H_2 formation heating

DR21/OrionBar models

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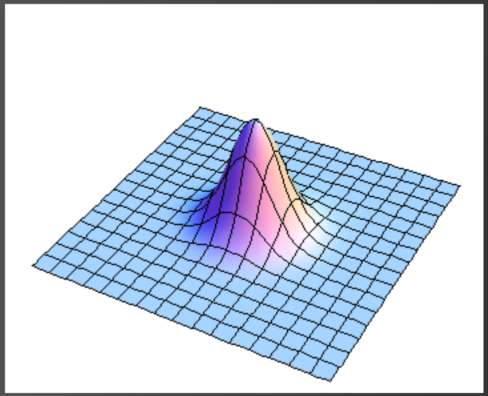
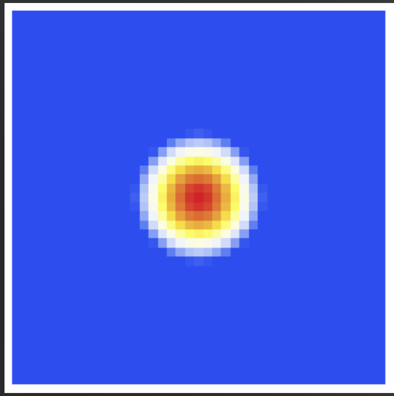
Outline

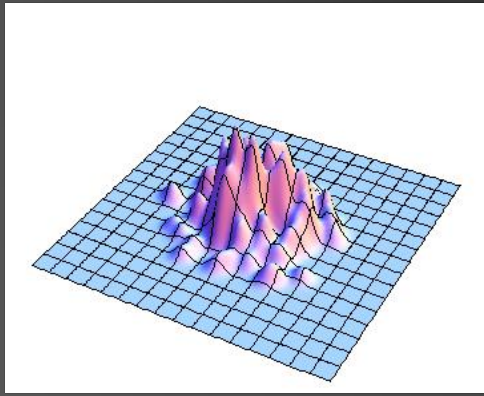
- Introduction
- DR21/ Orion bar models
- H_2 formation on grain surfaces
  - chemisorption vs. physisorption
  - H_2 formation efficiencies on different dust sorts
  - chemical H_2 heating & cooling
  - effects on clump structure
- Summary

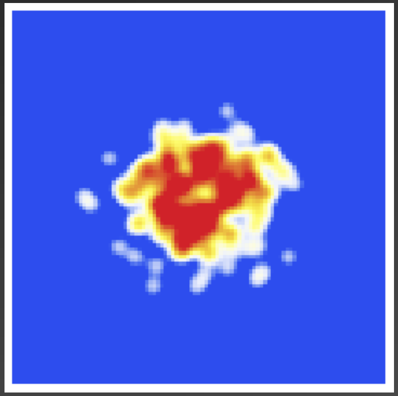
Clumpy Media





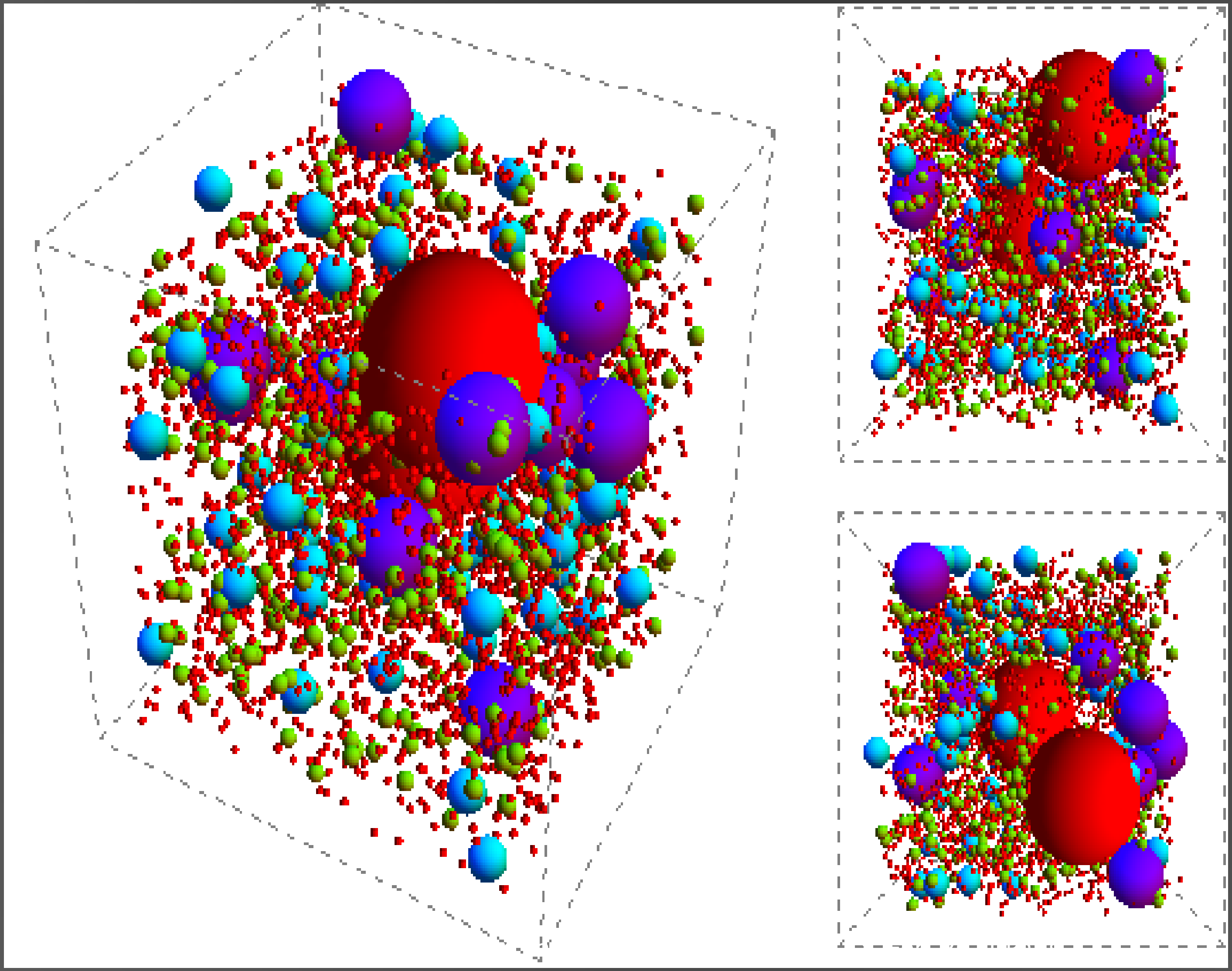
single clumps with Gaussian emission pattern





