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Water Molecules in Carbon 70, $(H_2O)_3@C_{70}$

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Abstract

Endohedral fullerene studies are the fascinating one, particularly with Carbon 60 and Carbon 70. Water molecules inside fullerenes alter their cage structure, reorientations make them to play a lot in charge distribution. In this line we are presenting our work on Carbon 70 with three water molecules inside. Ab initio SCF calculations are carried out for the fullerene Carbon 70 and Carbon 70 with three water molecules. Carbon 70 is a rugby ball structure, when three water molecules are added inside it, dissociation of charges takes place. Unusual flip flop circular hydrogen bond formation takes place inside Carbon 70. The dipole moment of endohedral C_{70} with three water molecules has been found to be 0.53 Debye, 0.49 Debye and 0.71 Debye respectively for STO-3G, 3-21G and 6-31G basis sets. Total energies for this molecule are reported in addition to the Hydrogen bond length and bond angles of the three water molecules trapped inside C_{70}.

Keywords

Carbon 70, $(H_2O)_3@C_{70}$: Endohedral Fullerene, *Ab Initio*, Self Consistent Field, Dipole Moment

1. Introduction

Theoretical predictions of buckyball molecules appeared in literature between 1960 and 1970. Carbon 70 was discovered in 1985 by Robert Curl, Harold Kroto and Richard Smalley using laser evaporation of graphite. They found C_n clusters ($n > 20$) of which the most common were C_{60} and C_{70}. For this discovery they have been awarded Nobel Prize in 1996. Carbon 70 molecule, which is one type of fullerene is a cage like fused ring structure, resembles like a rugby ball. C_{70} 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. First lanthanum C_{60} complex was synthesized in 1985 and called as La@C_{60} [1]. C_{60} with one water molecule [2] [3] [4] and three water molecule [5] [6] are reported. Also, C_{70} with two water molecules [7] is also reported. In this work three water molecules that are included inside C_{70} are reported and can be called as $(H_2O)_3@C_{70}$. Calculations are carried out at SCF *ab-initio* STO-3G, 3-21G and 6-31G basis sets.

2. Methods of Calculation

Computations of Self Consistent Field *ab-initio* calculations are carried out with STO-3G, 3-21G and 6-31G basis sets. Computations package, Firefly [8] [9] and Avogadro [10] are used.

3. Results

The structure of fullerene C_{70} and the structure of Carbon 70 with three waters molecules inside are shown in **Figure 1** and **Figure 2** respectively. Optimized geometry calculations are carried out at SCF *ab-initio* STO-3G, 3-21G and 6-31G basis sets. Total energies of these molecules are given in **Table 1** in atomic units.

Optimized C_{70} with 3 water molecules at 3-21G basis set is reported in the **Figure 2**. Cyclic hydrogen bonds involving flipping action inside Carbon 70 with 3 water molecules at 3-21G basis set with bond lengths and oxygen angles is shown in **Figure 3**. The bond length of one oxygen atom to the hydrogen atom of other water molecule and vice versa is 1.52 Å, 1.53 Å and 1.64 Å and the angle with respect to the oxygen of each water molecule is 57.55˚, 64.96˚ and 57.48˚ respectively.

Structure of C_{70} with 3 H2O molecules optimised at 3-21G basis set

Cyclic water molecules having anchored and deflected with one hydrogen atom in each molecule, angles formed among water molecules after optimisation at 3-21G basis set are shown in **Figure 4**. The angles in respect of anchored and deflected hydrogen atom in each water molecule are 49.41˚, 79.65˚ and 50.93˚, 60.67˚, 61.88˚ and 57.46˚ respectively. The angle of water molecule is of 109.82˚, 105.69˚ and 107.15˚.

The optimized structure at 6-31G basis set of C_{70} with 3 water molecules reported and the conformation of water molecules with hydrogen bonding in cyclic manner along with their bond lengths and oxygen bond angles are shown in **Figure 5**, **Figure 6(a)** and **Figure 6(b)** respectively. The bond length of one oxygen atom to the hydrogen atom of other water molecule and vice versa is 1.63 Å, 1.63 Å and 1.70 Å and the angle with respect to the oxygen of each water molecule is 57.64˚, 65.85˚ and 56.51˚ respectively.

