Thermochemistry and thermodynamics of promising hydrogen carriers

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The main difficulty in using hydrogen as an alternative fuel is the problem of achieving both a high gravimetric and a high volume density for hydrogen. The most efficient technology of the storage and a consequent use of hydrogen is the one that involves organic compounds, which are capable of the hydrogen accumulation by creating bonds with the hydrogen. The release of hydrogen from the storing compound is achieved by the reverse reaction dehydrogenation with formation of the original liquid organic hydrogen carrier. Thus, the cycle «accumulation – release» for hydrogen that can be done with liquid organic hydrogen carrier can be repeated many times.

So far, many studies have been conducted to find a suitable compound with a low melting point, high hydrogen storage capacity, moderate reaction temperature and pressure among various compounds. Among these properties, the enthalpy of dehydrogenation, is an important parameter, which defines the energy cost for the reaction and is related to the necessary dehydrogenation temperature [1].

In this paper, aromatic and heterocyclic compounds were considered as promising hydrogen carriers. The aim of the work was to develop research related to the search for systems of reverse accumulation and release of hydrogen, the study of their thermodynamic and thermochemistry properties. The series of experiments was carried out for each system to study the equilibrium of the hydrogenation-dehydrogenation reaction. Extensive thermochemical studies of these compounds were carried out, including vapor pressure measurements and combustion calorimetry. The data obtained are compared with the results of a theoretical study of the same reactions using quantum chemical methods. In addition, the report will demonstrate the effectiveness of each system in terms of the concept of hydrogen storage.

1. C. Tang, S. Fei, G. David Lin, Y. Liu, Natural liquid organic hydrogen carrier with low dehydrogenation energy: A first principles study // Int. J. Hydrogen Energy. V.45, 56. 2020. P. 32089-32097.

Acknowledgments. This research was supported by the Government of Russian Federation (decree №220 of 9 April 2010) agreement №14.Z50.31.0038.