Digest Journal of Nanomaterials and Biostructures Vol. 4, No.3, September 2009, p. 487-493

COMPUTER CALCULATION OF THE EDGE WIENER INDEX OF AN INFINITE FAMILY OF FULLERENES

M. GHORBANI, M. B. AHMADI, M. HEMMASI*
Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-51167, I. R. Iran
Department of Mathematics, University of Shiraz, Shiraz 71454, I. R. Iran

The edge-Wiener index of G is defined as the sum of the distances between all pairs of edges of G. In this paper, the first and the second edge-Wiener index of an infinite family of fullerenes is computed.

(Received June 2, 2009; accepted July 19, 2009)

Keywords: Fullerene, Edge-Wiener index.

1. Introduction

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by V(G) and E(G), respectively. If x and y are two vertices of G then d(x,y) denotes the length of a minimal path connecting x and y. A topological index for G is a numeric quantity that is invariant under automorphisms of G. The oldest topological index is the Wiener index which introduced by Harold Wiener.[1] This index is defined as the sum of all distances between vertices of G, i.e. $W(G) = \sum_{x,y \in V(G)} d(x,y)$. The most important works on computing topological indices of nanostructures were done by Diudea and his co-authors.[2-7].

Also, the edge-Wiener index of G is defined as the sum of the distances (in the line graph) between all pairs of edges of G, i.e., $W_e(G) = \sum_{\{e,f\} \subseteq E(G)} d(e,f)$, where the distance between two edges is the distance between the corresponding vertices in the line graph of G[8]. The first edge-Wiener index is:

$$W_{e_0}(G) = \sum_{\{e,f\} \subseteq E(G)} d_0(e,f),$$

where $d_0(e,f) = \begin{cases} d_1(e,f)+1 & e \neq f \\ 0 & e = f \end{cases}$ and $d_1(e,f) = \min\{d(x,u), d(x,v), d(y,u), d(y,v)\}$

such that $e = xy$ and $f = uv$. This version satisfy in $W_{e_0}(G) = W(L(G))$. The second edge-

*Corresponding author: hg.paper@gmail.com

Wiener index is:

$$W_{e_4}(G) = \sum_{\{e,f\}\subseteq E(G)} d_4(e,f),$$

where $d_4(e,f) = \begin{cases} d_2(e,f) & e \neq f \\ 0 & e = f \end{cases}$ and $d_2(e,f) = \max\{d(x,u), d(x,v), d(y,u), d(y,v)\}$ such that $e = xy$ and $f = uv$.

Example1. Suppose K_n denotes the complete graph on *n* vertices and C_n be a cycle of length n. Then, we have $W_{e_0}(K_3) = 6$, $W_{e_0}(K_4) = 36$, $W_{e_0}(K_5) = 120$, $W_{e_0}(C_4) = 16$, $W_{e_0}(C_5) = 30$, $W_{e_0}(C_6) = 54$, $W_{e_1}(K_3) = 6$, $W_{e_1}(K_4) = 30$, $W_{e_1}(K_5) = 90$, $W_{e_1}(C_4) = 24$, $W_{e_1}(C_5) = 40$ and $W_{e_1}(C_6) = 78$. By continue this process one can see that $W_{e_0}(C_n) = \begin{cases} \frac{n^3}{4} & 2 \mid n \\ \frac{n^3 - n}{4} & 2 \nmid n \end{cases}$,

$W_{e_1}(C_n) = \begin{cases} \frac{(n+2)^2}{4} - 3 & 2 \mid n \\ \frac{(n+2)^2 - 17}{4} & 2 \nmid n \end{cases}$, $W_{e_0}(K_n) = n(n-1)^2(n-2)/2$ and $W_{e_0}(K_n) = \frac{n^2(n-1)^2}{4} - \frac{n(n-1)}{2}$.

Example2. Suppose S_n denotes the Star graph on n+1 vertices. Then for every $e,f \in E(S_n)$, $d_0(e,f) = d_4(e,f)$ and so $W_{e_0}(S_n) = W_{e_1}(S_n) = (n-1)(n-2)$.

