Photodissociation under varying dust absorption conditions

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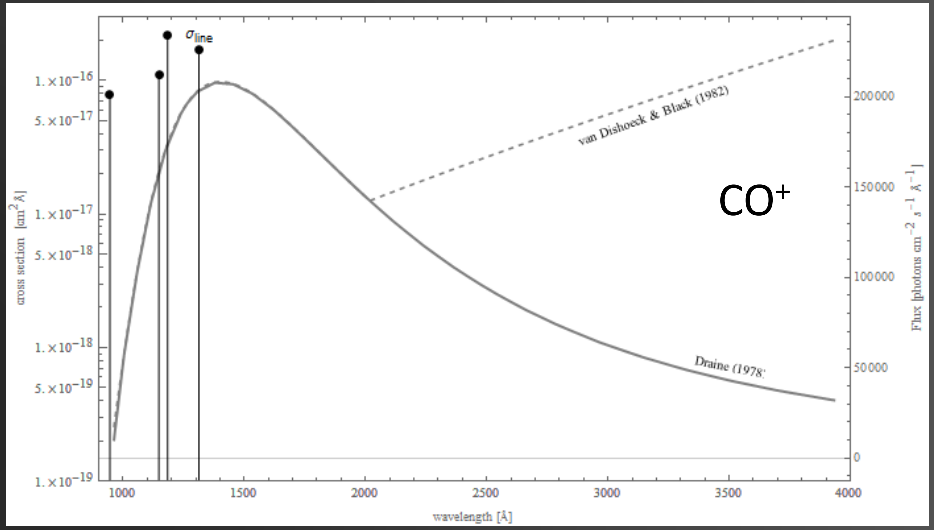
Motivation

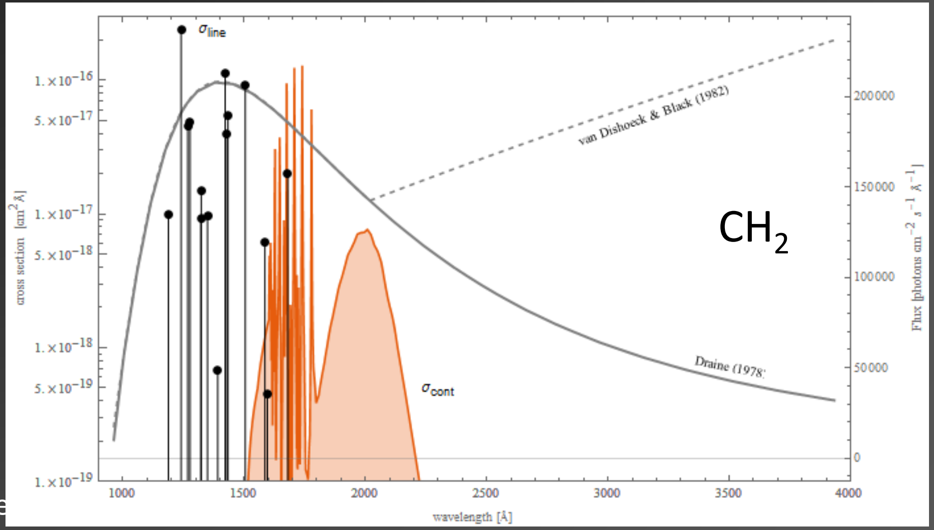
- Photodissociation and –ionization (PD&I) are important processes under various astronomical conditions (HII regions, PDRs, XDRs, accretion disks, …).
- The detailed physical conditions governing the PD&I are subject to significant local variations:
  - FUV/UV illumination
  - dust properties
- Numerical models computing PD&I have to account for these variations.

Introduction

- Photodissociation of species j:

$$\Gamma_j(\vec{r}) = 4\pi \int_{\nu_{min}}^{\nu_{max}} J_j(\vec{r},\nu)\, \sigma_j(\nu)\, d\nu$$





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- UMIST2012: 335 photodiss. reactions (including ^{13}C and ^{18}O isotopologues)

5882	13CH4+	PHOTON	13CH3+	H		5.33E-11	0.00	2.7	10	41000
5883	CH4	PHOTON	CH2	H2		9.80E-10	0.00	2.6	10	41000
5883	13CH4	PHOTON	13CH2	H2		9.80E-10	0.00	2.6	10	41000
5884	CH4	PHOTON	CH3	H		2.20E-10	0.00	2.6	10	41000
5884	13CH4	PHOTON	13CH3	H		2.20E-10	0.00	2.6	10	41000
5885	CH4	PHOTON	CH4+	ELECTR		6.80E-12	0.00	3.9	10	41000
5885	13CH4	PHOTON	13CH4+	ELECTR		6.80E-12	0.00	3.9	10	41000
5886	CH4	PHOTON	CH	H2	H	2.20E-10	0.00	2.6	10	41000
5886	13CH4	PHOTON	13CH	H2	H	2.20E-10	0.00	2.6	10	41000
5887	CH	PHOTON	C	H		9.20E-10	0.00	1.7	10	41000
5887	13CH	PHOTON	13C	H		9.20E-10	0.00	1.7	10	41000
5888	CH	PHOTON	CH+	ELECTR		7.60E-10	0.00	3.3	10	41000
5888	13CH	PHOTON	13CH+	ELECTR		7.60E-10	0.00	3.3	10	41000
5889	CN-	PHOTON	CN	ELECTR		2.22E-09	0.00	2.0	10	41000
5890	CN	PHOTON	N	C		2.90E-10	0.00	3.5	10	41000
5890	13CN	PHOTON	N	13C		2.90E-10	0.00	3.5	10	41000
5891	CNO	PHOTON	CN	O		1.00E-11	0.00	2.0	10	41000
5891	CN18O	PHOTON	CN	18O		1.00E-11	0.00	2.0	10	41000
5891	13CNO	PHOTON	13CN	O		1.00E-11	0.00	2.0	10	41000
5891	13CN18O	PHOTON	13CN	18O		1.00E-11	0.00	2.0	10	41000
5892	CO+	PHOTON	C+	O		1.00E-10	0.00	2.5	10	41000
5892	C18O+	PHOTON	C+	18O		1.00E-10	0.00	2.5	10	41000
5892	13CO+	PHOTON	13C+	O		1.00E-10	0.00	2.5	10	41000
5892	13C18O+	PHOTON	13C+	18O		1.00E-10	0.00	2.5	10	41000
5893	CO2	PHOTON	CO	O		8.90E-10	0.00	3.0	10	41000
5893	CO18O	PHOTON	CO	18O		4.45E-10	0.00	3.0	10	41000
5893	CO18O	PHOTON	C18O	O		4.45E-10	0.00	3.0	10	41000
5893	13CO2	PHOTON	13CO	O		8.90E-10	0.00	3.0	10	41000
5893	13CO18O	PHOTON	13CO	18O		4.45E-10	0.00	3.0	10	41000
5893	13CO18O	PHOTON	13C18O	O		4.45E-10	0.00	3.0	10	41000
5894	CO	PHOTON	O	C		2.00E-10	0.00	3.5	10	41000
5894	C18O	PHOTON	18O	C		2.00E-10	0.00	3.5	10	41000
5894	13CO	PHOTON	O	13C		2.00E-10	0.00	3.5	10	41000
5894	13C18O	PHOTON	18O	13C		2.00E-10	0.00	3.5	10	41000
5895	CP	PHOTON	C	P		1.00E-09	0.00	2.8	10	41000

