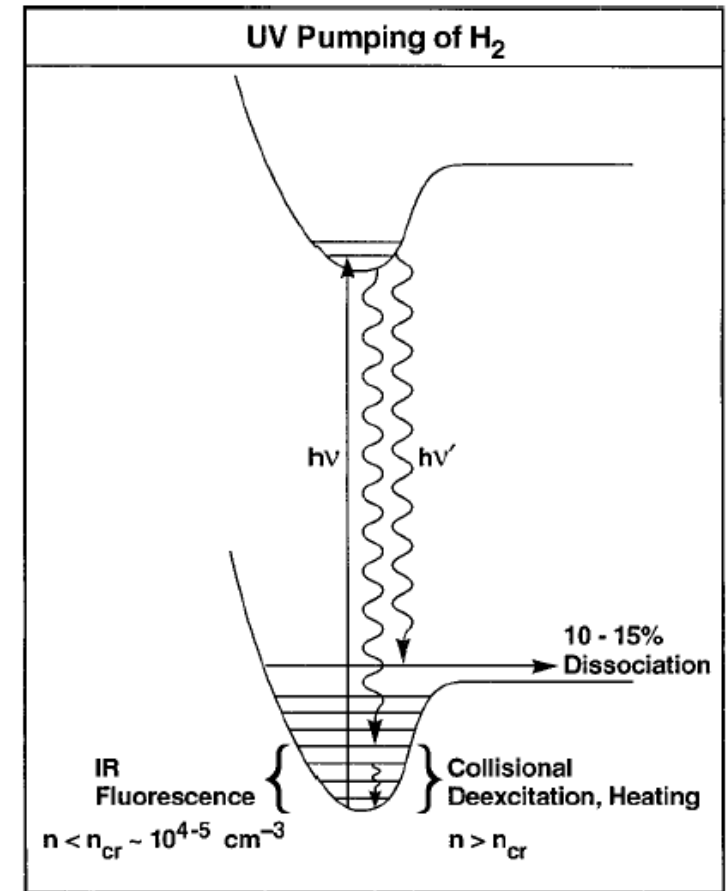# H$_2$ vibratonal heating (and cooling)

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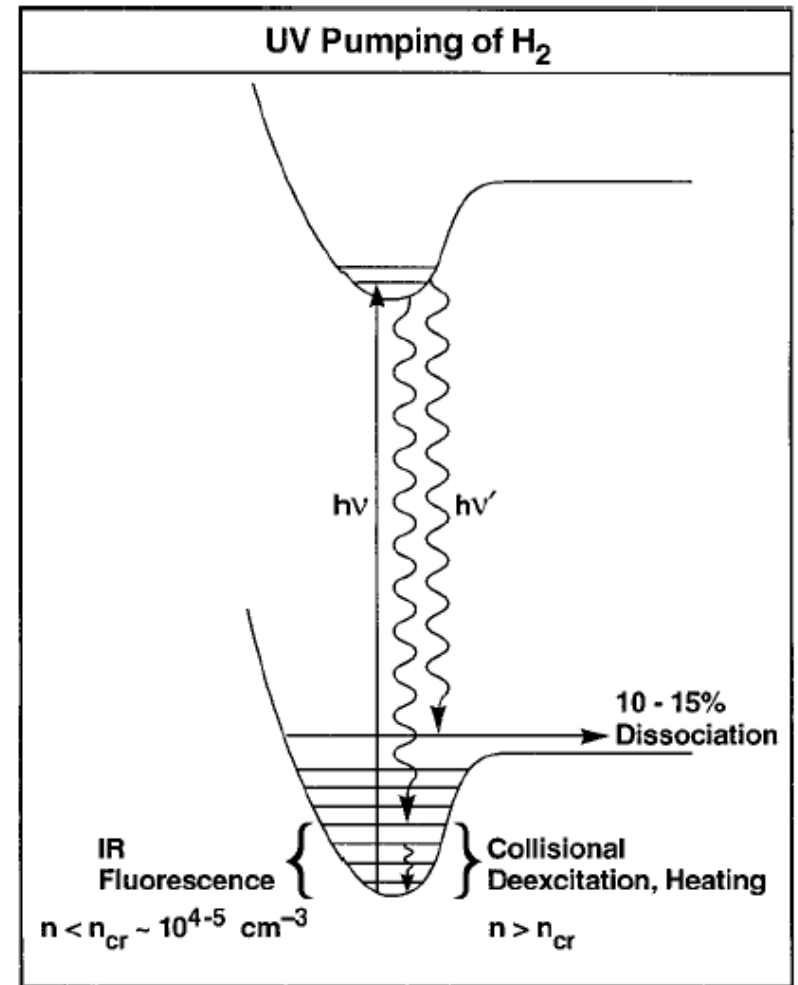

Hollenbach & Tielens (1999)

Basic principle

- UV radiative excitation of H_2 to an electronically excited state

- De-excitation by UV emission to a vibrationally (and rotationally) excited state

- De-excitation of the vibration level by spontaneous emission and collisions

- Collisions heat the gas

Complications:

- UV radiation may dissociate directly

- The electronically excited state may result in a dissociation.

