Chemical modeling crisis in PDR models

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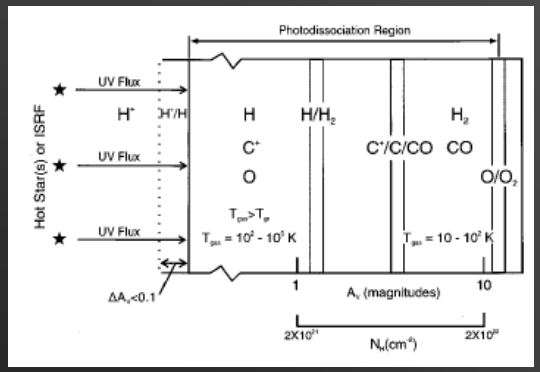
Outline

- Introduction
- Refit to problematic UMIST rates
  - negative γ
  - multiple temperature regimes
- 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

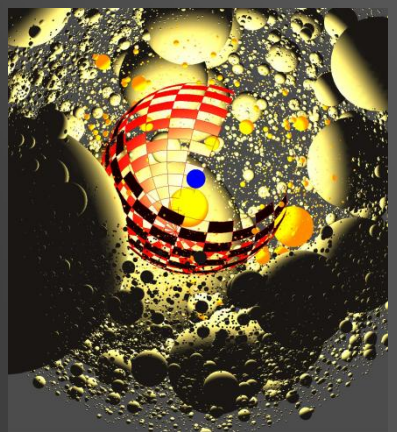
Introduction

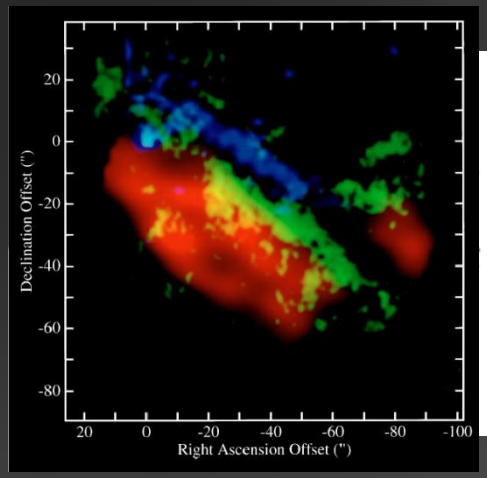
Numerical PDR models of proved to be a valuable tools in analyzing and understanding the local conditions in massive star forming regions.

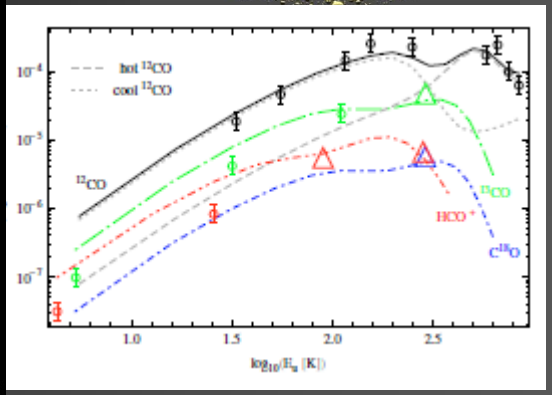
(Talk by Paola Caselli)



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







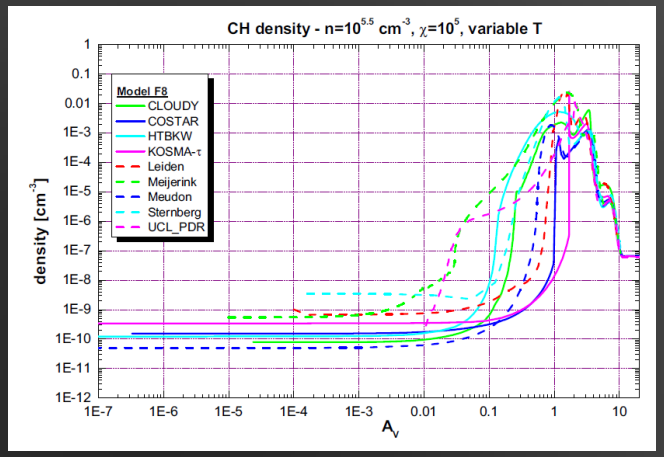
Ossenkopf et al, 2010, A&A 518, L79v

Introduction

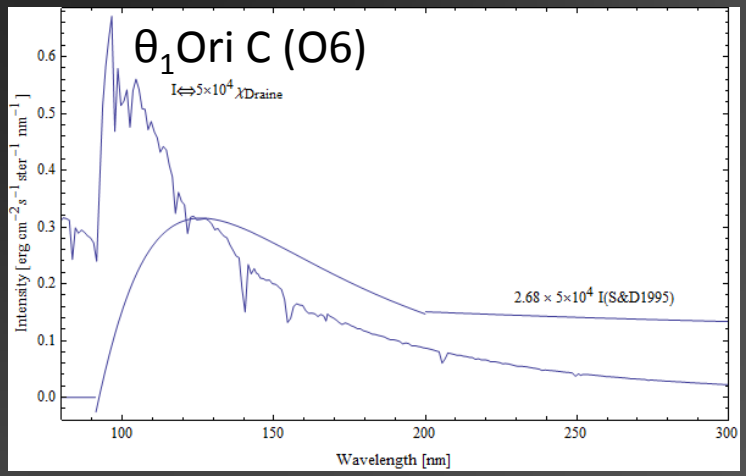
Yet, here be dragons...

- complex physics / chemistry

- complex/unknown local conditions

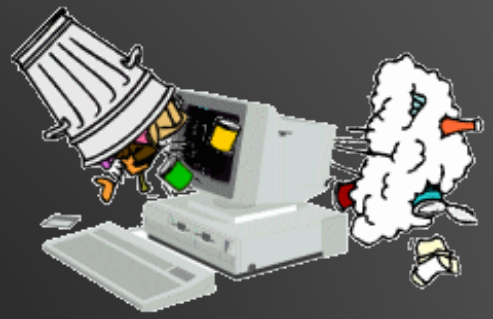


Röllig et al. 2007, A&A, 467



Introduction

and unfortunately, deficient input data



- missing experimental data
- inter/extrapolation

Refit to problematic reaction rates

Refit to problematic reaction rates

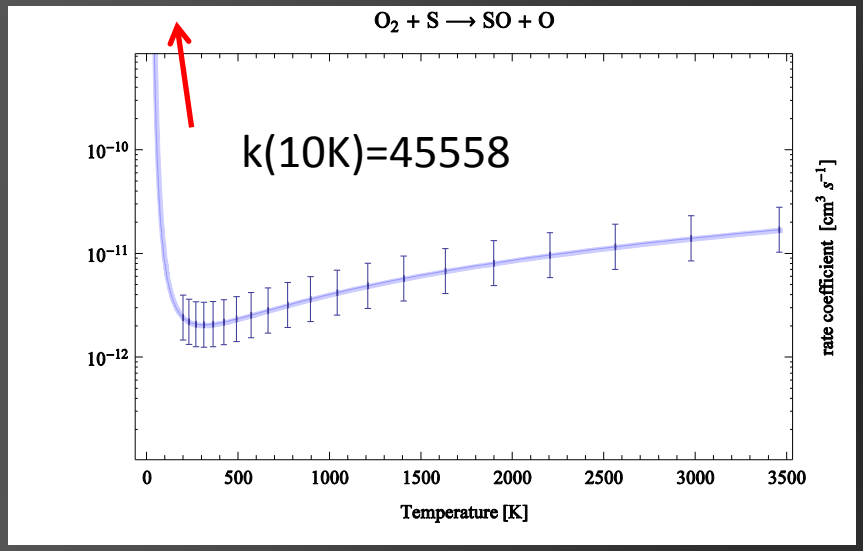
- chemical reaction rate coefficients are usually parametrized using few parameters (which are tabulated in chemical databases), e.g. α, β, γ

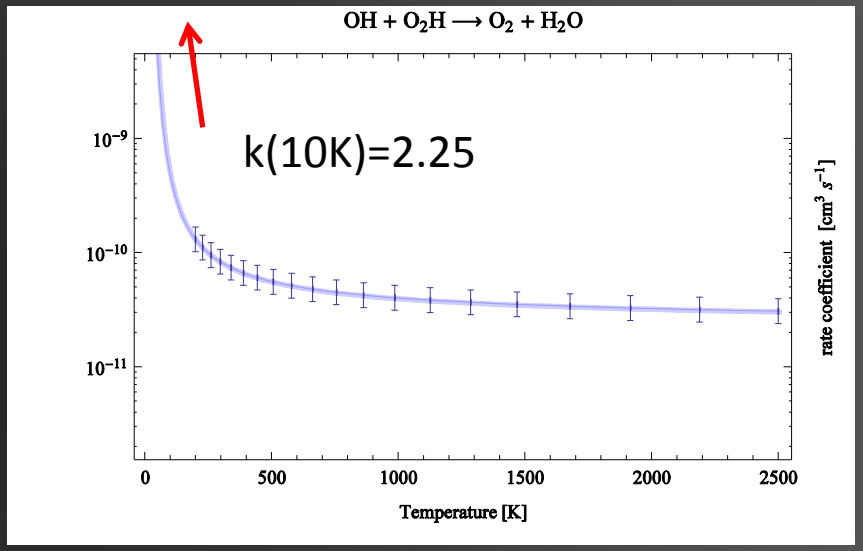
$$k = \alpha(T/300)^{\beta}\exp(-\gamma/T) \quad \mathrm{cm}^3\ \mathrm{s}^{-1}$$

1	H	CH	C	H2	2.70e-11	0.38	0.0C	300 2000BHG93
2	H	CH2	CH	H2	6.64e-11	0.00	0.0L	300 2500ANIST
3	H	NH	N	H2	1.73e-11	0.50	2400.0L	80 300C
4	H	CH3	CH2	H2	1.00e-10	0.00	7600.0L	300 2500ANIST
5	H	NH2	NH	H2	5.25e-12	0.79	2200.0L	73 300C
6	H	NH2	NH	H2	1.05e-10	0.00	4450.0M	1100 3000ANIST
7	H	CH4	CH3	H2	5.94e-13	3.00	4045.0L	300 2500ANIST
8	H	OH	O	H2	6.99e-14	2.80	1950.0L	300 2500ANIST
9	H	NH3	NH2	H2	7.80e-13	2.40	4990.0M	200 2500CNIST
10	H	H2O	OH	H2	1.59e-11	1.20	9610.0L	250 3000ANIST

- α, β, γ from best fit to experimental data within the experiments temperature range!

