دراسة التردد الاهتزازي والخصائص الكهربائية للفوليرين C_{30}, C_{50}, C_{60} and C_{70}

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اهمية البحث: على الرغم من اسمها غير المعتاد وقصر وقتها نسبيًا في ساحة البحث ، إلا أن هناك العديد من استخدامات الفوليرين الممكنة. هذه ما يسمى بتآصل الكربون (بالإضافة إلى الجرافيت والجرافين والماس المعروف حتى الآن) تتكون من جزيئات الكربون في شكل أشكال مختلفة مثل كرة مجوفة أو أنبوب أو إهليلجي. هذه الحقيقة جعلتها مثيرة للاهتمام للغاية للعلم والصناعات ، حيث أن المتآصلات المعروفة الأخرى لها العديد من الاستخدامات التجارية المختلفة. بناءً على الشكل الجزيئي ، يمكن تقسيم هذه الجزيئات إلى كروية (تسمى أيضًا باكمينستر فوليرينز أو كرات بوكي) وأسطوانية (تسمى الأنابيب النانوية أو أنابيب البوكي). نظرًا لخصائصها ، تم فحص كرات بوكي وأنابيب البوكي بشكل مكثف خاصة لتطبيقاتها التقنية المحتملة في تكنولوجيا النانو وعلوم المواد والإلكترونيات ولكن أيضًا في صناعة المستحضرات الصيدلانية ومستحضرات التجميل وأخيراً وليس آخراً في الطب.

مشكلة البحث: من اهم المشاكل التي تواجهنا في البحث هي قلة الموارد المالية لمواصلة البحث وكذلك قلة المعلومات العلمية والكوادر المتخصصة والمختبرات العملية واجهزة القياس المتطورة في هذا التخصص من العلوم (النانوتكنلوجي) وخاصة تعتبر (علوم النانوتكنلوجي) من العلوم الحديثة في العالم المتقدم وما زلنا في (العراق)نبحر في بداياته بعد ان قطع العالم الخارجي اشواطا طويلة فيه واصبحت التطبيقات النانوية جزءا من حياتهم اليومية ،لذلك احسن وسيلة لدراسة هذه العلوم في بلادنا كانت باستخدام البرامج الحاسوبية المتقدمة كبرامج الكم الشبة تجريبية وطرقها المعروفة والتي تفي بالغرض ولو لشئ بسيط .في بحثنا هذا تم تمثيل وتكوين Fullerenes C30 و C50 و C60 و C70 باستخدام برنامج Avogadro v. 4.8.6 ثم نقله إلى برنامج Hyperchem v.8 وبرامج Webmo v 21.0.010e لاستخراج الحسابات و الخواص الفيزيائية مثل الطاقة الكلية وطاقة الترابط والطاقة الإلكترونية والطاقة النووية وحرارة التكوين والعزم ثنائي القطب. وحساب الترددات الاهتزازية وشدة الجهد والجهد الالكتروستاتيكي. وحساب مستويات الطاقة ، HOMO و LUMO ، وقم بتمثيلها في شكل رسوم بيانية توضيحية

الملخص: تم تمثيل وتكوين Fullerenes C30 و C50 و C60 و C70 باستخدام برنامج Avogadro v. 4.8.6 ثم نقله إلى برنامج Hyperchem v.8 وبرامج Webmo v 21.0.010e لاستخراج

الحسابات و الخواص الفيزيائية مثل الطاقة الكلية وطاقة الترابط والطاقة الإلكترونية والطاقة النووية وحرارة التكوين وعزم ثنائي القطب. حساب الترددات الاهتزازية لأن الفوليرينات (C30 و C50 و C60 و C70) مركبات غير خطية ، لذلك نلاحظ أن C30 بها 84 تردد اهتزازي ، و C50 بها 144 تردد اهتزازي ، و C60 بها 174 تردد اهتزازي ، و C70 بها 204 تردد اهتزازي الترددات وشدة الجهد والجهد الالكتروستاتيكي، وحساب مستويات الطاقة HOMO و LUMO ، وتمثيلها على شكل رسوم بيانية توضيحية.

