Rotational Transitions of HOC+ Induced by Collision with He at Low Temperatures

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The HOC+ molecule has for long been detected in several regions of the interstellar medium (ISM). The collisional ro-vibrational rate coefficients of this molecule with the most common colliders in the ISM are then required for applying nonlocal thermal equilibrium models. However, this molecule has a low bending frequency (249 cm-1), and the use of the rigid rotor approximation is therefore limited to low collision energies. Also, the complete determination of the ro-vibrational rate coefficients of HOC+ in collision with He requires including the bending motion in the analytical model of the potential energy surface (PES) of the system. The first goal of this work is then to develop the first rigid bender four-dimensional PES for the interaction between HOC+ and He. To this aim, a large grid of ab initio energies are computed at the CCSD(T)-F12b/aug-cc-pVQZ level of theory and an analytical representation of the PES is obtained using a combination of least square and reproducing kernel Hilbert space procedures. The global minimum of this PES is found to be reached for a linear configuration of the complex. In the second part of this study, rigid rotor close-coupling calculations are performed at low collision energy, and the calculated rate coefficients are compared to those previously determined for the collisions of He with its HCO+ isomer. Copyright © 2019 American Chemical Society.