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

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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.

*Keywords*
nanostructures
algorithm for construction
nanosheet
relocation of nanocones

## 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.

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## 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 discussion. 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.

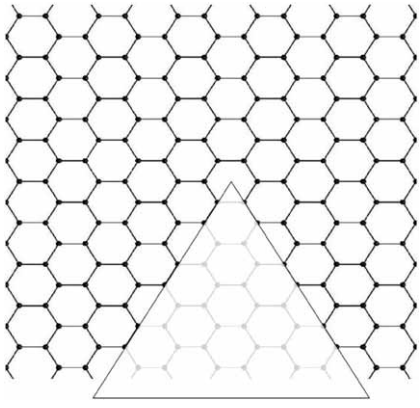

Figure 1. Nanosheet with cutting triangular zone.

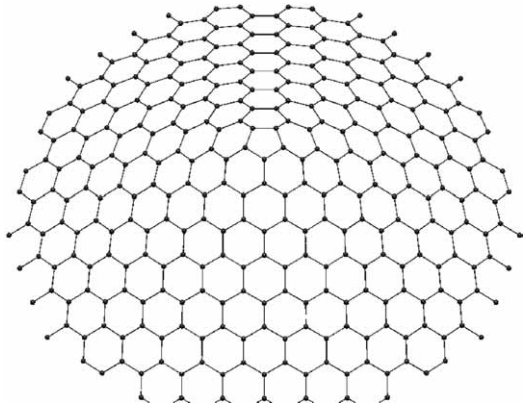

Figure 2. Nanocone.

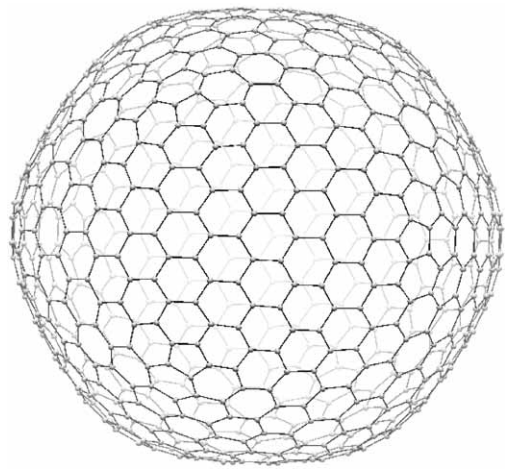

Figure 3. A cage-like structure with twelve pentagons.

## 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.

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

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:

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

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

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

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

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

…

## 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:

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

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 |

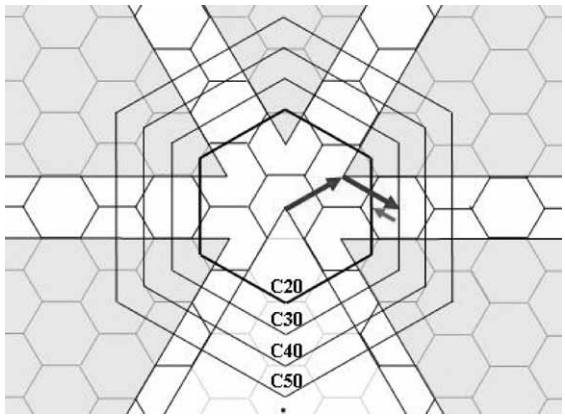


Figure 4. 2D model for first sequence of first series.

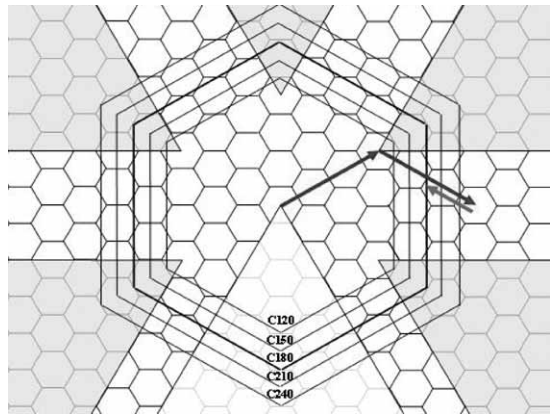


Figure 6. 2D model for third sequence of first series.

