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The adjacency matrix of three sequences of fullerenes

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Abstract. When we study chemical graphs, the adjacency matrix is an important invariant of a graph with chemical meaning. In this paper, the general form of the adjacency matrices of three sequences of fullerenes will be determined.

Keywords: Adjacency matrix, C_{12m+2}, C_{12m+4}, C_{12m+6}.

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1. Introduction and preliminaries

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. A fullerene graph is the molecular graph of a fullerene molecule. It is a cubic planar graph having pentagonal or hexagonal faces. Let p, h, n and m be the number of pentagons, hexagons, carbon atoms and bonds between them, in a given fullerene F. Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is $n = \dfrac{5p+6h}{3}$, the number of edges is $m = \frac{5p+6h}{2} = 3/2n$ and the number of faces is $f = p + h$. By the Eulers formula $n - m + f = 2$, one can deduce that $\frac{(5p+6h)}{3} - \frac{(5p+6h)}{2} + p + h = 2$, and therefore $p = 12$, $v = 2h + 20$ and $e = 3h + 30$. This implies that such molecules made up entirely of n carbon atoms and have 12 pentagonal

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and $(n/2-10)$ hexagonal faces, where $20 \leqslant n(\neq 22)$ is an even integer [3, 7]. An $n \times n$ matrix $A=[a_{i,j}]$ is called symmetric if $a_{ij}=a_{ji}$ and centrosymmetric when its entries satisfy $a_{ij}=a_{n-i+1,n-j+1}$ for $1 \leqslant i,j \leqslant n$ [5]. Using this property can see that the distance matrix of C_{10n} fullerene is centrosymmetric and by centrosymmetric of the graph C_{10n}, the number of weiner is calculated [2].

Let X be an $n-$vertex simple graph containing n vertices $u_1, u_2, ..., u_n$. The adjacency matrix $A(X)=[t_{ij}]$ is a matrix for which $t_{ii}=0$, $1 \leqslant i \leqslant n$, and $t_{ij}=1$, $i \neq j$, if and only if u_i and u_j are adjacent. We use Biggs's book [1] for important properties of this matrix.

A circulant matrix is a matrix where each row vector is rotated one element to the right relative to the preceding row vector. The centrosymmetricity of these matrices are proved and an upper bound for the energy of these matrices is given [4]. By proving centrosymmetricity of the adjacency matrix of the graph C_{10n}, a lower bound for its energy is given [6]. Determining the adjacency matrix in graph theory is always important. If this matrix is available the graphical parameters of a graph such as the characteristic polynomial, distance matrix, Wiener index, eigenvectors, etc can be calculated. In [4, 6], the authors paid special attention to obtaining the adjacency matrix of the fullerene graphs by using the properties of distance matrix and the centrisymetry property of the graph. Since these properties are not valid for all fullerene graphs, we have presented the general method to obtain the adjacency matrix of this type of graph.

The purpose of this article is to provide a general method for determining the adjacency matrix of a sequence of infinite fullerene graphs, where the adjacency matrix of three of them is given here. The authors have presented an algorithm similar to this method to obtain the adjacency matrix of a set of hexagonal systems. See [8] for more details.

2. Adjacency Matrices of C_{12m+2}

In [2], an infinite sequence of fullerenes was presented. The aim of this section is to calculate the adjacency matrices of these fullerenes in general. This fullerene, $C_n = C_{12m+2}$, has exactly $n=12m+2$, $m \geqslant 2$, vertices and it is depicted in Figure 1. Suppose that $A_{n\times n}=[a_{i,j}], 1 \leqslant i,j \leqslant n$, is the adjacency matrix of C_n. To calculate the adjacency matrix of C_n, we have to determine all entries which are equal to one and we will do as follows. Define the value t as $t=\frac{n-50}{12}, n \geqslant 51$. We have shown the labeling on the Figure 1 that the $(i,i+1); 1 \leqslant i \leqslant n-1, i \neq 20, 26, 38$ pairs of their value in the adjacency matrice is equal to 1. Pairs $(51,62),(63,74),...$ whose components are arithmetic sequences with the first sentence 51 and the common difference of 12 and their second component are also forming arithmetic sequences with the first sentence 62 and the common difference of 12, whose value in the adjacency matrix is equal to 1, i.e in pairs:

$$(39+12k, 50+12k); 1 \leqslant k \leqslant t$$

Pairs $(40,53),(52,65),...$, the first component of which is the formation of an arithmetic sequence with the first sentence 40 and the second component, also form an arithmetic sequence with the first sentence 53, whose value in the adjacency matrix is equal to 1, i.e.

