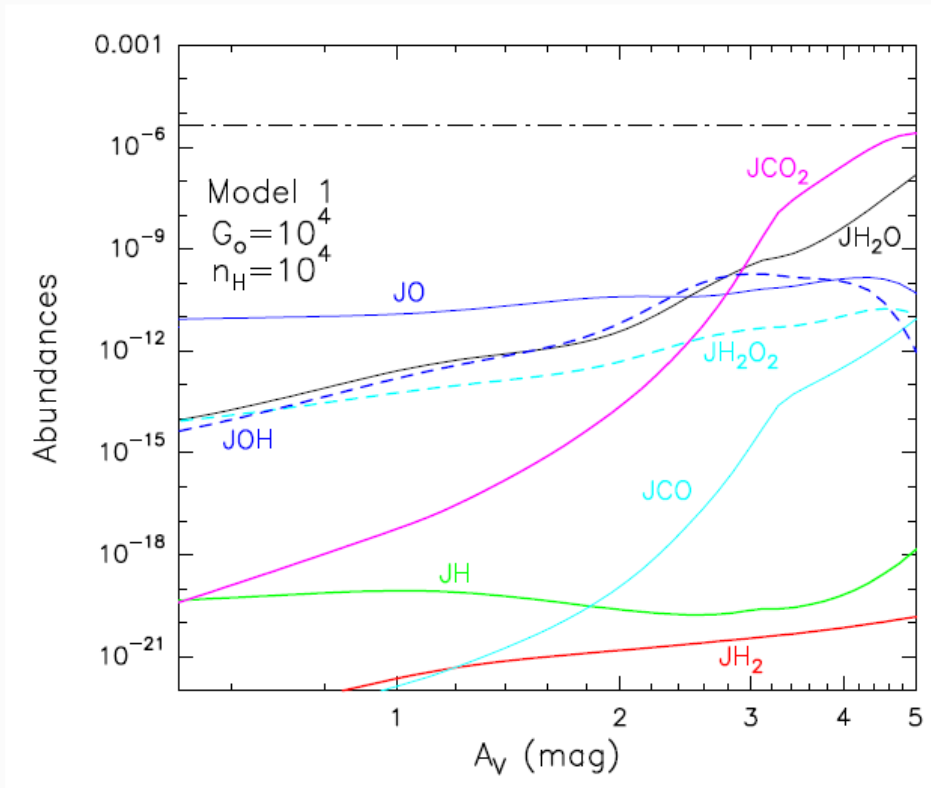


Full Surface Chemistry Upgrade

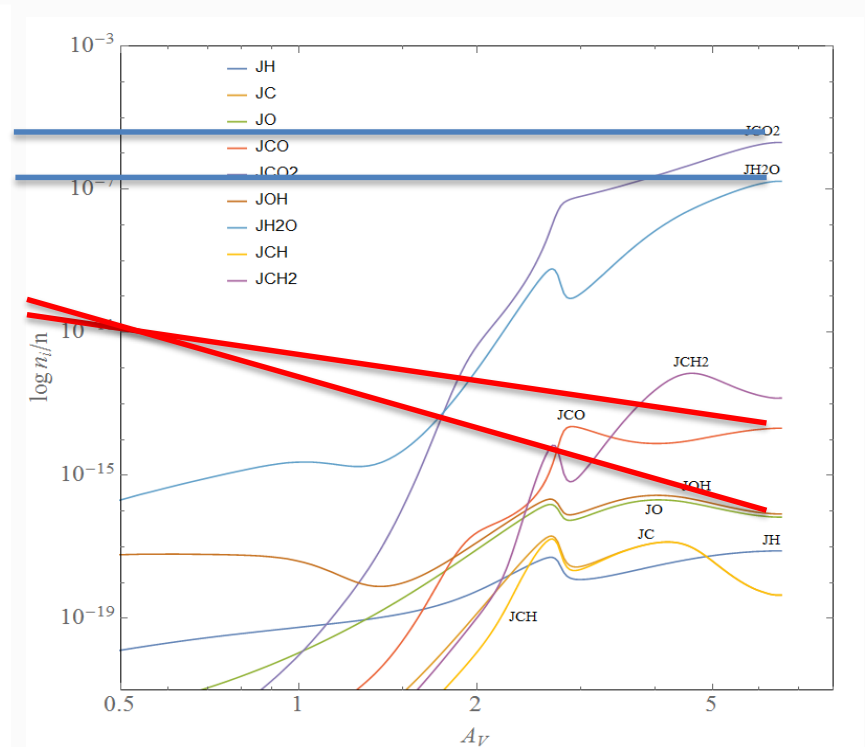
- surface-surface processes (Langmuir-Hinshelwood)
- exoenergetic reactions may lead to desorption of the product (Minissale et al. 2015, Cazaux et al. 2016)



