EXPERIMENTAL DETECTION AND THEORETICAL CHARACTERIZATION OF THE H_2-NH(X) VAN DER WAALS COMPLEX

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The H_2-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_2-NH(X), with a well depth of D_e=116 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_2 bond (C_{2v} point group). For this geometry the well depth is 73 cm^{-1}. Laser excitation spectra for the complex show transitions to the H_2+NH(A) dissociative continuum. The onset of the continuum establishes a binding energy of D_0=32$\pm$2 cm^{-1} for H_2-NH(X). Fluorescence from bound levels of H_2-NH(A) was not detected, most probably due to rapid reactive decay (H_2-NH(A) $\rightarrow$ H+NH_2). The complex appears to be a promising candidate for studies of the photo-initiated H_2+NH abstraction reaction under conditions were the reactants are pre-aligned by the van der Waals forces.