Ab initio Study of Dissociative Electron Attachment to ClCN and BrCN

J. ROYAL, Department of Applied Science, University of California at Davis, California 95616, A. E. OREL — ClCN and BrCN are pseudobihalogens, that is both CN and Cl/Br have positive electron affinities. This means that dissociative electron attachment is possible into two final fragment channels, CN\(^{-}\) and Cl\(^{-}\)/Br\(^{-}\). The resonance parameters for this system are obtained from electron scattering calculations using the Complex Kohn Variational method. These resonance parameters are used as input into both a time-dependent wave packet calculation and a time-independent calculation using the discrete variable representation and exterior complex scaling. The calculated cross sections will be reported and compared to available experiment. Work supported by the NSF PHY-02-44911 and from The Center for Biophotonics, an NSF Science and Technology Center PHY 0120999.

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