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Theoretical and Quantitative Structural Relationship Study on Fullerenes Polarizabilities on the basis of Monopole-Dipole Interactions Theorem

AVAT (ARMAN) TAHERPOUR[1]* and NOSRATOLLAH MAHDIZADEH[1,2]

[1]Chemistry Department, Faculty of Science, Islamic Azad University, P.O. Box 38135-567, Arak, Iran.
[2]Chemistry Department, Payame-Noor University, Islamabad-Gharb, Iran.
*Sabbatical address: Chemistry Department, School of Science and Technology,
The University of New England (UNE), Armidale-NSW 2351, Australia.
E-mail: avatarman.taherpour@gmail.com; ataherpour@iau-arak.ac.ir; (ataherpo@une.edu.au).

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ABSTRACT

Study about properties of fullerenes with medicinal and electronic applications have been made the highly useful and effective results for applications in different areas of science. Since the discovery of fullerenes (C_n), one of the main classes of carbon compounds, the unusual structures and physiochemical properties of these molecules have been discovered, and many potential applications and physicochemical properties have been introduced. Up to now, various empty carbon fullerenes with different numbers "n" had been obtained. The linear uniform field electric dipole polarizability tensors of fullerenes in the range C_{20} through C_{240} were calculated by the Olson Sundberg atom monopole-dipole interaction (AMDI) theory, Zhang et al. and Shanker and Applequist studies using the monopole and dipole polarizabilities of the carbon atom found previously to fit polarizability tensors of aromatic hydrocarbons. Topological indices are digital values that are assigned based on chemical composition. These values are purported to correlate chemical structures with various chemical and physical properties. They have been successfully used to construct effective and useful mathematical methods to establish clear relationships between structural data and the physical properties of these materials. In this study, were extended the calculation of the parameters concern to atom monopole-dipole moment such as *AMDI* (in Å^3, Atom monopole-dipole interaction theory; α_1 to α_3 and α), *Ellipsoid* (in Å^3, α_1 to α_3 and α) and semi-axes a,b,c of a thin ellipsoidal shell of uniform thickness (in Å, *abc* α_1 to α_3) for C_{20} through C_{300}.

Keywords: Fullerenes; Polarizability, Atom monopole-dipole interaction (AMDI) theory; Ellipsoid; Semi-axes a,b,c ellipsoidal shell; Molecular topology.

INTRODUCTION

The science and technology of nanoscale materials was applied in studies of nanotechnology and the results have been applied in many areas of sciences such as computers, microchips, sensors, actuators and machines fall. The role of computational nanotechnology has become important in the sustainable development of nanotechnology. The rapid increase in computing power has been used for large-scale and high-accuracy simulations. It makes increasingly possible for nano scale modeling to also be predictive. Fullerenes are a class caged molecules containing only hexagonal and pentagonal inter-atomic bonding networks (1–17). Study of the electronic properties of these materials such as the dipole polarizability has made highly useful and effective results in applications in different areas of science (1, 2, 17, 18).

Since the discovery of fullerenes [19], many studies have been undertaken to characterize the physical properties of these molecules [20]. Among these properties, the dielectric response of fullerenes and carbon onions is of great interest for their possible use in composite materials for the coating of electronic circuits [20]. The lattice and electronic structures of fullerenes will greatly change with the increase of their carbon number and thus will have a large effects on their physicochemical properties.

There are important theoretical studies on geometry of fullerenes "C_n" in the chemical literatures. The geometry optimization of fullerenes C_{20} through C_{240} had been performed with the second generation reactive empirical bond order potential energy, before [21,22,26]. The molecular polarizability of spherical and icosahedral fullerenes was found to vary linearly with the cube of their mean radius.[21,26] Many articles deal with the polarizability and optical properties of hyper fullerenes. Gueorguiev et al. give results for icosahedral fullerenes based on linear combination of atomic orbitals (LCAO) approximation, classic, and semi-classic calculations [21,23,26] . The results obtained give approximately a linear behavior versus R^3 where R is the averaged radius for optimized fullerenes.[21,23,26] Mayer et al. had been applied the Renormalized Monopole–Dipole Model (RMDM) developed to hyperfullerenes, carbon onions and fullerene-based molecules. [21,24,26] In addition to dipole excitation, the model included a free-charge response characteristic of metallic structures or the delocalized ð-electrons and so provides a significant improvement with respect to the classical dipolar interaction model, while keeping reasonable the calculation time.[21,26]

