

Cyclic voltammetry and digital simulation of the electroreduction of ortho- and meta-nitro aryl 1,4-dihydropyridines

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Cyclic voltammetry (CV) and digital simulation methods are utilized to elucidate the mechanism of electrochemical reduction of a series of nitro aryl 1,4-dihydropyridines in protic (aqueous) and mixed media. The experimental voltammograms show different behavior for the reduction of these compounds. In protic media, one cathodic and one anodic peak are observed, but in mixed media a new redox couple appears, indicating a change in the redox mechanism. We have determined that the position of the nitro group (ortho-, meta-) in nitroaromatics directly affects both the electron transfer rate (heterogeneous rate constant, k^0 , k^1) and the energetics of the electron transfer (E° values). According to this study, the splitting observed in the cyclic voltammograms, when aprotic solvent or inhibitors are added to a nitroaromatic aqueous solution, is due to a) a change in the kinetics of the first electron transfer reaction (k^0) from an irreversible to a reversible process, b) to a change in