Influence of H2 formation on PDR model results

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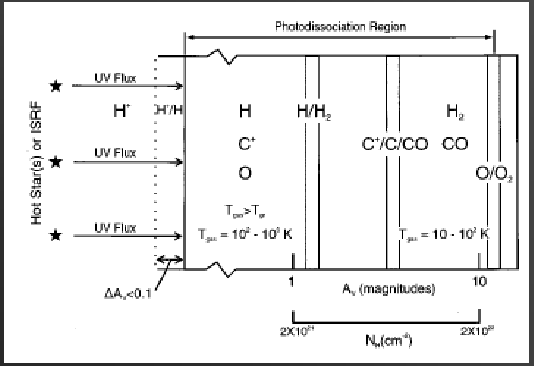
Outline

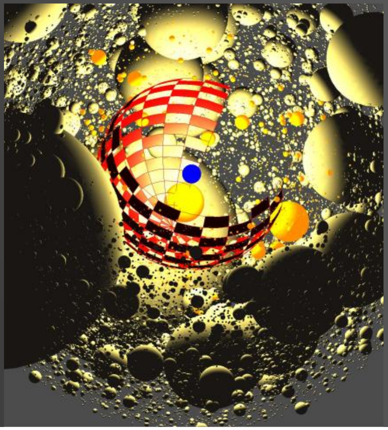
- H_2 formation on grain surfaces
  - chemisorption vs. physisorption
  - H_2 formation efficiencies on different dust sorts
  - chemical H_2 heating & cooling
  - effects on clump structure

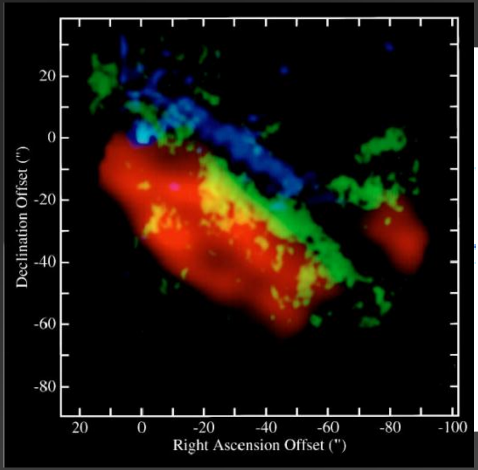
Introduction

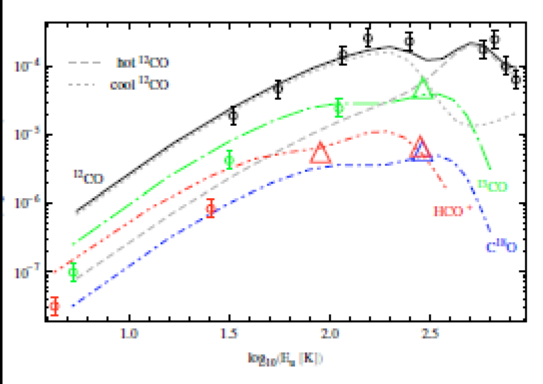
Numerical PDR models of proved to be a valuable tools in analyzing and understanding the local conditions in massive star forming regions.



Hollenbach & Tielens, 1999, R.o.m.P., 71







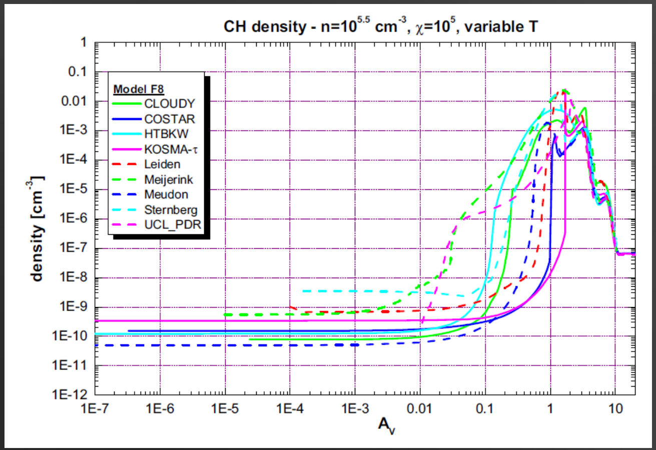
Ossenkopf et al, 2010, A&A 518, L79v

Introduction

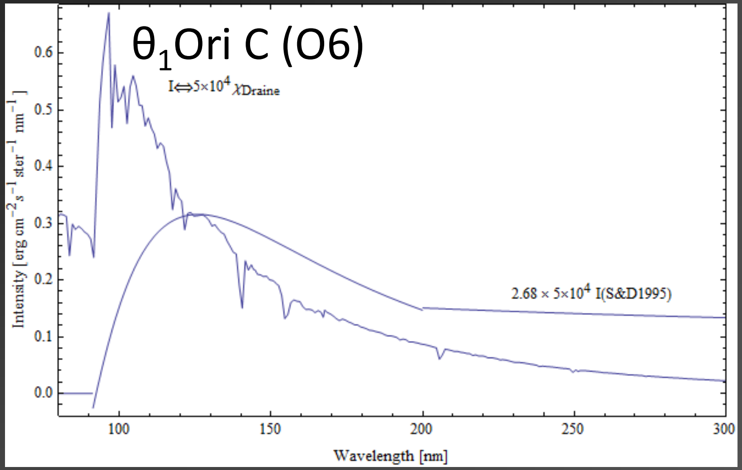
Yet, here be dragons...

- complex physics / chemistry

- complex/unknown local conditions



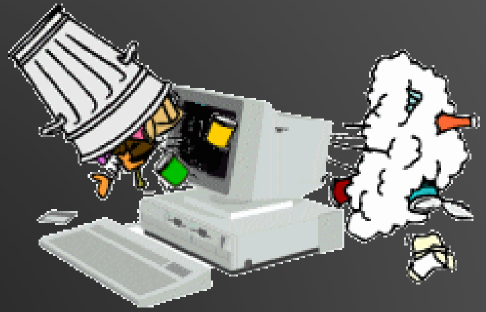
Röllig et al. 2007, A&A, 467



Introduction

and unfortunately, deficient input data

- missing experimental data
- inter/extrapolation



"OK, if you're so smart, *you* manage the portfolio!"