Chemical details with impact

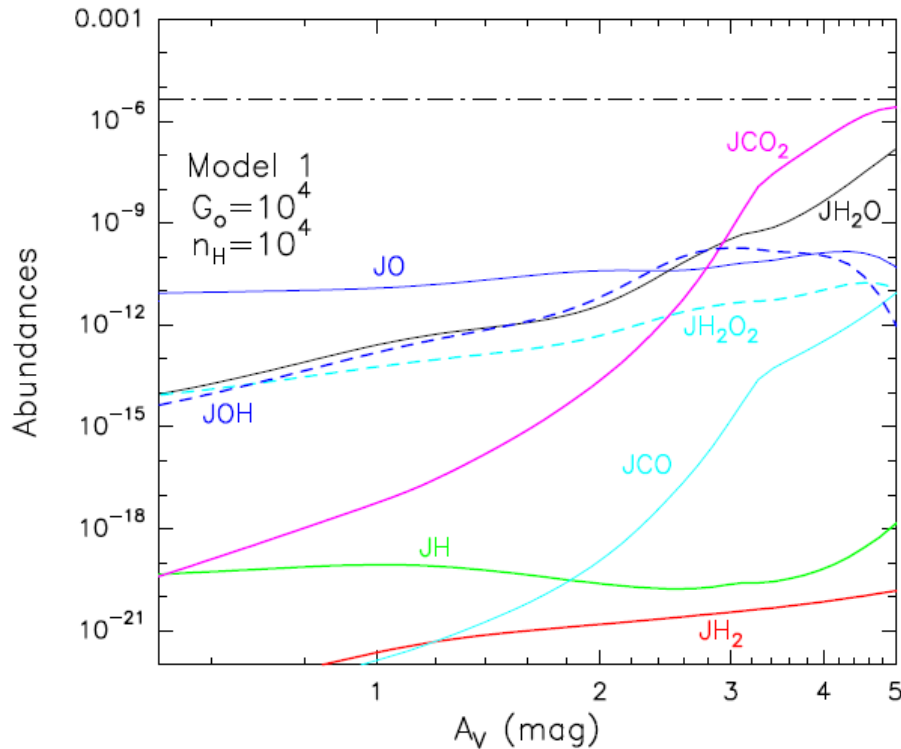


Esplugues et al. 2016



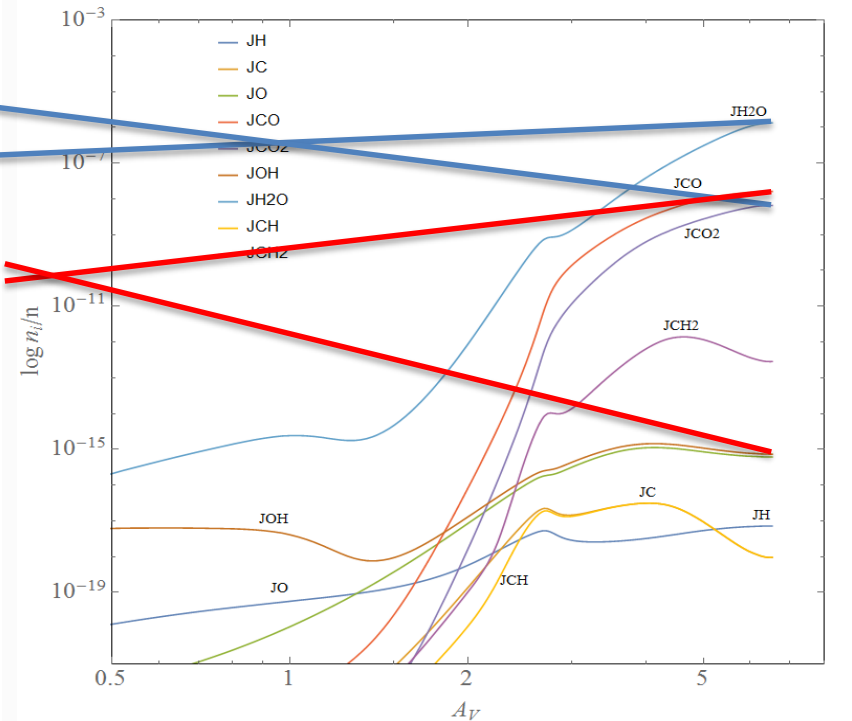
KOSMA- τ with „comparable“ setup

Chemical details with impact



