Prediction of the Number of Carbon Atoms in Various Nanostructures by Using Geometrical Approach

Hosein Sabaghian-Bidgoli,[a,*] Gholamreza Vakili-Nezhaad,[b] and Mehdi Vahidipour[a]

[a]*Department of Computer Engineering, Faculty of Engineering, University of Kashan, Kashan 87317-51167, I. R. Iran*

[b]*Department of Chemical Engineering, Faculty of Engineering, University of Kashan, Kashan 87317-51167, I. R. Iran*

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With the growth of nanotechnology, many attempts have been made on the chemical and physical properties of nanostructures. Due to relation between physical properties and geometrical structure, understanding of the geometrical structure is very important. Moreover, this can be useful for finding unknown structures that have not been produced in laboratory yet. In the present work, first we have investigated the structure of some nanostructures from the geometrical point of view. Then an algorithm is proposed for discovering the number of carbon atoms in various nanotubes and fullerenes. In the presented algorithm, a nanosheet in 2D space is considered as a start point. Creating twelve nanocones in nanosheet makes it a nanostructure. Different nanostructures are produced by relocation of nanocones. The result shows that the number of carbon atoms in different nanostructures is a sequence that has infinite harmonies and follows a simple formula. Each harmony is an arithmetic progression.

INTRODUCTION

After discovering some important carbon nanostructures such as carbon nanotubes and fullerenes[1–6] many efforts have been made on the mathematical properties of these structures from geometrical point of view. The geometrical methods have been applied to predict, investigate and clarify the new structures of carbon nanostructures. For example by using the Euler's formula Iijima predicted the basic characters of fullerene, *i.e.*, the existence of twelve pentagons before the clarification of the C_{60} structure.[3] More general morphology of these carbon nanostructures has been investigated.[7–11] For example in the work of Fujita *et al.*[8] an arbitrary fullerene can be specified by proper distribution of twelve pentagons on a honeycomb lattice. In another work[7] based on the differential geometry, it has been clarified that the topological defects (pentagons and heptagons) in a hexagonal graphitic network give rise to a non-zero curvature in the three-dimensional structure formed by the network and it has been shown that how the topological defects affect the carbon nanostructure morphology. In the present work first the structure of some nanostructures has been investigated from geometrical point of view, and then an algorithm is proposed for discovering the number of carbon atoms in different nanotubes and fullerenes. In the following sections we describe the details of the proposed method and the algorithm of the computer program and the calculated results are presented.

* Author to whom correspondence should be addressed. (E-mail: hsabaghianb@kashanu.ac.ir)

METHOD DESCRIPTION

In each carbon nanostructure studied here, one carbon atom has three chemical bound. Most of these nanostructures have a cage-like structure with twelve pentagons surrounded by 5 hexagons. Here we consider a plane connected structure. Consider many number of carbon atoms located in an infinite two dimensional network. Each carbon atom has 3 connected bounds in this network. The result will be a sheet with infinite number of regular hexagons. This plane is called nano-sheet. We are going to build a fullerene by proper cutting and rotating the nano-sheet.

For this purpose, as it can be seen from Figure 1, we cut a 60° angle in the nanosheet. It's important to consider that the apex of this angle concise on the center of the specified hexagon which we want to convert that to a pentagon. After cutting two edges of the angle must be concised. Consequently the nanosheet in 2D space changes to a nano-cone in 3D space. As shown in Figure 2 in the nanocone there is only one pentagon in the center surrounded by many hexagons. As it has been proved theoretically in the work of M. Hayashi[7] by creating twelve nanocones in the nano-sheet, we have made a closed cage-like structure (see Figure 3). Because of the symmetry of this structure we choose one half of it for our further dis-
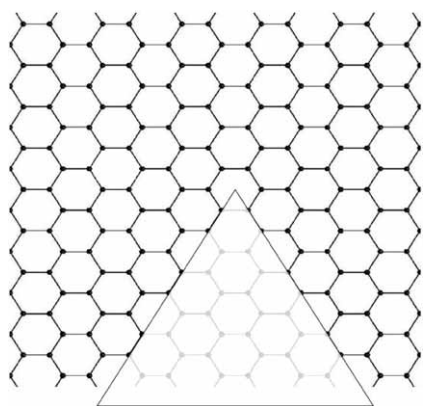

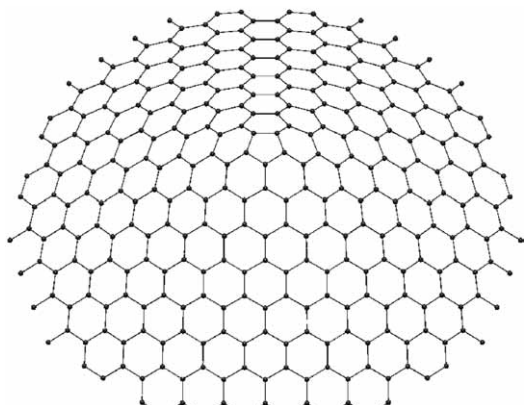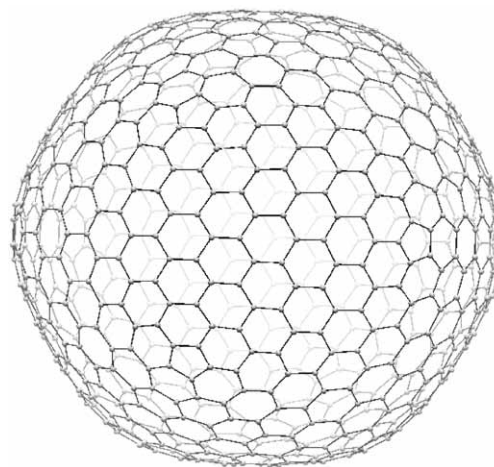Figure 1. Nanosheet with cutting triangular zone.

Figure 2. Nanocone.