superposition of 200 Gaussian clumps

Clumpy Clouds via Superposition of Individual Clouds



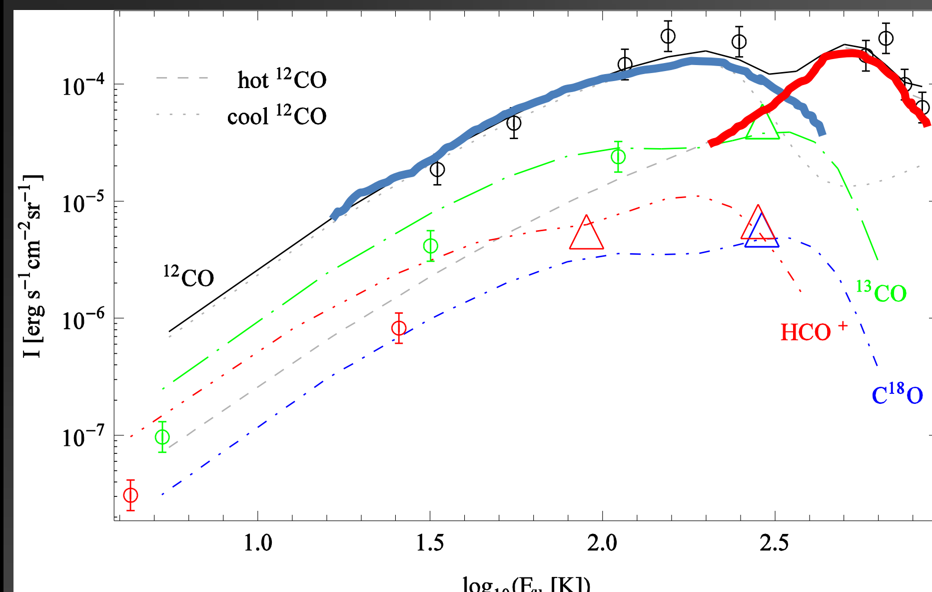
$dN/dM \sim M^{-1.8}$

$M/M_\odot$	N
100	2
10	13
1	80
0.1	502
0.01	3170

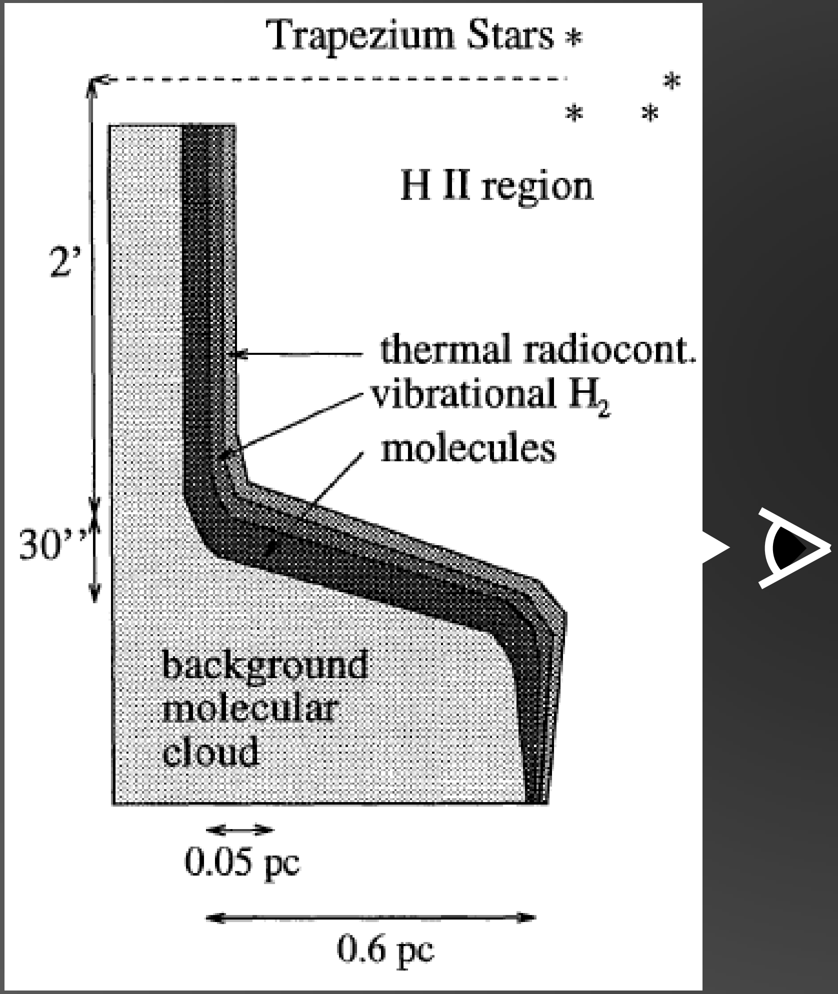
$M_{tot}=673\ M_\odot$

DR21 Geometry/Model

	ensemble 1 (hot)	emsemble 2 (cool)
mass [$M_\odot$]	150	830
mean density [cm^{-3}]	1.3×10^6	1.1×10^6
FUV intensity	1×10^5	3×10^2
mass range [$M_\odot$]	0.01-80	0.001-10



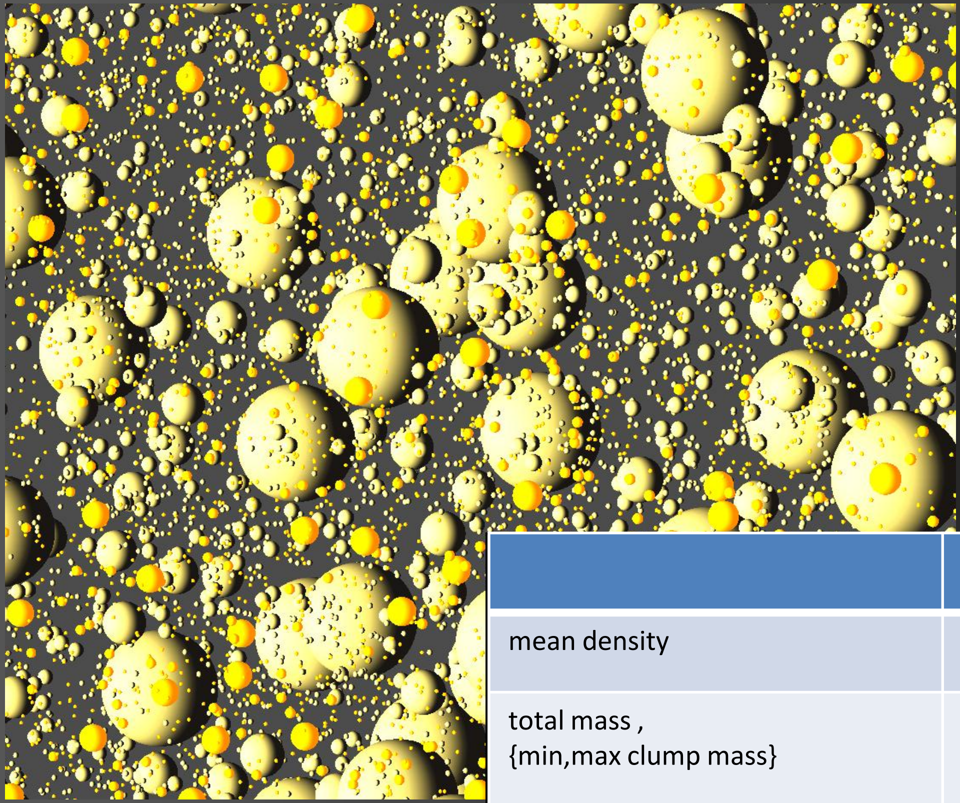
Orion Bar Geometry

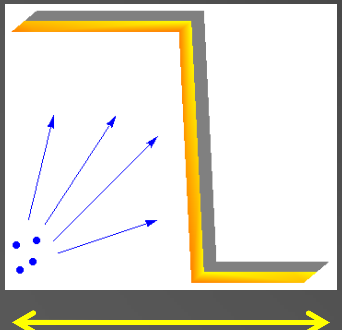


R. Visser, E. Van Dishoeck et al.

- Model: clumpy PDR
  (Hogerheijde et al. 1995)
  - $n_{clump} = 1\times10^6$ cm^{-3}
  - $n_{interclump} = 3\times10^4$ cm^{-3}
  - $G_0 = 4\times10^4$
    (Tielens & Hollenbach 1985)

Orion Bar Model

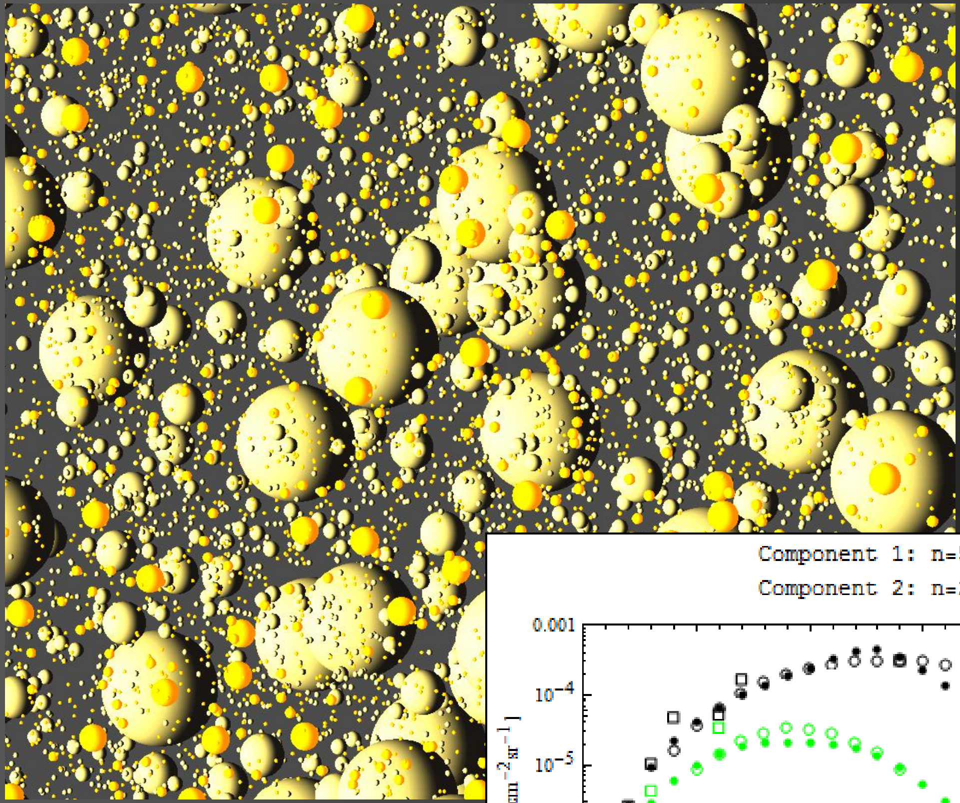


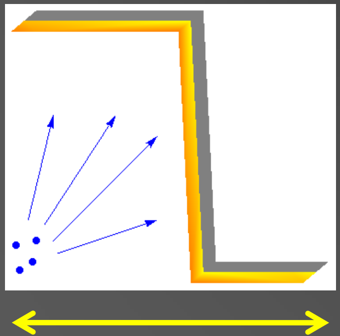


old Fit attempt (Jan 2011)