Structure of C_{70} with 3 H2O molecules optimised at 6-31G basis set

Cyclic water molecules having anchored and deflected with one hydrogen atom in each molecule and the angles formed among water molecules after optimized at 6-31G basis set. The angles in respect of anchored and deflected hydrogen atom in each water molecule are 49.08˚, 85.29˚ and 45.63˚, 60.76˚, 61.24˚ & 58.00˚ and the angle of water molecule is of 112.17˚, 107.37˚ and 109.48˚ respectively shown in **Figure 7(a)** and **Figure 7(b)**.

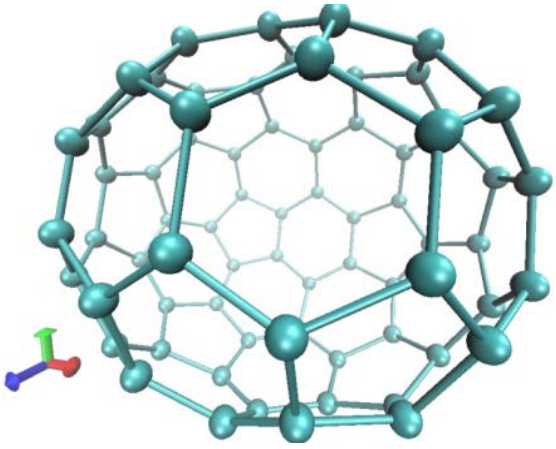


Figure 1. Carbon 70.

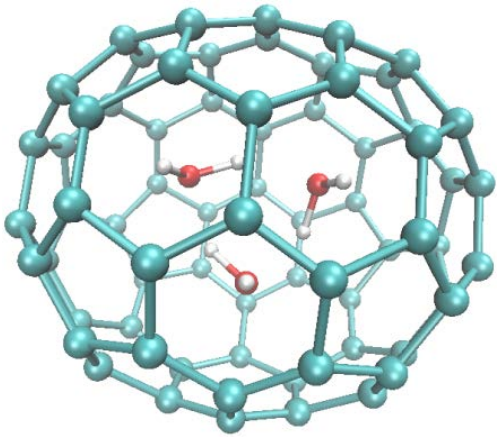
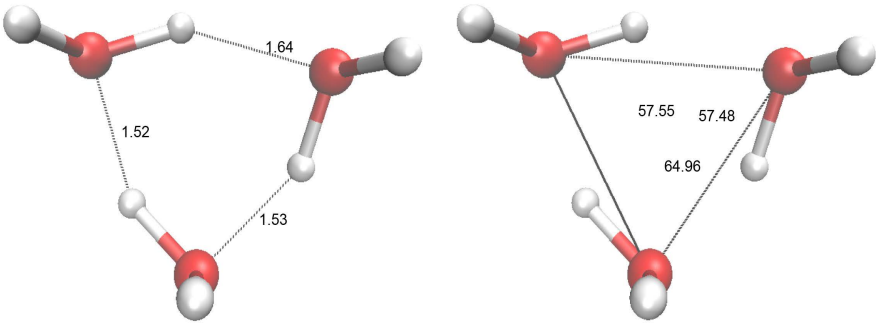


Figure 2. Optimised Structure of Carbon 70 with three water molecules at 3-21G basis set.

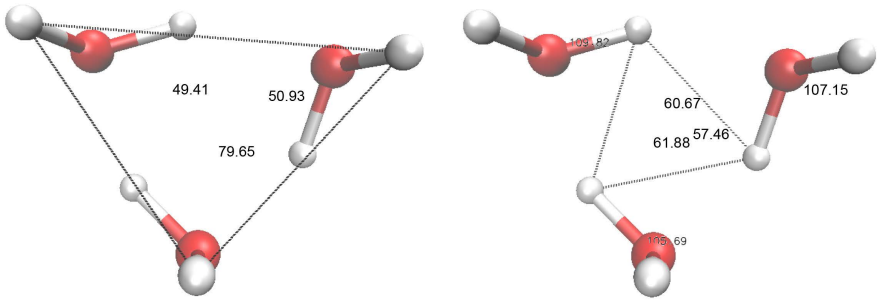
Table 1. Total energy of the molecules in atomic units (AU).