Figure 3. A cage-like structure with twelve pentagons.

cussion. There are 6 pentagons in one half of cage-like structure includes one at the center surrounded by five other pentagons. Relative positions of these six pentagons to each other can produce three different categories of structures. The first one includes a series of structures in which the neighbors of the central pentagon are located along with the perpendicular bisectors of each edge of the central pentagon. In the second series, the neighbors of the central pentagon are located along with the apex of it. In the third series, we don't have the geometrical properties of the two series mentioned above. In this work we are going to predict the number of carbon atoms existing in the first two series introduced here.

THE FIRST SERIES

As shown in Figure 4 for generating the central pentagon in the center of nanosheet white triangular zone is used. For generating other five pentagons, five neighbor hexagons are selected and five other triangular zones are used. These triangles are drawn with dark color in this figure. Depending to the distance between of surrounding pentagons from the central, different sets are made. Figure 4 shows the first set in which surrounded pentagons are immediate neighbors of the central pentagon. For determination of the cutting edge of the structure we use a specified hexagon namely half-cage cut-hexagon. It is a hexagon that contains half number of carbon atoms participate in a cage-like structure. By using the symmetry of the structure the second half is exactly the same. Through this way we have made a sequence of numbers by enlarging the cut-hexagon.

Here we introduce a well known homologue series of carbon nanostructures which have been named by fullerenes. Fullerenes are cage-like carbon nanostructures with different number of carbon atoms. The smallest of these structures is C_{20}. C_{20} is a symmetric fullerene contains twelve pentagons. C_{20} as well as other fullerenes can be

obtained from Figure 4 in the following manner. Smallest half-cage cut-hexagon contains ten carbon atoms which labeled as C_{20} in Figure 4. Therefore we can conclude that the number 20 is the first term of the sequence. Enlarging the cut-hexagon generates the next members of the sequence, *i.e.* C_{30}, C_{40}, C_{50}, C_{60}, C_{70} *etc*. This sequence of numbers can be expressed by the following expression which is an arithmetic progression with 20 as first term and 10 as common difference.

$$C_{(20 + 10N)}, \; N = 0, 1, 2, 3 \ldots \tag{1}$$

As the number N approaches to the very large numbers the corresponding structures form a new class of carbon nanostructures which are named as $(n,0)$ zig-zag nanotubes[12] which n is an integer multiplier of 5.

In the next step as illustrated in Figure 5 position of five pentagons is considered a little far from central pentagon. By doing this step a new set of nanostructures are made with larger diameters. The only thing that changes in these sequences is the distance of the central pentagon from the others. Considering the above explanations C_{60} will be the smallest structure of the new sequence (see Figure 5). It is worth while to mention the generated C_{60} in this sequence is not the well known buckminsterfullerene, C_{60} (Ref. 13) which is completely spherical. The

only spherical structure in this sequence is C_{80}. C_{100}, C_{120}, C_{140}, C_{160}, are the next structures of this sequence. Similarly this new sequence is an arithmetic progression with 60 as first term and 20 as common difference can be expressed by the following expression:

$$C_{(60 + 20N)}, \; N = 0, 1, 2, 3 \ldots \tag{2}$$

In the similar manner (see Figures 6 and 7) additional sequences are made with the following expressions:

$$C_{(120 + 30N)}, \; N = 0, 1, 2, 3 \ldots \tag{3}$$

$$C_{(200 + 40N)}, \; N = 0, 1, 2, 3 \ldots \tag{4}$$

$$C_{(300 + 50N)}, \; N = 0, 1, 2, 3 \ldots \tag{5}$$

…

A GENERAL FORMULA FOR THE FIRST SERIES

First term of each sequence in the series include 20, 60, 120, 200, 300, is also an arithmetic progression except that its common difference is a variable that can be calculated by the following expression:

$$20 + J*20 \quad \text{with} \quad J = 1, 2, 3, 4 \ldots \tag{6}$$

TABLE I. Predicted number of carbon atom for first series

|																			
20	60	120	200	300	420	560	720	900	1100	1320	1560	1820	2100	2400	2720	3060	3420	3800	4200
30	80	150	240	350	480	630	800	990	1200	1430	1680	1950	2240	2550	2880	3230	3600	3990	4400
40	100	180	280	400	540	700	880	1080	1300	1540	1800	2080	2380	2700	3040	3400	3780	4180	4600
50	120	210	320	450	600	770	960	1170	1400	1650	1920	2210	2520	2850	3200	3570	3960	4370	4800
60	140	240	360	500	660	840	1040	1260	1500	1760	2040	2340	2660	3000	3360	3740	4140	4560	5000
70	160	270	400	550	720	910	1120	1350	1600	1870	2160	2470	2800	3150	3520	3910	4320	4750	5200
80	180	300	440	600	780	980	1200	1440	1700	1980	2280	2600	2940	3300	3680	4080	4500	4940	5400
90	200	330	480	650	840	1050	1280	1530	1800	2090	2400	2730	3080	3450	3840	4250	4680	5130	5600
100	220	360	520	700	900	1120	1360	1620	1900	2200	2520	2860	3220	3600	4000	4420	4860	5320	5800
110	240	390	560	750	960	1190	1440	1710	2000	2310	2640	2990	3360	3750	4160	4590	5040	5510	6000
120	260	420	600	800	1020	1260	1520	1800	2100	2420	2760	3120	3500	3900	4320	4760	5220	5700	6200
130	280	450	640	850	1080	1330	1600	1890	2200	2530	2880	3250	3640	4050	4480	4930	5400	5890	6400
140	300	480	680	900	1140	1400	1680	1980	2300	2640	3000	3380	3780	4200	4640	5100	5580	6080	6600
150	320	510	720	950	1200	1470	1760	2070	2400	2750	3120	3510	3920	4350	4800	5270	5760	6270	6800
160	340	540	760	1000	1260	1540	1840	2160	2500	2860	3240	3640	4060	4500	4960	5440	5940	6460	7000
170	360	570	800	1050	1320	1610	1920	2250	2600	2970	3360	3770	4200	4650	5120	5610	6120	6650	7200
180	380	600	840	1100	1380	1680	2000	2340	2700	3080	3480	3900	4340	4800	5280	5780	6300	6840	7400
190	400	630	880	1150	1440	1750	2080	2430	2800	3190	3600	4030	4480	4950	5440	5950	6480	7030	7600
200	420	660	920	1200	1500	1820	2160	2520	2900	3300	3720	4160	4620	5100	5600	6120	6660	7220	7800
210	440	690	960	1250	1560	1890	2240	2610	3000	3410	3840	4290	4760	5250	5760	6290	6840	7410	8000
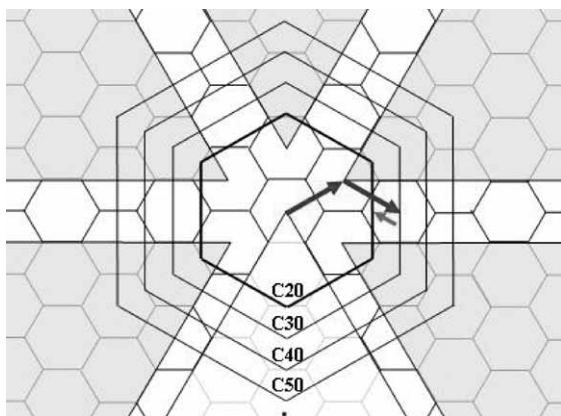
Figure 4. 2D model for first sequence of first series.
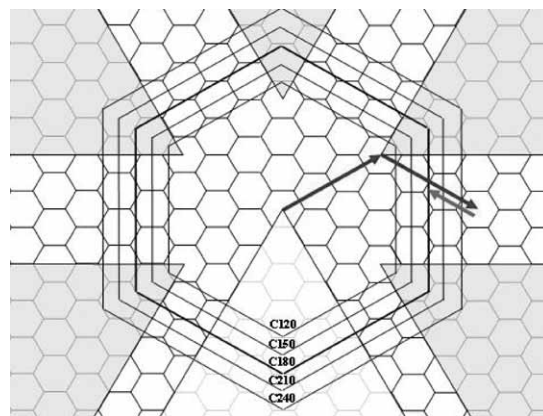