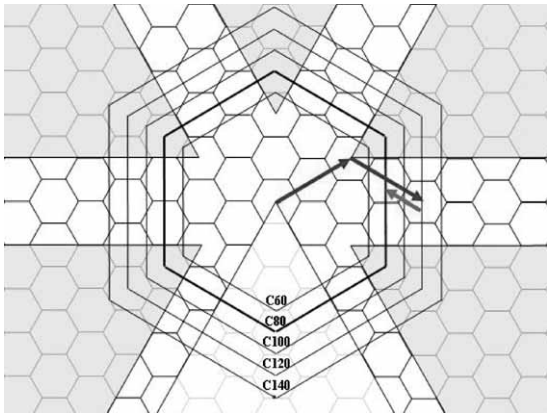


Figure 5. 2D model for second sequence of first series.

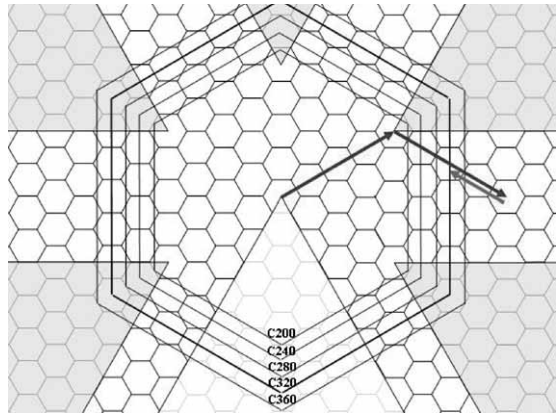


Figure 7. 2D model for fourth sequence of first series.

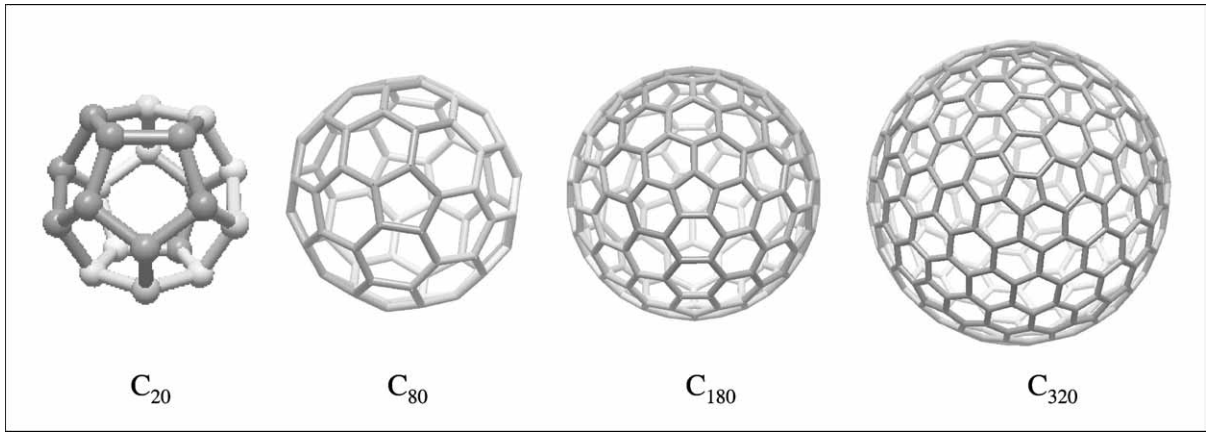


Figure 8. 3D shape of some spherical Fullerene of series one.

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:

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

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

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

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

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

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.