The linear uniform field electric dipole polarizability tensors of the fullerenes C_{20} through C_{240} were calculated by the Olson-Sundberg atom monopole-dipole interaction (AMDI) theory, using the monopole and dipole polarizabilities of the carbon atom found previously to fit polarizability tensors of aromatic hydrocarbons.[26,27] The molecular structures were taken to be the predicted results by Zhang and co-workers with respect to the molecular dynamics energy optimization.[26,28-30] The isotropic mean polarizabilities calculated for C_{60} and C_{70} are comparable to experimental data from solid film studies and quantum mechanical calculations.[26,31-43] Polarizability tensors were calculated for conducting ellipsoidal shells which have the same moment of inertia tensor as the corresponding fullerenes by Shanker and Applequist.[26] The results of the polarisability calculations were substantially smaller than the AMDI-polarizabilities for the smaller fullerenes, but the two calculations tend to converge for the larger molecules.[26-30, 34-44]

Graph theory has been found to be a useful tool in assessing the *QSAR* (Quantitative Structure Activity Relationship) and *QSPR* (Quantitative Structure Property Relationship).[45-53] Numerous studies in the above areas have also used what are called topological indices (TI).[54-57] It is important to use effective mathematical methods to make good correlations between the data corresponding to several chemical properties. One of the useful numerical and structural values in unsaturated compounds like fullerenes is the number of carbon atoms (C_n). To establish a good structural relationship between the structures of fullerenes (n) with the structural mechanical properties here was utilized the number of carbon atoms of the fullerenes "n." The relationship between this index with diameter (h_o, A°), volume (V_o, A^{o3}) molecular energy, endurance load and compressive stiffness of empty fullerenes (n = 20, 60, 80, and 180) were presented before. The results were extended for other empty fullerenes up to C_{300}. [46,58]

In this study, the relationship between the number of carbon atoms of fullerenes (C_n) index and polarizability of the fullerenes are presented on the basis of the Olson-Sundberg AMDI theory [27], Zhang et al. [28-30], Shanker and Applequist studies.[26-

[30] Here, were extended the calculation of the parameters concern to atom monopole-dipole moment such as AMDI (in Å^3, Atom monopole-dipole interaction theory; α_1 to α_3 and α), Ellipsoid (in Å^3, α_1 to α_3 and α) and semi-axes a,b,c of a thin ellipsoidal shell of uniform thickness (in Å, *abc* α_1 to α_3) for C_{120} through C_{300}, **6-15**.

Graphing and mathematical method

The number of carbon atoms of the fullerenes (C_n) was utilized as a structural index for fullerenes. All graphing operations were performed using the *Microsoft Office Excel-2003* program. The number of carbon atoms of these fullerenes (C_n) seems to be a useful numerical and structural value for the empty fullerenes. For modeling, both linear (MLR: Multiple Linear Regressions) and nonlinear (ANN: Artificial Neural Network) models were examined in this study. Some of the other indices were examined and the best results and equations for extending the physicochemical data were chosen.

