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Quantum and semiclassical cross section of dissociative electron attachment to polyatomic molecules.[1] HARINDRANATH AMBALAMPITIYA, ILYA FABRIKANT, University of Nebraska - Lincoln — The exact treatment of dissociative electron attachment (DEA)[1] to a polyatomic molecule is computationally challenging when the target molecule has more than one vibrational mode. The local approximation (or the boomerang model) has been applied to a few polyatomic molecules in the past. However, in many situations, particularly at low electron energies, the local approximation breaks down, and DEA cross sections should be calculated using the non-local complex potential (NLCP)[2] theory. In this report we develop the NLCP theory with inclusion of more than one mode of vibrations in the target molecule. In addition to the full quantum treatment, we also develop a semiclassical approach to computing multimode DEA cross section by expressing the electron capture amplitudes and the matrix elements of the Green's function by their semiclassical approximations. We then apply these theories to a generic molecule of the type CY_3X and include only the symmetric C-X and CY_3 deform ("umbrella") vibrations. Finally, we present and compare the DEA cross sections for CF_3Cl obtained via both non-local and semiclassical approaches. [1]I. I. Fabrikant *et al.*, Adv. At., Mol., Opt. Phys. 66, 545 (2017). [2] J. N. Bardsley, J. Phys. B: At. Mol. Phys. 1, 349 (1968).

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