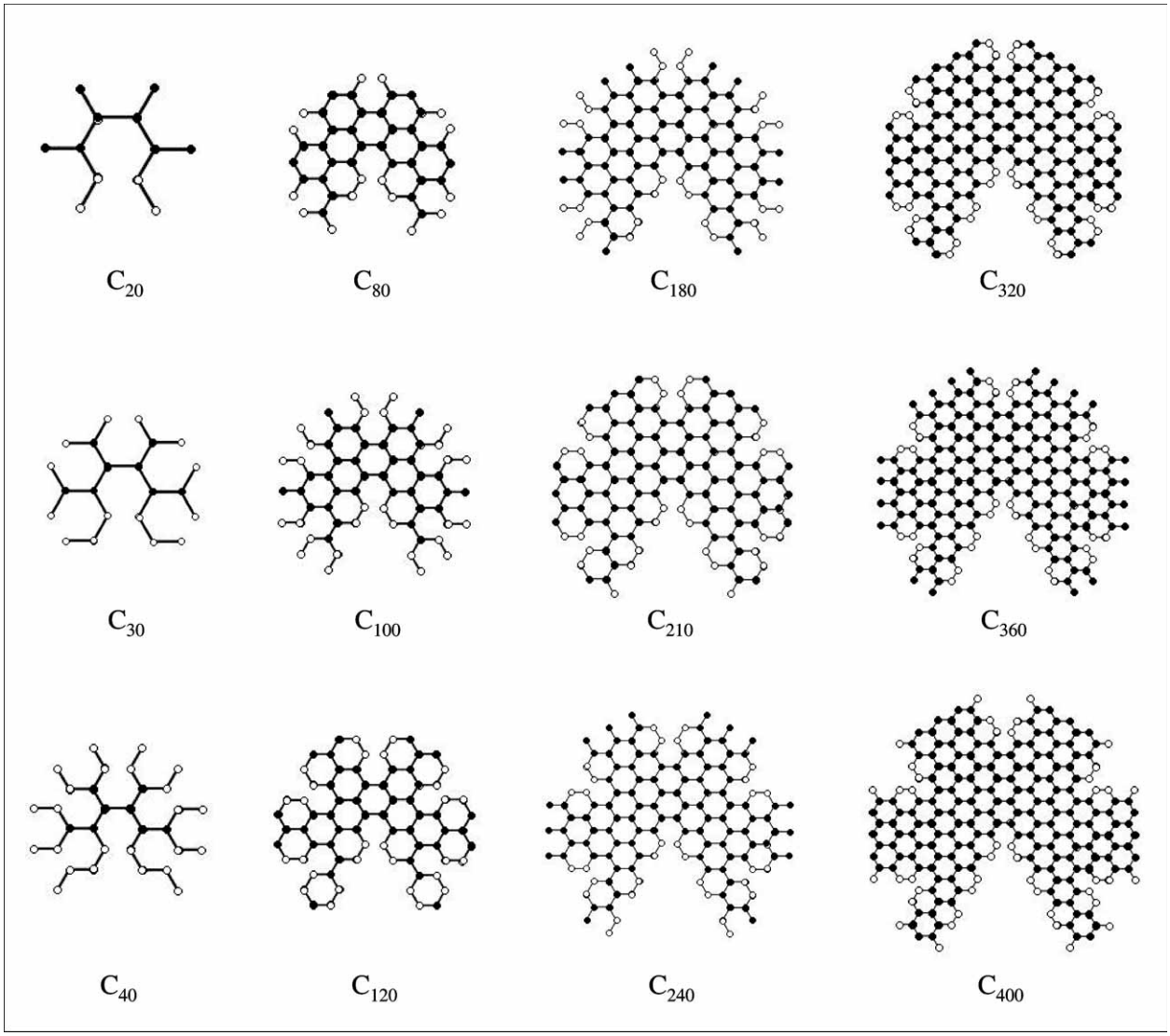


Figure 9. 2D shape for one half of various nanostructure of series one.

