BONDING AND DYNAMICS OF CN−Rg AND C_2−Rg COMPLEXES

MICHAEL C. HEAVEN, *Department of Chemistry, Emory University, Atlanta, GA 30322*.

The van der Waals complexes of CN and C_2 with rare gas atoms (Rg) are of interest from the perspectives of their bonding characteristics and predissociation dynamics. Matrix isolation data indicate that that the bonding ranges from a weak van der Waals interaction for the Ne complexes to incipient chemical bonding for Xe. The low-lying vibronic states of CN and C_2 are interleaved, which facilitates electronic energy transfer. Consequently, electronic predissociation of CN−Rg and C_2−Rg complexes provides a useful means to examine the detailed dynamics of electronic energy transfer. Predissociation processes for CN−Rg complexes have been characterized using double resonance techniques. The final state distributions exhibit symmetry preferences that yield insights concerning the topologies of the relevant potential energy surfaces. In addition, bond energies can be deduced from the predissociation dynamics. Data for the binary complexes CN−Rg (Rg=Ne, Ar, Kr, and Xe) and C_2−Rg will be presented, along with theoretical analyses based on $ab\ initio$ potential energy surfaces.