RESULTS AND DISCUSSIONS

The fullerenes possess a large number of conjugated ð-electrons, but are composed of only carbon atoms and therefore do not have any residual infrared absorption that the polymers have.[59] Naturally, these properties make the fullerenes very exciting materials for their potential applications in nonlinear optical devices. The lattice and electronic structures of fullerenes will greatly change with the increase of their carbon number and thus will have a large effect on their polarizability properties. [59-61] Therefore, it is interesting to investigate theoretically this effect from the viewpoint of *AMDI* (in Å^3, Atom monopole-dipole interaction theory; α_1 to α_3 and α), *Ellipsoid* (in Å^3, α_1 to α_3 and α) and semi-axes a,b,c of a thin ellipsoidal shell of uniform thickness (in Å, *abc* α_1 to α_3) for C_{20} through C_{300}.[26] Study on the comparison of the AMDI results with the conducting ellipsoid and monopole interaction treatments by Olson-Sundberg AMDI theory [27], Zhang et al. [28-30], Shanker and Applequist studies.[26-30], had given some insight into the behavior of the AMDI model.[26] The near parallel behavior of the three models is consistent with the major role of charge mobility in all three.[26] The values for the higher members of the series of the fullerenes had made this suggestion that charge mobility becomes the dominant mechanism of polarization with increasing size of the fullerenes in the AMDI model.[26] However, it was shown that the role of induced dipoles is substantial, especially for the lower members of fullerenes. It can be seen from the comparison of the AMDI and monopole interaction data (see Table-1 from ref.[26]). Shanker and Applequist have investigated AMDI, ellipsoid and semi-axes a,b,c of a thin ellipsoidal shell of uniform thickness for fullerenes C_{20} through C_{240}.[26] The AMDI model had treated the molecule (here fullerene) as an array of point atoms which interact with each other by way of the electrostatic potentials and fields of their induced electric monopoles and dipoles in the presence of an external field.[26] The molecular polarizabilities were calculated from the charges and dipole moments induced in the atoms with respect to a uniform external field, by Shanker and Applequist.[26] In their model the fullerene molecule was approximated by an equivalent thin shell ellipsoid whose thickness was uniform.[26] To obtain the moment of inertia of such an ellipsoid, they had investigated that it is important to note the moments of inertia of a solid ellipsoid of mass M. These values were obtained as: [26,62]

I_1=M (b^2+c^2) D 5 Eq.-1
I_2=M (a^2+c^2) D 5 Eq.-2
I_3=M (a^2+b^2) D 5 Eq.-3

where a,b,c are the semi-axis lengths along principal axes 1,2,3, respectively. The character of *ñ* is the density, so that M=4*ðñabc*/3. The moment of inertia of a thin shell of uniform thickness and mass *m* was then obtained by taking differentials of I_1, I_2, I_3 and M at equal differentials *da*, *db*, *dc*.[26,62] Here, by utilizing the relationship between number of carbon atoms of the fullerenes and the parameters concern to atom monopole-dipole moment such as AMDI (in Å^3, Atom monopole-dipole interaction theory; α_1 to α_3 and α), Ellipsoid (in Å^3, α_1 to α_3 and α) and semi-axes a,b,c of a thin ellipsoidal shell of uniform thickness (in Å, *abc* α_1 to α_3) for C_{20} through C_{240} were extended the results for the bigger fullerenes C_{120} through C_{300} **6-15**.

In Table-1 was demonstrated the values

of *AMDI* (in Å^3 Atom monopole-dipole interaction theory; α_1 to α_3 and α), *Ellipsoid* (α_1 to α_3 and α) and *Semi-axes* of a thin ellipsoidal shell of uniform thickness (in Å, *abc,* α_1 to α_3) of the selected fullerenes **1-5** from the results that was obtain for the fullerenes C_{20} to C_{240} by Olson-Sundberg AMDI theory [27], Zhang et al. [28-30], Shanker and Applequist studies[26-30]. These data were extracted from reference [26]. Table-2 shows the equations of polarizabilities and semi-axes of the fullerenes in accordance with the values of AMDI, Ellipsoid and Semi-axes of a thin ellipsoidal shell of uniform thickness which they have been reported in reference [26] In Table-3 has shown the calculated values of *AMDI* (in Å^3 Atom monopole-dipole interaction theory; α_1 to α_3 and α), *Ellipsoid* (α_1 to α_3 and α) and *Semi-axes* of a thin ellipsoidal shell of uniform thickness (in Å, *abc,* α_1 to α_3) of fullerenes C_{120}, C_{132}, C_{140}, C_{146}, C_{150}, C_{160}, C_{162}, C_{276}, C_{288} and C_{300} (**6-15**) by using equations 4 to 14. The data of the fullerenes **1-5** which they have demonstrated again from reference [26] in Table-1, and the obtained results for fullerenes **6-15** by the use of equations 4-14 (see Table-2), show increasing the values of AMDI, Ellipsoid and Semi-axes of a thin ellipsoidal shell of uniform thickness values of the fullerenes C_{20} to C_{240}, by increasing the number of carbon atoms at the structures of the fullerenes.[26-30] All of the equations 4-14, the lines of best fit are *Nieperian* logarithmic behavior curve. Equations 4-7 describe Fig.-1 and show the *Nieperian* logarithmic behavior of the relationship between the numbers of carbon atoms versus the *AMDI* (in Å^3 Atom monopole-dipole interaction theory; α_1 to α_3 and α) values in the fullerene structures C_{20} to C_{240}. The R-squared values (R^2) for these four graphs are equal to 0.9989, 0.9932, 0.9991 and 0.9993 for AMDI α_1 to α_3 and α, respectively. By utilizing the equations it is possible to achieve a good approximation for extending the determination of the *AMDI* polarizabilities (α_1 to α_3 and α) for the fullerenes [26-30], **6-15** and other fullerenes C_n. See Fig 2, Tables 1 and 3.

