Abstract:

In the last three decades, the studies of organometallic complexes containing heavy metals of element f (lanthanides and actinides) have been widely explored; this field is experiencing a remarkable state of progress on the experimental and theoretical levels, particularly for bimetallic complexes. This type of complexes recently synthesized with interesting properties, such as magnetic properties which are of great interest from the point of view of fundamental research and technological application as single molecular magnet or SMM which are integrated in the development of digital information storage.

One of the main goals of this field is to understand the factors that control and affect the interactions between the magnetic sites of two metals linked by an aromatic ligand. For this we need to know the electronic and magnetic structures of these objects. Theoretically, the use of relativistic density functional theory gives many possibilities to study those chemical systems that contain a large number of electrons.

The study of f-element complexes shows that they have structural and electronic properties not known in transition metal chemistry, these properties indicating metal-ligand interactions depending on the relativistic effects of heavy metals.

Most important think in these studies is to understand the role of the d and f valence orbitals of the metal to create metal-ligand bond and the nature of the metal bond in these complexes so as to rationalize their physical and chemical properties. But there are always difficulties found in carrying out the experimental studies due to many obstacles such as radiotoxicity and the scarcity of the raw material and sometimes the high budget. Carry out theoretical studies. Nevertheless, it remains to find solutions concerning calculation methods and computer tools, for example systems involving a very high number of electrons require very large memory capacities and a very high calculation time that can reach several months for a single complex. Without forgetting the correlations problems and relativistic effects.

The present work has been developed since 2014, we are interested in applying the density functional theory (DFT) in the study of the modeling and the determination of the magnetic properties of bi-nuclear organometallic complexes of element f, as well as theoretical studies applied in the form of theoretical calculations at the level of the ADF calculation program (Amsterdam density functional).