Esplugues et al. 2016

→ significantly different ice composition



KOSMA- τ with „comparable“ setup

plus

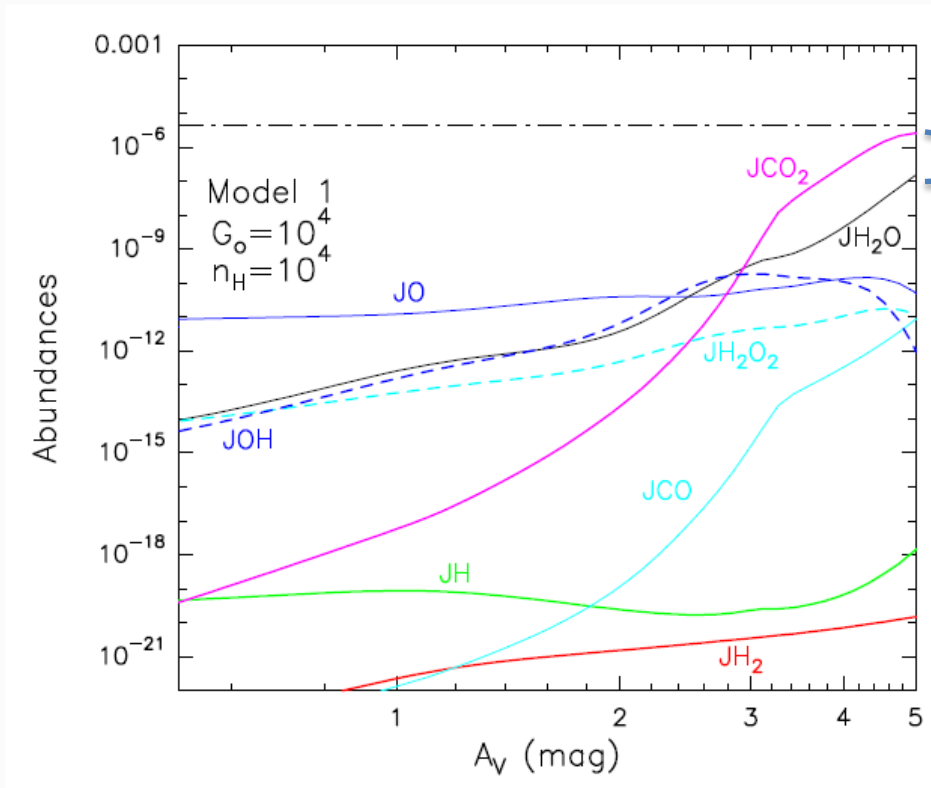
(theoretical BRs)

JCO + JO → CO₂ (22%)

JCO + JO → JCO₂ (78%)

