

THERMODYNAMIC ANALYSIS OF MODERN APPROACHES TO UNDERSTANDING THE NATURE OF DEEP EUTECTIC SOLVENTS

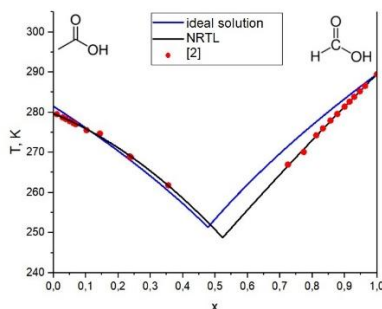
Misikov G.Kh., Petrov A.V., Toikka A.M.

Saint Petersburg State University

198504, Saint Petersburg, Peterhof, Univeritetsky pr., 26

Although the deep eutectic solvents are already being studied for more than twenty years, the determination of which mixtures should be referred as deep eutectic ones remains as contestable as, in some cases, arbitrary. Up to now, there are several approaches proposed to distinguish deep eutectic solvents from other mixtures. For example, the presence of relatively strong hydrogen bonds in the mixture is believed to be marker for a “deep eutectic”; however, some researchers. e.g. [1], highlight that such an approach seems to be controversial as well.

In this work, the comparative analysis of melting diagrams, phase equilibria and physico-chemical properties for a number of binary mixtures, both deep eutectic and common ones, was carried out, e.g. see Fig. Based on the literature data, the modeling of thermodynamic properties was performed using several well-known approaches and equations (regular solution, Wilson equation, NRTL, UNIQUAC).



Melting diagram of the systems formic acid – acetic acid

1. Martins M.A.R., Pinho S.P., Coutinho J.A.P. Insights into the Nature of Eutectic and Deep Eutectic Mixtures // J. Solution. Chem. 2019. Vol. 49, P. 962–982. <https://doi.org/10.1007/s10953-018-0793-1>

2. Timmermans J. The Physico-chemical Constants of Binary Systems in Concentrated Solutions. Volume 2. Two Organic Compounds., Interscience Publishers, Inc., New York, 1959.

The work was carried out with the financial support of the Russian Science Foundation, project 25-23-00021.