Molecules	STO-3G Basis Set	3-21 G Basis set	6-31 G Basis set
CARBON 70	−2618.357389	−2843.170273	2649.574118
$(H_2O)_3@C_{70}$	−2635.636499	−2862.366387	−2877.425062



(a) (b)

Figure 3. (a) Hydrogen Bond lengths in Å and (b) Oxygen bond angles in °.



(a) (b)

Figure 4. (a) Angles of anchored hydrogen atoms and (b) Angles of deviated hydrogen atoms of water molecules encapsulated in C_{70}.

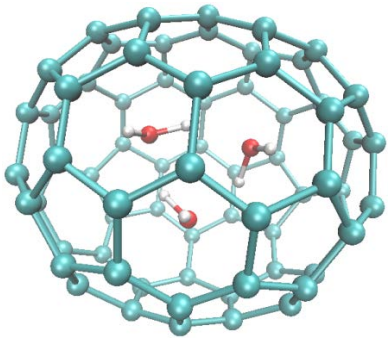
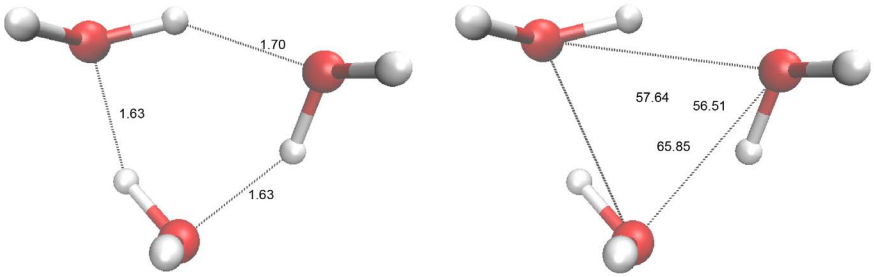
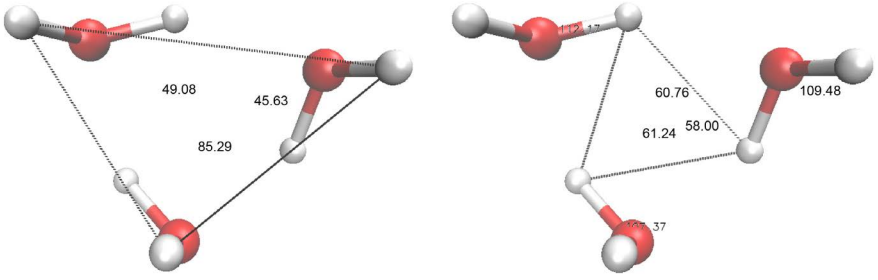


Figure 5. Optimised structure of C_{70} encapsulated with three water molecules at 6-31G basis set.



(a) (b)

Figure.6. (a) Hydrogen bond lengths and (b) Oxygen bond angles.



(a) (b)

Figure 7. (a) Angles of anchored hydrogen atoms and (b) Angles of deviated hydrogen atoms of water molecules encapsulated in C_{70}.

4. Discussion

The pentagons and hexagons of the rugby ball structure of fullerene C_{70} as shown Figure 1 are adopted to have the usual bond lengths and bond angles as reported experimentally. Due to the inclusion of water molecules as shown in Figure 2, C_{70} structure is slightly modified and the formation of dipole moment is seen. Dipole moment has been found to be 0.53 Debye, 0.49 Debye and 0.71 Debye respectively for STO-3G, 3-21G and 6-31G basis sets. Dipole moment is the indication of conductivity and magnetism. Three water molecules inside C_{70} interact with each other through hydrogen bonding. One hydrogen of the water molecule interact with Oxygen of other water molecule respectively through bonding in cyclic, which makes themselves as a cyclic water trimer. Water trimer exhibits ortho metastable configuration inside C_{70}, rather para configuration when it is outside the rugby ball [11].

