Syntheses of half-sandwich nickel and iron complexes presenting hyperpolarizable thiophene based ligands

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The search for new organometallic materials with second-order nonlinear optical (SONLO) properties is currently the subject of considerable interest due to their potential technologic applications in photonic devices for telecommunications and optical computing.¹ The main studies have been made in push-pull systems in which the metal center, bonded to a hyperpolarizable organic conjugated backbone, acts as an electron releasing or withdrawing group. In spite of the research in this field, an improved understanding of the relationship between the molecular structure and the microscopic optical nonlinearities is crucial for a broadening of reflection and



incorporation of novel molecules. Experimental work on η^5 -monocyclopentadienylmetal complexes with benzene-based nitrile chromophores showed the fundamental role played by the organometallic fragment on the SONLO response.² Also, recent results seem to demonstrate that NMR spectroscopic data can be used as a probe on the SONLO properties of these complexes, since a quantitative correlation was found.³ However, it is important to check if such correlation can be used in compounds with different chromophores, namely thiophene derivatives. Thiophene based chromophores were already recognized to have real merits in NLO properties. Thus, we report herein the preliminary results concerning the synthesis and spectroscopic characterization of new compounds derived from FeCpDPPE (DPPE=1,2-bis(diphenylphosphino)ethane) and NiCpPPh₃ organometallic fragments possessing different thiophene based chromophores. (examples of target molecules are depicted in figure). Spectroscopic data will be analyzed in order to give an insight on the NLO properties of these compounds.

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