We encourage the reader to consult[9-11] and references therein for background material as well as basic computational techniques. Our notation is standard and mainly taken from standard books of graph theory and the books of Trinajestic[12-17].

2. Main results and discussion

The fullerene era was started in 1985 with the discovery of a stable C_{60} cluster and its interpretation as a cage structure with the familiar shape of a soccer ball, by Kroto and his co-authors.[18] The well-known fullerene, the C_{60} molecule(figure 1), is a closed-cage carbon molecule with three-coordinate carbon atoms tiling the spherical or nearly spherical surface with a truncated icosahedral structure formed by 20 hexagonal and 12 pentagonal rings.[19] 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 = (5p+6h)/3, the number of edges is m = (5p+6h)/2 = 3/2n and the number of faces is f = p + h. By the Euler's formula n − m + f = 2, one can deduce that (5p+6h)/3 – (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 having 12 pentagonal and (n/2 – 10) hexagonal faces, where n ≠ 22 is a natural number equal or greater than 20.[20-23]

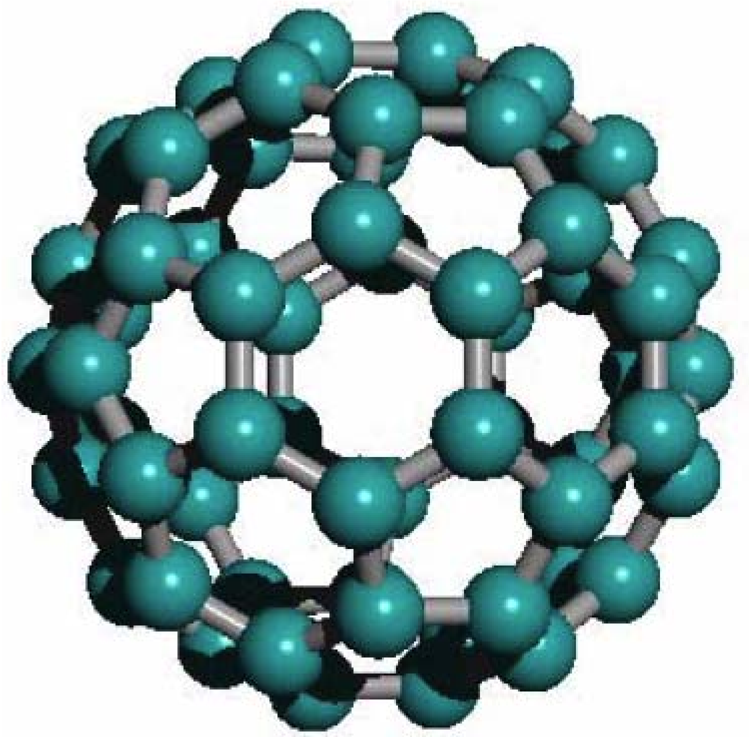

Fig. 1. Fullerene graph C_{60}

The adjacency matrix of a molecular graph G with n vertices is an n × n matrix A = [a_{ij}] defined by: a_{ij} = 1, if vertices i and j are connected by an edge and, a_{ij} = 0, otherwise. The distance matrix D = [d_{ij}] of G is another n × n matrix defined by d_{ij} is the length of a minimum path connecting vertices i and j, i ≠ j, and zero otherwise.

In this section, a computer program is presented which is useful for computing the edge-Wiener index of a connected graph. To do this, we first draw the molecule by HyperChem[24] and then compute the distance matrix of the molecular graph by TopoCluj.[25] Finally, we prepare a GAP[26] program for computing the first and the second edge- Wiener indices of any connected graph G. We apply this program to compute the first and the second edge-Wiener index of the molecular graph of fullerene C_{12n+4}, Figure 2. In Table 1, we calculate the first and the second edge- Wiener indices of C_{12n+4}, for $2 \leq n \leq 14$. Then by curve fitting method, we will find a polynomial of degree ≤ 12, through the values of Table 1. This polynomial will be the edge-Wiener index of fullerene C_{12n+4}.