- There are **many** possible transitions between the ro-vibrational levels.

Hollenbach & Tielens (1999)

Advantages of the H$_2$ molecule

- Vibration levels close to a harmonic oscillator, i.e. almost equidistant: $\Delta E = 4450 \pm 1500$ K for $v \leq 10$

- Only 15 vibrational levels

- Rotational transitions only with $\Delta J = 2$. All rotational transition coefficients are by far smaller than the vibrational coefficients.

- The main gas heating originates from vibrational transitions.

- Dominant spontaneous emission between neighbouring vibrational levels.

- Dominant collisional transitions as well between neighbouring levels.

Molecular hydrogen, H$_2$
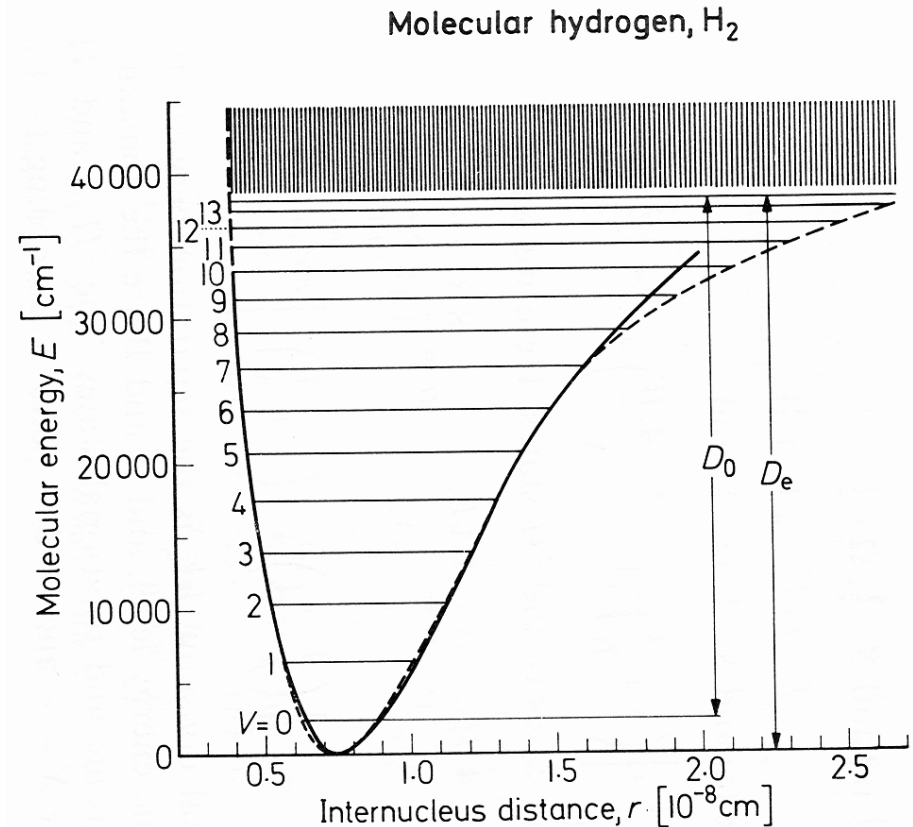
The two-level approximation

Hollenbach, Tielens, Burton (1985-1999)

Basic idea:
Put all excited levels into one virtual level at the average energy.

- Recombination heating is treated as separate process, so that re-combination virtually populates only the ground state.

- The resulting energy barrier of about 23000 K is so large that no exciting collisions occur.

