Combined DFT and spectroscopic study of biologically active Cu-, Ni-, Co-Quinolone complexes with phenantroline

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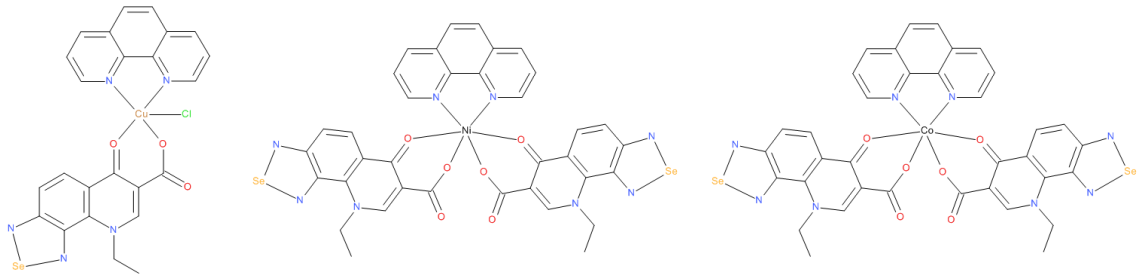
Quinolones are generally used against many gram positive and gram negative bacteria.[1] It has been shown that the presence of selenium in the quinolone structure can positively affect its biological impact.[2] Newly synthesized [3] biologically active copper (**1**), nickel (**2**), and cobalt (**3**) complexes with selenadiazoloquinolone ligands have been studied by theoretical calculations and in situ EPR/UV-vis-NIR spectroelectrochemistry. Structure of these complexes is shown in Figure 1. Due to the complicated structure of coordination polyhedron (*i.e.* three bidentate ligands in the case of **2** and **3**) a considerable attention has been paid to the conformation analysis of the studied systems. Calculated results were compared with the experimentally obtained X-ray geometries. Non-relativistic Fermi contact terms as well as relativistic hyperfine coupling constants and g-tensors are presented and compared with in situ EPR experiment.



1 **2** **3**

Figure 1: Structure of systems under study.

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