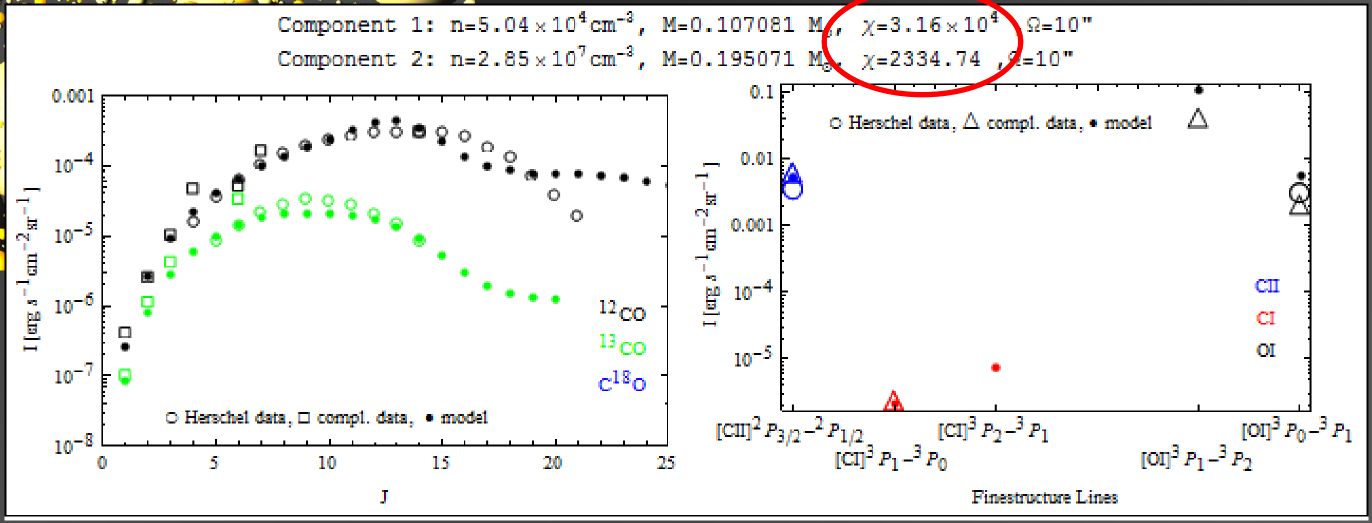
	component 1	component 2
mean density	1e6 cm^{-3}	1e6 cm^{-3}
total mass , {min,max clump mass}	0.4 $M_\odot$ {0.001 $M_\odot$, 10 $M_\odot$}	0.1 $M_\odot$ {0. 1 $M_\odot$, 10 $M_\odot$}
FUV (Draine)	5.7e5	3.3e4
area filling (1)	1.9	0.3
volume filling (2)	0.056	0.014

Orion Bar Model

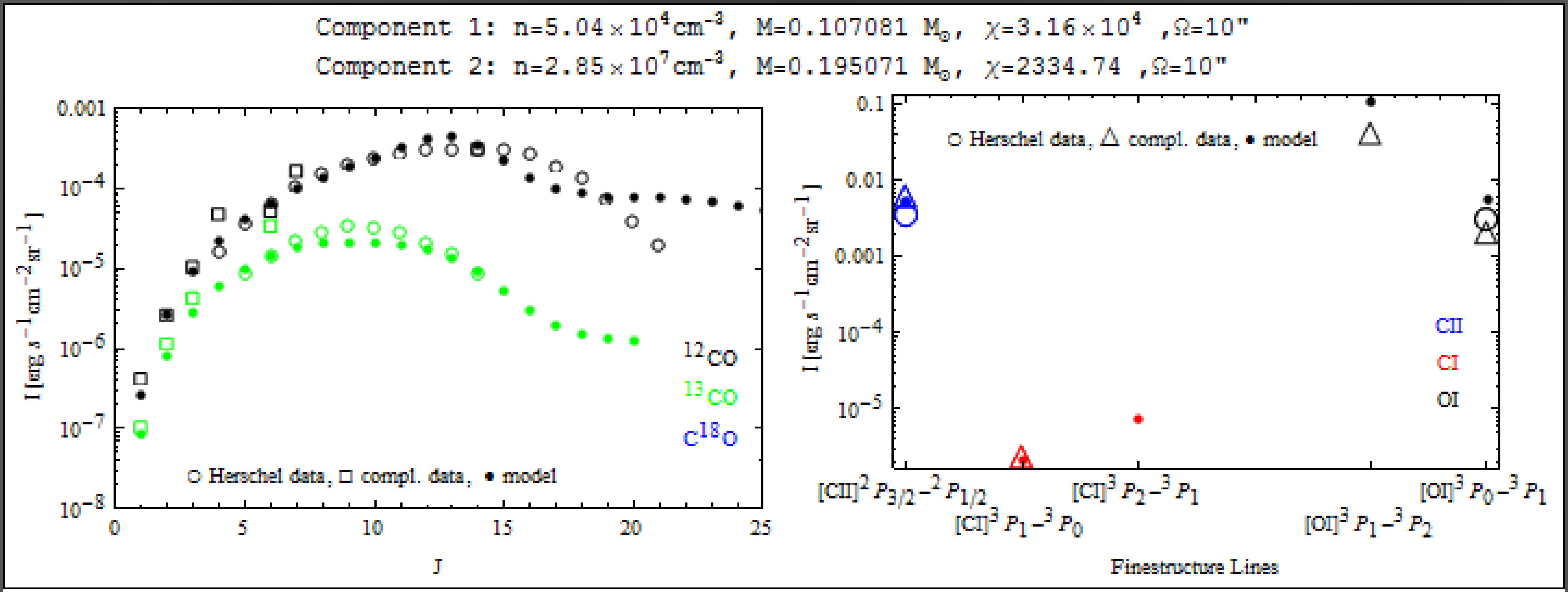




newer Fit attempt (May 2011)



Orion Bar Model



- accounting for chemisorption in H_2 formation
- dust content different from MRN
  - $\Rightarrow$ larger dust surface to form H_2 on
- newest CO rates

H_2 formation on grain surfaces

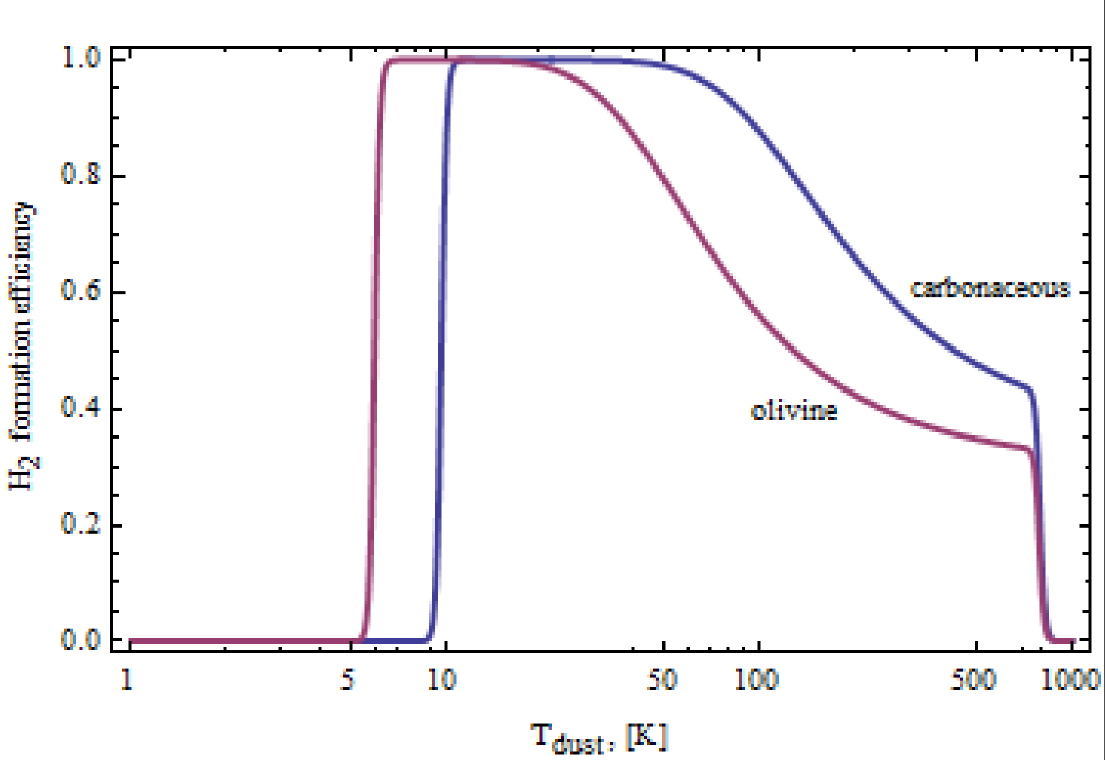
H_2 formation on grain surfaces

- H atoms hitting grain surfaces can stick weakly (physisorption) or strongly (chemisorption) bound.
- T_d>100 K desorption overcomes binding and H_2 formation efficiency →0
- Chemisorbed H atoms can effectively form H_2 up to T>500K
- we implemented the formalism presented by Cazaux & Tielens (2002,2004) in the KOSMA-τ chemistry.