snippet from the UMIST table

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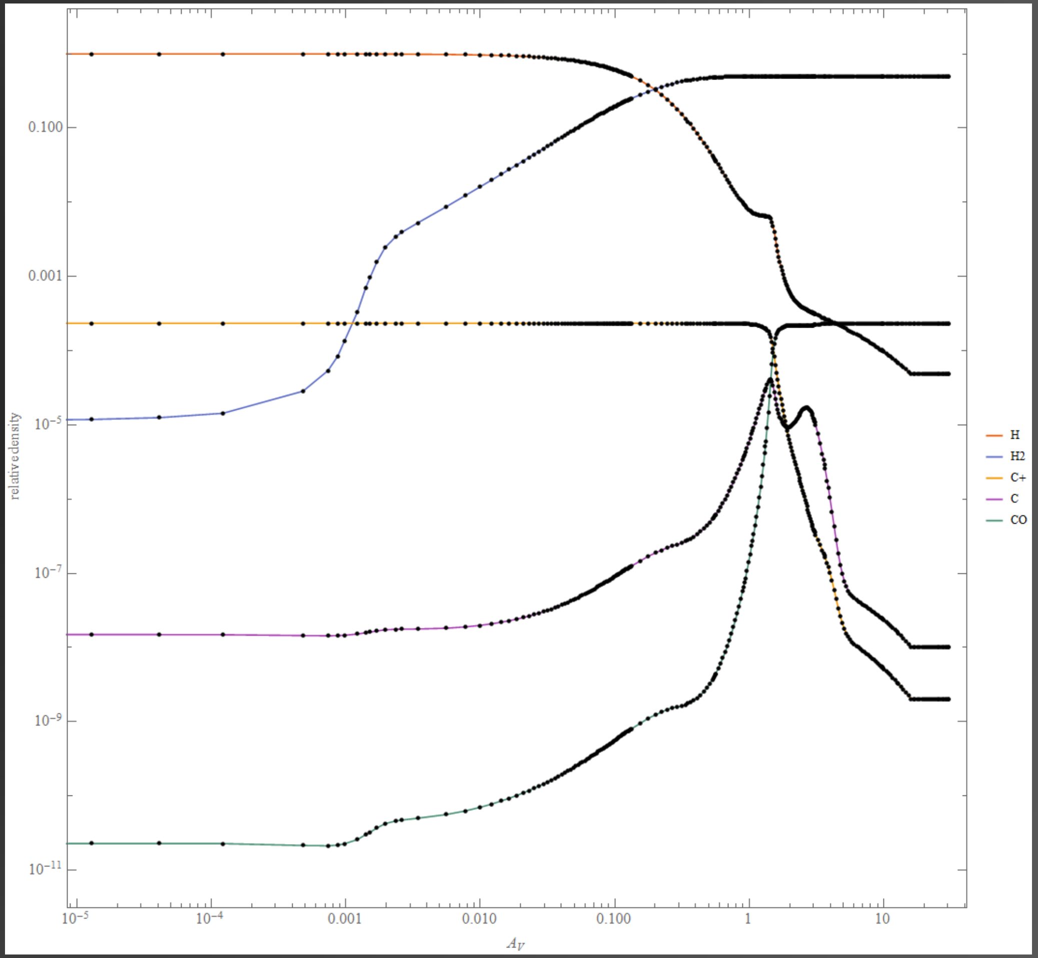

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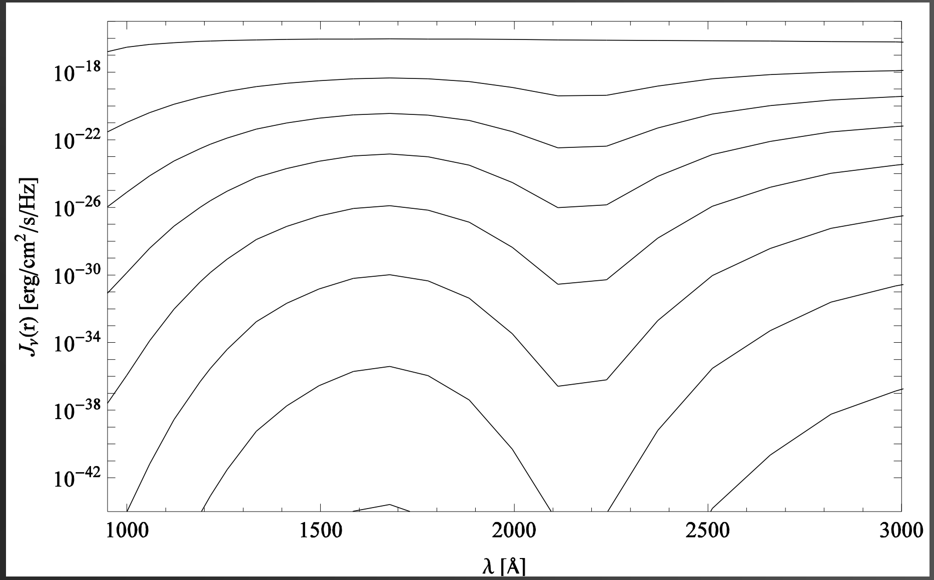

