Cathodic behavior of 2,3-dihydrooxoisoaporphines comportamiento catódico de 2,3-dihidro-oxoisoaporfinas

Sobarzo-Sánchez, Eduardo

Olea-Azar, Claudio

Alarcón, Jaime

Opazo, Lucía

Cassels, Bruce K.

The electrochemical behavior of two representative 2,3-dihydro-7H-dibenzo[de,h]quinolin-7-ones was determined using cyclic voltammetry in DMSO as solvent and rationalized by quantum chemical calculations using ab initio and DFT methods. The ESR spectra of the radicals obtained by electrolytic reduction were characterized and analyzed. Calculations at the HF/3-21G and DFT-B3LYP/6-311 ++G** levels were carried out to obtain the optimized structure, hyperfine coupling constants and to determine the values and to visualize the LUMO and SOMO energy levels, respectively. The calculated electron affinities are in agreement with the reduction potentials measured for both heterocyclic compounds.