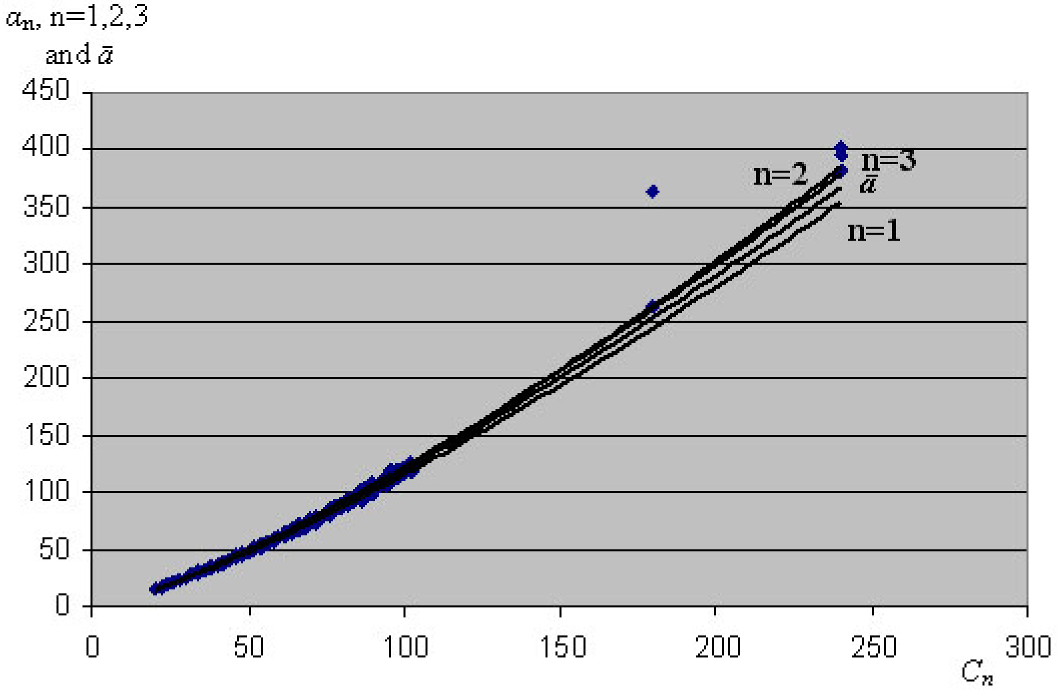

Fig.1: The relationship between the number of carbon atoms "n" and the values of polarizabilities in *AMDI* (in Å^3, Atom monopole-dipole interaction theory; α_1 to α_3 and α) method for fullerenes C_{20} to C_{240}. The values of *AMDI* of C_{20} to C_{240} is from Ref.[26].