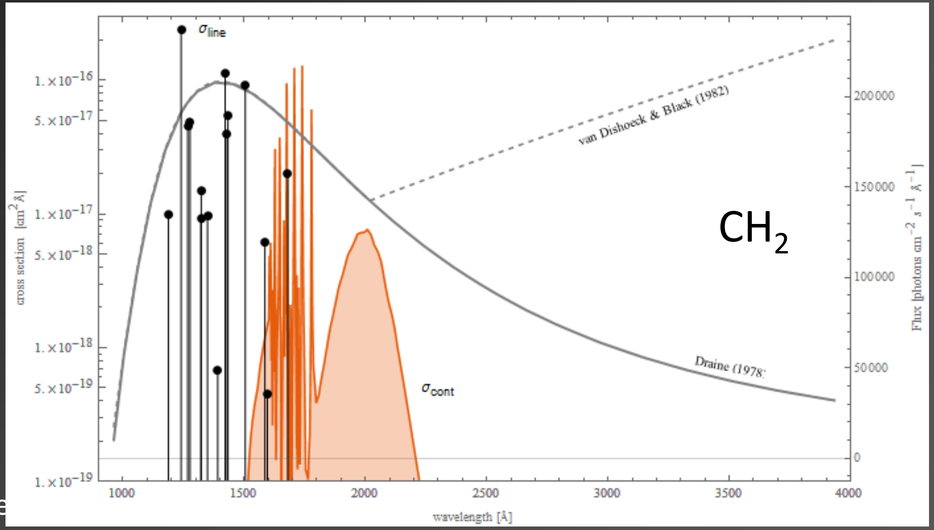

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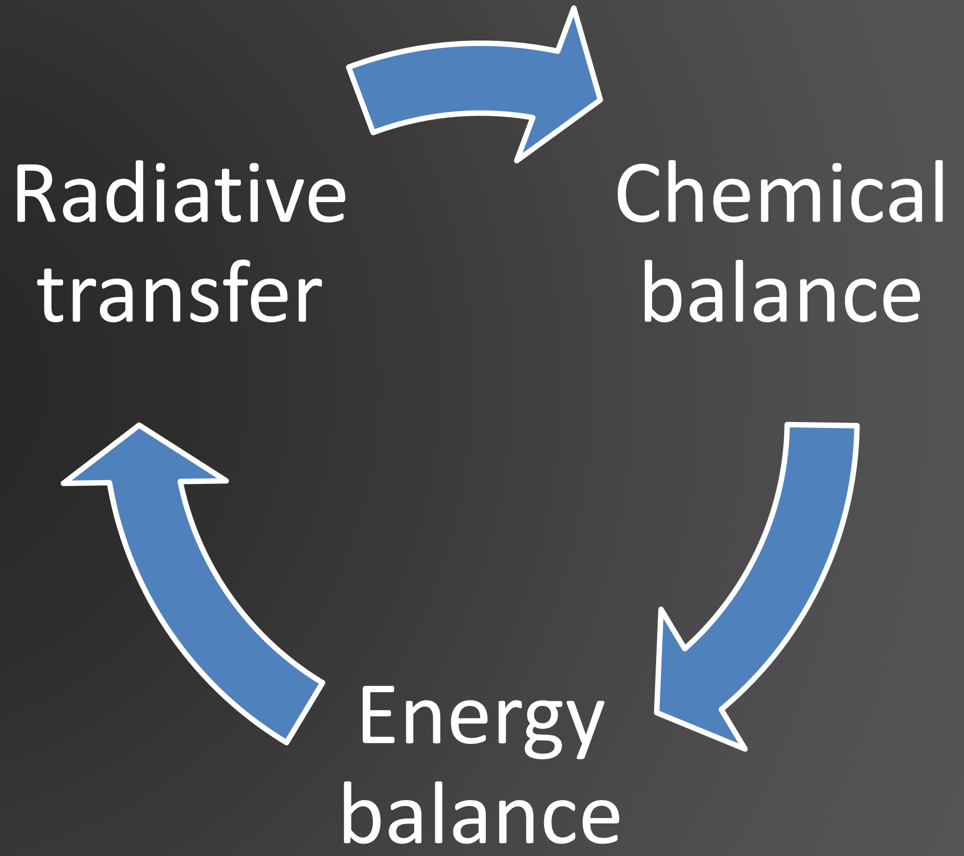

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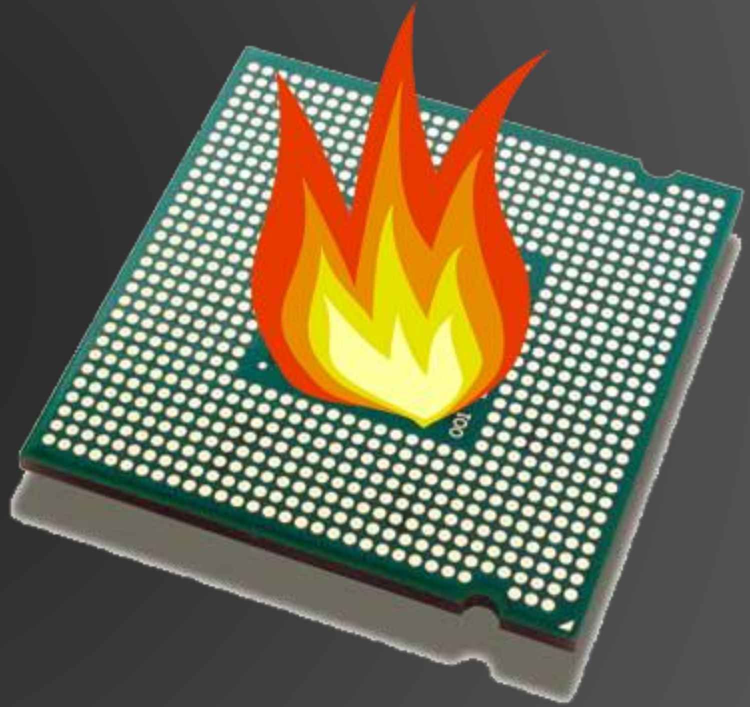
- Significant CPU workload



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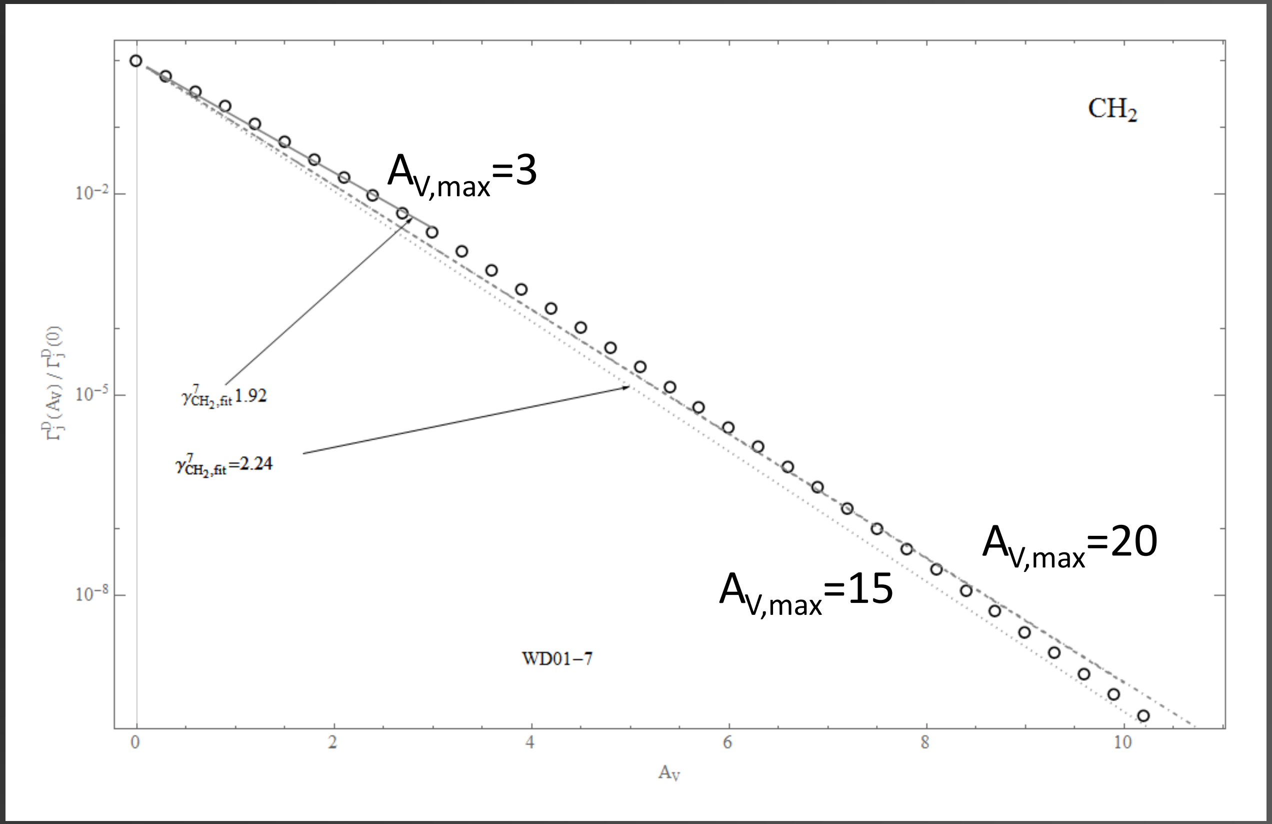

