

Studies on the solvatochromic effect and NLO response in new symmetric bimetallic Rhenium compounds

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Abstract

In the search of novel coordination complexes with enhanced nonlinear optical activity, symmetrical bimetallic Rhenium complexes incorporating polypyridine plane bridging ligands are reported. The complexes studied were of the type $(\text{Re}(\text{CO})(3)\text{Cl})(2)\mu\text{-N}^{\langle \wedge \rangle \text{N}}$, with $\text{N}^{\langle \wedge \rangle \text{N}}$ 2,3-Dicarboxypyrazino[2,3-f][4,7]phenanthrolinecarboxylic (L1), or 2,3-Diethoxycarbonylpyrazino[2,3-f][4,7]phenanthroline (L2). Specifically, the physicochemical, solvatochromic, and nonlinear optical behaviour of the complexes were measured. DFT calculations were also performed, in order to improve the understanding of the observed phenomena.

Spectroscopic characterization shows absorption bands at low energy associated to a charge transfer that involves the electronic transition from the Rhenium center and Chloride ligand towards the bridging ligand ($\text{Re}(d) + \text{Cl}(n) \rightarrow \text{L1}(\pi^*)$; $\text{Re}(d) + \text{Cl}(n) \rightarrow \text{L2}(\pi^*)$) in both complexes. These bands are strongly dependent on the polarity of the solvent. This behaviour indicates a redistribution of the electronic density, mainly observed in the complex with L1. As expected, a relationship between solvatochromic effect and NLO response of the analyzed complexes was observed. The bimetallic complexes show a high NLO response, that is a noteworthy effect considering the symmetrical arrangement of the bimetallic complexes herein reported, the non-centro symmetry of these molecules being due to the carboxylic and ester groups only. (C) 2020 Elsevier Ltd. All rights reserved.

Palabras clave

Palabras clave de autor: [Rhenium complexes](#); [Bridging ligand](#); [Metal to ligand charge transfer](#); [Solvatochromic effect](#); [Nonlinear optics](#)

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