

Nonlinear optical response of octupolar Zn(II) complexes incorporating highly aromatic polypyridinic ligands: Insights into the role of the metal center

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© 2017 Elsevier B.V. In this work, the linear and nonlinear optical properties of a series of octupolar Zn(II) complexes with highly aromatic polypyridine ligands are investigated. The effect of the metal center on the spectroscopic properties of octupolar Zn (II) complexes are explored and compared to its respective free ligands. DFT and TD-DFT calculations were performed to gain more insights about the electronic and structural properties of these compounds. The aromaticity index of ligands and its modulation by Zn(II) in complexes was also theoretically studied. Quadratic hyperpolarizabilities ($\chi^{(2)}$) were determined by using the Hyper-Light Scattering (HLS) technique at 1.06 μm . Results show that $\chi^{(2)}$ values of the octupolar Zn(II) complexes are around three times higher than those of their respective ligands, which correlates with the number of ligands directly coordinated to the metal center. These results show how Zn(II) plays a positive structural role in the elaboration of highly tra