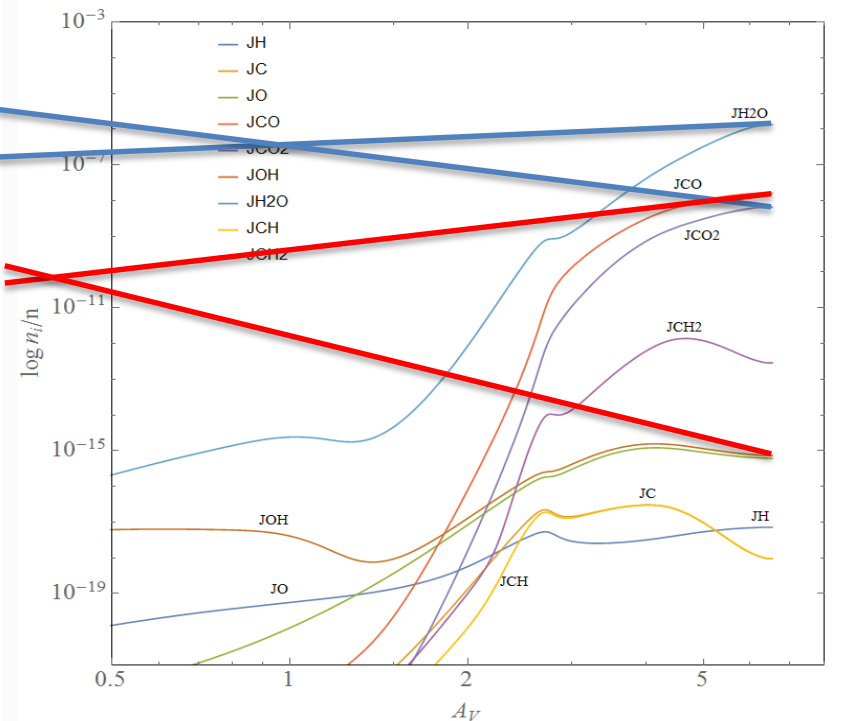


Chemical details with impact



Esplugues et al. 2016

→ significantly different ice composition



KOSMA- τ with „comparable“ setup

plus

(measured BRs)

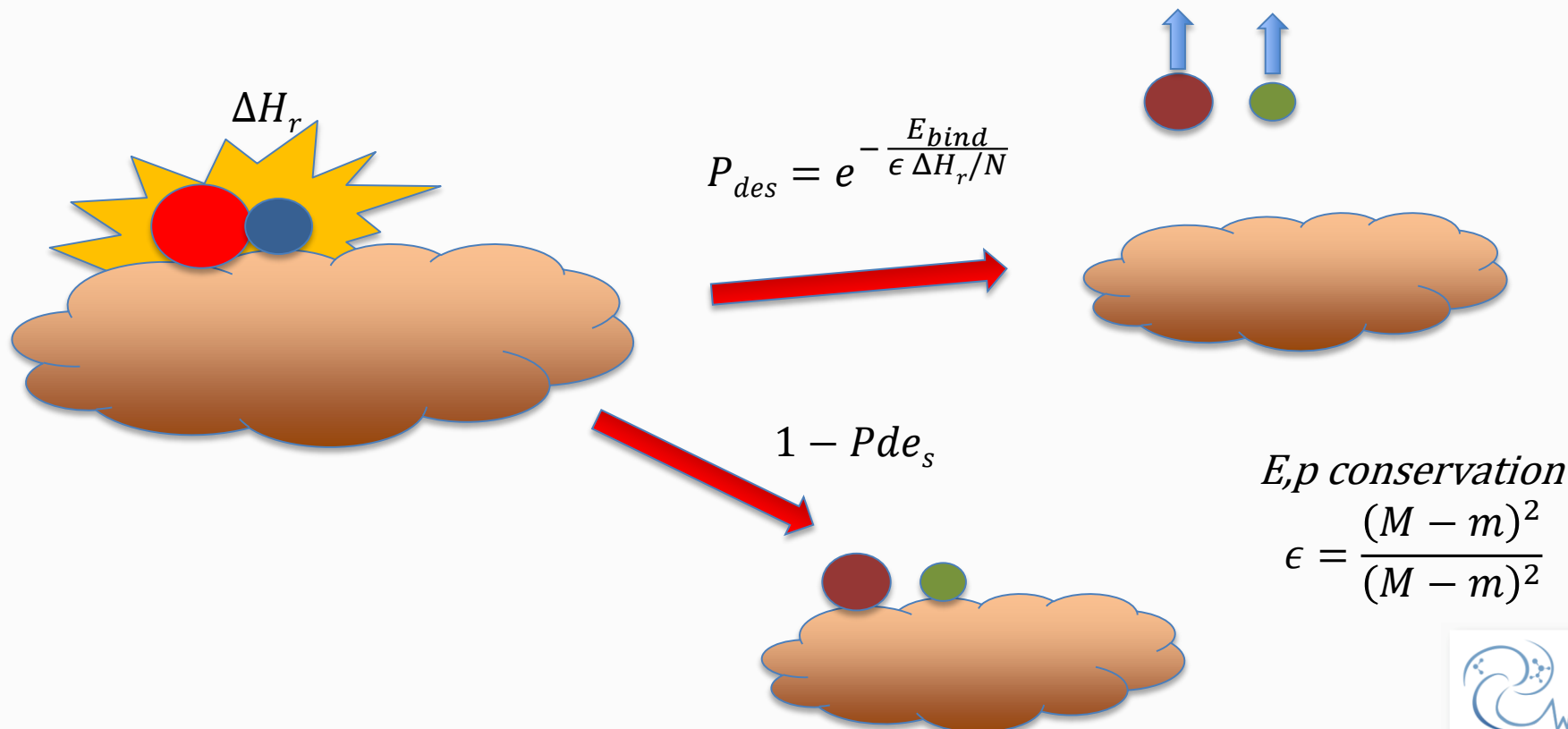
$JCO + JO \rightarrow CO_2$ (4%)

