Natural Bond Analysis (NBO) and Quantum Theory Atoms in Molecules

Analysis of Platinabenzene (C₅H₅Pt)Cp

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The molecular structure of platinabenzene (C₅H₅Pt)Cp was calculated by the B3LYP density functional model using LANL2DZ basis set for Pt and 6-31G (d,p) for other atoms. The results from atoms in molecules theory (AIM) and natural bond orbital (NBO) analysis have provided new insights into Pt–ligand bonding, the hybridization of atoms and the electronic structure of the title molecule.

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

The main goal of the present work is to provide investigate the nature of bonding in an platinabenzene, 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.

REFERENCES