

We can say that these studies are mainly devoted to the quantification of the spin-spin exchange coupling constant within the bimetallic molecular complexes of uranium (IV) and (V), the study of the properties and magnetic behavior and the modeling of the coupling of these complexes containing two metallic centers of uranium bound together by an aromatic bridging ligand, which exhibits anti and ferromagnetic exchange interactions.

Therefore, our objective is to understand the role of metal f orbitals in the creation of metal-ligand chemical bonds and the properties of the compounds studied. The method used is based on the theory of the functional of the density "DFT", by taking into account the relativistic effects by the approximation ZORA (Zeroth Order Regular Approximation) coupled with the method of the broken symmetry of the spin "BS". This DFT/ZORA/BS method has proven itself for this type of study and treatment of the properties of this type of system.

After several years of work, we were able to collect and extract the results obtained in this thesis which consists of several parts, which include an introduction and a general conclusion with four talking chapters on our research subject.

The first chapter entitled (Theoretical and methodological aspect) contains the theoretical aspects and the methodology of quantum chemistry, the important relativistic effects, the approximations and the approaches for this study to carry out.

The second chapter takes up the concepts and the fundamental relations of the theories applied in quantum chemistry, which allowed us to obtain these results, and which explains the field of the magnetic fields and the exchange coupling, the different approaches which helped us to model and study the magnetic coupling as the method of broken symmetry BS (Broken symmetry), the methods and the techniques of the realization of the calculations. This chapter entitled (Molecular magnetism, general concept).

Constitute the essence of the results obtained within the framework of this doctoral thesis. The third chapter entitled (relativistic DFT study of magnetic coupling in the diuranium U(IV)-U(IV) ethynediyl-bispyrazine and imino-amido quinoid complexes.) we were interested in studying the ferro or antiferromagnetic magnetic character of di-uranium U(IV) of the $5f^2-5f^2$ configuration, linked by two different types of aromatic bridge. the model ethynediyl-bispyrazine diuranium $[\text{Cp}_3\text{U}]_2(\text{ethyne-1,2-diyl})\text{bis}(\text{pyrazi-4-ide})$ an unsynthesized typical example showing significant magnetic properties, the second complex is imino-amido quinoid diuranium which is recently synthesized and which gives results and behaviors in agreement with experimental, these two complexes present an