This study is in line with our previous work on circular and linear hydrogen bonds on molecules [5] [6] [12] [13] [14] [15]. Fullerenes and Endohedral fullerenes will find a lot of applications in conductivity, magnetism, drug delivary, photovoltics 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.

3-21 G basis set Calculation on $(H_2O)_3@C_{70}$

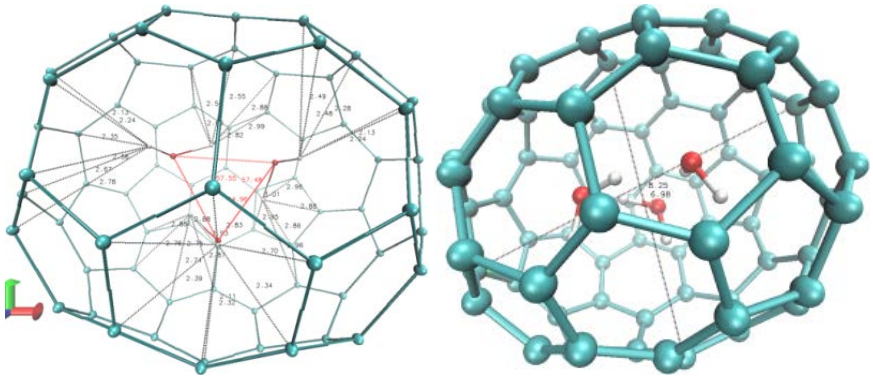
One hydrogen atom of all the three water molecules (H-O-H) encapsulated in the endohedral fullerene is anchored with respect to H-O- in a triangle forming among themselves, as shown in Figure 4(a), in an angle H-H-H is 49.41˚, 79.65˚ and 50.93˚ respectively which are altogether and considerably different from the same anchored angle of H-H-H in $(H_2O)_3@C_{60}$ [5] [6] *i.e.* 61.89˚, 57.17˚ and 60.94˚. On the other hand, the other hydrogen atom is deflected in all the three water molecules with respect to -O-H and the angle between the deflected hydrogens is 60.67˚, 61.88˚ and 57.46˚ respectively, as shown in Figure 4(b), which are very little change similarities from the angle of H-H-H in $(H_2O)_3@C_{60}$ [5] [6] *i.e.* 59.90˚, 60.26˚ and 59.84˚. The bond length between the deflected hydrogen atom of one water molecule and the oxygen of the second water molecule, deflected hydrogen of second water molecule and the oxygen of the third water molecule and deflected hydrogen of third water molecule and the oxygen of the first water molecule have been observed respectively as 1.52 Å, 1.53 Å and 1.64 Å as shown in Figure 3(a). The ab-initio calculations of Fullerene C_{70}, Water trimer and Water trimer encapsulated fullerene in three different levels of basis sets, STO-3G, 3-21G and 6-31G, using RHF have been taken place and their optimised and the total energy for stabilizing the molecules is presented as shown in the Table 1. Water molecules in the endohedral fullerene adopt an angle is 109.82˚, 105.69˚ and 107.15˚ and their bond length as defined in the Figure 3(b) and Table 2 respectively. The angles of each of the water molecules and their bond lengths are having little deviation from their corresponding experimental values for gas phase, O-H length is 0.95718 Å and the H-O-H angle is 104.474˚ [16] and liquid water, O-H length 0.991 Å, H-O-H angle 105.5˚ and 106.0˚ [17] [18].

Table 2. Bond length (Å) and Bond angles (˚) of three water molecules in C_{70} encapsulated, optimized at 3-21G basis set and 6-31G basis set.