$JCO + JO \rightarrow JCO_2$ (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)

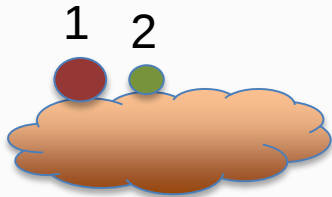


Full Surface Chemistry Upgrade

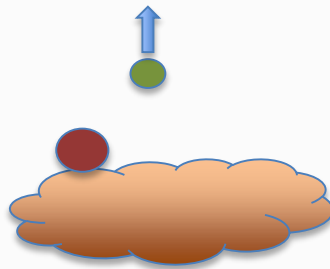
- So far assumed that all products desorb with full reaction enthalpy
- Now, we assume that formation **energy is distributed across products**

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

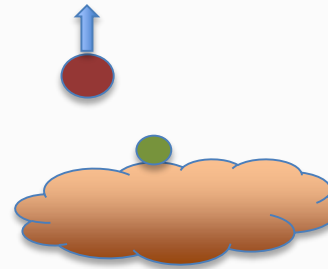
$$(1-P_{des,1}) \times (1-P_{des,2})$$



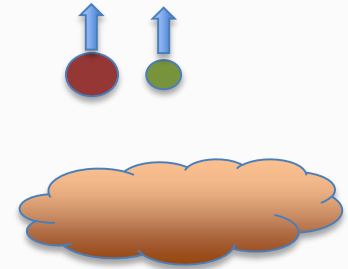
$$(1-P_{des,1}) \times P_{des,2}$$



$$P_{des,1} \times (1-P_{des,2})$$

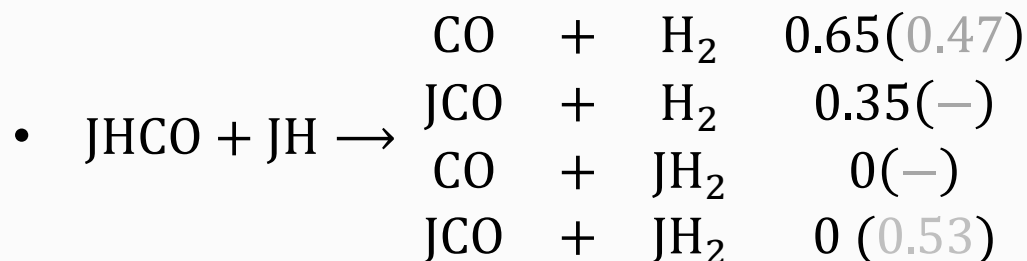
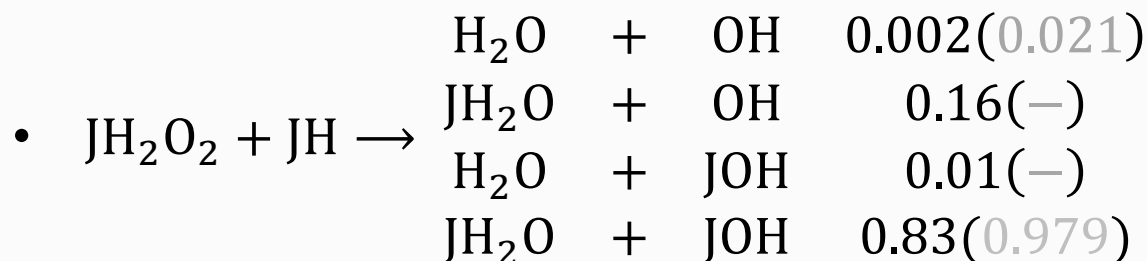
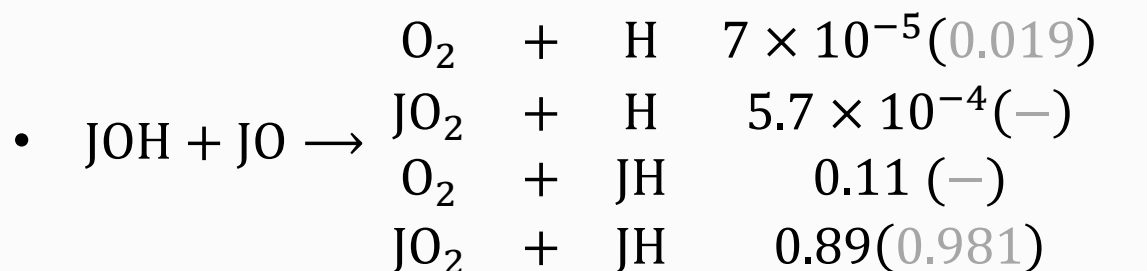


