Molecular encapsulation of 5-nitroindazole derivatives in 2,6-dimethyl-?-cyclodextrin: Electrochemical and spectroscopic studies

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Four different 5-nitroindazole derivatives (1-4) and its inclusion with Heptakis(2,6-di-O-methyl)-?-cyclodextrin (DM?CD) were investigated. The stoichiometric ratios and stability constants describing the extent of formation of the complexes were determined by phase-solubility measurements obtaining in all cases a type-AL diagram. Also electrochemical studies were carried out, where the observed change in the EPC value indicated a lower feasibility of the nitro group reduction. The same behavior was observed in the ESR studies. The detailed spatial configuration is proposed based on 2D NMR methods. These results are further interpreted using molecular modeling studies. The latter results are in good agreement with the experimental data.