Photo-rates in ProDiMo

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The general definition of a photo-rate is

$$R_{\rm ph} \;=\; \frac{1}{h}\int \sigma(\lambda)\,\lambda u_\lambda\,d\lambda \tag{1}$$

1 Delta peak cross section

Let's first consider the most simple case $\sigma(\lambda) = \sigma_0\delta(\lambda-\lambda_0)$ where the absorption is centered around a very narrow spectral band

$$R_{\rm ph} \;=\; \frac{1}{h}\sigma_0\,\lambda_0 u_{\lambda_0} \tag{2}$$

1.1 UMIST

Consider this photo-rate in a standard ISM radiation field $\lambda u_\lambda^{\rm ISM}$ which is shielded by some column of ISM dust

$$R^{\rm ISM}_{\rm ph} \;=\; \frac{1}{h}\sigma_0\,\lambda_0 u^{\rm ISM}_{\lambda_0}\exp(-\tau^{\rm ISM}_{\lambda_0}) \tag{3}$$

The visual extinction is defined as auxiliary variable

$$A_V^{\rm ISM} = 2.5\log e\,\tau_V^{\rm ISM} \tag{4}$$

with visual optical depth $\tau_V^{\rm ISM} = \frac{\kappa_V^{\rm ISM}}{\kappa_{\lambda_0}^{\rm ISM}}\tau_{\lambda_0}^{\rm ISM}$. This yields

$$\begin{aligned} R^{\rm ISM}_{\rm ph} \;&=\; \underbrace{\frac{1}{h}\sigma_0\,\lambda_0 u^{\rm ISM}_{\lambda_0}}_{\alpha}\exp\Big(-\underbrace{\frac{1}{2.5\log e}\frac{\kappa^{\rm ISM}_{\lambda_0}}{\kappa^{\rm ISM}_V}}_{\gamma}A_V^{\rm ISM}\Big) && (5)\\ &=\; \alpha\exp(-\gamma A_V^{\rm ISM}) && (6)\end{aligned}$$

as given by UMIST. Remarks

- Small $\gamma < 1$ in UMIST are because of ionisation by soft radiation and because ISM dust shows an opacity decrease toward longer wavelength $\kappa^{\rm ISM}_{\lambda_0} < \kappa^{\rm ISM}_V$, e. g. $\gamma = 0.5$ for H^- bf.
- The unshielded rate α depends on the assumptions made by UMIST about the ISM irradiation at λ_0. Not only about the spectral slope, but first of all about the absolute strength at λ_0.
- λ_0 is not known from the UMIST database, but we can calculate the likewise unknown ISM dust opacity at centre wavelength λ_0 from γ according to Eq. (5)

$$\kappa^{\rm ISM}_{\lambda_0} \;=\; 2.5\log e\;\gamma\;\kappa^{\rm ISM}_V \tag{7}$$

1.2 ProDiMo

In arbitrary radiation fields, but slab symmetry, we can still use Eq. (3)

$$R_{\rm ph} \;=\; \frac{1}{h}\sigma_0\,\lambda_0 u_{\lambda_0}\exp(-\tau_{\lambda_0}) \tag{8}$$

We define another auxiliary variable here, namely the UV optical depth as

$$\tau_{\rm UV} = \frac{\kappa_{\rm UV}}{\kappa_{\lambda_0}}\tau_{\lambda_0} \tag{9}$$

and use Eqs. (8)

$$R_{\rm ph} \;=\; \underbrace{\frac{1}{h}\sigma_0\,\lambda_0 u^{\rm ISM}_{\lambda_0}}_{=\,\alpha}\;\frac{u_{\lambda_0}}{u^{\rm ISM}_{\lambda_0}}\;\exp\Big(-\frac{\kappa_{\lambda_0}}{\kappa_{\rm UV}}\tau_{\rm UV}\Big) \tag{10}$$

