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Theoretical Study of Structural Parameters, Chemical Reactivity and Spectral and Thermodynamical Properties of Organometallic Complexes Containing Zinc, Nickel and Cadmium with Nitrilotriacetic Acid and Tea Ligands: Density Functional Theory Investigation

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Abstract : The pollution of water resources is characterized by the presence of microorganisms, chemicals, or industrial waste. Generally, this waste generates effluents containing large quantities of heavy metals, making the water unsuitable for consumption and causing the death of aquatic life and associated biodiversity. Currently, it is very important to assess the impact of heavy metals in water pollution as well as the processes for treating and reducing them. Among the methods of water treatment and disinfection, we mention the complexation of metal ions using ligands which serve to precipitate and subsequently eliminate these ions. In this context, we are interested in the study of complexes containing heavy metals such as zinc, nickel, and cadmium, which are present in several industrial discharges and are discharged into water sources. We will use the ligands of triethanolamine (TEA) and nitrilotriacetic acid (NTA). The theoretical study is based on molecular modeling, using the density functional theory (DFT) implemented in the Gaussian 09 program. The geometric and energetic properties of the above complexes will be calculated. Spectral properties such as infrared, as well as reactivity descriptors, and thermodynamic properties such as enthalpy and free enthalpy will also be determined.

Keywords : heavy metals, NTA, TEA, DFT, IR, reactivity descriptors
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