antiferromagnetic behavior, we carried out calculations DFT/ZORA/B3LYP coupled with the approach Broken Symmetry (BS) to try to explain the magnetic behavior of two compounds.

We have enriched our theoretical study with a fourth chapter under the title (Electronic structure and magnetic properties of bridged diuranium(V) naphthalene and stilbene-diimide complexes: a theoretical study.) which speaks about the study of the other two molecular pentavalent systems U(V) uranium bis metal of the $5f^1$-$5f^1$ configuration. In this chapter we have provided a theoretical study of two paramagnetic complexes naphthalene-diimide $[(MeC_5H_4)_3UV]_2(\mu\text{-}1,5\text{-}N_2C_{10}H_6]$ and stilbene-diimide $[(MeC_5H_4)_3UV]_2(\mu\text{ -}1,2\text{- }(4\text{-}NC_6H_4)_2\text{-}C_2H_2]$, and which have no systematic theoretical study to date. These systems were synthesized and rationalized from an experimental result obtained by Rosen et al.in 1989 but their magnetic behaviors were not entirely demonstrated by susceptibility measurements Both complexes exhibit antiferromagnetic behavior in the U(V)—L—U(V) superexchange interaction.

The results obtained confirm the effectiveness of the method used in all respects, since it is consistent with the published experimental results.

Keywords: magnetic properties, spin-spin coupling, DFT, spin broken symmetry, organometallic compounds, uranium.