Electronic Properties and Vibrational Frequenies of Fullerenes C_{30},C_{50},C_{60} and C_{70}

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Abstract:

Fullerenes C_{30}, C_{50}, C_{60} and C_{70} were represented and configured using the Avogadro v. 4.8.6 program and then transferred to the Hyperchem v.8 program and Webmo v 21.0.010e programs to extract the calculations and physical properties such as Total Energy, Bonding Energy, Electronic Energy, Nuclear Energy, Heat of Formation and Dipole Moment. Calculating the Vibrational Frequencies because fullerenes (C_{30}, C_{50}, C_{60} and C_{70}) were non-linear, so we note that C_{30} has 84 vibrational frequencies, C_{50} has 144 vibrational frequencies, C_{60} has 174 vibrational frequencies, and C_{70} has 204 vibrational frequencies, and the intensity of the voltage and Electrostatic effort. Calculate the energy levels, HOMO and LUMO, and represent them in the form of illustrative graphs

Keywords:

Graphite ,Diamond., Fullerenes, C_{30},C_{50},C_{60} and C_{70}, Vibrational Frequency, Electrical Properties, Mega tubes, Bucky ball clusters.

Introduction:

Carbon, the common element and widely distributed in nature, is known to exist in several forms viz. graphite and diamond. Fullerenes are fourth allotropic form of carbon. In Comparison with graphite and diamond with extended solid state structures, fullerenes are spherical molecules which have solubility in various organic solvents. This property can be used for different chemical manipulation. A fullerene is a carbon cage structure having fused ring system which consists of pentagons and hexagons. The first proposal of buck ball was given by Eiji Osawa, Japan. He recognized that corannulene, a cyclopentane ring fused with 5 benzene rings was a part of football framework and hypothesized that entire structure could exist. In 1985, the group of scientists Richard Smalley, Robert Curl, James Heath,Sean O'Brien, and Harold Kroto synthesized the first fullerene molecule, Buckminsterfullerene.
(C_{60}) at Rice University. These scientists named newly discovered molecule in honor of arc- hitect R. Buckminster Fuller who created geodesic dome with same shape.[1,2]

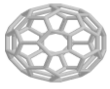
Fullerenes, first reported by Curl,Kroto and Smalley over 20 years ago [3] , are highly symmetric cage-shaped molecules that consist only of carbon atoms. They have been thoroughly studied during the last two decades. Since the preparation of fullerene C_{60} in multigram amounts in 1990 [4] , a wide variety of chemically modified fullerenes have been synthesized and outstanding structural [5] , magnetic [6] , superconducting [7] , electrochemical [8] and photo physical [9] properties reported [10] . Many polymer scientists shifted their attention to this fi eld. They tried to use this molecule as a building block to construct novel materials with unusual properties. The combination of fullerenes and polymer chemistry is a new interdisciplinary field in which all knowledge on the synthesis and study of natural as well as artificial macromolecules can be applied to fullerenes to achieve novel fullerene - based architectures with

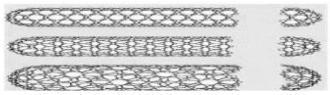
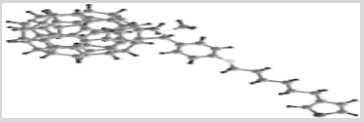
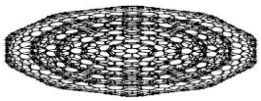
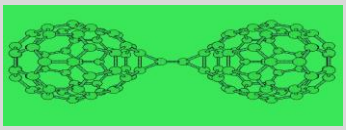
unprecedented properties and realistic applications. Because of their original structure, three - dimensional fullerenes as well as polymers are intrinsically useful scaffolds for the construction of high molecular weight structures. As we shall see later, the unique molecular structures of C_{60} can not only provide each of the carbon entities with special physicochemical properties but they also allow controlled structural modifications, leading to the formation of various advanced composite materials with appropriate polymers for many potential applications. Therefore, a combination of both systems has led to a wide variety of new materials that show appealing features based on the possibility of tuning their properties by modifying the chemical nature of the components or the chemical linkage between them. The present chapter summarizes some of the important issues on the preparation of advanced composite materials based on polymers containing fullerene C_{60}.During the rapid development of fullerene chemistry, many types of polymeric derivatives have been prepared. Numerous chapters and reviews have been published on fullerenes [11] : some focus on their physical properties, others on their synthesis. Our aim here to give a detailed account of progress, especially recent progress, on the synthesis and properties of electro active fullerene – containing polymers: photo induced electron transfer, organic solar cells, potential C_{60}-polymers for photodynamic cancer therapy and so on.

