Study of the CF+ formation from the HF + C+ → CF+ + H reaction at energies of astrophysical interest and the interaction of vibrating CF+ with He.

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Abstract

The recent detections of the carbon monofluoride cation (CF+) in galactic and extragalactic regions have increased the interest in the chemistry of this system. This species considered the second reservoir of fluorine in regions where C+ is abundant, has been proposed as a tracer of C+ in photo-dissociation regions and dense core environments [1, 2]. Furthermore, a correct interpretation of the astronomical observations requires the rate coefficients with the most common colliders in the ISM (e.g. He, H2, H). The CF+ molecule can be formed from the reaction of HF with C+ [3]. However, in exothermic reactions like HF + C+ → CF+ + H, even from the ground vibrational state of the reactant diatomic molecule (e.g. HF), the product diatom (e.g. CF+) can be in an excited vibrational state [4]. Therefore, this work focuses on the study of the CF+ formation from the HF + C+ reaction and the interaction of vibrating CF+ with He. First, we develop a potential energy surface (PES) for the HF + C+ at the MRCI+Q/aug-cc-pVQZ level of theory, where the correct R-4 asymptotic behavior is taking into account in the fitting procedure. The dynamics of the system is studied using quasi-classical trajectory and time-independent quantum reactive scattering calculations. The results using both, classical and quantum methods, are compared. Second, the He + CF+ interaction in full dimensionally at the close-coupling level is investigated. A set of CCSD(T)/aug-cc-pv5z ab-initio interaction energies was computed, and a new three-dimensional potential energy surface (PES) is represented using a reproducing kernel Hilbert space (RKHS). The vibrational quenching cross sections were found to be at least six orders of magnitude lowers than the pure rotational cross sections at collision energies lower than 1000 cm-1. Finally, the hyperfine rate coefficients are explored. The data here computed can be useful for the determination of the interstellar conditions where this molecule has been detected.

References

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