

A Computational Study to Determine Thermodynamic Properties for Hydrogen Production From Sodium Borohydride Reaction

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INTRODUCTION & AIM

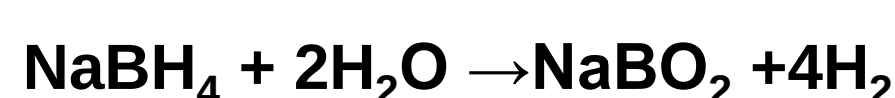
✓ **NaBH₄ hydrolysis reaction** is preferred due to its advantages. It can be possible to reach **high hydrogen generation rates under mild conditions** with this reaction [1].

✓ **Quantum Chemical Methods** can be applied to a process to define its **thermodynamic properties**. In this way, it is possible to determine the **enthalpy and free energy of a given reaction**. Via GaussView Software, one can reach these values via **non-empirical** ways [2].

✓ *In this study, the aim was to determine the thermodynamic properties of the NaBH₄ hydrolysis reaction. The study was based on only computational studies.*

METHOD

✓ Thermochemical values were computed in **Gaussian software**. First, every reactant and product was drawn. Regarding their calculation results, the Free Energy and Enthalpy of the reaction were determined. NaBH₄ hydrolysis reaction was as follows:



RESULTS & DISCUSSION

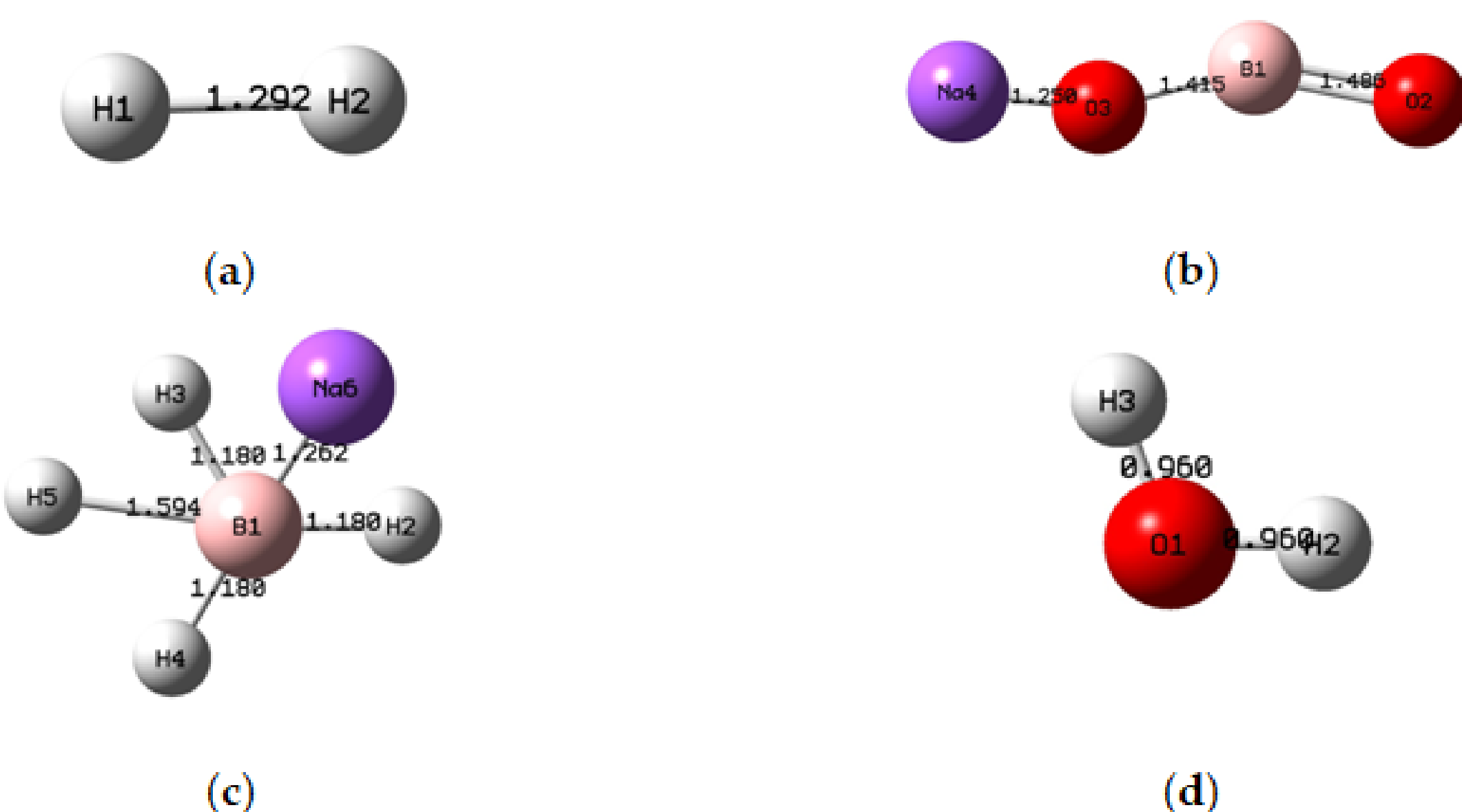


Figure 1. Related Molecules for NaBH₄ reaction (a) Hydrogen; (b) Sodium metaborate; (c) Sodium borohydride; (d) Water.

✓ For Gaussian calculations, firstly, **molecules were drawn based on the reaction in GaussView**. In Fig. 1, images of each molecule with bond lengths in Å.

✓ Calculations were done via the **Hartree-Fock Method** for each **molecule**. Basis Set was selected as **6-31G(d)**. Reaction conditions were assumed as 298 K and 1 atm.

Table 1. Calculated thermochemistry values from Gaussian for sodium borohydride hydrolysis. All values are in Hartrees. (298 K, 1 atm).