3-21 G basis set		6-31 G basis set	
Water Molecule	**Bond Angle in ˚/ Bond Length in Å**	**Water Molecule**	**Bond Angle in ˚/ Bond Length in Å**
$H_{11} - O_1 - H_{12}$	109.82˚ 107.15 0.96 0.99	$H_{11} - O_1 - H_{12}$	112.17˚ 0.94 0.96
$H_{21} - O_2 - H_{22}$	105.69˚ 0.99 0.96	$H_{21} - O_2 - H_{22}$	107.37˚ 0.96 0.95
$H_{31} - O_3 - H_{33}$	107.15˚ 0.96 0.99	$H_{31} - O_3 - H_{33}$	109.48˚ 0.96 0.94
$O_1 - O_2 - O_3$	57.55˚ 2.53 2.36	$O_1 - O_2 - O_3$	57.64˚ 2.57 2.35
$O_2 - O_3 - O_1$ $O_3 - O_1$	64.96˚ 2.53	$O_2 - O_3 - O_1$ $O_3 - O_1$	65.852˚ 2.38
$O_3 - O_1 - O_2$	57.48˚	$O_3 - O_1 - O_2$	56.51˚
$O_1 - H_{21}$	1.64	$O_1 - H_{21}$	1.70
$O_2 - H_{31}$	1.52	$O_2 - H_{31}$	1.63
$O_3 - H_{11}$	1.53	$O_3 - H_{11}$	1.63
$H_{12} - H_{22} - H_{33}$ Anchored	49.41˚ 2.55 2.50	$H_{12} - H_{22} - H_{33}$ Anchored	49.08˚ 3.29 2.36
$H_{22} - H_{33} - H_{12}$ Anchored	79.65˚ 3.23	$H_{22} - H_{33} - H_{12}$ Anchored	85.29˚ 2.50
$H_{33} - H_{12} - H_{22}$ Anchored	50.93˚	$H_{33} - H_{12} - H_{22}$ Anchored	45.63˚
$H_{12} - H_{22} - H_{33}$ Deflected	60.87 1.89 1.81	$H_{12} - H_{22} - H_{33}$ Deflected	60.76˚ 1.97 1.91
$H_{22} - H_{33} - H_{12}$ Deflected	61.88 1.87	$H_{22} - H_{33} - H_{12}$ Deflected	61.24˚ 1.96
$H_{33} - H_{12} - H_{22}$ Deflected	57.46	$H_{33} - H_{12} - H_{22}$ Deflected	58.00˚

All the three water molecules are stabilized by interacting with their hydrogens among themselves and also with carbons of fullerenes C_{70}. Four hydrogens of two water molecules are interacting with six membered ring of C_{70} and two hydrogens of one water molecule is interacting with five membered ring of the C_{70} as shown in **Figure 8(a)**. The overall optimized fullerene C_{70} structure is related to oval in shape and the diameter of the fullerene alongside of the oval is 8.25 Å and their minimum diameter other than the oval side is 6.98 Å as shown in **Figure 8(b)**. The spatial orientation of atoms (anchored hydrogens, deviated hydrogens and oxygens) in all the three water molecules within C_{70} are altogether are in different planes and parallel to each other.

The hydrogen atoms and oxygen atoms of all the three water molecules are stabilized by maximally interacting with six membered rings of the fullerene molecule in range of the distance from 2.5 Å to 2.9 Å. Graphical representations of the molecule are referred by Visual Molecular Dynamics software Package [19].

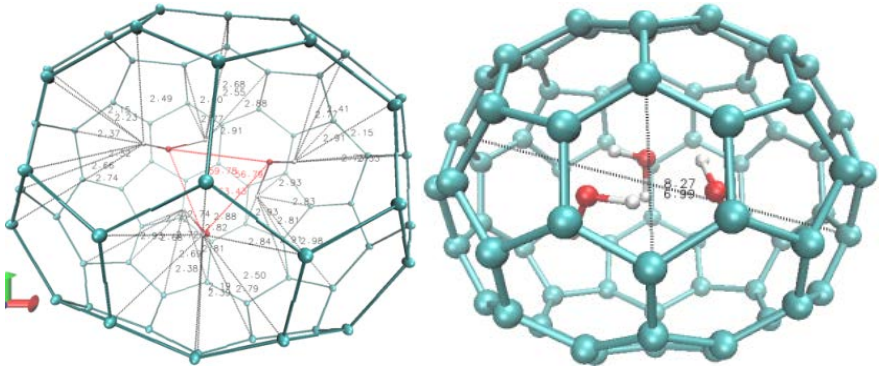


(a) (b)

Figure 8. (a) Length of C_{70} optimised at 3-21G and (b) Interactions of the six hydrogens of 3 waters molecules with C_{70}.