H_2 formation efficiency

$$\epsilon_{H_2} = \left(\frac{\mu F}{2\beta_{H_2}} + 1 + \frac{\beta_{H_P}}{\alpha_{pc}} \right)^{-1}$$

Cazaux & Tielens 2004, ApJ 604



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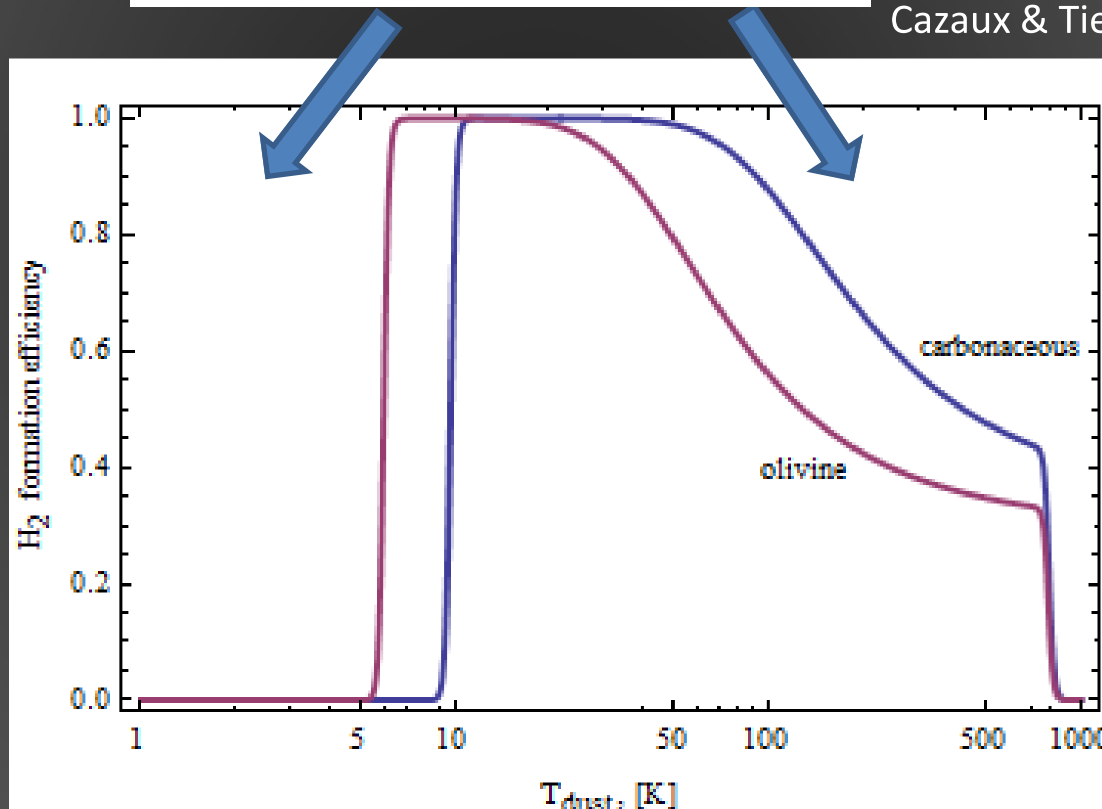

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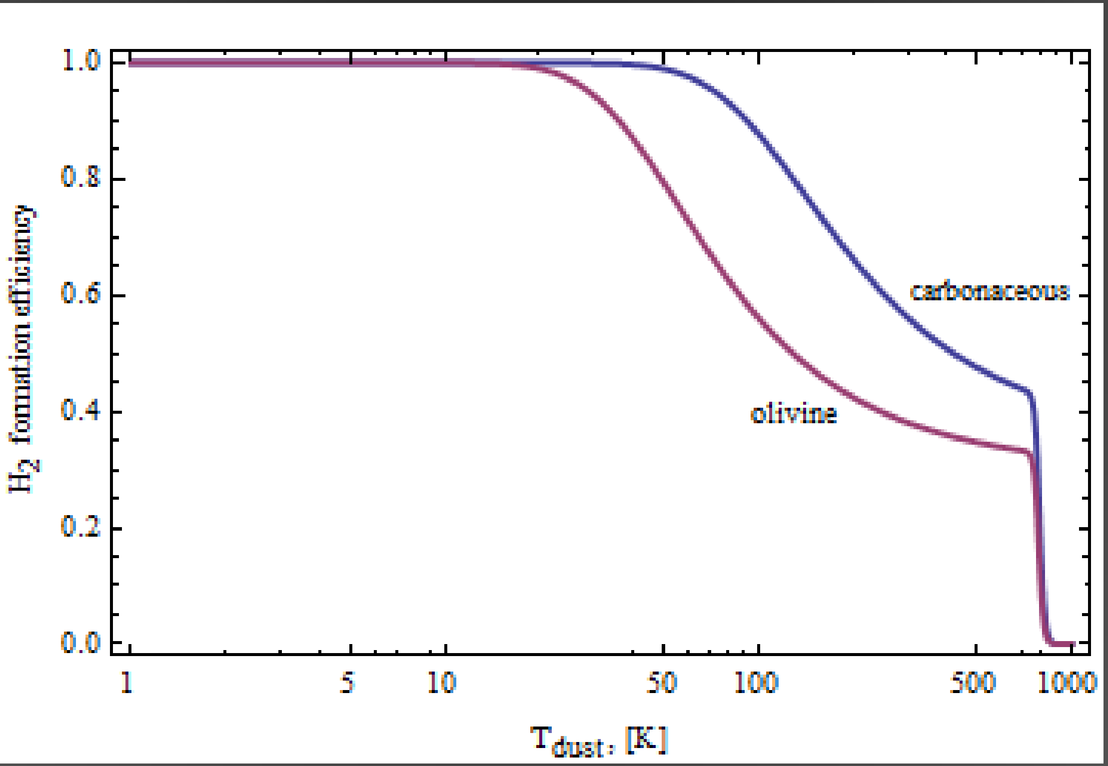

