NMR Theoretical Studies of Trapped Cations inside Fullerenes

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Abstract

To probe the ability of Cations to enter, we have calculated the charge and NMR parameters of a direct diffusion pathway for H^+, Li^+, Na^+, K^+ Cations to move through the C_{60}, C_{70} and C_{80} fullerenes with density functional theory (DFT) technique. These Cations could easily diffuse along the central axis of C_{60}, C_{70} and C_{80} fullerenes with distance of 4.9,3.678,2.433,1.249 and in the center of cage system. In this work, the charge and NMR calculations with B3LYP/6-31+G**/6-31++G** levels have indicated that the Cationic fullerene cages are very stable molecules and do not have the reactivity associated with ordinary empty fullerenes.

A common feature of these curves has characterized by three local minima which has located near the H^+, Li^+, Na^+, K^+ that hydrogen, lithium and sodium Cations had a good agreement and potassium Cation had a little deviation in NMR parameters. Also, In all FH^+, FLi^+, FNa^+, and FK^+ systems, the charge has transferred between ion and fullerene and then fullerene has been achieved the positive charge. These compounds can be miniaturized electronics beyond the micro electromechanical scale currently used in electronics.

Keywords: Fullerene; C_{60}, C_{70} and C_{80}; H^+, Li^+, Na^+, K^+ Cations charge; DFT; NMR

Introduction

A fullerene is any molecule composed entirely of carbon, in the form of a hollow sphere, ellipsoid, or tube. Spherical fullerenes are also called buckyballs and they resemble the balls used in association football. Cylindrical ones are called carbon nanotubes or buckytubes. Fullerenes are similar in structure to graphite, which is composed of stacked graphene sheets of linked hexagonal rings; but they may also contain pentagonal (or sometimes heptagonal) rings [1].

The first fullerene to be discovered, and the family's namesake, buckminsterfullerene (C_{60}), was prepared in 1985 by Richard Smalley, Robert Curl, James Heath, Sean O'Brien, and Harold Kroto at Rice University. The name was homage to Buckminster Fuller, whose geodesic domes it resembles. The structure was also identified some five years earlier by Sumio Iijima, from an electron microscope image, where it formed the core of a "bucky onion" [2]. Fullerenes have since been found to occur in nature [2]. More recently, fullerenes have been detected in outer space [3]. According to astronomer Letizia Stanghellini, "It's possible that buckyballs from outer space provided seeds for life on Earth" [3].

Fullerenes are stable, but not totally unreactive. The sp^2-hybridized carbon atoms, which are at their energy minimum in planar graphite, must be bent to form the closed sphere or tube, which produces angle strain. The characteristic reaction of fullerenes is electrophilic addition at 6,6-double bonds, which reduces angle strain by changing sp^2-hybridized carbons into sp^3-hybridized ones. The change in hybridized orbitals causes the bond angles to decrease from about 120° in the sp^2 orbitals to about 109.5° in the sp^3 orbitals. This decrease in bond angles allows for the bonds to bend less when closing the sphere or tube, and thus, the molecule becomes more stable.

Other atoms can be trapped inside fullerenes to form inclusion compounds known as endohedral fullerenes [4]. Recent evidence for a meteor impact at the end of the Permian period was found by analyzing noble gases so preserved [5]. Metallofullerene-based inoculates using the rhonditic steel process are beginning production as one of the first commercially-viable uses of buckyballs. Fullerene purification remains a challenge to chemists and to a large extent determines fullerene prices. So-called endohedral fullerenes have ions or small molecules incorporated inside the cage atoms. Fullerene is an unusual reactant in many organic reactions such as the Bingel reaction discovered in 1993. Carbon nanotubes were recognized in 1991[6].

Minute quantities of the fullerenes, in the form of C_{60}, C_{70}, C_{76}, and C_{84} molecules, are produced in nature, hidden in soot and formed by lightning discharges in the atmosphere. In 1992, fullerenes were found in a family of minerals known as Shungites in Karelia, Russia. In 2010, fullerenes (C_{60}) have been discovered in a cloud of cosmic dust surrounding a distant star 6500 light years away [7]. Another

common fullerene is C_{70} [7], but fullerenes with 72, 76, 84 and even up to 100 carbon atoms are commonly obtained.