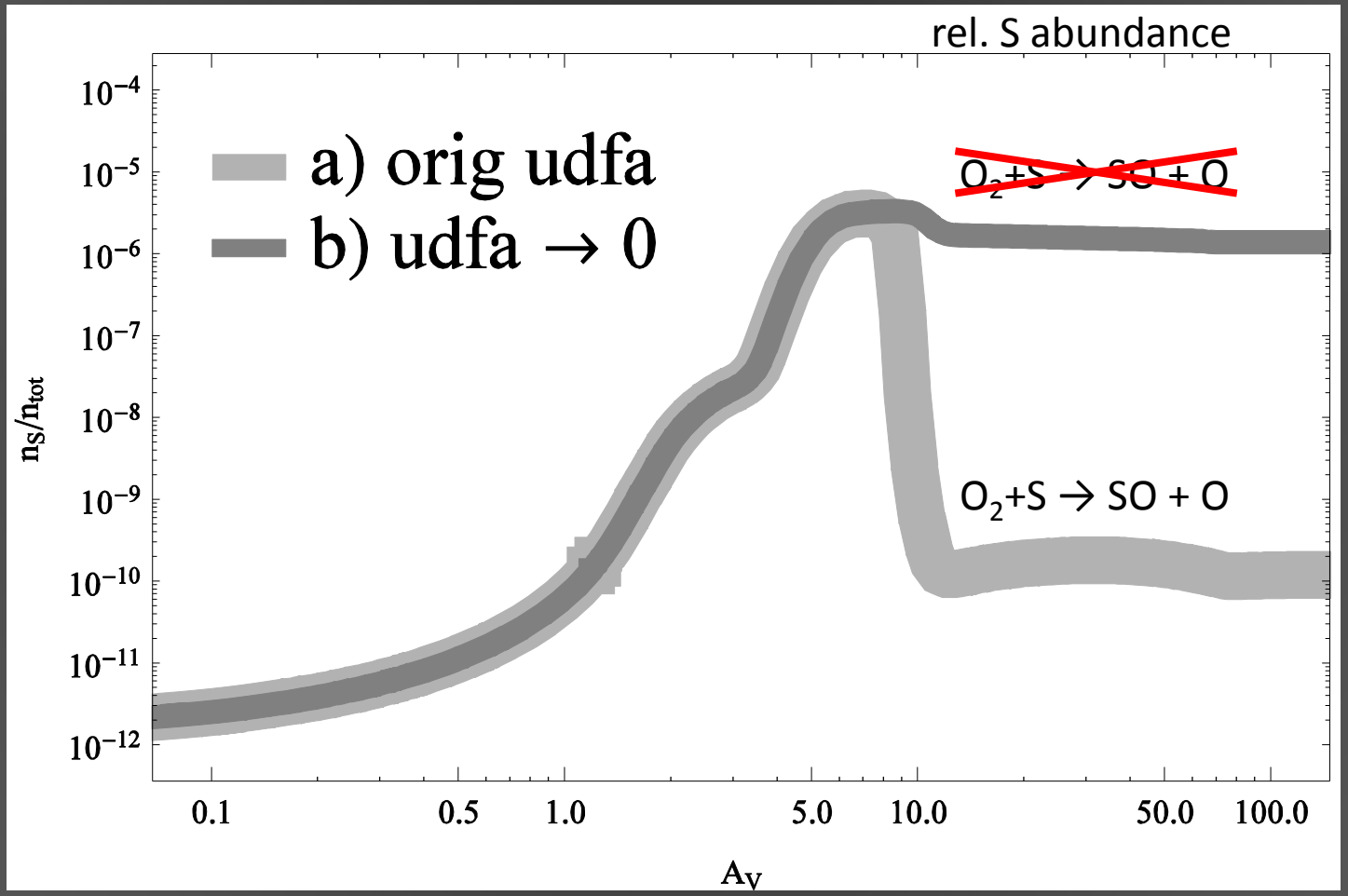
Negative γ





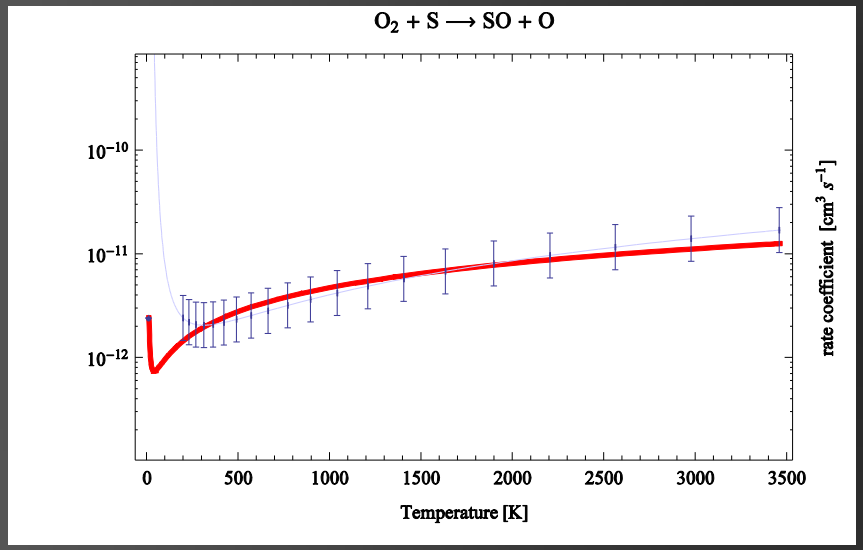
- Outside their temperature regime, the rate coefficient may become unrealistically large
- one suggested remedy: k(10K)→0

