

论文

用活度相互作用系数描述多元体系热力学

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摘要: 基于MacLaurin级数推出了可用于同时计算熔体中溶质和溶剂活度系数的解析表达式,其特点是保留了热力学的一致性,且比传统的Wagnerε公式更精确.另外,在本文研究的体系内,高阶活度相互作用系数对体系的热力学性质影响很小

关键词: 热力学 活度 模型

THERMODYNAMIC DESCRIPTION OF MULTICOMPONENT SYSTEMS BY INTERACTION PARAMETERS

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Abstract: Novel analytical expressions for calculating activity coefficients of solvent and solutes are given in the present study which is based on the MacLaurin infinite series. These new expressions have thermodynamic consistency and more accuracy in comparison with traditional used Wagner's ε formalism. The another advantage of this treatment is found in a rather small influence of the higher order interaction parameters upon the properties of the studied systems.

Keywords: thermodynamics activity model

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