This class of novel molecules comprises 80 carbon atoms (C_{80}) forming a sphere which encloses a complex of three metal atoms and one nitrogen atom [8]. Transport of molecules through molecular pores is essential for many biological and technical processes [9]. Pores in zeolites [10] and biological channels [11-13] are often too narrow for ions or small molecules to pass each other, but wide enough to be conducted in a single-file arrangement. Molecular transport through the sequasi-one-dimensional pores is highly collective, since motion of a molecule requires concomitant motion of all molecules in the file [9,14].

Some early attempts to design channels for transport of ions and molecules involved the preparation of cylindrical structures or compounds that looked cylindrical [12,15]. Carbon nanostructure, a new form of element carbon, is composed of grapheme sheets rolled into closed concentric cylinders with diameter of the order of nanometers and length of micrometers. Since its discovery by Iijima [16], extensive applications have been found in physical, chemical, biological and material science fields. Also, Single-walled nanotubes are the most likely candidate for miniaturizing electronics beyond the micro electromechanical scale currently used in electronics [17].

The most basic building block of these systems is the electric wire, and SWNTs can be excellent conductors [18,19]. One useful application of SWNTs is in the development of the first intramolecular field effect transistors (FET). Production of the first intramolecular logic gate using SWNT FETs has recently become possible as well [20]. To create a logic gate, you must have both a p-FET and an n-FET. Because SWNTs are p-FETs when exposed to oxygen and n-FETs otherwise, it is possible to protect half of an SWNT from oxygen exposure, while exposing the other half to oxygen. This results in a single SWNT that acts as a NOT logic gate with both p and n-type FETs within the same molecule.

Ab initio investigations of Lithium diffusion in carbon nanotube systems [21,22], the potential energy curves for H_2 penetration into the open-ended nanotube [23,24] and molecular dynamics (MD) simulation of water inside single-walled carbon nanotubes [17,25-28] have been reported. In this study, to probe the ability of along the central axis of C_{60}, C_{70} and C_{80} fullerenes with distance of 4.9,3.678,2.433,1.249 and in the center of cage, we have calculated the NMR parameters of a diffusion pathway for each of ions to move through the inside of C_{60}, C_{70} and C_{80} fullerenes.

Since the H^+, Li^+ and Na^+ ions used in this study generally transfer electron density to a localized region on the fullerenes [22,29,30], we have investigated the change of partial charges distribution in effect of transport of Cations, too. All calculations in this work were performed with 6-31+G** and 6-31++G** basis set of B3LYP level of the Gaussian03W suite of software [31].

Computational Method

There are many calculations that have been done using ab-initio quantum methods applied to fullerenes. By DFT and TD-DFT methods one can obtain IR, Raman and UV spectra. Results of such calculations can be compared with experimental results.

In order to investigate the movement of ions through Fullerenes, we calculated the potential energy of a diffusion pathway for H^+, Li^+, Na^+ and K^+ Cations along the central axis of C_{60}, C_{70} and C_{80} fullerenes with distance of 4.9,3.678,2.433,1.249 and in the center of cage, as shown in Figure 1. Because of the large size of fullerenes (C_{60}, C_{70} and C_{80}, respectively), high level calculations of the full system were impractical. For this, we adopt the 6-31+G** and 6-31++G** basis sets of B3LYP method of the Gaussian 03 program package [31].
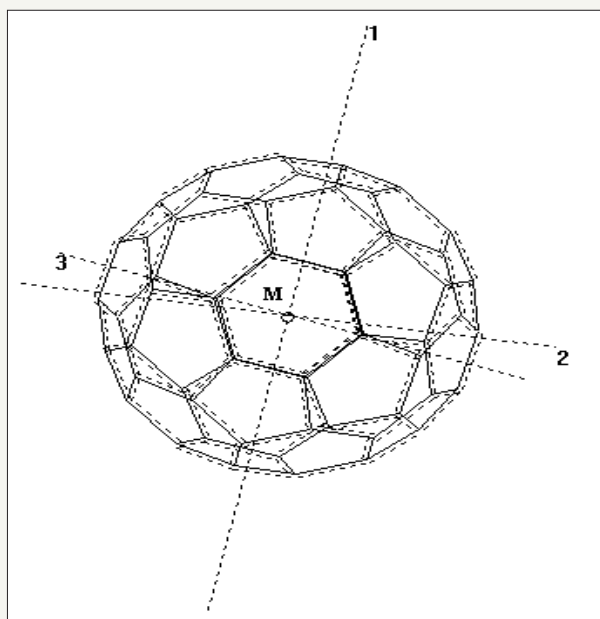

Figure 1: Configuration of Cation penetration (M=H^+,Li^+,Na^+,K^+) into the optimized C_{60}, C_{70},C_{80} fullerenes.