symbols: explicit Γ integration
lines: α exp(-γ AV) fit

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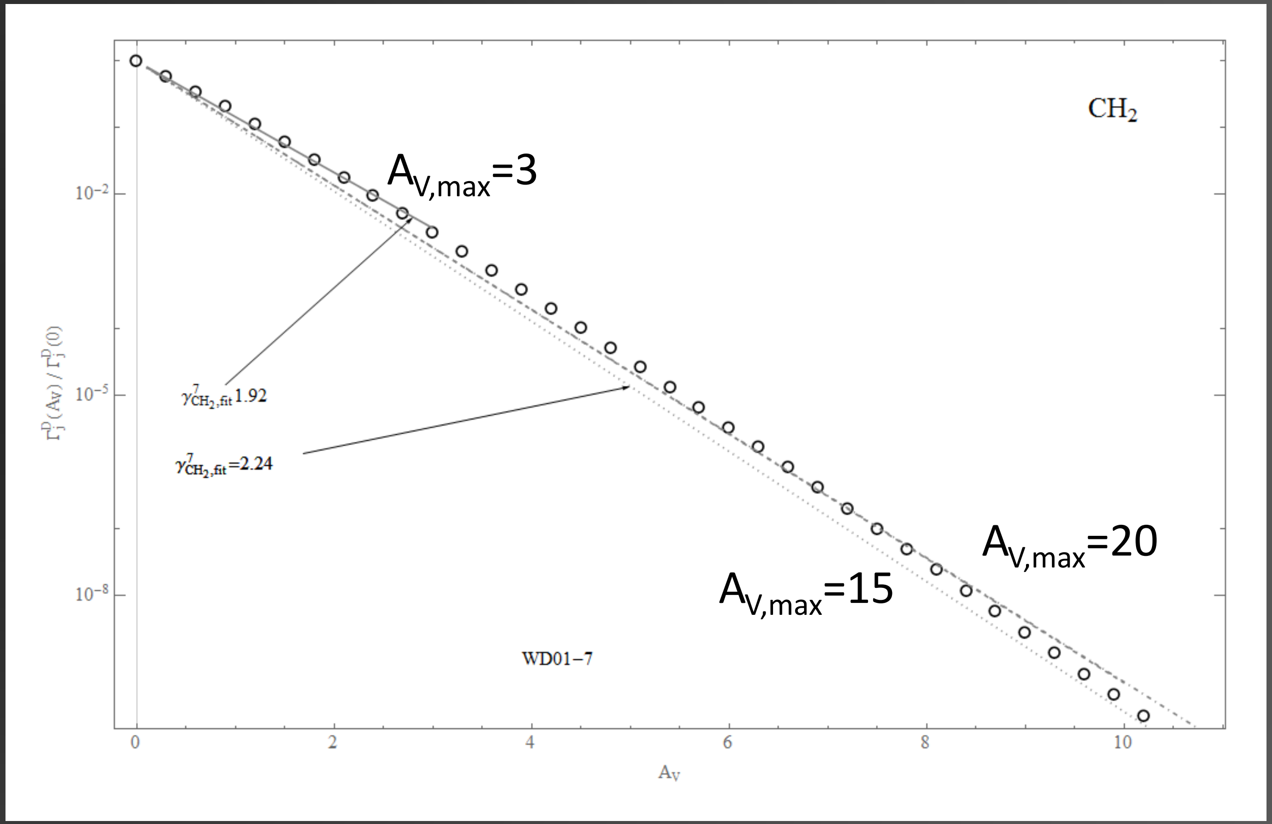

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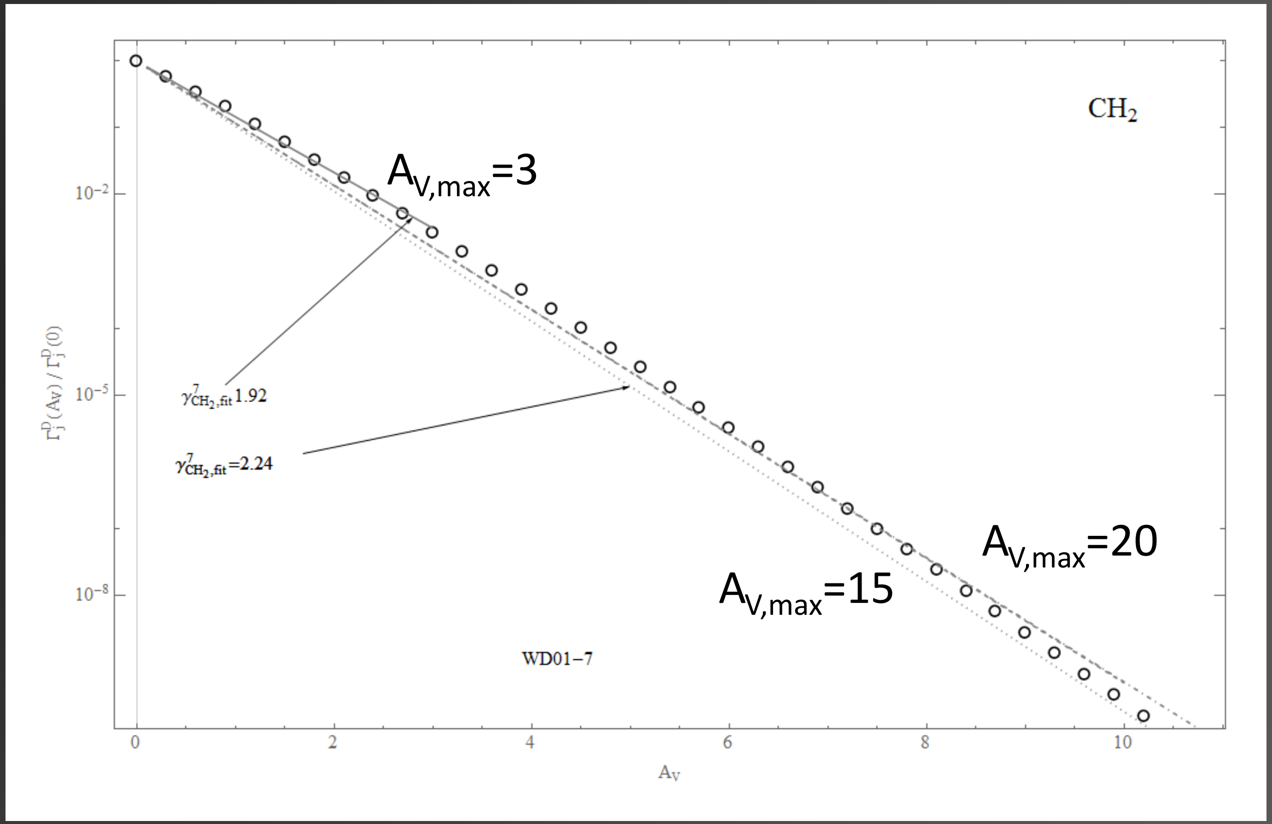

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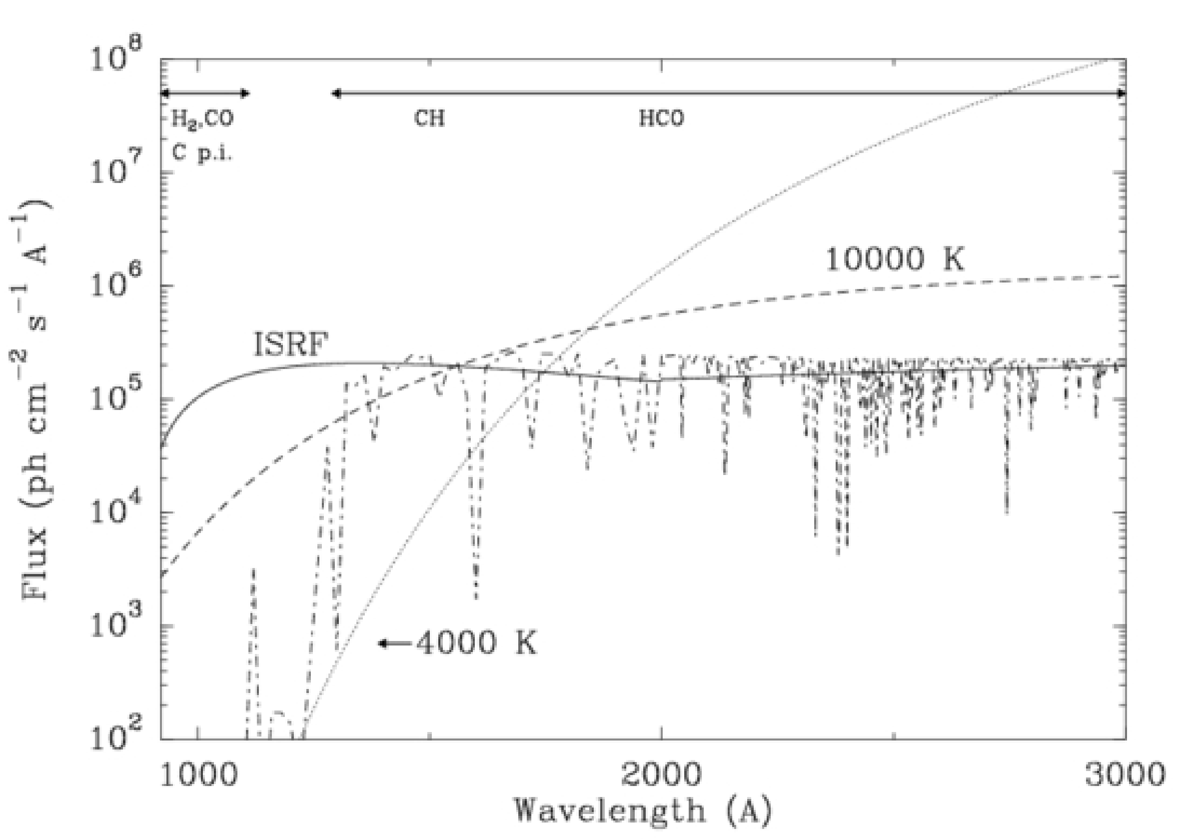

