Rotational relaxation of CF+(X1?) in collision with He(1S)

Denis-Alpizar O.

Inostroza N.

Palacio J.C.C.

The carbon monofluoride cation (CF+) has been detected recently in Galactic and extragalactic regions. Therefore, excitation rate coefficients of this molecule in collision with He and H2 are necessary for a correct interpretation of the astronomical observations. The main goal of this work is to study the collision of CF+ with He in full dimensionality at the close-coupling level and to report a large set of rotational rate coefficients. New ab initio interaction energies at the CCSD(T)/aug-cc-pv5z level of theory were computed, and a three-dimensional potential energy surface was represented using a reproducing kernel Hilbert space. Close-coupling scattering calculations were performed at collisional energies up to 1600 cm-1 in the ground vibrational state. The vibrational quenching cross-sections were found to be at least three orders of magnitude lower than the pure rotational cross-sections. Also, the collisional rate coefficients were reported for the lowest 20 rotational states of CF+ and an even propensity rule was found to be in action only for j > 4. Finally, the hyperfine rate coefficients were explored. These data can be useful for the determination of the interstellar conditions where this molecule has been detected. © 2016 The Authors.

Astrochemistry

ISM: molecules

Molecular data

Molecular processes

Scattering