Poster Presentation

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Investigating valence tautomerism presence in compounds of Co and naphthoquinone

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The search for new functional materials involves the development of bistable molecules exhibiting different electronic states with distinct properties at the ambient condition (temperature, pressure, illumination) of application. Coordination compounds, which present electron transfer between metal ion and an organic ligand associated with a change in electron multiplicity of the metal ion, are named valence tautomers(VT)[1]. The chemical equilibrium between two distinct electronic states in VT can be induced by temperature and pressure change as well as by soft X-ray and light irradiation. Thermodynamic and structural data highlighting the mechanisms of the valence tautomerism interconversion can be found in the literature for materials build up with cobalt and benzoquinones such as the 3,5-di-t-butyl-semiquinonate. However, to the best of our knowledge, there is no example of compounds showing VT build up with cobalt and naphthoquinones. In the present work 2-hydroxy-1,4-naphthoquinone (law) has been used as redox active ligands in the search for new VT compounds with cobalt. Three new coordination compounds of cobalt and 2-hydroxy-1,4-naphthoquinone (law), [Co(law)2(im)2], [Co(law)2(phen)] e [Co(law)2(bpy)] were synthesized and characterized by infrared (IR), UV-vis spectroscopy, electron paramagnetic resonance (EPR) and cyclic voltammetry. The three dimensional structures were determined using single crystal X-ray diffraction techniques. However, within the investigated temperature range neither X-ray diffraction nor EPR data showed the presence of VT in the materials, mainly due to the electrochemical properties of the 2-hydroxy-1,4-naphthoquinone. Nevertheless the structural features of the compounds as well as their supramolecular packing motifs suggest that naphthoquinones can be an alternative for the synthesis of compounds showing valence tautomerism[3].

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