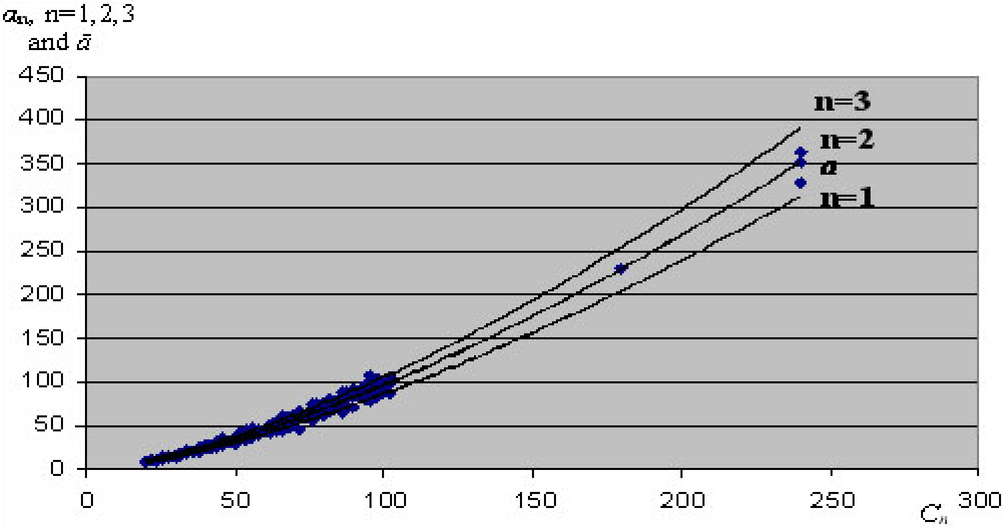

Fig. 2: The relationship between the number of carbon atoms "n" and the values of polarizabilities in *Ellipsoid* (in Å^3, α_1 to α_3 and α) method for fullerenes C_{20} to C_{240}. The values of *Ellipsoid* of C_{20} to C_{240} is from Ref.[26].

Fig 2 demonstrates four *Nieperian* logarithmic behavior curves relevant to relationships between the numbers of carbon atoms and the values of *Ellipsoid* (α_1 to α_3 and α) of C_{20} to C_{240}. Equations 8–11 describe Fig.-2 and show the *Nieperian* logarithmic behavior of the relationship. By the equations it is possible to achieve to the good approximations for extending the determination of *Ellipsoid* (α_1 to α_3 and α) in the bigger fullerenes C_{120} to C_{300}, **6-15** and other fullerenes C_n. In Fig.-2, the R-squared values (R^2) for these four graphs are equal to 0.9953, 0.9960, 0.9955 and 1.0 for *Ellipsoid* α_1 to α_3 and α, respectively. The predicted values of the α_1 to α_3 and α for **6-15** were calculated by the use of equations 8–11 (see Fig 2 and Tables 1 and 3).

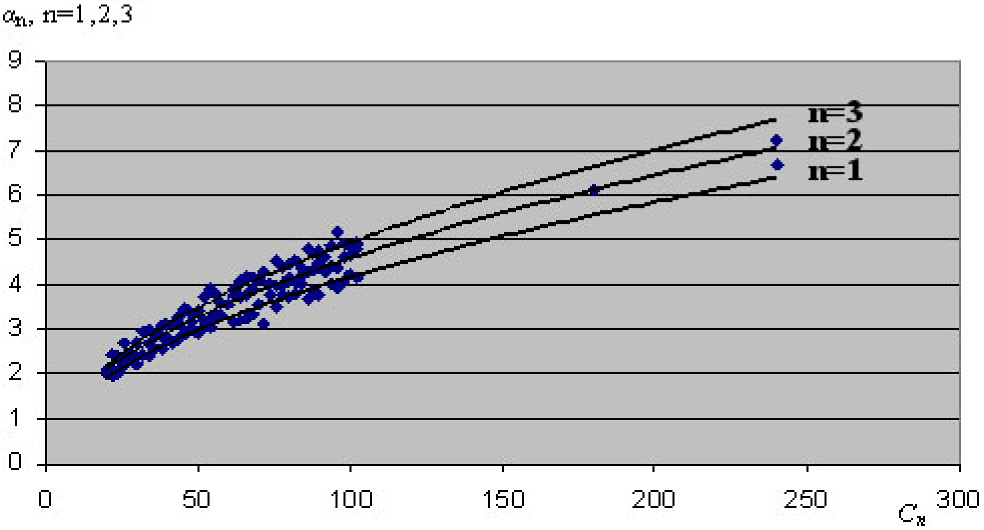

Fig.3: The relationship between the number of carbon atoms "n" and the valuesof polarizabilities in *Semi-axes* of a thin ellipsoidal shell of uniform thickness (in Å, *abc,* α_1 to α_3) for fullerenes C_{20} to C_{240}. The values of *Semi-axes* of C_{20} to C_{240} is from Ref.[26].