H_2 formation on grain surfaces

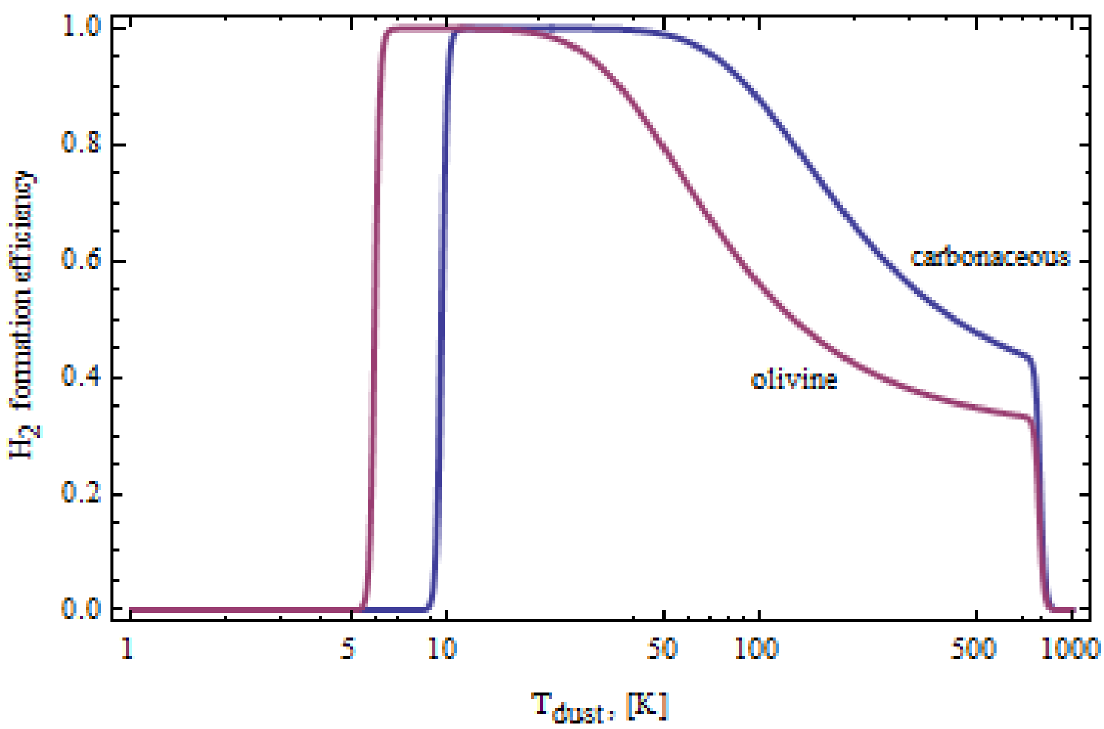
H_2 formation on grain surfaces

- 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_d>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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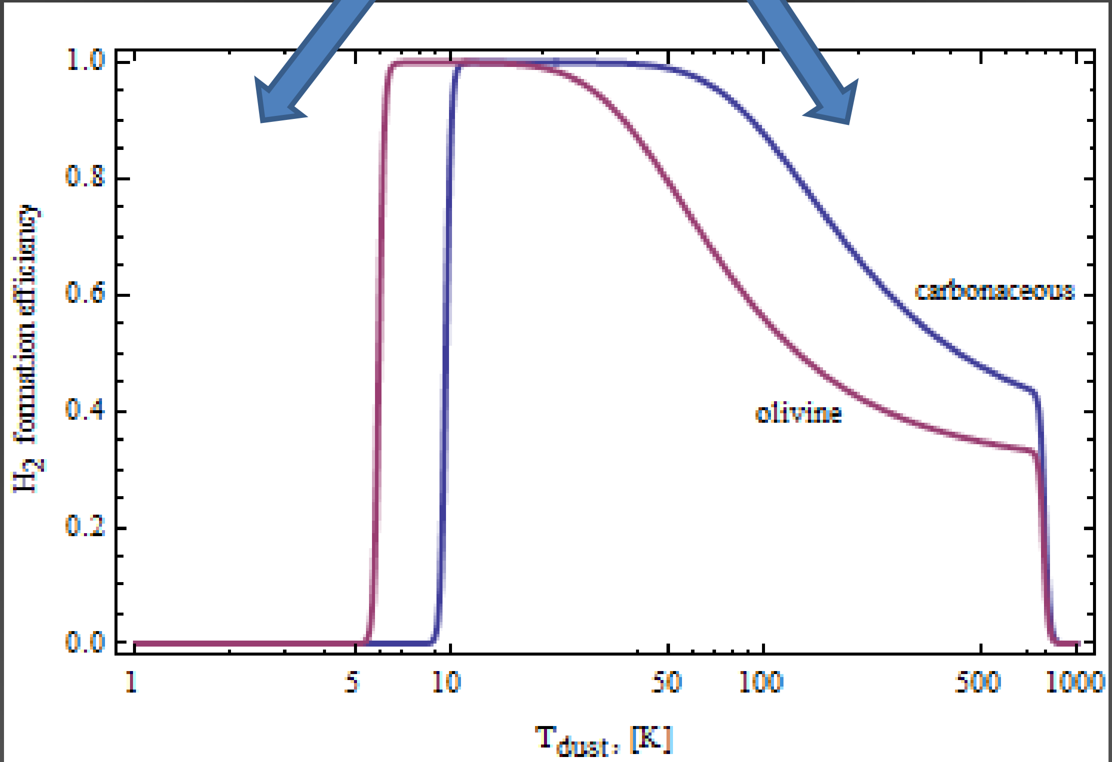

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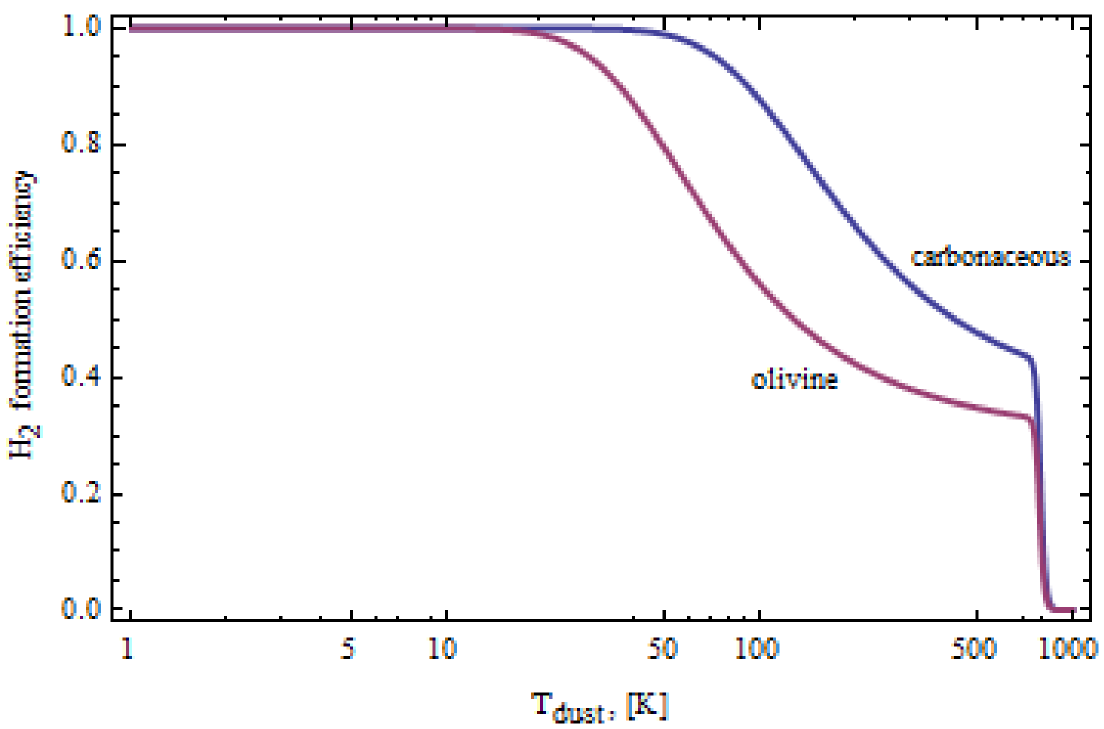

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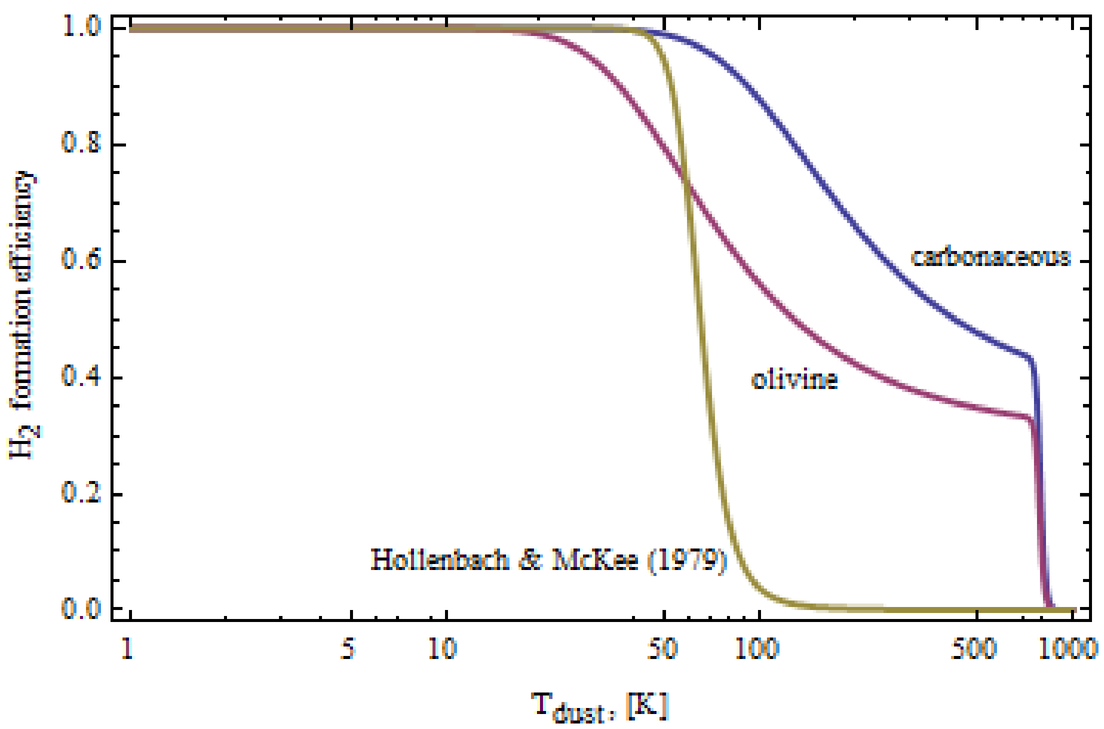
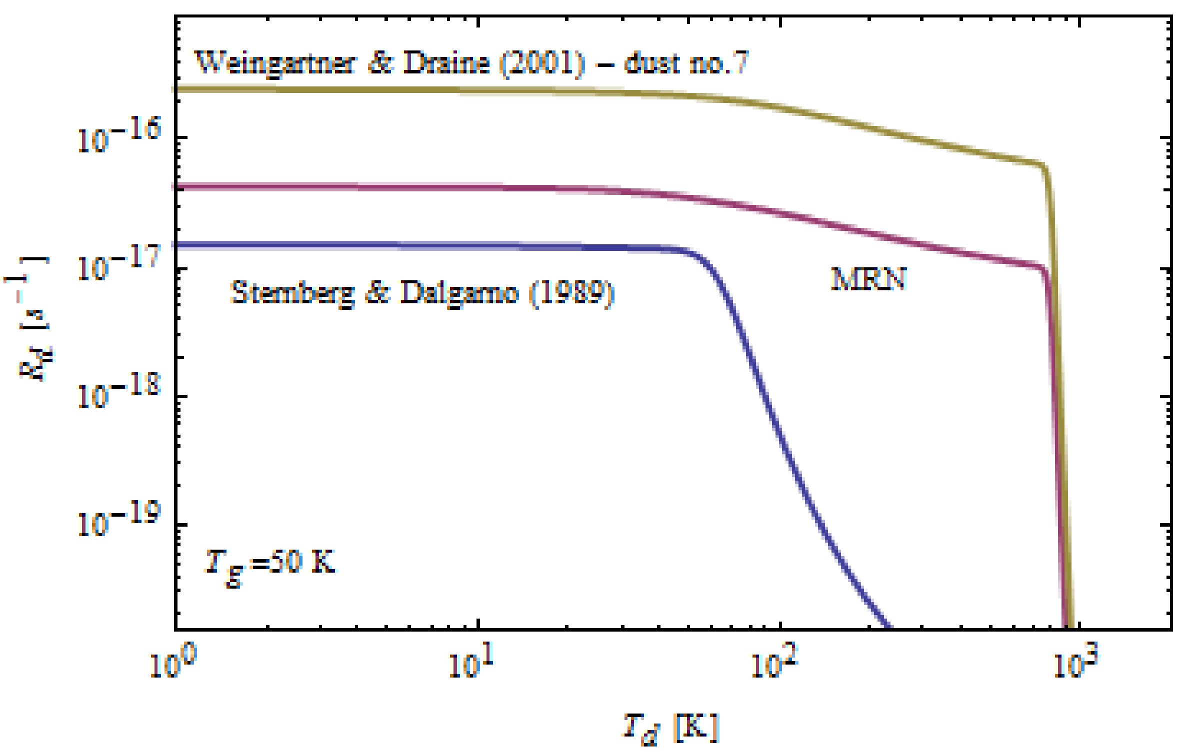