By the calculation, the first edge-Wiener index of fullerene C_{12n+4} is computed as $W_{e_0}(C_{12n+4}) = a_{12}n^{12} + a_{11}n^{11} + a_{10}n^{10} + \cdots + a_1 n + a_0$, where
a_{12}=-7.73275078830634386189941 7455E-6, a_{11} =7.4249438832772166105499438833 E-4,
a_{10}= -0.03199037330981775426219870664, a_9=0.81670524691358024691358 02469,
a_8=-13.74000385802469135802469135 8025, a_7= 160.2235763888888888888888888889,
a_6=-1325.580640064667842445620223398, a_5= 7823.881327160493827160493 82710,
a_4=-32613.33490005878894767783656 6725, a_3=93511.0584567901234567901234 5679,
a_2=-172645.8124579124579124579124 5791, a_1=187523.5191919191919191919191 919 and
a_0=-88892. The second edge-Wiener index of fullerene C_{12n+4} is computed as
$W_{e_4}(C_{12n+4}) = a_{12}n^{12} + a_{11}n^{11} + a_{10}n^{10} + \cdots + a_1 n + a_0$, where
a_{12}=-2.1486358291913847469403024959E-5, a_{11}=0.0021194584736251402918069584 73625,
a_{10}=-0.09395052542621987066431510 87595, a_9=2.4710289902998236331569664903,
a_8=-42.876345623897707231040564 37389, a_7=516.0807060185185185185185185 1852,
a_6=-4408.673514568636096413874191652, a_5=26863.39465663580246913580246 9136,
a_4=-115532.7360475455614344503233 3921, a_3=341024.9050242504409171075837743,
a_2=-651211.620120250120250120250 12025, a_1=724107.14646464646464646464646 46 and
a_0=-351288.

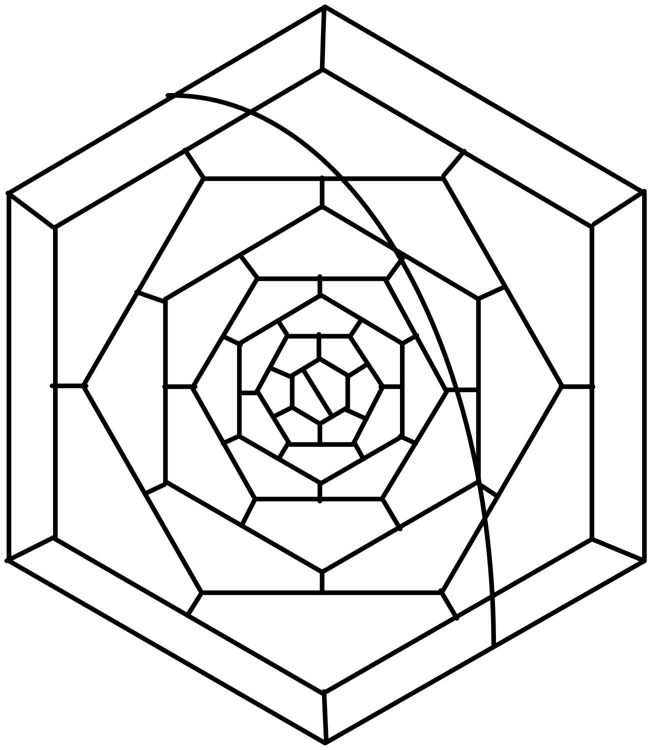

Fig. 2. The molecular graph of fullerene C_{12n+4}.

Table1. Values of the first and the second edge-Wiener of C_{12n+4} ($2 \leq n \leq 14$).

n	$W_{e_0}(C_{12n+2})$	n	$W_{e_0}(C_{12n+2})$	n	$W_{e_4}(C_{12n+2})$	n	$W_{e_4}(C_{12n+2})$
2	4752	9	195849	2	5484	9	217574
3	12414	10	260544	3	14342	10	287840
4	24812	11	338418	4	28460	11	371930
5	42926	12	430764	5	48914	12	471140
6	67848	13	538878	6	76760	13	586766
7	100794	14	664056	7	113330	14	720104
8	143028			8	159836		