Figure 6. 2D model for third sequence of first series.
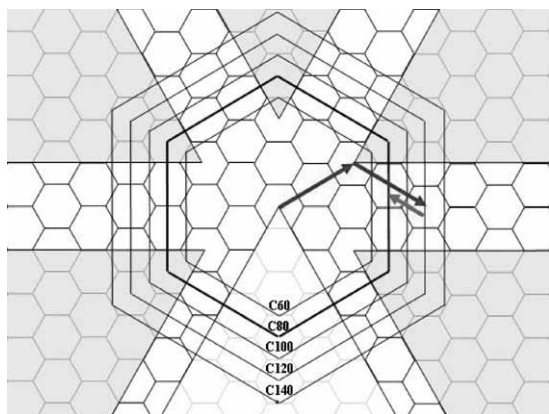

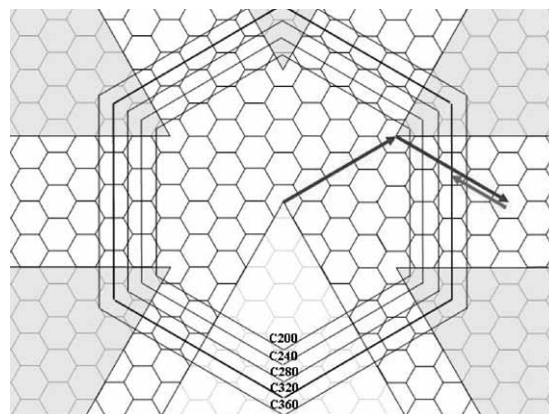Figure 5. 2D model for second sequence of first series.
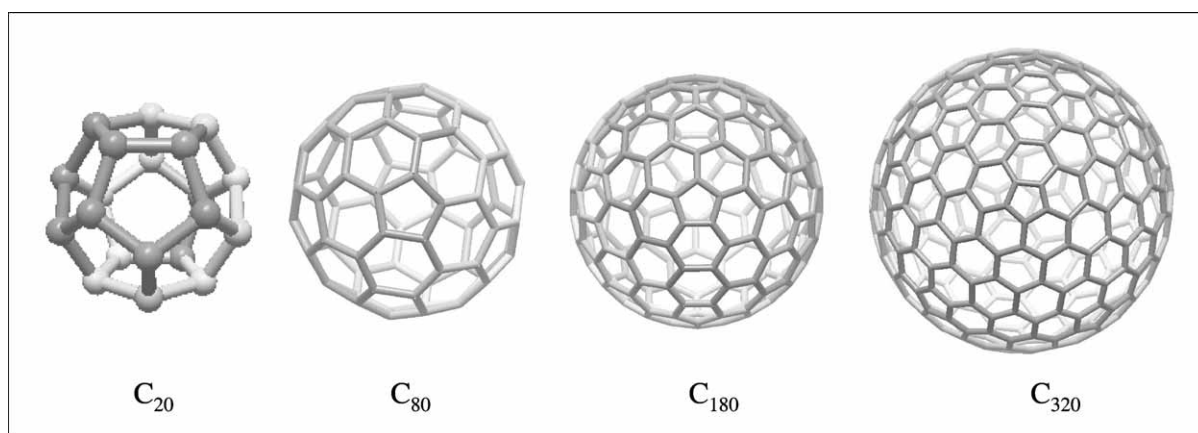

Figure 7. 2D model for fourth sequence of first series.

Figure 8. 3D shape of some spherical Fullerene of series one.

Therefore the first term of the sequences in the series can be obtained by the following manner:

$$20 + (20 + 1*20) = 60$$

$$60 + (20 + 2*20) = 120$$

$$120 + (20 + 3*20) = 200$$

$$200 + (20 + 4*20) = 300$$

$$300 + (20 + 5*20) = 420$$

$$420 + (20 + 6*20) = 560$$

Thus this series can be considered as a 2D sequence that can be expressed by the following general formula:

$$10j(i + j) \qquad (7)$$

Where i and j denote respective rows and columns of Table I. This table shows the first 20×20 of this 2D sequence.

