

Simplified model to treat the dissociative electron attachment of complex molecules

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We present a theoretical approach to evaluate cross sections for dissociative electron attachment to polyatomic molecules. Starting from the Bardsley-O'Malley theory developed for diatomic targets, we extend the formalism of resonant scattering to polyatomic molecules. Variation of resonance energies with respect to normal coordinates of the molecules allows us to introduce a generalized dissociation coordinate. Using the local complex potential model, the present *ab initio* model gives a reasonable estimate for dissociative attachment cross sections with modest computational efforts. The model is applied to the H₂CN and NO₂ molecules. The former molecule is considered as a precursor in the formation of the CN⁻ anion observed in the IRC +10216 carbon star. The computed rate coefficient suggests that the dissociative electron attachment of H₂CN may not be an efficient reaction to form CN⁻ in the circumstellar envelope of IRC +10216. The NO₂ molecule is important in depollution of combustion and in decontamination of food. The obtained cross section for NO₂ agrees well with experimental results.

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