

Thermodynamic Study of Yttrium Boranate - $\text{Y}(\text{BH}_4)_3$

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The storage of hydrogen is a necessary step to achieve the transition of the German energy sector from fossil fuels to renewable energy sources [1]. Transition metal boranates may contribute to reach this goal. Yttrium boranate, $\text{Y}(\text{BH}_4)_3$, is such a candidate. Several investigations concerning the decomposition of this boranate can be found in the literature, but there is no agreement on the final decomposition products [2]. In addition, no investigations concerning the thermodynamic data of the compound exist, despite their necessity for the detailed understanding of the decomposition reactions. Therefore, we conducted a calorimetric study to provide these data and employed them in thermodynamic equilibrium calculations to study the decomposition and the rehydrogenation behaviour of Yttrium boranate.

Because there are several problems by using a wet chemical route to produce $\text{Y}(\text{BH}_4)_3$, we applied a metathesis synthesis by ball milling of YCl_3 with three equivalents of LiBH_4 adapted from [3]. The obtained mixture of $\text{Y}(\text{BH}_4)_3$ with three equivalents of LiCl was used for all further investigations.

The heat capacity of the compound was measured between 2 K and 300 K using a Quantum Design Physical Property Measurements System and between 280 K and 380 K using a Setaram DSC-111. The Debye temperature and absolute entropy at 298.15 K were determined from the low temperature measurements. TG-DSC-MS measurements and Hess law were employed to determine the enthalpy of formation at 298.15 K, which is comparable to the respective value estimated from DFT calculations [4].

In addition, there is no consent in the literature on the final decomposition products. Therefore, thermodynamic equilibrium calculations were used to shed light on the thermodynamically favoured decomposition reactions. An evaluation of possible decomposition reactions to various products (YH_2 , YH_3 , B, H_2 , YB_2 , YB_4 , YB_6) was carried out using data from our own experiments, own DFT calculations and the literature.

References

- [1] Bundesministerium für Wirtschaft und Energie (BMWi), *Die Nationale Wasserstoffstrategie*, 2020, zu finden unter https://www.bmbf.de/bmbf/shareddocs/downloads/files/die-nationale-wasserstoffstrategie.pdf?__blob=publicationFile&v=1.
- [2] K. Suárez-Alcántara, J. R. Tena García, *Materials* **2021**, *14*, 2561–2616.
- [3] M. B. Ley, M. Paskevicius, P. Schouwink, B. Richter, D. A. Sheppard, C. E. Buckley, T. R. Jensen, *Dalton Trans.* **2014**, *43*, 13333–13342.
- [4] Y. Nakamori, K. Miwa, A. Ninomiya, H. Li, N. Ohba, S.-i. Towata, A. Züttel, S.-i. Orimo, *Phys. Rev. B* **2006**, *74*, 1-9.