

Collisional excitation of H₂CO deuterated isotopologues by molecular hydrogen

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The deuteration fractionation is the molecular abundance ratio of a given hydrogenated molecule and its deuterated counterpart. It is a useful quantity to trace the physical and chemical evolution of star-forming regions [1]. The interpretation of observational spectra through radiative transfer modeling is the knowledge base for determining these abundances. Accurate rate coefficients, induced by collisions with H₂, are required to interpret spectra of these deuterated species. In this work, we focus on the deuterated isotopologues of formaldehyde (H₂CO), being an important precursor to the formation of interstellar complex organic molecules such as methanol [2]. We report the first rate coefficients for rotational transitions of HDCO and D₂CO in collision with both *ortho*- and *para*-H₂. Based on an accurate five-dimensional potential energy surface [3], collisional cross sections and rate coefficients are computed with the time-independent close-coupling method over a temperature range of 5–300 K. Our calculations include the first 60 energy levels of *ortho*-D₂CO and *para*-D₂CO; and the first 100 levels of HDCO. General propensity rules are discussed. We found a significant isotopic substitution effect in the rate coefficients. The present collisional data have found good agreement with pressure broadening experiments. The impact of the new set of collisional data will be investigated in radiative transfer modeling of the HDCO and D₂CO emissions seen toward star-forming sources.

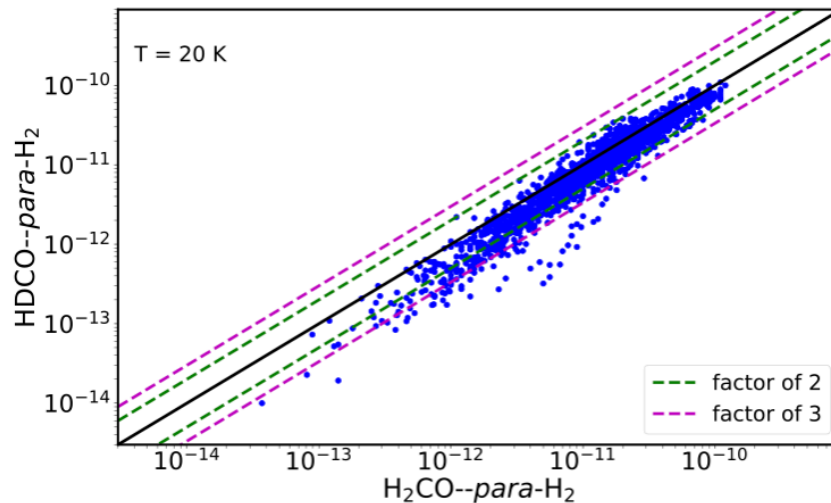


Figure 1: Systematic comparison of rate coefficients at 20 K between H₂CO and HDCO transitions induced by collisions with *para*-H₂.

References

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