

Host-guest interaction between new nitrooxoisoaporphine and β -cyclodextrins: Synthesis, electrochemical, electron spin resonance and molecular modeling studies

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A new nitrooxoisoaporphine derivative was synthesized and characterized by cyclic voltammetry and electron spin resonance. Its aqueous solubility was improved by complexes formation with β -cyclodextrin, heptakis(2,6-di-O-methyl)- β -cyclodextrin and (2-hydroxypropyl)- β -cyclodextrin. In order to assess the inclusion degree reached by nitrooxoisoaporphine in cyclodextrin cavity, the stability constants of formation of the complexes were determined by phase-solubility measurements obtaining in all cases a type-AL diagram. Moreover, electrochemical studies were carried out, where the observed change in the EPC value indicated a lower feasibility of the nitro group reduction. Additionally, a detailed spatial configuration is proposed for inclusion of derivative within the cyclodextrin cavity by 2D NMR techniques. Finally, these results are further interpreted by means of molecular modeling studies. Thus, theoretical results are in complete agreement with the experimental data. © 2012 Elsevier