$$(40+12k, 53+12k); 0 \leqslant k \leqslant t-1$$

Also, the above discussion can be expressed for the following sequences as well.

$$(42+12(k-1), 55+12(k-1)); 1 \leqslant k \leqslant t$$
$$(44+12(k-1), 57+12(k-1)); 1 \leqslant k \leqslant t$$

$$(46 + 12(k-1), 59 + 12(k-1)); 1 \leqslant k \leqslant t$$
$$(48 + 12(k-1), 61 + 12(k-1)); 1 \leqslant k \leqslant t$$

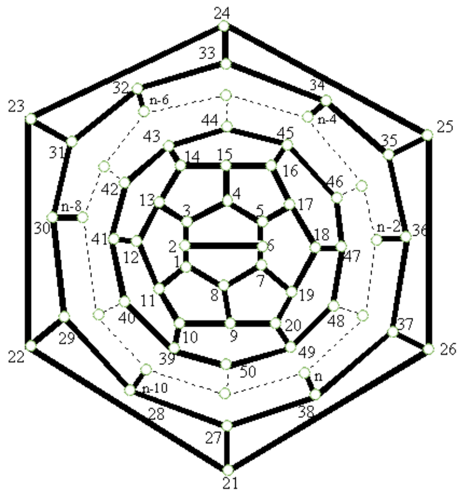

Figure 1. The Fullerene C_{12m+2}

In Table 1, other pairs, which are not considered in the algorithm, for which the corresponding entries of the adjacency matrix are one are given. Since only the upper (lower) ends (main diameter) are specified and the adjacency matrix is symmetric, we replace the above matrix with $A = A + A^t$.

Table 1. Some entries whose values in the adjacency matrix are equal to 1.

(1, 11)	(1, 8)	(2, 6)	(3, 13)	(4, 15)
(5, 17)	(7, 19)	(9, 20)	(10, 39)	(12, 41)
(14, 43)	(16, 45)	(18, 47)	(20, 49)	(21, 27)
(21, 26)	(22, 29)	(23, 31)	(24, 33)	(25, 35)
(26,37)	(27, 38)	(39, 50)	(28, n - 10)	(30, n - 8)
(32, n - 6)	(34, n - 4)	(36, n - 2)	(38, n)	

Otherwise, we consider $(i, j) = 0$ for each i, j. Graphs C_{26} and C_{38} do not follow the above algorithm. The graph C_{38} is drawn in Figure 3.

3. Adjacency Matrices of C_{12m+4}

In this section and the next section, we will describe the adjacency matrix of two graphs C_{12m+4} and C_{12m+6} in a brief manner and refrain from repeated explanations. The fullerene, $C_n = C_{12m+4}$, has exactly $n = 12m + 4$, $m \geqslant 2$, vertices and it is depicted in Figure 4.

Suppose that $B_{n \times n} = [a_{i,j}], 1 \leqslant i, j \leqslant n$, is the adjacency matrix of C_{12m+4}. We first present a labeling of the graph which is important in our calculations. In Figure 5, forty vertices are labeled by the numbers 1, 2, ..., 40. This part of the graph is common in all members of this sequence of the fullerenes. The other part of the graph is similar to Figure 2. For the first part of the graph, all adjacencies are determined in Figure 5 and there is nothing for it. Hence, we can assume that $n \geqslant 52$. Define $t = [\frac{n-50}{12}]$, where

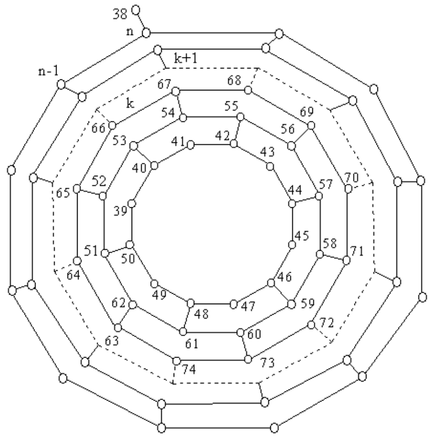

Figure 2. The Second Part of C_n.

