

二氧六环-水体系的 ^1H 和 ^{17}O NMR研究

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摘要 本工作用配位平衡和快交换方法定量描述了二氧六环水体系中 ^1H 和 ^{17}O 化学位移随浓度的变化. 讨论了未配位水的结构破坏程度及其存在形式.

关键词 [二元体系](#) [水](#) [核磁共振谱法](#) [浓度](#) [质子磁共振谱法](#) [化学位移](#) [氧同位素](#) [二氧六环](#)

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^1H and ^{17}O NMR study of the dioxane-water system

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Abstract ^1H and ^{17}O NMR of the dioxane (DO)-water system were studied. The complex equilibrium constants in this system were obtained from the ^1H chem. shift variation of DO with its concentration. With these equilibrium constants the equilibrium concns. of each species in all the samples were calculated. The variations of ^1H and ^{17}O chem. shifts of water were analyzed with the fast exchange method. The ^1H and ^{17}O chem. shifts of free water in this system are linearly related to the natural logarithm of its concns. from which the degree of structural break of water by DO was evaluated.

Key words [BINARY SYSTEM](#) [WATER](#) [NMR SPECTROMETRY](#) [CONCENTRATION](#) [PROTON](#) [MAGNETIC RESONANCE SPECTROMETRY](#) [CHEMICAL SHIFT](#) [OXYGEN ISOTOPES](#) [DIOXANE](#)

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