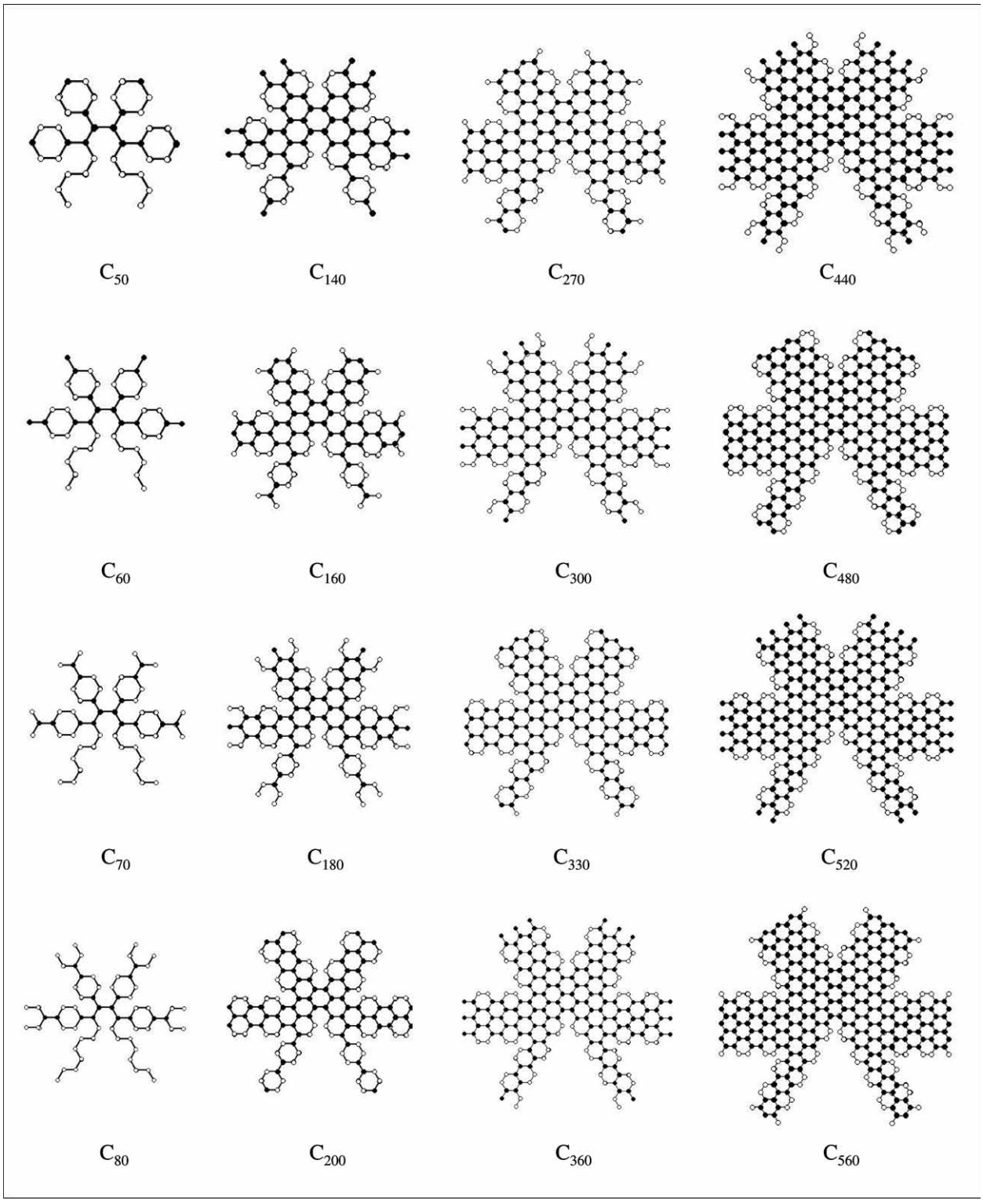


Figure 9. (continued)

## 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 Buckminsterfullerene. This structure is a completely spherical carbon nanostructure.

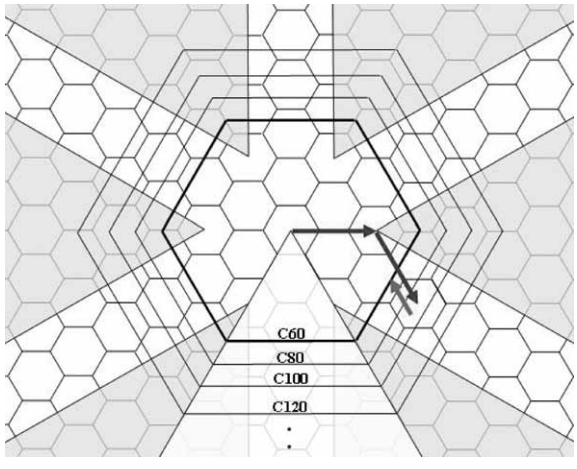


Figure 10. 2D model for first sequence of second series.

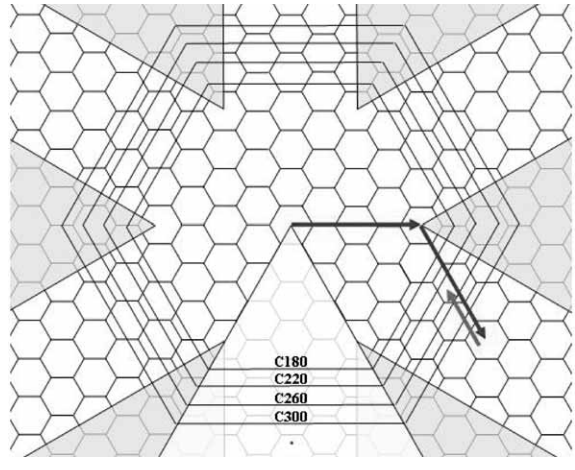


Figure 11. 2D model for second sequence of second series.

