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Natural Bond Orbital (NBO) Population Analysis of Iridabenzene $(C_5H_5Ir)(PH_3)_3$

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Abstract

The molecular structure of iridabenzene $(C_5H_5Ir)(PH_3)_3$ was calculated by the B3LYP density functional model using LANL2DZ basis set for Ir and 6-31G(d) for other atoms. The results from natural bond orbital (NBO) analysis have provided new insights into Ir–ligand bonding, the hybridization of atoms and the electronic structure of the title molecule. The NBO calculations show that σ(Ir-C2) bonds are formed from an $sd^{1.18}$ hybrid on iridium atom π(Ir–C3) bond is formed from an $sd^{5.21}$. Also, these calculations determined that strongest electron donation occurs from a lone pair orbital on the phosphorous atoms, LP(1)P to the antibonding acceptor σ*(Ir–C) orbitals.

Keywords: *Density functional theory (DFT), Metallabenzenes, Iridabenzene, Natural bond orbital (NBO).*

Introduction

For the past decade the synthesis of metallabenzenes have been examining [1-7] and their valence isomers starting from (Z)-3-(2-iodoethenyl)cyclopropenes [8-12]. Recently, the direct synthesis of a series of iridabenzenes from nucleophilic 3-vinylcyclopropenes reported. From experimental and theoretical examinations, it is obersrved that the actual experimental knowledge concerning iridabenzenes compounds is still relatively limited due to the subtle nature of such compounds.

The objective of the present work is to investigate the nature of bonding in an iridabenzene (Figure 1), by using natural bond orbital (NBO) analysis. We have shown that the results from NBO calculations can provide the detailed insight into the electronic structure of molecule.

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