One of the most important properties of this table is that the numbers on its main diameter produce symmetrical spherical fullerenes. These numbers are shaded in table. Smaller fullerenes have more spherical shape which shaded darker. Figure 8 shows some of these fullerene shapes in 3D space. Figure 9 demonstrates 2D shapes of some nanostructures.

THE SECOND SERIES

In this section other series of sequences are proposed. Method is similar to the previous section. As it was mentioned before here 5 surrounding pentagons are placed along with the apex of the central pentagon. By referring to Figures 10, 11 and 12 if a line is drawn from the center of central pentagon to each its apex, passes from the apex of the cut-triangle. By doing similar steps as presented before we can obtain the new series of sequences. Common statement of these sequences is given below:

$$C_{(60 + 20N)}, \ N = 0, 1, 2, 3 \dots \tag{8}$$

$$C_{(180 + 40N)}, \ N = 0, 1, 2, 3 \dots \tag{9}$$

$$C_{(360 + 60N)}, \ N = 0, 1, 2, 3 \dots \tag{10}$$

$$C_{(600 + 80N)}, \ N = 0, 1, 2, 3 \dots \tag{11}$$

$$C_{(900 + 400N)}, \ N = 0, 1, 2, 3 \dots \tag{12}$$

In these statements when N approaches to very large number we will obtain some important carbon nanotubes which are named as (n,n) arimchair nanotubes.[12] Again similar to series one n is an integer multiplier of 5.

