RO-VIBRATIONAL EIGENSTATES OF H_2CN VAN DER WAALS COMPLEX

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$Ab\ initio$ 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.