6-31 G basis set Calculation $(H_2O)_3@C_{70}$

One hydrogen atom of all the three water molecules (H-O-H) encapsulated in the endohedral fullerene is anchored with respect to H-O- in a triangle among themselves in an angle H-H-H is 49.08, 85.29˚ and 45.63˚ respectively which are about 12.81˚, 28.12˚ and 15.31˚ differ from the same angle of H-H-H in $(H_2O)_3@C_{60}$ [5] [6] as shown in **Figure 6(b)**. On the other hand, the other hydrogen atom is deflected in all the three water molecules with respect to -O-H and the angle between the deflected hydrogens is 60.76˚, 61.24˚ and 58.00˚ respectively which are very little change similarities, as shown in **Figure 7**, from the angle of H-H-H in $(H_2O)_3@C_{60}$ [5] [6]. The bond length between the deflected hydrogen atom of one water molecule and the oxygen of the second water molecule, deflected hydrogen of second water molecule and the oxygen of the third water molecule and deflected hydrogen of third water molecule and the oxygen of the first water molecule have been observed respectively as 1.63 Å, 1.63 Å and 1.70 Å respectively as shown in **Figure 6(a)**. The ab-initio calculations of Fullerene C_{70}, Water trimer and Water trimer encapsulated fullerene in three different levels of basis sets, STO-3G, 3-21G and 6-31G, using RHF have been taken place and their optimized and the total energy for stabilizing the molecules is presented as shown in the **Table 1**. Water molecules in the endohedral fullerene adopt an angle is 112.17˚, 107.34˚ and 109.48˚ and their bond length as defined in **Figure 7** and **Table 2**. All the three water molecules are stabilized by interacting with their hydrogens among themselves and also with carbons of fullerenes C_{70}. Four hydrogens of two water molecules are interacting with six membered ring of C_{70} and two hydrogens of one water molecule is interacting with partially with both the five and six membered ring of the C_{70} as shown in **Figure 9(a)**. The overall optimized fullerene C_{70} structure optimized at 631-G is also related to oval in shape and the maximum diameter of the fullerene alongside of the oval is 8.26 Å and their maximum diameter other than the oval side is 6.98 Å as shown in **Figure 9(b)**. The spatial orientation of atoms (*i.e.* anchored hydrogen, deviated hydrogen and oxygen) in all the three water molecules within C_{70} are altogether existing in different planes and parallel to each other.



(a) (b)

Figure 9. (a) Length of C_{70} optimised at 6-31G and (b) Interactions of the six hydrogen of 3 waters molecules with C_{70}.

Comparison of optimised C_{70} with three water molecules at 3-21G and 6-31G basis sets

Comparing the endohedral fullerene $(H_2O)_3@C_{70}$ structure at 3-21G and 6-31G basis sets, it is found that having maximum similarities. In contrary the water molecules adopts their position among themselves are meagerly deflective through their oxygen and hydrogen bonds as show in **Figure 10** & **Figure 11**. There is also a dissimilarity of their bond lengths. The orientations of the water molecules encapsulated in C_{60} [5] [6] with comparison of the water molecules encapsulated in C_{70} optimized both at 3-21G and 6-31G basis sets are considerably different in their various angles and bond lengths as discussed. The hydrogen and oxygen bond deviations in respect of the water molecules optimized at 3-21G and 6-31G basis set is shown in **Figure 10** & **Figure 11**.

The spacial orientation of atoms (*i.e.* anchored hydrogen, deviated hydrogen and oxygen) in all the three water molecules within C_{70} level are altogether existing in different planes and parallel to each other separately but high probable similarities could be observed among the water molecules at 3-21 G and 6-31 G by measuring the differences as detailed in **Table 3**.

The length of deviations among bond lengths and angles of all the three water molecules in C_{70} is as shown in **Figure 12** and in **Table 3**.

