Recombination Cooling in ProDiMo

Peter Woitke, May 2009

1 Photo-processes and related heating and cooling rates

Consider a pair of photo-process as

$$\mathrm{AB} + h\nu \underset{k_r}{\overset{k_f}{\rightleftharpoons}} \mathrm{A} + \mathrm{B} \tag{1}$$

As main application in mind, we will consider the photo-ionisation and direct recombination of H^- (AB=H^-, A=H, B=e^-), but the following method may also be applicable to a pair of photo-dissociation and radiative association processes (?). The forward rate coefficient k_f is given by

$$k_f = 4\pi \int\limits_{\nu_\mathrm{thr}}^{\infty} \frac{J_\nu}{h\nu}\,\sigma^\mathrm{f}(\nu)\,d\nu \ , \tag{2}$$

such that $n_\mathrm{AB}\,k_f$ [$\mathrm{cm^{-3}s^{-1}}$] is the number of photoionisations per volume and time. $\sigma^\mathrm{f}(\nu)$ is the photo cross section [$\mathrm{cm^2}$] of AB for the forward reaction (only continuous cross sections considered here). Energy conservation implies that

$$h\nu = E_b + E_\mathrm{th} \tag{3}$$

where $E_b = h\nu_\mathrm{thr}$ is the binding energy of AB, ν_thr is the threshold frequency, and E_th is the excess thermal energy $\frac{1}{2}m_e v^2$ liberated by the photo-reaction.

Hence, the *ionisation heating rate* $\Gamma[\mathrm{erg\,s^{-1}cm^{-3}}]$ is given by

$$\Gamma = n_\mathrm{AB}\; 4\pi \int\limits_{\nu_\mathrm{thr}}^{\infty} J_\nu\,\frac{\nu-\nu_\mathrm{thr}}{\nu}\,\sigma^\mathrm{f}(\nu)\,d\nu \ . \tag{4}$$

The reverse process, the recombination cooling rate, is slightly more difficult to understand. A direct recombination destroys one thermal electron, so the cooling rate should be of order $n_\mathrm{A}n_\mathrm{B}k_r(T_\mathrm{g})\langle E_\mathrm{th}\rangle$, where the recombination rate coefficient is given by an Arrhenius law with fit coefficients α, β, γ as

$$k_r(T_\mathrm{g}) = \alpha\left(\frac{T_\mathrm{g}}{300\,\mathrm{K}}\right)^\beta \exp\left(-\frac{\gamma}{T_\mathrm{g}}\right) \ . \tag{5}$$

In order to investigate the details of $\langle E_\mathrm{th}\rangle$, we consider the pair of photo-processes (1) in the case of thermodynamical equilibrium, where $J_\nu = B_\nu(T_\mathrm{g})$ and where every reaction is in detailed balance with its direct reverse, i. e.

$$n^\star_\mathrm{AB} k_f\big|_{J_\nu=B_\nu(T_\mathrm{g})} = n^\star_\mathrm{A} n^\star_\mathrm{B} k_r(T_\mathrm{g}) \ . \tag{6}$$

Thus, we find the recombination rate coefficient to be

$$k_r(T_\mathrm{g}) = \frac{n^\star_\mathrm{AB}}{n^\star_\mathrm{A} n^\star_\mathrm{B}}\; 4\pi \int\limits_{\nu_\mathrm{thr}}^{\infty} \frac{B_\nu(T_\mathrm{g})}{h\nu}\,\sigma^\mathrm{f}(\nu)\,d\nu \ , \tag{7}$$