H_2 formation rate

total formation rate depends on total dust surface

$$R_d = \frac{1}{2} n(H) v_H n_d \boxed{\sigma_d} \epsilon_{\mathrm{H}_2} S_H$$



H_2 formation rate

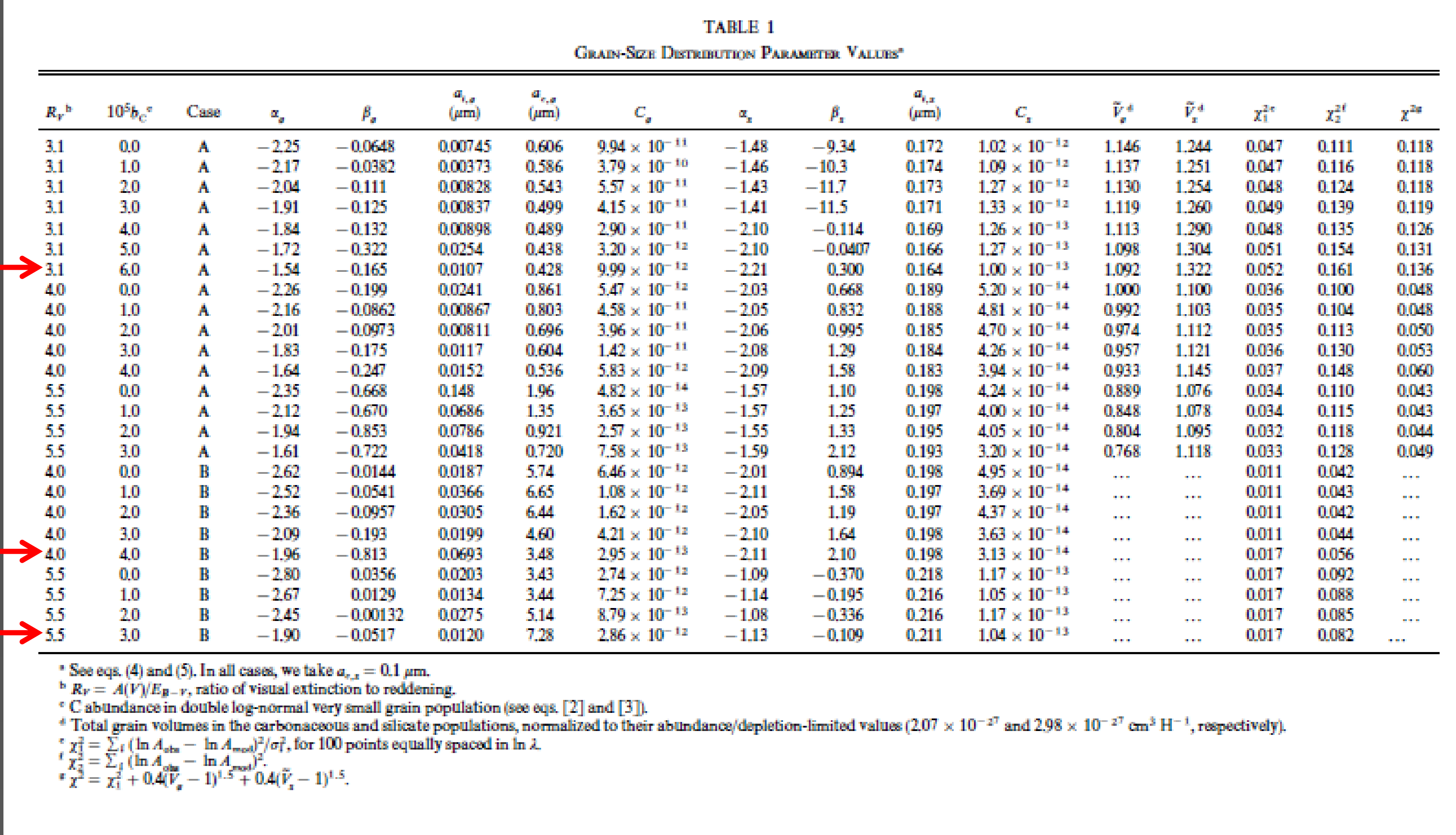


TABLE 1

GRAIN-SIZE DISTRIBUTION PARAMETER VALUES[a]