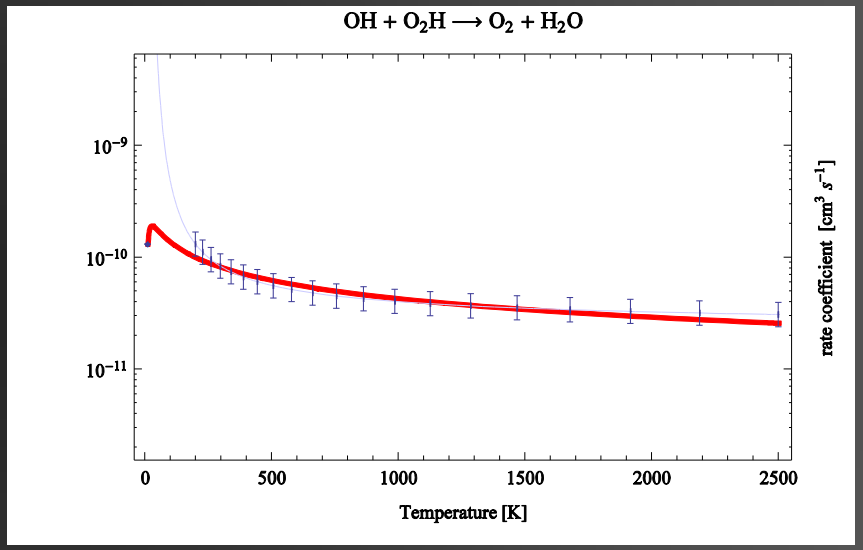
Negative γ



KOSMA-τ model result

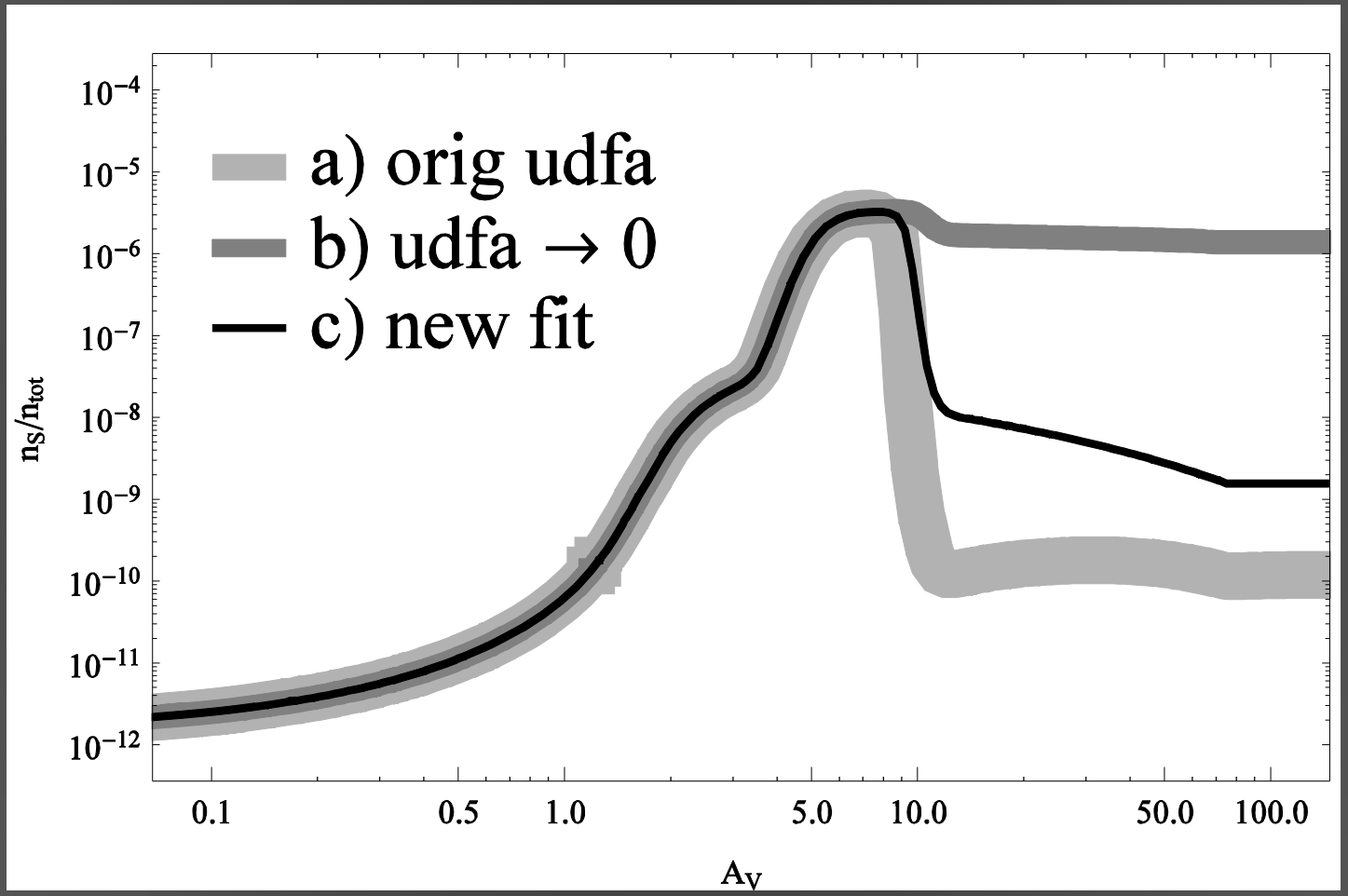
Negative γ





- forcing the fit with an artificial, low T „data point“
- stay inside the original error bars as much as possible
- choice of k(10K) is arbitrary and a possibly large error source!

Negative γ


a) orig udfa
b) udfa → 0
c) new fit
n_S/n_{tot}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
0.1
0.5
1.0
5.0
10.0
50.0
100.0
A_V

Negative γ

Educts				Products			α_{old}	β_{old}	γ_{old}	T_{min}	T_{max}	α_{new}	β_{new}	γ_{new}	[Error]
C	+	O_2	⟶	CO	+	O	2.48(–12)	1.54	–613	295	8000	9.94(–12)	1.05	–42.48	–0.42, 0.26
N	+	OH	⟶	NO	+	H	4.06(–11)	0.05	–78	103	2500	5.73(–11)	–0.15	1.34	–0.19, 0.09
NH	+	NH	⟶	NH_2	+	N	1.03(–14)	3.07	–1123	300	3000	1.81(–13)	1.80	–70.03	–0.47, 0.36
NH	+	NO_2	⟶	N_2O	+	OH	1.44(–13)	0	–1140	200	300	1.06(–11)	–5.36	168	–0.07, 0.04
CH_3	+	NH_2	⟶	CH_2	+	NH_3	4.76(–17)	5.77	–151	300	2000	4.07(–17)	5.85	–205	–0.03, 0.03
O	+	NH_2	⟶	HNO	+	H	4.56(–11)	0	–10	200	3000	4.72(–11)	–0.02	0.38	–0.01, 0.01
O	+	OH	⟶	O_2	+	H	1.77(–11)	0	–178	158	5000	3.35(–11)	–0.28	4.30	–0.29, 0.15
O	+	O_2H	⟶	O_2	+	OH	3.17(–11)	0	–174	200	2500	5.76(–11)	–0.30	7.48	–0.17, 0.09
O	+	HS	⟶	SO	+	H	8.25(–11)	0.17	–254	298	2000	1.74(–10)	–0.20	5.70	–0.12, 0.06
O	+	NO_2	⟶	O_2	+	NO	6.5(–12)	0	–120	200	2500	9.82(–12)	–0.21	5.16	–0.12, 0.06
NH_2	+	OH	⟶	H_2O	+	NH	7.78(–13)	1.50	–230	250	3000	1.35(–12)	1.25	–43.45	–0.14, 0.07
OH	+	C_2H_2	⟶	CO	+	CH_3	6.51(–18)	4.00	–1006	500	2500	4.75(–17)	3.16	–128	–0.18, 0.10
OH	+	H_2CO	⟶	HCO	+	H_2O	2.22(–12)	1.42	–416	200	3000	7.76(–12)	0.82	–30.62	–0.35, 0.21
OH	+	HNO	⟶	NO	+	H_2O	4.44(–12)	1.37	–169	298	4000	6.17(–12)	1.23	–44.29	–0.09, 0.04
OH	+	O_2H	⟶	O_2	+	H_2O	3.66(–11)	–0.13	–244	200	2500	8.58(–11)	–0.56	14.76	–0.23, 0.13
NH_3	+	CN	⟶	HCN	+	NH_2	3.41(–11)	–0.90	–9.90	25	761	3.73(–11)	–1.08	10.00	–0.23, 0.09
C_2H	+	C_2H_2	⟶	H_2CCCC	+	H	1.31(–10)	0	–25	143	3400	1.44(–10)	–0.05	0.80	–0.05, 0.02
CN	+	CH_3CH_3	⟶	C_2H_5	+	HCN	4.8(–12)	2.08	–484	185	1140	2.34(–11)	1.02	–34.95	–0.28, 0.17
CN	+	O_2	⟶	NO	+	CO	5.01(–12)	–0.46	–8	13	1565	5.12(–12)	–0.49	–5.16	–0.11, 0.02
CN	+	O_2	⟶	OCN	+	O	1.86(–11)	–0.13	–40	13	4526	2.02(–11)	–0.19	–31.91	–0.30, 0.07
CN	+	NO_2	⟶	NO	+	OCN	3.93(–11)	0	–199	297	2500	7.02(–11)	–0.27	8.27	–0.11, 0.06
C_2H_3	+	O_2	⟶	H_2CO	+	HCO	4.62(–12)	0	–171	200	362	8.87(–12)	–0.73	22.67	–0.02, 0.01
C_2H_3	+	O_2	⟶	O_2H	+	C_2H_2	2.16(–14)	1.61	–193	300	3500	3.15(–14)	1.45	–51.97	–0.09, 0.04
HCO	+	O_2	⟶	O_2H	+	CO	1.58(–12)	1.24	–353	200	2500	4.64(–12)	0.70	–25.61	–0.29, 0.17
O_2	+	S	⟶	SO	+	O	4.74(–13)	1.41	–439	200	3460	1.76(–12)	0.81	–30.75	–0.38,0.24

Röllig 2011, A&A 530, 9

Multiple temperature regimes

- For some reactions rate coefficients have been determined for multiple temperature regimes
- Each temp. range results in one entry in a chemical database

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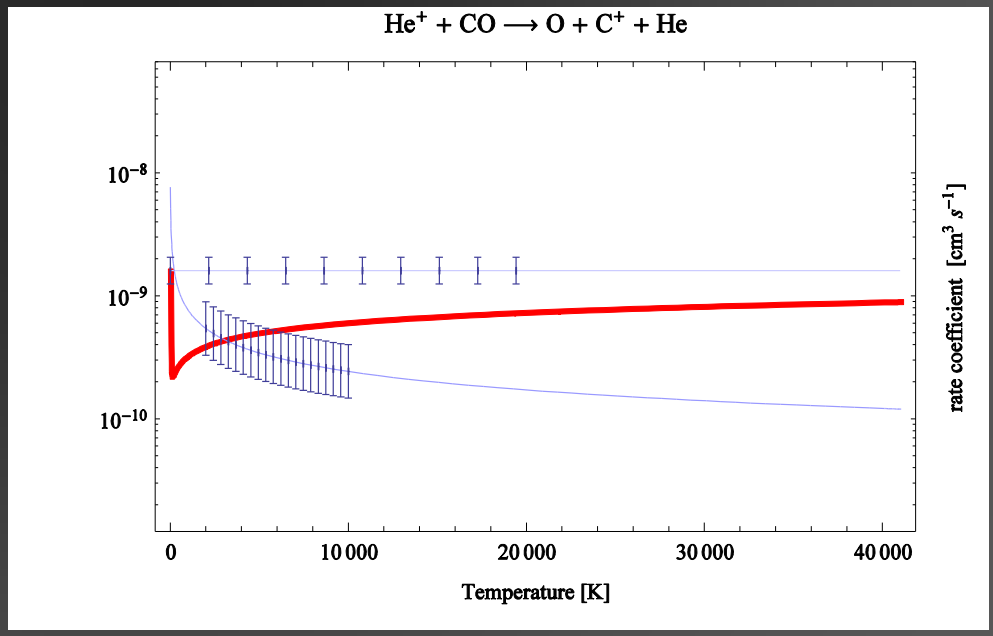

