

## DFT investigation: Molecular and electronic properties of homogeneous trinuclear complexes of formulas $M_3(\text{Ant})_2$ , $M_3(\text{CO})_2(\text{Ant})_2$ ( $M = \text{Ti, Cr, Fe and Ni}$ )

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**Abstract.** The theoretical calculations applied in this study were carried out on homogeneous trimetallic complexes of  $M_3(\text{Ant})_2$  ( $M = \text{Ti, Cr, Fe, Ni}$ ), ( $\text{C}_{14}\text{H}_{10} = \text{Ant} = \text{l'anthracene}$ ) via the functional GGA BP86 using density functional theory (DFT) to elucidate the mode of coordination that governs this type of complexes as well as the metal-metal bonding order, this depending on the nature of the metal. Also the substituted complexes of the  $M_3(\text{CO})_2(\text{Ant})_2$  type will be analyzed after the introduction of carbonyl ligands, in order to see the effect of this substitution on the formation where the breaking of existing metal bonds in the trimetallic compound, and on the stabilization of this type of substituted complexes.

**Keywords:** Anthracene ligand, electronic configuration, NBO analysis.

### Introduction

Neutral anthracene ( $\text{C}_{14}\text{H}_{10} = \text{Ant}$ ) is a 14-electron polycyclic molecule  $\pi$  composed of three C6 benzene rings (Scheme 1) and promises a particularly strong communication between three  $\pi$ -coordinated metal centers. A theoretical study with a complete rationalization concerning the neutral sandwich complexes  $M_3(\text{Ant})_2$  ( $M = \text{Ti, Cr, Fe, Ni}$ ) was carried out using calculations of the theory of the density functional (DFT) applied to the atoms metal sandwiched between two anthracene ligands, which have not been isolated so far. The density functional theory (DFT) method using the BP86 non-local density functional approximation [1-2] which combines the Becke exchange function in 1988 with that of corrected correlation Perdew The 1986 gradient is valuable for determining electronic structures, geometric parameters, bonding analysis, and other properties based on various workings of organometallic and inorganic systems [3-4]. BP86 calculations were performed assuming the Frozen-Core approximation up to 1s for C, 3p for first-row metals. The complete geometrical optimizations were carried out using the analytical gradient method implemented by Versluis and Ziegler. High spin calculations were performed for all open-layer systems. Frequency calculations [4] were performed on all the compounds studied to verify that the optimized structures are minimums of energy. Representation of