Table-1: The values of *AMDI* (in Å^3 Atom monopole-dipole interaction theory; α_1 to α_3 and α), *Ellipsoid* (α_1 to α_3 and α) and *Semi-axes* of a thin ellipsoidal shell of uniform thickness (in Å, *abc,* α_1 to α_3) of fullerenes C_{20} to C_{240}. T hese data were extracted from reference [26].

NoFullerenes		AMDI (Å^3)				Ellipsoid (Å^3)				Semi-axes (Å)		
		α_1	α_2	α_3	α	α_1	α_2	α_3	α	α_1	α_2	α_3
1	60	60.75	60.75	60.75	60.75	44.74	44.74	44.74	44.74	3.55	3.55	3.55
2	70	72.39	72.42	76.46	73.76	51.81	51.93	62.47	55.40	3.54	3.55	4.13
3	76	79.73	82.26	86.92	82.97	54.61	63.48	74.72	64.27	3.50	3.98	4.54
4	82	88.96	90.79	94.88	91.54	64.85	70.67	80.05	71.86	3.82	4.09	4.55
5	86	93.06	97.20	102.56	97.61	64.74	77.55	89.28	77.19	3.68	4.29	4.81

Table-2: The equations of polarizabilities and semi-axes of Fullerenes; *AMDI* (in Å^3 Atom monopole -dipole interaction theory;α_1 to α_3 and α), *Ellipsoid* (α_1 to α_3 and α) and *Semi-axes* of a thin ellipsoidal shell of uniform thickness (in Å, *abc,* α_1 to α_3).

Equations	Y-value*	R^2	$Y = a(n)^b$	
			a	*b*
Eq.-4	α_1-AMDI	0.9989	0.3251	1.2755
Eq.-5	α_1-AMDI	0.9932	0.2869	1.3139
Eq.-6	α_3-AMDI	0.9991	0.3232	1.2891
Eq.-7	α-AMDI	0.9993	0.3214	1.2843
Eq.-8	α_1-Ellipsoid	0.9953	0.0991	1.4698
Eq.-9	α_2-Ellipsoid	0.9960	0.1087	1.4743
Eq.-10	α_3-Ellipsoid	0.9955	0.1087	1.4937
Eq.-11	α-Ellipsoid	1	0.1058	1.4793
Eq.-12	α_1-*abc*	0.9694	0.4474	0.4854
Eq.-13	α_2-*abc*	0.9755	0.4844	0.4888
Eq.-14	α_3-*abc*	0.9739	0.4840	0.5049

*Y-values are the values of *AMDI*, *Ellipsoid* polarizabilities and *semi-axes* of Fullerenes.

Table-3: The calculated values of *AMDI* (in Å^3 Atom monopole-dipole interaction theory; α_1 to α_3 and α), *Ellipsoid* (α_1 to α_3 and α) and *Semi-axes* of a thin ellipsoidal shell of uniform thickness (in Å, *abc,* α_1 to α_3) of fullerenes C_{120}, C_{132}, C_{140}, C_{146}, C_{150}, C_{160}, C_{162}, C_{276}, C_{288} and C_{300} (6-15) by using equations 4 to 14. See Table-2.

