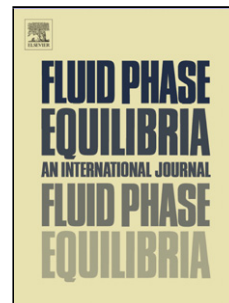


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Thermodynamic evaluation and optimization of the CH₃COOLi-CH₃COOK-CH₃COOCs system using the Modified Quasichemical Model

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Abstract :

A complete critical evaluation of all available phase diagram and thermodynamic data has been performed for all condensed phases of the CH₃COOLi-CH₃COOK-CH₃COOCs system, and optimized model parameters have been found which best reproduce all available experimental data simultaneously. The CH₃COOLi-CH₃COOK-CH₃COOCs 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% CH₃COOLi + 32.3 mol% CH₃COOK + 45.3 mol% CH₃COOCs). This relatively low liquidus temperature makes the ternary mixture an interesting alternative to ionic liquids.

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