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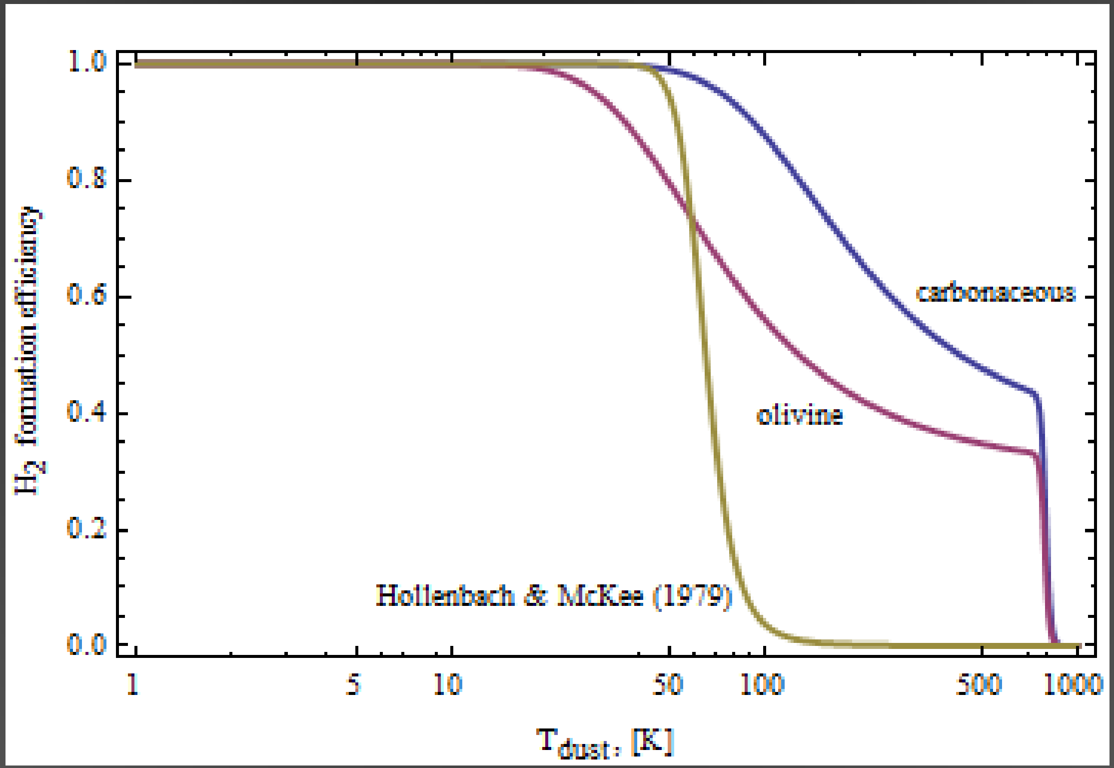
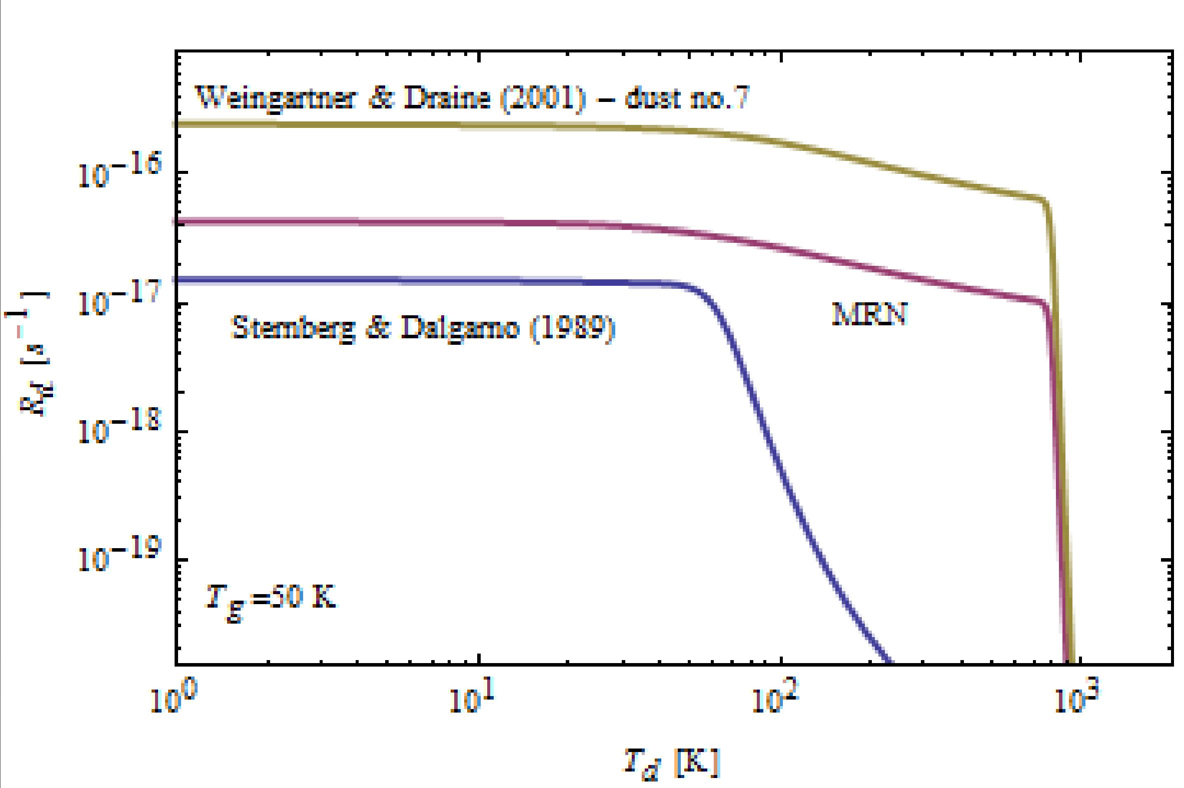


H_2 formation rate

total formation rate depends on total dust surface

$$R_d = \frac{1}{2} n(H) v_H n_d \sigma_d \epsilon_{H_2} S_H$$



H_2 heating/cooling

- H_2 binding energy 4.5 eV
  → H_2 formation heating
- kinetic H_2 dissociation cooling
  (Lepp & Shull, 1983, ApJ 270, 578)

$$H_2 + H \rightarrow H + H + H - 4.5\text{eV}$$

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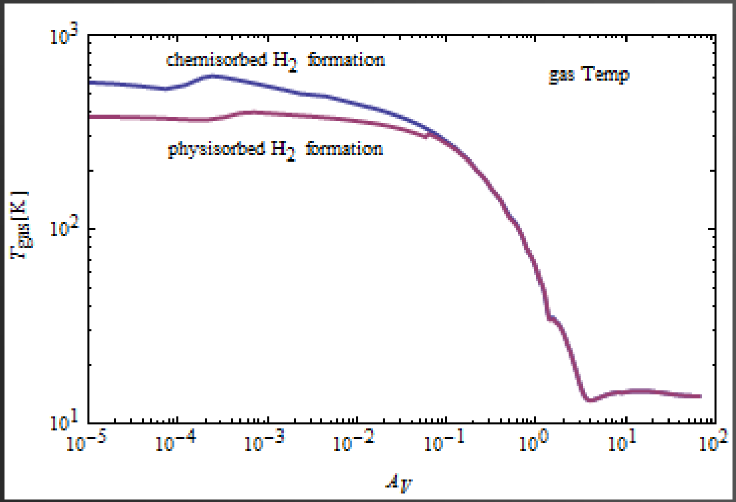

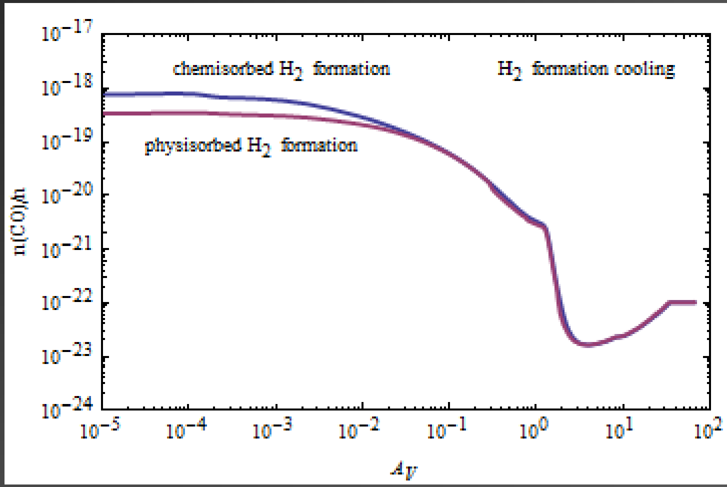

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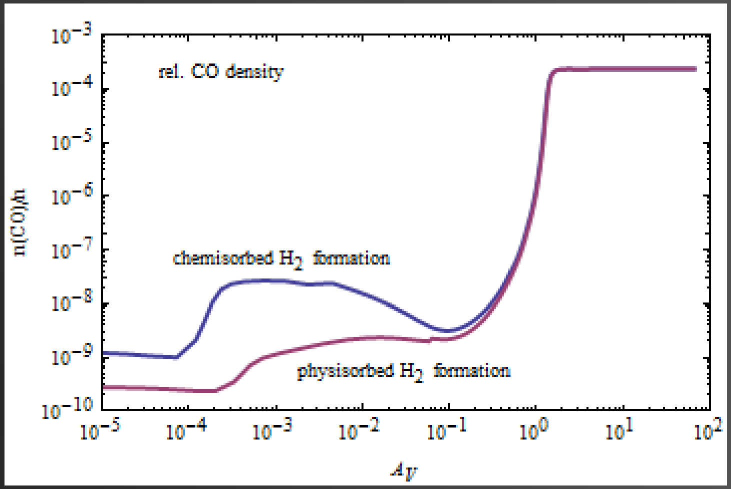
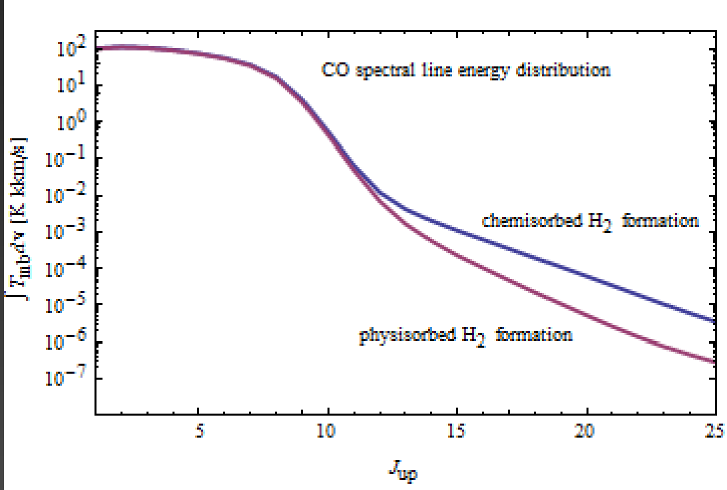
- large effect on H-H_2 transition region chemistry





