MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **65** (2011) 183-192

ISSN 0340 - 6253

Computing the Vertex PI and Szeged Polynomials of Fullerene Graphs C_{12n+4}

Modjtaba Ghorbani

Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran, 16785 – 136, I R. Iran
E-mail: mghorbani@srttu.edu

(Received June 1, 2009)

Abstract

The topological index PI_v is defined as $PI_v(G)= \sum_{e=uv\in E(G)}n_u(e|G)+ n_v(e|G)$ where $n_u(e|G)$ is the number of vertices of G lying closer to u and $n_v(e|G)$ is the number of vertices of G lying closer to v. In this paper, some GAP programs are prepared to compute the vertex PI and Szeged polynomials of an infinite family of fullerenes named C_{12n+4}.

1. Introduction

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.[1] The well-known fullerene, the C_{60} molecule, 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.[2] 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 $n \neq 22$ is a natural number equal or greater than 20.[3-6]

Mathematical calculations are necessary to explore important concepts in chemistry. Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is an important tool for studying molecular structures. This theory had an important effect on the development of the chemical sciences.

We first describe some notations that will be kept throughout. Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which being represented by V(G) and E(G), respectively. A topological index of a graph G is a numeric quantity related to G. The oldest topological index is the Wiener index which introduced by Harold Wiener.[7]

Khadikar[8,9] defined a new topological index and named it Padmakar-Ivan (PI) index. This newly proposed topological index does not coincide with the Wiener index for acyclic molecules. It is defined as $PI(G) = \sum_{e=uv\in E(G)}[m_u(e|G)+ m_v(e|G)]$, where $m_u(e|G)$ is the number of edges of G lying closer to u than to v and $m_v(e|G)$ is the number of edges of G lying closer to v than to u. Edges equidistant from both ends of the edge uv are not counted. Ashrafi,[10] introduced a vertex version of PI index, named the vertex PI index and abbreviated by PI_v. This new index is defined as $PI_v(G) = \sum_{e=uv\in E(G)}[n_u(e|G)+ n_v(e|G)]$, and the Vertex PI polynomial is defined as $PI_v(G,x)= \sum_{e=uv\in E(G)}x^{nu(e|G)+\ nv(e|G)}$ where $n_u(e|G)$ is the number of vertices of G lying closer to u and $n_v(e|G)$ is the number of vertices of G lying closer to v.

The Szeged index is another topological index, introduced by Ivan Gutman.[11-14] To define the Szeged index of a graph G, we consider the values $n_u(e|G)$ and $n_v(e|G)$ defined in last paragraph. Then the Szeged index of the graph G is defined as $Sz(G) = \sum_{e=uv\in E(G)}n_u(e|G)n_v(e|G)$ and the Szeged polynomial is defined as $Sz(G) = \sum_{e=uv\in E(G)} x^{nu(e|G)nv(e|G)}$. Notice that vertices equidistant from u and v are not taken into account.

Ashrafi et al.[15-18] have calculated the Vertex PI and Szeged polynomials of some Fullerenes. The aim of this paper is to compute the vertex PI and Szeged polynomials of an infinite family of fullerenes. Throughout this paper, our notation is standard.[19]

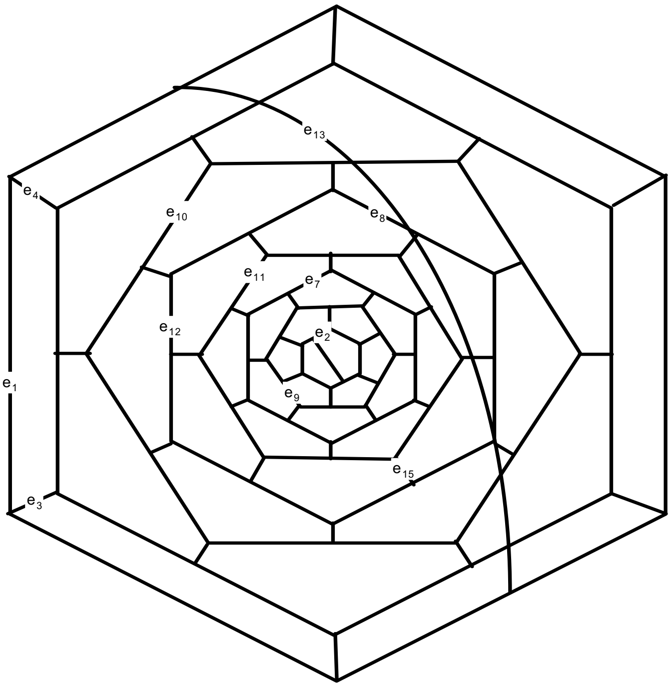

Figure1. The Fullerene Graph C_{12n+4}.