Multiple temperature regimes

- For some reactions rate coefficients have been determined for multiple temperature regimes
- Each temp. range results in one entry in a chemical database
- Moving from one temp. regime to another numerically problematic

```
C+      e-      C       PHOTON      4.67e-12   -0.60       0.0  C  10          7950        BNP97
C+      e-      C       PHOTON      1.23e-17    2.49  -21845.6  C  7950        21140       BNP97
C+      e-      C       PHOTON      9.62e-08   -1.37  115786.2C    21140       41000       BNP97
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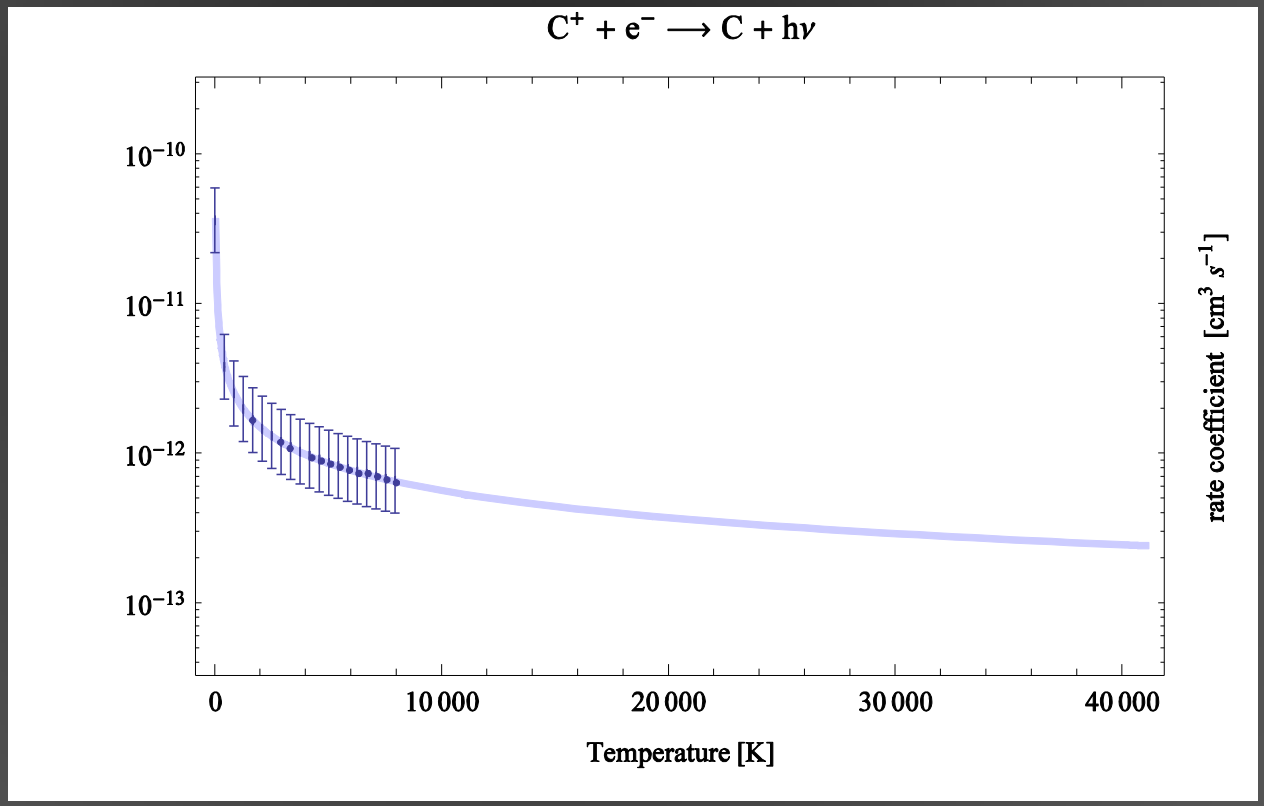

