

COMPUTATIONAL ANALYSIS OF AROMATIC THIOMORPHOLINE BORANE AS A HYDROGEN STORAGE MATERIAL

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Abstract

Efficient and cost-effective hydrogen storage remains a significant challenge for utilization of hydrogen as a fuel source. In response, the search for new chemical hydrides has become a major focus. Molecular complexes such as ammine boranes serve as promising hydrogen storage materials, releasing multiple equivalents of molecular hydrogen (H₂) upon decomposition. In this work, a detailed theoretical analysis of aromatic thiomorpholine borane (ATMB), a cyclic amine-borane, was conducted to assess its potential as a hydrogen storage material. Thermochemical parameters, B-N bond dissociation energies and the potential energy surface associated with dehydrogenation pathways were calculated by using the CBS-QB3 level of theory. The computed Gibbs free energy changes indicate the thermodynamic feasibility of hydrogen release from ATMB. Furthermore, the enthalpy of dehydrogenation at 298 K was found to be -50.7 kJmol⁻¹, suggesting that the hydrogen elimination process is exothermic - a desirable feature for practical hydrogen storage systems. Transition state structures were identified for both non-catalyzed and borane (BH₃)-catalyzed dehydrogenation pathways. The results show that BH₃ significantly lowers the activation barrier to 41 kJmol⁻¹. This value is much lower than the B-N bond dissociation energy of 94 kJmol⁻¹. Therefore, BH₃ plays an essential catalytic role in facilitating hydrogen release. This study represents the first theoretical investigation of ATMB as a hydrogen storage candidate and provides valuable insights into the design and development of efficient hydrogen storage materials.

Keywords: *Aromatic Thiomorpholine Borane, Hydrogen Storage, Catalytic Dehydrogenation, B-N Bond Dissociation Energy*