Distance matrix and diameter of two infinite family of fullerenes

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Let G be a molecular graph. The distance d(u,v) between two vertices u and v of G is the minimum length of the paths connecting them. The greatest distance between any two vertices of G called the diameter of G. In this paper the diameter of two infinite families of fullerenes are computed.

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1. Introduction

The discovery of buckminsterfullerene which has a nanometer-scale hollow spherical structure in 1985 by Kroto and Smalley revealed a new form of existence of carbon element other than graphite, diamond and amorphous carbon [1,2]. Now a day, fullerenes with a wide range of numbers of carbon atoms have been produced in experiment and so theoretical study of this new materials are more and more important in chemistry.

From a theoretical point of view, fullerenes are molecules in the form of polyhedral closed cages made up entirely of n three coordinate carbon atoms and having 12 pentagonal and (n/2 – 10) hexagonal faces, where n is equal or greater than 20**.** If F is a fullerene graph with exactly v vertices, e edges and f faces then by Euler formula, v – e + f = 2. Suppose F has exactly p pentagons and h hexagons. Then v = (5p+6h)/3, e = (5p+6h)/2 = 3/2v and f = p + h. Therefore, p = 12, v = 2h + 20 and e = 3h + 30. We encourage the reader to consult papers by Fowler and his co-authors, references therein and his book for background material, as well as basic computational methods about fullerene graphs [3−5].

We now describe some notations which will be kept throughout. If x and y are two vertices of a molecular graph G then d(x,y) denotes the length of a minimal path connecting x and y. The Wiener index of graph G [6] is defined as the sum of distances between vertices of G. The Wiener index is a useful number associated to the structure of a molecule. Such numbers which has good applications in chemistry, usually named a topological index. The Diameter of G, diam(G), is defined as diam(G) = Max$\{d(u,v) \mid u,v \in V(G)\}$. In other words, a graph's diameter is the largest number of vertices which must be traversed in order to travel from one vertex to another.

Computing Wiener index of nanostructures began with the work of Diudea and his team [7-10] and then continued by one of the present authors (ARA) [11,12].

The aim of this paper is to study the diameter of two infinite families of fullerenes. A computer program is also prepared for computing this number. Our notation is standard and mainly taken from standard books of graph theory and the books of Trinajestic [13].

2. Results and discussion

The matrix $[d_{ij}]$ is consisting of all distances between vertices of a graph G is known as the distance matrix. In the paper [14−18], we compute some distance based topological indices of fullerenes. In this section, we continue this program and consider the problem of computing diameter of fullerenes into account.

Example 1. Consider fullerene graph C_{20}, Fig. 1. From Table 1, one can see that the diameter of this fullerene is equal to 5.

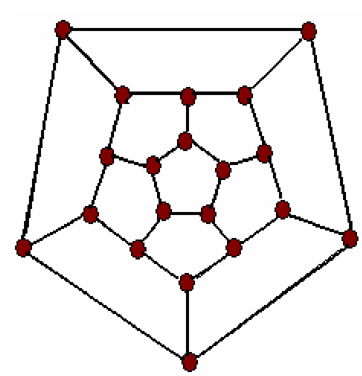

Fig. 1. The Fullerene C_{20}.

Theorem 1. Let G be a connected graph and diam(G) denoted to the diameter of G. Then we have:$W(G) \le 1/2(n-1)\,[2 + (n-2) \times d(G)]$.

Proof. It is easy to see that the distance matrix of G satisfied the following matrix in equation:

$$\begin{bmatrix} 0 & 1 & d(1,3) & \ldots & d(1,n) \\ & 0 & 1 & \ddots & \vdots \\ & & 0 & \cdots & d(i,n) \\ & & & 0 & 1 \\ & & & & 0 \end{bmatrix} \le \begin{bmatrix} 0 & 1 & d(G) & \ldots & d(G) \\ & 0 & 1 & \ddots & \vdots \\ & & 0 & 1 & d(G) \\ & & & 0 & 1 \\ & & & & 0 \end{bmatrix}$$

and this completes the proof.

Table 1. The distance matrix of C_{20}.