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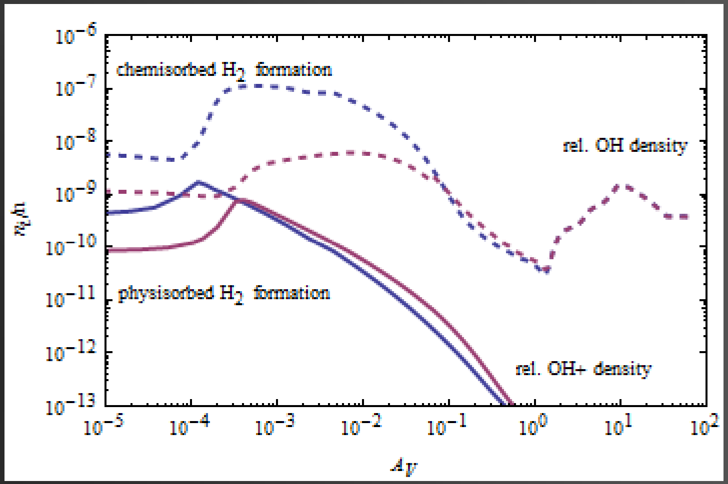
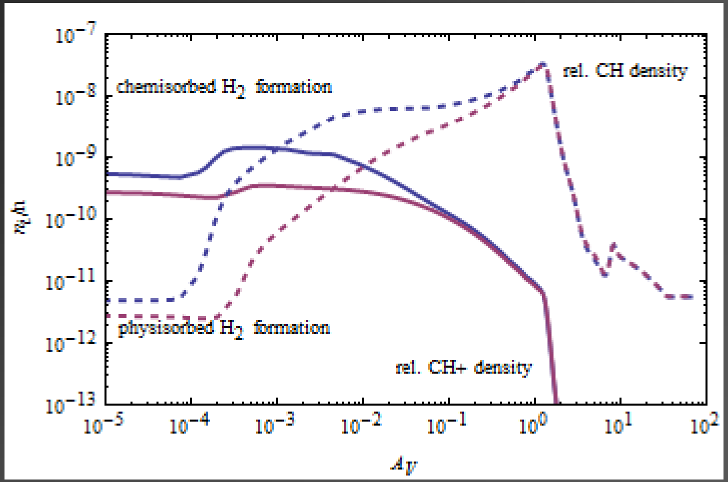
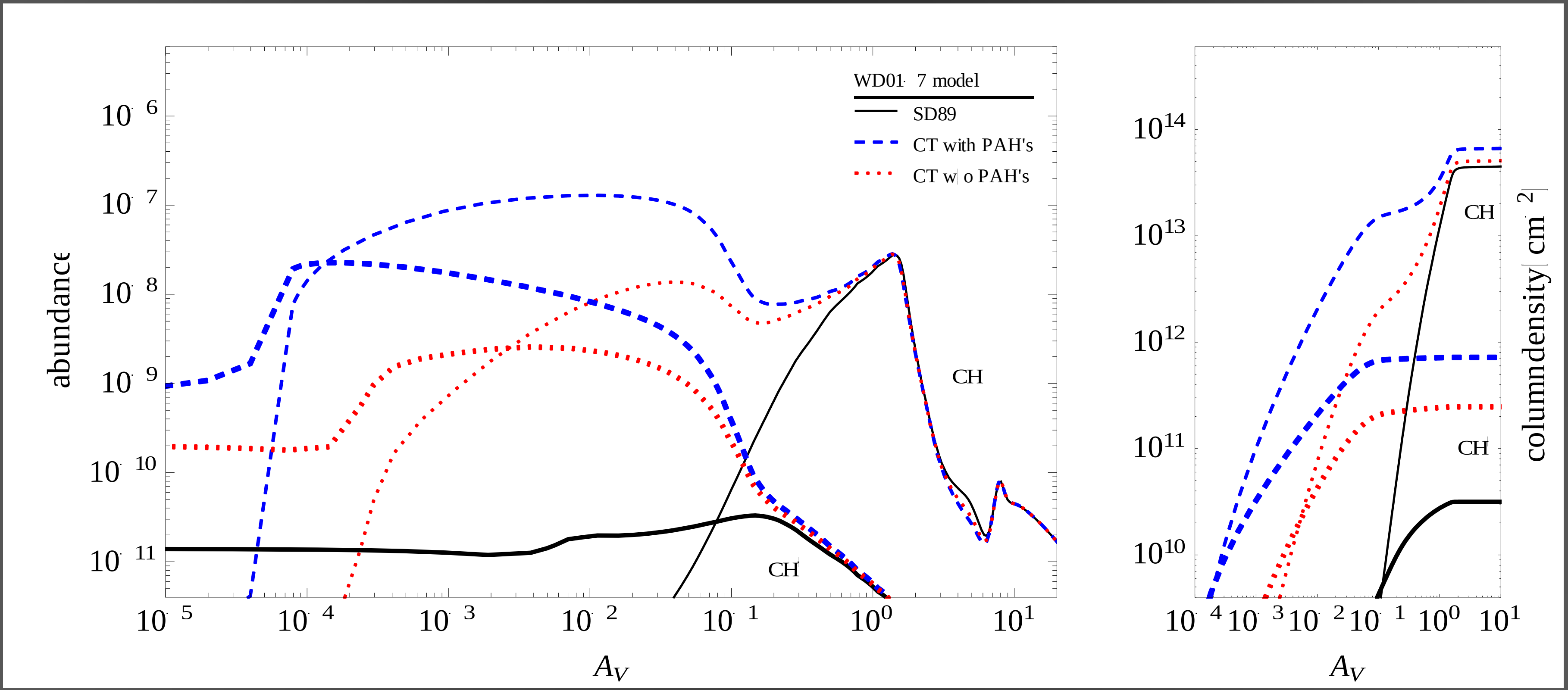
- large effect on H-H_2 transition region chemistry
- chemistry ↔ physics





H_2 Formation on PAHs?