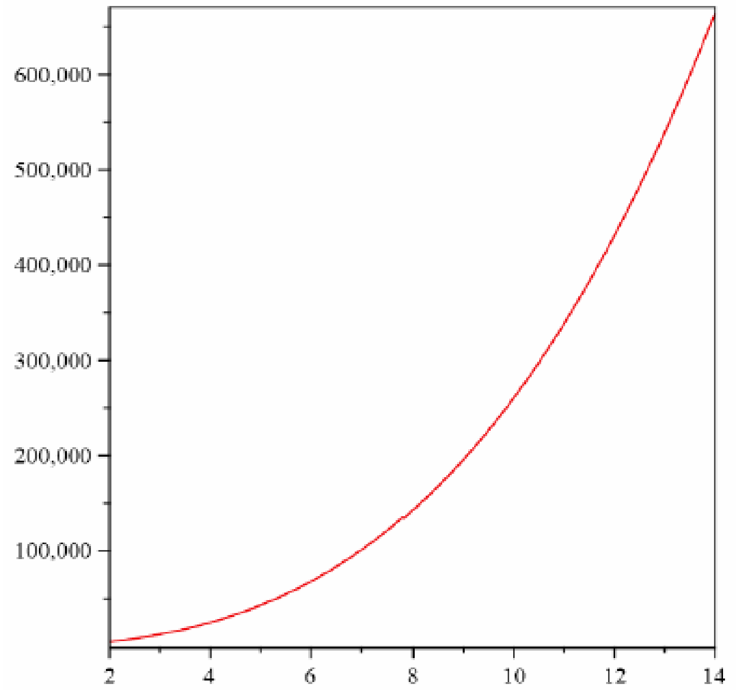

Fig. 3. The curve of W_{e_0} *for* $2 \leq n \leq 14$

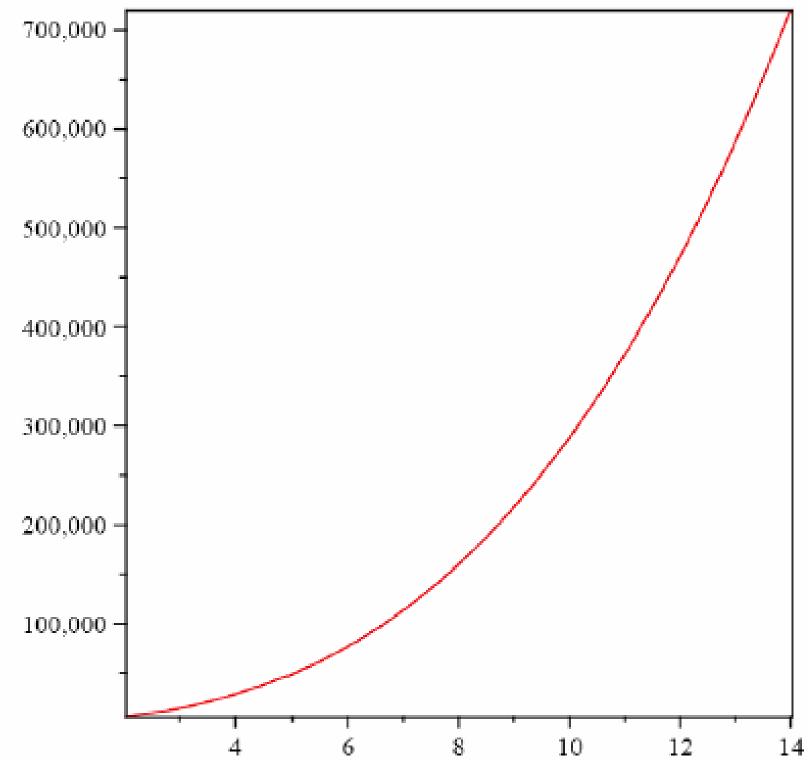

Fig. 4. The curve of W_{e_4} *for* $2 \leq n \leq 14$.