- 10 % of the molecules are disso-ciated by the UV pumping, $R_D = 1/9 R_{pump}$
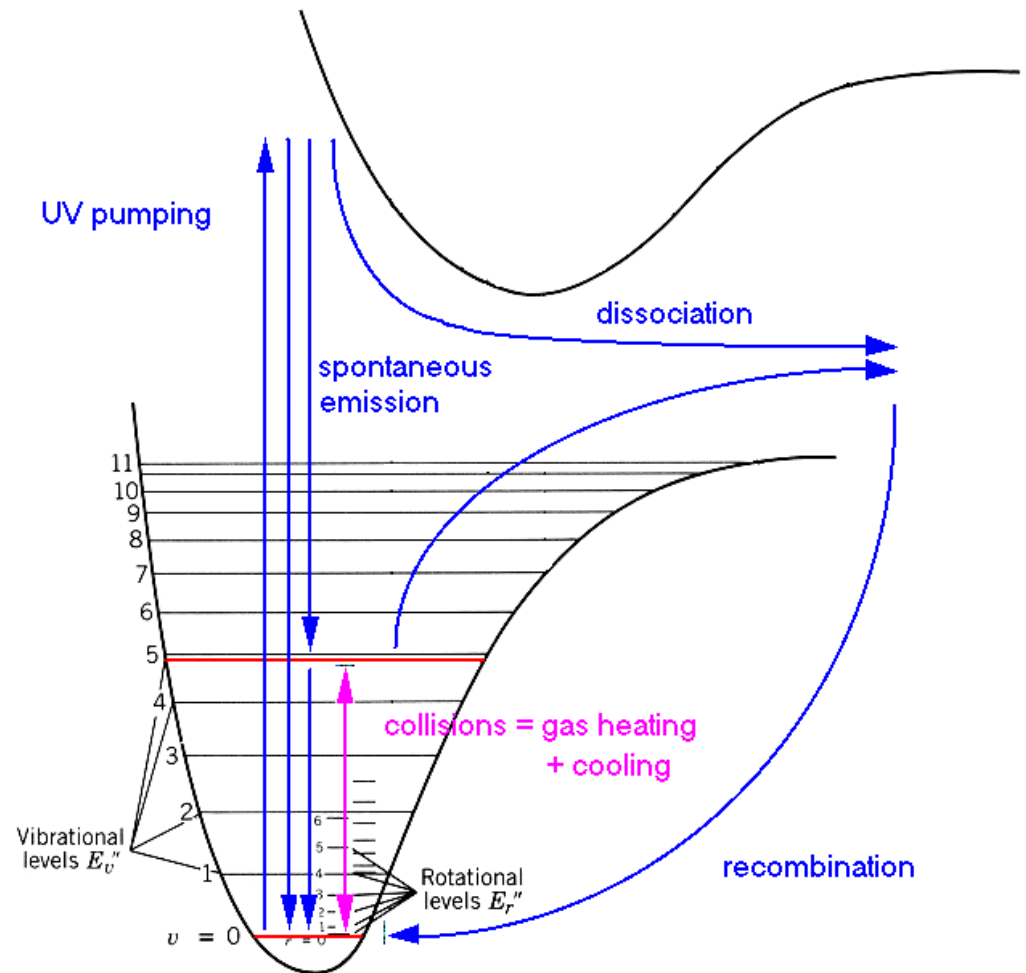
The two-level approximation

Balance equations:

$$n_{H_2}^* \left(\gamma_{\text{down}} n_{\text{gas}} + A + R_D^* \right) = n_{H_2} \times R_{\text{pump}}$$

$$n_{H_2} \left(R_{\text{pump}} + R_D \right) = n_H R_{\text{recomb}} n_{\text{gas}} + n_{H_2}^* \left(\gamma_{\text{down}} n_{\text{gas}} + A \right)$$

Level population:

$$n_{H_2}^* = \frac{9 n_H R_{\text{recomb}} n_{\text{gas}}}{\gamma_{\text{down}} n_{\text{gas}} + A + 10 \times R_D^*}$$

Resulting heating rate:

