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Molecular and Electronic Structure of Chromium (III) Cyclopentadienyl Complexes

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Abstract : Here we show that the reduction of [Cr(ArN(CH2)3NAr)2Cl2] (1) where (Ar = 2,6-Pri2C6H3) and in presence of NaCp (2) (Cp= C5H5 = cyclopentadien), with a center coordination η5 interaction between Cp as co-ligand and chromium metal center, this was optimization by using density functional theory (DFT) and then was comparing with experimental data, also other possibility of Cp interacted with ion metal were tested like η1 ,η2 ,η3 and η4 under optimization system. 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 [Cr(ArN(CH2)3NAr)2(η5-Cp)] (Ar = 2,6-Pri2C6H3 and Cp= C5H5) was found to be thermally more stable than others of chromium cyclopentadienyl. 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 : Chromium(III) cyclopentadienyl complexes, DFT, MO, HOMO, LUMO
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