R_V[b]	$10^5 b_C$[c]	Case	α_g	β_g	$a_{t,g}$ (μm)	$a_{c,g}$ (μm)	C_g	α_s	β_s	$a_{t,s}$ (μm)	C_s	$\tilde{V}_g$[d]	$\tilde{V}_s$[d]	χ_1^2[e]	χ_2^2[f]	χ^2[g]
3.1	0.0	A	−2.25	−0.0648	0.00745	0.606	9.94×10^{-11}	−1.48	−9.34	0.172	1.02×10^{-12}	1.146	1.244	0.047	0.111	0.118
3.1	1.0	A	−2.17	−0.0382	0.00373	0.586	3.79×10^{-10}	−1.46	−10.3	0.174	1.09×10^{-12}	1.137	1.251	0.047	0.116	0.118
3.1	2.0	A	−2.04	−0.111	0.00828	0.543	5.57×10^{-11}	−1.43	−11.7	0.173	1.27×10^{-12}	1.130	1.254	0.048	0.124	0.118
3.1	3.0	A	−1.91	−0.125	0.00837	0.499	4.15×10^{-11}	−1.41	−11.5	0.171	1.33×10^{-12}	1.119	1.260	0.049	0.139	0.119
3.1	4.0	A	−1.84	−0.132	0.00898	0.489	2.90×10^{-11}	−2.10	−0.114	0.169	1.26×10^{-13}	1.113	1.290	0.048	0.135	0.126
3.1	5.0	A	−1.72	−0.322	0.0254	0.438	3.20×10^{-12}	−2.10	−0.0407	0.166	1.27×10^{-13}	1.098	1.304	0.051	0.154	0.131
3.1	6.0	A	−1.54	−0.165	0.0107	0.428	9.99×10^{-12}	−2.21	0.300	0.164	1.00×10^{-13}	1.092	1.322	0.052	0.161	0.136
4.0	0.0	A	−2.26	−0.199	0.0241	0.861	5.47×10^{-12}	−2.03	0.668	0.189	5.20×10^{-14}	1.000	1.100	0.036	0.100	0.048
4.0	1.0	A	−2.16	−0.0862	0.00867	0.803	4.58×10^{-11}	−2.05	0.832	0.188	4.81×10^{-14}	0.992	1.103	0.035	0.104	0.048
4.0	2.0	A	−2.01	−0.0973	0.00811	0.696	3.96×10^{-11}	−2.06	0.995	0.185	4.70×10^{-14}	0.974	1.112	0.035	0.113	0.050
4.0	3.0	A	−1.83	−0.175	0.0117	0.604	1.42×10^{-11}	−2.08	1.29	0.184	4.26×10^{-14}	0.957	1.121	0.036	0.130	0.053
4.0	4.0	A	−1.64	−0.247	0.0152	0.536	5.83×10^{-12}	−2.09	1.58	0.183	3.94×10^{-14}	0.933	1.145	0.037	0.148	0.060
5.5	0.0	A	−2.35	−0.668	0.148	1.96	4.82×10^{-14}	−1.57	1.10	0.198	4.24×10^{-14}	0.889	1.076	0.034	0.110	0.043
5.5	1.0	A	−2.12	−0.670	0.0686	1.35	3.65×10^{-13}	−1.57	1.25	0.197	4.00×10^{-14}	0.848	1.078	0.034	0.115	0.043
5.5	2.0	A	−1.94	−0.853	0.0786	0.921	2.57×10^{-13}	−1.55	1.33	0.195	4.05×10^{-14}	0.804	1.095	0.032	0.118	0.044
5.5	3.0	A	−1.61	−0.722	0.0418	0.720	7.58×10^{-13}	−1.59	2.12	0.193	3.20×10^{-14}	0.768	1.118	0.033	0.128	0.049
4.0	0.0	B	−2.62	−0.0144	0.0187	5.74	6.46×10^{-12}	−2.01	0.894	0.198	4.95×10^{-14}	…	…	0.011	0.042	…
4.0	1.0	B	−2.52	−0.0541	0.0366	6.65	1.08×10^{-12}	−2.11	1.58	0.197	3.69×10^{-14}	…	…	0.011	0.043	…
4.0	2.0	B	−2.36	−0.0957	0.0305	6.44	1.62×10^{-12}	−2.05	1.19	0.197	4.37×10^{-14}	…	…	0.011	0.042	…
4.0	3.0	B	−2.09	−0.193	0.0199	4.60	4.21×10^{-12}	−2.10	1.64	0.198	3.63×10^{-14}	…	…	0.011	0.044	…
4.0	4.0	B	−1.96	−0.813	0.0693	3.48	2.95×10^{-13}	−2.11	2.10	0.198	3.13×10^{-14}	…	…	0.017	0.056	…
5.5	0.0	B	−2.80	0.0356	0.0203	3.43	2.74×10^{-12}	−1.09	−0.370	0.218	1.17×10^{-13}	…	…	0.017	0.092	…
5.5	1.0	B	−2.67	0.0129	0.0134	3.44	7.25×10^{-12}	−1.14	−0.195	0.216	1.05×10^{-13}	…	…	0.017	0.088	…
5.5	2.0	B	−2.45	−0.00132	0.0275	5.14	8.79×10^{-13}	−1.08	−0.336	0.216	1.17×10^{-13}	…	…	0.017	0.085	…
5.5	3.0	B	−1.90	−0.0517	0.0120	7.28	2.86×10^{-12}	−1.13	−0.109	0.211	1.04×10^{-13}	…	…	0.017	0.082	…

[a] See eqs. (4) and (5). In all cases, we take $a_{r,s} = 0.1$ μm.

[b] $R_V = A(V)/E_{B-V}$, ratio of visual extinction to reddening.

[c] C abundance in double log-normal very small grain population (see eqs. [2] and [3]).

[d] Total grain volumes in the carbonaceous and silicate populations, normalized to their abundance/depletion-limited values (2.07×10^{-27} and 2.98×10^{-27} cm^3 H^{-1}, respectively).

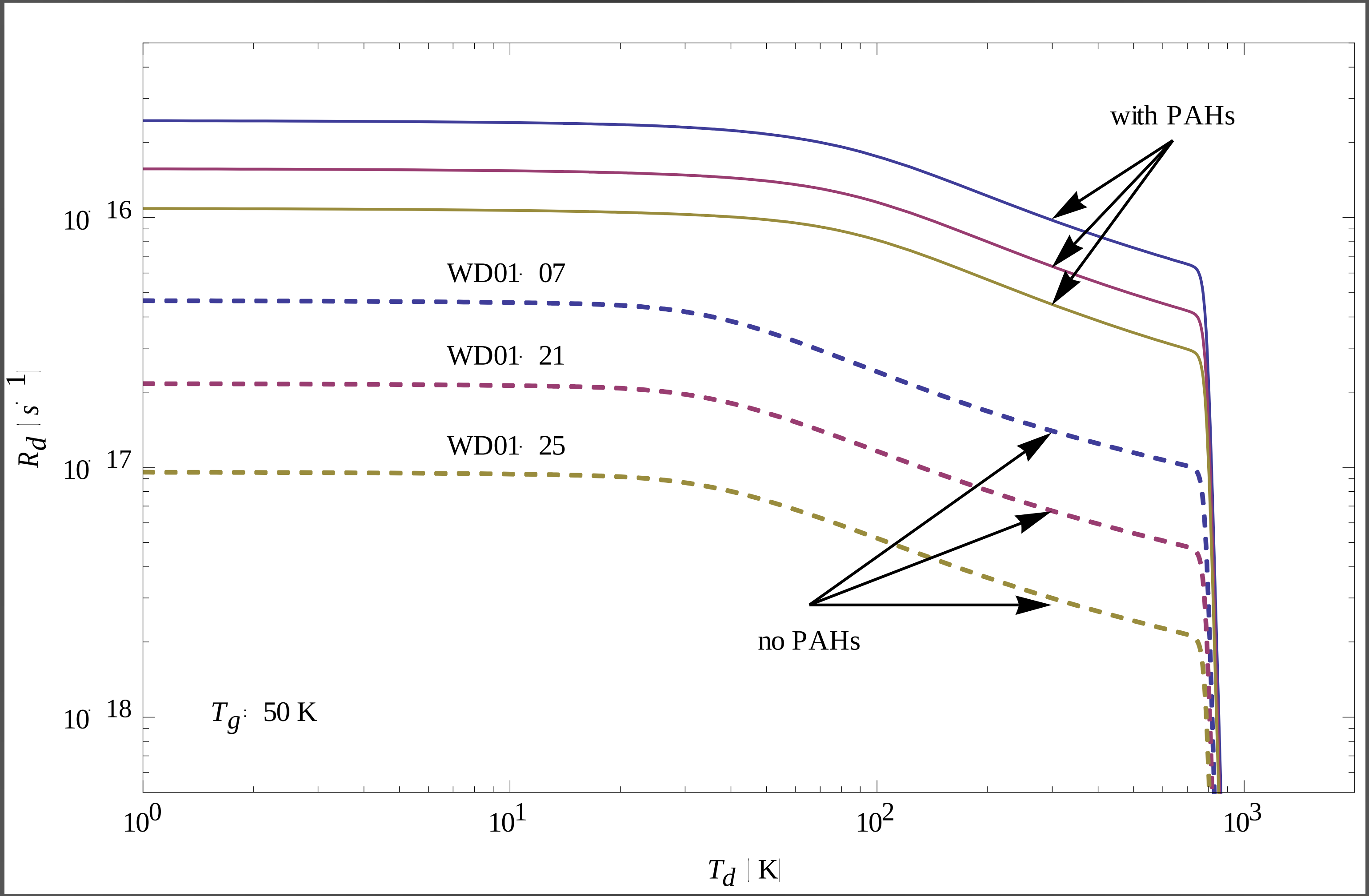
[e] $\chi_1^2 = \sum_i (\ln A_{\rm obs} - \ln A_{\rm mod})^2/\sigma_i^2$, for 100 points equally spaced in $\ln \lambda$.

[f] $\chi_2^2 = \sum_j (\ln A_{\rm obs} - \ln A_{\rm mod})^2$.

[g] $\chi^2 = \chi_1^2 + 0.4(\tilde{V}_g - 1)^{1.5} + 0.4(\tilde{V}_s - 1)^{1.5}$.