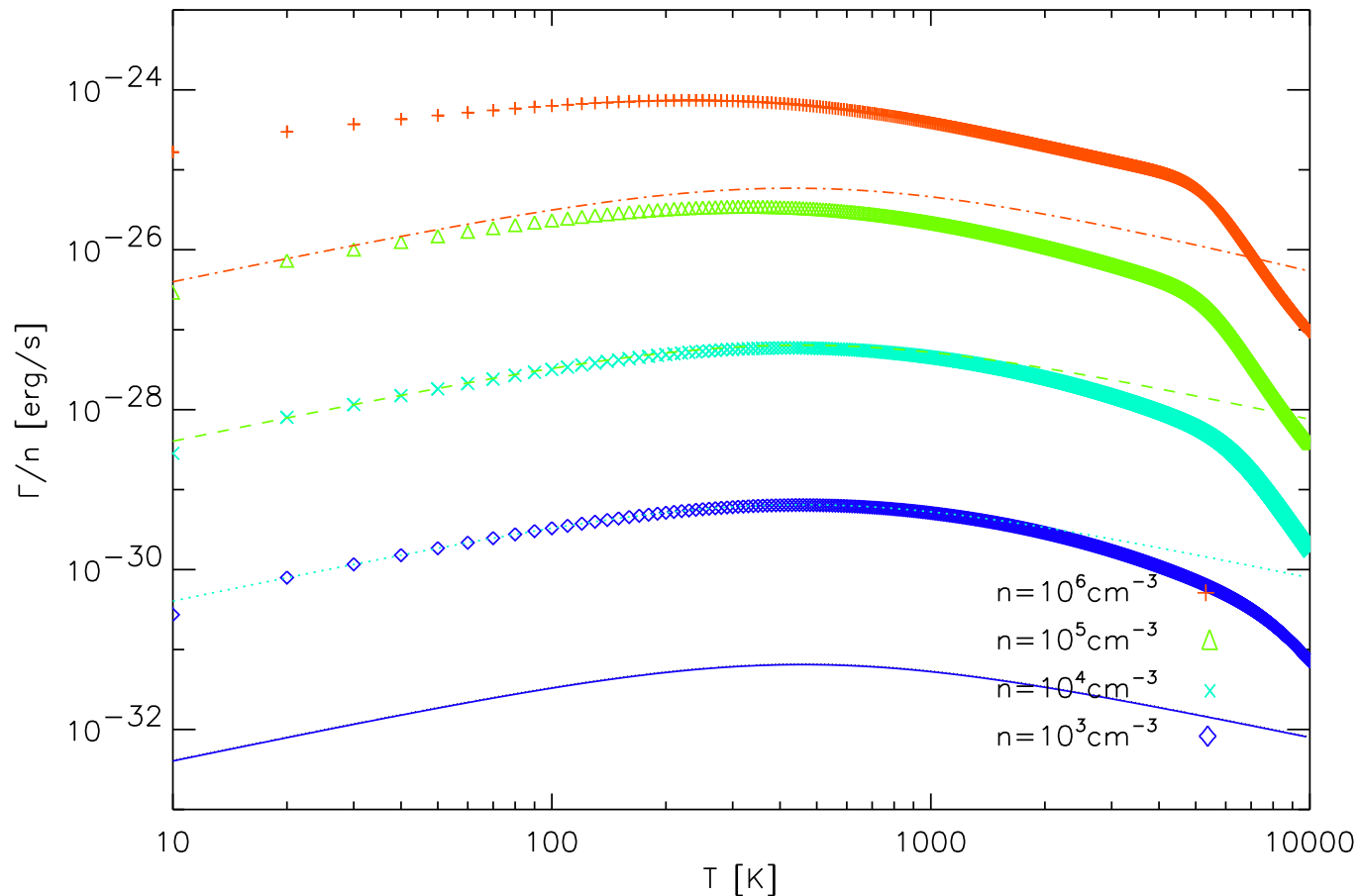$$\Gamma = \Delta E \, \gamma_{\text{down}} n_{\text{gas}} n_{H_2}^*$$

Advantage of the two-level approch:

Analytic solution – enables deeper insight into the governing physical rules.

**Disadvantage of the two-level approch:**

It is quantitatively wrong.

Comparison with the full treatment

Heating rate at the surface of a PDR from the analytic two-level solution (lines) and from the numeric model treating the full vibrational level structure of H_2 (dots) for a radiation field of $\chi = 10^6$ Draine fields and various densities.

