First principles study on the dehydrogenation of ethylene diamine monoborane adducts and its cyclic products

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Dehydrogenation of Ethylene diamine mono borane (EDMB) adducts and its derivatives by substituting (R1/R2=H, CH_3, Cl, F, NH_2, OCH_3 and CN) have been performed to explore the potential candidate towards liquid organic hydrogen carrier (LOHC). Thermochemical properties such as energy, enthalpy and free energy change of these EDMB adducts and its dehydrogenated cyclic products (Monomer, Dimer and Trimer) were investigated. The free energy barrier calculation performed for the selected EDMB adducts such as 1. Cl/CN, 2. Cl/OCH_3, 3. F/CN, 4. F/OCH_3 5. F/F, 6. NH_2/H for cyclic monomer formation, 1. H/CH_3, 2. H/CN, 3. Cl/H, 4. NH_2/H for cyclic dimer formation and 1. H/Cl, 2. H/F, 3. NH_2/H shows promising candidate for chemical hydrogen storage. Electrostatic surface potential and Frontier molecular orbitals also reveals the same through electron redistribution and HOMO-LUMO gap were noticed.