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Dissociative Electron Attachment to ClCN and BrCN J. ROYAL,

A.E. OREL, Department of Applied Science, University of California at Davis, California 95616 — ClCN and BrCN are pseudobihalogens. They have the interesting property that since both fragments, CN and Cl/Br, have positive electron affinities, two fragment channels are open. This means that dissociative electron attachment is possible into both CN⁻ and Cl⁻/Br⁻ channels. The resonance parameters for these systems are obtained from electron scattering calculations using the Complex Kohn variational method. These resonance parameters are used as input into a full three dimensional wave packet calculation using the multi-configuration time-dependent Hartree (MCTDH) method. The resonances leading to dissociation into the product channels will be discussed and 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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