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DMF-H_2O缔合体系的**~1HNMR**研究

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摘要　　DMF水溶液是一种生物分子水溶液的简单生化模型。测量了DMF-H_2O体系不同温度下全浓度范围的~1H NMR数据，对体系中的缔合情况进行了讨论，基于H_2O, H_2O·DMF, (H_2O)_2和(DMF)_2·H_2O的缔合平衡建立了化学缔合模型，采用最 小二乘法拟合实验数据，联合遗传算法和Levenberg- Marquardt算法对模型参数进 行全局寻优求解得不同温度的缔合平衡常数K，再根据不同温度的K求得缔合平衡的 ΔH和ΔS。为了更好地理解DMF水溶液中分子间的相互作用，还测量了298K下DMF- CCl_4和DMF-BuOH体系全浓度范围的~1H NMR数据作为比较，结合NMR的基本原理对各DMF溶液体系~1H NMR的实验现象进行了分析和解释，认为水溶液的特殊结构、氢键和DMF酰胺基的共轭体系是影响DMF-H_2O体系~1H NMR的主要因素。

关键词　 二甲基甲酰胺　 水　 质子磁共振谱法　 缔合

分类号　 0645

~1H NMR Studies of DMF-H_2O Association System

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Abstract Dimethylformamide (DMF) aqueous solution is a kind of simple biochemical model of biological molecular aqueous solutions. In this paper, ~1H NMR of DMF-H_2O system was measured at different temperatures to discuss molecular interactions in the mixtures. The association system was modeled on the equilibrium among H_2O, H_2O· DMF, (H_2O)_2 and (DMF)_2·H_2O and calculated by nonlinear least- square fitting. Association equilibrium constant K and the corresponding ΔH and ΔS were obtained by combined GA and levenberg- marquardt algorithm. In addition, DMF-CCl_4 and DMF-BuOH systems were also studied in order to further understand the nature of interactions in DMF-water mixture. Some peculiar phenomena were found and considered to be mainly caused by the special structure of liquid water, the hydrogen-bonding interactions and the conjugate system of amide.

Key words DIMETHYLFORMAMIDE WATER 1HNMR ASSOCIATION

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