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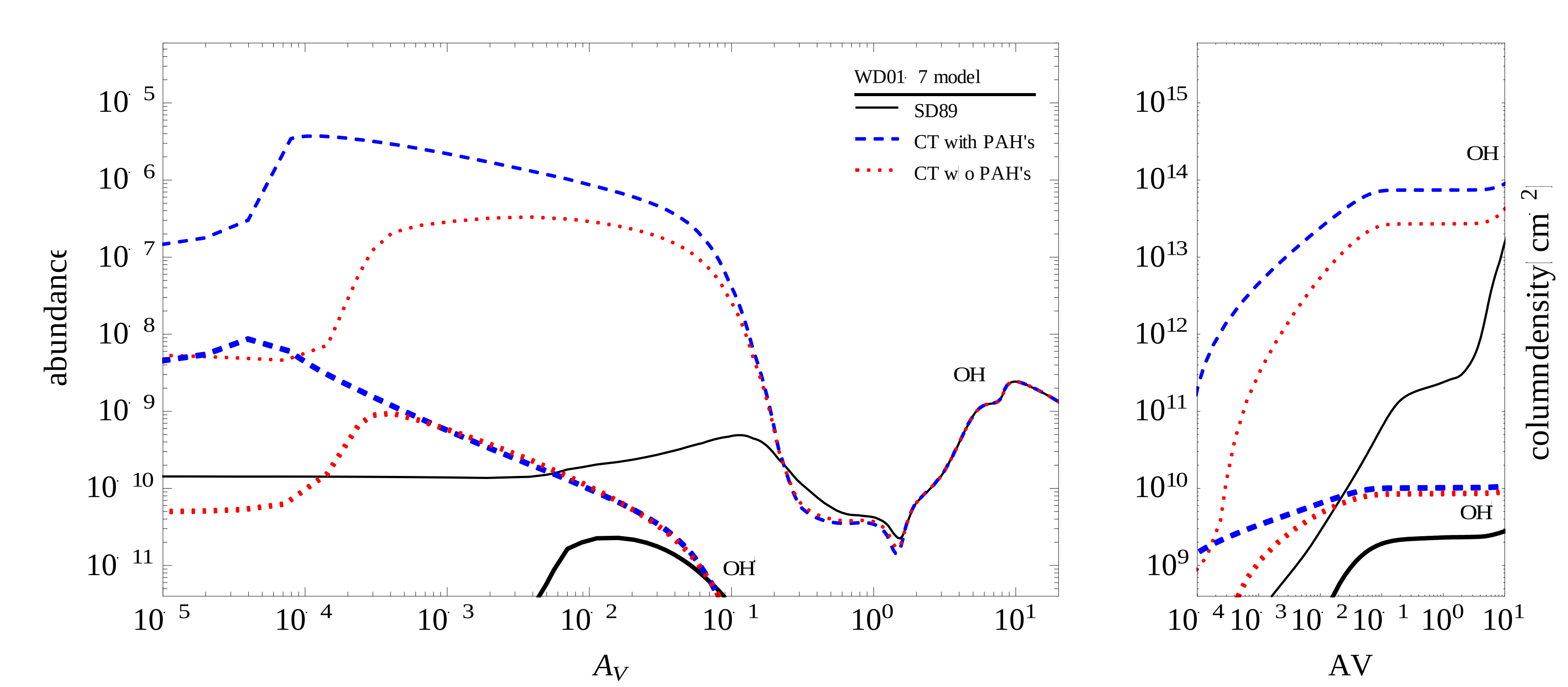
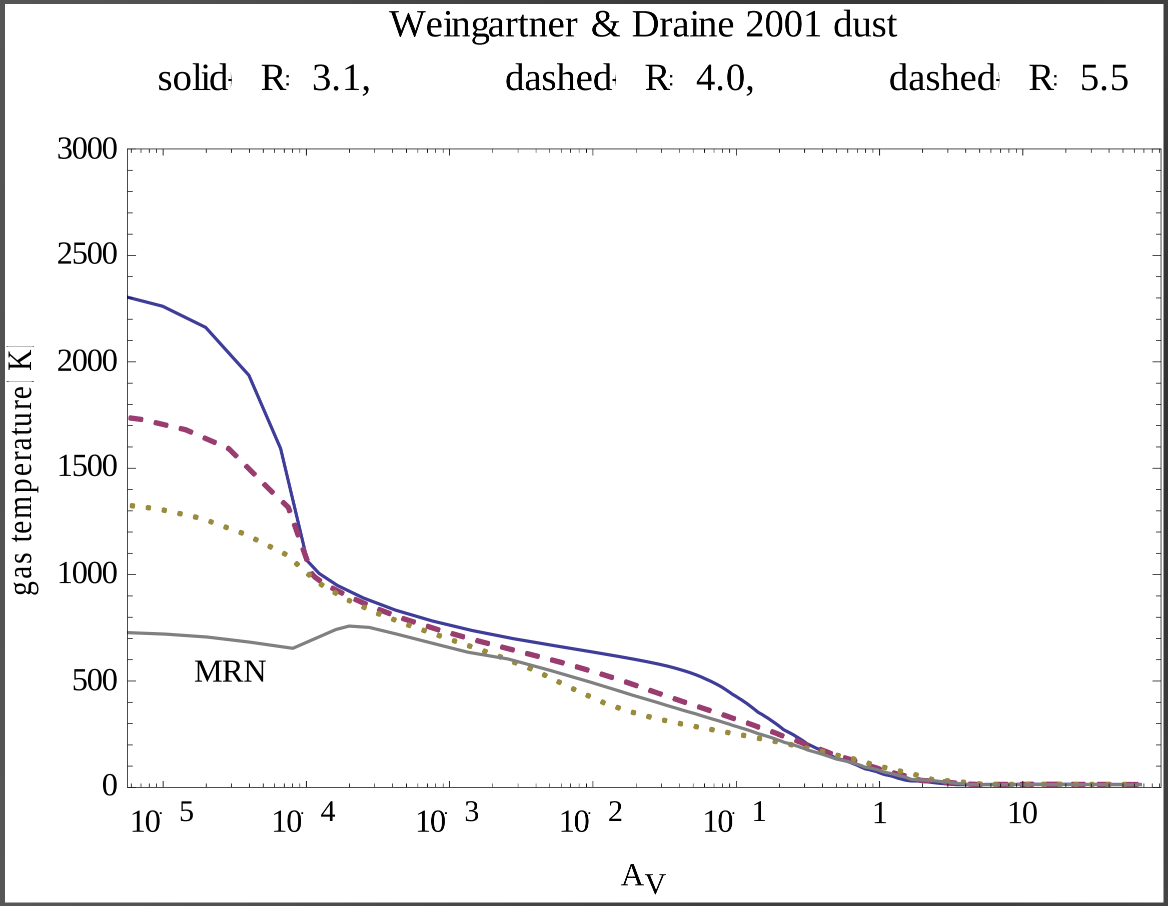


Variation of Dust Properties



detailed dust properties:

- FUV attenuation capabilities
- photodiss. rates (λ depend.)
- PE heating properties

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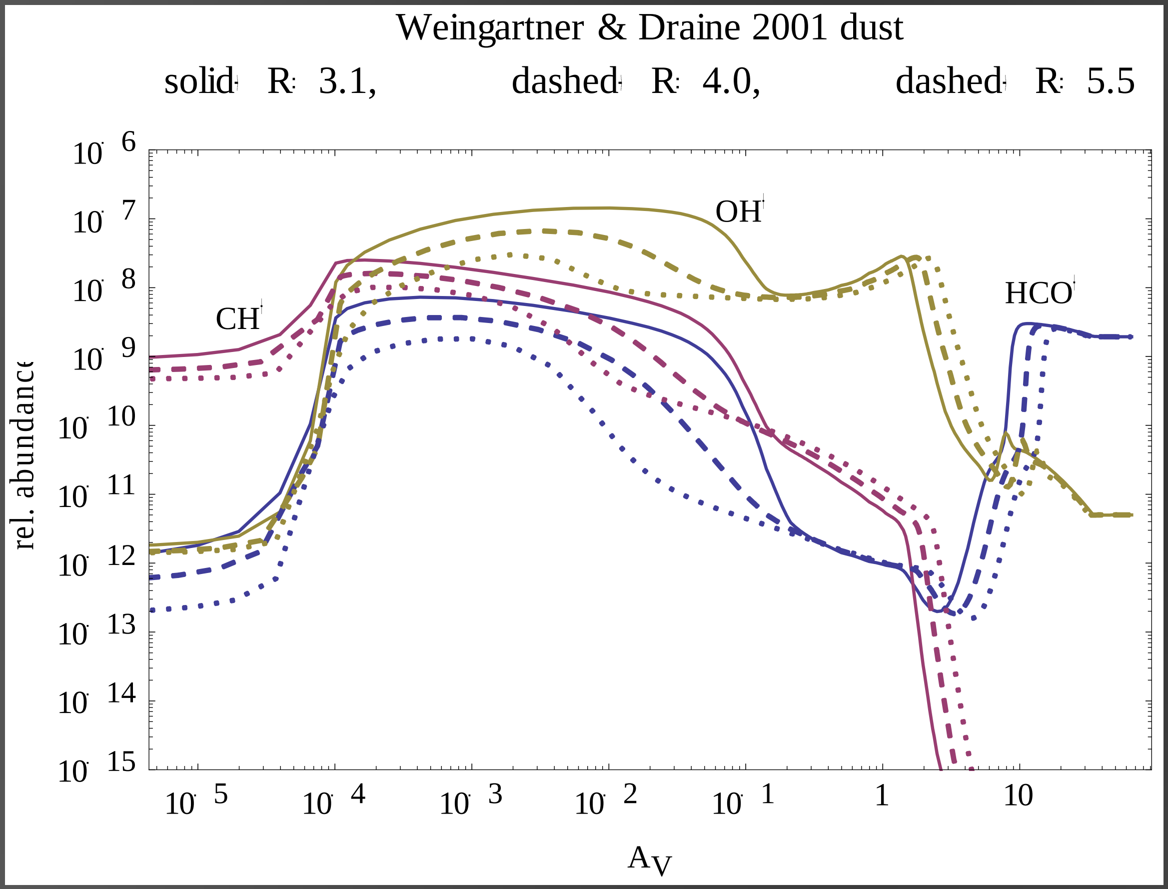

