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Semi-Empirical Calculations on Carbon70 with Trimer Water Molecules

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Abstract: Quantum mechanical Semi-Empirical calculations are carried out for the fullerene carbon70 and carbon70 with three water molecules. Carbon70 is a rugby ball structure, when three water molecules are added inside it, dissociation of charges takes place. Endohedral C70 shows semiconductor and magnetic properties, which is reflected in the form of dipole moment. Total energies and dipole moments are reported for this molecule at the Semi-Empirical MNDO, AM1and PM3 calculations.

Index Terms: Carbon70; $(H_2O)_3@C_{70}$, Endoheral fullerene, Semi-empirical: MNDO, AM1 and PM3.

1. INTRODUCTION

Theoretical predictions of buckyball molecules appeared in literature between 1960 and 1970. Carbon70 was discovered in 1985 by Robert Curl, Harold Kroto and Richard Smalley using laser evaporation of graphite and found C_n clusters (n>20) of which the most common were C_{60} and C_{70}. For this discovery they have been Nobel Prize in 1996. Carbon70 molecule, which is one type of fullerene is a cage like fused ring structure, resembles like a rugby ball. Fullerene70 is made by 25 hexagons and 12 pentagons. Endohedral fullerenes also called as endofullerenes are fullerenes that have additional atoms, ions, clusters enclosed within their inner spheres. The first lanthanum C60 complex was synthesized in 1985 and called as La@C_{60} [**1**]. C60 with one water molecule [2] and three water molecule [**3**] is reported. Also C70 with two water molecules [**4**] are reported. In this work three water molecules are included inside the fullerene70 is reported and can be called as $(H_2O)_3@C_{70}$. The Quantum Mechanical Semi-Empirical calculations are carried out at MNDO, AM1 and PM3 levels.

2. METHOD OF CALCULATIONS

Computations of Quantum Mechanical Semi-empirical calculations are carried out with MNDO, AM1 and PM3 methods by using the quantum computations package, Firefly [**5, 6]** and Avogadro [**7].** Calculations are carried out at the Research Center, KG Reddy College of Engineering and Technology. Telangana-501504, India.

3. RESULTS AND DISCUSSION

The structure of fullerene70 is shown in Figure.1 and the structure of Carbon70 with three waters is shown in Figure.2. Quantum Mechanical Semi-empirical calculations are carried out at MNDO, AM1 and PM3 levels. Total energies of these molecules are given in Table.1 in atomic units

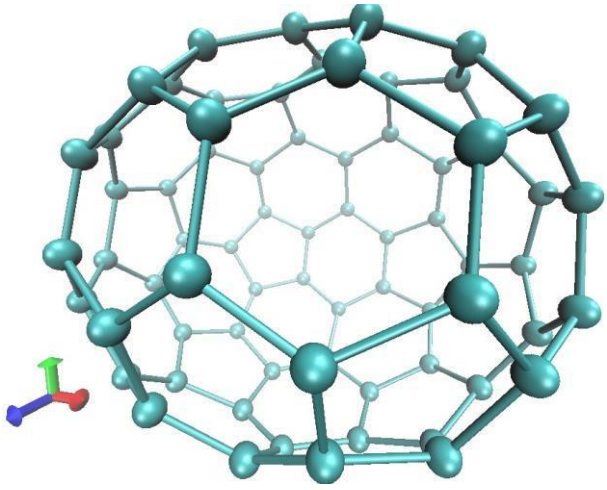

Figure.1. Carbon70

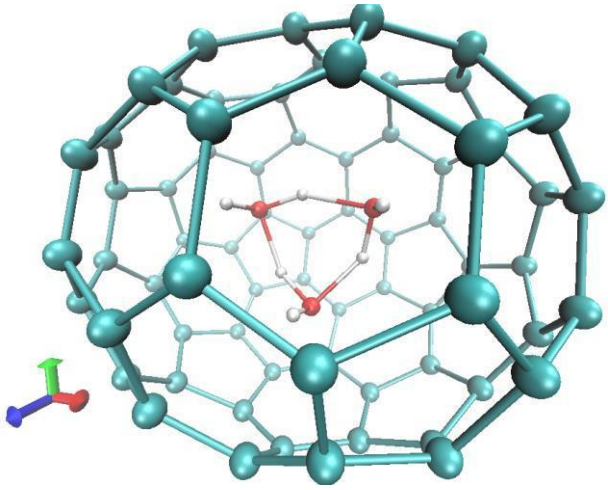

Figure. 2. Carbon70 with three water molecules.

Bond length of hydrogen attached with Oxygen and angle of hydrogens of each water molecule are

reported in the Figure.2. Cyclic hydrogen bonds inside Carbon70 is shown in Figure.3.

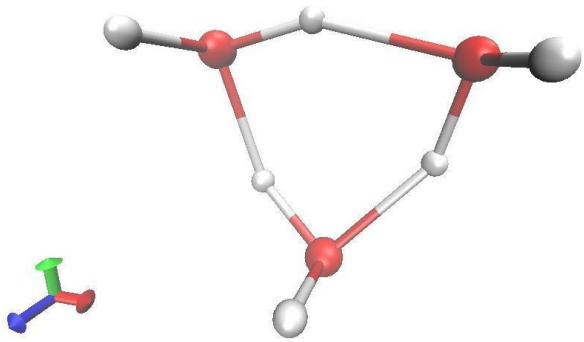

Figure.3. Cyclic hydrogen bonds inside Carbon70

The pentagons and hexagons of the rugby ball structure of fullerene70, figure-1, are adopted to have the usual bond lengths and bond angles as reported experimentally. Due to the inclusion of water molecules, figure-2, C70 structure is slightly modified and the formation of dipole moment is seen. The dipole moment has been found to be 0.16, 0.16 and 0.22 debye respectively for AM1, MNDO and PM3 calculation. Dipole moment is the indication of conductivity and magnetism. Three water molecules inside C70 interact with each other through hydrogen bonding, one hydrogen of the water molecule with Oxygen of other water molecule respectively bonding in cycle, which makes themselves as a cyclic water timer. Water trimer exhibits ortho configuration inside C70, rather para configuration when it is outside the rugby ball. Total energies in Table-1 indicate the stability of C70 and $(H_2O)_3@C_{70}$.

Fullerenes and Endohedral fullerenes will find lot of applications in conductivity, magnetism and storing atoms and molecules. It seems to be finding applications in sensing, cosmetics and medicinal fields. This kind of studies will help to achieve the above applications. Applications

Table.1 Total Energy in Atomic Units.

Semi-Empirical levels	**CARBON70**	**$(H_2O)_3@C_{70}$**
MNDO	-327.544880	-365.927338
AM1	-328.160130	-366.510703
PM3	-303.784505	-339.508700

4. CONCLUSION

Quantum mechanical Semi-empirical Calculations by MNDO, AM1 and PM3 levels on fullerenes and endohedral fullerenes shows a promising beginning to find out the equilibrium geometries. Charges need refinements. This result is in line with *ab-initio* and experimental values. It also shows that the need of higher level *ab-initio* and DFT calculations to correlate with experimental values particularly dipole moment. This kind of studies will help to achieve the applications in the field of sensors, medicine, magnetism and storage.

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