Next, we use Eq.(4) to replace $\tau_{\rm UV}$ by the visual extinction $A_V^{\rm ISM} = 2.5\log e\,\frac{\kappa_V^{\rm ISM}}{\kappa_{\rm UV}^{\rm ISM}}\tau_{\rm UV}$ as would be present if the dust had interstellar transport coefficients

$$\begin{aligned}
R_{\rm ph} \;&=\; \alpha\,\frac{u_{\lambda_0}}{u^{\rm ISM}_{\lambda_0}}\exp\Big(-\frac{\kappa_{\lambda_0}}{\kappa_{\rm UV}}\,\frac{\kappa^{\rm ISM}_{\rm UV}}{\kappa^{\rm ISM}_V}\,\frac{1}{2.5\log e}A_V^{\rm ISM}\Big) &(11)\\
&=\; \alpha\,\frac{u_{\lambda_0}}{u^{\rm ISM}_{\lambda_0}}\exp\Big(-\frac{\kappa_{\lambda_0}}{\kappa_{\rm UV}}\,\frac{\kappa^{\rm ISM}_{\rm UV}}{\kappa^{\rm ISM}_{\lambda_0}}\,\underbrace{\frac{\kappa^{\rm ISM}_{\lambda_0}}{\kappa^{\rm ISM}_V}\,\frac{1}{2.5\log e}}_{=\,\gamma}\,A_V^{\rm ISM}\Big) &(12)\\
&=\; \alpha\,\underbrace{\frac{u_{\lambda_0}}{u^{\rm ISM}_{\lambda_0}}}_{\approx\,\chi_0}\exp\Big(-\underbrace{\frac{\kappa_{\lambda_0}/\kappa^{\rm ISM}_{\lambda_0}}{\kappa_{\rm UV}/\kappa^{\rm ISM}_{\rm UV}}}_{\approx\,1}\;\gamma A_V^{\rm ISM}\Big) &(13)\\
&\approx\; \alpha\,\chi_0\exp\Big(-\gamma A_V^{\rm ISM}\Big) &(14)
\end{aligned}$$

Equation (14) demonstrates the following

- As long as the relative opacity ratio $\frac{\kappa_{\lambda_0}/\kappa^{\rm ISM}_{\lambda_0}}{\kappa_{\rm UV}/\kappa^{\rm ISM}_{\rm UV}} \approx 1$, and $\frac{u_{\lambda_0}}{u^{\rm ISM}_{\lambda_0}} \approx \chi_0$, we can use the UMIST parameter α and γ according to Eq. (14), ...
- ... if we use $A_V^{\rm ISM}$ and not A_V !
- Otherwise, we can't. I do not see how this could be justified. Can you?
- The ratio $u_{\lambda_0}\,/\,u^{\rm ISM}_{\lambda_0}$ can easily differ substantially from $\chi_0 = \int_{91.2\,\rm nm}^{205\,\rm nm}\lambda u^\star_\lambda\,d\lambda \;/\; \int_{91.2\,\rm nm}^{205\,\rm nm}\lambda u^{\rm ISM}_\lambda\,d\lambda$, even if λ_0 is well inside the interval 91.2 nm ... 205 nm, because $u^\star_\lambda$ is a steep function of λ, whereas $u^{\rm ISM}_\lambda$ isn't (may go the other way!). The only solution I see is to integrate properly over the stellar spectrum

$$R_{\rm ph} \approx \alpha^\star\exp\Big(-\frac{\kappa_{\lambda_0}/\kappa^{\rm ISM}_{\lambda_0}}{\kappa_{\rm UV}/\kappa^{\rm ISM}_{\rm UV}}\;\gamma A_V^{\rm ISM}\Big)\quad\text{with}\quad \alpha^\star = \frac{1}{h}\int\sigma(\lambda)\,\lambda u^\star_\lambda\,d\lambda \tag{15}$$

- The relative opacity ratio in the exponent is a problem because it sits in the exponent! For larger than ISM grains, the slope in the UV is small, but for ISM grains it isn't! This is just expressed by the parameter γ. It simply makes no sense to introduce A_V in the first place. It would be better to keep it as

$$R_{\rm ph} = \alpha^\star\;\exp\Big(-\frac{\kappa_{\lambda_0}}{\kappa_{\rm UV}}\tau_{\rm UV}\Big) \tag{16}$$

  and $\frac{\kappa_{\lambda_0}}{\kappa_{\rm UV}}$ stays in the memory as additional parameter for every photo-reaction.

- For both solutions, we must have $\sigma(\lambda)$, or at least an estimate of the center wavelength λ_0.