Types of Fullerenes:

Fullerenes can be found in many forms in nature, as shown in the following table(1)

Table(1): Represents the different types of Fullerenes

S.N.	Type	Description	Representation
1	Bucky ball clusters [12]	Bucky ball clusters	

2	Nanotubes [13]	Hollow tubes of very small dimensions with single or multiple walls, used in electronics industry.	
3	Mega tubes [14]	Varying in dimensions than nanotubes as larger in diameter with walls of different thickness; application in transport of a variety of molecules of different sizes.	
4	Polymers [15]	Chain, two or three dimensional, formed under high pressure and temperature conditions.	
5	Nano"onions" [16]	Spherical particles having multiple layers which surrounds buckyball core. Typical diameter is 3-5 nm; proposed for lubricants	
6	Linked "ball-and-chain" dimers [17]	Two buck balls linked by a carbon chains	

there are two important facts that are considered to be barriers to fullerene applications. The first one is relative insolubility and instability of fullerenes to water. This however is being successfully overcome with the development of numerous water-soluble fullerene derivatives. The second and more important limitation is the high cost of fullerenes. Compared to gold that is available at the cost of $10/g, the cost of fullerenes, as listed on web, varies from $45 to $1000/g, depending on degree of purification. This high cost, which is mainly attributed to very high temperature involved in the production process, is restricting the numerous potential applications of fullerenes[18]

The C_{50} fullerene has been investigated by several experimental methods.[19,20,21] In 1993, von Helden et al.[21,22] reported that the fraction of C_{50} fullerene structures observed was nearly up to 90% by collisional heating

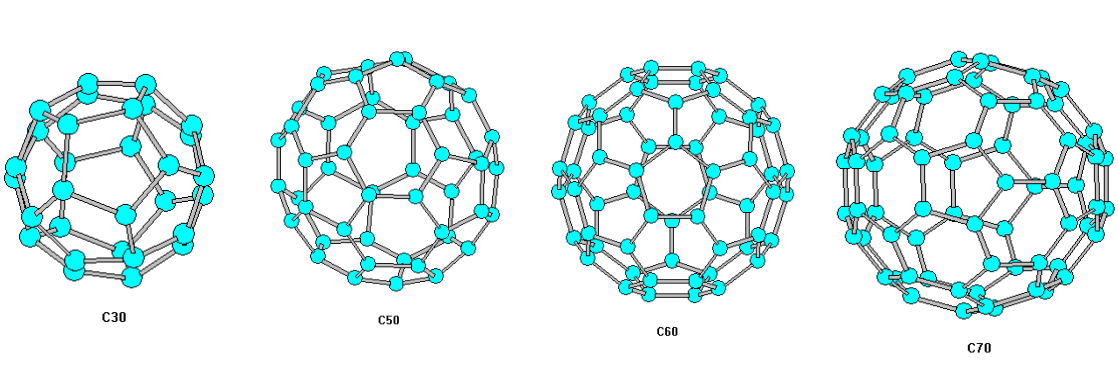
of the carbon rings in the gas phase (the gas-phase ion chromatography method).[21] Xie et al.[23] reported the first production of a decachlorofullerene $C_{50}Cl_{10}$, which is structurally one of the fullerene C_{50} derivatives, and demonstrated a possible way for the preparation of the C_{50} fullerene molecule. The abovementioned observations have proposed the fullerene C_{50} as an exciting system to be investigated by both experimental and theoretical methods in order to evaluate its chemical and physical properties.

