The Nitrogen Hydride Clusters NHn (n=1-5) and their Anions: Structures and Electron Affinities

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Abstract

The molecular structures and electron affinities of the NHn/NHn–(n=1-5) species were examined using hybrid Hartree-Fock/density functional theory(DFT). The basis set used in this work was of double-ζ plus polarization quality with additional diffuse s- and p-type functions, denoted DZP++. Seven different density functionals (B3LYP, BLYP, BHLYP, BP86, B3P86, BPW91 and B3PW91) were used in this work. The ground state structures of the NH_n(n=1-5) were explored in this work. The NH has a $X^2\pi$ ground state, the NH2 has an open C_{2V}(ozone-like) structure. For the NH3, C3V structure is turned to be ground state. The NH4 has D3h structure, and the NH5 has C3V structure. The most reliable adiabatic electron affinities, obtained at the DZP++ B3LYP and BPW91 level of theory, is 0.439(0.445)eV and 0.423(0.430)eV for NH, 0.700(0.714)eV and 0.712(0.725)eV for NH2, -0.818(-0.777)eV and -0.820(-0.780)eV for NH3, 0.168(0.191)eV and 0.123(0.127)eV for NH4, -0.802(-0.778)eV and -0.800(-0.785)eV for NH5. The B3P86 and B3PW91 bond lengths of the NH atom, NH2 molecules and NH3 molecules predicted by this work are in reasonable agreement with the experimental results. The dissociation energies predicted by the BHLYP method are the most reliable. For the vibrational frequencies of nitrogen hydride, the BP86 and BPW91 methods produce good predictions compared with the limited experiments.

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