Weingartner and Draine, 2001, ApJ 548

H_2 formation rate



H_2 heating/cooling

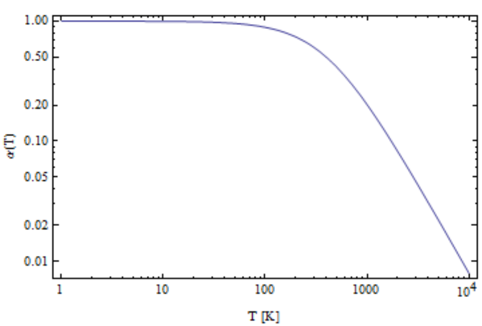
- H_2 binding energy 4.5 eV
  → H_2 formation heating
- kinetic H_2 dissociation cooling
  (Lepp & Shull, 1983, ApJ 270, 578)

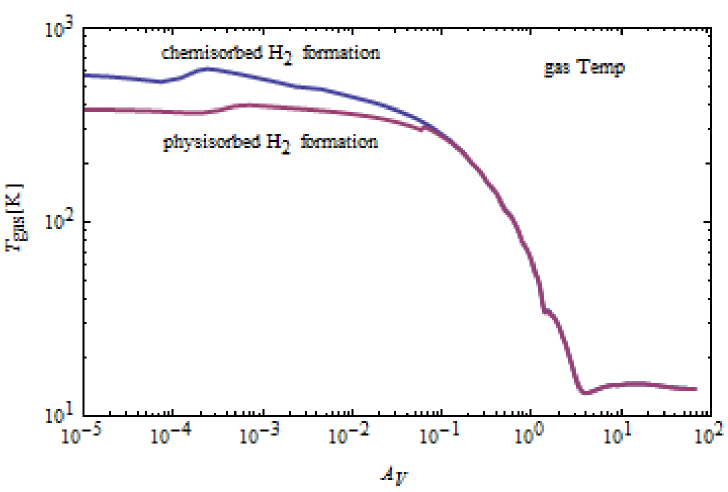
  $H_2 + H \rightarrow H + H + H - 4.5\text{eV}$

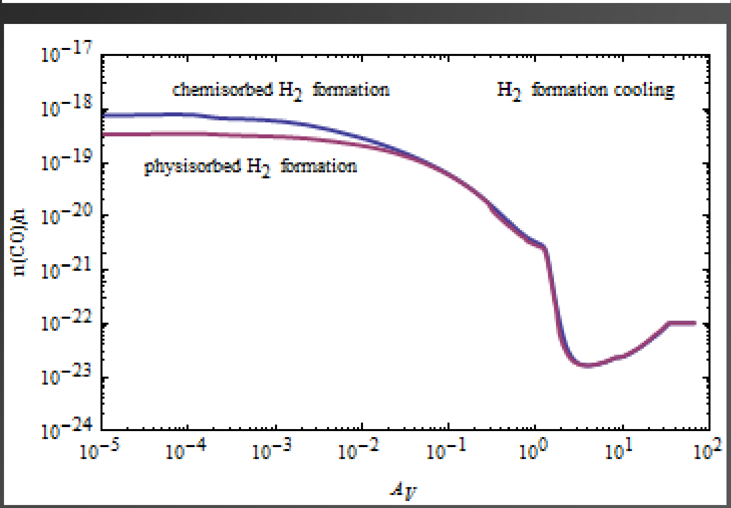
  $H_2 + H_2 \rightarrow H_2 + H + H - 4.5\text{eV}$

Alternatively: sticking coeff.

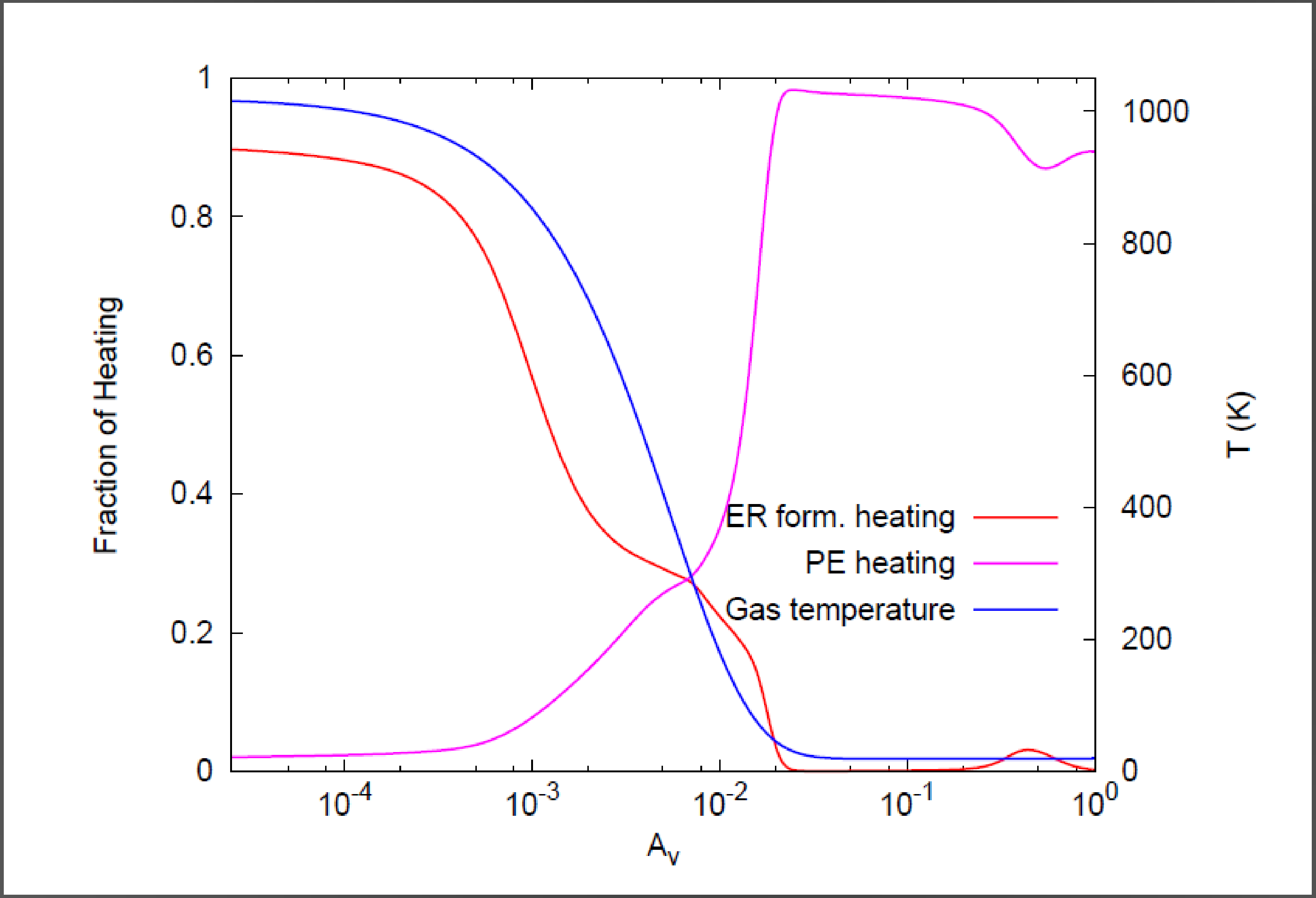
$$\alpha(T) = \frac{1}{1+\left(\frac{T}{T_2}\right)^{\beta}}.$$







H_2 heating/cooling



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H_2 heating/cooling

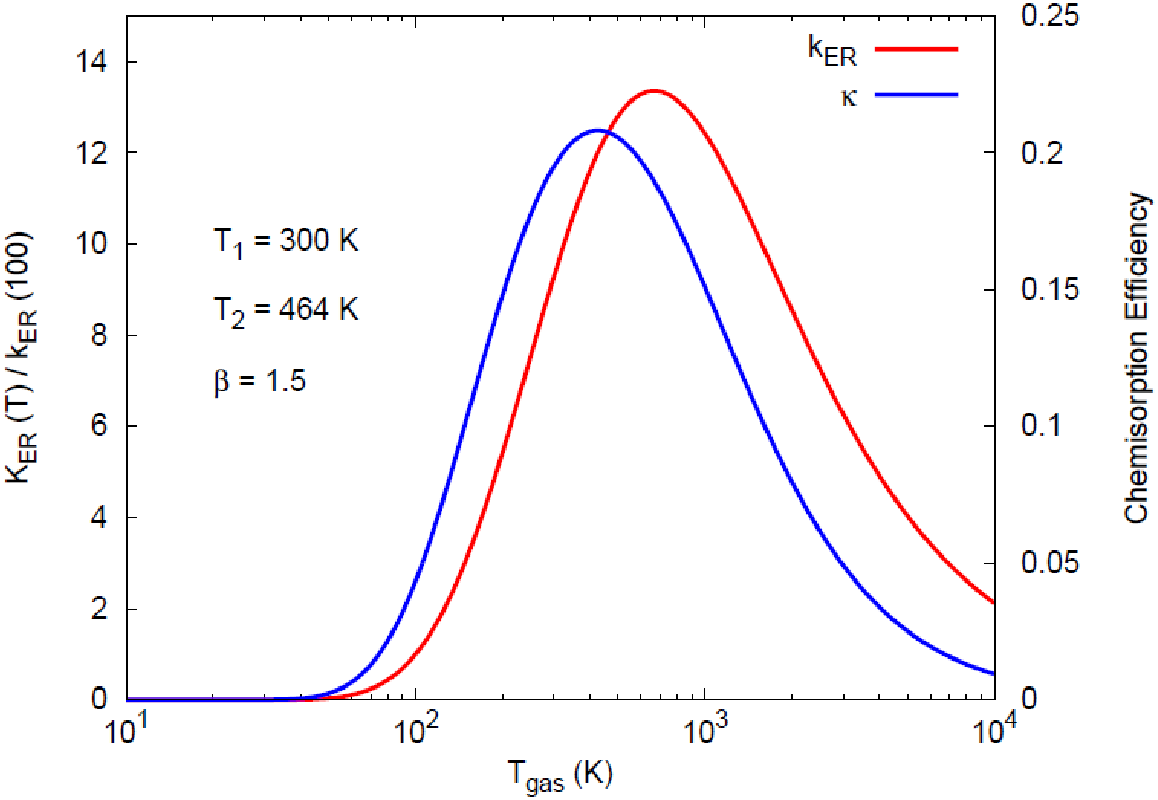

Figure C.1. Left axis: Variation of k_{ER} with gas temperature T (relative to the one at 100 K). Right axis: chemisorption efficiency κ (see text).