- Introducing the proper physical $A_V = 2.5\log e\,\tau_V$ does not help, but makes things worse: Applying the same formalism results is

$$R_{\rm ph} = \alpha\ \chi_0 \exp\Big(- \frac{\kappa_{\lambda_0}/\kappa_{\lambda_0}^{\rm ISM}}{\kappa_V/\kappa_V^{\rm ISM}}\ \gamma A_V\Big) \tag{17}$$

  The ratio $(\kappa_{\lambda_0}/\kappa_{\lambda_0}^{\rm ISM})/(\kappa_V/\kappa_V^{\rm ISM})$ is even worse determined as compared to $(\kappa_{\lambda_0}/\kappa_{\lambda_0}^{\rm ISM})/(\kappa_{\rm UV}/\kappa_{\rm UV}^{\rm ISM})$ because, in most cases, λ_0 is in the UV and not in the visual. And the more these wavelength are apart (for unknown λ_0) the larger the error is if putting this ratio to 1.

- It is insightful to combine Eq. (17) with Eq. (7)

$$R_{\rm ph} = \alpha\ \chi_0 \exp\Big(- \underbrace{\frac{\kappa_{\lambda_0}}{\kappa_V}\ \frac{1}{2.5\log e}}_{\gamma^\star} A_V\Big) \tag{18}$$

  Equation (7) is a implicit equation for λ_0. If one would use it to determine λ_0 and then calculate the disk opacities at that wavelength, one would get a pretty good alternative, I think.

2 The general case

2.1 UMIST

The full rate in a standard ISM radiation field shielded by some column of ISM dust is

$$R_{\rm ph}^{\rm ISM} = \frac{1}{h}\int \sigma(\lambda)\,\lambda u_\lambda^{\rm ISM} \exp(-\tau_\lambda^{\rm ISM})\,d\lambda \tag{19}$$

Introducing $A_V^{\rm ISM}$ results in

$$R_{\rm ph}^{\rm ISM} = \frac{1}{h}\int \sigma(\lambda)\,\lambda u_\lambda^{\rm ISM} \exp\Big(- \frac{1}{2.5\log e}\frac{\kappa_\lambda^{\rm ISM}}{\kappa_V^{\rm ISM}} A_V^{\rm ISM}\Big)\,d\lambda \tag{20}$$

$$= \underbrace{\frac{1}{h}\int \sigma(\lambda)\,\lambda u_\lambda^{\rm ISM}\,d\lambda}_{\alpha}\ \underbrace{\frac{\int \sigma(\lambda)\,\lambda u_\lambda^{\rm ISM} \exp\Big(- \frac{1}{2.5\log e}\frac{\kappa_\lambda^{\rm ISM}}{\kappa_V^{\rm ISM}} A_V^{\rm ISM}\Big)\,d\lambda}{\int \sigma(\lambda)\,\lambda u_\lambda^{\rm ISM}\,d\lambda}}_{\exp(-\gamma A_V^{\rm ISM})} \tag{21}$$

I do not see any further possible simplification for abritrary $A_V^{\rm ISM}$ and

$$\exp(-\gamma A_V^{\rm ISM}) = \frac{1}{h\alpha}\int \sigma(\lambda)\,\lambda u_\lambda^{\rm ISM} \exp\Big(- \frac{1}{2.5\log e}\frac{\kappa_\lambda^{\rm ISM}}{\kappa_V^{\rm ISM}} A_V^{\rm ISM}\Big)\,d\lambda \tag{22}$$

states an implicit equation for the function $\gamma{=}\gamma(A_V^{\rm ISM})$ that has be to fitted numerically, provided that $\sigma(\lambda)$, $\kappa_\lambda^{\rm ISM}$, and $u_\lambda^{\rm ISM}$ are known. However, for small $A_V^{\rm ISM} \ll 1$, with $\exp(-x){\approx}1{-}x$, I get the following result

$$\gamma = \frac{1}{2.5\log e}\ \frac{\int \sigma(\lambda)\,\lambda u_\lambda^{\rm ISM}\frac{\kappa_\lambda^{\rm ISM}}{\kappa_V^{\rm ISM}}\,d\lambda}{\int \sigma(\lambda)\,\lambda u_\lambda^{\rm ISM}\,d\lambda} \tag{23}$$

which states a generalization of Eq. (5) for the definition of γ. Equating these two equations gives us a hint how to define an effective opacity at aborption center wavelength λ_0:

$$\frac{\kappa^{\rm ISM}_{\lambda_0}}{\kappa^{\rm ISM}_V} \approx \frac{\int\sigma(\lambda)\,\lambda u^{\rm ISM}_\lambda \frac{\kappa^{\rm ISM}_\lambda}{\kappa^{\rm ISM}_V}\,d\lambda}{\int\sigma(\lambda)\,\lambda u^{\rm ISM}_\lambda\,d\lambda} \tag{24}$$

