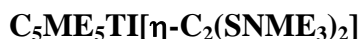


THE NATURE OF THE METAL-ACETYLIDE INTERACTION IN THE TERNARY TRANSITION METAL ACETYLIDE COMPLEX



A. May¹, N. Ouddai¹ and A. Ounissi^{2,*}

1Laboratoire de Chimie des Matériaux et des Vivants: Activité, Réactivité Univ Hadj-Lakhdar Batna, Algeria

2. Laboratoire d'Electronique Avancée University Hadj-Lakhdar Batna, Algeria

Ounissi_abdelhamid@hotmail.com

Abstract

The metal–acetylide bonding in the transition metal acetylide $\text{C}_5\text{Me}_5\text{Ti}[\eta\text{-C}_2(\text{SnMe}_3)_2]$ complex have been studied at the density functional theory (DFT) level using natural bond orbital (NBO)[1], energy decomposition analysis (EDA)[2], atoms in molecule (AIM)[3] and electron localization function (ELF)[4] methods. The NBO analyses show that there is a single bond between each M-C_{acetylide} bond, and all of them are polarized toward the C atoms. These bonds were associated with the intermediate atomic interaction type in terms of the Bader topological theory, whereas, both EDA and ELF methods support the classification of the metal-C_{acetylide} bonding as mainly ionic.

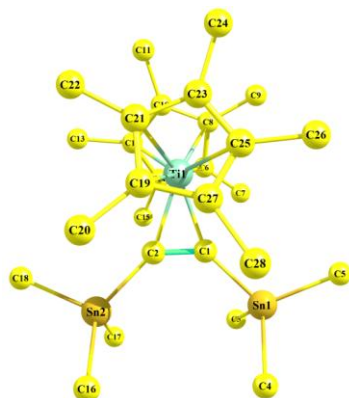


Figure 1: Molecular structure of the parent complex

$\text{C}_5\text{Me}_5\text{Ti}[\eta\text{-C}_2(\text{SnMe}_3)_2]$. The hydrogen are removed for clarity

Keywords:

Transition metal acetylide, polymetallic acetylide compounds, (NBO), (EDA), (AIM), (ELF) methods

REFERENCES

1. J. P. Foster, F. Weinhold, J. Am. Chem. Soc., 102, 7211(1980).
2. T. Ziegler, A. Rauk, Inorg. Chem., 18, 1558(1979).
3. R. F. W. Bader, Chem. Rev., 91, 893(1991).
4. A. D. Becke, K. E. J. Edgecombe, Chem. Phys., 92, 5397(1990).