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Study of IPR Fullerenes by PI Index

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The PI index is a Wiener-Szeged-like topological index developed recently. The PI index of a graph G is the sum over all edges uv of G of number of edges which are not equidistant to u and v. In some earlier papers it is proved that this topological index correlates some chemico-physical properties of molecules. In this paper, we generalized our earlier results for computing PI index of fullerenes. We conjecture that the PI index of fullerenes is a polynomial of degree 2 in terms of the number of carbon atoms.

Keywords: PI Index, Fullerene.

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.[1,2] 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.[3] Using the Euler's formula, one can see that every fullerene molecule with n carbon atoms have exactly 12 pentagons and $(n/2-10)$ hexagons, where $n \neq 22$ is a natural number equal or greater than 20.

We first describe some notations which will be kept throughout. This index is defined as the sum of the minimum distances between all pairs of vertices. Khadikar[4] defined a new topological index and named it Padmakar-Ivan (PI) index. It is defined as $PI(G) = \sum_{e=uv\in E(G)}[m_u(e)+m_v(e)]$, where $m_u(e)$ is the number of edges of G lying closer to u than to v and $m_v(e)$ 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.

Suppose G is a graph, $e = xy$, $f = uv \in E(G)$ and $w \in V(G)$. Define $d(w,e) = \text{Min}\{d(w,x), d(w,y)\}$. We say that e is parallel to f if $d(u,e) = d(v,e)$. The set of all edges parallel to e is denoted by $P(e)$ and $N(e) = |P(e)|$. If e is parallel to f then we write $e \parallel f$. It is easy to see that the relation of parallelism is reflexive but not symmetric or transitive. To compute the PI index of the graph G, we define $N(e) = |P(e)| = |E(G)| - (m_u(e)+m_v(e))$. This implies that $PI(G) = |E(G)|^2 - \sum_{e\in E(G)} N(e)$. We use this simple equation freely throughout the paper.

In recent years, some authors[5–17] considered the problem of computing topological indices of fullerenes and nanotubes. In this article, we continue this program to calculate the PI index of an infinite family of IPR fullerenes, Figure 1.

2. RESULTS AND DISCUSSION

The first author of this paper,[15] introduced two infinite families of fullerenes and computed the number of their carbon atoms. Suppose $G[m,n]$ denotes the first series of fullerenes in the mentioned paper above. It is shown that the fullerene molecule $G[m,n]$ has exactly $10m(m+n)$ carbon atom. In an earlier paper,[17] the authors proved that $PI(G[m,1]) = 225m^2+95m+620$. It is easy to see that the fullerenes $G[m,1]$ are not IPR. On the other hand, for $n \geq 2$ the fullerenes $G[m,n]$ are IPR. The aim of this section is computing the PI index of these IPR fullerenes.

We apply a C program to compute the adjacency and distance matrices of the fullerene $G[m,n] = C_{10n(n+m)}$, $n \geq 2$. In Table I, we calculate the PI index of $G[m,n]$, for $1 \leq m \leq 37$ and $1 \leq n \leq 7$. Then by curve fitting method, we will find a polynomial of degree ≤ 6, through the values of Table I. This polynomial will be the PI index of IPR fullerenes under consideration. Our method is general and can be applied to compute other topological indices of fullerenes.

Curve fitting is finding a curve which has the best fit to a series of data points and possibly other constraints. We are interested in curve fitting by polynomial functions. We

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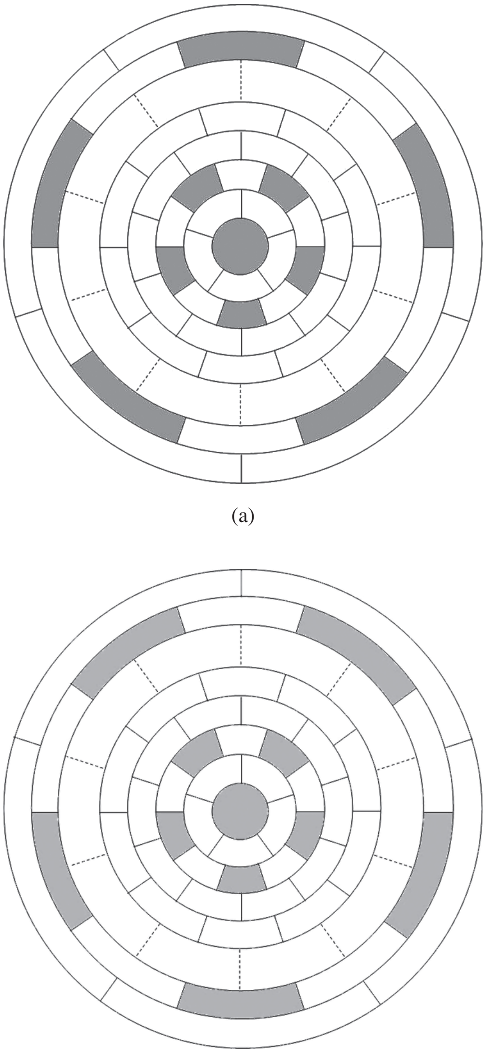