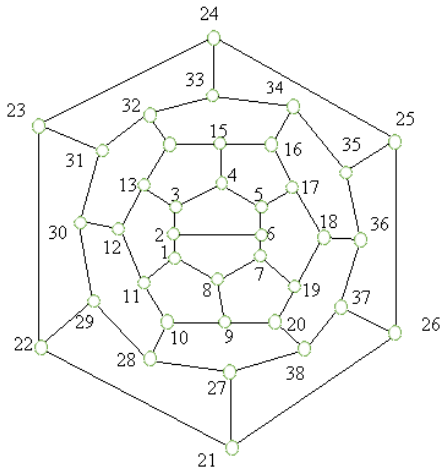

Figure 3. The Graph C_{38}.

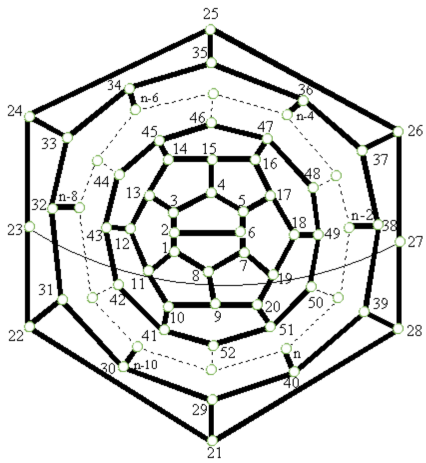

Figure 4. The Fullerene C_{12m+4}

$[x]$ denotes the integer part of x and gives the largest integer less than or equal to x. If $1 \leqslant k \leqslant t$ then all entries corresponding to the following seven sets of ordered pairs are equal to one:

$$
\begin{gathered}
(52,53),\ (64,65),\ \ldots,\ (52+12(k-1),\ 53+12(k-1)),\\
(42,55),\ (54,67),\ \ldots,\ (42+12(k-1),\ 55+12(k-1)),\\
(44,57),\ (56,69),\ \ldots,\ (44+12(k-1),\ 57+12(k-1)),\\
(46,59),\ (58,71),\ \ldots,\ (46+12(k-1),\ 59+12(k-1)),\\
(48,61),\ (60,73),\ \ldots,\ (48+12(k-1),\ 61+12(k-1)),\\
(50,63),\ (62,75),\ \ldots,\ (50+12(k-1),\ 63+12(k-1)),\\
(41,52),\ (53,64),\ \ldots,\ (41+12(k),\ 52+12(k)).
\end{gathered}
$$

Furthermore, $a_{i(i+1)} = 1$, for all integers i such that $1 \leqslant i \leqslant n-1$ and $i \notin \{20, 28, 40\}$. Since the adjacency matrix of a graph is symmetric and all entries on the main diagonal are zero, our process completes our calculations for the adjacency matrix of C_{12m+4}. In Table 2, other pairs for which the corresponding entries of the adjacency matrix are one are given.

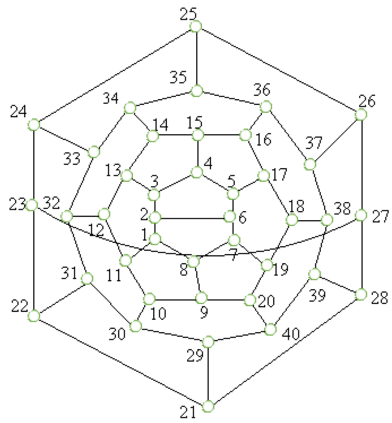

Figure 5. The Graph C_{40}.

Table 2. Some entries whose values in the adjacency matrix are equal to 1.

(1, 11)	(2, 6)	(1, 8)	(3, 13)	(4, 15)
(5, 17)	(7, 19)	(9, 20)	(10, 41)	(12, 43)
(14, 45)	(16, 47)	(18, 49)	(20, 51)	(21, 29)
(21, 28)	(22, 31)	(24, 33)	(25, 35)	(26, 37)
(28, 39)	(23, 27)	(29, 40)	(41, 52)	(30, n - 10)
(32, n - 8)	(34, n - 6)	(36, n - 4)	(38, n - 2)	(40, n)

4. Adjacency Matrices of C_{12m+6}

According to the previous section, we obtain the adjacency matrix of the fullerene graph $C_n = C_{12m+6}$, which has exactly $n = 12m + 6$, $m \geqslant 2$ vertices. It is shown in Figure 6 along with its labeling. First, like the previous two kinds of graphs, we present a labeling of the graph. In Figure 7, the eighty six vertices are labeled by the numbers 1, 2, ..., 86. This part of the graph is common in all members of this sequence of the fullerenes. The other part of the graph is similar to Figure 2. For the first part of the graph, all the adjacencies are determined in Figure 7. Hence, we can assume that $n \geqslant 86$.

