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Vibrational and NMR Properties of 2,2′-Biquinolines: Experimental and Computational Spectroscopy Study

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Experimental (IR, Raman and NMR) techniques and quantum chemical (DFT) methods have been applied to investigate the vibrational and NMR properties of a new ligand based on 2,2′-biquinoline (*bq*) functionalized with polar hydrophilic tetraethylene glycol monomethylether (TEG) chains (*bq_TEG*). Vibrational and NMR spectra of the ligand have been explained based on DFT computational data obtained at B3LYP/6-311+G(d,p) level of theory. For the spectroscopic analysis we started from the parent molecule 2,2′-biquinoline and explained the changes in the spectra of *bq_TEG* in close relation to the corresponding spectra of *bq*. Our data point to a *trans* conformation of *bq_TEG* in solid state, as wells as in liquid phase. The excellent agreement between the experimental and computed data allowed for a reliable assignment of the vibrational and NMR spectra, both for *bq* and *bq_TEG*.

Keywords: 2,2′-Biquinoline, Ligand, FTIR, Raman, NMR, DFT.

1. INTRODUCTION

N∧N-chelating oligopyridines are a well-known class of ligands used in supramolecular chemistry to obtain functional materials with targeted properties like luminescence, magnetism, catalytic activity, etc. The most studied ligands from this class are based on 2,2′-bipyridine [1, 2] and 1,10-phenanthroline [3, 4]. On the other hand, 2,2′-biquinoline (*bq* in Chart 1) is a more sterically demanding ligand, which can be successfully used in obtaining transition metal complexes with remarkable biological activities [5–8]. However, for applications in biomedical fields, water soluble coordination complexes are highly researched. Previously we reported on the synthesis and characterization of a new ligand, namely ditetraethylene glycol monomethylether 2,2′-biquinoline-4,4′-dicarboxylate (*bq_TEG* in Chart 1) based on 2,2′-biquinoline functionalized with polar hydrophilic chains (*TEG*: tetraethylene glycol monomethylether) which showed good potential in obtaining Zn(II) and Cu(II) species soluble in aqueous media [9]. Giving the difficulty of inducing water solubility in such systems we considered that an accurate investigation of the structural and electronic properties of this ligand is essential.

N-containing functional groups such as pyridinic or phenanthrolinic, are important reactive centres in controlled catalytic edges carbonaceous materials like functionalized graphenes [1], *N*-carbon materials [11, 12] etc. being extensively studied both experimental and using density functional theory calculations [13]. Therefore, we consider that the accurate investigations of spectral properties of ligands based on 2,2′-biquinolines can bring important developments in the field of carbonaceous materials and in the coordination chemistry of N∧N-chelators, metal organic frameworks (MOFs) prepared with the latter being also excellent precursors for the former [14–16]. On this background, herein we present the Fourier transform infrared (FTIR), Raman and Nuclear Magnetic Resonance (NMR) spectroscopic and DFT theoretical studies for the ligands *bq* and *bq_TEG*. Although the synthesis

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