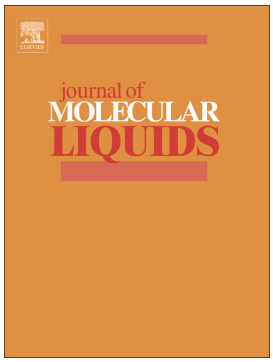

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Effect of Electrolytes on the Solubility and Solution thermodynamics of 1-Amino-4-Hydroxy-9,10-Anthraquinone, an Analogue of Anthracycline Anticancer Drugs, in Aqueous Ethanol Media Using Theoretical and UV-Vis Spectroscopic Study

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Abstract

The solubility of 1-amino-4-hydroxy-9,10-anthraquinone (AHAQ) in binary solvents (ethanol water mixtures) was determined at 298.15 K under atmospheric pressure using a thermostatted reactor and analytical 'UV-Vis spectroscopic method'. The structure of the molecule was optimized using theoretical studies to compute molecular dimension and the dipole moment which are essential in determining different thermodynamic parameters of solvation. The effects of binary solvents compositions and presence of electrolytes such as NaCl and KCl on the solubility were analyzed. Using the measured solubilities, the thermodynamic properties of dissolution of AHAQ such as Gibbs free energies of solutions, Gibbs free energetics due to cavity forming and dipole-dipole interactions, transfer enthalpy of dissolution, and chemical transfer energetics were calculated.

Keywords: AHAQ, solubility, electrolytes, transfer free energetics.

Abbreviations: 1-Amino-4-hydroxy-9,10-anthraquinone : AHAQ