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H_2 heating/cooling

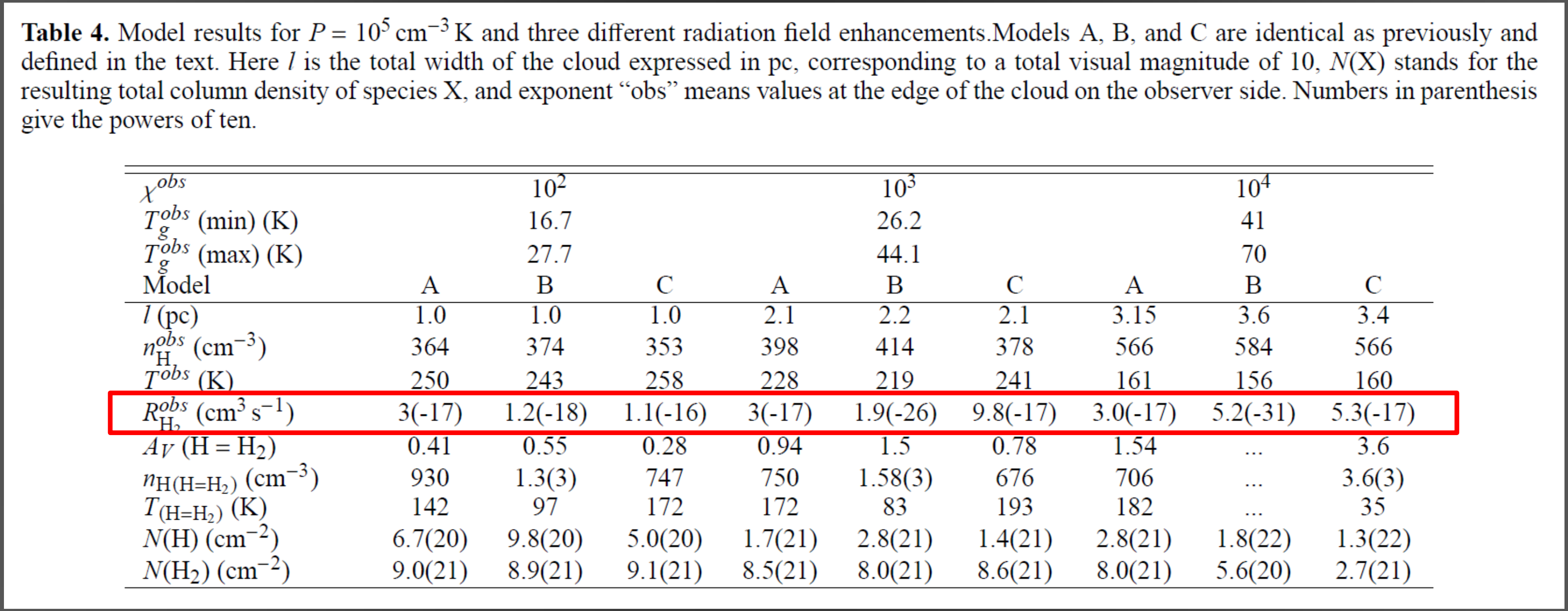

Table 4. Model results for $P = 10^5$ cm^{-3} K and three different radiation field enhancements.Models A, B, and C are identical as previously and defined in the text. Here l is the total width of the cloud expressed in pc, corresponding to a total visual magnitude of 10, N(X) stands for the resulting total column density of species X, and exponent "obs" means values at the edge of the cloud on the observer side. Numbers in parenthesis give the powers of ten.

χ^{obs}		10^2			10^3			10^4	
T_g^{obs} (min) (K)		16.7			26.2			41	
T_g^{obs} (max) (K)		27.7			44.1			70	
Model	A	B	C	A	B	C	A	B	C
l (pc)	1.0	1.0	1.0	2.1	2.2	2.1	3.15	3.6	3.4
$n_{\rm H}^{obs}$ (cm^{-3})	364	374	353	398	414	378	566	584	566
T^{obs} (K)	250	243	258	228	219	241	161	156	160
$R_{\rm H_2}^{obs}$ (cm^3 s^{-1})	3(-17)	1.2(-18)	1.1(-16)	3(-17)	1.9(-26)	9.8(-17)	3.0(-17)	5.2(-31)	5.3(-17)
A_V (H = H$_2$)	0.41	0.55	0.28	0.94	1.5	0.78	1.54	...	3.6
$n_{\rm H(H=H_2)}$ (cm^{-3})	930	1.3(3)	747	750	1.58(3)	676	706	...	3.6(3)
$T_{\rm (H=H_2)}$ (K)	142	97	172	172	83	193	182	...	35
N(H) (cm^{-2})	6.7(20)	9.8(20)	5.0(20)	1.7(21)	2.8(21)	1.4(21)	2.8(21)	1.8(22)	1.3(22)
N(H$_2$) (cm^{-2})	9.0(21)	8.9(21)	9.1(21)	8.5(21)	8.0(21)	8.6(21)	8.0(21)	5.6(20)	2.7(21)