Given the many benefits and uses of Fullerenes in nature, many researchers and scientists have inspired to study its properties and types, such as C_{20},C_{30},C_{50},C_{60},C_{70}, C_{80}, C_{180}, C_{240}, C_{260}, C_{320}, C_{500} and C_{720}. …..etc.**(Adhikari and Chowdhury ,……2011)**,They were able to use molecular mechanics simulations to achieve the natural frequency and vibration patterns of the fullerene family molecules. Using the UFF model, C60 results were obtained using molecular mechanics and the calculation of the modulus of elasticity and Poisson's ratio. The obtained results give a clear picture of the frequency change across the entire fullerene family.[24] **(Hainam Do and Nicholas A. Besley…..,2010),**They were able to calculate the vibrational frequencies and their associated spectroscopy of large carbon systems lies within the limits of the size of the system that can be studied in scalar quantitative chemical methods. For C_{60} and G in nanotubes, the expected frequencies of the higher-frequency constant modes are very high, and significant deviation is observed in the calculated and experimental vibrational frequencies of the active IR and Raman modes. Power modulation to reproduce the experimental vibrational frequencies reduces the error in the calculated frequencies but it was found that to achieve satisfactory agreement with the ex- it is necessary to consider the low frequency (<1200 cm−1) and the high frequency modes separately. This gives an RMS error of 45 cm^{-1} for the active IR and Raman C_{60} modes and results in reasonable experimental agreement for Infrared spectrum of C_{70}, G-band, and RBM of nanotubes.[25] **(Yu. I. Prylutskyy et al……..,2014)**, From the research that was done, they were able to conclude that the surface hydroxyl of C_{60} molecules is the most likely mechanism of pristine C_{60}/C_{60} fullerene aggregate stability in water, regardless of the method of C_{60} hydrated fullerene solution preparation. And that water surface C_{60} macromolecules is the most likely mechanism for pristine C_{60}/C_{60} fullerene aggregate stability in water, being independent of the C_{60}FAS preparation method. General hydroxylation in

the case of C_{60} fullerene in water has been observed by several workers in the past [26,27,28] for different methods of hydrated fullerene solution preparation although the exact role played by hydroxyl for the stability of C_{60}FAS has so far been unclear. Covalent attachment, revealed by the present work, gives a deeper insight into this problem. However, further studies are needed to clarify the mechanism by which this attachment occurs.[29]**(Sumbul Firdaus et al……,2015)**,They concluded through their experiments that Primase provides a starting point for RNA (or DNA) for DNA polymerase to start the synthesis of new DNA strands, but this may be affected by the activity of Primase by the action of fullerenes (C30, C40 & C50). While the interaction of fullerenes with other enzymes (helicases, ssb protein, dna polδ, dna pol, ligase, DNA clip, and topoisomerases) significantly reduced the docking points. Apart from the replication factor RPA14 enzymes Upon docking with the ssDNA-fullerene complex it shows a significant decrease in the degree of docking, which means that RPA14 will not be able to destabilize the unwanted secondary.[30] In view of the great importance of fullerenes and their wide uses and in several areas of life such as C_{30}, C_{50}, C_{60} and C_{70}, we have studied some of their important properties to know the advantages that these compounds enjoy,

MATERIALS:

The structures of Fullerenes (C_{30},C_{50},C_{60} and C_{70}) were designed primarily using Avogadro v 4.8.6,Hyperchem v 8 and Web Mo v 21.0.010e (Figure 1). The optimization and natural bond orbital calculations were done with Avogadro v 4.8.6.



Figure(1): represent shapes of Fullerenes (C_{30}, C_{50}, C_{60} and C_{70}).

we calculated some important physical properties for them, as in the table (1) the following

Table(1): represents the values of some physical properties of(C_{30},C_{50},C_{60} and C_{70})

Feature	Molecule			
	C_{30}	C_{50}	C_{60}	C_{70}
Total Energy (kcal/mol)	-81211.02	-135960.8	-163347	-190629.7
Binding Energy (kcal/mol)	-4258.766	-7707.038	-9442.684	-11074.43
Electronic Energy (kcal/mol)	-765122.1	-1731069	-2310337	-2941575
Nuclear Energy (kcal/mol)	683911.1	1595108	2146990	2750946

Through table (1), we note that the decrease in the values of some physical properties of Fullerenes(C_{30},C_{50},C_{60} and C_{70}) such as Total Energy, Binding Energy and Electronic Energy is offset in Nuclear Energy as a result of the increase in the number of Carbon atoms (30 to 70) with high effectiveness and a significant impact on the properties of different materials, also Heat of formation(kcal/mol) and the Dipole moment(Debye) were also calculated in table(2).

