Solid-liquid equilibrium in the system 2-Keto-L-gulonic acid + sodium hydroxide + water

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Introduction

2-Keto-L-gulonic acid (HKGA) is a key intermediate of the L-Ascorbic acid (Vitamin C) production process. The HKGA production process is one of the exemplary processes within the EU Horizon 2020 research project PRODIAS (Processing Diluted Aqueous Systems). After the fermentation HKGA is present within a highly diluted aqueous solution that also contains a large variety of process- and product-related impurities, including sodium salts. Crystallization offers a possibility to recover and simultaneously purify biotechnologically produced HKGA.

Regarding the crystallization of HKGA the knowledge of the solubilities of HKGA and its sodium salt NaKGA in water are of crucial importance. Within PRODIAS, physico-chemical properties relevant for the purification process of HKGA are experimentally measured and modeled. This work presents the experimental elucidation of the solid-liquid equilibrium in the system HKGA + NaKGA + water between 2 and 39.6 °C as well as the development of a thermodynamic model to describe the solid-liquid equilibrium.

Solid-liquid experiments

Procedure:
Preparation of synthetic solid-liquid samples by mixing HKGA, NaOH and water

- Isothermal equilibration at temperatures ranging from 2.0 °C to 39.6 °C

Analysis:
- Analysis of clear supernatant and wet solid residue
- Determination of concentrations of Na+ and HKGA ions by ion chromatography
- Determination of solubility and composition of the crystal phase

The properties of the ternary solid-liquid system HKGA + NaKGA + water are described by three equilibrium processes (chemical reactions and phase transitions) (see Fig. 2).

Fig. 1: Left: Phase diagram of the ternary system HKGA + NaOH + water. The dashed line marks the binary system NaKGA + water. The synthetic samples (circles) are located in the gray area. Right: Enlarged depiction of the gray area. The continuous line represents the solubility line in an eutectic system. The dashed lines mark the boundaries of the two-phase and three-phase regions.

The solid-liquid model

The ternary system HKGA + NaKGA + water is depicted in Fig. 2. The ternary solubility diagram is obtained from the binary systems HKGA + NaKGA at 1000/3.0 and NaKGA + H2O at 1000/3.0.

Results:
- Very good agreement of calculated composition of the liquid phase with experimental results
- No necessity for binary or higher Pitzer interaction parameters

The developed model offers a valuable tool for the HKGA crystallization process development

Summary and outlook

The solid-liquid equilibrium of the ternary system HKGA + NaKGA + water was experimentally determined at temperatures between 2.0 °C and 39.6 °C. A thermodynamic model was developed including an extended Debye–Hückel activity coefficient model. The predicted solubilities of HKGA and NaKGA in water as well as the crystallizing phase show very good agreement with experimental data. The model will be extended to multi-component systems in further steps to investigate e.g. the influence of other acids and salts on the solid-liquid equilibrium.


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ABOUT THE PROJECT

- Start date: 1st January 2015
- Duration: 48 months, until 31st December 2018
- Budget: 14 million €
- Project web site: www.spire2030.eu/prodias/

The research project receives funding from the European Community’s Framework Programme for Research and Innovation Horizon 2020 (2014-2020) under grant agreement n° 637077.