d(x,y)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0	1	2	2	1	1	2	3	3	2	2	2	3	4	3	4	5	4	3	3
2	1	0	1	2	2	2	1	2	3	3	3	2	2	3	4	5	4	3	3	4
3	2	1	0	1	2	3	2	1	2	3	4	3	2	2	3	4	3	3	4	5
4	2	2	1	0	1	3	3	2	1	2	3	4	3	2	2	3	3	4	5	4
5	1	2	2	1	0	2	3	3	2	1	2	3	4	3	2	3	4	5	4	3
6	1	2	3	3	2	0	2	4	4	2	1	1	3	5	3	3	4	3	2	2
7	2	1	2	3	3	2	0	2	4	4	3	1	1	3	5	4	3	2	2	3
8	3	2	1	2	3	4	2	0	2	4	5	3	1	1	3	3	2	2	3	4
9	3	3	2	1	2	4	4	2	0	2	3	5	3	1	1	2	2	3	4	3
10	2	3	3	2	1	2	4	4	2	0	1	3	5	3	1	2	3	4	3	2
11	2	3	4	3	2	1	3	5	3	1	0	2	4	4	2	2	3	3	2	1
12	2	2	3	4	3	1	1	3	5	3	2	0	2	4	4	3	3	2	1	2
13	3	2	2	3	4	3	1	1	3	5	4	2	0	2	4	3	2	1	2	3
14	4	3	2	2	3	5	3	1	1	3	4	4	2	0	2	2	1	2	3	3
15	3	4	3	2	2	3	5	3	1	1	2	4	4	2	0	1	2	3	3	2
16	4	5	4	3	3	3	4	3	2	2	2	3	3	2	1	0	1	2	2	1
17	5	4	3	3	4	4	3	2	2	3	3	3	2	1	2	1	0	1	2	2
18	4	3	3	4	5	3	2	2	3	4	3	2	1	2	3	2	1	0	1	2
19	3	3	4	5	4	2	2	3	4	3	2	1	2	3	3	2	2	1	0	1
20	3	4	5	4	3	2	3	4	3	2	1	2	3	3	2	1	2	2	1	0

In what follows, diam(G) denotes the diameter of a graph G.

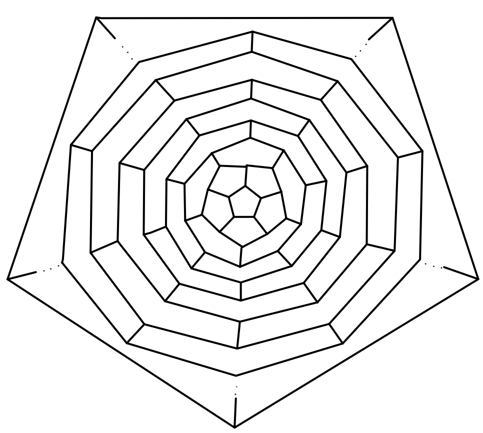

Fig. 2. The molecular graph of the Fullerene C_{10n}.

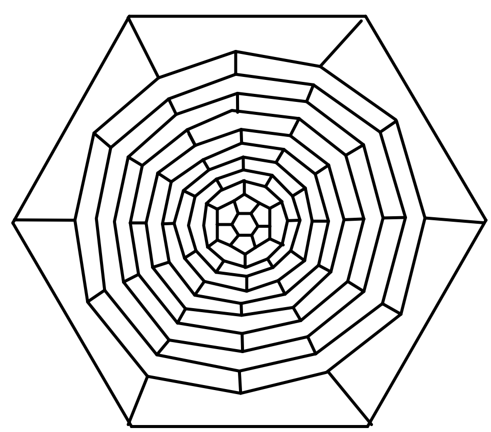

Fig. 3. The molecular graph of the Fullerene C_{12n}.

Corollary. Let G be a connected graph and diam(G) ≥ 3. Then we have:

W(G) ≤ (3n−5) + [(n−3)(n−2) × d(G)] /2.

Proof. It is easy to see that for distance matrix we have:

$$(d_{ij}) \le \begin{bmatrix} 0 & 1 & 2 & \cdots & \cdots & \cdots & d(G) \\ & 0 & 1 & 2 & \ddots & \ddots & \vdots \\ & & 0 & 1 & 2 & \ddots & \vdots \\ & & & 0 & 1 & 2 & d(G) \\ & & & & 0 & 1 & 2 \\ & & & & & 0 & 1 \\ & & & & & & 0 \end{bmatrix}$$

and this completes the proof.

Theorem 2. The diameter of the fullerene graph C_{12n}, $n \ge 6$, is $d(G) = 2n-1$.

Proof. From Fig. 4, one can see that the blue columns are exceeded by one if n is exceeded by one. Also, $\max\{d(x,y) | x,y \in V(G)\}$ is d(u,v) as shown in Fig. 5. So, in each case d(u,v) is change to d(u,v) + 2. In Table 2, the exceptional cases are also investigated, proving the result.

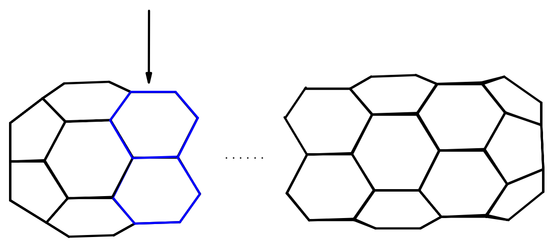

Fig. 4. The Fullerene graph C_{12n}.

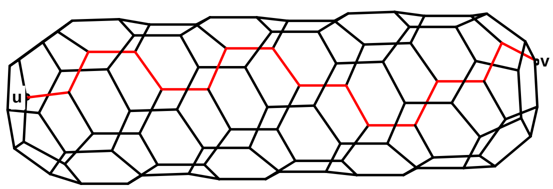

Fig. 5. Diameter of the Fullerene graph C_{12n}.

Table 2. The Exceptional Cases of diam(G) for n = 2, 3, 4, 5.

