DFT INVESTIGATION OF NEW MIXED AMINO ACIDS COMPLEXES OF MANGANESE (Mn) WITH PARACETAMOL AS LIGAND

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Ternary complexes present several areas of interest due to the diversity of their structures and their properties. These complexes have many applications, particularly in biology and medicine.

The compounds on which our work relates are the ternary complexes based on Manganese, which is an essential transition metal in the metabolic processes, due to its better biological activity. In this work, we have carried out an experimental study of new Mn(II) complexes with paracetamol as main ligand and various amino acids (Histidine and Proline) as secondary ligand. The studied complexes were synthesized at the level of the coordination chemistry laboratory and characterized by infrared and UV-visible spectroscopies. The antioxidant power of these systems has evaluated by the DPPH method. These complexes have also been studied theoretically using density functional theory (DFT) for the aim to define geometric structures, calculate energetic properties, reactivity descriptors, and spectral properties. Theoretical evaluation of the antioxidant power by the HAT mechanism has also carried out.

In this study we have recorded coherence between the experimental work and the theory computation