HEAT EFFECTS OF PHASE AND CHEMICAL PROCESSES IN A MULTICOMPONENT SYSTEM WITH CHEMICAL INTERACTION

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The study of thermochemical behavior of reacting systems in the chemical equilibrium is an important task from both basic and applied point of view. Correct thermochemical data in the case of simultaneous phase and chemical processes are of particular importance for chemical technology and fundamental problems of thermodynamics: the problems of separating the thermal effects of mixing and chemical reactions are non-trivial. A fairly limited number of modern studies are devoted to these complex problems, although experimental information on the thermochemical characteristics of multicomponent systems with chemical interaction is necessary not only for the development of appropriate databases, but also for understanding the nature of the processes.

In work detailed experimental data on excess enthalpies in binary systems acetic acid - ethyl alcohol, ethyl alcohol - water, acetic acid - ethyl acetate, acetic acid - water at 313.15 K were obtained [1]. Data on the heats of mixing in the quaternary system acetic acid - ethanol - ethyl acetate - water 313.15 K were obtained (Fig. 1). Data on the chemical equilibrium in the system with the reaction of ethyl acetate synthesis at 313.15 K [2] were obtained (Fig. 2). There were obtained data on the heat of reaction for the synthesis of ethyl acetate at 313.15 K using the developed technique that allows to take into account the totality of thermal effects accompanying the mixing and synthesis process.

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Figure 1. Dependence of the excess enthalpy of the quaternary system on the chemical equilibrium compositions represented in the transformed α -variables.



Figure 2. Chemical equilibrium surface in the acetic acid-ethanol-ethyl acetate-water system at 323.15 K: composition points determined by gas chromatography • and NMR •

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- [2] Golikova A, Samarov A, Trofimova M, Rabdano S, Toikka M, Pervukhin O, et al., J Solution Chem, 2017, 46, 374.