

**Title:** Synthesis of new Fe(II) and Ru(II) eta(5)-monocyclopentadienyl compounds showing significant second order NLO properties

**Author(s):** Valente, Andreia <sup>[1]</sup>; Royer, Sophie <sup>[2]</sup>; Narendra, Milan <sup>[1]</sup>; Silva, Tiago J. L. <sup>[1,3]</sup>; Mendes, Paulo J. G. <sup>[3]</sup>; **Robalo, M. Paula** <sup>[2,4]</sup>; Abreu, Manuel <sup>[5]</sup>; Heck, Juergen <sup>[6]</sup>; Garcia, M. Helena <sup>[1]</sup>

**Source:** Journal of Organometallic Chemistry **Volume:** 736 **Pages:** 42-49

**DOI:** 10.1016/j.jorganchem.2013.02.028 **Published:** Jul 15 2013

**Document Type:** Article

**Language:** English

**Abstract:** A series of new ruthenium(II) complexes of the general formula [Ru(eta(5)-C5H5)(PP)(L)][PF6] (PP = DPPE or 2PPH(3), L = 4-butoxybenzotrile or N-(3-cyanophenyl)formamide) and the binuclear iron(II) complex [Fe(eta(5)-C5H5)(PP)(mu-L)(PP)(eta(5)-C5H5)Fe][PF6](2) (L = (E)-2-(3-(4-nitrophenyl)allylidene)malononitrile, that has been also newly synthesized) have been prepared and studied to evaluate their potential in the second harmonic generation property. All the new compounds were fully characterized by NMR, IR and UV-Vis spectroscopies and their electrochemistry behaviour was studied by cyclic voltammetry. Quadratic hyperpolarizabilities (beta) of three of the complexes have been determined by hyper-Rayleigh scattering (HRS) measurements at fundamental wavelength of 1500 nm and the calculated static beta(0) values are found to fall in the range 65-212 x 10(-30) esu. Compound presenting beta(0) = 212 x 10(-30) esu has revealed to be 1.2 times more efficient than urea standard in the second harmonic generation (SHG) property, measured in the solid state by Kurtz powder technique, using a Nd:YAG laser (1064 nm). (C) 2013 Elsevier B.V. All rights reserved.

**Author Keywords:** Cyclopentadienyl complexes; Quadratic hyperpolarizabilities; Hyper-Rayleigh scattering; Kurtz powder technique; Second-order nonlinear optical

**KeyWords Plus:** Nonlinear-Optical Properties; Hyper-Rayleigh Scattering; Ray Crystal-Structure; Organometallic Compounds; 2ND-Harmonic Generation; Organic Materials; Powder Technique; Metal-Complexes; Hyperpolarizabilities; Derivatives

**Reprint Address:** Garcia, MH (reprint author) - Univ Lisbon, Ctr Ciencias Mol & Mat, Fac Ciencias, P-1749016 Lisbon, Portugal.

**Addresses:**

[1] Univ Lisbon, Ctr Ciencias Mol & Mat, Fac Ciencias, P-1749016 Lisbon, Portugal

[2] Inst Super Tecn, Ctr Quim Estrutural, P-1049001 Lisbon, Portugal

[3] Univ Evora, Ctr Quim Evora, P-7002554 Evora, Portugal

[4] Inst Super Engn Lisboa, Area Dept Engn Quim, P-1959007 Lisbon, Portugal

[5] Univ Lisbon, Dept Fis, Fac Ciencias, Lab Opt Lasers & Sistemas, P-1749016 Lisbon, Portugal

[6] Univ Hamburg, Inst Anorgan & Angew Chem, D-20146 Hamburg, Germany

**Funding:**

Funding Agency	Grant Number
Portuguese Foundation for Science and Technology	PTDC-QUI-66148-2006 PEst-OE/QUI/UI0536/2011 SFRH/BPD/80459/2011

**Publisher:** Elsevier Science SA

**Publisher Address:** Po Box 564, 1001 Lausanne, Switzerland

**ISSN:** 0022-328X

**Citation:** VALENTE, Andreia; ROYER, Sophie; NARENDRA, Milan; SILVA, Tiago J. L.; MENDES, Paulo J. G.; ROBALO, M. Paula; ABREU, Manuel; HECK Juergen; GARCIA, M. Helena - Synthesis of new Fe(II) and Ru(II) eta(5)-monocyclopentadienyl compounds showing significant second order NLO properties. Journal of Organometallic Chemistry. ISSN 0022-328X. Vol. 736 (2013), p. 42-49.