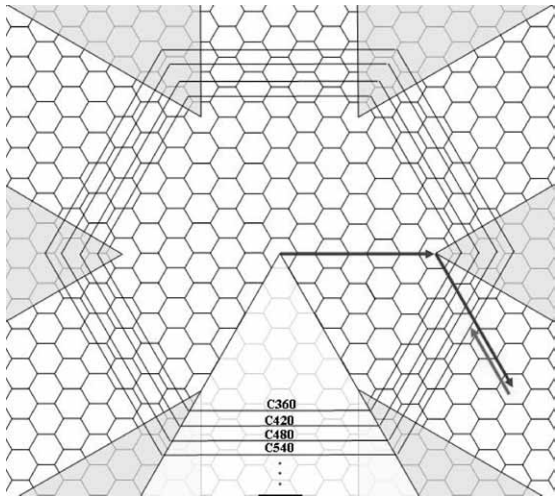


Figure 12. 2D model for third sequence of second series.

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

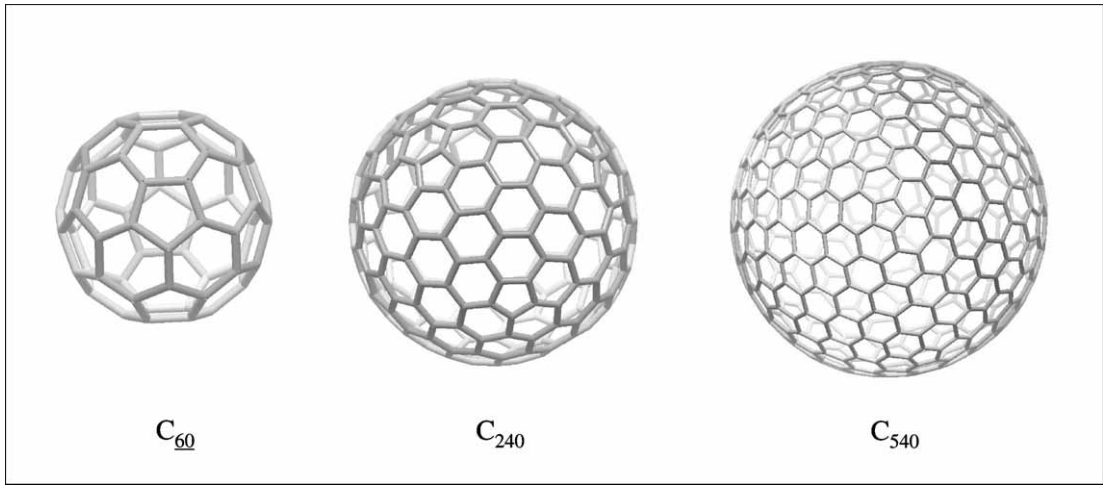


Figure 13. 3D shape of some spherical Fullerene of series two.

