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Gaseous complex hydrides NaMH4 and Na2MH5 (M = B, Al) as hydrogen storage materials: a quantum chemical study

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Abstract

Metal hydrides are feasible for energy storage applications as they are able to decompose with hydrogen gas release. In this work, gaseous complex sodium hydrides, NaMH4 and Na2MH5 (M = B or Al), have been investigated using DFT/B3P86 and MP2 methods with 6-311++G(d,p) basis set; the optimized geometry, vibrational spectra and thermodynamic (TD) properties have been determined. Based on TD approach, a stability of the hydrides to different dissociation channels is analysed; the enthalpies of formation ΔfH°(0) of gaseous species have been obtained: − 1 ± 17 kJ mol−1 (NaBH4), 91 ± 14 kJ mol−1 (NaAlH4), − 13 ± 16 kJ mol−1 (Na2BH5), and 71 ± 16 kJ mol−1 (Na2AlH5). The complex hydrides are confirmed to produce gaseous products with hydrogen gas release at elevated temperature, whereas heterophase reactions, with NaH and B/Al products in condensed state, are predicted to occur spontaneously at lower temperature.

Keywords

Complex metal hydrides; Hydrogen storage; Thermodynamic properties