

Modulated Structure of $[\text{FeCl}(\text{DMPE})_2(\text{NCC}_6\text{H}_4\text{NO}_2)][\text{PF}_6]$ a Material for Use in NLO

Leo Straver^a, V. Petricek^b, M. T. Duarte^c, M. F. M. da Piedade^c, M. P. Robalo^c, A. P. S. Teixeira^c, M. H. Garcia^c, ^a*Bruker AXS B.V., Delft, Netherlands.* ^b*Acad Sci Czech Republ, Inst Phys, Prague, Czech Republic.* ^c*Centro de Química Estrutural, IST, Lisboa, Portugal.* E-mail: leo.straver@bruker-axs.nl

It is well known the recent interest in the nonlinear optical (NLO) properties of organometallic complexes [1,2]. Most efficient NLO-active complexes have a dipolar composition, with an electron-donating group linked by a π -conjugated bridge to an electron-accepting group. Our studies on complexes with this composition have been focused on metal σ -nitriles, for which the second-order NLO responses have been determined [3,4]. Since, it is also of interest to assess the importance of co-ligands in the donor metal coordination sphere, our attention has turned to an alternative coordinated Fe(II) system, namely trans-chloro(diphosphine)iron nitriles. In the solid state our main interest is to align the molecules and avoid centrosymmetric space groups. When trying to solve the structure of the title complex we had several difficulties and the structure proved to be modulated. Refinements are being done using JANA and final results will be presented in this work.

[1] Whittall I.R., et al, *Adv. Organomet. Chem.*, 1999, **43**, 349. [2] Goovaerts E., et al, *Handbook of Advanced Electronic and Photonic Materials*, Ed. H.S. Nalwa, 2001, **9**, Ch. 3, 127. [3] Wenseleers W. et al, *J. Mater.Chem.*, 1998, **8**, 925. [4] Garcia M.H., Robalo M.P., Teixeira A.P.S., Piedade M.F.M., Duarte M.T., Dias A.R., *J. Organomet. Chem.*, 2001, **632**, 145.

Keywords: NLO, organometallic compound, modulated structure