$$P_{des,1} \times P_{des,2}$$



Röllig et al., in prep

Some example branching rates



BRs depend on the energy redistribution.

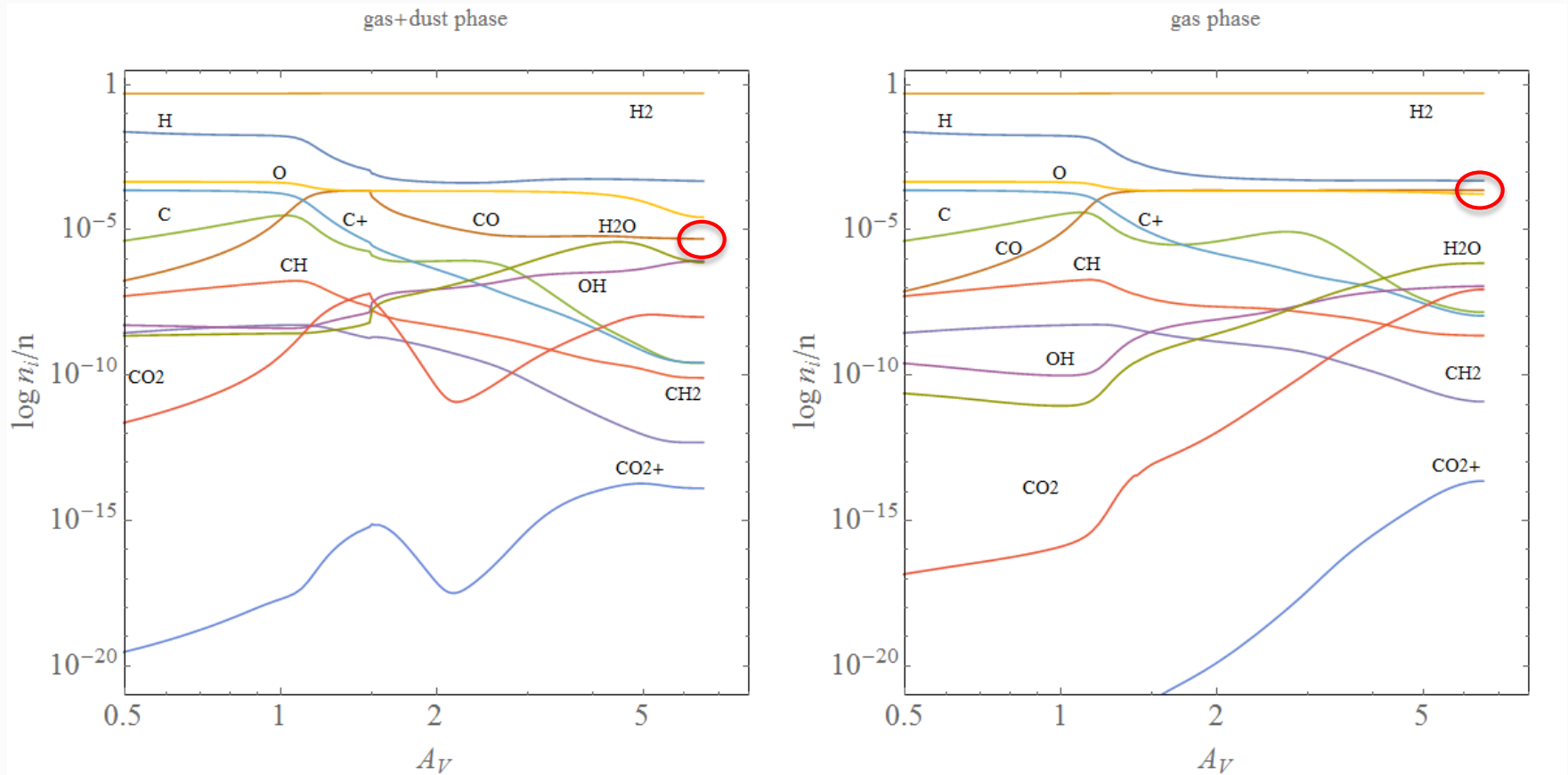
Other distribution schemes?

