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PROGRAM

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NOVEL TETRAZINE ORGANOMETALLIC COMPLEXES FOR NONLINEAR OPTICAL SWITCHING: A COMBINED DENSITY FUNCTIONAL THEORY AND EXPERIMENTAL STUDY

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Over the past decade, mono- and bi- and oligonuclear organometallic complexes have been deal of great interest by material chemists and engineers since they were envisaged as powerful candidates for quantum computing, molecular devices and more interestingly as molecular switches.[1]The definition of molecular switch implies that a compound should have two interconvertable stable forms that have a significant difference in the magnitude of, at least, one of their physico-chemical properties. [2]In the case of organometallic complexes the most expedite way to achieve such interconversion is by redox means, where one takes advantage of the different oxidations states allowed by a single or multiple metal centers that interact with each other, and with the ligands therein.

It is known that the choice of an appropriate π-bridging system between the metal centers is crucial to obtain the adequate electronic environment for efficient metal-to-metal and metal-to-ligand interactions, and hence fine tune their optical properties. Mixed-valance metal complexes, particularlly Fe(II)/Fe(III) and Ru(II)/Ru(III) systems [3,4],have been successfully synthesized as stable species that possess strong MLCT and IVCT absorption bands in visible and NIR regions, respectively.[5, 6]This is the case of the $[(H_3N)_5Ru(m\text{-}pz)Ru(NH_3)_5]^{5+}$ ion (pz=pyrazine) and related compounds. Substituted 1,2,4,5-tetrazine (tz) strongly enhance both the stability and the MLCT and IVCT phenomenon's since they act as a strong π-acceptor and can stimulate the metal-to-metal interaction.[6]

In this work, we present our ongoing studies in the use of substituted 1,2,4,5-tetrazine (tz) ligands as the π-bridge between two transition metal centers, both experimentally and by means of Density Functional Theory (DFT). Synthesis and characterization of the complexes are presented. The DFT calculations were used to evaluate the nature of the electronic transitions as well as the switching of the NLO properties. The compounds showed to be great candidates for NLO switching.

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