

THERMODYNAMICS AND CHEMICAL ...

标题: 二元体系C-H和N-拉伸振动九波干涉现象

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关键词: 红外光谱; 干涉现象; 二元体系

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 include water/2-propanol, water/1,4-dioxane, water/ethylacetate (EAC), 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: [vapor-liquid equilibrium](#); [infinite dilution activity coefficient](#); [binary systems](#); [linear expansion system](#)

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

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