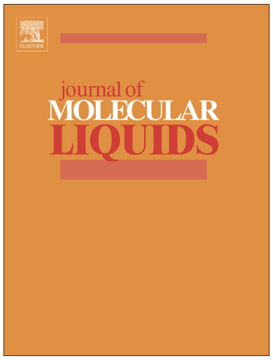

Spectral and proton transfer behavior of 1,4-dihydroxylanthraquinone in aqueous and confined media; molecular modelling strategy

Mohandoss Sonaimuthu, Suganya Bharathi Balakrishnan, Sakthi Velu Kuppu, Giri Babu Veerakanellore, Stalin Thambusamy

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Spectral and proton transfer behavior of 1,4-dihydroxylanthraquinone in aqueous and confined media; Molecular modelling strategy

Mohandoss Sonaimuthu [a,b], Suganya Bharathi Balakrishnan [a], Sakthi Velu Kuppu [a], Giri Babu Veerakanellore[c] and Stalin Thambusamy [a]*

[a]Department of Industrial Chemistry, School of Chemical Sciences, Alagappa University, Karaikudi- 630 003, Tamilnadu, India.
[b]Department of Chemistry, National Sun Yat-Sen University, 70, Lien-Hai Road, Kaohsiung-80424, Taiwan.
[c]Department of Chemistry, University of Miami, Coral Gables, Miami, Florida-33146, USA.

**Corresponding author (Stalin Thambusamy)*
E-mail: stalin.t@alagappauniversity.ac.in, drstalin76@gmail.com.

Abstract

The formation of supramolecular complex between the various ionic solutions of 1,4-dihydroxyanthraquinone (1,4-DHAQ) and hydrophobic cavity of β-cyclodextrin (β-CD) was studied by UV–visible, fluorescence spectroscopy and cyclic voltammetry methods. The stoichiometric ratio of the inclusion complex was found to be 1:1 and the binding constant of the inclusion complex at 303 K were calculated using Benesi–Hildebrand plot and the inclusion interaction was examined and the thermodynamic parameter (ΔG) of inclusion process is also determined. The oxidation and reduction reactions specific to 1,4-DHAQ is quasi-reversible occur in a complex mechanism. The stable inclusion of 1,4-DHAQ in β-CD is proved by the significant changes of redox activity characteristic for 1,4-DHAQ and good electrochemical stability of the complex. On the other hand, the solid complex prepared between β-CD and 1,4-DHAQ were characterized by FT-IR, XRD, DSC, SEM and ^{1}H NMR methods. The β-CD and 1,4-DHAQ inclusion complex obtained by molecular docking studies in good correlation with the results obtained through experimental methods using PatchDock and FireDock servers. The