INFRARED SPECTRA AND *AB INITIO* POTENTIAL ENERGY SURFACES FOR ACETYLENE COMPLEXED TO Mg ATOMS AND CLUSTERS

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We have recently developed a technique to measure high-resolution infrared spectra of molecules attached to metal atoms and clusters. Using this technique, the spectrum of the CH stretching band of the acetylene-Mg van der Waals complex has been measured in superfluid liquid ^{4}He droplets. A pure b-type band was observed, indicating that the vibrationally averaged structure of the complex is T-shaped, with the Mg atom binding to the π-cloud of the acetylene. Spectral bands corresponding to acetylene-Mg_n (n=2-4) complexes were also observed. Structural interpretations based on these spectra will be discussed. High level [CCSD(T)/6-311++G(3df,3pd)] *ab initio* potential energy surfaces were also constructed for these complexes, and structural predictions based on these calculations will be compared with the experimentally determined structures.