Questions & Concerns

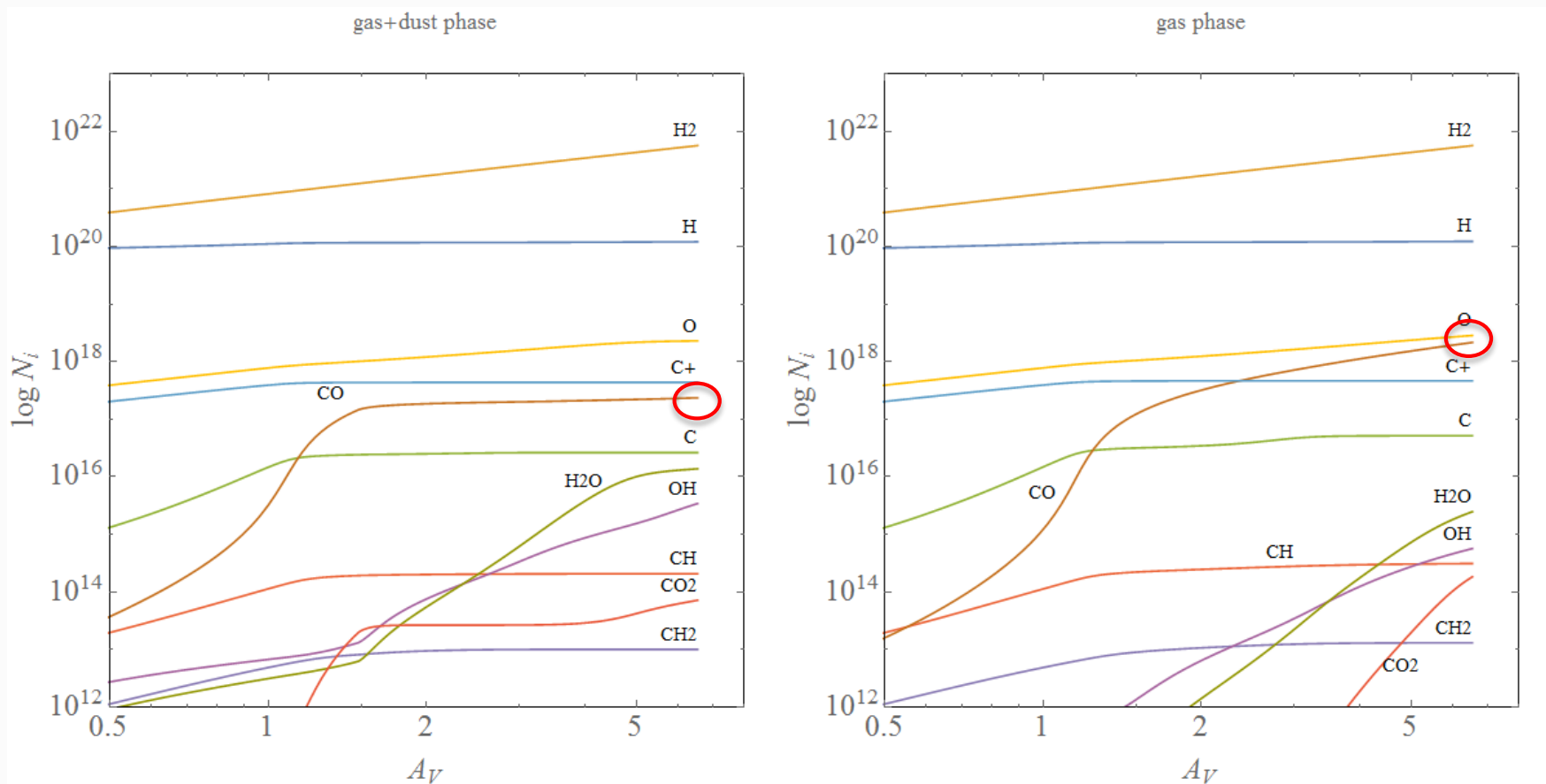
- Binding energies – Yes, but which one? (see Wakelam et al. 2017)
- How about surfaces of very small grains? PAHs?
 - Very important for H₂ formation
 - excitation of small hydrocarbons, H₂, high-J CO
- Cross sections of surface photo-processes
 - Important for PDRs because of FUV attenuation/shielding
 - 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