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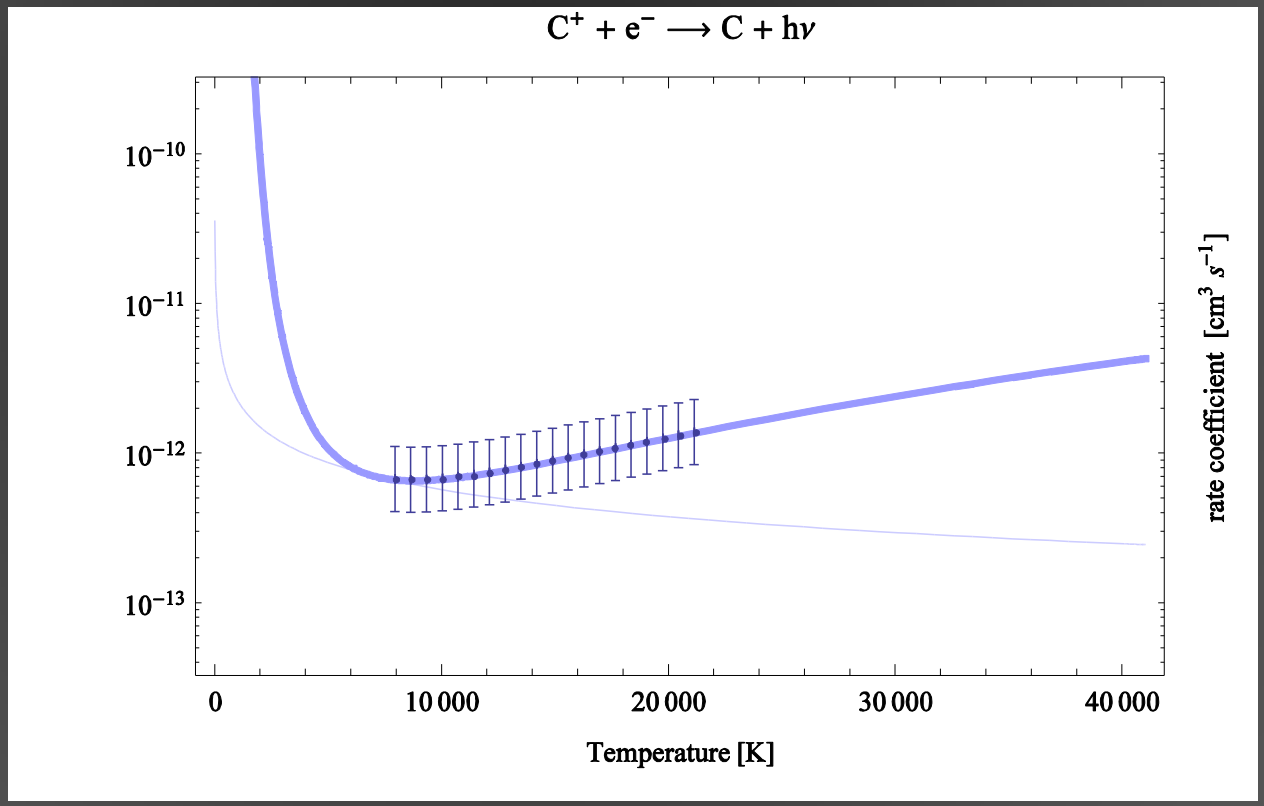

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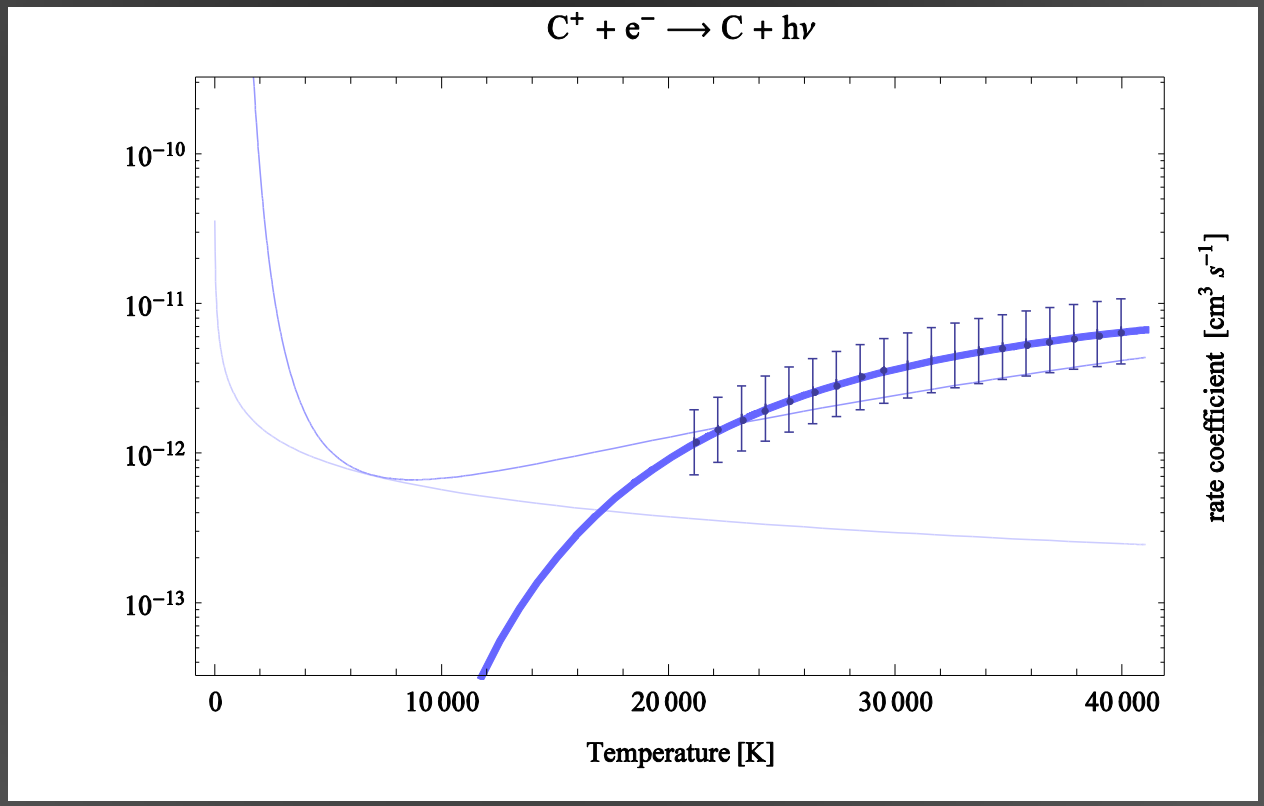

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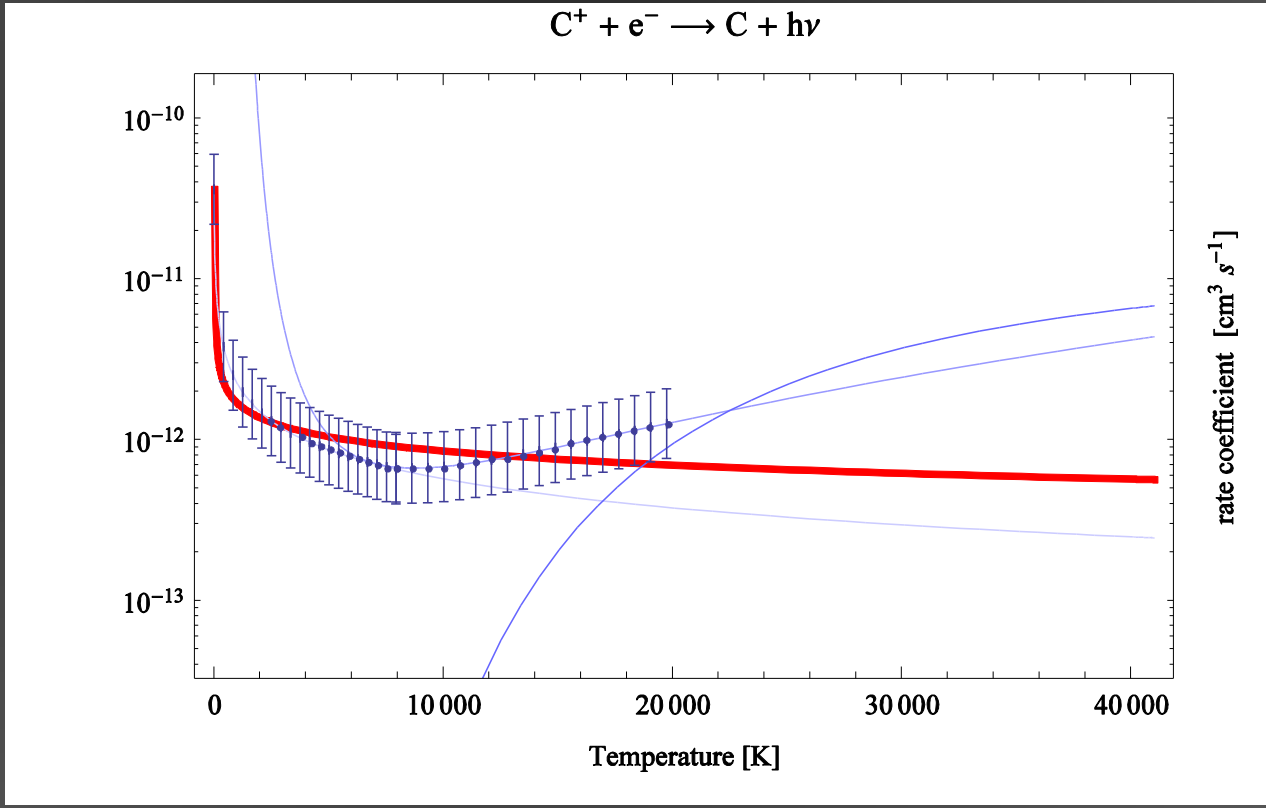

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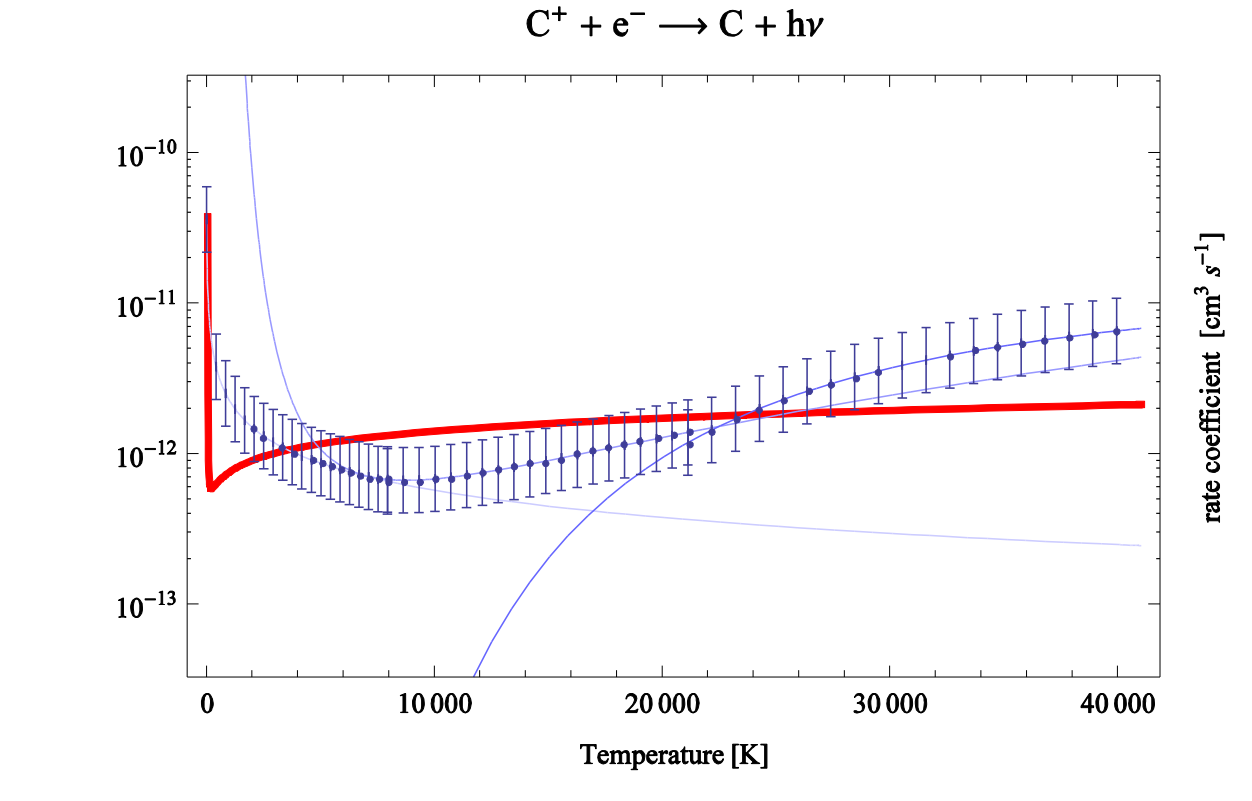
If your application requires temperatures up to 40000 K, the error grows sigificantly



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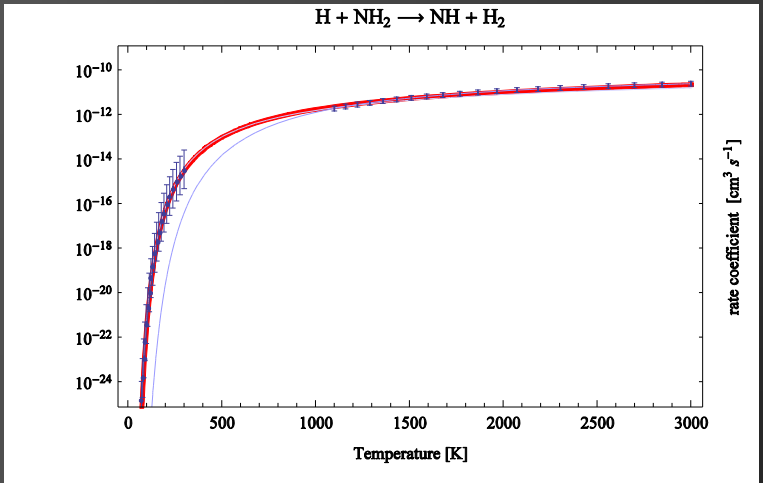
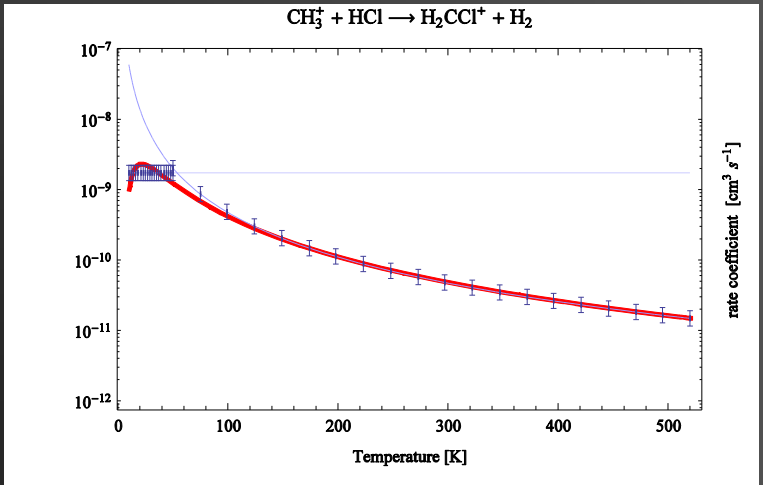
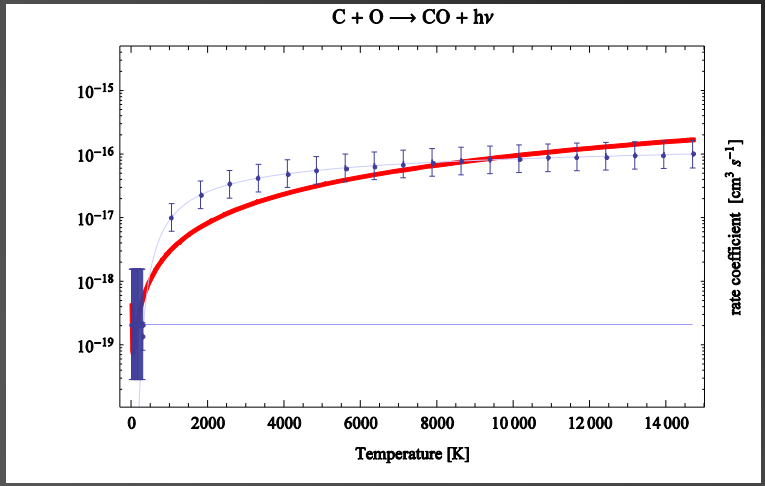