C_{20} C_{80} C_{180} C_{320}

C_{30} C_{100} C_{210} C_{360}

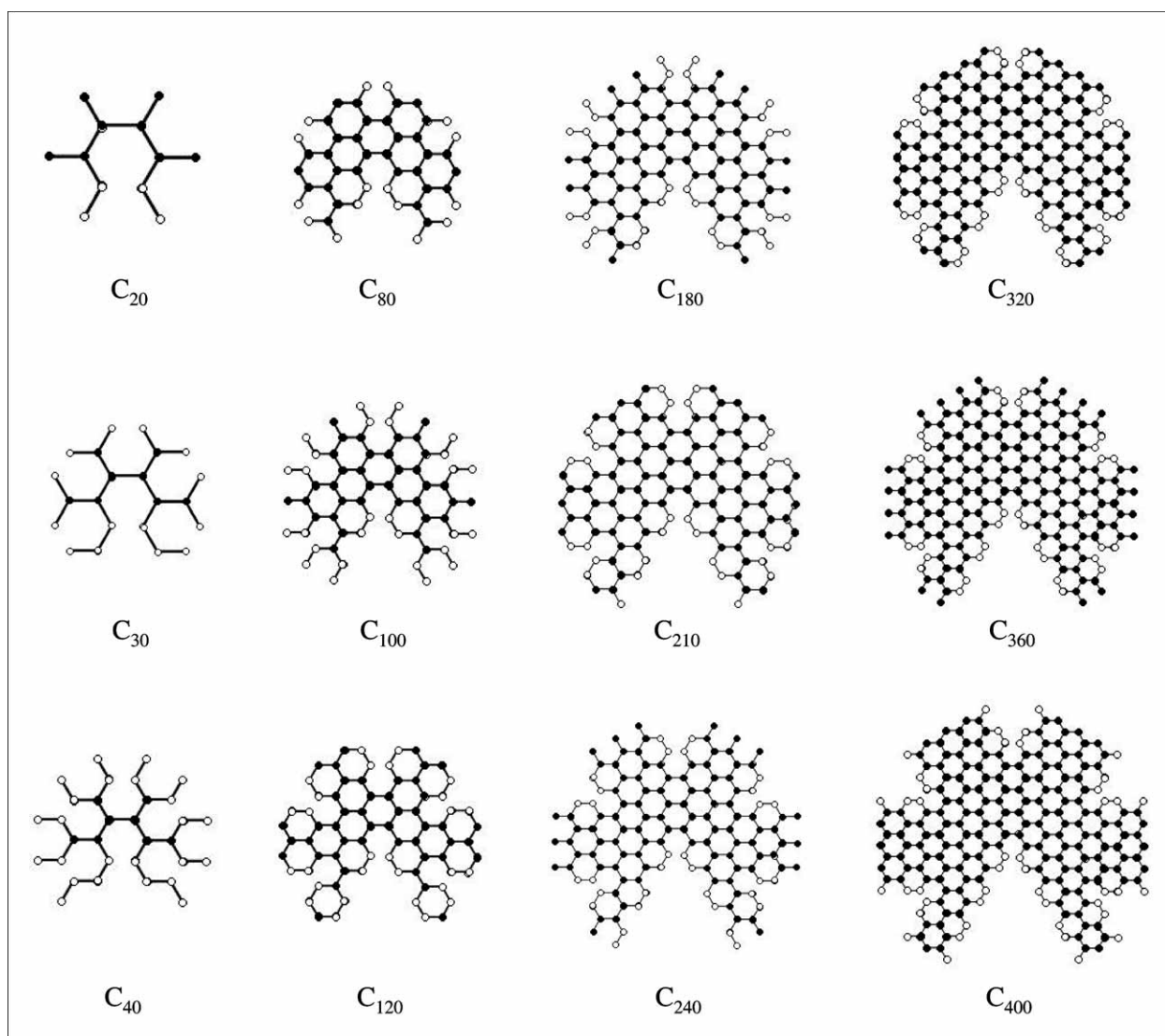C_{40} C_{120} C_{240} C_{400}

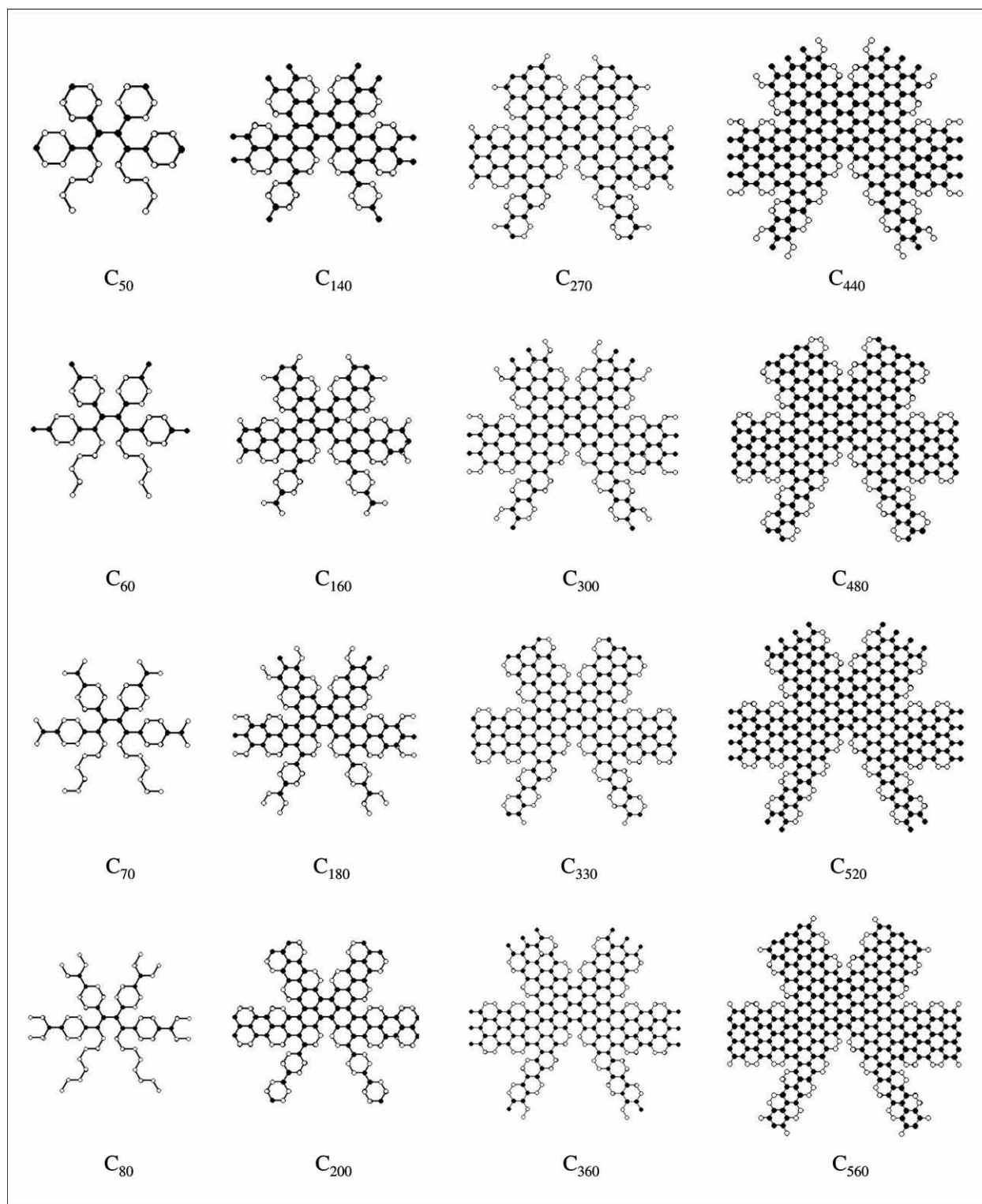Figure 9. 2D shape for one half of various nanostructure of series one.

Figure 9. (continued)

A GENERAL FORMULA FOR THE SECOND SERIES

Similar to the previous section first term of each sequence is an arithmetic progression with the following variable common difference:

$$60 + J*60 \text{ with } J = 1, 2, 3, 4 \ldots \quad (13)$$

Thus this series can be considered as a 2D sequence that can be expressed by the following general formula:

$$10j(2i + 3j + 1) \quad (14)$$

TABLE II. Predcted number of carbon atom for second series

60	180	360	600	900	1260	1680	2160	2700	3300	3960	4680	5460	6300	7200	8160	9180	10260	11400	12600
80	220	420	680	1000	1380	1820	2320	2880	3500	4180	4920	5720	6580	7500	8480	9520	10620	11780	13000
	240																		
100	260	480	760	1100	1500	1960	2480	3060	3700	4400	5160	5980	6860	7800	8800	9860	10980	12160	13400
120	300	540	840	1200	1620	2100	2640	3240	3900	4620	5400	6240	7140	8100	9120	10200	11340	12540	13800
140	340	600	920	1300	1740	2240	2800	3420	4100	4840	5640	6500	7420	8400	9440	10540	11700	12920	14200
			960																
160	380	660	1000	1400	1860	2380	2960	3600	4300	5060	5880	6760	7700	8700	9760	10880	12060	13300	14600
180	420	720	1080	1500	1980	2520	3120	3780	4500	5280	6120	7020	7980	9000	10080	11220	12420	13680	15000
200	460	780	1160	1600	2100	2660	3280	3960	4700	5500	6360	7280	8260	9300	10400	11560	12780	14060	15400
					2160														
220	500	840	1240	1700	2220	2800	3440	4140	4900	5720	6600	7540	8540	9600	10720	11900	13140	14440	15800
240	540	900	1320	1800	2340	2940	3600	4320	5100	5940	6840	7800	8820	9900	11040	12240	13500	14820	16200
260	580	960	1400	1900	2460	3080	3760	4500	5300	6160	7080	8060	9100	10200	11360	12580	13860	15200	16600
							3840												
280	620	1020	1480	2000	2580	3220	3920	4680	5500	6380	7320	8320	9380	10500	11680	12920	14220	15580	17000
300	660	1080	1560	2100	2700	3360	4080	4860	5700	6600	7560	8580	9660	10800	12000	13260	14580	15960	17400
320	700	1140	1640	2200	2820	3500	4240	5040	5900	6820	7800	8840	9940	11100	12320	13600	14940	16340	17800
									6000										
340	740	1200	1720	2300	2940	3640	4400	5220	6100	7040	8040	9100	10220	11400	12640	13940	15300	16720	18200
360	780	1260	1800	2400	3060	3780	4560	5400	6300	7260	8280	9360	10500	11700	12960	14280	15660	17100	18600
380	820	1320	1880	2500	3180	3920	4720	5580	6500	7480	8520	9620	10780	12000	13280	14620	16020	17480	19000
											8640								
400	860	1380	1960	2600	3300	4060	4880	5760	6700	7700	8760	9880	11060	12300	13600	14960	16380	17860	19400
420	900	1440	2040	2700	3420	4200	5040	5940	6900	7920	9000	10140	11340	12600	13920	15300	16740	18240	19800
440	940	1500	2120	2800	3540	4340	5200	6120	7100	8140	9240	10400	11620	12900	14240	15640	17100	18620	20200

