State-to-state rate coefficients for HCS+in rotationally inelastic collisions with H2at low temperaturas

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Abstract

HCS+ ions have been detected in several regions of the interstellar medium (ISM), but an accurate determination of the chemical-physical conditions in the molecular clouds where this molecule is observed requires detailed knowledge of the collisional rate coefficients with the most common colliders in those environments. In this work, we study the dynamics of rotationally inelastic collisions of HCS+ + H2 at low temperature, and report, for the first time, a set of rate coefficients for this system. We used a recently developed potential energy surface for the HCS+-H2 van der Waals complex and computed state-to-state rotational rate coefficients for the lower rotational states of HCS+ in collision with both para-and ortho-H2, analysing the influence of the computed rate coefficients on the determination of critical densities. Additionally, the computed rate coefficients are compared with those obtained by scaling the ones from HCS+ in collision with He (an approximation that is sometimes used when data is lacking), and large differences are found. Furthermore, the approximation of using the rates for the HCO+ + H2 collision as a rough approximation for those of the HCS+ + H2 system is also evaluated. Finally, the complete set of de-excitation rate coefficients for the lowest 30 rotational states of HCS+ by collision with H2 is reported from 5 to 100 K.

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Author keywords

astrochemistry; ISM: molecules; molecular data; molecular processes; scattering