DFT Study of Half Sandwich of Vanadium (IV) Cyclopentadienyl Complexes

Authors : Salem El-Tohami Ashoor

Abstract : A novel new vanadium (IV) complexes incorporating the chelating diamido cyclopentadienyl {ArN(CH2)3NAr)}2-((ηn-Cp)Cp)} (Ar = 2,6-Pri2C6H3)(Cp = C5H5 and n = 1,2,3,4 and 5) have been studied with calculation of the properties of species involved in various of cyclopentadienyl reaction. These were carried out under investigation of density functional theory (DFT) calculation, and comparing together. Other methods, explicitly including electron correlation, are necessary for more accurate calculations; MB3LYP (Becke) (Lee–Yang–Parr) level of theory often being used to obtain more exact results. These complexes were estimated of electronic energy for molecular system, because it accounts for all electron correlation interactions. The optimised of [V(ArN(CH2)3NAr)2Cl(η5-Cp)] (Ar = 2,6-Pri2C6H3 and Cp= C5H5) was found to be thermally more stable than others of vanadium cyclopentadienyl. In the meantime the complex [V(ArN(CH2)3NAr)2Cl(η1-Cp)] (Ar = 2,6-Pri2C6H3 and Cp= C5H5) which is showed a low thermal stability in case of the just one carbon of cyclopentadienyl can be insertion with vanadium metal centre. By using Dewar-Chatt-Duncanson model, as a basis of the molecular orbital (MO) analysis and showed the highest occupied molecular orbital (HOMO) and lowest occupied molecular orbital LUMO.

Keywords : vanadium (IV) cyclopentadienyl complexes, DFT, MO, HOMO, LUMO
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