A GAP Program For Computing The Edge Wiener Index Of Graphs

```
f:= function(M)
local l, s, ss, e, i, j, a, b;
l:=Length(M);s:=0;ss:=0;e:=[];
for i in [1..l]do
for j in[i+1..l] do
if M[i][j]=1 then
Add(e,[i,j]);
fi;
od;
od;
for a in e do
for b in e do
if a<> b then
s:=s+Minimum(M[a[1]][b[1]],M[a[1]][b[2]],M[a[2]][b[1]],M[a[2]][b[2]])+1;
ss:=ss+Maximum(M[a[1]][b[1]],M[a[1]][b[2]],M[a[2]][b[1]],M[a[2]][b[2]]);
fi;
od;
od;
Print("************************************","\n");Print("\n");
Print("The first edge - Wiener number is: ", s);Print("\n");Print("\n");
Print("The second edge - Wiener number is: ", ss);Print("\n");
Print("************************************","\n");
return;
end;
```

References

[1] H. Wiener, J. Am. Chem. Soc. **69**, 17 (1947).
[2] M. V. Diudea, M. Stefu, B. Pârv, P. E. John, Croat Chem Acta **77**, 111 (2004).
[3] M. V. Diudea, B. Parv, E. C. Kirby, MATCH Commun. Math. Comput. Chem. **47**, 53 (2003).
[4] M. V. Diudea, Bull Chem Soc Japan **75**, 487 (2002).
[5] M. V. Diudea, MATCH Commun. Math. Comput. Chem. **45**, 109 (2002).
[6] M. V. Diudea, P. E. John, MATCH Commun. Math. Comput. Chem. **44**, 103 (2001).
[7] M. V. Diudea, E. C. Kirby, Fullerene Sci Technol **9**, 445 (2001).
[8] A. Iranmanesh, I. Gutman, O. Khormali, A. Mahmiani, MATCH Commun. Math. Comput. Chem. 61 (3), 663 (2009).
[9] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Zigert, Acta Appl. Math. **72**, 247 (2002).
[10] M. Ghorbani and A. R. Ashrafi, J. Comput. Theor. Nanosci. **3**, 803 (2006).
[11] A. R. Ashrafi, M. Ghorbani, MATCH Commun. Math. Comput. Chem, **60**, 359 (2008)
[12] N. Trinajstic, Chemical Graph Theory, CRC Press, Boca Raton, FL (1992).
[13] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Zigert, Acta Appl. Math. **72**, 247 (2002).
[14] A.R. Ashrafi, M. Ghorbani, M. Jalali, Digest Journal of Nanomaterials and Biostructures , **3**(4), 245 (2008).
[15] M. Ghorbani, M. Jalali, Digest Journal of Nanomaterials and Biostructures, **3(**4), 269 (2008).
[16] A. R. Ashrafi, M. Ghorbani, Digest Journal of Nanomaterials and Biostructures, **4**(2), 389 (2009).
[17] M. A. Alipour, A. R. Ashrafi, Digest Journal of Nanomaterials and Biostructures, **4**(1), 1 (2009).
[18] H.W. Kroto, J. R. Heath, S.C. O'Brien, R.F. Curl, R.E. Smalley, Nature **318** (1985) 162
[19] H.W. Kroto, J.E. Fichier, D.E. Cox, The Fullerene, Pergamon Press, New York, 1993
[20] W. Mirvold, B. Bultena, S. Daugherty, B. Debroni, S. Girn, M. Minchenko, J. Woodcock and

P. W. Fowler, MATCH Commun. Math. Comput. Chem. **58** (2007) 235
[21] P. W. Fowler, D. Horspool, W. Mirvold, Chem. Eur. J. **13** (2007) 2208
[22] P. W. Fowler, D. E. Manolopoulos, An Atlas of Fullerenes, Oxford Univ. Press, 1995.
[23] G. Brinkman, P. W. Fowler, MATCH Commun. Math. Comput. Chem. **58** (2007) 423
[24] HyperChem package Release 7.5 for Windows, Hypercube Inc., 1115 NW 4th Street, Gainesville, Florida 32601, USA 2002.
[25] M. V. Diudea, O. Ursu, Cs. L. Nagy, TOPOCLUJ, Babes-Bolyai University, Cluj 2002.
[26] M. Schönert, H.U. Besche, Th. Breuer, F. Celler, B. Eick, V. Felsch, A. Hulpke, J. Mnich, W. Nickel, G. Pfeiffer, U. Polis, H. Theißen and A. Niemeyer, GAP, Groups, Algorithms and Programming, Lehrstuhl De für Mathematik, RWTH, Aachen, 1995.