**Abstract**

A theoretical study on the intermolecular dihydrogen bonding (DHB) of ground state B3N3H6···HM (Li, Na, and K) complexes were investigated by B3LYP and MP2 methods with 6-311++G\*\* basis set. Thermodynamic parameters (entropy, enthalpy, heat capacity and Gibbs free energy) of the complexes were calculated at diferent temperatures in the gas phase. The vibrational analysis of N–H···H–M DHB bond formation reveals that the calculated N–H and M–H stretching frequencies undergo red and blue shifts, respectively. The calculated interaction energies correlate well with the geometrical parameters wherein the shortest H···H intermolecular distance is obtained for B3N3H6···HK complex. The chemical shift of 1 H, 11B and 15N NMR predict large variation for B3N3H6···HK complex which has large protonic hydrogen than the hydridic hydrogen. Furthermore, natural bond orbital and quantum theory of atoms in molecule analyses were carried out to explore the non-covalent interaction along with the molecular electrostatic potential to predict the reactive sites of electrophilic and nucleophilic attack.