RO-VIBRATIONAL EIGENSTATES OF H_2CN VAN DER WAALS COMPLEX

A. L. KALEDIN, M. C. HEAVEN, E. KRYACHKO, and J. BOWMAN, *Cherry L. Emerson Center for Scientific Computation and Department of Chemistry Emory University, Atlanta, GA 30322*.

Ab initio calculations have been performed on the H_2...CN Van der Waals complex. An analytical potential, which included functions up to fourth order Legendre polynomial, was fitted to the 3D potential energy surface calculated at Gauss-Legendre quadrature points. This analytical potential will be used to solve for the bound ro-vibrational eigenstates of the Van der Waals complex in order to analyze experimentally observed rotational structure. Details of the potential energy surface and results of ro-vibrational energy level calculations will be presented.