Define $t = [\frac{n-86}{20}]$. If $1 \leqslant k \leqslant t$ then all entries corresponding to the following eleven sets of ordered pairs are equal to one:

$$(80,101),\ (100,121),\ \ldots,\ (80 + 20(k-1),\ 101 + 20(k-1)),$$
$$(82,103),\ (102,123),\ \ldots,\ (82 + 20(k-1),\ 103 + 20(k-1)),$$
$$(84,105),\ (104,125),\ \ldots,\ (84 + 20(k-1),\ 105 + 20(k-1)),$$
$$(86,87),\ (106,107),\ \ldots,\ (86 + 20(k-1),\ 87 + 20(k-1)),$$
$$(68,89),\ (88,109),\ \ldots,\ (68 + 20(k-1),\ 89 + 20(k-1)),$$
$$(70,91),\ (90,111),\ \ldots,\ (70 + 20(k-1),\ 91 + 20(k-1)),$$
$$(72,93),\ (92,113),\ \ldots,\ (72 + 20(k-1),\ 93 + 20(k-1)),$$
$$(74,95),\ (94,115),\ \ldots,\ (74 + 20(k-1),\ 95 + 20(k-1)),$$
$$(76,97),\ (96,117),\ \ldots,\ (76 + 20(k-1),\ 96 + 20(k-1)),$$
$$(78,99),\ (98,119),\ \ldots,\ (78 + 20(k-1),\ 99 + 20(k-1)),$$
$$(67,86),\ (87,106),\ \ldots,\ (67 + 20(k),86 + 20(k)).$$

Also, $a_{i(i+1)} = 1$, for all integers i such that $1 \leqslant i \leqslant n-1$ and $i \notin \{44, 66\}$. Since the adjacency matrix of a graph is symmetric and all entries on the main diagonal are zero, our process completes our calculations for the adjacency matrix of C_n. In Table 3, other

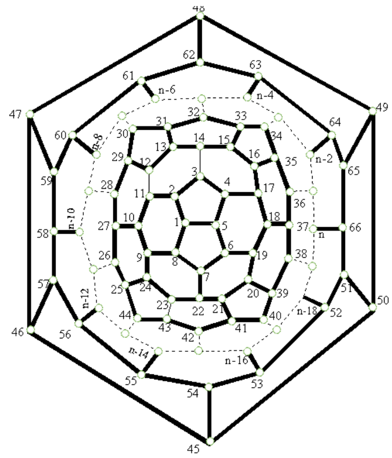

Figure 6. The Fullerene C_{12m+6}

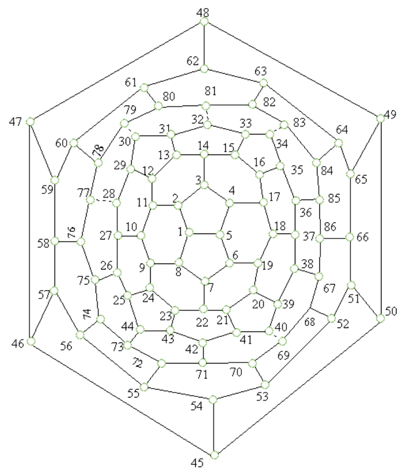

Figure 7. The Graph C_{86}.

pairs for which the corresponding entries of the adjacency matrix are one are given.

Table 3. Some entries whose values in the adjacency matrix are equal to 1.

(1, 8)	(1, 5)	(2, 11)	(3, 14)	(4, 17)
(6, 19)	(7, 22)	(9, 24)	(10, 27)	(12, 29)
(13, 31)	(15, 33)	(16, 35)	(18, 37)	(20, 39)
(21, 41)	(23, 43)	(25, 44)	(54, 45)	(57, 46)
(59, 47)	(62, 48)	(65, 49)	(66, 51)	(40, 69)
(42, 71)	(44, 73)	(26, 75)	(28, 77)	(30, 79)
(32, 81)	(34, 83)	(36, 85)	(38, 67)	(45, 50)
(67, 86)	(52, n - 18)	(53, n - 16)	(55, n - 14)	(56, n - 12)

Finally, all the adjacency matrices of the described graphs can be obtained with the algorithms presented in this article from software such as Mathematica. We refrain from displaying the matrices here due to their large size.

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