How to take H_2 excited levels into account

Case 1: $50 < T_k < 500$ K

Hydrogen molecules (H_2) exist in two isomeric forms: para-hydrogen with total nuclear spin $I = 0$ and ortho-hydrogen with $I = 1$. In the ground electronic and vibrational state[1], the rotational levels of para-H_2 have even values of the angular momentum j while the levels of ortho-H_2 have odd j values. The ground-state of ortho-H_2 (j=1) lies 170 K above the ground-state of para-H_2 ($j = 0$).

In cold environments where the kinetic temperature T_k is lower than $\sim$50 K and in the absence of radiative pumping, only the ground-state of the two nuclear spin isomers are significantly populated so that only para-$H_2(j = 0)$ and ortho-$H_2(j = 1)$ need to be considered as collision partners. Moreover, the rate coefficients for ortho-$H_2(j = 1)$ are generally larger than those for para-$H_2(j = 0)$, by up to an order of magnitude.

At higher kinetic temperatures $T_k > 50$ K or in the presence of radiative pumping, H_2 molecules in excited levels $j = 2, 3$, etc. can become significant new colliders. It has been generally found, however, that the dominant collisional rate coefficients for $H_2(j > 1)$ differ by less than 20-30% from those for $H_2(j = 1)$ (e.g. Daniel et al. 2014 and references therein). This result holds for targets in their ground vibrational state and for target rotational levels or kinetic temperatures below ~ 500 K, i.e. below the opening of the H_2 level $j = 2$ at 510 K. In these conditions, rotation-rotation transfers between the target species and H_2 are negligible so that H_2 remains mostly in the same rotational state during the collision (i.e. $j \to j$).

EMAA provides de-excitation rate coefficients (in cm^3s^{-1}) due to collisions with 'para-H_2' and 'ortho-H_2' which in practice correspond to $H_2(j = 0 \to 0$) and $H_2(j = 1 \to 1)$, respectively (except otherwise stated). In order to include excited levels of H_2, rate coefficients for e.g. $H_2(j = 2 \to 2)$) can be assumed to be approximately equal to those for $H_2(j = 1 \to 1)$. **Thus, in radiative transfer calculations, the volume density (in cm^{-3}) affected to the 'para-H_2' collider should be that of $H_2(j = 0)$ while the volume density affected to the 'ortho-H_2' collider should be that of the sum of all levels of H_2 with $j > 0$.** A simple solution to estimate the H_2 level populations is to further assume that these levels are thermalized at the kinetic temperature, with a fixed or thermalized ortho-to-para ratio.

References
Daniel F., Faure A., Wiesenfeld L., Roueff E., Lis D. C, Hily-Blant P., *MNRAS* **444** 2544-2554 (2014)
Faure A., Lique F., Wiesenfeld L., *MNRAS* **460** 2103-2109 (2016)

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[1] The first vibrational level of H_2 opens at 4161.2 cm^{-1}.