Rotational relaxation of CF+ by collision with para-H2

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The recent detections of CF+ and its proposition as a tracer of fluorine and C+ in the interstellar medium (ISM) have increased the interest in this system. For a correct interpretation of physical-chemical conditions of the regions where this molecule is observed, its collisional rate coefficients with the most common colliders of the ISM are required. The main goal of this work is to study the collision of CF+ with para-H2 (j = 0) and report a large set of rotational rate coefficients for this system. A new averaged potential energy surface (PES) from ab initio energies at the CCSD(T)-F12/aug-cc-pVTZ level of theory was developed for this work. Close-coupling scattering calculations were performed for the lowest 20 rotational levels of CF+. The rotational rate coefficients from 10 K to 300 K are reported. Discrepancies of these new rates with those estimated from CF+ + He were found for both magnitude and propensity rules. For CF+ + para-H2, ?j =-1 have the most significant values, and the rates decrease with the increment of ?j. The new data here determined can be useful for modeling the conditions of the ISM where CF+ has been observed.

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ISM: molecules

molecular data

molecular processes

scattering