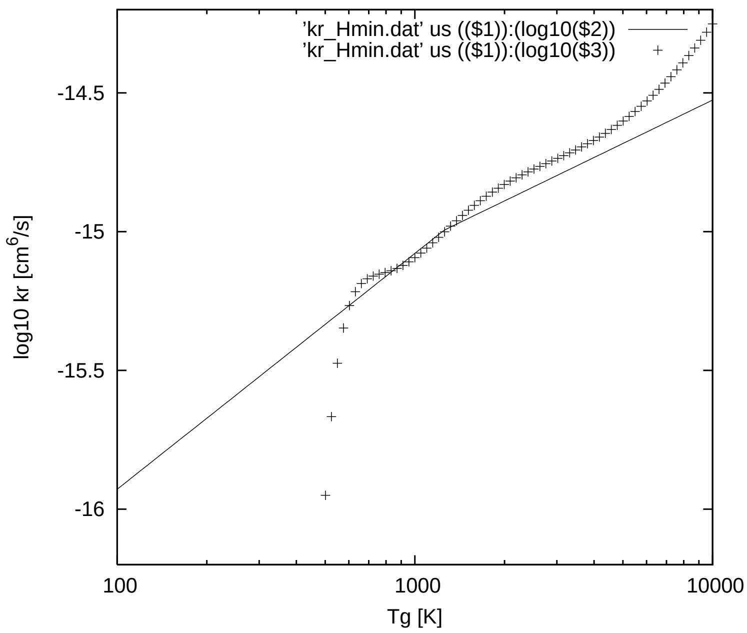

Figure 1: Comparison of the recombination rate coefficient $k_r(T_{\rm g})$ of $\rm H^-$ according to Eq. (5) with data from UMIST 2006 (full line) and according to Eq. (7) with photo cross-sections data from Leiden's photoionisation database and thermo-chemical data from the JANAF tables (1985), involving a polynomial fit of $k_p(T_{\rm g})$ between 1000 K and 6000 K.

which is known as the bound-free Milne relation. Equation (7) allows us to calculate the *recombination cooling rate* $\Lambda[\rm erg\,s^{-1}cm^{-3}]$ analogous to Eq. (4)

$$\Lambda = n_{\rm A} n_{\rm B}\,\frac{n^\star_{\rm AB}}{n^\star_{\rm A} n^\star_{\rm B}}\,4\pi\int\limits_{\nu_{\rm thr}}^{\infty} B_\nu(T_{\rm g})\,\frac{\nu-\nu_{\rm thr}}{\nu}\,\sigma^{\rm f}(\nu)\,d\nu\ , \tag{8}$$

Obviously, $\Gamma = \Lambda$ in thermodynamical equilibrium, as required from first principles. The fraction $n^\star_{\rm AB}/(n^\star_{\rm A} n^\star_{\rm B})$ can, in principal, be determined from thermochemical data.

$$p^\star_{\rm AB} = p^\star_{\rm A}\,p^\star_{\rm B}\,k_p(T_{\rm g}) \tag{9}$$

which relates the partial pressures in thermodynamical equilibrium. $k_p(T_{\rm g})$ is the equilibrium constant of $\rm H^-$. Figure 1 shows an attempt to use Eq. (7) directly to calculate the recombination rate coefficient k_r which clearly shows some numerical problems at low temperatures where the integral goes to zero and the fraction $\frac{n^\star_{\rm AB}}{n^\star_{\rm A} n^\star_{\rm B}}$ goes to infinity. Also, the range of validity of the polynomial fit of k_p is clearly too narrow.

Therefore, we will rely on Eq. (5) rather than on Eq. (7) to compute the recombination rate coefficient k_r, also because these rates are deeply imbedded in ProDiMo's treatment of chemistry. However, we will indirectly use Eq. (7), in form of Eq. (8), to get a handle on $\langle E_{\rm th}\rangle$. Inserting Eq. (6) into Eq. (8) results in

$$\Lambda = \frac{n_{\rm A}\,n_{\rm B}\,k_r(T_{\rm g})}{k_f\big|_{J_\nu=B_\nu(T_{\rm g})}}\,4\pi\int\limits_{\nu_{\rm thr}}^{\infty} B_\nu(T_{\rm g})\,\frac{\nu-\nu_{\rm thr}}{\nu}\,\sigma^{\rm f}(\nu)\,d\nu\ , \tag{10}$$

where k_r is computed from Eq. (5). ProDiMo uses directly Eq. (10) to calculate recombination cooling rates. Figure 2 shows the results for $\rm H + e^- \rightarrow H^- + h\nu$, with the cross section data from Fig. 3, in units of $n_{\rm A} n_{\rm B} k_r(T_{\rm g}) kT_{\rm g}$, showing that the mean thermal energy destroyed by a direct recombination is roughly given by $\langle E_{\rm th}\rangle \approx (1.5-2.5)kT_{\rm g}$.

