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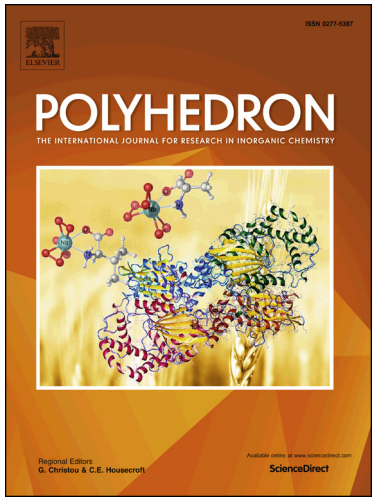

THERMODYNAMICS OF DISSOLUTION OF FERROCENE IN COMMERCIAL MIXED SOLVENTS CONTAINING WATER AND 2-PROPANOL

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THERMODYNAMICS OF DISSOLUTION OF FERROCENE IN COMMERCIAL MIXED SOLVENTS CONTAINING WATER AND 2-PROPANOL

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Abstract

The solubility of ferrocene in commercial mixed solvents containing 50, 70, and 91% 2-propanol and water has been determined as a function of temperature. From the solubility data, the values of ΔH, ΔS, and ΔG for the dissolution process have been determined. For 50% 2-propanol, the values obtained for ΔH, ΔS, and ΔG are 31.54±1.58 kJ mol^{-1}, 62.78±3.14 J mol^{-1} K^{-1}, and 12.82± 0.64 kJ mol^{-1}, respectively. When the solvent is 70% 2-propanol, the values are (in the same order) are 23.29± 1.16 kJ mol^{-1}, 46.58±2.33 J mol^{-1} K^{-1}, and 9.40±0.47 kJ mol^{-1}, and for 91% alcohol they are 22.70±1.34 kJ mol^{-1}, 53.39±2.67 J mol^{-1} K^{-1}, and 6.78±0.34 kJ mol^{-1}. Although values for ΔH for dissolution of ferrocene in 70 and 91% 2-propanol are of similar magnitudes, the values for ΔG are quite different and show the greater solubility in 91% 2-propanol. The thermodynamic quantities for dissolution in 50% 2-propanol shows the lower solubility in that solvent and the hydrophobic nature of ferrocene.

Key words: ferrocene, solubility, 2-propanol, thermodynamics, mixed solvents, solvation

1. Introduction

Ferrocene is one of the most commonly encountered organometallic compounds. Its synthesis is described as an experiment to be carried out in advanced teaching laboratories [1]. Applications of ferrocene include its use as a fuel additive [2], and the ferrocenyl group is a constituent in compounds having medicinal properties [3,4]. The latter include ferroquine and the closely related compound chloroquine, both of which have antimalarial activity [5,6]. In fact, a considerable number of compounds that contain the ferrocene moiety are of considerable interest as a result of their having therapeutic properties. For example, complexes of gold have been shown to be effective in treatment of rheumatoid arthritis, and they have also shown antitumor activity [7]. Because ferrocene has attributes that result in it having potential uses when dissolved in organic solvents, there have been many studies on such systems. Although the ferrocene molecule is nonpolar and the compound is insoluble in water, it readily dissolves in organic solvents, including hydrocarbons [8-13]. A great deal of important work has also been done on the theory of solutions of ferrocene in numerous solvents in an effort to determine quantitative relationships between solubility and molecular characteristics of the solvent [14-16].

In view of the many potential applications of ferrocene, it is not surprising that there have been numerous of studies dealing with its solubility in a wide variety of solvents, including some mixed solvents [10,16]. The heat of solution of ferrocene in methanol has been reported to be 17.5 kJ mol^{-1} [9] and that when ethanol is the solvent has been reported as 20.6 kJ mol^{-1} [10]. In general, there is a considerable lack of data corresponding to thermodynamics of dissolution of

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