Comparison with the full treatment
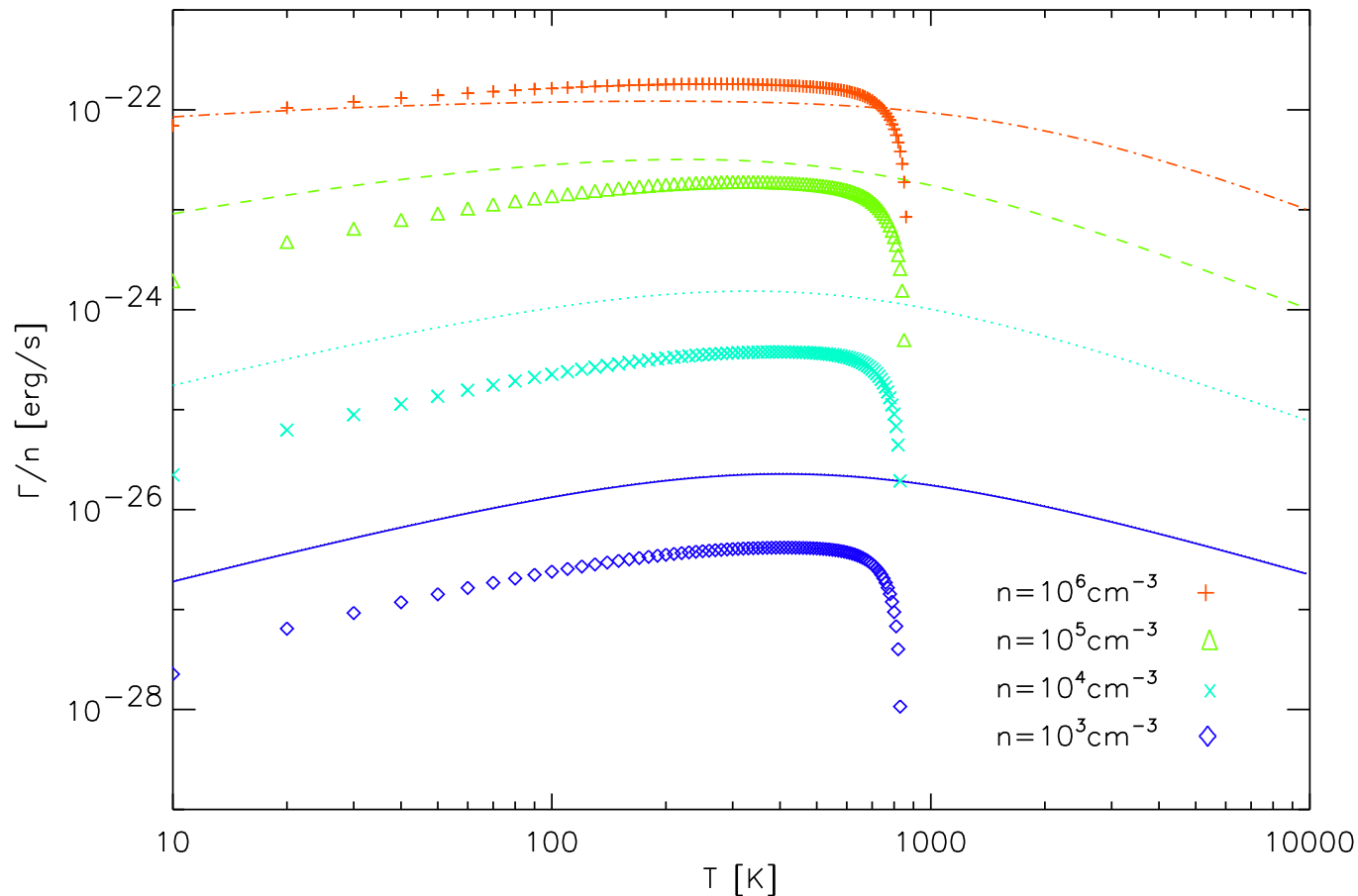
Comparison for $\chi = 1$.

Main problem:

The huge energy gap between ground state and the virtual excited level prevents collisional cooling. In the real system cooling by transitions to the first vibrationally excited state start to dominate at $T \geq 800$ K (see Sternberg & Dalgarono 1989).