No	Fullerenes	AMDI (Å^3)				Ellipsoid (Å^3)				Semi-axes (Å)		
		α_1	α_2	α_3	α	α_1	α_2	α_3	α	α_1	α_2	α_3
6	120	145. 90	154. 73	154. 79	150. 43	112. 73	126. 35	138. 64	125. 96	4. 57	5. 03	5. 43
7	132	164. 74	175. 37	175. 03	170. 02	129. 69	145. 41	159. 86	145. 03	4. 77	5. 27	5. 69
8	140	177. 60	189. 46	188. 82	183. 37	141. 40	158. 59	174. 54	158. 22	4. 92	5. 42	5. 87
9	146	187. 35	200. 20	199.31	193. 52	150.40	168. 71	185. 83	168. 35	5. 03	5. 53	5. 99
10	150	193. 92	207. 44	206. 38	200. 35	156.49	175 .57	193. 49	175. 22	5. 09	5. 61	6. 07
11	160	210. 56	1034. 08	224. 29	217. 67	172.06	193. 09	213. 07	192. 77	5. 25	5. 79	6. 28
12	162	213. 92	229. 52	227.91	221. 17	175. 23	196. 66	217. 06	196. 35	5. 29	5. 82	6. 32
13	276	422. 08	3222. 11	452. 95	438. 43	383. 46	431. 38	481. 08	431. 84	6. 85	7. 56	8. 26
14	288	445. 63	488. 79	478. 49	263. 07	408. 21	459. 32	512. 65	459. 90	6. 99	7. 71	8. 44
15	300	469. 44	515. 73	504. 35	487. 99	433. 46	487. 81	544. 89	488. 53	7. 13	7. 87	8. 62

Similar to Fig 2 and 3, in Fig.-4 the lines of best fit are *Nieperian* logarithmic behavior curve. Four *Nieperian* logarithmic behavior curves relevant to relationships between the numbers of carbon atoms and the values of *Semi-axes* of a thin ellipsoidal shell of uniform thickness (in Å, *abc,* α_1 to α_3) were shown in Fig.-3. Equations 12-13 describe Fig.-3. By the equations it is possible to achieve to the good approximations for extending the determination of *Semi-axes* (in Å, *abc,* α_1 to α_3) of the fullerenes C_{120}, C_{132}, C_{140}, C_{146}, C_{150}, C_{160}, C_{162}, C_{276}, C_{288} and C_{300} (**6-15**) and other bigger fullerenes C_n. In Fig.-3, the R-squared values (R^2) for these four graphs are equal to 0.9694, 0.9755 and 0.9739 for *Semi-axes* (in Å, *abc,* α_1 to α_3), respectively. The predicted values of the α_1 to α_3 for **6-15** were calculated by the use of equations 12–14 (see Fig 3, Tables 1 and 3). The number of carbon atoms in the structures of the fullerenes (C_n) shows a good relationship with their *AMDI* (in Å^3 Atom monopole-dipole interaction theory; α_1 to α_3 and α), *Ellipsoid* (α_1 to α_3 and α) and *Semi-axes* of a thin ellipsoidal shell of uniform thickness (in Å, *abc,* α_1 to α_3) polarizability values on the basis of the Olson-Sundberg AMDI theory, Zhang et al., Shanker and Applequist studies.[26-30] Table 3 show the calculated values of AMDI, *Ellipsoid* and *Semi-axes* of a thin ellipsoidal shell of C_{20} to C_{240} on the basis [26-30] that the selected data were shown in Tables 1, 2 and fig 1-3. The explained polarizability data for **6-15** and other fullerenes C_n were obtained by extension values of C_{20} to C_{240} fullerenes which they reported before.[26]

CONCLUSION

The science and technology of nano-scale materials was applied in studies of nanotechnology and the results have been applied in many areas of sciences such as computers, microchips, sensors, actuators and machines Study on the useful applications of graph theory have made the different mathematical methods for finding the relationship between several data of the material properties. In this study, the relationships between the number of carbon atoms of fullerenes (C_n) index and AMDI, Ellipsoid and Semi-axes of a thin ellipsoidal shell polarizability of the fullerenes C_{20} to C_{240} are presented on the basis of the Shanker and Applequist studies were demonstrated. By the use of the results and the equations 4-14 of this model it is possible to achieve the good approximations for extending the AMDI, Ellipsoid and Semi-axes of a thin ellipsoidal shell polarizabilities values for bigger fullerenes C_n such as **6-15**.

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