For beginning, the structure of free C_{60}, C_{70} and C_{80} fullerenes were full optimized, then all carbon atoms coordinates were kept frozen and a single ion was moved with about 0.6 Å steps along the central axis of the tube from -10°A to 10°A respect to the fullerene center of mass and NMR parameters and charges were calculated with the super molecular approach on using the hybrid exchange-functional B3LYP/6-31+G**/6-31++G** levels of theory [32].

Figure 2 shows curves of potential energy as a function of

distance between the center of mass of the nanotube and ion (R/Å) for each of Cations in all hollow spheres. Carbon nanostructures reveal diverse electrical properties depending on the diameter, length and chirality [33]. Besides, in the nanostructure-ion systems, the charge can transfer between ion and nanostructure. For example, using the fullerene C_{60} model, Pavanello et al. [34] determined that a charge transfer between lithium and external surface of C_{60} is possible.

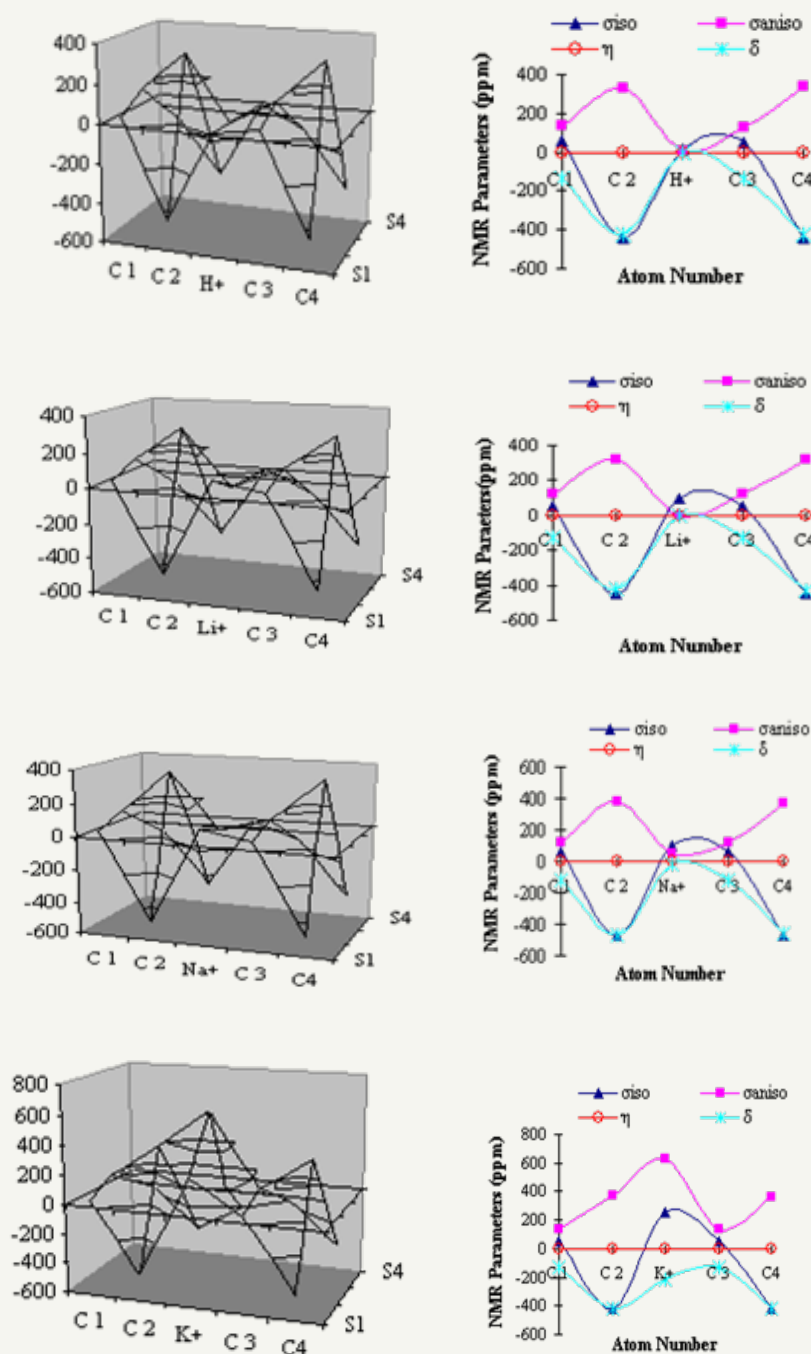
Figure 2: The calculated NMR parameters for H$^+$, Li$^+$, Na$^+$ and K$^+$ Cations entering into various fullerenes (C_{60}, C_{70} and C_{80}) are given in B3LYP/6-31+G**,6-31++G** (two basis sets had the same results).