(a)

(b)

Fig. 1. Two configurations of IPR fullerenes: (a) C_{40n+40} fullerenes. (b) C_{40n+20} fullerenes.

search for the best polynomial to fit data of Table I. By these calculations, the PI indices of these fullerenes are computed as follows:

$$PI(G[m,1]) = PI(C_{10m+10}) = 225m^2+95m+620 \quad m\geq 4$$

$$PI(G[m,2]) = PI(C_{20m+40}) = 900m^2+2140m+5730 \quad m\geq 9$$

$$PI(G[m,3]) = PI(C_{30m+90}) = 2025m^2+8835m+23950 \quad m\geq 14$$

$$PI(G[m,4]) = PI(C_{40m+160}) = 3600m^2+22880m+69680 \quad m\geq 19$$

$$PI(G[m,5]) = PI(C_{50m+250}) = 5625m^2+46975m+162180 \quad m\geq 24$$

Table I. The PI Index of $G[m,n]$, $n\geq 2$.

	n						
m	1	2	3	4	5	6	7
1	660	6640	27580	79310	181850	362090	650850
2	1560	12120	44100	115330	249680	475450	827540
3	2850	19090	64560	159070	328930	605830	1026320
4	4600	27780	88130	210060	419780	752560	1247910
5	6720	38380	115820	266150	522060	915750	1492130
6	9290	50630	147440	329720	631900	1095300	1758520
7	12310	64640	182980	400050	753530	1286010	2047260
8	15780	80410	222980	477570	885960	1493440	2350460
9	19700	97890	266760	562740	1029480	1716150	2676890
10	24070	117130	314240	654830	1184390	1955260	3024110
11	28890	138170	365860	754650	1350560	2210600	3393450
12	34160	161010	421450	861290	1528730	2481950	3784720
13	39880	185650	480990	974300	1717720	2770130	4198200
14	46050	212090	544540	1094720	1918630	3074370	4634040
15	52670	240330	612100	1222310	2130290	3395830	5091720
16	59740	270370	683710	1357060	2351710	3732900	5572500
17	67260	302210	759370	1498920	2584650	4086990	6074990
18	75230	335850	839080	1647880	2828830	4456600	6600850
19	83650	371290	922840	1804000	3084330	4840060	7147950
20	92520	408530	1010650	1967280	3351100	5240020	7718060
21	101840	447570	1102510	2137760	3628980	5656230	8309330
22	111610	488410	1198420	2315440	3918010	6088770	8919310
23	121830	531050	1298380	2500320	4218190	6537760	9551620
24	132500	575490	1402390	2692400	4529580	7002850	10206120
25	143620	621730	1510450	2891680	4852180	7483990	10882760
26	155190	669770	1622560	3098160	5186030	7981190	11581980
27	167210	719610	1738720	3311840	5531130	8494490	12303200
28	179680	771250	1858930	3532720	5887480	9023890	13046470
29	192600	824690	1983190	3760800	6255080	9569450	13811590
30	205970	879930	2111500	3996080	6633930	10131170	14598600
31	219790	936970	2243860	4238560	7024030	10709090	15407520
32	234060	995810	2380270	4488240	7425380	11303210	16238390
33	248780	1056450	2520730	4745120	7837980	11913530	17091210
34	263950	1118890	2665240	5009200	8261830	12540050	17966040
35	279570	1183130	2813800	5280480	8696930	13182770	18862880
36	295640	1249170	2966410	5558960	9143280	13841690	19781770
37	312160	1317010	3123070	5844640	9600880	14516810	20722710

$$PI(G[m,6]) = PI(C_{60m+360}) = 8100m^2+83820m+326570 \quad m\geq 29$$

$$PI(G[m,7]) = PI(C_{70m+490}) = 11025m^2+136115m+593230 \quad m\geq 34$$

$$PI(G[m,8]) = PI(C_{80m+640}) = 14400m^2+206560m+997900 \quad m\geq 39$$

$$PI(G[m,9]) = PI(C_{90m+810}) = 18225m^2+297855m+1581460 \quad m\geq 44$$

$$PI(G[m,10]) = PI(C_{100m+1000}) = 22500m^2+412700m+2391090 \quad m\geq 49$$

From these calculations, one can see that the coefficient of m^2 is satisfied by the polynomial $225n^2$ and the coefficient of m is satisfied by $450n^3-375n^2+20n$, where n is a natural number. But we cannot find a good polynomial for the constant terms of these equations. On the

