ESR and electrochemical studies of 2-acylpyridines and 6,6?-diacyl-2,2?-bipyridines

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The ESR spectra of radicals obtained by electrolytic reduction of 2-acylpyridines and 6,6?-diacyl-2,2?-bipyridines were measured in dimethylsulfoxide (DMSO) and analyzed by quantum chemical calculations. The electrochemistry of these compounds was characterized using cyclic voltammetry, in DMSO solvent. The results showed a two step reduction mechanism, first wave was assigned to the generation of the correspondent free radical species, and the second wave was assigned to the dianion derivatives. AM1 and DFT calculations were performed to obtain the optimized geometries, theoretical hyperfine constants, and spin distributions, respectively. The theoretical results are in complete agreement with the experimental ones.