Title: Thermodynamic evaluation and optimization of the CH_3COOLi-CH_3COOK-CH_3COOCs system using the Modified Quasichemical Model

Author: Gildas K. Gbassi Christian Robelin

PII: S0378-3812(15)30013-3
DOI: http://dx.doi.org/doi:10.1016/j.fluid.2015.06.044
Reference: FLUID 10659

To appear in: *Fluid Phase Equilibria*

Received date: 6-6-2015
Revised date: 25-6-2015
Accepted date: 26-6-2015

Please cite this article as: G.K. Gbassi, C. Robelin, Thermodynamic evaluation and optimization of the CH_3COOLi-CH_3COOK-CH_3COOCs system using the Modified Quasichemical Model, *Fluid Phase Equilibria* (2015), http://dx.doi.org/10.1016/j.fluid.2015.06.044

Thermodynamic evaluation and optimization of the CH_3COOLi-CH_3COOK-CH_3COOCs system using the Modified Quasichemical Model

Gildas K. Gbassi [a] and Christian Robelin [b,*]

[a] *Department of Chemistry, Faculty of Pharmacy, Université Félix Houphouët Boigny, BPV 34 Abidjan 01, Côte d'Ivoire.*

[b] *Centre for Research in Computational Thermochemistry (CRCT), Department of Chemical Engineering, École Polytechnique, C.P. 6079, Succursale ''Downtown'', Montreal (Quebec), Canada, H3C 3A7.*

*Corresponding author. Tel.: +1 (514) 340 4711 ext. 4304; Fax: +1 (514) 340 5840;
E-mail address: christian.robelin@polymtl.ca (C. Robelin).

Abstract :

A complete critical evaluation of all available phase diagram and thermodynamic data has been performed for all condensed phases of the CH_3COOLi-CH_3COOK-CH_3COOCs system, and optimized model parameters have been found which best reproduce all available experimental data simultaneously. The CH_3COOLi-CH_3COOK-CH_3COOCs system may be used in supported molten salt catalysis. The Modified Quasichemical Model for short-range ordering was used for the molten salt phase. No ternary model parameters were required for the liquid phase; the optimized binary parameters suffice to reproduce satisfactorily the available experimental data for the ternary system using a standard symmetric interpolation method. The calculated (predicted) minimum liquidus temperature corresponds to a ternary eutectic at T = 368 K, with a liquid composition of (22.4 mol% CH_3COOLi + 32.3 mol% CH_3COOK + 45.3 mol% CH_3COOCs). This relatively low liquidus temperature makes the ternary mixture an interesting alternative to ionic liquids.