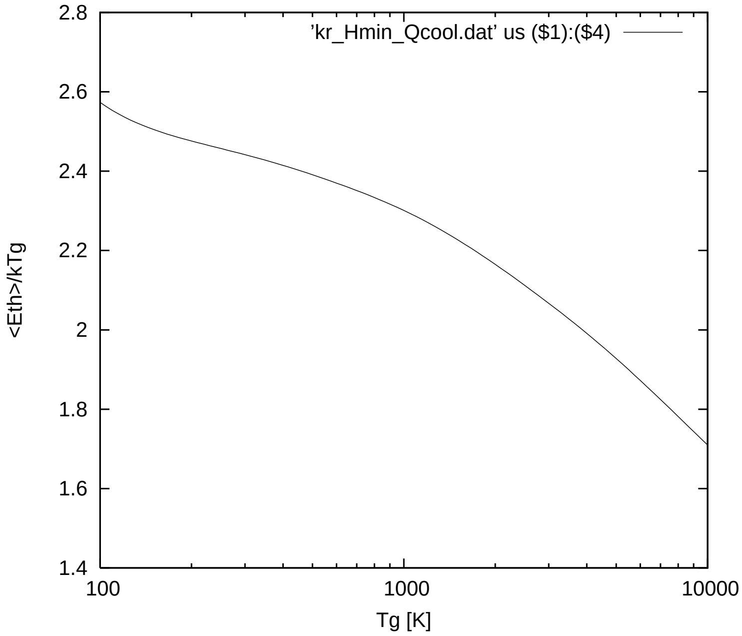

Figure 2: Mean thermal energy $\langle E_{\rm th}\rangle$ destroyed by a direct recombination of $\mathrm{H} + \mathrm{e}^- \rightarrow \mathrm{H}^- + \mathrm{h}\nu$ in units of $kT_{\rm g}$, according to Eq. (10).

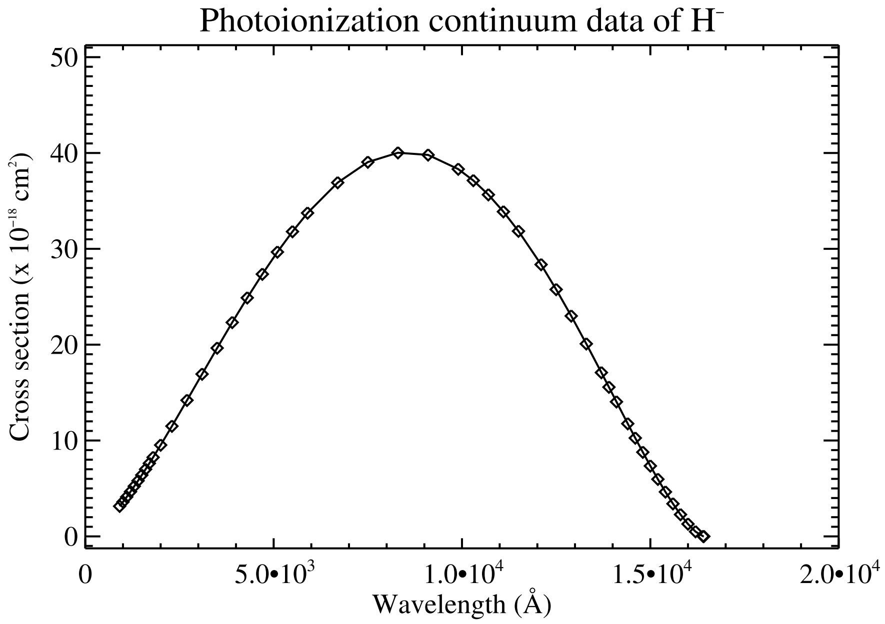

Figure 3: Bound-free ionisation cross-section $\sigma^f(\lambda)$ of the negative hydrogen ion H^- from Leiden's photoionisation database. Binding energy of H^- is $E_b = 0.755\,eV$, which corresponds to threshold wavelength $\lambda_{\rm thr} = 1.642\mu$m.

