Molecular Hydrogen

The self-shielding of H_2 can be treated (Tielens & Hollenbach 1985) through a one-line approximation, $R_{\rm diss} = R_0\beta(\tau)e^{-kA_V}$ with $k \approx 1.8$ for the FUV dust opacity. This is an approximation of the full H_2 treatment as in Black & van Dishoeck (1987) or Sternberg & Dalgarno (1989). One has

$$\beta(\tau) = \{\tau^{-1}[ln(\tau/\sqrt{\pi})]^{-0.5} + (b/\tau)^{0.5}\}erfc(\tau b\pi^{-1}v_1^{-2})^{0.5},$$

for the optical depth $\tau > 10$, $b = 9.2 \times 10^{-3}/\delta v$, $v_1 = 500/\delta v$, δv the turbulent Doppler line width in km/s, and with an approximate power series expansion for $\tau \leq 10$

$$\beta(\tau) = \Sigma_{n=0}^{\infty}\frac{(-1)^n\tau^n}{n!(n+1)^{1/2}\pi^{n/2}}.$$

Note that there is a correction for a sphere versus a slab geometry caused by the dust attenuation length of UV photons that is different (see Jürgen's comments) and that it is difficult to find a simple scaling for shielding effects because $G_0/n_{\rm H}$ alone does not determine the H-H_2 transition if the chemical and thermal balance are treated self-consistently.

An important issue is the impact of line overlap. It is unclear at this point in time whether the Draine & Bertoldi (1996) treatment of H_2 line overlap is sufficient when compared to Gary's 'big molecule' computation. This should be resolved. It is also important to assess the contribution of the many atomic lines that Gary includes and others do not (see also Gary's and Jacques' contributions in Marco's powerpoint presentation). In any case, for $G_0/n_{\rm H} > 1$ the importance of self-shielding is diminished and dust attenuation plays a greater role, rendering the one-line approximation better (see also Mark's and Jacques' comments in Marco's powerpoint presentation).

Photorates with Depth

As to photorates, one should determine thin rates with

$$\int I(\lambda)\sigma(\lambda)d\lambda,$$

where σ is the cross section for the photo-process, I is the radiation field and λ is the wavelength. The use of a fit is dangerous when the impinging radiation field is scaled only with total energy, say between 6-13.6 eV, while its spectral content also changes. It is important to realize that the impinging radiation field cannot always be parameterized accurately with the Draine or Habing radiation field because of the temperature of the illuminating star or the presence of strong absorption features when the stellar radiation field traverses circumstellar and interstellar matter (see John's comments).

Line Transfer

Finally, for line transfer it is important to realize that the geometry can have a big impact on the level populations. For example, an optically thick, effectively thin line has more population in its upper level for a sphere than for a slab, for the same temperature distribution, because the warm edge of a PDR subtends a larger solid angle in the spherical case. When the line optical depth becomes much larger than one, for an effectively thin line, significant differences can occur in the rate of convergence for Monte Carlo versus ALI methods. Any numerical tests in this respect should concentrate on the level populations rather than just the radiation temperature or total intensity.