Rotational relaxation of HCO^+ and DCO^+ by collision with H_2

Denis-Alpizar, O.
Stoecklin, T.
Dutrey, A.
Guilloteau, S.

Abstract
The HCO+ and DCO+ molecules are commonly used as tracers in the interstellar medium. Therefore, accurate rotational rate coefficients of these systems with He and H2 are crucial in non-local thermal equilibrium models. We determine in this work the rotational de-excitation rate coefficients of HCO+ in collision with both para- and ortho-H2, and also analyse the isotopic effects by studying the case of DCO+. A new four-dimensional potential energy surface from ab initio calculations was developed for the HCO+-H2 system, and adapted to the DCO+-H2 case. These surfaces are then employed in close-coupling calculations to determine the rotational de-excitation cross-sections and rate coefficients for the lower rotational states of HCO+ and DCO+. The new rate coefficients for HCO+ + para-H2 were compared with the available data, and a set of rate coefficients for HCO+ + ortho-H2 is also reported. The difference between the collision rates with ortho- and para-H2 is found to be small. These calculations confirm that the use of the rate coefficients for HCO+ + para-H2 for estimating those for HCO+ + ortho-H2 as well as for DCO+ + para-H2 is a good approximation.

Author keywords
Astrochemistry
ISM: molecules
molecular data
molecular processes
scattering