AB INITIO INVESTIGATION OF THE ELECTRONIC GROUND STATE OF THE NH–N₂ COMPLEX

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The NH–N₂ 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 Dₑ=199 cm⁻¹ and Rₑₑ=4.3 Å. The secondary minimum corresponds to a T-shaped geometry of C₂ᵥ symmetry, where the nitrogen atom of the H-N moiety points toward the center of mass of the N₂ unit, aligned with the α-inertial axis of the complex. The binding energy and Rₑₑ value for the secondary minimum were 117 cm⁻¹ and 3.7 Å, respectively. Results of the current work on the NH–N₂ complex will be discussed and compared to results of our previous work on the HN–H₂ complex.