Where i and j denote respective rows and columns of Table II. This table shows the first 40×20 matrix of this 2D sequence.
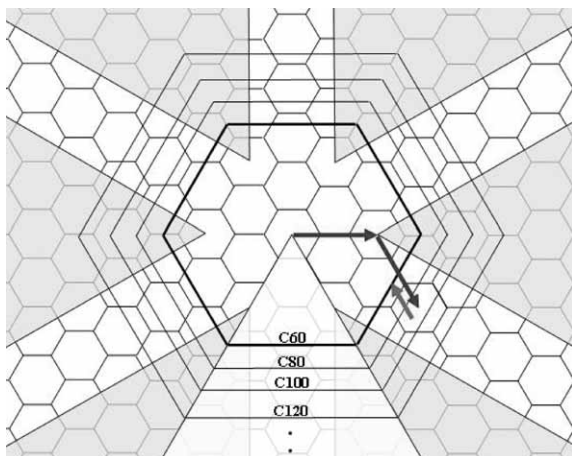
The first term of the first sequence in this series is 60 corresponding to C_{60} which is named Buckminster-fullerene. This structure is a completely spherical carbon nanostructure.

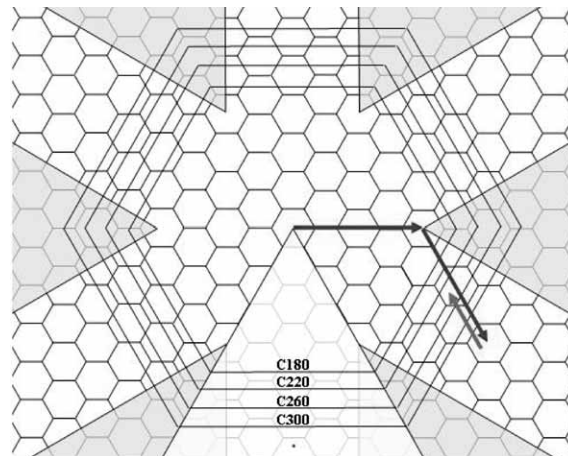Figure 10. 2D model for first sequence of second series.

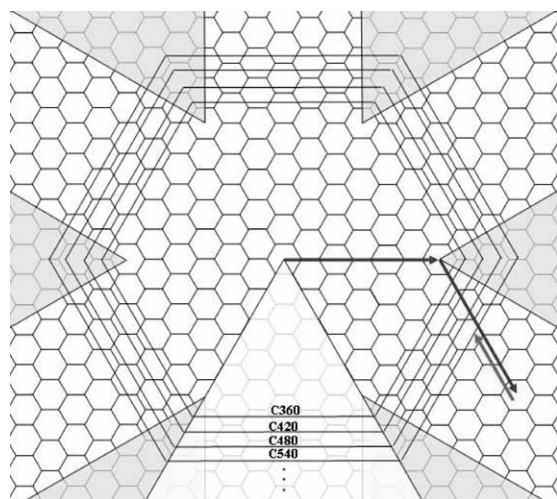Figure 11. 2D model for second sequence of second series.

Figure 12. 2D model for third sequence of second series.

One point should be noticed is that in this spectrum for all sequences one number can be inserted between with the average value of two consequent numbers. Location

of these numbers in the table is left blank except symmetrical spherical fullerenes which are shaded in the table. Similar to Table I smaller fullerenes are more spherical and are shaded darker in Table II. Figure 13 shows some of these fullerene shapes in 3D space. Figure 14 demonstrates 2D shapes of some nanostructures.

CONCLUSION

In this work we classified nanostructures from geometrical point of view and proposed a 2D topological model for two big series of these regular structures. Each series has a large number of sets. This approach provides the facility to imagine connectivity structure of nanostructures and determining the number of carbon atoms for all members of these sets. The obtained numbers for each set satisfy an arithmetic progression. Two program source codes have been presented for generating two series of sequences. The results can be useful for educational purposes, prediction of new structures in laboratory which have not been produced yet, finding coordination of all
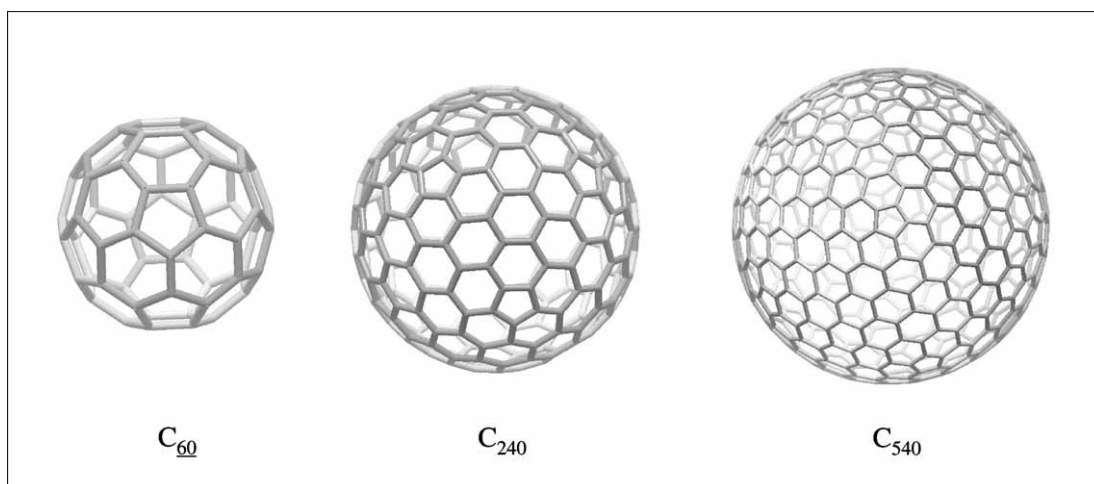

