

Structural and electronic study at the DFT and TD-DFT level of new gold (III) complexes of bio-pharmacological interest.

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Abstract :

The last decade has witnessed a significant increase in the biological applications of metal complexes due to their key role in therapy [1]. Indeed, these metal ions are known for their ability to bind with nucleic and change their conformations and biological functions. The effectiveness of platinum complexes as anti-cancer agents can be listed as one of the most remarkable successes among inorganic drugs [2]. Gold (III) complexes are iso-structural and iso-electronic with platinum (II) complexes [3]. These complexes generally have interesting cytotoxic and anticancer properties, but their development has so far been severely hampered by their stability in the physiological environment [4].

As part of this work we carried out a theoretical study of the new gold (III) complexes [5]. This theoretical study will allow us to focus on the entire structural and electronic properties as well as their thermodynamic stability and reactivity in order to understand and then propose the right molecules likely to be potential drugs candidates. This work is carried out at the DFT and TD-DFT level with bases 6-311+G (d,p) for light atoms and LANL2DZ for the metal ion. The theoretical results will be compares with those obtained experimentally.

Keywords: coordination metals, gold (III) complexes, DFT and TD-DFT.