5. Conclusion

SCF ab initio Calculations on fullerenes C_{70} and endohedral fullerene $(H_2O)_3@C_{70}$ shows a promising beginning to find out the structural reorientation in equilibrium geometries. Spacial orientations of atoms in water molecules within C_{70} show three different planes. Charges need refinements. This result is in line with our previous *ab-initio* calculation with $(H_2O)_3@C_{60}$. The study on seven endofullerene, $M@C_{60}$), Where M = H2O, Li+, Na+, K+, Be2+, Mg2+, and Ca2+ were also reported [20] and concluded that all of the endofullerenes are more stable than pure C60. Coupled translational and rotational motions of H2 molecules in C_{70} and C60 has been reported [21] with the predictions that at most two H2 molecules can stably occupy C_{70} and just one can be accommodated by C_{60} which are

Table 3. Length of deviations in bond length and bond angles of trimer water molecules in C_{70} encapsulated at 3-21G and 6-31G basis set.

Water Molecule	H–H		O–O
	1	2	
1	0.05	0.11	0.10
2	0.20	0.07	0.15
3	0.15	0.20	0.92

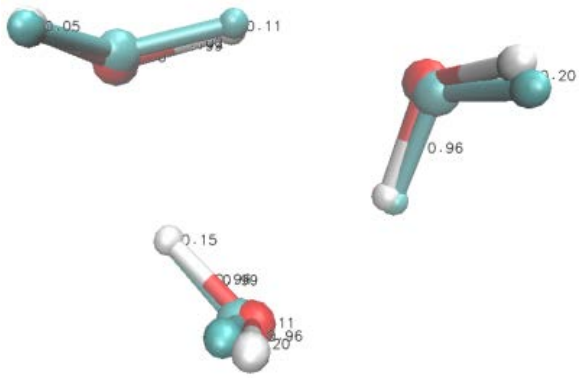


Figure 10. Orientation of water molecules inside C_{70}, Optimised at 3-21G and 6-31G basis sets.

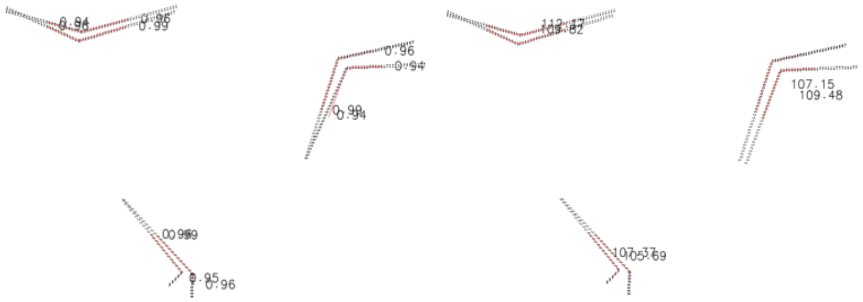


Figure. 11. Bond length (Å) and Angle (˚) of water molecules inside C_{70} at 3-21G and 6-31G basis sets.

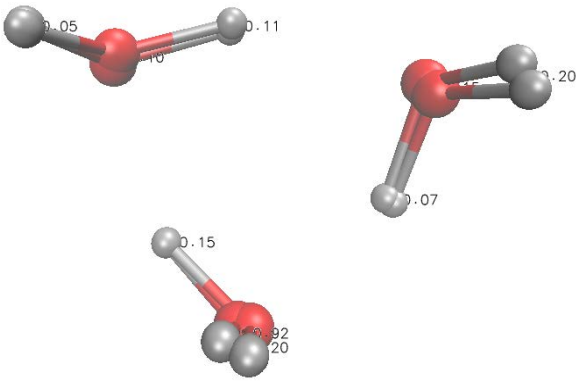


Figure 12. Deviations of bond length in Å and bond angle in degrees among three water molecule inside C_{70}, optimized at 3-21G basis set and 6-31G basis set.

in accord with the experimental preparation of $(H_2)n@C_{70}$ (n) 1, 2) 4 and $H_2@C_{60}$ [22] [23]. At the same Experimental value of dipole moment of one water encapsulated fullerene also supports this kind of work, but a lot of experimental work should be carried out for further endeavours. This kind of studies will help endohedral fullerenes to achieve the applications in the field of sensors, super conductivity, medicine, magnetism, storing, photovoltic and drug delivery, etc.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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