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Electron Affinities, Solvation Energies and Redox Potentials of Some Chalcones: Substituents` Effect and Correlation with Semi-Empirical MO Energies

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Abstract: Experimental and theoretical investigations were carried out on 2 sets of chalcones. Set 1 has an OH group on ring A and Set 2 does not, and both have different substituents on ring B at different positions. The experimental investigations comprised cyclic voltammetric (CV) studies to determine the reactivity in terms of redox potentials in DMF at room temperature (23 \pm 1 °C). Electrochemical parameters from cyclic voltammograms were used to evaluate the reversibility of electron transfer, standard reduction potentials, solvation energies, electron affinities, diffusion coefficients, critical scan rates and heterogeneous electron transfer rate constants. Heterogeneous electron transfer rate constants were determined experimentally by Gileadi's method for the Set 2 chalcones only. Computational studies included the use of MO theory with semi-empirical AM1 and PM3 approximations for the determination of optimized geometries and the energies of lowest unoccupied molecular orbital (E_{LUMO}). An attempt was also made to correlate the experimental and theoretical parameters

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