Table(2): represents the values of Heat of Formation for C_{30},C_{50},C_{60} and C_{70}

Feature	Molecule			
	C_{30}	C_{50}	C_{60}	C_{70}
Heat of Formation (kal/mol)	817.9344	837.462	850.7167	887.871
Dipole moment (Debye)	$2\chi10^{-4}$	$4.4\chi10^{-4}$	$9\chi10^{-4}$	$28\chi10^{-4}$

1-Vibrational Frequency:

The vibrational frequencies of the four fullerenes (C_{30}, C_{50}, C_{60} and C_{70}) were calculated according to the general rule (3N-6) because all fullerenes are nonlinear and as in the following table (3)

Table(3): represents No.Vibrational Frequency of C_{30},C_{50},C_{60} and C_{70}

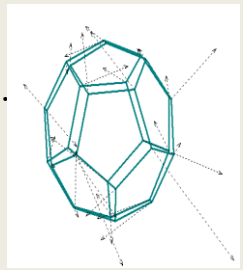
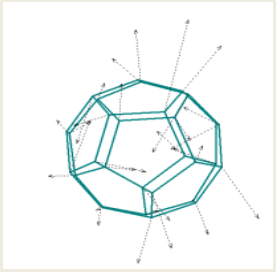
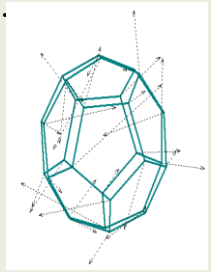
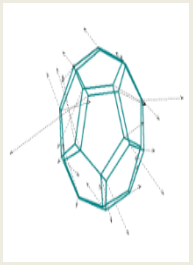
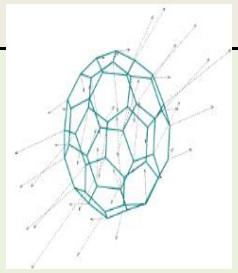
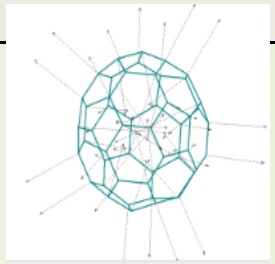
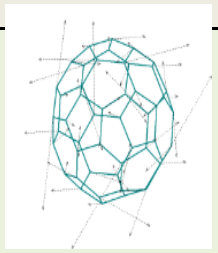
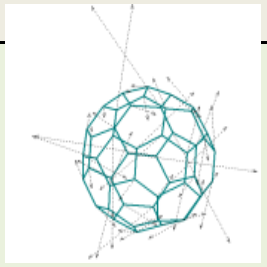
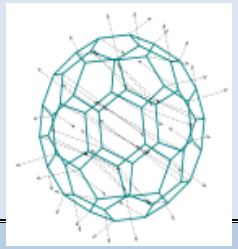
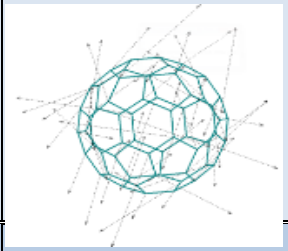
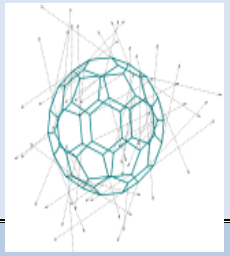
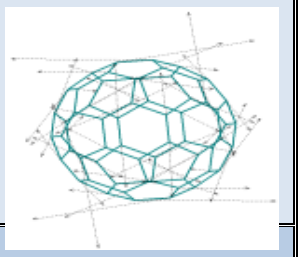
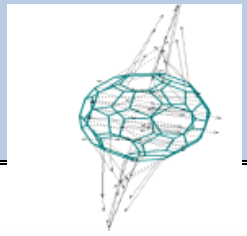
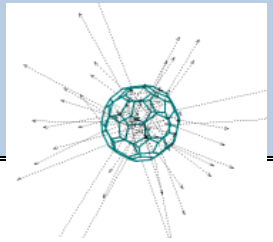
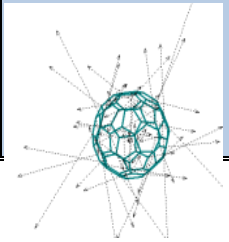
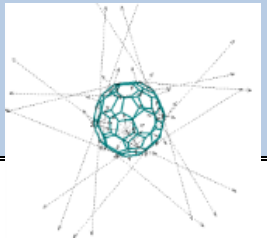
Feature	Molecule			
	C_{30}	C_{50}	C_{60}	C_{70}
No.Vibrational Frequency of Fullerenes according 3N-6	84	144	174	204