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The availability of methods with small scaling law such as DFT allows reasonable accuracy for sufficiently large model system. For examples, Zhao et al. [35] has performed SCF pseudo potential plane-wave calculation based on local density approximation (LDA) on a periodic Li5C40 system that represents Li-intercalated CNT ropes. Yang and co-workers employed LDA calculations using an electron core potential to study Li_2C_{120}, Li_2C_{132} and $Li_2C_{120}H_{12}$ that model the Li intercalation in open, closed and H-saturated CNTs, respectively [36].

Therefore, structures of fullerene with various metallic Cations could fully relax during the several optimization processes. Electrical resistance Properties of the structures are calculated using prior calculation. But in NMR scrutiny used prior method with 6-31g**, 6-31+G** and 6-31++G** basis sets that two basis sets 6-31+G**, 6-31++G** is had good agreement together in all cases. Hence, we extracted the partial charges and NMR parameters of atoms in C_{60}, C_{70} and C_{80} models and hollow sphere-Cation systems.

Results and Discussion

The discovery of fullerenes greatly expanded the number of known carbon allotropes, which until recently were limited to graphite, diamond, and amorphous carbon such as soot and charcoal. Buckyballs and buckytubes have been the subject of intense research, both for their unique chemistry and for their technological applications, especially in materials science, electronics, and nanotechnology. We have described the interaction potentials of Cations penetration into the indicated fullerenes. To interpret the diameter dependent penetration, we have presented the three kind C_{60}, C_{70} and C_{80} fullerenes (Figure 1).

The aim of this section was to first discuss the different aspects of the electronic structure of the H^+, Li^+, Na^+ and K^+ Cations along the central axis of C_{60}, C_{70} and C_{80} fullerenes with distance of 4.9,3.678,2.433,1.249 and in the center of cage system for further validation of theoretical results to increase their usefulness in practical applications or for pre-experimental modeling with charge measurement of charges of interaction between Cations and carbons in hollow spheres of C_{60}, C_{70} and C_{80} fullerenes (Figure 1) . Second, we have explored the electromagnetic nature of these systems by calculating the following parameters, which provide valuable information on the interaction characteristics (Table 1).

Table 1: Shows the charge of Cations and total charge of hollow sphere (C_{60}, C_{70} and C_{80}) -Cation systems at situations of Cations along central axis of cages.

