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

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The equilibrium geometry of the ground electronic state of C_3Ar 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.