

## EXPERIMENTAL DETECTION AND THEORETICAL CHARACTERIZATION OF THE H<sub>2</sub>-NH(X) VAN DER WAALS COMPLEX

W. M. FAWZY, G. KERENSKAYA, and M. C. HEAVEN, *Department of Chemistry and Cherry L. Emerson Center for Scientific Computation, Emory University, Atlanta, GA 30322.*

The H<sub>2</sub>-NH(X) van der Waals complex has been examined using ab initio theory and detected via fluorescence excitation spectroscopy of the  $A^3\Pi - X^3\Sigma^-$  transition. Electronic structure calculations show that the minimum energy geometry corresponds to collinear H<sub>2</sub>-NH(X), with a well depth of  $D_e=116\text{ cm}^{-1}$ . The potential energy surface supports a secondary minimum for a T-shaped geometry, where the H atom of NH points towards the middle of the H<sub>2</sub> bond ( $C_{2v}$  point group). For this geometry the well depth is  $73\text{ cm}^{-1}$ . Laser excitation spectra for the complex show transitions to the H<sub>2</sub>+NH(A) dissociative continuum. The onset of the continuum establishes a binding energy of  $D_0=32\pm 2\text{ cm}^{-1}$  for H<sub>2</sub>-NH(X). Fluorescence from bound levels of H<sub>2</sub>-NH(A) was not detected, most probably due to rapid reactive decay (H<sub>2</sub>-NH(A)  $\rightarrow$  H+NH<sub>2</sub>). The complex appears to be a promising candidate for studies of the photo-initiated H<sub>2</sub>+NH abstraction reaction under conditions where the reactants are pre-aligned by the van der Waals forces.