2.2 ProDiMo

In arbitrary radiation fields and slab symmetry we write

$$R_{\rm ph} = \frac{1}{h}\int\sigma(\lambda)\,\lambda u^\star_\lambda \exp(-\tau_\lambda)\,d\lambda\ . \tag{25}$$

The UV dust opacity in ProDiMo is defined as band-mean according to

$$\kappa_{\rm UV} = \frac{1}{\lambda_2 - \lambda_1}\int_{\lambda_1}^{\lambda_2}\kappa_\lambda\,d\lambda \tag{26}$$

with $\lambda_1 = 91.2\,$nm and $\lambda_2 = 205\,$nm, and the unattenuated UV strength is defined as

$$\chi_0 = \int_{\lambda_1}^{\lambda_2}\lambda u^\star_\lambda\,d\lambda \ \Big/ \int_{\lambda_1}^{\lambda_2}\lambda u^{\rm ISM}_\lambda\,d\lambda\ , \tag{27}$$

Putting $\tau_{\rm UV}$ into Eq. (25) we find

$$\begin{aligned}
R_{\rm ph} &= \frac{1}{h}\int\sigma(\lambda)\,\lambda u^\star_\lambda \exp\Big(-\frac{\kappa_\lambda}{\kappa_{\rm UV}}\tau_{\rm UV}\Big)\,d\lambda && (28)\\
&= \underbrace{\frac{1}{h}\int\sigma(\lambda)\,\lambda u^\star_\lambda\,d\lambda}_{\alpha^\star}\ \underbrace{\frac{\int\sigma(\lambda)\,\lambda u^\star_\lambda \exp\Big(-\frac{\kappa_\lambda}{\kappa_{\rm UV}}\tau_{\rm UV}\Big)\,d\lambda}{\int\sigma(\lambda)\,\lambda u^\star_\lambda\,d\lambda}}_{\exp(-\beta^\star\,\tau_{\rm UV})} && (29)\\
&= \alpha^\star\exp(-\beta^\star\,\tau_{\rm UV}) && (30)
\end{aligned}$$

Again, this doesn't help much for the definition of $\beta^\star$, unless we consider small $\tau_{\rm UV} \ll 1$

$$\beta^\star = \frac{\displaystyle\int\sigma(\lambda)\,\lambda u^\star_\lambda \frac{\kappa_\lambda}{\kappa_{\rm UV}}\,d\lambda}{\displaystyle\int\sigma(\lambda)\,\lambda u^\star_\lambda\,d\lambda} \tag{31}$$

Remarks

- $\beta^\star$ is a "colour correction". It accounts for the deeper penetration of star light into the disk, if the typical wavelength of molecular absorption is longer than typical UV, and vice versa.
- We do not need χ nor A_V in general.
- Eqs. (30) and (31) are a generalisation of Eq. (16).
- If $\sigma(\lambda)$ is known, $\alpha^\star$ and $\beta^\star$ can be pre-calculated straightforwardly for every photo-reaction, unless we allow for position-dependent dust opacities ($\rightarrow$ dust settling).

The **big big** question now is: *Whether and how can we use χ_0 and the UMIST coefficients α and γ in cases where we have no informations about $\sigma(\lambda)$?*