A: R=const, B: only LH, C=LH+ER

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H$_2$ heating/cooling

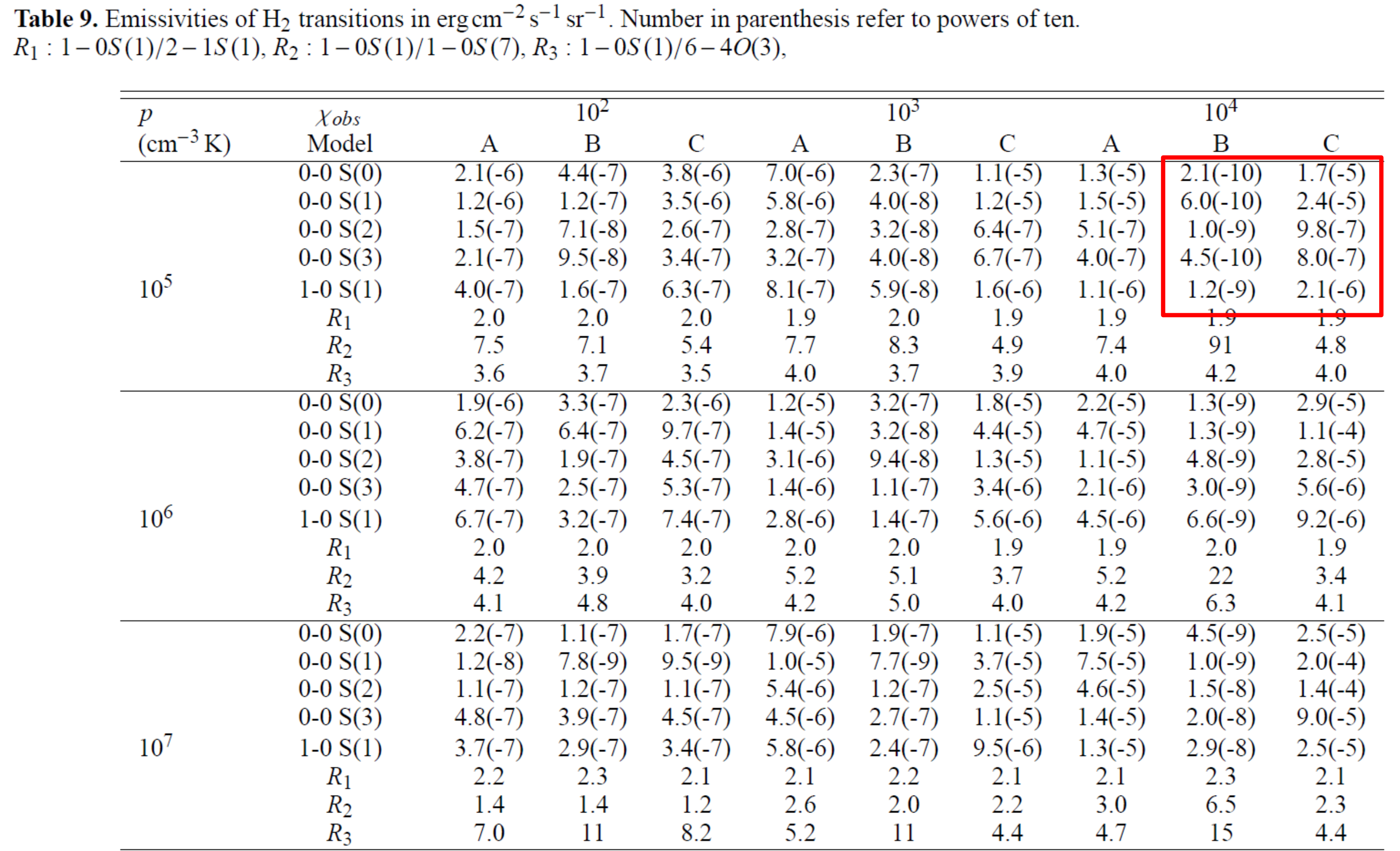

Table 9. Emissivities of H$_2$ transitions in erg cm^{-2} s^{-1} sr^{-1}. Number in parenthesis refer to powers of ten.
$R_1 : 1-0S(1)/2-1S(1)$, $R_2 : 1-0S(1)/1-0S(7)$, $R_3 : 1-0S(1)/6-4O(3)$,

p	χ_{obs}	10^2			10^3			10^4		
(cm^{-3} K)	Model	A	B	C	A	B	C	A	B	C
10^5	0-0 S(0)	2.1(-6)	4.4(-7)	3.8(-6)	7.0(-6)	2.3(-7)	1.1(-5)	1.3(-5)	2.1(-10)	1.7(-5)
	0-0 S(1)	1.2(-6)	1.2(-7)	3.5(-6)	5.8(-6)	4.0(-8)	1.2(-5)	1.5(-5)	6.0(-10)	2.4(-5)
	0-0 S(2)	1.5(-7)	7.1(-8)	2.6(-7)	2.8(-7)	3.2(-8)	6.4(-7)	5.1(-7)	1.0(-9)	9.8(-7)
	0-0 S(3)	2.1(-7)	9.5(-8)	3.4(-7)	3.2(-7)	4.0(-8)	6.7(-7)	4.0(-7)	4.5(-10)	8.0(-7)
	1-0 S(1)	4.0(-7)	1.6(-7)	6.3(-7)	8.1(-7)	5.9(-8)	1.6(-6)	1.1(-6)	1.2(-9)	2.1(-6)
	R_1	2.0	2.0	2.0	1.9	2.0	1.9	1.9	1.9	1.9
	R_2	7.5	7.1	5.4	7.7	8.3	4.9	7.4	91	4.8
	R_3	3.6	3.7	3.5	4.0	3.7	3.9	4.0	4.2	4.0
10^6	0-0 S(0)	1.9(-6)	3.3(-7)	2.3(-6)	1.2(-5)	3.2(-7)	1.8(-5)	2.2(-5)	1.3(-9)	2.9(-5)
	0-0 S(1)	6.2(-7)	6.4(-7)	9.7(-7)	1.4(-5)	3.2(-8)	4.4(-5)	4.7(-5)	1.3(-9)	1.1(-4)
	0-0 S(2)	3.8(-7)	1.9(-7)	4.5(-7)	3.1(-6)	9.4(-8)	1.3(-5)	1.1(-5)	4.8(-9)	2.8(-5)
	0-0 S(3)	4.7(-7)	2.5(-7)	5.3(-7)	1.4(-6)	1.1(-7)	3.4(-6)	2.1(-6)	3.0(-9)	5.6(-6)
	1-0 S(1)	6.7(-7)	3.2(-7)	7.4(-7)	2.8(-6)	1.4(-7)	5.6(-6)	4.5(-6)	6.6(-9)	9.2(-6)
	R_1	2.0	2.0	2.0	2.0	2.0	1.9	1.9	2.0	1.9
	R_2	4.2	3.9	3.2	5.2	5.1	3.7	5.2	22	3.4
	R_3	4.1	4.8	4.0	4.2	5.0	4.0	4.2	6.3	4.1
10^7	0-0 S(0)	2.2(-7)	1.1(-7)	1.7(-7)	7.9(-6)	1.9(-7)	1.1(-5)	1.9(-5)	4.5(-9)	2.5(-5)
	0-0 S(1)	1.2(-8)	7.8(-9)	9.5(-9)	1.0(-5)	7.7(-9)	3.7(-5)	7.5(-5)	1.0(-9)	2.0(-4)
	0-0 S(2)	1.1(-7)	1.2(-7)	1.1(-7)	5.4(-6)	1.2(-7)	2.5(-5)	4.6(-5)	1.5(-8)	1.4(-4)
	0-0 S(3)	4.8(-7)	3.9(-7)	4.5(-7)	4.5(-6)	2.7(-7)	1.1(-5)	1.4(-5)	2.0(-8)	9.0(-5)
	1-0 S(1)	3.7(-7)	2.9(-7)	3.4(-7)	5.8(-6)	2.4(-7)	9.5(-6)	1.3(-5)	2.9(-8)	2.5(-5)
	R_1	2.2	2.3	2.1	2.1	2.2	2.1	2.1	2.3	2.1
	R_2	1.4	1.4	1.2	2.6	2.0	2.2	3.0	6.5	2.3
	R_3	7.0	11	8.2	5.2	11	4.4	4.7	15	4.4