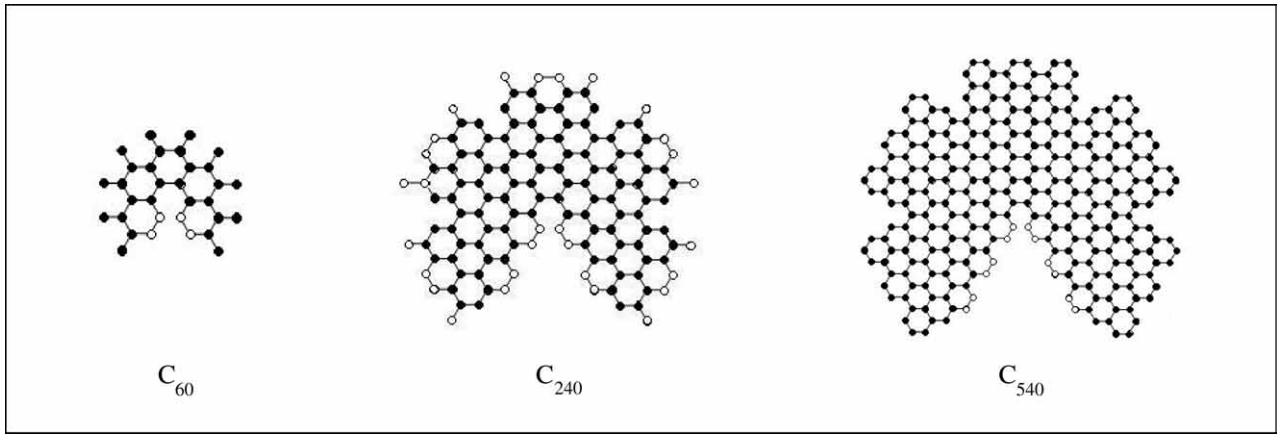


Figure 14. 2D shape for one half of various nanostructure of series two.

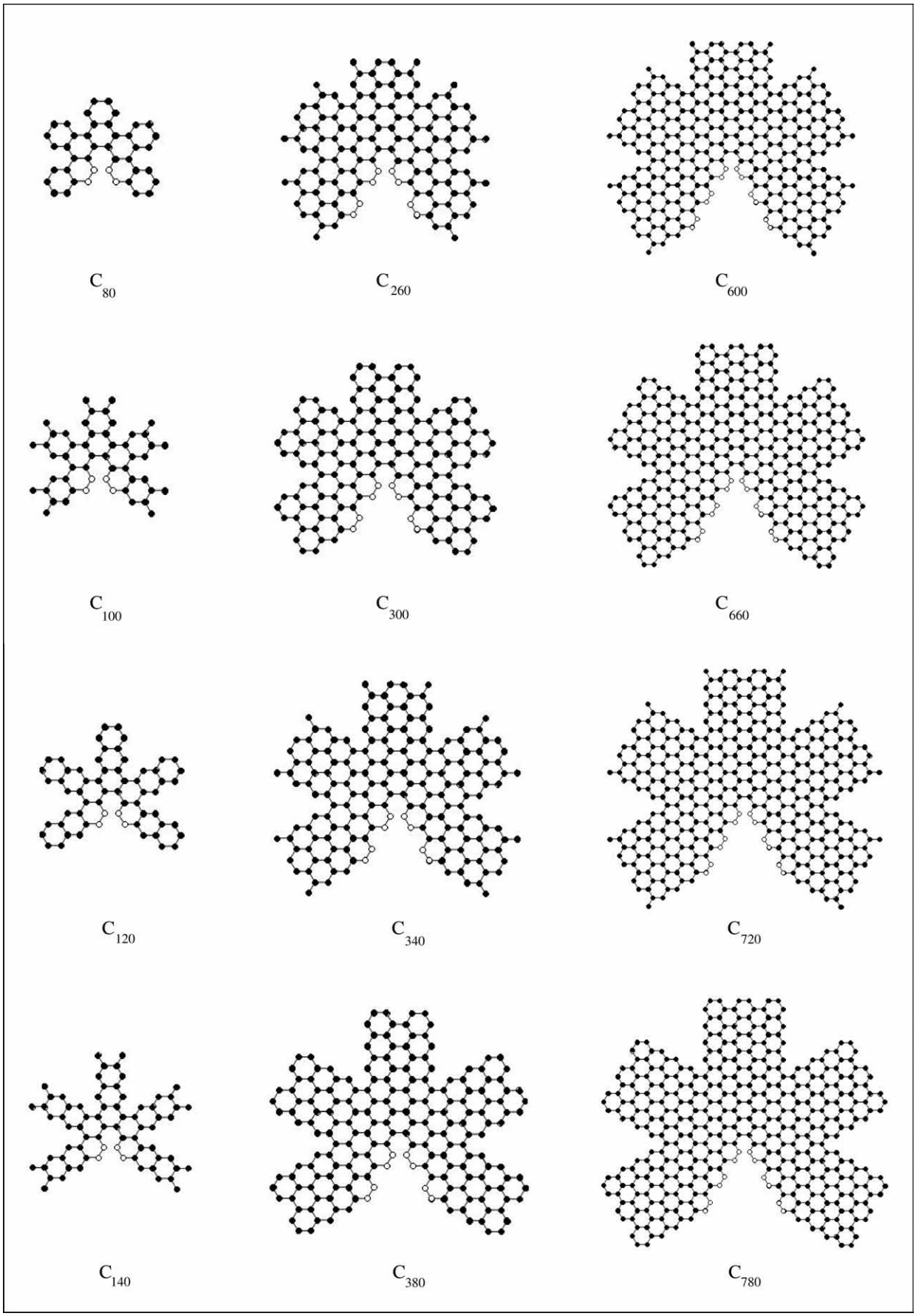


Figure 14. (continued)

