

Collisional Quenching of Rotationally Excited CS ($^1\Sigma^+$) by H^+

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Rate coefficients for state-to-state rotational transitions in H^+ collision with CS have been obtained using accurate quantum dynamical close-coupling calculations useful in understanding the CS chemistry in interstellar space and studying molecular properties near quantum degeneracy. Charge transfer processes have been investigated using time-dependent wave packet dynamics between one-dimensional ground and low-lying excited states potential energy curves of H approach towards CS^+ . [1] Accurate three dimensional *ab initio* potential energy surfaces have been computed for the ground state and low-lying excited states of $H^+ - CS (^1\Sigma^+)$ system using MRCI/aug-cc-pVQZ methods. Rotational excitation and quenching integral cross sections have been computed at low and ultra low collision energies, respectively. Resonances have been observed at very low energies typically below 50 cm^{-1} . Among all the transitions, $\Delta j=+1$ and $\Delta j=-1$ are found to be predominant for excitation and quenching, respectively. Quenching cross section in the ultracold region is found to obey Wigner's threshold law. The excitation cross section obtained using vibrationally averaged potential show rotational rainbow maximum for $j'=2$ state. Mean lifetime of rotationally excited CS trap estimated using unimolecular kinetics is found to be 550 ns with effective quenching rate of $2 \times 10^7\text{ s}^{-1}$ due to the H^+ collision at microkelvin temperature indicating good collisional quenching efficiency of the system.

References

(1) Kaur, R.; Kumar, T. J. D. *Mol. Phys.* **2015**, 113, 3271-3281.