P115a Collisional excitation of H_2CO 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 cheminal evolution of star-forming regions. The interpretation of observational spectra through radiative transfer modeling is the knowledge base for determining these abundances. Accurate rate coefficients, induced by collisions with H_2, are required to interpret spectra of these deuterated species. In this work, we focus on the deuterated isotopologues of formaldehyde (H_2CO), being an important precursor to the formation of interstellar complex organic molecules such as methanol. We report the first rate coefficients for rotational transitions of HDCO and D_2CO in collision with both ortho- and para-H_2. Based on an accurate five-dimensional potential energy surface, 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-D_2CO and para-D_2CO; 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 D_2CO emissions seen toward star-forming sources.