Can we save the two-level treatment?
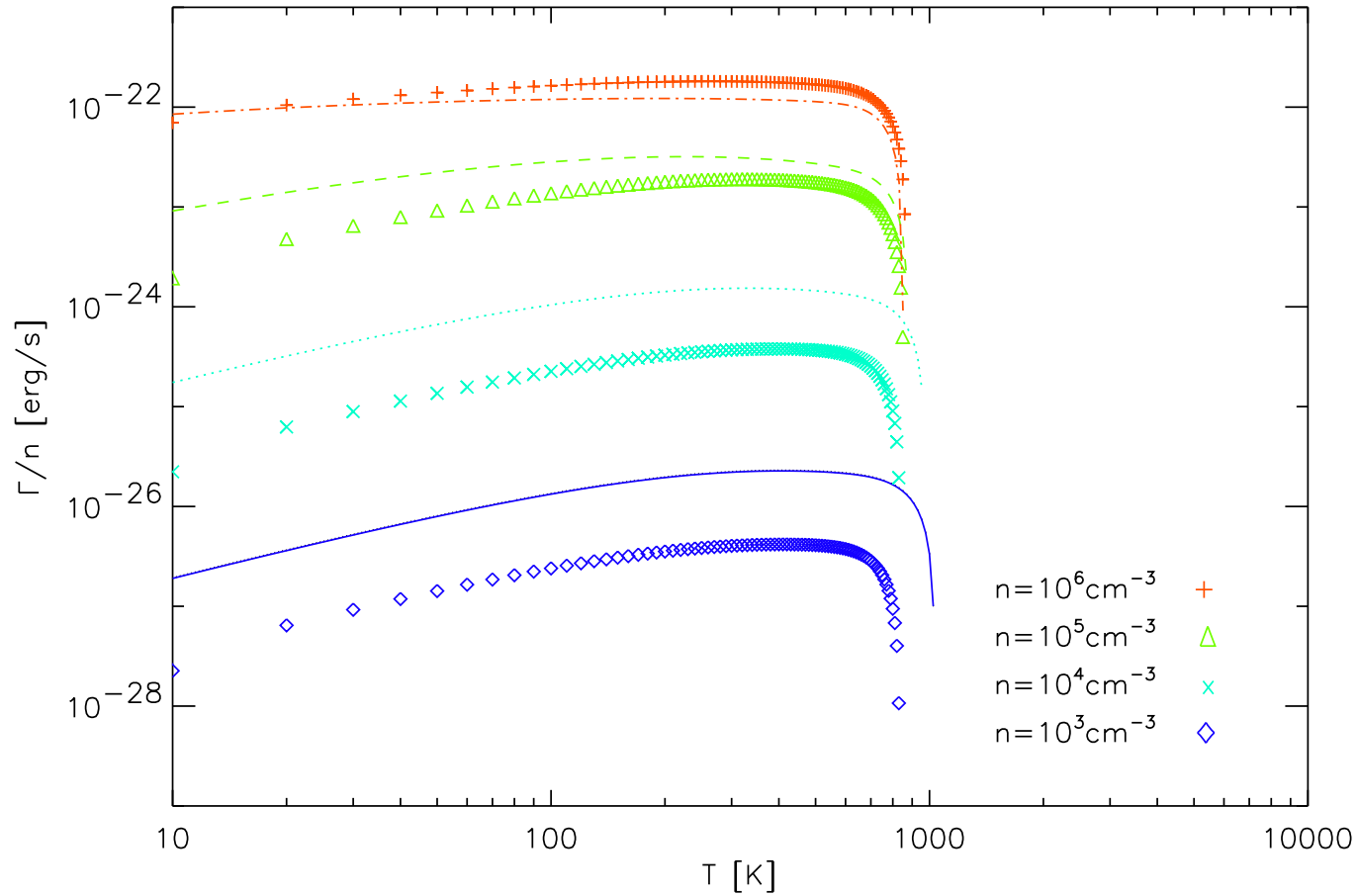
First step:

Add cooling

- 99 % of the H_2 is in the ground state. Only transitions from this state may contribute significantly to cooling.

- The effective cooling arises from those upward transitions that are eaten up by spontaneous emission or dissociation.

Cooling rate:

$$\Gamma_{\text{cool}} = -\Delta E_{1,0} \gamma_{1,0} \, \exp\left(\frac{-\Delta E_{1,0}}{kT}\right) \, n_{\text{gas}} n^*_{H_2} \frac{A_{1,0} + R_{D,1}}{\gamma_{1,0} n_{\text{gas}} + A_{1,0} + R_{D,1}}$$

Influence of cooling

H_2 vibrational heating rate at the surface of a PDR including the effect of vibrational cooling for a radiation field of $\chi = 1$.

Can we save the two-level treatment?

Second step:

Define the actually equivalent two-level molecule

Consider heating rate from the full system:

$$\Gamma = n_{\mathrm{H}_2} \sum_j \sum_{i \geq j} \frac{R_{\mathrm{pump}}(i) \times \Delta E(j)}{1 + [A(j) + R_{\mathrm{D}}(j)] / [\gamma(j) n_{\mathrm{gas}}]}$$

Equivalent two-level system heating:

$$\Gamma = n_{\mathrm{H}_2} \frac{R_{\mathrm{pump,tot}} \times \Delta E_{\mathrm{eff}}}{1 + [A_{\mathrm{eff}} + R_{\mathrm{D,eff}}] / [\gamma_{\mathrm{eff}} n_{\mathrm{gas}}]}$$

Determine constants from asymptotic behaviour

$n_{\text{gas}} \to \infty$:

$$R_{\text{pump,tot}} \times \Delta E_{\text{eff}} = \sum_j \sum_{i \geq j} R_{\text{pump}}(i) \times \Delta E(j)$$

