

# An efficient statistical method to compute molecular collisional rate coefficients

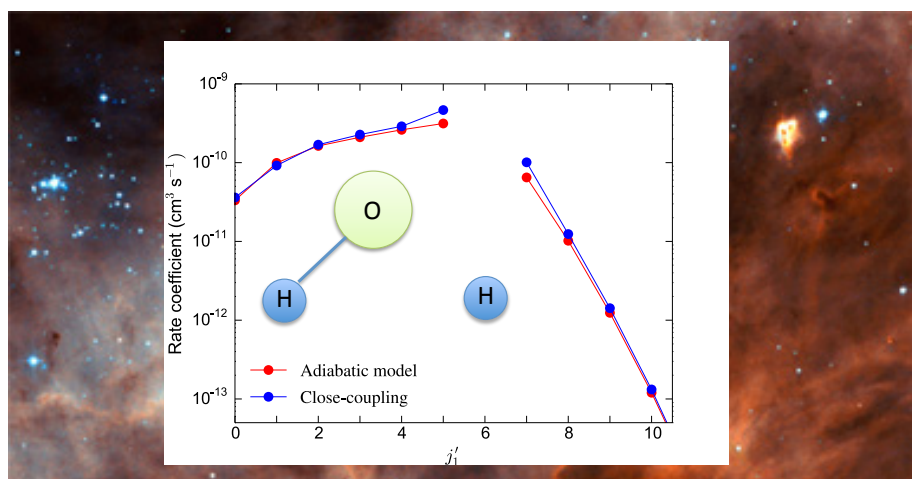
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Our knowledge about the “cold” universe often relies on molecular spectra. A general property of such spectra is that the energy level populations are rarely at local thermodynamic equilibrium. Solving the radiative transfer thus requires the availability of collisional rate coefficients with the main colliding partners over the temperature range 10–1000 K. These rate coefficients are notoriously difficult to measure and expensive to compute. In particular, very few reliable collisional data exist for inelastic collisions involving reactive radicals or ions. We have explored the use of a fast quantum statistical method [1] to determine molecular collisional excitation rate coefficients. The method is benchmarked against accurate (but costly) rigid-rotor close-coupling calculations. For collisions proceeding through the formation of a strongly bound complex, the method is found to be highly satisfactory up to room temperature. Its accuracy decreases with decreasing potential well depth and with increasing temperature, as expected. This new method opens the way to the determination of accurate inelastic collisional data involving key reactive species such as  $\text{H}_3^+$ ,  $\text{H}_2\text{O}^+$ , and  $\text{H}_3\text{O}^+$  for which exact quantum calculations are currently not feasible.



## Références

[1] Loreau et al., ApJL, 853, L5 (2018)