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RESEARCH NOTES

SAFT缔合模型关联含水体系的^{1}H NMR

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摘要 ^1H NMR chemical shifts of binary aqueous mixtures of acylamide, alcohol, dimethyl sulphoxide (DMSO), and acetone are correlated by statistical associating fluid theory (SAFT) association model. The comparison between SAFT association model and Wilson equation shows that the former is better for dealing with aqueous solutions. Finally, the specialties of both models are discussed.

关键词 核磁共振技术, 水溶液, 氢键, 缔合性, 温度, 热力学性质,

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Correlation of ^1H NMR Chemical Shift for Aqueous Solutions by Statistical Associating Fluid Theory Association Model

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Abstract ^1H NMR chemical shifts of binary aqueous mixtures of acylamide, alcohol, dimethyl sulphoxide (DMSO), and acetone are correlated by statistical associating fluid theory (SAFT) association model. The comparison between SAFT association model and Wilson equation shows that the former is better for dealing with aqueous solutions. Finally, the specialties of both models are discussed.

Key words Statistical associating fluid theory (SAFT), association model; NMR; chemical shift; aqueous solution,

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