$\implies \qquad \Delta E_{\text{eff}} = 9920 \text{ K}$

$n_{\text{gas}} \to 0, \chi \to \infty$:

$$\frac{\gamma_{\text{eff}} R_{\text{pump,tot}} \Delta E_{\text{eff}}}{R_{\text{D,eff}}} = \sum_j \sum_{i \geq j} \frac{R_{\text{pump}}(i) \Delta E(j) \gamma(j)}{R_{\text{D}}(j)}$$
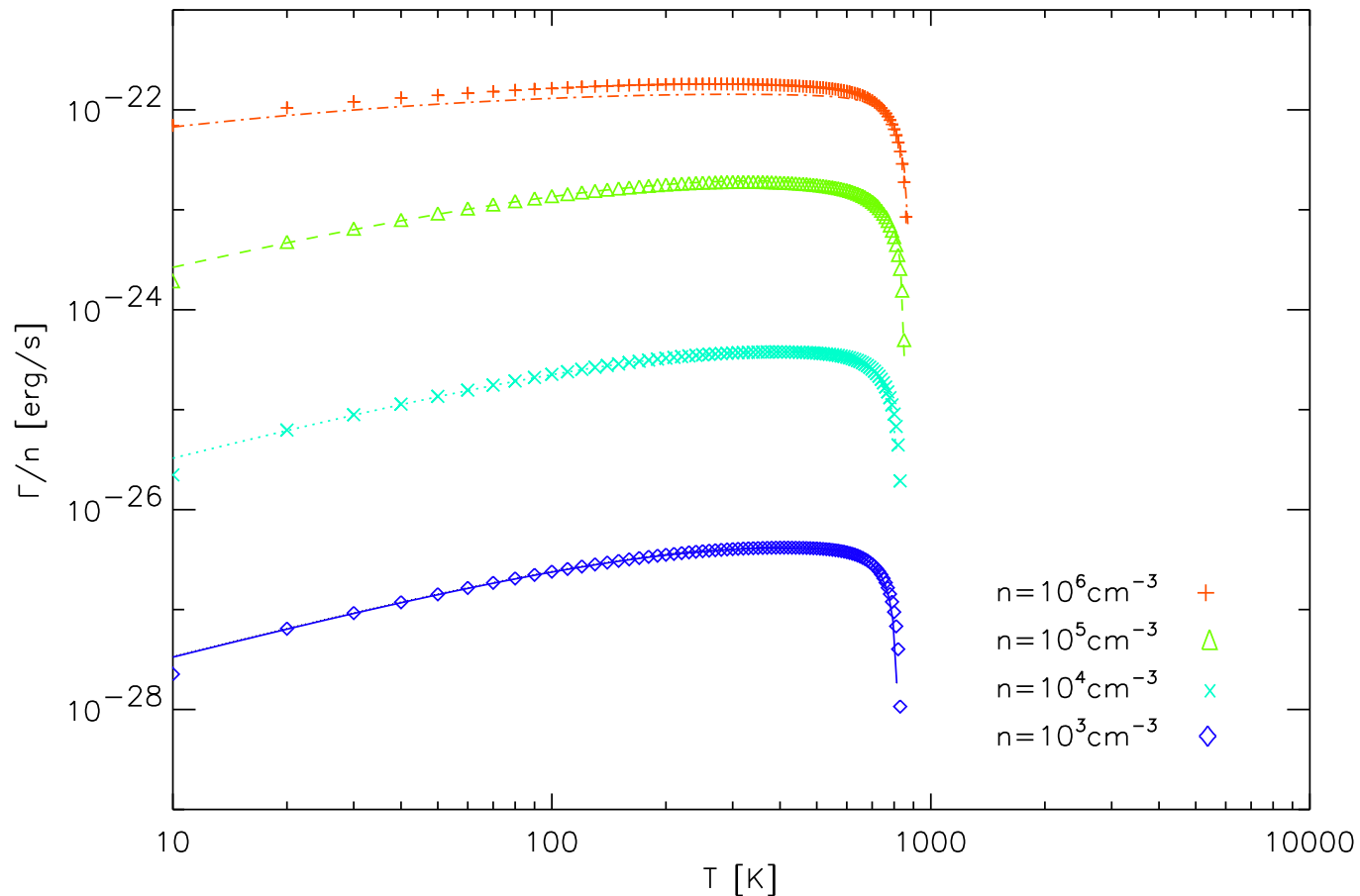
$\implies \qquad \gamma_{\text{eff}} = \gamma_{1,0}, \; R_{\text{D,eff}} = 9.1 \, 10^{-13} \text{s}^{-1} \chi$