2 How does recombination cooling work?

Equations (4) and (10) are sufficient to calculate ionisation heating and recombination cooling rates, and ProDiMo uses them directly. However, these equations need some interpretation to understand what's going on. In kinetic chemical equilibrium, free electrons are destroyed and created at the same rate, and whether H^- bound-free and free-bound transitions cause radiative heating or cooling is given by the *difference between the thermal energies of created and destroyed free electrons.*

Let's assume that reaction (1) is in kinetical equilibrium, i. e. $n_{\rm AB} k_f = n_{\rm A} n_{\rm B} k_r$ (other reaction channels like $H^- + H \leftrightarrow H_2 + e^-$ are ignored in this section). What's the net (heating – cooling) rate $Q_{\rm net} = \Gamma - \Lambda$?

$$Q_{\rm net} = n_{\rm AB}\, 4\pi \int\limits_{\nu_{\rm thr}}^{\infty} J_\nu \frac{\nu - \nu_{\rm thr}}{\nu}\, \sigma^{\rm f}(\nu)\, d\nu \;-\; n_{\rm A} n_{\rm B} k_r \langle E_{\rm th}\rangle \tag{11}$$

Using the assumption of detailed kinetic equilibrium we find

$$Q_{\rm net} = n_{\rm AB} k_f \Big(\langle E_{\rm abs}\rangle - \langle E_{\rm th}\rangle \Big) \tag{12}$$

where

$$\langle E_{\rm abs}\rangle = \frac{\int_{\nu_{\rm thr}}^{\infty} J_\nu \frac{h\nu - E_b}{h\nu}\, \sigma^{\rm f}(\nu)\, d\nu}{\int_{\nu_{\rm thr}}^{\infty} J_\nu \frac{1}{h\nu}\, \sigma^{\rm f}(\nu)\, d\nu} = \frac{\int_{\nu_{\rm thr}}^{\infty} J_\nu\, \sigma^{\rm f}(\nu)\, d\nu}{\int_{\nu_{\rm thr}}^{\infty} J_\nu \frac{1}{h\nu}\, \sigma^{\rm f}(\nu)\, d\nu} - E_b \tag{13}$$

is the mean excess photon energy $\langle h\nu\rangle - E_b$ as weighted by the photo-cross section in a given radiation field J_ν. It is instructive to consider a dilute Planckian radiation field $J_\nu = W\, B_\nu(T_{\rm rad})$ in the Wien limit ($h\nu \gg kT_{\rm rad}$), i. e. $J_\nu \approx W\, \frac{2h\nu^3}{c^2} \exp(-h\nu/kT_{\rm rad})$. For this case, we can derive

$$\frac{\partial k_f}{\partial T_{\rm rad}} = \frac{\partial}{\partial T_{\rm rad}} 4\pi \int\limits_{\nu_{\rm thr}}^{\infty} W\, \frac{2h\nu^3}{c^2} \exp\Big(-\frac{h\nu}{kT_{\rm rad}}\Big) \frac{1}{h\nu}\, \sigma^{\rm f}(\nu)\, d\nu \tag{14}$$

$$= \frac{4\pi}{kT_{\rm rad}^2} \int\limits_{\nu_{\rm thr}}^{\infty} W\, \frac{2h\nu^3}{c^2} \exp\Big(-\frac{h\nu}{kT_{\rm rad}}\Big)\, \sigma^{\rm f}(\nu)\, d\nu \tag{15}$$

Identifying the terms in Eq. (13), we find

$$\langle E_{\rm abs}\rangle = \frac{kT_{\rm rad}^2 \frac{\partial k_f}{\partial T_{\rm rad}}}{k_f} - E_b \tag{16}$$