Fullerene	C_{24}	C_{36}	C_{48}	C_{60}
diam(G)	5	7	8	10

Theorem 3. The diameter of the fullerene graph C_{10n}, $n \ge 5$, is $d(G) = 2n-1$.

Proof. From Fig. 6, one can see that the pink columns are exceeded by one if n is exceeded by one. Also, $\max\{d(x,y) | x,y \in V(G)\}$ is d(u,v) as shown in Fig. 7. So, in each case d(u,v) is change to d(u,v) + 2. We now apply the Table 3 to complete the proof.

Table 3. The Exceptional Cases of diam(G) for n = 2, 3, 4.

Fullerene	C_{20}	C_{30}	C_{40}
diam(G)	5	6	8

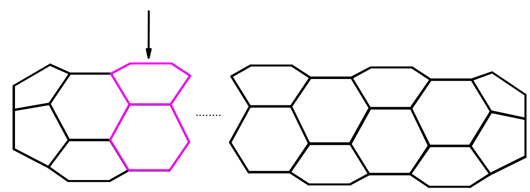

Fig. 6. The Fullerene Graph C_{10n}

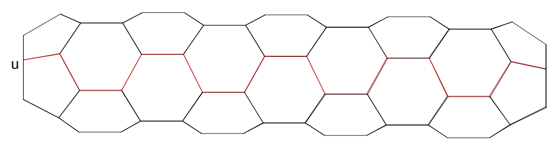

Fig. 7. The diameter of Fullerene graph C_{10n}.

A Gap Program for Computing Diameter of Graph

```
f:= function(A)
        local n, b,bb,bbb,b1,bb1,bbb1,s,x,y,k,B,i,j,t,tt; n:=Length(A);
        b:=[];bb:=[];bbb:=[];b1:=[];bb1:=[];bbb1:=[];s:=0;tt:=[];
 for x in [1..n] do
        for y in [1..n] do
                for k in [1..n] do
B:=A^k;
                        if B[x][y]<>0 then
                                AddSet(b,k);break;
                        fi;
                od;
        if y<=x then Add(bb,0);
```

```
else
                              Add(bb,b[1]);
                              fi;
          b:=[];
          od;
          Add(bbb,bb);bb:=[];
od;
for i in bbb do
           for j in i do
                    s:=s+j;
          od;
od;
t:=bbb+TransposedMat(bbb);
          for i in t do
                    for j in i do
                              Add(tt,j);
                    od;
          od;
Print("******************************************","\n");
          Print("diameter of G= ");
                    Print (Maximum(tt));Print("\n");
Print("******************************************","\n");
          return;
end;
```

References

[1] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, R. E. Smalley, Nature 318, 162 (1985).
[2] H. W. Kroto, J. E. Fichier, D. E. Cox, "The Fullerene", Pergamon Press, Inc., New York, 1993.
[3] W. Mirvold, B. Bultena, S. Daugherty, B. Debroni, S. Girn, M. Minchenko, J. Woodcock, P. W. Fowler, MATCH Commun. Math. Comput. Chem. **58**, 235 (2007).
[4] P. W. Fowler, D. E. Manolopoulos, An Atlas of Fullerenes, Oxford Univ. Press, Oxford, 1995.
[5] P. W. Fowler, D. Horspool, W. Mirvold, Chemistry, An European Journal **13**, 2208 **(**2007).
[6] H. Wiener, J. Am. Chem. Soc. **69**, 17 (1947).
[7] P. E. John, M. V. Diudea, Croat. Chem. Acta **77**, 127 (2004).
[8] M. V. Diudea, P. E. John, MATCH Commun. Math. Comput. Chem. **44**, 103 (2001).
[9] M. V. Diudea, M. Stefu, B. Pârv, P. E. John, Croat. Chem. Acta **77**, 111 (2004).
[10] M. V. Diudea, I. Silaghi-Dumitrescu, B. Parv, MATCH Commun. Math. Comput. Chem. **44**, 117 (2001).
[11] S. Yousefi, H. Yousefi-Azari, M. H. Khalifeh, A. R. Ashrafi, Int. J. Chem. Mod. **1**, 149 (2008).
[12] S. Yousefi, A. R. Ashrafi, Studia Universitatis Babes-Bolyai Chemia **53**, 111 (2008).
[13] N. Trinajstic, Chemical Graph Theory, CRC Press, Boca Raton, FL, 1992.
[14] A. R. Ashrafi, MATCH Commun. Math. Comput. Chem. 53, 161 (2005).
[15] A. R. Ashrafi, M. Jalali, M. Ghorbani, M. V. Diudea, MATCH Commun. Math. Comput. Chem. **60**, 905 (2008).
[16] M. Ghorbani, A. R. Ashrafi, J. Comput. Theor. Nanosci. **3**, 803 (2006).
[17] A. R. Ashrafi, M. Ghorbani, M. Jalali, J. Theor. Comput. Chem. **7,** *2*21 (2008).
[18] A. R. Ashrafi, M. Ghorbani, MATCH Commun. Math. Comput. Chem. **60**, 359 (2008).

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