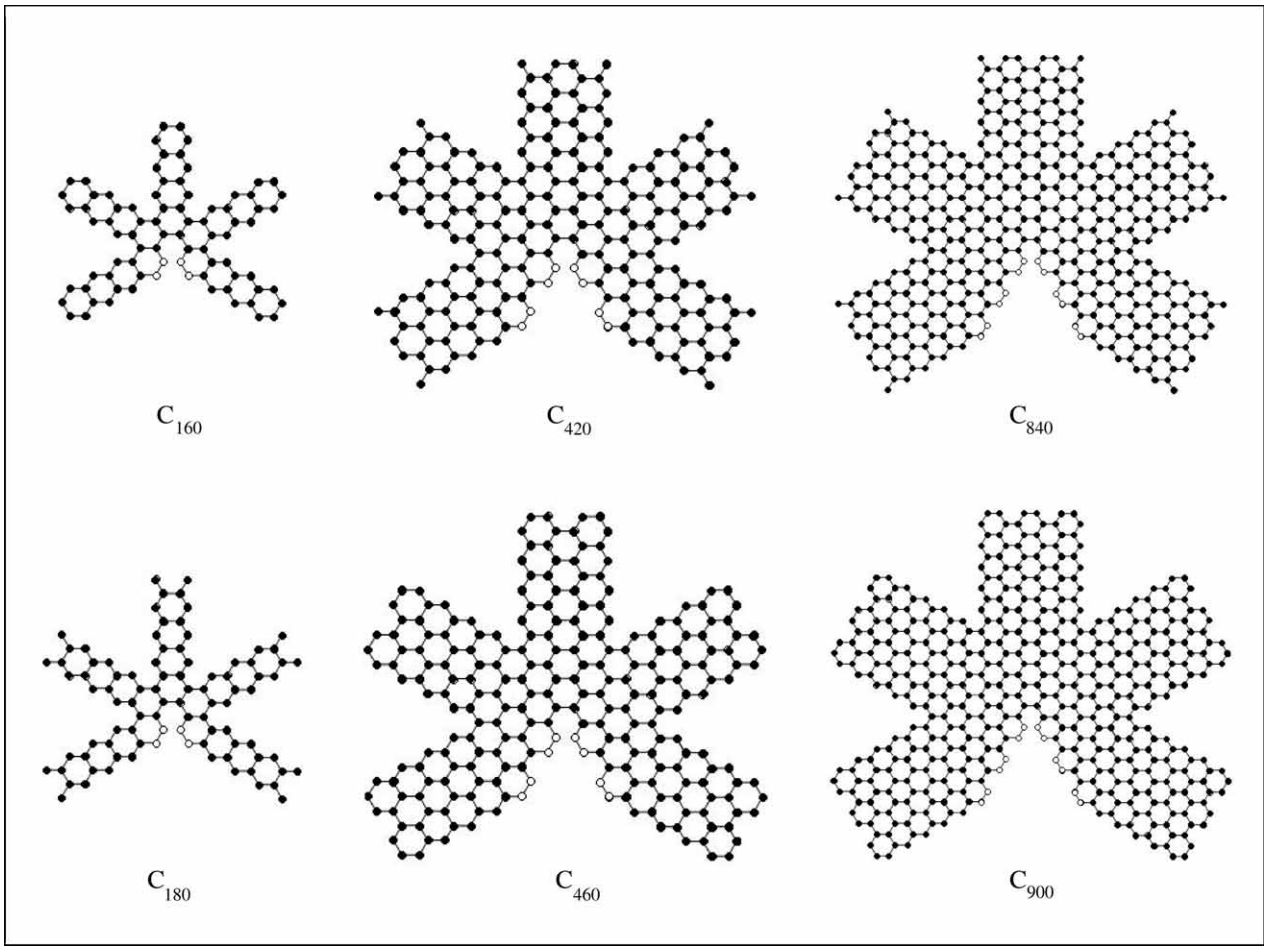


Figure 14. (continued)

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

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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.