

CYCLIC VOLTAMMETRY STUDIES OF η^5 - MONOCYCLOPENTADIENYLIRON COMPLEXES

P. Mendes¹, M.H. Garcia², A. R. Dias²

¹*Centro de Química de Évora, Departamento de Química da Universidade de Évora, Colégio Luís António Verney, Rua Romão Ramalho 59, 7000-671 Évora, PORTUGAL*
²*Centro de Química Estrutural, Instituto Superior Técnico, Av. Rovisco Pais, 1049-001 Lisboa Codex, PORTUGAL*

Recently, organometallic complexes have emerged as potential building blocks for second-order nonlinear optical (SONLO) materials in view of their potential application in the area of integrated optics [1]. Organometallic complexes can possess low energy, sometimes intense, electronic charge transfer excitations that are responsible for the NLO response. Most of these electronic transitions are MLCT or LMCT excitations which energy can be related to the HOMO-LUMO gaps.

Experimental work on η^5 -monocyclopentadienylmetal complexes with *p*-substituted benzonitrile chromophores showed the fundamental role played by the organometallic fragment, namely their electronic richness, in the second-order nonlinear optical response [2]. In addition, the first hyperpolarizability was found to decrease with increasing conjugation length of the chromophores, being the larger values associated to the lower HOMO-LUMO gaps [3,4]. For similar η^5 -monocyclopentadienyliron complexes possessing thiophene based conjugated backbone, an inverse trend on experimental first hyperpolarizability with increasing conjugation length was observed [5].

In order to obtain a deeper insight into the electronic richness of the organometallic moiety and to get an evaluation of the corresponding HOMO-LUMO gaps and the connection with NLO properties, the electrochemical behavior of the compounds $[\text{FeCp}(\text{P_P})(\text{NC}\{\text{SC}_4\text{H}_2\}_n\text{NO}_2)]^+$ (P_P=DPPE, (+)-DIOP; n=1-3) were studied by cyclic voltammetry in dichloromethane and acetonitrile.

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