Nonlocal complex potential theory of dissociative electron attachment: Inclusion of two vibrational modes

HARINDRANATH AMBALAMPITIYA, ILYA FABRIKANT, University of Nebraska - Lincoln — Dissociative electron attachment (DEA) process is important for many applications in plasma industry and radiation damage [1]. Theory of DEA to polyatomic molecules often includes a single vibrational mode in the target molecule, with all the other modes being “frozen”. In the local approximation [2] of DEA, the nuclear motion of the intermediate negative-ion state is described by a Schrödinger equation with a local complex potential which is an approximation to a non-local energy-dependent complex operator [3]. Previous non-local DEA calculations assumed only one nuclear degree of freedom in the target molecule. In the present paper we extend the non-local theory by inclusion of two or more degrees of freedom in the target molecule. The theory is then applied to DEA to the CF₃Cl molecule by inclusion of the C-Cl symmetric stretch and CF₃ “umbrella” modes. The DEA cross section for specific vibrational states and temperature-averaged cross sections are obtained and compared with the previous theoretical results and experiments. ¹ I. I. Fabrikant et al., Adv. At., Mol., Opt. Phys. 66, 545 (2017). ² D. T. Birtwistle and A. Herzenberg, J. Phys. B: At. Mol. Phys. 4, 53 (1971). ³ J. N. Bardsley, J. Phys. B: At. Mol. Phys. 1, 349 (1968)

¹National Science Foundation

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Date submitted: 27 May 2019

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