2. Computational Details

It is a well-known fact that for an acyclic graph T, Sz(T) = W(T). On the other hand, an acyclic graph T does not have cycles and thus $m_u(e|G) + m_v(e|G) = |V(T)|$. Thus $PI_v(T) = |V(T)|\cdot|E(T)|$. Since a fullerene graph F has 12 pentagonal faces, $PI_v(F) < |V(F)|\cdot|E(F)|$. The aim of this section is computing vertex PI and Szeged polynomial (and then the vertex PI and Szeged indices) of the fullerene graph C_{12n+4}, Figure 1. We now assume that G is a graph, E = E(G) and V = V(G). Define $N(e) = |V| - (n_u(e|G)+n_v(e|G))$. Then $PI_v(G) = \sum_{e=uv}[|V| - N(e)] = |V||E| - \sum_{e=uv} N(e)$.

If G is bipartite then N(e) = 0 and so $PI_v(G) = |V||E|$. This shows that the vertex PI index is the same for bipartite graphs with n vertices and m edges. On the other hand, the vertex PI index of graphs with exactly n vertices has maximum value, for bipartite graphs. We encourage the reader to consult ref. [20], for mathematical properties as well as computational techniques of Szeged polynomial of graphs.

3. Result and discussion

In this section, by using a GAP program[21] we compute the vertex PI and Szeged indices of graphs. Here, GAP stands for Groups, Algorithms and Programming. The name was chosen to reflect the aim of the system, which is a group of theoretical software for solving computational problems in computational group theory. Because of including GRAPE for working with graphs, GAP is useful also for working with graphs. This software was constructed by GAP's team in Aachen.[23] Our program is accessible from the author upon request.

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, $i \neq j$, and zero otherwise.

To compute the vertex PI and Szeged indices of molecular graphs, we first draw it by HyperChem.[22] Then we apply TopoCluj software of Diudea and his team[23] to compute distance matrices of the molecular graph under consideration. We now upload D in our GAP program to compute the vertex PI and Szeged indices of a molecular graph. Using this program we obtain ten exceptional cases that n = 28, 40, 52, 64, 76, 88, 100, 112, 124 and 136. Our method can be applied to compute the vertex PI and Szeged indices of nanotubes and tori studied by Diudea and his co-authors.[24-29] In the mentioned paper Diudea and his team computed Wiener index of these nanostructures.

If n ≥ 11 then we have the following general formula for computing the vertex PI and Szeged polynomials of fullerene C_{12n+4}, Figure 1.

Theorem. The vertex PI and Szeged indices of C_{12n+4} fullerenes are computed as follows:

$$PI_v(C_{12n+4},x) = (18n-128)x^{12n+4} + 32x^{12n+3} + 48x^{12n+2} + 16x^{12n+1} + 8x^{12n} + 8x^{12n-4} + 8x^{12n-8} + 4x^{12n-20} + 8x^{37} + 2x^{34}.$$

and

$$Sz(C_{12n+4},x) = \begin{cases} 8x^{342} + 2x^{289} + 8x^{396n-990} + 8x^{408n-1088} + \\ 12x^{384n-896} + 8x^{504n-1596} + 16x^{504n-1680} + 12x^{528n-1760} + \\ 8x^{192n-320} + 4x^{108n-261} + 8x^{168n-308} + 8x^{300n-625} + \\ 8x^{324n-702} + 8x^{312n-624} + 12x^{816n-4352} + 12x^{36n^2+24n+4} + \\ 12x^{672n-2912} + 8x^{396n-1056} + 24x^{744n-3658} + 12x^{240n-320} + \\ 8x^{624n-2496} + 24x^{888n-5180} + 16x^{612n-2499} \\ +6(3+(-1)^i)\sum_{i=1}^{n-13} x^{(74+6i)(12n-70-6i)} & n \text{ is even} \\ 8x^{342} + 2x^{289} + 8x^{396n-990} + 8x^{408n-1088} + \\ 12x^{384n-896} + 8x^{504n-1596} + 16x^{504n-1680} + 12x^{528n-1760} + \\ 8x^{192n-320} + 4x^{108n-261} + 8x^{168n-308} + 8x^{300n-625} + \\ 8x^{324n-702} + 8x^{312n-624} + 12x^{816n-4352} + 6x^{36n^2+24n+4} + \\ 12x^{672n-2912} + 8x^{396n-1056} + 24x^{744n-3658} + 12x^{240n-320} \\ +8x^{624n-2496} + 24x^{888n-5180} + 16x^{612n-2499} \\ +6(3+(-1)^i)\sum_{i=1}^{n-13} x^{(74+6i)(12n-70-6i)} & n \text{ is odd} \end{cases}$$

Proof. From Figure 1, one can see that there are fifteen types of edges of fullerene graph C_{12n}. We name them $e_1, e_2, \ldots, e_{15}$ as see shown in Figure 1.