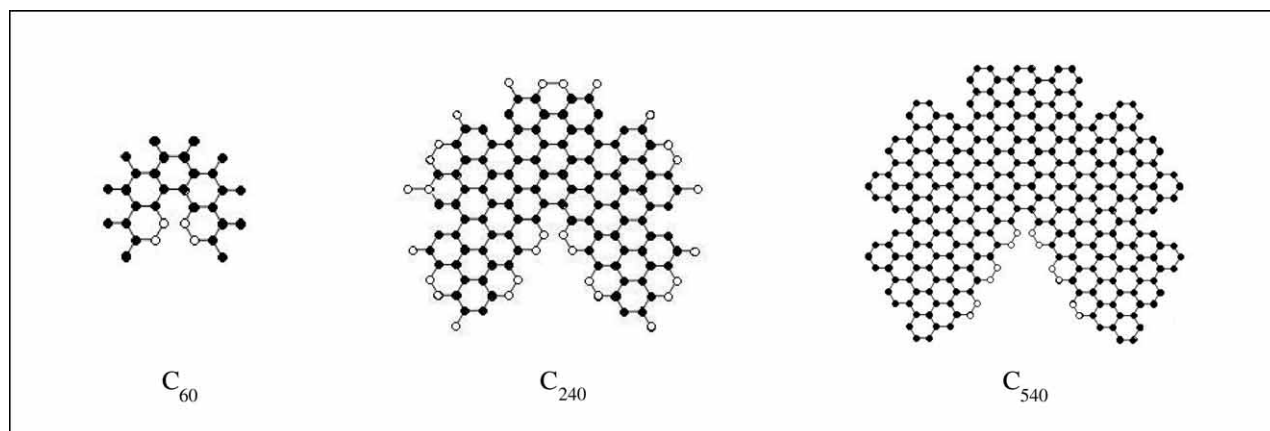Figure 13. 3D shape of some spherical Fullerene of series two.