A: R=const, B: only LH, C=LH+ER

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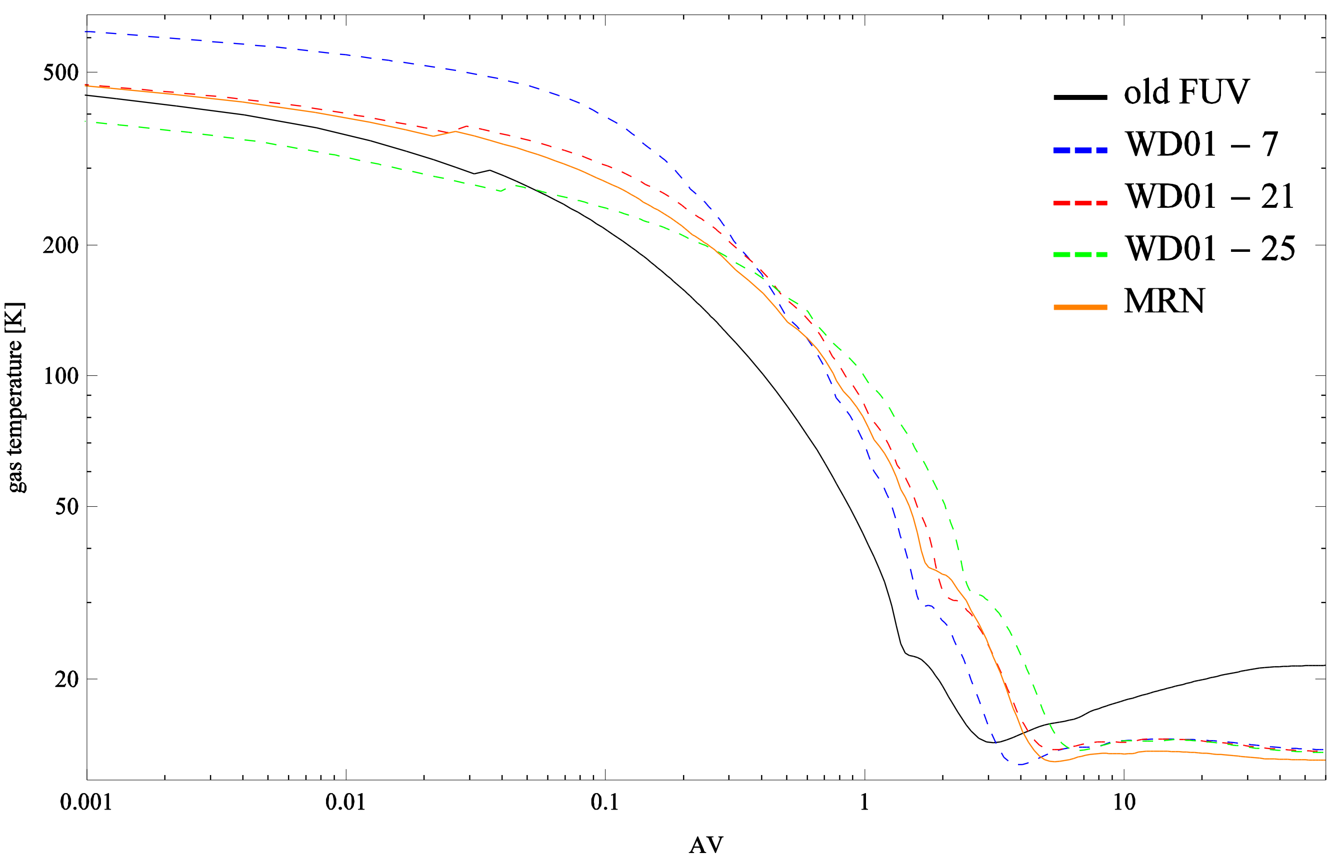
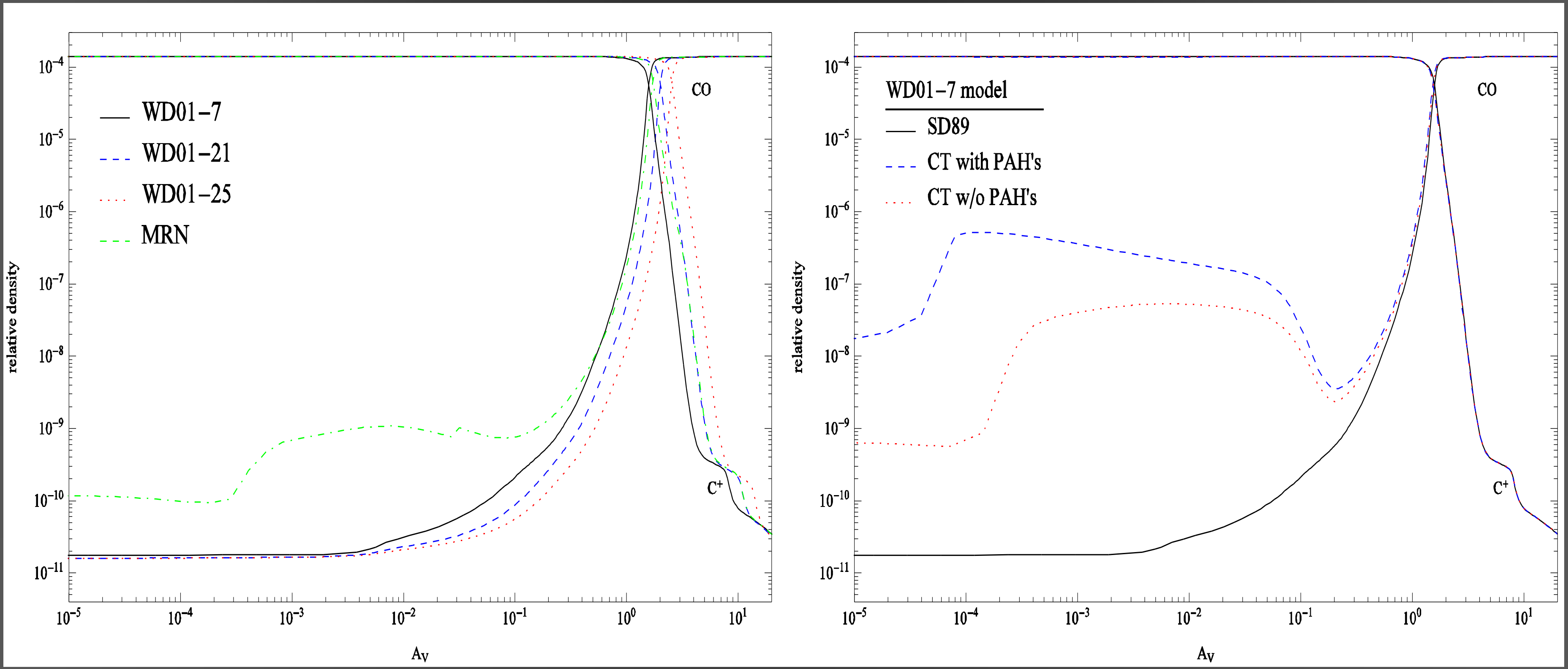
Dust influence



Dust influence

radiative transfer effect

H_2 chemistry effect



Dust influence

- 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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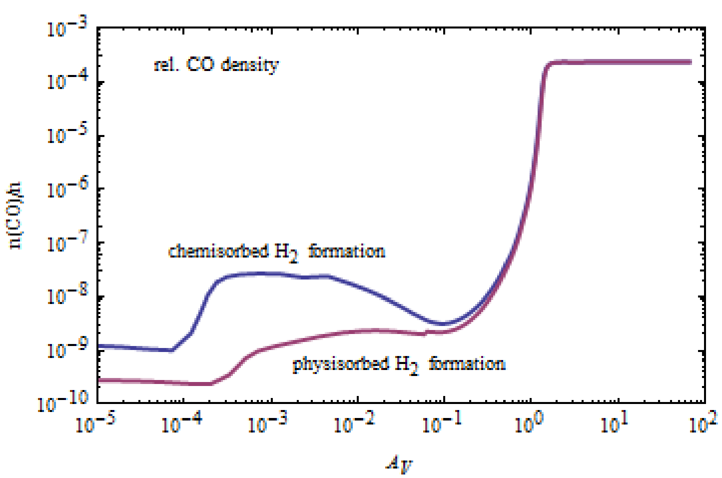
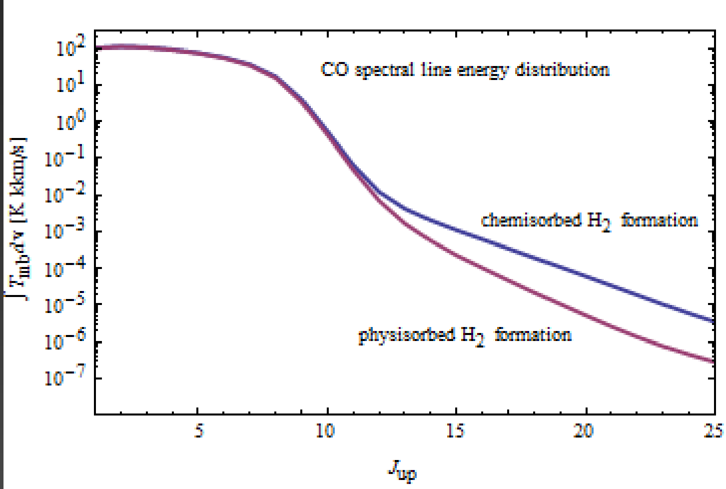
- large effect on H-H_2 transition region chemistry





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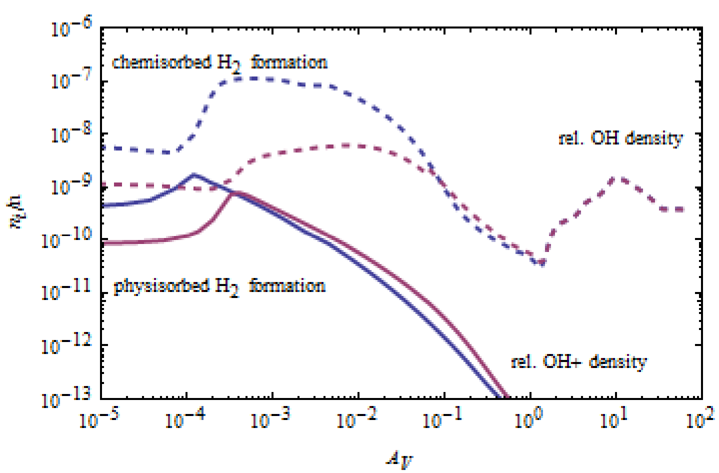

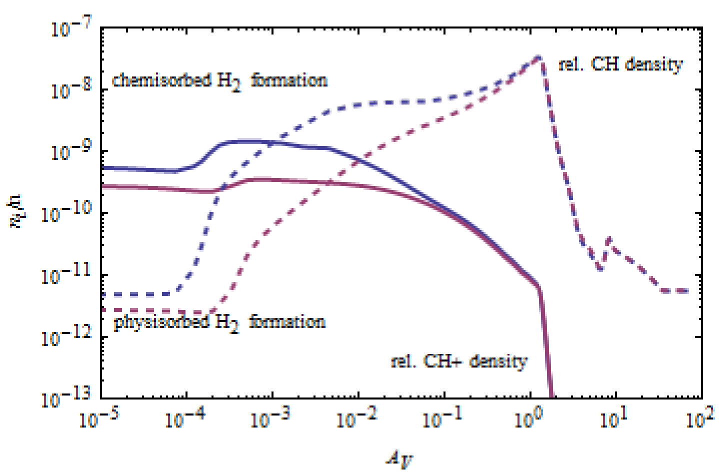

Summary

- Great need for reliable (astrochemistry) data
- Lab results need to be robust against different modeling applications
- Growing understanding of dust properties and H_2 formation process dramatically influences model results
- chemistry and physics strongly connected to each other