

## Accepted Manuscript

Theoretical studies on aminoborane oligomers

Ch. Bheema Lingam, Surya P. Tewari

PII: S2210-271X(13)00334-4

DOI: <http://dx.doi.org/10.1016/j.comptc.2013.07.046>

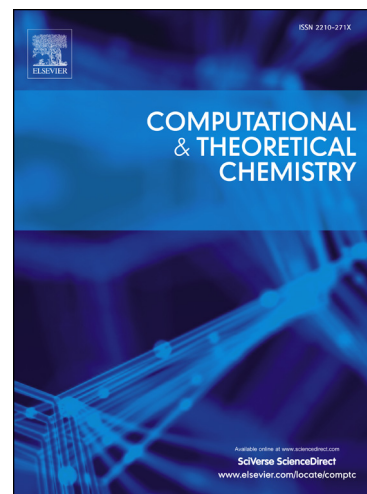
Reference: COMPTC 1216

To appear in: *Computational & Theoretical Chemistry*

Received Date: 3 April 2013

Revised Date: 31 July 2013

Accepted Date: 31 July 2013



Please cite this article as: Ch. Bheema Lingam, S.P. Tewari, Theoretical studies on aminoborane oligomers, *Computational & Theoretical Chemistry* (2013), doi: <http://dx.doi.org/10.1016/j.comptc.2013.07.046>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

# Theoretical studies on aminoborane oligomers

Ch. Bheema Lingam\* and Surya P. Tewari

*School of Physics and Advanced Centre of Research in High Energy Materials (ACRHEM), University of Hyderabad, Prof. C. R. Rao Road, Gachibowli, Andhra Pradesh, Hyderabad- 500 046, India.*

---

## Abstract

Aminoborane oligomers,  $(\text{NH}_2\text{BH}_2)_n$  are the possible dehydrogenation products of  $\text{NH}_3\text{BH}_3$  and  $\text{NH}_4\text{BH}_4$ , which are promising materials for chemical hydrogen storage. The structure and reaction stabilities of  $\text{H}(\text{NH}_2\text{BH}_2)_n\text{H}$  ( $n = 1 - 4$ ) 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 ( $\Delta E_{(\text{LUMO}-\text{HOMO})}$ ) 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 ( $\text{NH}_3\text{BH}_3$ ) and ammonium borohydride ( $\text{NH}_4\text{BH}_4$ ) are fascinating hydrogen storage materials with 19.6 wt% and 24.5 wt% of hydrogen content, respectively [1–10]. The dehydrogenation of  $\text{NH}_3\text{BH}_3$  and  $\text{NH}_4\text{BH}_4$  by catalytic and thermal decomposition results the polyaminoboranes  $(\text{NH}_2\text{BH}_2)_n$ , which are again promising materials for chemical hydrogen

Download English Version:

<https://daneshyari.com/en/article/5394021>

Download Persian Version:

<https://daneshyari.com/article/5394021>

[Daneshyari.com](https://daneshyari.com)