http://home.strw.leidenuniv.nl/~ewine/photo

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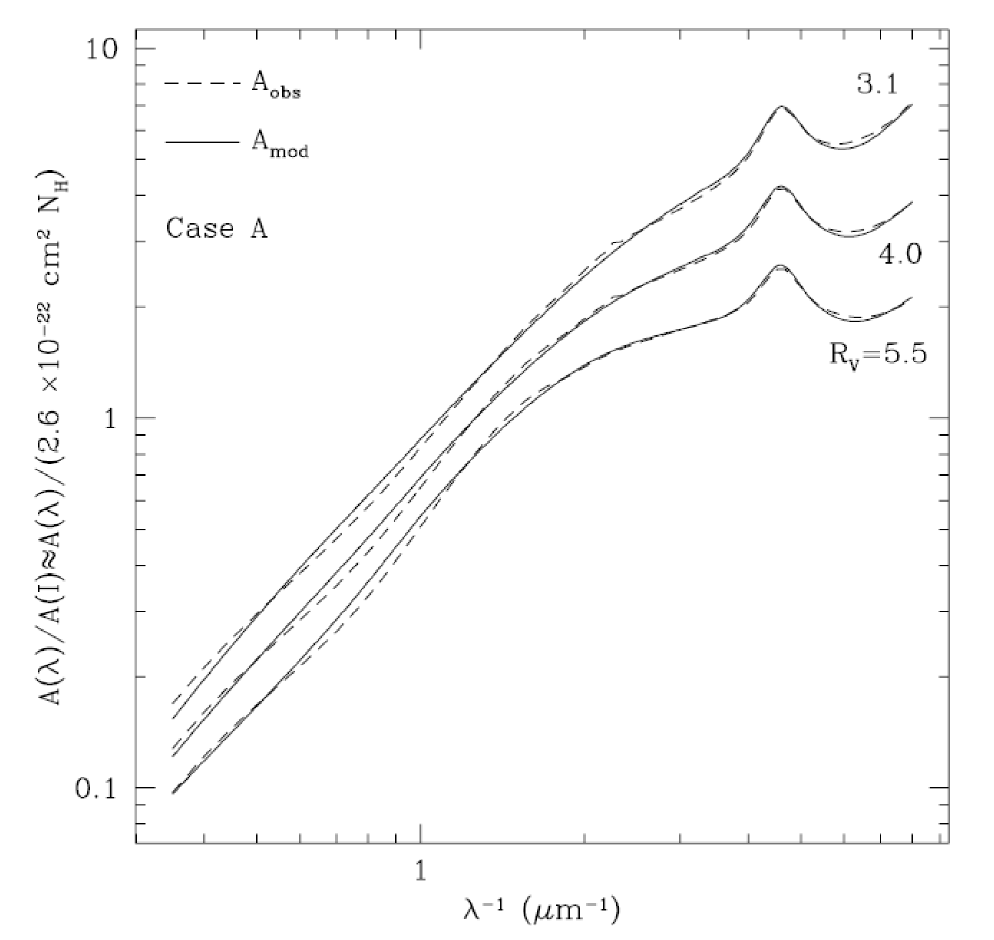

Weingartner & Draine 2001, ApJ 548, 296

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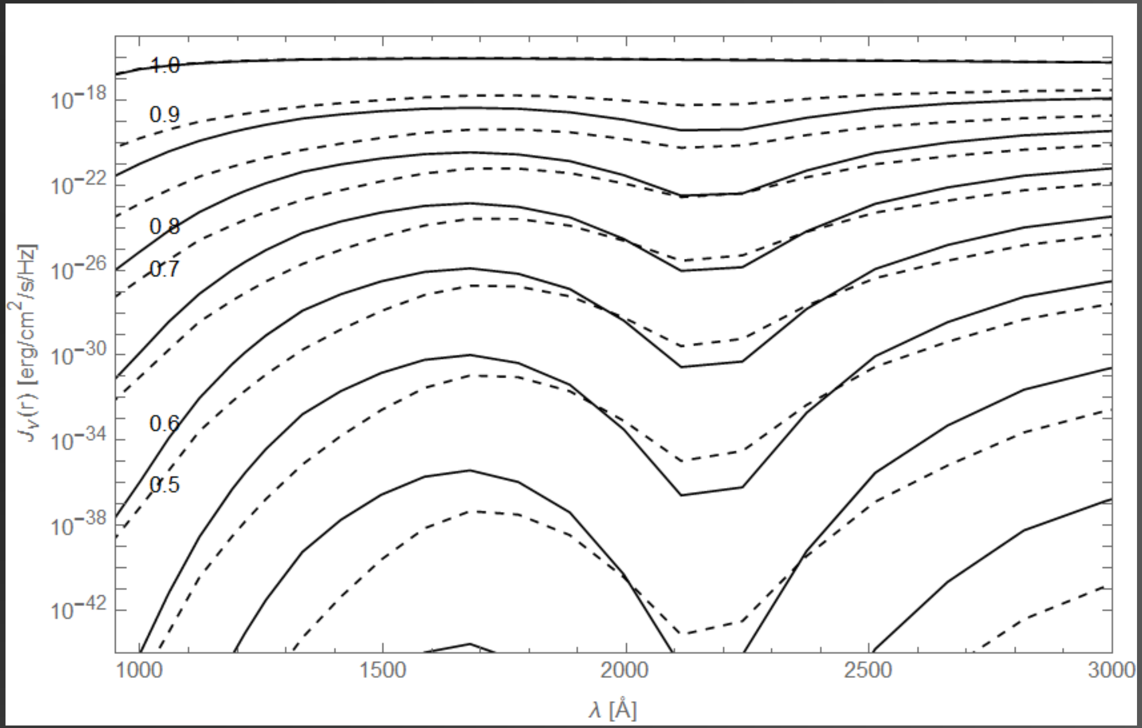
$J_j(\vec{r}, \nu)$ for different relative cloud radii