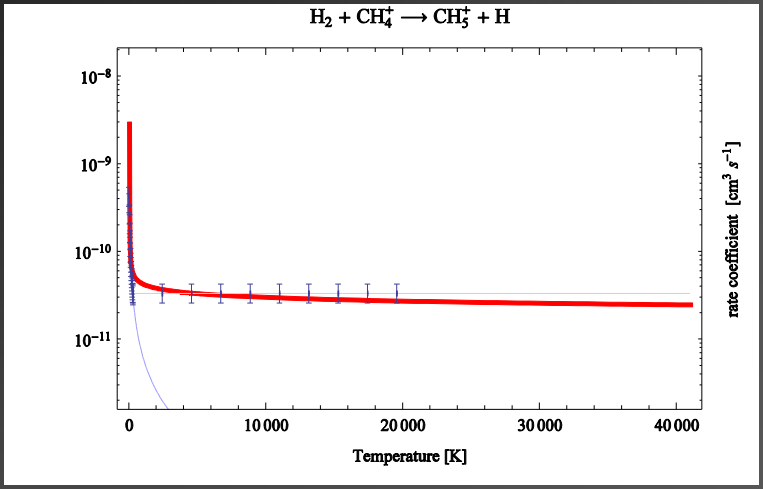








H_2 formation on grain surfaces

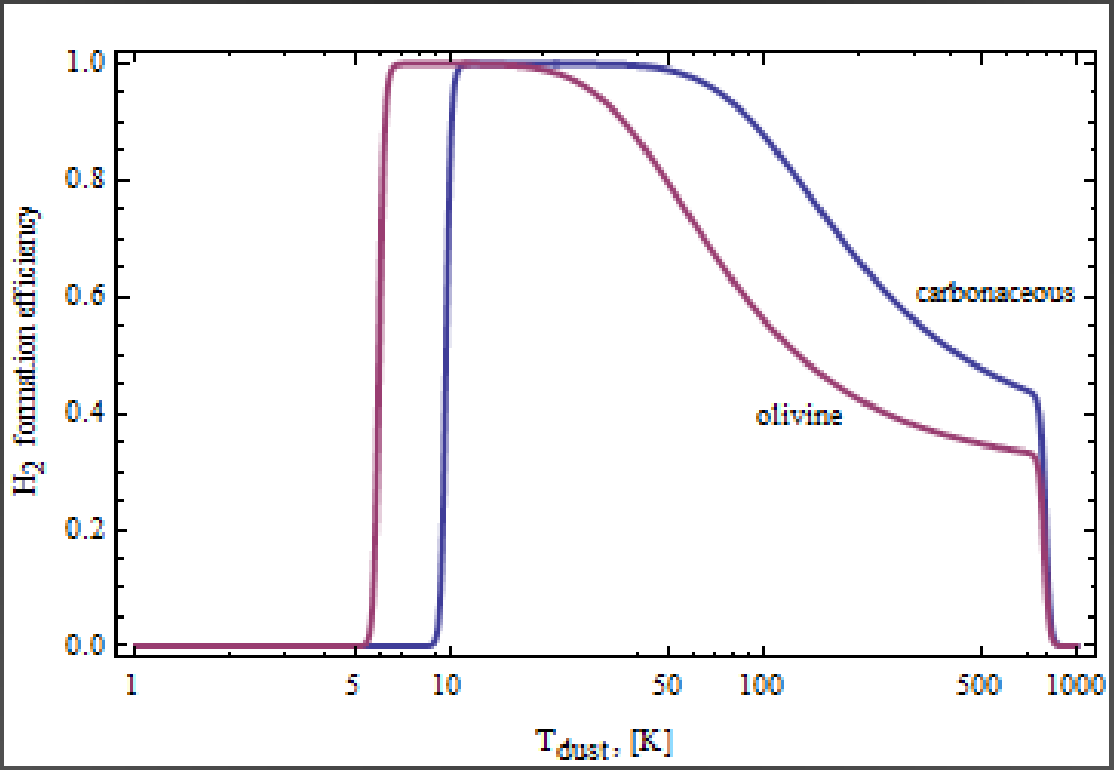
H_2 formation on grain surfaces

- 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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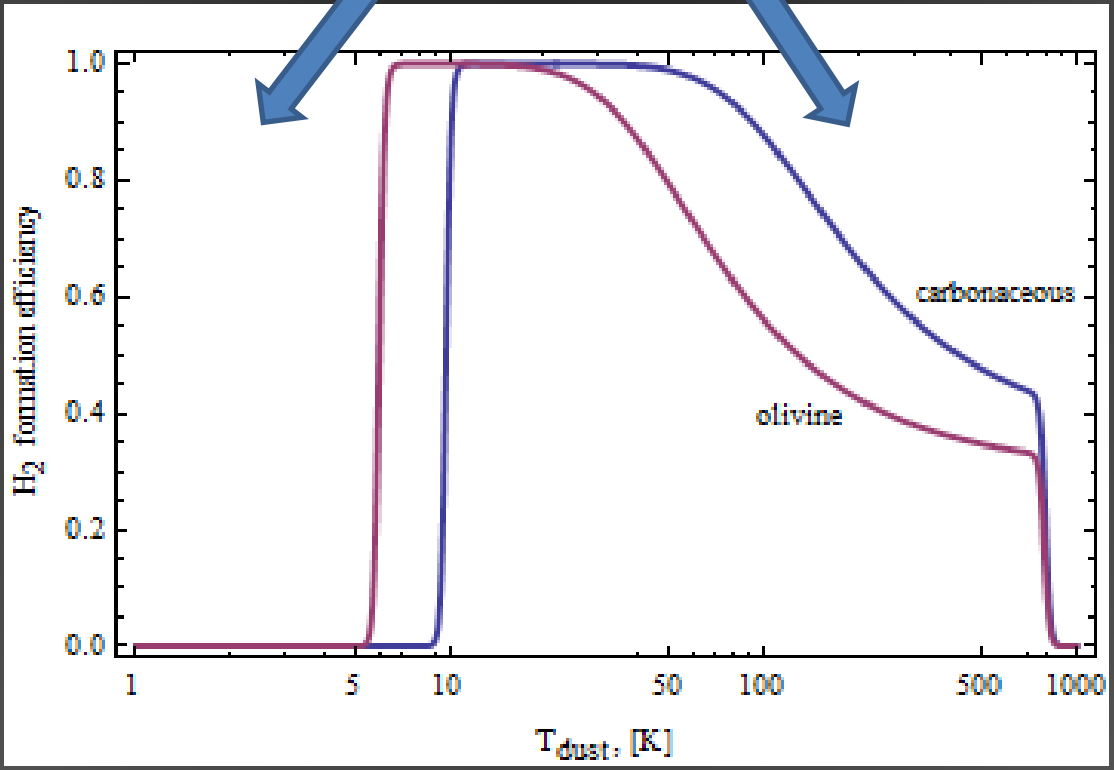

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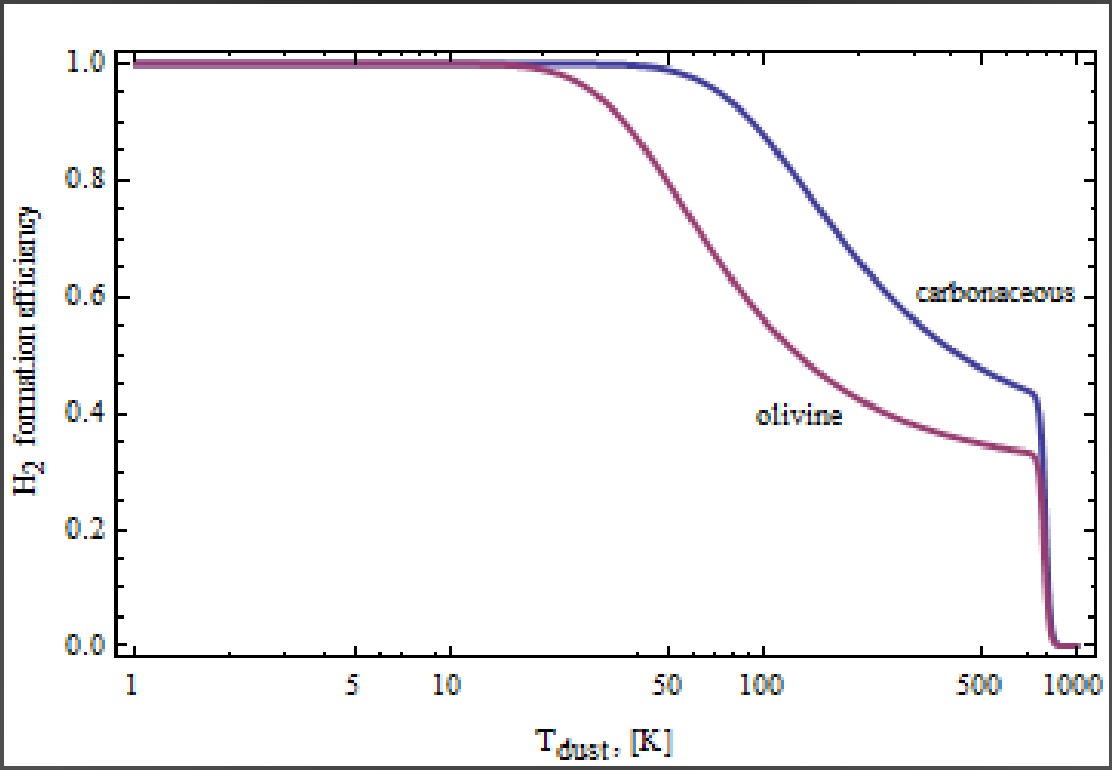

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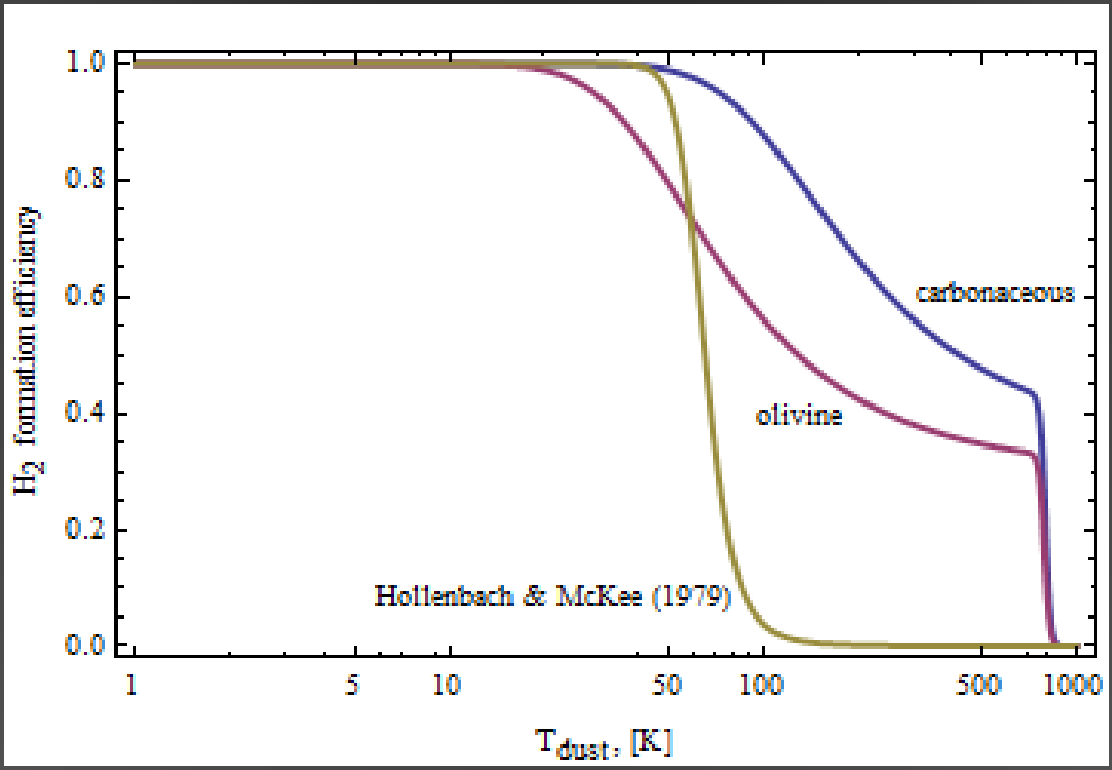
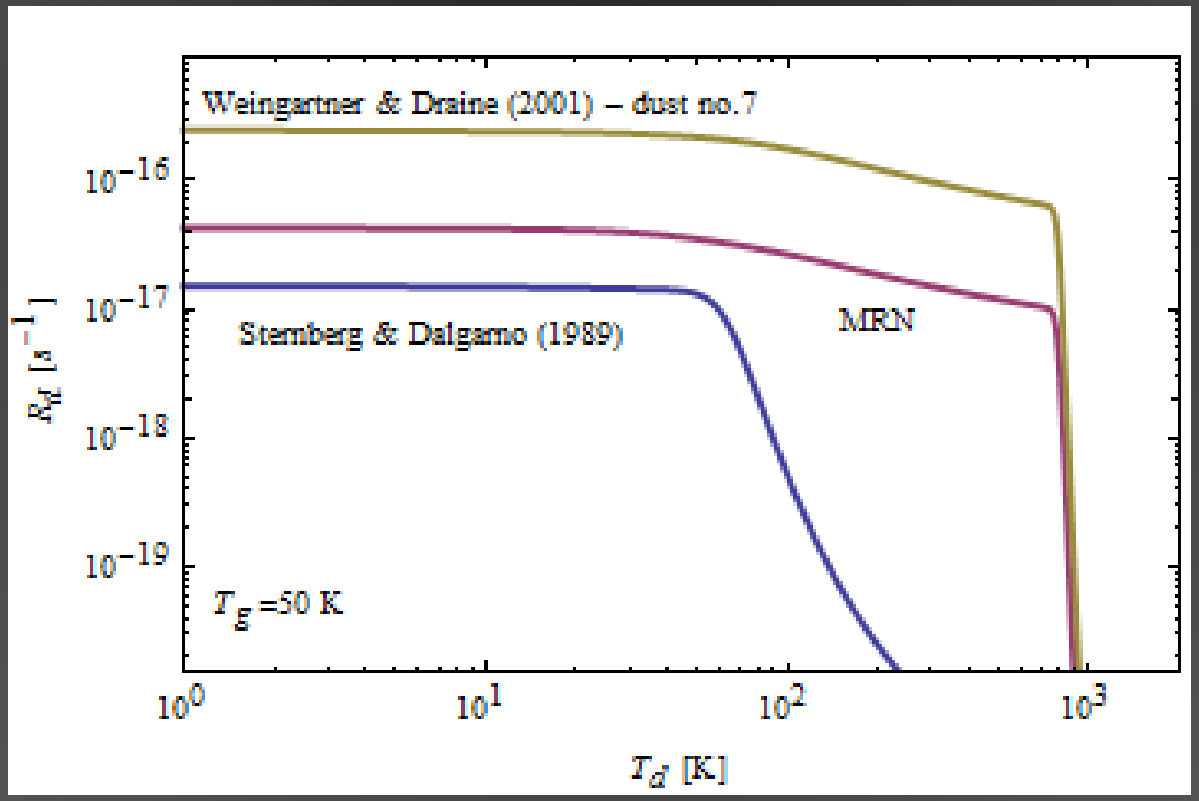


H_2 formation rate

total formation rate depends on total dust surface

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