	NaBH ₄	H ₂ O	NaBO ₂	H ₂
ε ₀	-187.976351	-76.009862	-335.860216	-1.037482
ε _{ZPE}	0.050072	0.022129	0.009946	0.000000
E _{tot}	0.053187	0.024963	0.013374	0.002360
H _{corr}	0.054131	0.025907	0.014318	0.003305
G _{corr}	0.027274	0.004514	-0.015115	-0.012532
ε ₀ +ε _{ZPE}	-187.926279	-75.987733	-335.850270	-1.037482
ε ₀ +E _{tot}	-187.923163	-75.984899	-335.846842	-1.035121
ε ₀ +H _{corr}	-187.922219	-75.983954	-335.845898	-1.034177
ε ₀ +G _{corr}	-187.949077	-76.005348	-335.875331	-1.050014

Table 2. Entropy and heat capacity values for molecules in NaBH₄ hydrolysis.

Thermodynamic Property	Unit	Compound			
		NaBH ₄	H ₂ O	NaBO ₂	H ₂
Entropy (S)	Cal/mol.K	56.526	45.027	61.947	33.331
Heat Capacity (C _v)		8.052	5.986	9.134	4.968

✓ As a result of the computations utilizing the values in Table 1, **Enthalpy and Free Energy of the reaction were found as -58.0315 kcal/mol and -72.6141kcal/mol, respectively**. This meant that this reaction was exothermic because of the negative sign of enthalpy. The enthalpy value coincided with the literature [3]. Besides that, the negative sign of Gibbs Energy was related to a spontaneous reaction.

✓ The **experimental data were found for Hydrogen as 53.14 J/gK for entropy and 10.16 J/gK for constant volume heat capacity** in the literature [4]. So, the computational data in Table 2 nearly coincided with the experimental data.

CONCLUSION & FUTURE WORK

✓ There is scarce information about thermodynamics studies for a given reaction via Gaussian software. So, this study can be accepted as novel.

✓ This approach can be applied to any reactions in the future because of the decrease in the number of chemicals and energy use in the research.

REFERENCES

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