solid: WD-7, R_V=3.1 (diffuse gas)
dashed: MRN

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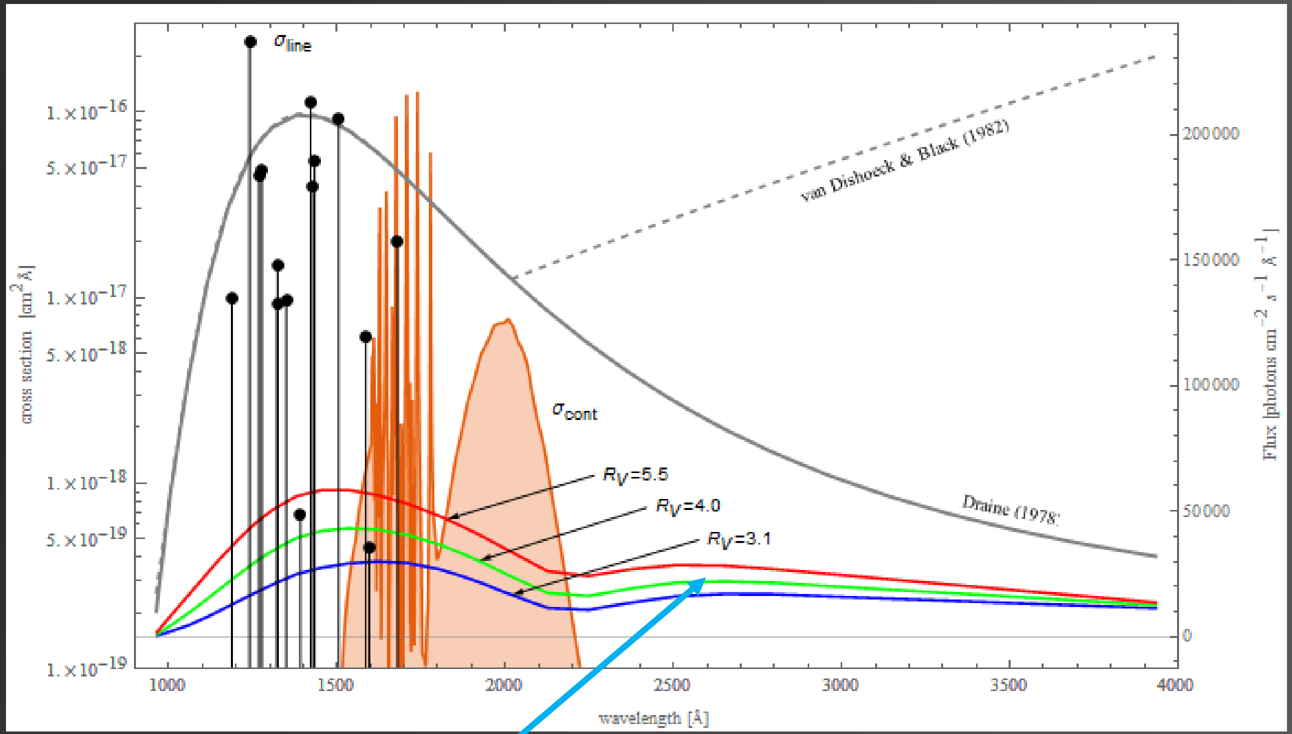

J(r,ν) at r=0.9 R_{max}

$$R_V = A(V) / E(B_V)$$

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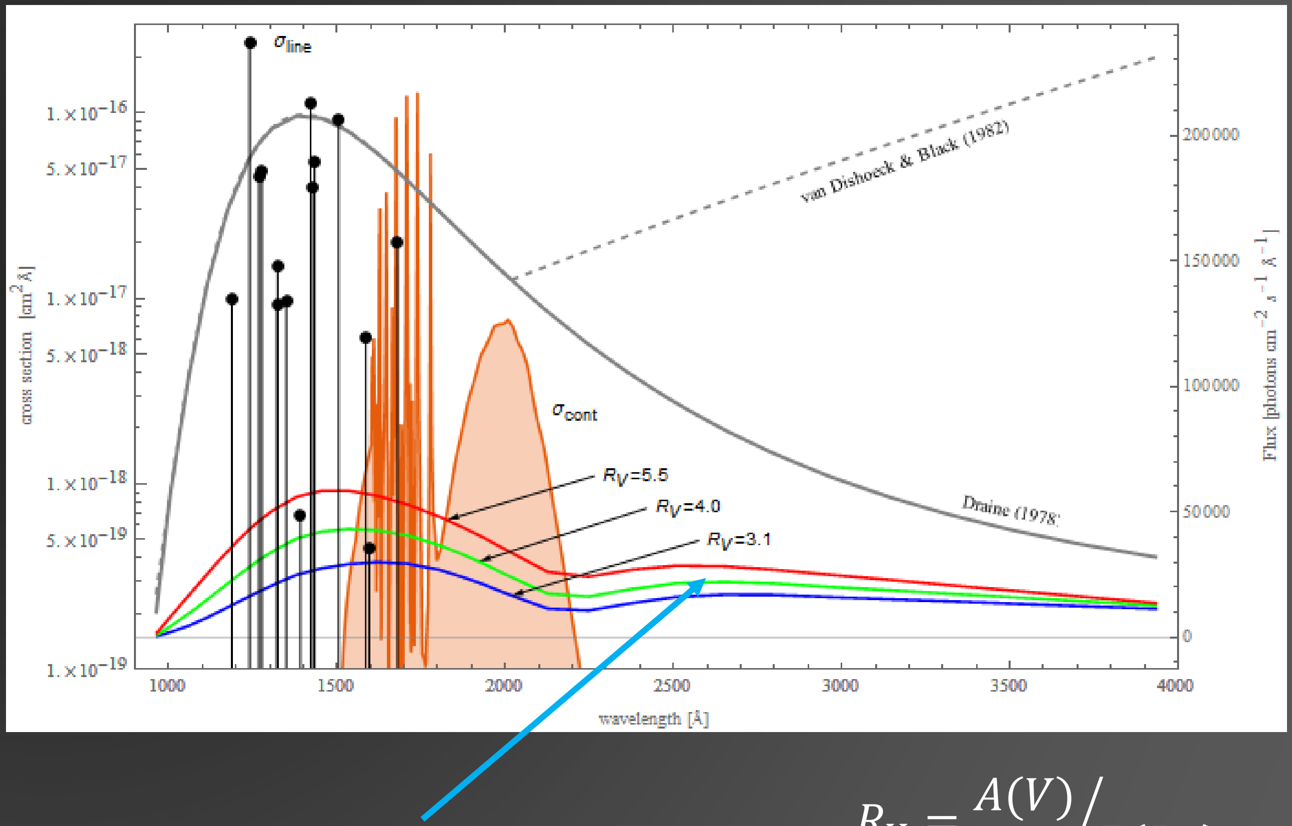
- detailed information on photodissociation cross-section not available for all species



