HYPERFINE EXCITATION OF $HC^{17}O^+$ WITH p-H_2 COLLISIONS

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The formyl ion (HCO^+) is one of the most abundant ions in molecular clouds and represents an excellent candidate to trace dense molecular gas through the evolutionary stages of the interstellar medium (ISM). For this reason, the accurate rotational rate coefficients of HCO^+ and its isotopes with the most abundant perturbing species in the ISM are crucial in non-local thermal equilibrium (LTE) models and deserve special attention. To this end, many efforts have been made in order to retrieve accurate collisional parameters of HCO^+ interacting with the He and H_2 colliders as well as for some of its isotopologues[a,b]. However, in spite of laboratory and observational studies on $HC^{17}O^+$[c,d], to the best of our knowledge, an accurate characterization of its collisional parameters has not been carried out yet. Although rarer, the $HC^{17}O^+$ isotope assumes a prominent role to avoid problems due to the optical thickness of the parent species emissions. With the aim of filling this lack, this work reports the first calculations of hyperfine resolved rate coefficients for the excitation of $HC^{17}O^+$ by p-H_2 ($J = 0$).

We characterized the potential energy surface of the HCO^+ and H_2 collisional system by means of the CCSD(T)-F12a/aug-cc-pVQZ level of theory. The interaction energy has been averaged over five H_2 orientations and then fitted as an expansion of angular functions. Finally, state-to-state rate coefficients between the lower hyperfine levels have been computed using recoupling techniques for temperature ranging from 5 to 100 K.

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