Table 1. Computing $n_u(e)$ and $n_v(e)$ for Different Edges.

Edges	n_u, n_v, Co	*Number*
e_1	18, 19, 12n-33	8
e_2	16, 12n-20 , 8	8
e_3	9, 12n-29, 24	4
e_4	14, 12n-22, 12	8
e_5	25, 12n-25, 4	8
e_6	27, 12n-26, 3	8
e_7	26, 12n-24, 2	8
	34, 12n-32, 2	8
	42, 12n-40, 2	16
	56, 12n-52, 0	12
	62, 12n-59, 1	24
	68, 12n-64, 0	12
	74, 12n-70, 0	24
	80, 12n-76, 0	12
	86, 12n-82, 0	24
	92, 12n-88, 0	12
e_8	33, 12n-30, 1	8
e_9	33, 12n-32, 3	8
e_{10}	42, 12n-38, 0	8
e_{11}	52, 12n-48, 0	8
e_{12}	51, 12n-49, 2	16
e_{13}	17, 17, 12n-34	2
e_{14}	32, 12n-28, 0	12
e_{15}	33, 12n-30, 1	8
e_{16}	44, 12n-40, 0	12

By using these calculations and Table 2 for exceptional cases, the proof is completed.

Table 2. Some Exceptional Cases of Fullerenes.

Edges	C_{28}			C_{40}			C_{52}			C_{64}			C_{76}		
e_1	8	12	8	13	15	12	16	17	19	18	19	27	18	19	39
e_2	12	10	6	20	13	7	29	15	8	40	16	8	52	16	8
e_3	9	9	10	9	13	18	9	22	21	9	32	23	9	43	24
e_4	13	11	4	20	13	7	29	14	9	39	14	11	50	14	12
e_5	9	12	7	15	18	7	19	27	6	23	37	4	24	47	5
e_6	10	13	5	17	19	4	26	21	5	35	24	5	46	26	4
e_7	12	12	4	16	20	4	20	28	4	23	37	4	25	48	3
e_8	-	-	-	20	20	0	20	32	0	20	44	0	20	56	0
e_9	-	-	-	17	19	4	23	26	3	27	34	3	30	43	3
e_{10}	-	-	-	16	20	4	24	24	4	32	28	4	41	31	4
e_{11}	-	-	-	-	--	-	23	23	6	29	32	3	31	42	3
e_{12}	-	-	-	-	-	-	32	20	0	32	32	0	32	44	0
e_{13}	-	-	-	-	-	-	26	23	3	32	29	3	36	38	2
e_{14}	-	-	-	-	-	-	28	20	4	34	27	3	36	36	4
e_{15}	-	-	-	-	-	-	-	-	-	44	20	0	38	38	0
e_{16}	-	-	-	-	-	-	-	-	-	37	23	4	42	31	3
e_{17}	-	-	-	-	-	-	-	-	-	23	37	4	31	44	1
e_{18}	10	10	8	18	15	7	27	21	4	37	23	4	47	24	5
e_{19}	-	-	-	-	-	-	-	-	-	-	-	-	43	30	3
e_{20}	-	-	-	-	-	-	-	-	-	-	-	-	56	20	0
e_{21}	-	-	-	-	-	-	-	-	-	-	-	-	47	24	5
e_{22}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
e_{23}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
e_{24}	--	-	-	-	-	-	-	-	-	-	-	-	-	-	-
e_{25}	-	-	-	-	-	-	-	-	-	--	-	-	-	-	-
e_{26}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
e_{27}	12	12	4	16	16	8	17	17	18	17	17	30	17	17	42

Table 2. (Continue)

