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

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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 ¹H 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

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