$$R_V = {A(V)}/{E(B_V)}$$

Rescaling of γ

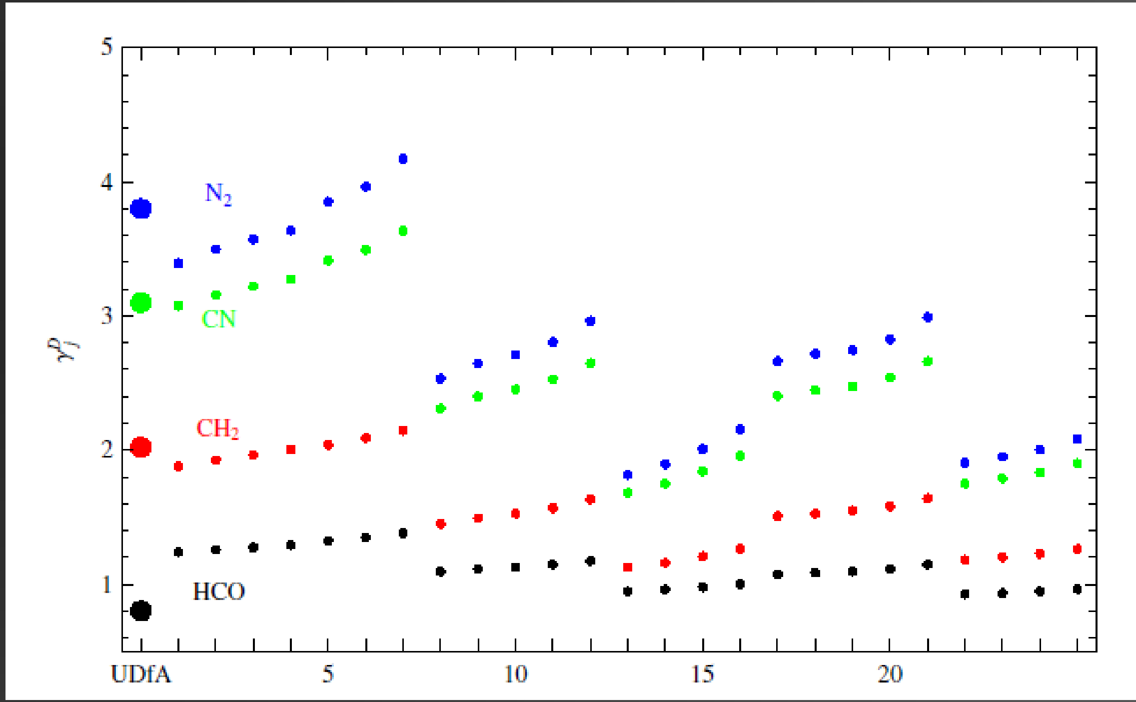
- frequency dependence of $J_j(\vec{r},\nu) \times \sigma_j(\nu)$ contained in γ
- dust extinction changes slowly across $\vec{r},\nu,$ and dust properties

- Idea: for a given γ_j (e.g. from UMIST) and unknown γ_j^D (target dust content D) find a scaling relation $\gamma_j \to \gamma_j^D$

Rescaling of γ

- Least-squares fit $\Gamma_j(A_V)/\Gamma_j(0) = e^{-\gamma_j^D A_V}$ to derive γ_j^D for all j and D

γ_j^D for 25 different dust models from W&D 2001



large dots: UMIST γ
x-axis: entry # in W&D 2001

Rescaling of γ

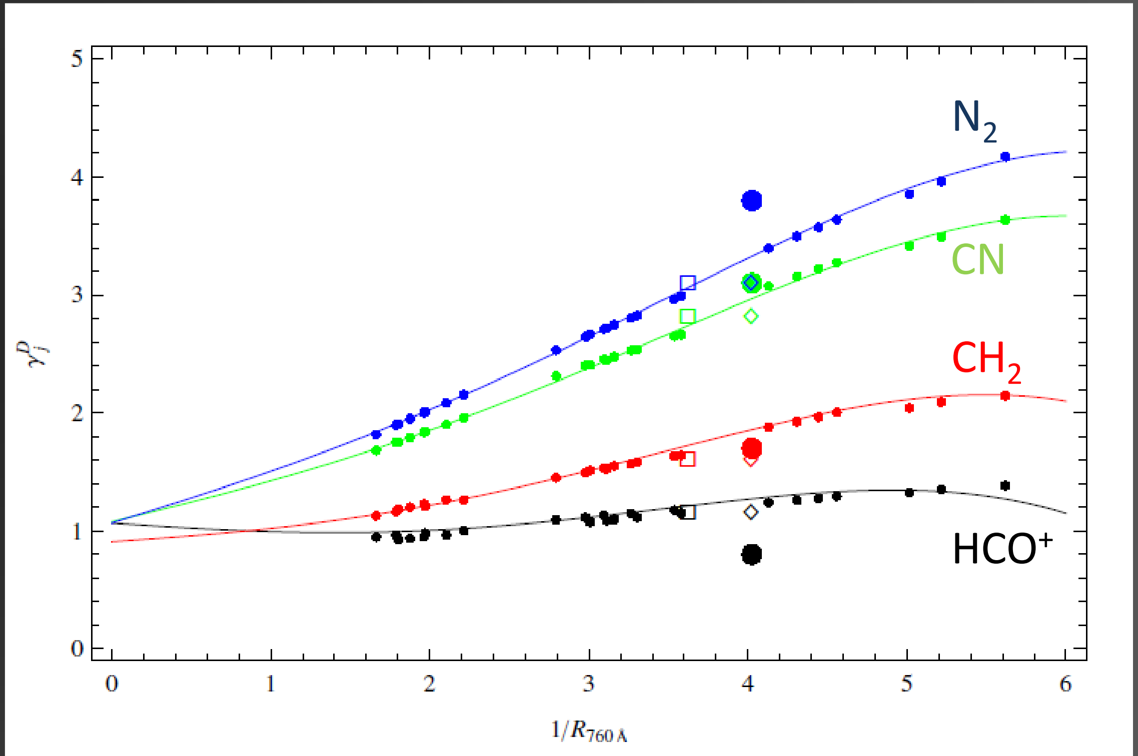
- Least-squares fit $\Gamma_j(A_V)/\Gamma_j(0) = e^{-\gamma_j^D A_V}$ to derive γ_j^D for all j and D
- find the dust model property best correlated to γ_j^D

$$\frac{1}{R_\lambda} = \left(\frac{A(V)}{A(\lambda) - A(V)}\right)^{-1} \quad for\ \lambda = 760\text{Å}$$

- Find parametrization w.r.t. $1/R_{760Å}$

$$\gamma_j^D = w_1 + w_2\left(\frac{1}{R^D_{760\ \text{Å}}}\right) + w_3\left(\frac{1}{R^D_{760\ \text{Å}}}\right)^3 + w_4\left(\frac{1}{R^D_{760\ \text{Å}}}\right)^4 + w_5\gamma_j + w_6\gamma_j^3 + w_7\gamma_j^4 + w_8\frac{\gamma_j}{R^D_{760\text{Å}}} + w_9\frac{\gamma_j^2}{R^D_{760\ \text{Å}}}.$$

γ_j^D for 25 different dust models from W&D 2001



large dots: UMIST γ , x-axis $1/R_{760Å}$

Rescaling of γ

- Details in Röllig et al. 2013, A&A, 549, A85

Fit parameter	
w_1	1.39460
w_2	–0.27655
w_3	0.02053
w_4	–0.00295
w_5	–0.45990
w_6	0.08725
w_7	–0.01616
w_8	0.24747
w_9	–0.01677

$$\gamma_j^D = w_1 + w_2\left(\frac{1}{R^D_{760\ \text{Å}}}\right) + w_3\left(\frac{1}{R^D_{760\ \text{Å}}}\right)^3 + w_4\left(\frac{1}{R^D_{760\ \text{Å}}}\right)^4$$
$$+w_5\gamma_j + w_6\gamma_j^3 + w_7\gamma_j^4 + w_8\frac{\gamma_j}{R^D_{760\text{Å}}} + w_9\frac{\gamma_j^2}{R^D_{760\ \text{Å}}}.$$

