Ultracold rotational quenching of NCCN collision with ^{3}He and ^{4}He

Sanchit, Apoorv Kushwaha, Rajwant Kaur and T. J. Dhilip Kumar
Department of Chemistry, Indian Institute of Technology Ropar, India
E-mail: sanchit.chhabra@iitrpr.ac.in

Abstract

Quantum mechanical scattering calculations[1] are performed for the rotational quenching of NCCN in collision with ^{3}He and ^{4}He using the close-coupling approach for collision energies between 10^{-6} and 200 cm^{-1}. Rotational quenching cross sections are computed in the ultracold region for rotational levels up to j = 8 using the He + NCCN potential energy surface[2] computed at CCSD(T)/aug-cc-pVQZ level of theory[3]. By averaging the cross sections over a Boltzmann distribution of velocities of the incoming ion, rate coefficients are obtained. Wigner threshold law[4] is found to be valid in ultracold regime where the cross-section exhibit inverse relation to kinetic energy. To further analyse the isotopic effect of He, we also computed the scattering lengths for rotational level of NCCN in the limit of zero temperature. The imaginary part of scattering length[5] is found to be very large for ^{3}He-NCCN. The results presented here will benefit future experimental studies of these or similar systems as methods to cool and trap neutral molecules.

Reference(s)

1. M. H. Alexander, and D. E. Manolopoulos, *J. Chem. Phys.* **86**, 2044 (1987).
2. S. Chhabra, A. Kushwaha, and T. J. Dhilip Kumar, *J. Chem. Phys.* 149, 174312 (2018).
3. T. H. Dunning Jr., *J. Chem. Phys.* **90**, 1007 (1989).
4. E. P. Wigner, *Phys. Rev.* **73**, 1002 (1948).
5. N. Balakrishnan, V. Kharchenko, R. C. Forrey, and A. Dalgarno, *Chem. Phys. Lett.* 280, 5 (1997).