

Formation of radical anions by electrochemical reduction of nitroimidazoles in aprotic solvents and mixed solvent

Norambuena, E.

Olea-Azar, C.

The EPR spectra of radicals obtained by electrochemical reduction of 2-nitroimidazole and 4-nitroimidazole were measured in mixed solvents. The behavior of the nitrogen coupling constants with the solvent composition is discussed in terms of equilibria between radicals in different solvents. The equilibrium constants of the DMSO/water system were determined. Molecular orbital calculations in the frame of LCAO-HMO method account correctly for the spin distribution of both compounds investigated.