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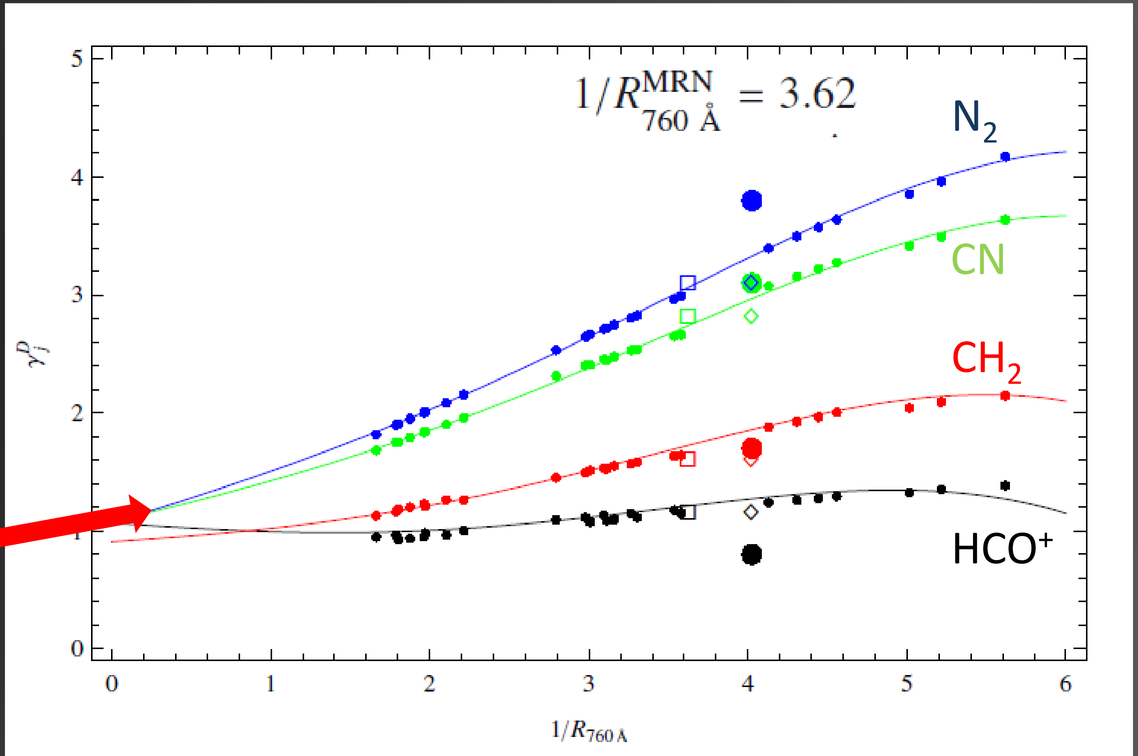
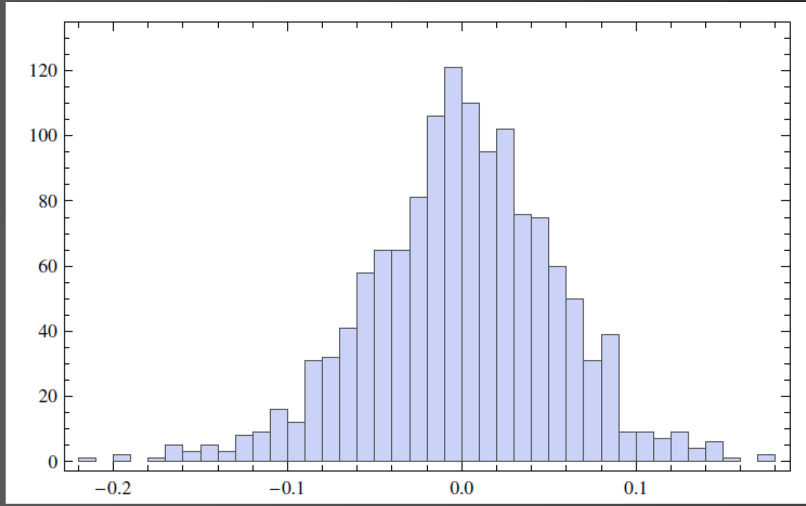


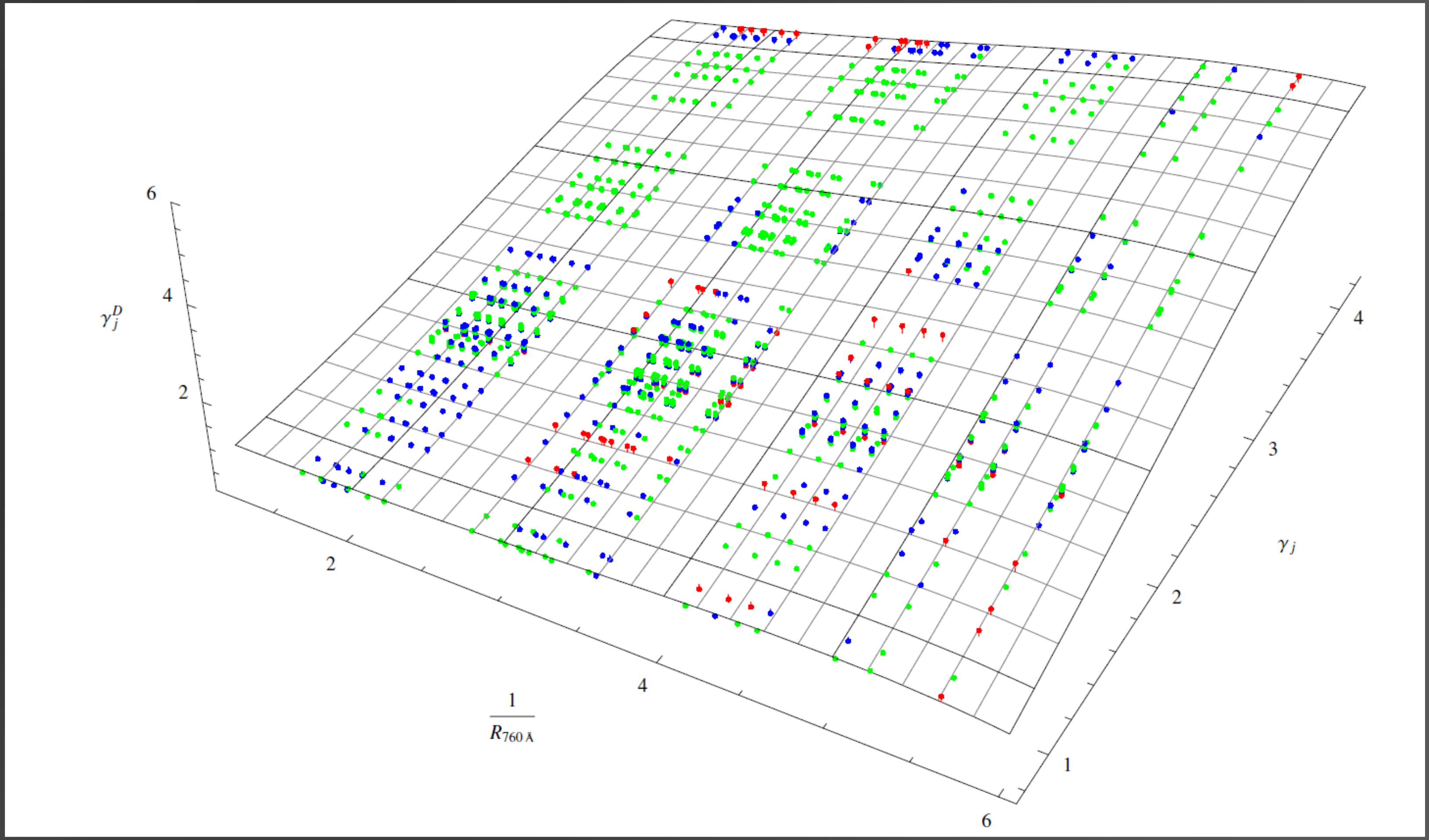
large dots: UMIST γ , x-axis $1/R_{760\text{Å}}$

Accuracy of the scaling

- rescaled γ_j^D are within a 5-10% level of acc.
- small error compared to chem. database unknowns
- „zero“ comp. costs



residuals γ_j^D-γ_j



absolute error: green 0.05, blue 0.1, red > 0.1 (max error < 0.22)

Summary

- Simple parametrized solution to map $\gamma_j \rightarrow \gamma_j^D$ for a given dust composition D.
- New mapped γ_j^D match the fully integrated and fitted $\gamma_j^{D,fit}$ at the 5-10% level.
- Fast and simple way to adapt the photodissociation calculations to altered dust properties.