Fullerene	C_{60}							
NMR Parameters	σ_{iso}		σ_{aniso}		η		δ	
Level Atom Number	B3LY-P/6-31+G**	B3LY-P/6-31++G**	B3LY-P/6-31+G**	B3LY-P/6-31++G**	B3LY-P/6-31+G**	B3LY-P/6-31++G**	B3LY-P/6-31+G**	B3LY-P/6-31++G**
	C_{60}							
C1	62.8359	62.8826	134.3619	134.3619	0.2288	0.2286	-145.874	-145.813
C2	-464.866	-464.794	403.8347	403.8347	0.0924	0.0923	-492.824	-492.926
Li	99.7341	99.731	1.2496	1.2496	0.0099	0.0103	-1.6608	-1.6491
C3	62.8228	62.8517	134.3729	134.3729	0.2287	0.2285	-145.862	-145.832
C4	-464.921	-464.879	403.882	403.882	0.0928	0.0925	-492.838	-492.87
	C_{70}							
C1	62.8359	55. 7788	134.4451	127.4725	0.2288	0.3184	-145.874	-128.91
C2	-464.866	-448.603	403.7959	323.6367	0.0924	0.0133	-492.824	-425.813
Li	99.7341	97.7596	1.258	1.9578	0.0099	1.5172	-1.6608	-1.037
C3	62.8228	55.8034	134.4229	127.4453	0.2287	0.3189	-145.862	-128.837
C4	-464.921	-448.764	403.9616	323.4737	0.0928	0.0124	-492.838	-425.974
	C_{80}							
C1	55.7787	55.4479	127.4728	126.7297	0.3184	0.3305	-128.91	-126.993
C2	-448.603	-448.401	323.6369	323.5058	0.0133	0.0223	-425.812	-422.729

Li	97.7596	97.5009	1.9578	2.6572	1.5172	1.9015	-1.037	-1.3787
C3	55.8035	55.8489	127.4449	127.9772	0.3189	0.3446	-128.837	-126.903
C4	-448.764	-449.599	323.4737	323.8406	0.0124	0.0204	-425.974	-423.121
				C₆₀				
C1	62.969	62.969	121.2711	121.2711	0.1587	0.1587	-139.541	-139.541
C2	-494.801	-494.801	494.9432	494.9432	0.1964	0.1964	-551.588	-551.588
Be	117.5442	117.5442	38.0898	38.0898	1.7333	1.7333	-12.7674	-12.7674
C3	62.9327	62.9327	121.2282	121.2282	0.1586	0.1586	-139.508	-139.508
C4	-494.973	-494.973	495.3515	495.3515	0.1973	0.1973	-551.591	-551.591
				C₇₀				
C1	119.7267	55.4122	55.4122	119.7271	0.297	0.297	-123.078	-123.078
C2	-473.201	382.6982	382.6982	382.697	0.0873	0.0873	-469.292	-469.291
Be	104.73	46.5874	46.5874	46.5886	2.7115	2.7115	-16.7362	-16.7365
C3	55.9182	120.7124	120.7124	120.7125	0.3144	0.3162	-122.45	-122.45
C4	-474.368	378.8439	378.8439	378.8437	0.0811	0.0811	-467.206	-467.206
				C₈₀				
C1	55.2798	55.2796	119.7095	119.7094	0.3154	0.3154	-121.341	-121.341
C2	-472.666	-472.666	377.2317	377.2328	0.0811	0.1038	-465.221	-465.221
Be	103.8243	103.8242	47.3187	47.3175	2.6822	2.6822	-17.1338	-17.1334
C3	55.8703	55.8696	120.8302	120.8301	0.3348	0.3348	-120.692	-120.693
C4	-473.925	-473.925	372.3987	372.3987	0.073	0.073	-462.709	-462.709
				C₆₀				
C1	61.1762	56.4495	142.1951	145.4579	0.2616	0.2506	-150.278	-155.072
C2	-456.963	-470.549	422.6444	406.342	0.1494	0.1251	-490.257	-481.529
Na	11.799	11.4407	4.4827	4.6796	0.0002	0.0095	-5.9756	-6.1803
C3	61.1518	55.7247	142.187	146.1629	0.2615	0.2485	-150.281	-156.085
C4	-457.026	-467.415	422.8011	417.5641	0.1498	0.1578	-490.286	-480.847
				C₇₀				
C1	54.5721	54.5706	135.619	135.6193	0.3656	0.3656	-132.409	-132.408
C2	-443.862	-443.866	332.1998	332.2003	0.042	0.042	-425.04	-425.041
Na	10.6688	10.6688	4.7192	4.7192	0.1988	0.1988	-5.2488	-5.2489
C3	52.7504	52.7485	132.0534	132.0471	0.3182	0.3182	-133.56	-133.559
C4	-439.665	-439.662	342.0236	342.0336	0.0758	0.0758	-423.873	-423.877
				C₈₀				
C1	336.7676	52.7353	52.7942	130.1132	0.3209	0.3264	-130.556	-130.788
C2	129.342	-445.445	-444.433	334.1012	0.057	0.051	-424.775	-424.212
Na	10.624	10.6558	4.7034	4.5571	0.2193	0.1796	-5.1432	-5.1508
C3	52.6318	51.835	132.9151	129.2435	0.3417	0.3065	-132.086	-131.896
C4	-438.081	-436.118	338.1488	344.6779	0.0732	0.0886	-420.102	-422.16
				C₆₀				
C1	58.6742	52.9451	141.6546	132.2658	0.2542	0.3207	-150.585	-133.525
C2	-435.818	-417.129	452.8176	369.006	0.2587	0.3241	-479.653	-414.975
K	264.8547	259.8272	615.6712	624.0286	2.9916	2.9552	-205.652	-210.365
C3	58.6365	53.9917	141.5431	132.8731	0.2542	0.3437	-150.473	-131.842

