中国化学工程学报 2007 15(1) 97-101 ISSN: 1004-6356 CN: 44-1963/R

THERMODYNAMICS AND CHEMICAL.....

利用二元体系的C-H红外光谱漂移代表平衡数据

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收稿日期 修回日期 网络版发布日期 接受日期

摘要 Prediction of vapor-

liquid equilibrium (VLE) is extremely necessary to separate liquid mixture in chemical production, especially when the required experimental data are difficult to measure, or the measurement is not economical. The infinite dilution activities can be used to predict VLE. However, it needs both the ends of the activities that are difficult to obtain for many systems. In the present study, a new model is proposed for correlating the frequency shift of C-H stretching band of IR spectra over the whole concentration. Investigated mixtures include water/2-propanol, water/N, N-dimethylformamide (DMF), water/methanol, water/ethanol, water/1, 4-dioxane, and water/dimethylsulfoxide (DMSO) systems. Simultaneous correlations of C-H frequency shift and VLE data are made. Furthermore, the VLE data were predicted with satisfactory results by the parameters obtained from IR spectra coupled with one of the infinite dilution activity coefficients.

关键词 IR; vapor-liquid equilibrium; infinite dilution activity coefficient; binary aqueous system;

分类号

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Prediction of vapor-liquid equilibrium data from C-H band shift of IR spectra in some binary systems

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Received Revised Online Accepted

Abstract Prediction of vapor-liquid equilibrium (VLE) is extremely necessary to separate liquid mixture in chemical production, especially when the required experimental data are difficult to measure, or the measurement is not economical. The infinite dilution activities can be used to predict VLE. However, it needs both the ends of the activities that are difficult to obtain for many systems. In the present study, a new model is proposed for correlating the frequency shift of C-H stretching band of IR spectra over the whole concentration. Investigated mixtures in-clude water/2-propanol, water/N, N-dimethylformamide (DMF), water/methanol, water/ethanol, water/1, 4-dioxane, and water/dimethylsulfoxide (DMSO) systems. Simultaneous correlations of C-H frequency shift and VLE data are made. Furthermore, the VLE data were predicted with satisfactory results by the parameters obtained from IR spectra coupled with one of the infinite dilution activity coefficients.

Key words IR; vapor-liquid equilibrium; infinite dilution activity coefficient; binary aqueous system;

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本刊中 朱宾 "IR; vapor-liquid equilibrium; infinite dilution activity coefficient; binary aqueous system"的 相关文章
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