Due to the huge amount of vibrational frequencies of fullerenes, models were taken from them and the choice was on the first mode because it represents the beginning of the case in which the particles suffer critical vibrational changes at zero energy and the vibrational frequency at the vibrational pattern No. 50 because it represents the middle of the vibrational changes experienced by the particles and the third was the vibrational pattern Number 100 because it represents the semi-stable state of the molecule after vibrational changes, and the fourth pattern is the last for the molecule, which represents the final state of the molecule. Note: First, that the vibrational frequencies of the C30 particle initially have a negative value, and this negative state continues to mode No. 26, which represents the first positive value, secondly, the C_{30} molecule (and it is the only one) does not have the 100th vibrational pattern because the highest vibrational pattern is at the 84th vibrational pattern. The selected vibration frequencies are shown in Table (4).

Table(4): Represents the selected vibrational frequencies of Fullerenes C_{30},C_{50},C_{60} and C_{70}

Mode No.	Feature	Molecule			
		C_{30}	C_{50}	C_{60}	C_{70}
1	Degeneracy	1	2	5	2
	Frequency(cm^{-1})	-8210.42	280.19	266.46	238.48
	Intensity(Km/mol)	33606.98	0.000	0.000	0.000
	Symmetry	1A	1E1"	1AG	1A'
26	Degeneracy	1			
	Frequency(cm^{-1})	140.49			
	Intensity(Km/mol)	2413.656			
	Symmetry	26A			
50	Degeneracy	3	3	5	3
	Frequency(cm^{-1})	939.70	170.52	700.21	626.75
	Intensity(Km/mol)	2902.57	0.000	0.000	1.798
	Symmetry	50A	4A"	10AU	26A'
84	Degeneracy	1			
	Frequency(cm^{-1})	7888.05			
	Intensity(Km/mol)	13592.125			
	Symmetry	84A			
100	Degeneracy		2	3	3
	Frequency(cm^{-1})		1386.56	1157.37	914.31
	Intensity(Km/mol)		0.000	0.000	0.942
	Symmetry		10E1"	21BU	49A'
144 (Last Mode of C50	Degeneracy		4		
	Frequency(cm^{-1})		1758.05		
	Intensity(Km/mol)		0.000		
	Symmetry		14A1"		
150	Degeneracy			3	
	Frequency(cm^{-1})			1708.14	
	Intensity(Km/mol)			18.406	
	Symmetry			26BU	
174 (Last Mode of C60)	Degeneracy			5	
	Frequency(cm^{-1})			1814.01	
	Intensity(Km/mol)			0.000	
	Symmetry			27A	
204 (Last Mode of C70)	Degeneracy				1
	Frequency(cm^{-1})				1830.21
	Intensity(Km/mol)				1.534
	Symmetry				88A'

Table(5):represents the vibrational frequencies of (C_{30},C_{50},C_{60} and C_{70}) and its kinematic representation by arrows.

Type of Fullerene	Vibratory State			
C_{30}	 Normal MODE: 1	 Normal MODE: 26	 Normal MODE: 50	 Normal MODE: 84
C_{50}	 Normal MODE: 1	 Normal MODE: 50	 Normal MODE: 100	 Normal MODE: 144
C_{60}	 Normal M ODE: 1	 Normal M ODE: 50	 Normal M ODE: 100	 Normal M ODE: 174
C_{70}	 Normal MODE: 1	 Normal MODE: 50	 Normal MODE: 100	 Normal MODE: 204

2-Levels Energies:

The energy levels of four fullerenes (C_{30},C_{50},C_{60} and C_{70}) were calculated, as well as the calculation of HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital). It is represented in the form of graphs and as in the table (7) and through the table (6) we note that C_{30} has 120 orbitals Molecular (60) HOMO and (60) LUMO,