We start all over again with Eq. (28) and insert ISM quantities

$$R_{\rm ph} = \frac{1}{h}\int \sigma(\lambda)\,\lambda u^\star_\lambda \exp\Big(-\frac{\kappa_\lambda}{\kappa_{\rm UV}}\tau_{\rm UV}\Big)\,d\lambda \tag{32}$$

$$= \frac{1}{h}\int \sigma(\lambda)\,\lambda u^\star_\lambda \exp\Big(-\frac{\kappa_\lambda}{\kappa_{\rm UV}}\,\frac{\kappa^{\rm ISM}_{\rm UV}}{\kappa^{\rm ISM}_V}\,\frac{1}{2.5\log e}A^{\rm ISM}_V\Big)\,d\lambda \tag{33}$$

$$= \alpha^\star \exp(-\delta^\star\gamma A^{\rm ISM}_V) \tag{34}$$

In order to determine $\delta^\star$, let's consider small A_V rightaway

$$R_{\rm ph} \approx \frac{1}{h}\int \sigma(\lambda)\,\lambda u^\star_\lambda \Big(1-\frac{\kappa_\lambda}{\kappa_{\rm UV}}\,\frac{\kappa^{\rm ISM}_{\rm UV}}{\kappa^{\rm ISM}_V}\,\frac{1}{2.5\log e}A^{\rm ISM}_V\Big)\,d\lambda \tag{35}$$

$$= \underbrace{\frac{1}{h}\int \sigma(\lambda)\,\lambda u^\star_\lambda\,d\lambda}_{=\alpha^\star} - \frac{1}{h}\int \sigma(\lambda)\,\lambda u^\star_\lambda\,\frac{\kappa_\lambda}{\kappa_{\rm UV}}\,\frac{\kappa^{\rm ISM}_{\rm UV}}{\kappa^{\rm ISM}_V}\,\frac{1}{2.5\log e}A^{\rm ISM}_V\,d\lambda \tag{36}$$

$$= \alpha^\star(1-\delta^\star\gamma A^{\rm ISM}_V) \tag{37}$$

Inserting the definition of γ (Eq. 23) yields

$$\alpha^\star\delta^\star\frac{\int \sigma(\lambda)\,\lambda u^{\rm ISM}_\lambda \frac{\kappa^{\rm ISM}_\lambda}{\kappa^{\rm ISM}_V}\,d\lambda}{\int \sigma(\lambda)\,\lambda u^{\rm ISM}_\lambda\,d\lambda} = \frac{1}{h}\int \sigma(\lambda)\,\lambda u^\star_\lambda\frac{\kappa_\lambda}{\kappa_{\rm UV}}\,\frac{\kappa^{\rm ISM}_{\rm UV}}{\kappa^{\rm ISM}_V}\,d\lambda \tag{38}$$

We can cancel $\kappa^{\rm ISM}_V$ and use the definition of the unattenuated stellar photo-rate $\alpha^\star$

$$\delta^\star = \frac{\kappa^{\rm ISM}_{\rm UV}}{\kappa_{\rm UV}}\;\frac{\int \sigma(\lambda)\,\lambda u^\star_\lambda\kappa_\lambda\,d\lambda \Big/ \int \sigma(\lambda)\,\lambda u^\star_\lambda\,d\lambda}{\int \sigma(\lambda)\,\lambda u^{\rm ISM}_\lambda\kappa^{\rm ISM}_\lambda\,d\lambda \Big/ \int \sigma(\lambda)\,\lambda u^{\rm ISM}_\lambda\,d\lambda} \tag{39}$$

This is the desired color correction for the application of the UMIST parameters, a generalization of Eq. (13).

The discussion of Eq. (39) is a bit irksome. To zero-order approximation, everything calcels and $\delta^\star\approx 1$, as long as the integral boundaries are situated in the UV. Since we only need this description if we do not have detailed cross sections $\sigma(\lambda)$ at hand, there is no point in trying to really use Eq. (39). However, Eq. (39) can be useful to check the errors made by assuming $\delta^\star\approx 1$. It gives a better feeling for the meaning of $\kappa_{\lambda_0}/\kappa^{\rm ISM}_{\lambda_0}$ in Eq. (13). In addition to the discussion after Eq. (13), which demonstrates the main effect, one can say that things get worse, because the reddish disk opacities are weighted by the reddish stellar irradiation, and the blueish ISM opacities with the blueish ISM irradiation. This gives more weight to the extremes and makes deviations from unity more likely.

In conclusion, the best way to use the UMIST rate coefficients still seems to be to assume $\alpha/\alpha^{\rm ISM}\approx\chi_0$ and $\delta^\star\approx 1$

$$R_{\rm ph} \approx \alpha\,\chi_0\,\exp(-\gamma A^{\rm ISM}_V) \tag{40}$$

although it is hard to justify.