Abstract

In this study, the ability of the Cu metal to form different coordination complexes with the ligand "quercetin" was investigated. Quercetin is an important flavonol, having a chemical formula of 3,3',4',5,7-pentahydroxyflavone. It is a highly utilized bio-flavonoid, used for the treatment of various inflammatory and metabolic disorders, but it is not produced by the human body. DFT was used to carry out computational studies on all the complexes and the functionl and the basis set used are B3LYP /def2-svp. Three different coordination schemes of the metal Cu and the ligand quercetin are discussed. It was found that Cu is able to form bonds with the ligand (quercetin) in various ways forming different geometries. The metal to ligand ratio can be 1:1 or 1:2. The geometry of the complexes formed can be a square planar complex or an octahedral complex, with water molecules binding to the metal. Our studies also show, how the UV-Vis spectrum obtained from TD-DFT changes with variation in the metal to ligand ratio. We also studied how the HOMO and LUMO orbitals vary for each complex and how their shape changes with respect to each geometry.