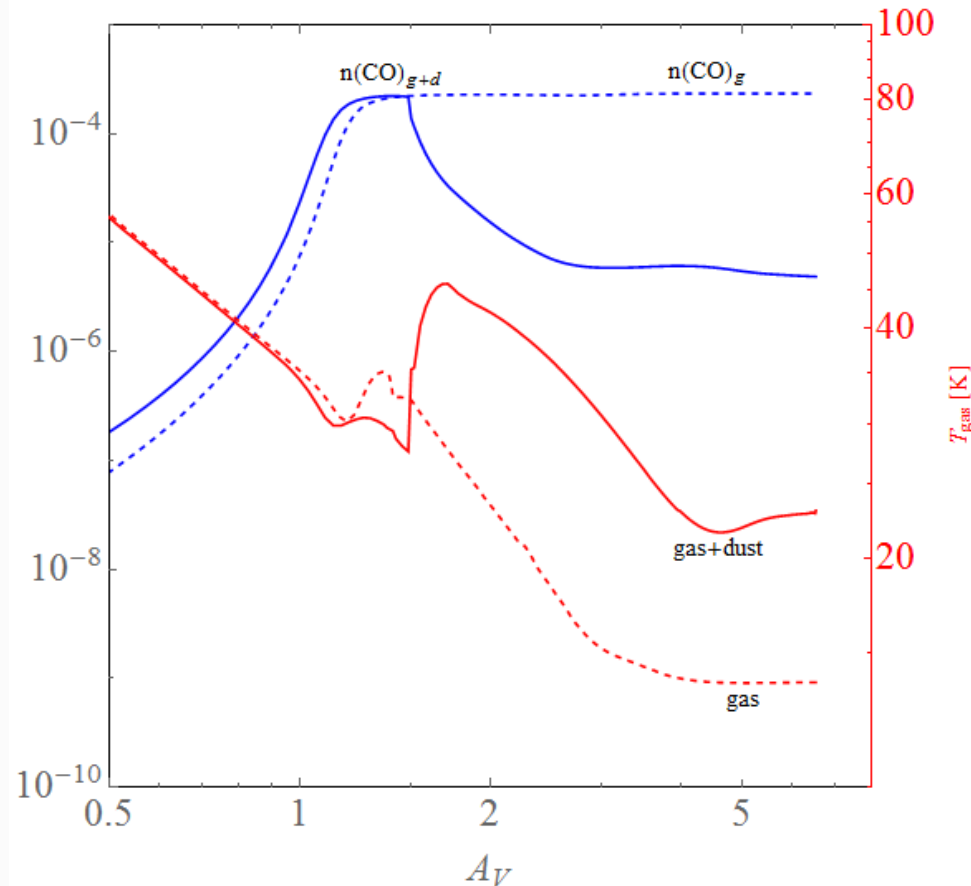
Line	$\int T_{mb} dv$ [K km/s]
CO J=1-0	5.8
CO J=2-1	7.3
CO J=3-2	4.3
CO J=4-3	1.4
[CII] 158 μ m	2.3
[CI] 609 μ m	8.7
[CI] 370 μ m	2.3

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 μ m	2.1
[CI] 609 μ m	9.5
[CI] 370 μ m	2.6

lower column densities
higher intensities !

Excitation matters



gas cooling is significantly reduced in the absence of CO

→ gas temperature increases

Questions & Concerns

- Densities and column densities are good for inter-model comparison but are no observables.
- Calibrate model against ‚derived‘ (column) densities? Which ones? Derived under which conditions?
 - We need to make sure that model (column) densities can be compared to ‚observed‘ ones.
- Alternatively one could apply radiative transfer and compare against measured intensities!
 - But then we need to know the density/temperature structure.

It might be time for a follow-up round of the PDR-Benchmark.

Thank you for your attention!

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