Figure 14. 2D shape for one half of various nanostructure of series two.
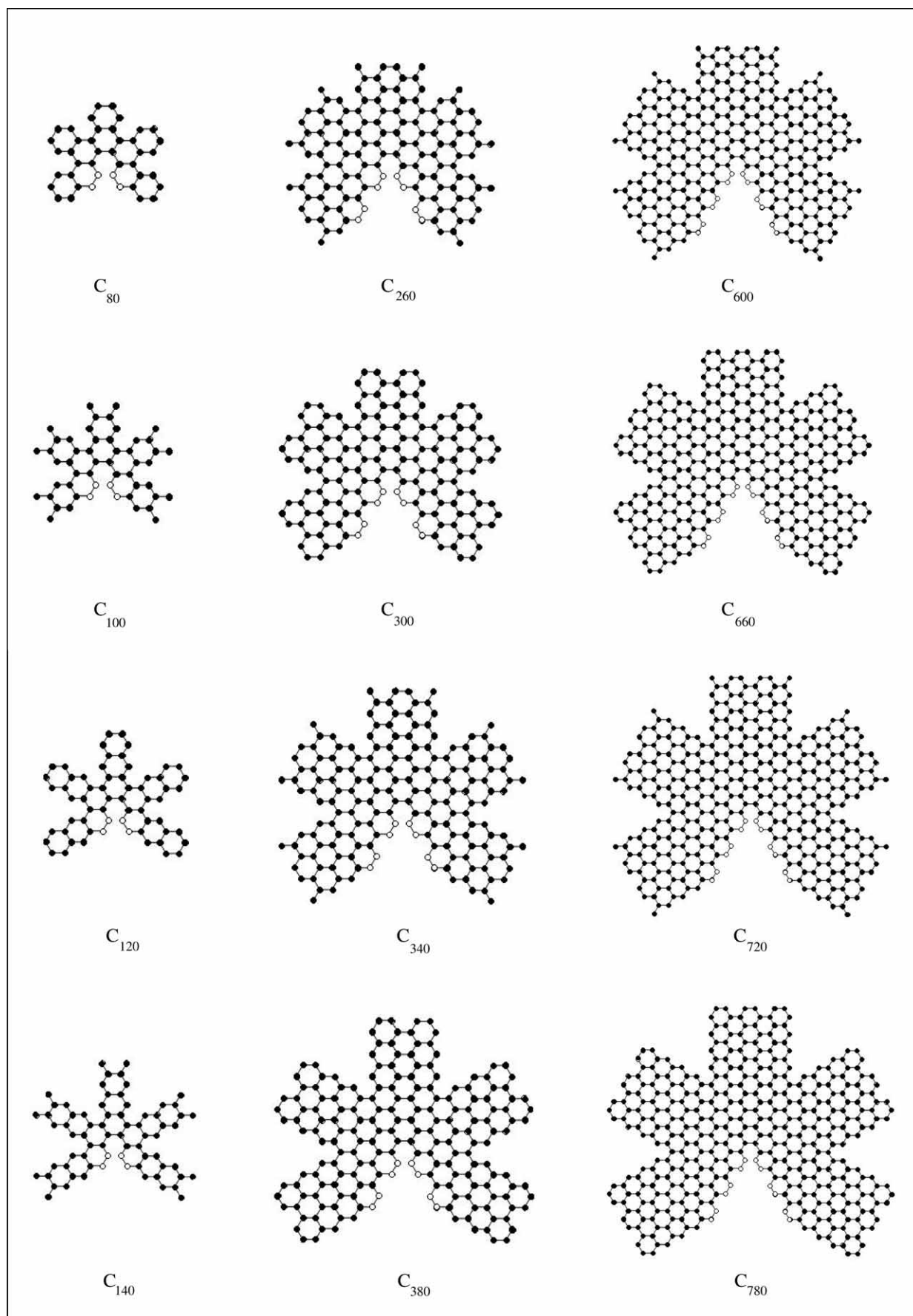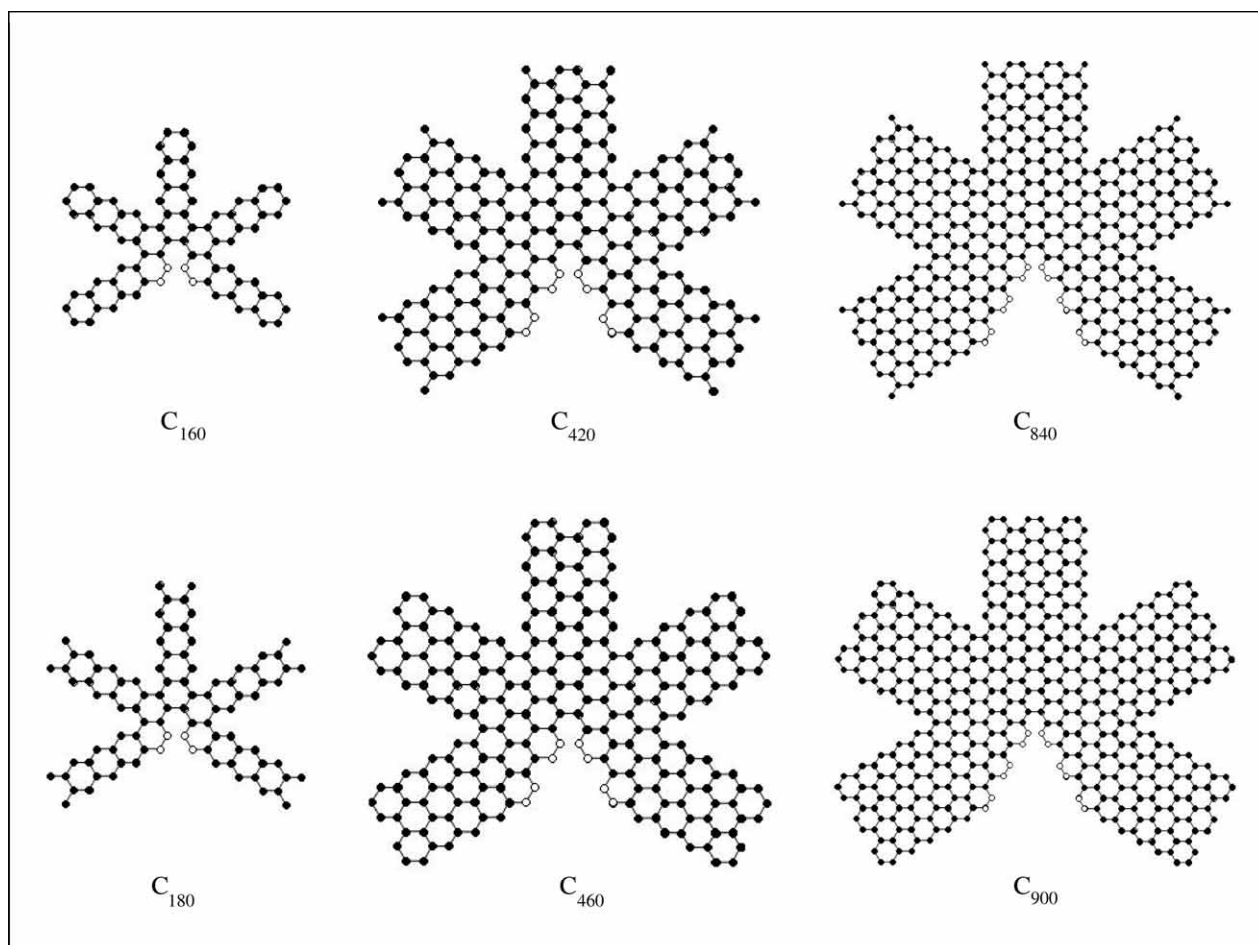
Figure 14. (continued)

Figure 14. (continued)

nodes in each nanostructure and drawing 3D shapes of various nanostructures. More extensive works are needed for generating the shape of some other nanostructures with different geometrical properties. This will be the subject of our further research work.

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SAŽETAK

Predviđanje broja ugljikovih atoma u raznim nanostrukturama korištenjem geometrijskog pristupa

Hosein Sabaghian-Bidgoli, Gholamreza Vakili-Nezgaad i Mehdi Vahidipour

Rast nanotehnologija je doveo do mnogih istraživanja kemijskih i fizikalnih svojstava nanostruktura. Kako su ova ovisna o geometriji, to su geometrijske studije vrlo važne. Štoviše, one mogu biti također od koristi u pronalaženju novih struktura koje još nisu dobivene u laboratoriju. U ovom radu prvo istražujemo neke nanostrukture s geometrijskog stanovišta. Nakon toga predlažemo algoritam za određivanje broja ugljikovih atoma u raznim nanocjevčicama i fullerenima, gdje krećemo od dvodimenzionalnog lista u koji zatim ugrađujemo dvanaest nanostožaca. Konačno se premještanjem nanosožaca dobivaju razne nanostrukture. Pokazano je da broj ugljikovih atoma u raznim nanostrukturama pokazuje pravilnosti koje se daju opisati jednostavnim formulama.