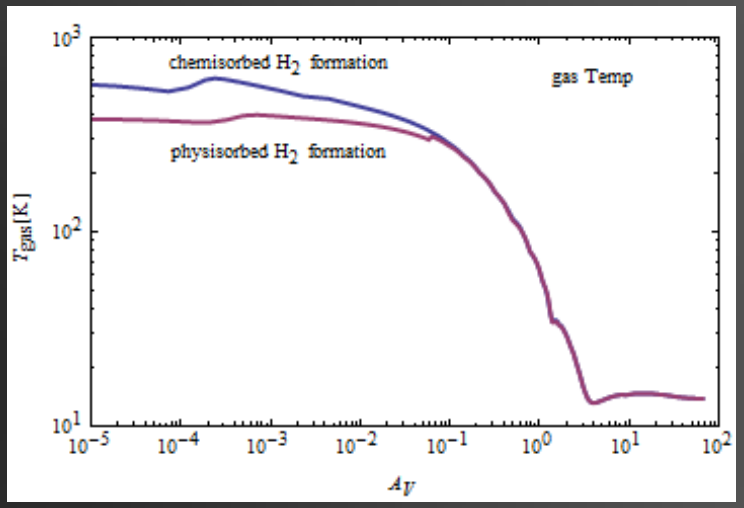


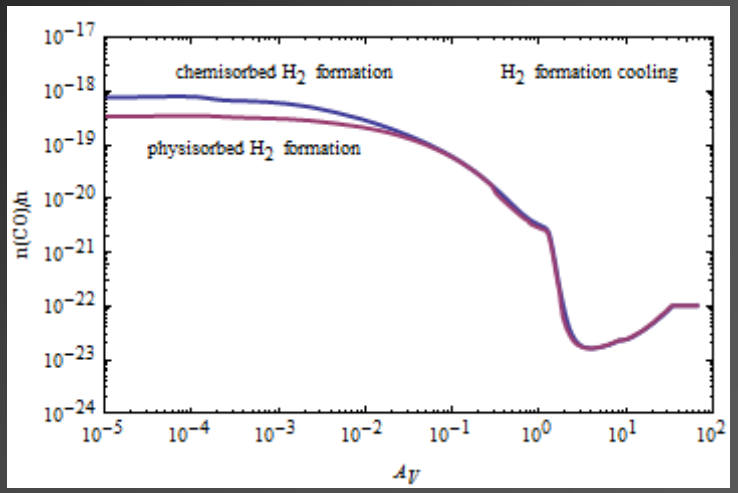
H_2 heating/cooling

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

  $H_2 + H \rightarrow H + H + H - 4.5eV$

  $H_2 + H_2 \rightarrow H_2 + H + H - 4.5eV$





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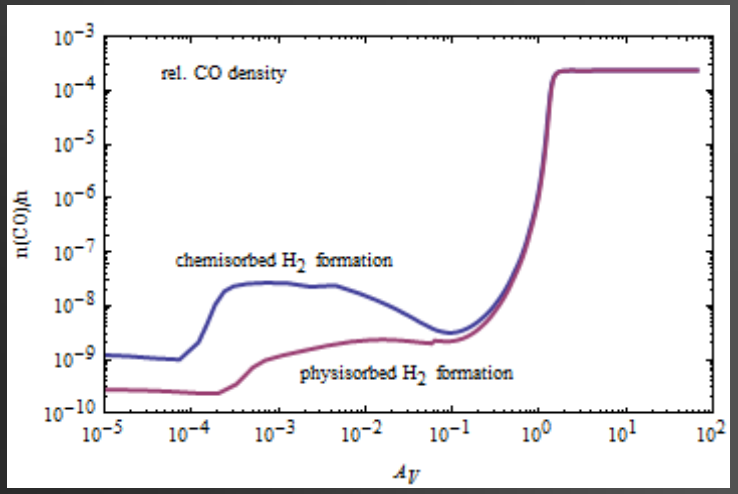
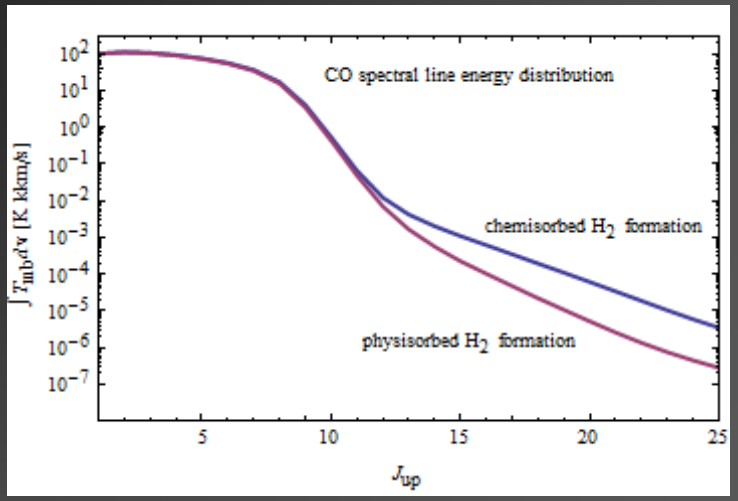
- H_2 binding energy 4.5 eV
  → H_2 formation heating
- kinetic H_2 dissociation cooling
  (Lepp & Shull, 1983, ApJ 270, 578)

  $H_2 + H \rightarrow H + H + H - 4.5eV$

  $H_2 + H_2 \rightarrow H_2 + H + H - 4.5eV$

- large effect on H-H_2 transition region chemistry





