

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

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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.

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