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MONOCYCLOPENTADIENYLRUTHENIUM COMPLEXES FOR SECOND-ORDER NLO PURPOSES

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Organometallic compounds have given rise to a great deal of interest owing to their application in the field of nonlinear optics (NLO) [1]. For second-order nonlinear optics (SONLO), strongly asymmetric systems are needed, which led to the development of typical push–pull systems in which the metal centre, bound to a highly polarizable conjugated backbone, acts as an electron releasing or withdrawing group. Among the organometallic compounds presenting this donor– π -system–acceptor feature, η^5 -monocyclopentadienyliron and ruthenium moieties were found to be much more efficient donor groups for second-order NLO purposes than the traditional organic donor groups, leading to higher first hyperpolarizabilities (β) [2]. Recent results on η^5 -monocyclopentadienyliron complexes presenting thiophene nitrile chromophores showed an enhanced SONLO performance when compared to that observed on analogue benzenoid structures. Also, the first hyperpolarizability of these complexes was found to be influenced by a compromise between the conjugation length of the chromophores and the metal-to-ligand charge-transfer [3].

In our continuous effort to understand the role played by the organometallic fragment on the SONLO properties and to establish detailed structure–NLO activity correlations, we now study a series of complexes of general formula $[RuCp(P_P)(NC{SC_4H_2}_nNO_2)][PF_6]$ (Fig. 1) (P_P=dppe, (+)-diop; n=1-3). Spectroscopic and electrochemical data will be used in order to evaluate the effect of the phosphine coligand and the length of the conjugated ligand on the second-order NLO response of the complexes. The results will be compared to those found in parent iron derivatives.

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