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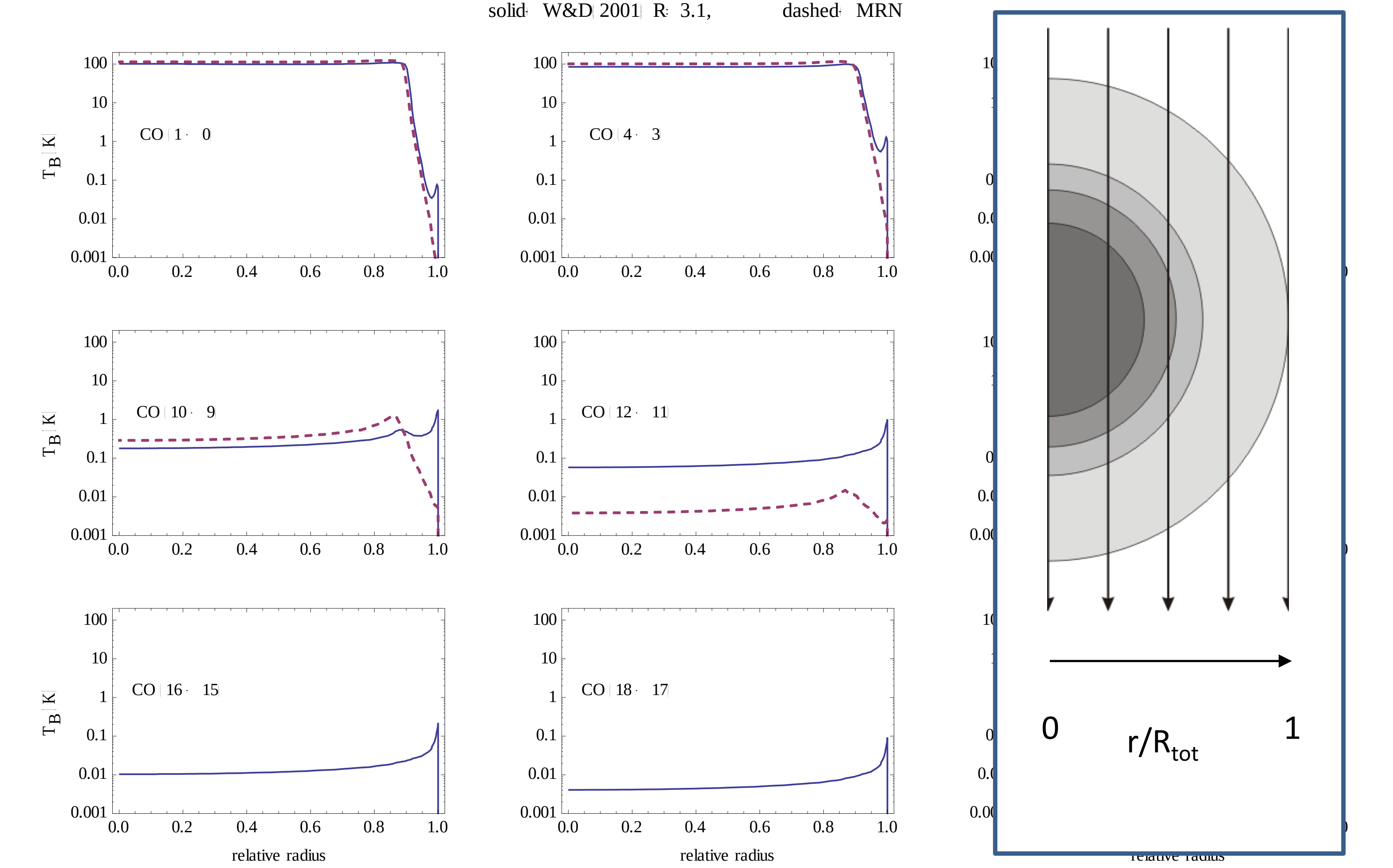
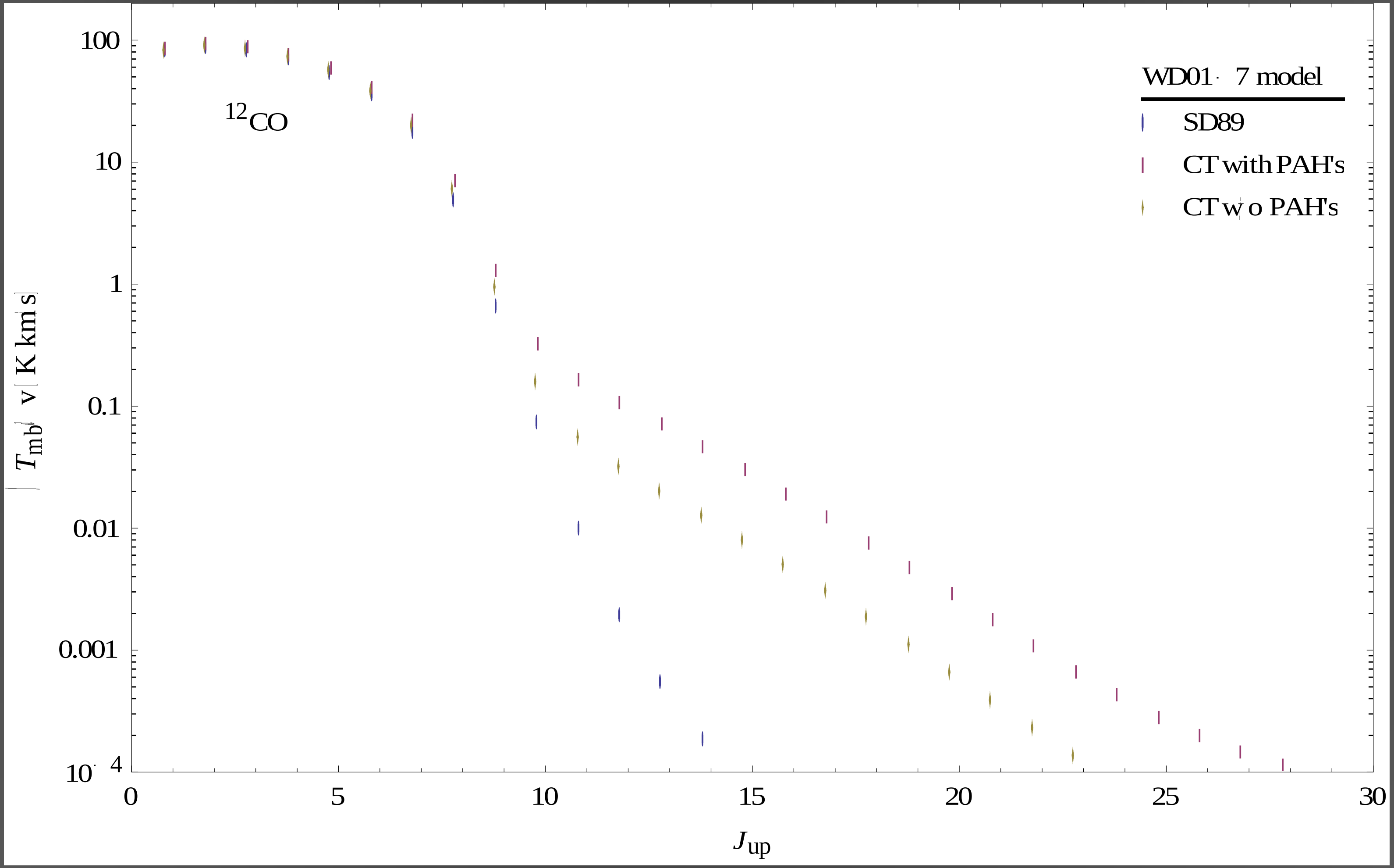
CO Brightness Temperatures



CO Surface Brightness



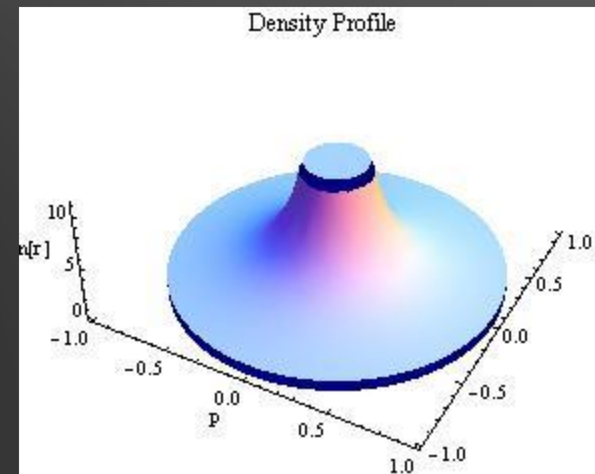
Summary

- Growing understanding of dust properties and H_2 formation process dramatically influences model results
- chemistry and physics strongly connected to each other
- Orion bar model fit approaches reasonable parameters
- J>15 CO transitions not reproduced

Modeling: KOSMA-τ PDR Code

- spherical geometry

$$n[r] == \begin{cases} n\left(\frac{r}{R}\right)^{-\alpha} & R\,R_{core} \le r \le R \\ n\,R_{core}^{-\alpha} & 0 \le r < R\,R_{core} \\ 0 & \text{True} \end{cases}$$



- isotropic illumination
- modular chemistry incl. isotopologues
- coupled with radiative transfer code (ONION, SimLine, etc.)
- self-consistently solves chemistry & energy balance

Modeling: KOSMA-τ PDR Code

Output:

- density profile of all contained species
- temperature profile (gas, dust)
- excitation conditions (T_{ex}, etc.)
- clump-averaged quantities
  - column densities
  - AV
  - optical depths
  - intensities