Development of a “Molecular Hook” group contribution approach for prediction of thermodynamic properties of substituted benzenes and amino alcohols

Irina V. Andreeva [a,b], Sergey P. Verevkin [a,b]

[a] *Institute of Chemistry, University of Rostock, 18059 Rostock, Germany*

[b] *Faculty of Interdisciplinary Research, Competence Centre CALOR, University of Rostock, 18051 Rostock, Germany*

The development of efficient chemistry-based technologies depends crucially on the availability of physico-chemical and thermodynamic data for the substances involved in the considered processes. Every year thousands of new compounds are synthesized, but in the same time they are characterized properly. It also refers to data on standard molar enthalpies of vaporization and formation, which are responsible for the energetics of chemical reactions and the temperature management. For this reason, the issue of how to predict these parameters becomes increasingly important and it is a task for scientists not only to develop new approaches to predict these exact parameters, but also to be responsible for verifying the accuracy of these methods.

In our current work we have investigated two sets of compounds, they were substituted benzenes and amino alcohols. The first set of the compounds is considered to be model substances appearing from the lignin valorization processes which are promising to be used in industry. Amino alcohols are used in the development of CO_2 capture and sequestration systems. The systematic studies these substances and determining their thermodynamic parameters is an important and challenging task.

In our work the enthalpies of vaporization, sublimation and formation were obtained measured using the transpiration technique and combustion calorimetry. Enthalpies of fusion and heat capacities were measured using differential scanning calorimetry. Based on our own data and data collected from literature, the group contribution approach “Molecular Hook” was developed to predict the thermodynamic properties of both sets of compounds. The key idea of this approach is to select a "hook" molecule with well-known thermodynamic property as a starting point for the estimation the same characteristic for a new similarly shaped molecule. The new structure is easily created by hanging additional fragments or functional groups such as OH, OCH_3 and etc. on the starting “hook”-molecule. For that matter, the energetic contributions of groups have been already known. Such approach is more reliable for predicting thermodynamic properties of medium-size and large molecules compared to the traditional group additivity method. The ability of the “molecular hook” approach to predict accurately thermodynamic data has been validated using our own experimental as well as the literature data.