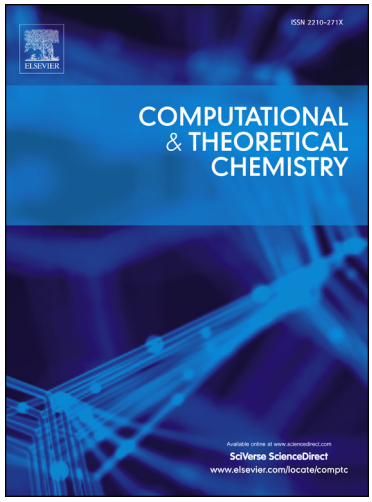

Theoretical studies on aminoborane oligomers

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Theoretical studies on aminoborane oligomers

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Abstract

Aminoborane oligomers, $(NH_2BH_2)_n$ are the possible dehydrogenation products of NH_3BH_3 and NH_4BH_4, which are promising materials for chemical hydrogen storage. The structure and reaction stabilities of $H(NH_2\ BH_2)_nH$ (n = 1 - 4) are calculated by density functional theory for the zigzag, square-wave linear chain structures, along with the coil and ring type structures. We compared the structure stabilities of these oligomers in the view of total energies and found that the coil structured oligomers are stable among other structured oligomers. The reaction stabilities are studied by calculating dipole moment, band gap ($\triangle E_{(LUMO-HOMO)}$) and electronegativity of these oligomers. The study reveals that the dimer ring structured oligomers are found to be more stable towards the reaction compared to all other structured oligomers with high band gap values. The molecular electrostatic potential (MEP) surfaces besides with infrared and Raman spectra of aminoborane oligomers are characterized. It is found that, the B-H bonds have maximum electrostatic potential and minimum for the N-H bonds. The bond dissociation energies of N-H and B-H bonds are calculated to understand their pyrolysis mechanism at molecular level. Comparing the bond dissociation energies of N-H and B-H bonds reveal that N-H bonds are weaker.

Key words: Density functional theory, stability, Bond dissociation energy, Molecular electrostatic potential
PACS:

1 Introduction

Ammonia borane (NH_3BH_3) and ammonium borohydride (NH_4BH_4) are fascinating hydrogen storage materials with 19.6 wt% and 24.5 wt% of hydrogen content, respectively [1–10]. The dehydrogenation of NH_3BH_3 and NH_4BH_4 by catalytic and thermal decomposition results the polyaminoboranes $(NH_2BH_2)_n$, which are again promising materials for chemical hydrogen