$n_{\text{gas}} \to 0, \chi \to 0$:

$$\frac{\gamma_{\text{eff}} R_{\text{pump,tot}} \Delta E_{\text{eff}}}{A_{\text{eff}}} = \sum_j \sum_{i \geq j} \frac{R_{\text{pump}}(i) \Delta E(j) \gamma(j)}{A(j)}$$
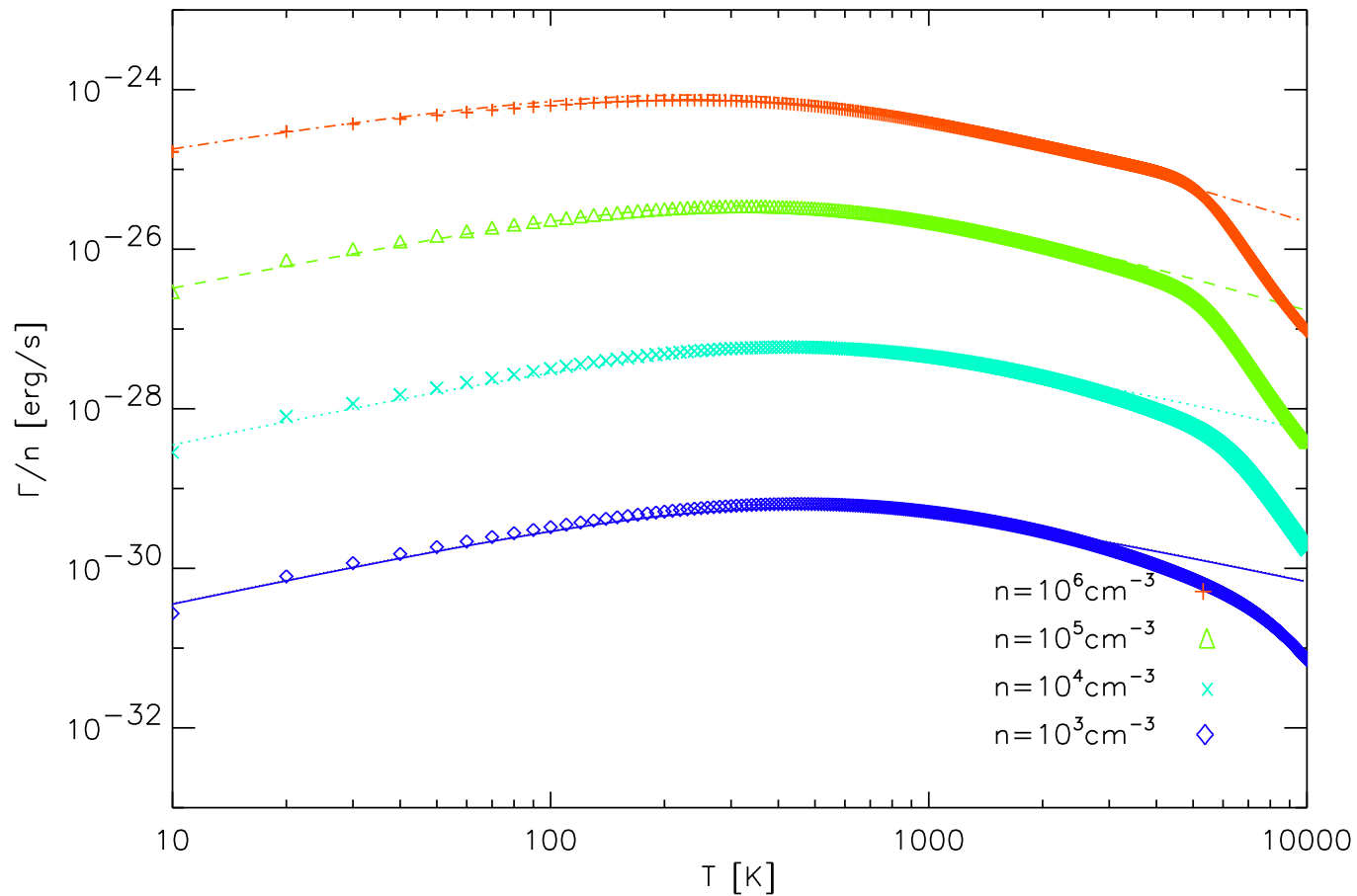
$\implies \qquad A_{\text{eff}} = 7.6 \, 10^{-6} \text{s}^{-1}$

Comparison with the full treatment

Heating rate at the surface of a PDR from the two-level solution with adjusted effective molecular parameters (lines) and from the numeric model treating the full vibrational level structure of H_2 (dots) for a radiation field of $\chi = 1$.

Comparison with the full treatment

Comparison for a radiation field of $\chi = 10^6$.

Conclusions

- It is actually possible to treat the energy balance with H_2 in terms of a two-level approximation:

  – Cooling and heating have to be treated independently

  – The constants for the cooling are determined by the lowest actual transition.

  – For the heating all transition parameters have to be computed as effective parameters (not only ΔE as by Burton et al.)

- The approximation works independently from the physical laws used for the temperature and radiation field dependence of γ, R_{pump}, and R_D.

- The approach can be applied in an equivalent way for the treatment of the full ro-vibrational system.

- **The error produced by the two-level approximation is small compared to the uncertainty of most of the entering quantities.**