

EXPERIMENTAL AND THEORETICAL INVESTIGATIONS OF COMPLEXES IN GROUNDWATER: DFT STUDIES

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Our study focuses on the determination of the physicochemical properties of water resources in the Algerian hydrographic basin and the reduction of the concentration of heavy metals Cu, Zn and Mn.

In order to propose a treatment method for resource waters found to be out of specification, we used the complexation method, which is known for its reliable results.

This mode of treatment is studied using molecular modeling at the level of density functional theory (DFT), to avoid waste of products during the experimental work and to encourage experimenters to exploit the models obtained and apply them.

Although the studied metal ions are negatively correlated with nitrate and chloride ions, complexes containing these ions are modeled and compared with other complexes to assess their chemical and biological reactivities.

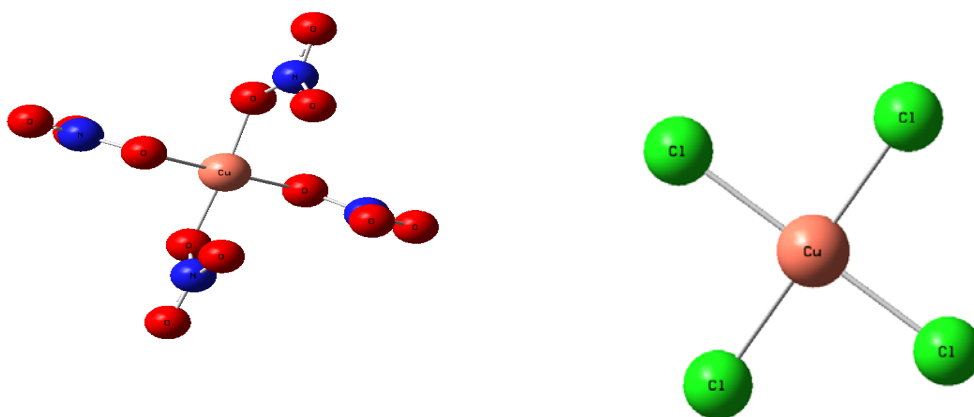


Figure 1: The structures of complexes we take as example the complexes of copper.