THE AB INITIO CALCULATION OF THE $C_3 - AR$ VAN DER WAALS COMPLEX

BON-GI LIN, SHIH-MING WEN, A. MEBEL, AND YEN-CHU HSU, *INSTITUTE OF ATOMIC AND MOLECULAR SCIENCES, ACADEMIA SINICA, P. O. BOX 23-166, TAIPEI 107, TAIWAN, R. O. C.*.

The equilibrium geometry of the ground electronic state of $C_3 Ar$ has been determined to be T-shaped at the level of CCSD(T)/cc-pVQZ: $\ell(C-C)$=1.298Å, $\angle C-C-C$=173.75°, $\ell(C_3-Ar)$=3.85Å, $\angle C_3-Ar$=90°. Its binding energy is about 130 $\mathrm{cm}^{-1}$and the vdW stretch is 30 cm^{-1}. The internal rotation of the complex is strongly coupled with the vdW stretch. Other conformers (two in-plane and one out-of-plane) have been identified as the C_3 moiety of the complex bends away from the equlibrium angle. The computation results will be used to qualitatively interpret our experimental observations.