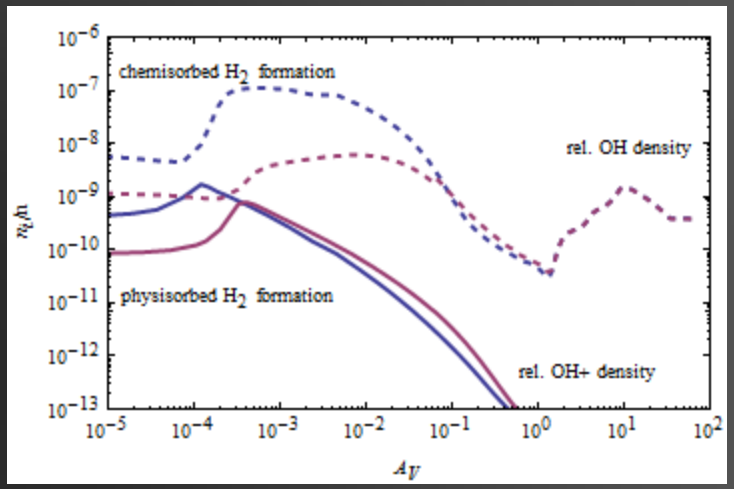
H_2 heating/cooling

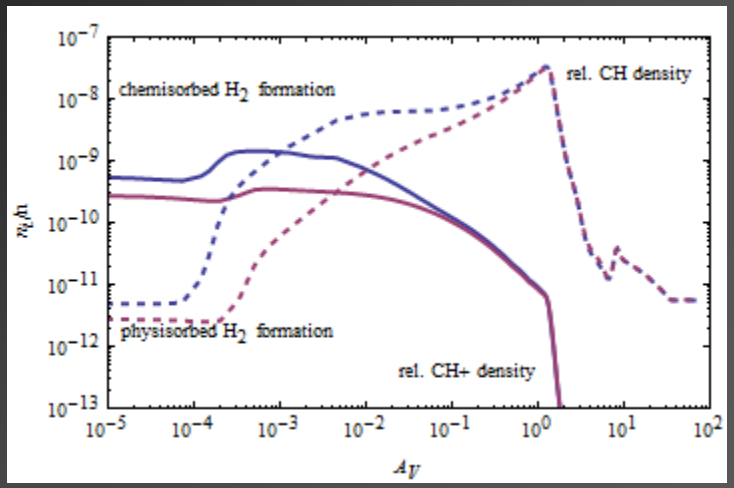
- H_2 binding energy 4.5 eV
  → H_2 formation heating
- kinetic H_2 dissociation cooling
  (Lepp & Shull, 1983, ApJ 270, 578)

  $H_2 + H \rightarrow H + H + H$

  $H_2 + H_2 \rightarrow H_2 + H + H$

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



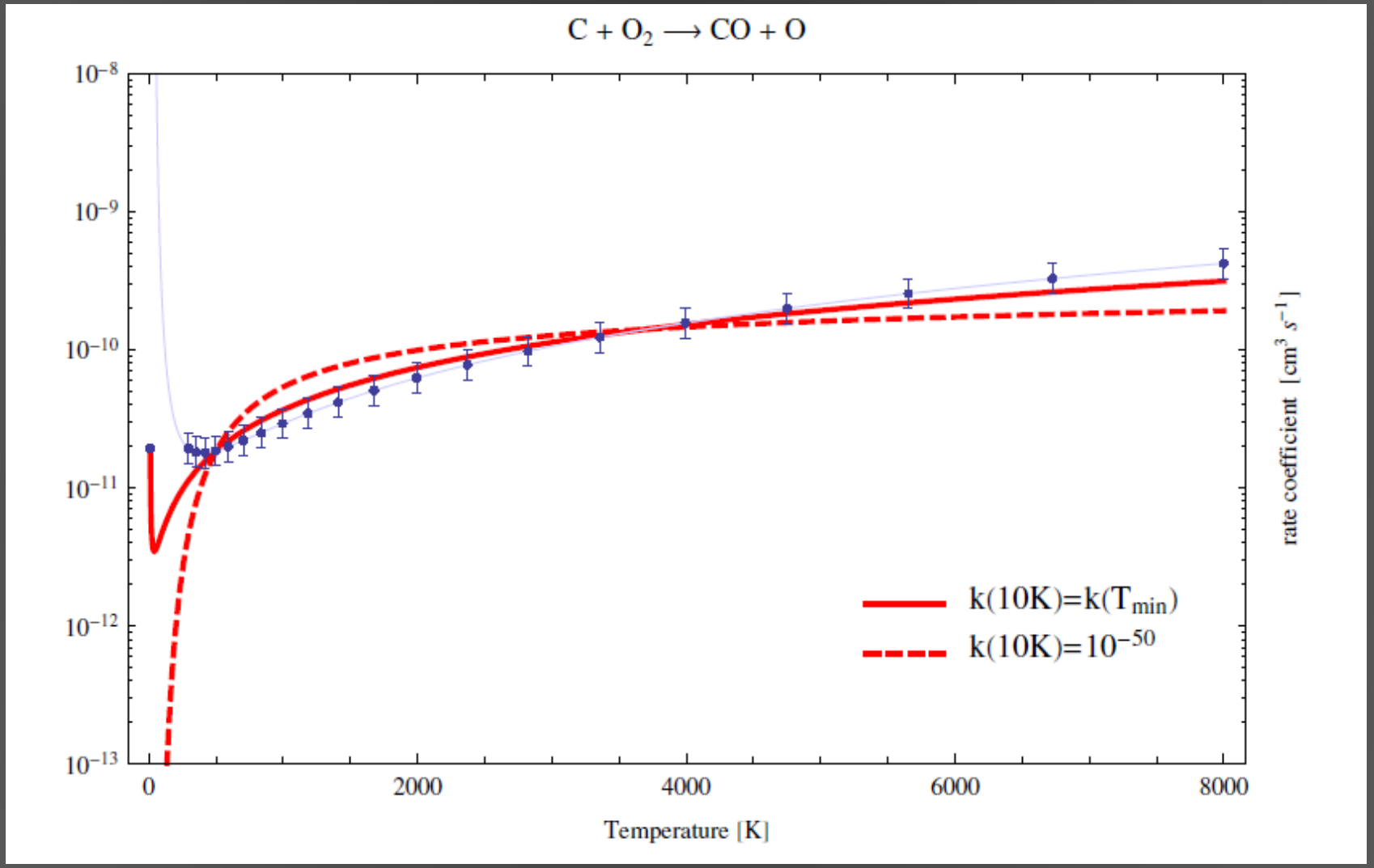


Summary

- 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

Thank you!

Negative γ


C + O2 ⟶ CO + O
10−8
10−9
10−10
10−11
10−12
10−13
0
2000
4000
6000
8000
Temperature [K]
rate coefficient [cm3 s−1]
k(10K)=k(Tmin)
k(10K)=10−50