AB INITIO INVESTIGATION OF THE ELECTRONIC GROUND STATE OF THE $NH-N_2$ COMPLEX

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The $NH-N_2$ van der Waals complex has been examined at the CCSD(T) level of theory using the aug-cc-pVDZ basis set. The full basis set superposition error correction was applied. Two minimum energy structures were located for the electronic ground state. The global minimum corresponds to a linear geometry of the complex (NH−N-N), with D_e=199 cm^{-1} and R_{cm}=4.3 Å. The secondary minimum corresponds to a T-shaped geometry of C_{2v} symmetry, where the nitrogen atom of the H-N moiety points toward the center of mass of the N_2 unit, aligned with the a-inertial axis of the complex. The binding energy and R_{cm} value for the secondary minimum were 117 cm^{-1} and 3.7 Å, respectively. Results of the current work on the $NH-N_2$ complex will be discussed and compared to results of our previous work on the $HN-H_2$ complex[a].

[a] Wafaa M. Fawzy, Galina Kerenskaya, and Michael C. Heaven, *J. Chem. Phys.* **122**, 144318, (2005).