Bonding and Electronic Structure In

\[ \text{[THF}_2\text{Lu]}_2(\mu-\eta^2:\eta^2\text{N}_2) \text{ L} = \text{N(SiMe}_3)_2 \text{ and C}_5\text{Me}_4\text{H} \]

Computational Analysis Of The Ligand Effect

D. Hannachi, A. May, A. Ounissi, H. Benflis et N. Ouddai

Laboratoire de Chimie des matériaux et des vivants : Activité, Réactivité, Université de Batna 05000 - Algérie.
ounissi_abdelhamid@hotmail.com

The purpose of our work is to present a theoretical comparative study of these compounds based on lutetium, according the nature of the surrounding ligands

\[ \text{[THF(C}_5\text{Me}_4\text{H})_2\text{Lu]}_2(\mu-\eta^2:\eta^2\text{N}_2) \] 1

\[ \text{[THF}\{\text{N(SiMe}_3)_2\}_2\text{Lu]}_2(\mu-\eta^2:\eta^2\text{N}_2) \] 2

Quantum calculations, carried out using DFT and TD-DFT methods, enabled us to establish a correlation between the structural arrangement of these compounds and their physical properties, in particular the luminescence. The effect of the surrounding ligands on the nitrogen-nitrogen bond of the bridge is well verified. The application of the DFT broken symmetry approach in the study of binuclear systems has been carried out in the aim of quantifying the exchange constants of which the determination using the traditional magnetochemical measurements is thought to be difficult. In the recent years the development of new luminescent materials are gaining more and more attention. The luminescent lanthanide complexes have attracted a lot of attention due to their potential applications in fluorescent materials, electroluminescent devices, and medicinal diagnostics, etc. Trivalence europium, terbium, samarium, and dysprosium are very good luminescent centers owing to their f-electronic configuration. Luminescent intensities of lanthanide complexes are dependent on organic ligands. J. Evans William, S. Lee David and al reported the synthesis and the X-ray structure of dilutetium complexes 1 and 2 in Refs 1-2, respectively (see scheme 1). In this paper, we apply a variety of DFT computational methods to questions of bonding and electronic structure in the dilutetium complexes 1 and 2.

\[ \text{[THF(C}_5\text{Me}_4\text{H})_2\text{Lu]}_2(\mu-\eta^2:\eta^2\text{N}_2) \] (1)

\[ \text{[THF}\{\text{N(SiMe}_3)_2\}_2\text{Lu]}_2(\mu-\eta^2:\eta^2\text{N}_2) \] (2)

REFERENCES