Table(6):represent Levels Energies of four fullerenes (C_{30},C_{50},C_{60} and C_{70})

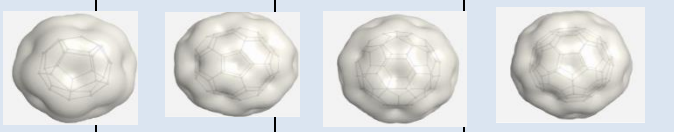
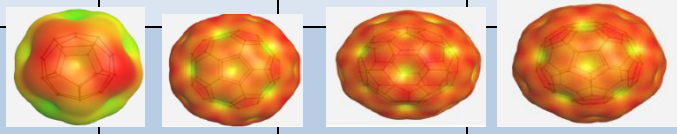
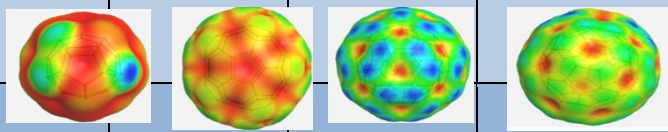
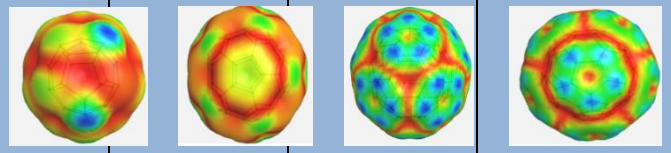
Energy-eV	Feature	C_{30}		C_{50}		C_{60}		C_{70}	
		No. Mode	Energy-eV	No. Mode	Energy-eV	No. Mode	Energy-eV	No. Mode	Energy-eV
								280	23.385
						240	59.611		
								193	0.060
				200	64.67			192	-0.388
						151	0.093		
		120	28.8			150	-4.976		
								141	-10.789 0
	LUMO			127	0.17				
		85	1.19	126	-0.45			140	-11.923
		84	-0.13						
						121	-10.31		
				101	-10.77	120	-11.351		
				100	-11.7				
	E_g	61	-10.751						
		60	-10.53						
		1	-30.36					1	-30.06
	HOMO			1	-31.30				
						1	-31.34		

C_{50} possesses 200 molecular orbital (100- HOMO and 100- LUMO), C_{60} possesses 240 molecular orbital (120-HOMO and 120- LUMO), and molecule C_{70} has 280 molecular orbital (140- HOMO and 140- LUMO), meaning that the more carbon atoms there are, the higher the energy levels, which leads to an increase in the molecular structure of the substance.

3-Electrical Properties:

The Charge Density and Electrostatic Potential for Fullerenes(C_{30},C_{50},C_{60} and C_{70})were calculated, Charge Density and Electrostatic Potential are very important and play a key role in the properties of materials and their interactions. Through the table(7), we notice the regular distribution of electrons around the about Fullerenes atoms .

Table(7):represent the shapes of Charge Density, Electrostatic Potential, HOMO and LUMO of Fullerenes (C_{30},C_{50},C_{60} and C_{70})

Feature	Molecule			
	C_{30}	C_{50}	C_{60}	C_{70}
1-CHARGE DENSITY				
2- Electrostatic-Potential				
3-HOMO				
				

4-LUMO				

Conclusion:

1-The increase number of carbon atoms in Fullerenes led to the increase of complexity of Fullerenes, and this is what we notice in the results mentioned in the tables.

2- By applying the equation for the vibrational frequencies (3N-6) of nonlinear particles (Fullerenes), they have very many vibrational frequencies, so a sample of the many readings was taken as the first frequency of all the Fullerenes. For C_{30}, the 26th frequency reading was taken because it is the starting point of the positive frequency value and all previous values are negative (due to the resistance it shows atoms for the sudden change of zero energy), and took the reading of the pattern number 50 for all Fullerenes and 84 for Fullerene C_{30} and reading number 100, 144, 174 and 204 because it is the last reading for C_{50}, C_{60}, C_{70} .

3- Through table(4), we notice some intensity values equal to zero as a result of the opposite direction of the forces, and their sum is zero, as in Table (5).

4-We notice from table (7) that as the number of carbon increases, the shapes become more complex, and this is what we see in the drawings of charge density, electrostatic potential, HOMO and LUMO.

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