C4	-435.824	-418.129	453.1034	366.7424	0.2591	0.1769	-479.799	-415.483
	C_{70}						
C1	52.6335	52.9451	132.1474	132.2658	0.3171	0.3207	-133.772	-133.525
C2	-417.337	-417.129	369.3955	369.006	0.1861	0.1856	-415.217	-414.975
K	257.7659	259.8272	624.6623	624.0286	2.9626	2.9552	-210.181	-210.365
C3	53.7841	53.9917	132.8798	132.8731	0.3434	0.3437	-131.884	-131.842
C4	-418.447	-418.129	366.8031	366.7424	0.175	0.1769	-418.447	-415.483
	C_{80}						
C1	53.1057	53.1057	131.6613	131.6613	0.3337	0.3337	-131.624	-131.624
C2	-417.395	-417.395	365.5737	365.5737	0.1826	0.1826	-412.138	-412.138
K	260.3325	260.3325	625.7481	625.7481	2.9428	2.9428	-211.604	-211.604
C3	54.0521	54.0521	132.1971	132.1971	0.3549	0.3549	-130.089	-130.089
C4	-418.26	-418.26	363.4695	363.4695	0.1744	0.1744	-412.624	-412.624

A common feature of these curves has characterized by three local minima which has located near the H+, Li+, Na+ and K+ that hydrogen, lithium and sodium Cations had a good agreement and potassium Cation had a little deviation in NMR parameters. The potential barrier between two minima have been decreased in C_2 and C_4 in all three C_{60}, C_{70} and C_{80} fullerenes (Figure 2). This is because the wave functions of carbon atoms and that of Cations do not overlap significantly for smaller fullerenes, in particular for small ions. These compounds can be miniaturized electronics beyond the micro electromechanical scale currently used in electronics.

In Table, has shown the change of charge distribution associated with moving the ions along the central axis of fullerenes: the charge of Cations and sum of charges distributed over all atoms of hollow spheres of C_{60}, C_{70} and C_{80}. In C_{60}, C_{70} and C_{80} the Cations had non-bonded interactions. Note that because of a mirror image charge which forms on the both side of fullerene center, we have shown half of fullerenes.

In all FH+ systems, the fullerene had much of positive charge that it increases when the diameter of fullerene increases and reach to +1.922 in the center of the C_{80} fullerene versus the -0.922 charge of H+ Cation. In the case of other Cations: the Li+, Na+ and K+ held the most of positive charge that this reach to about +1 with increase of the diameter of Cation and fullerene and with moving the Cation toward the center of hollow sphere.