Edges	C_{88}			C_{100}			C_{112}			C_{124}			C_{136}		
e_1	18	19	51	18	19	63	18	19	75	18	19	87	18	19	99
e_2	64	16	8	76	16	8	88	16	8	100	16	8	112	16	8
e_3	9	55	24	9	67	24	9	79	24	9	91	24	9	103	24
e_4	62	14	12	74	14	12	86	14	12	98	14	12	110	14	12
e_5	25	59	4	25	71	4	25	83	4	25	95	4	25	107	4
e_6	58	27	3	70	27	3	82	27	3	94	27	3	106	27	3
e_7	26	60	2	26	72	2	26	84	2	26	96	2	26	108	2
e_8	20	68	0	20	80	0	20	92	0	20	204	0	20	116	0
e_9	32	54	2	33	66	1	33	78	1	33	90	1	33	102	1
e_{10}	52	33	3	64	34	2	76	34	2	88	34	2	100	34	2
e_{11}	32	52	4	33	64	3	33	76	3	33	88	3	33	100	3
e_{12}	32	56	0	32	68	0	32	80	0	32	92	0	32	104	0
e_{13}	40	48	0	48	58	1	42	70	0	42	82	0	42	94	0
e_{14}	39	45	4	41	56	3	42	68	2	42	80	2	42	92	2
e_{15}	44	44	0	44	56	0	44	68	0	44	80	0	44	92	0
e_{16}	48	40	0	50	50	0	51	60	1	52	72	0	52	84	0
e_{17}	40	48	0	49	49	2	60	51	1	72	52	0	84	52	0
e_{18}	59	25	4	71	25	4	83	25	4	95	25	4	107	25	4
e_{19}	45	39	4	48	48	4	50	59	3	51	71	2	51	83	2
e_{20}	56	32	0	56	44	0	56	56	0	56	68	0	56	80	0
e_{21}	54	32	2	58	41	3	59	50	3	61	61	2	62	73	1
e_{22}	68	20	0	68	32	0	68	44	0	68	56	0	68	68	0
e_{23}	59	25	4	64	33	3	70	42	0	72	52	0	73	62	1
e_{24}	-	-	-	80	20	0	80	32	0	80	44	0	80	56	0
e_{25}	-	-	-	70	27	3	76	33	3	80	42	2	84	52	0
e_{26}	-	-	-	-	-	-	92	20	0	92	32	0	92	44	0
e_{27}	17	17	54	17	17	66	17	17	78	17	17	90	17	17	102

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 Fullerenes*, Pergamon Press, 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. Horspool, W. Mirvold, *Chem. Eur. J.* **13**, 2208 (2007).
5. P. W. Fowler, D. E. Manolopoulos, *An Atlas of Fullerenes*, Oxford Univ. Press, Oxford, 1995.
6. G. Brinkman, P. W. Fowler, *MATCH Commun. Math. Comput. Chem.*, **58**, 423 (2007)
7. H. Wiener, *J. Am. Chem. Soc.*, **69**, 17 (1947).
8. P. V. Khadikar, *Nat. Acad. Sci. Lett.*, **23**, 113 (2000).
9. P. E. John, P. V. Khadikar, J. Singh, *J. Math. Chem.*, **42**, 37 (2007).
10. M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, *Discr. Appl. Math.*, **157**, 804 (2009).
11. M. V. Diudea, I. Gutman, *Croat. Chem. Acta*, **71,** 21 (1998).
12. I. Gutman, *Graph Theory Notes of New York*, **27,** 9 (1994).
13. O. M. Minailiuc, G. Katona, M. V. Diudea, M. Strunje, A. Graovac, I. Gutman, *Croat. Chem. Acta*, **71**, 473 (1998).
14. I. Gutman, P. V. Khadikar, P. V. Rajput, S. Karmarkar, *J. Serb. Chem. Soc.*, **60**, 759 (1995).
15. A. R. Ashrafi, M. Ghorbani, *MATCH Commun. Math. Comput. Chem.*, **60**, 359 (2008).
16. M. Ghorbani, A. R. Ashrafi, *J. Comput. Theor. Nanosci.*, **3**, 803 (2006).
17. A.R. Ashrafi, M. Ghorbani, M. Jalali, *Digest J. Nanomat. Biostruct.,* **3**, 245 (2008).
18. M. Ghorbani, M. Jalali, *Digest J. Nanomat. Biostruct.*, **3**, 269 (2008).

19. A. R. Ashrafi, M. Jalali, M. Ghorbani, M. V. Diudea, *MATCH Commun. Math. Comput. Chem*., **60**, 905 (2008).
20. N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton**,** 1992.
21. H. Hosoya, *Discr. Appl. Math.*, **19**, 239 (1988).
22. 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, A. Niemeyer, *GAP, Groups, Algorithms and Programming*, Lehrstuhl D für Mathematik, RWTH, Aachen, 1995.
23. HyperChem package Release 7.5 for Windows, Hypercube Inc., 1115 NW 4th Street, Gainesville, Florida 32601, U. S. A. (2002).
24. M. V. Diudea, O. Ursu, C. L. Nagy, *TOPOCLUJ*, Babes-Bolyai University, Cluj **2002.**
25. M. V. Diudea, M. Stefu, B. Pârv, P. E. John, *Croat. Chem. Acta*, **77**, 111 (2004).
26. M. V. Diudea, B. Parv. E. C. Kirby, *MATCH Commun. Math. Comput. Chem.,* **47**, 53 (2003).
27. M. V. Diudea, *Bull. Chem. Soc. Japan*, **75**, 487 (2002).
28. M. V. Diudea, *MATCH Commun. Math. Comput. Chem.*, **45**, 109 (2002).
29. M. V. Diudea, P. E. John, *MATCH Commun. Math. Comput. Chem.*, **44**, 103 (2002).
30. M. V. Diudea, E. C. Kirby, *Fullerene Sci. Technol*., **9**, 445 (2002).