It is obvious and worthwhile that in all FH+ systems and FLi+ systems with small diameters, the charge transferred between Cation and fullerene and fullerene achieved the positive charge. This finding can be useful in the fuel hydrogen cells, Li batteries, nano electrode science and the processes of remove of charged pollutants.
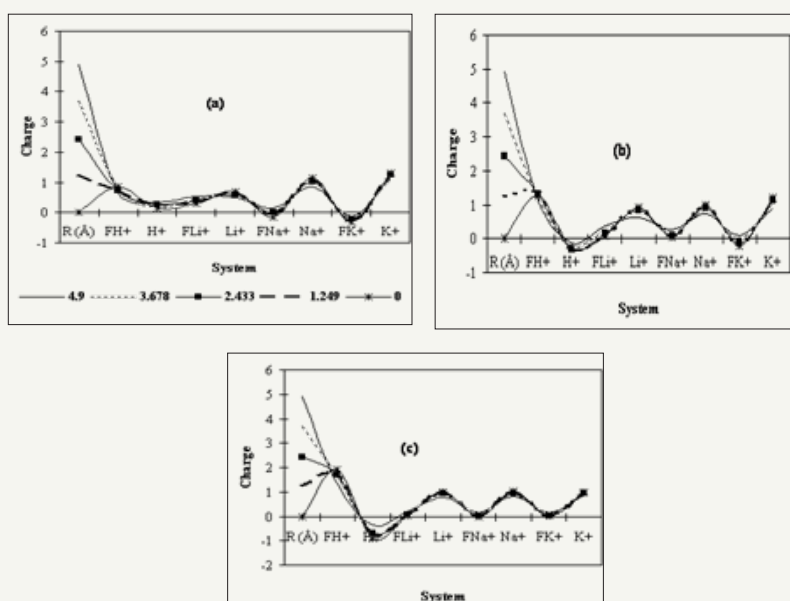

Figure 3: The charge of Cations of H+, Li+, Na+ and K+ single and systems in trapped of Fullerene at different distance (4.9, 3.678, 2.433, 1.249 and in the center of cage) as (a)C60 (b)C70 (c)C80 fullerenes.

In the all fullerenes (C_{60}, C_{70} and C_{80}), the charges of carbon atoms are negative. However, by entry of Cations, we have observed reduction of the charge of carbon atoms around of Cation (Figure 3). This fact has shown that Cations have maintained positive charges while transferring electron density to a localized region on the fullerenes. But in the C_{70} and C_{80} fullerene H^+ system, the charge of carbon atoms become more positive (Figure 3).

Figure 3 has evidenced the charge of Cations and total charge of hollow sphere (C_{60}, C_{70} and C_{80})-Cation systems at situations of Cations along central axis of cages. Endohedral fullerenes are fullerenes that have additional atoms, ions, or clusters enclosed within their inner spheres [37]. Doping fullerenes with electropositive metals takes place in an arc reactor or via laser evaporation. The metals can be transition metals like scandium, yttrium as well as lanthanides like lanthanum and cerium. Also possible are endohedral complexes with elements of the alkaline earth metals like barium and strontium, alkali metals like potassium and tetravalent metals like uranium, zirconium and hafnium.

Endohedral metallofullerenes are characterized by the fact that electrons will transfer from the metal atom to the fullerene cage and that the metal atom takes a position off-center in the cage [37]. The size of the charge transfer is not always simple to determine. In most cases it is between 2 and 3 charge units, in the case of the C_{60}, C_{70} and C_{80} fullerenes however it can be electrons such as in compounds which is better described as complex [38]. In this investigation, the Cationic fullerene cages have been very stable molecules and do not have the reactivity associated with ordinary empty fullerenes (Figure 3).

Conclusion

In this investigation, all computations on diffusion pathway for H^+, Li^+, Na^+, K^+ Cations to move through the C_{60}, C_{70} and C_{80} fullerenes with density functional theory (DFT) technique have carried out via Gaussian03 package at the level of density functional theory (DFT) using the hybrid exchange-functional B3LYP method at 6-31+G**, 6-31++G** standard basis sets that were sufficient for structural optimization of fullerenes, in summary we have concluded:

1. In the C_{60}, C_{70} and C_{80} fullerenes, the Cations had non-bonded interactions with these compounds.

2. Structures of the C_{60}, C_{70} and C_{80} fullerenes with various metallic cations are allowed to fully relax during the several optimization processes.

3. Electrical resistance Properties of the structures have calculated using prior calculation by measurement of charge transfer between of the C_{60}, C_{70} and C_{80} fullerenes and H^+, Li^+, Na^+, K^+ Cations.

4. In NMR scrutiny used prior method with 6-31+G**, 6-31++G** basis sets, good agreement together in results.

These compounds can be miniaturized electronics beyond the micro electromechanical scale currently used in electronics.

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