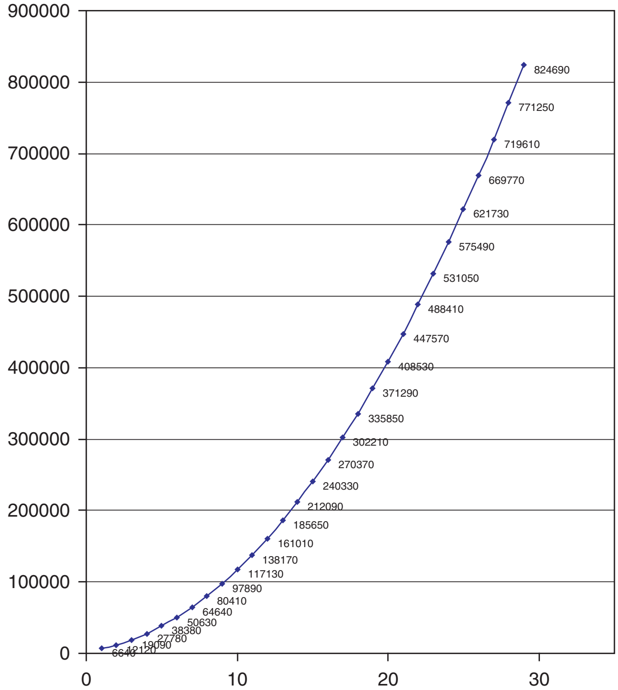

Fig. 2. Diagram of PI index of the fullerenes C_{20m+40}.

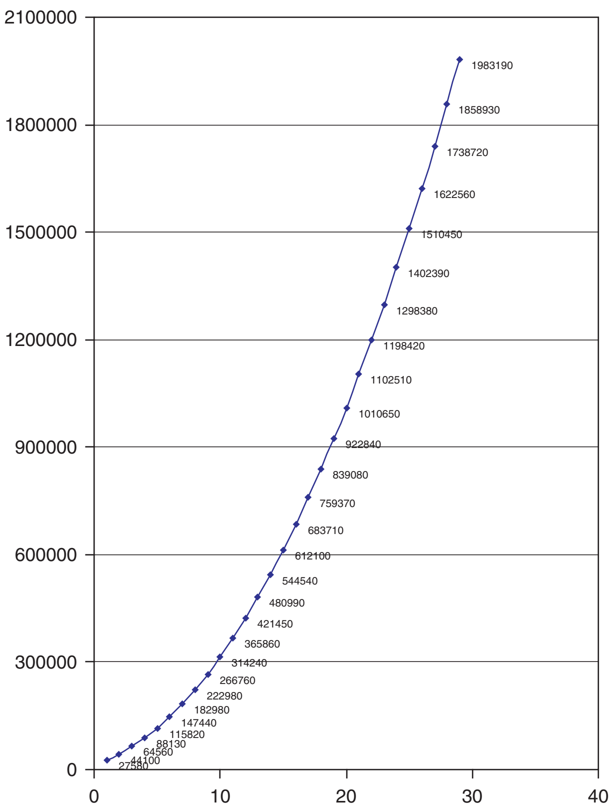

Fig. 3. Diagram of PI index of the fullerenes C_{30m+90}.

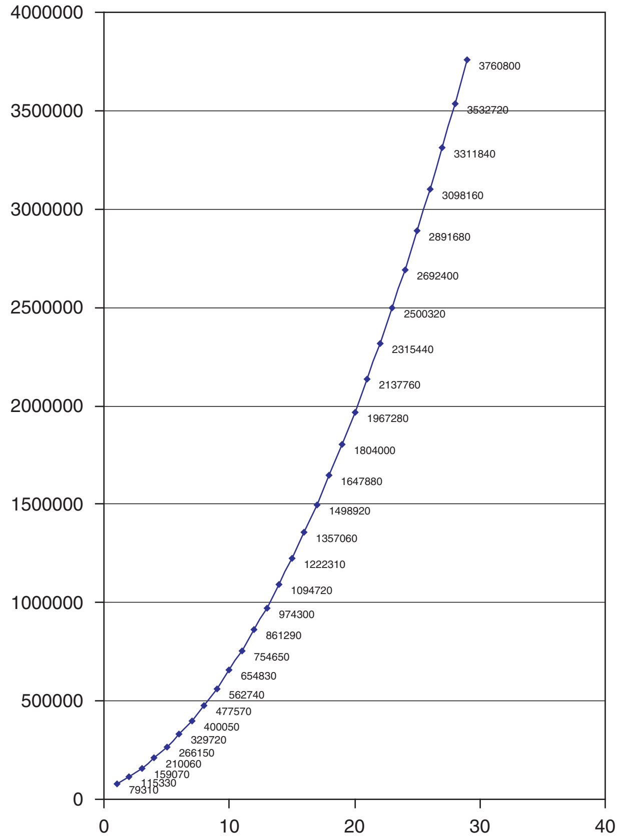

Fig. 4. Diagram of PI index of the fullerenes $C_{40m+160}$.

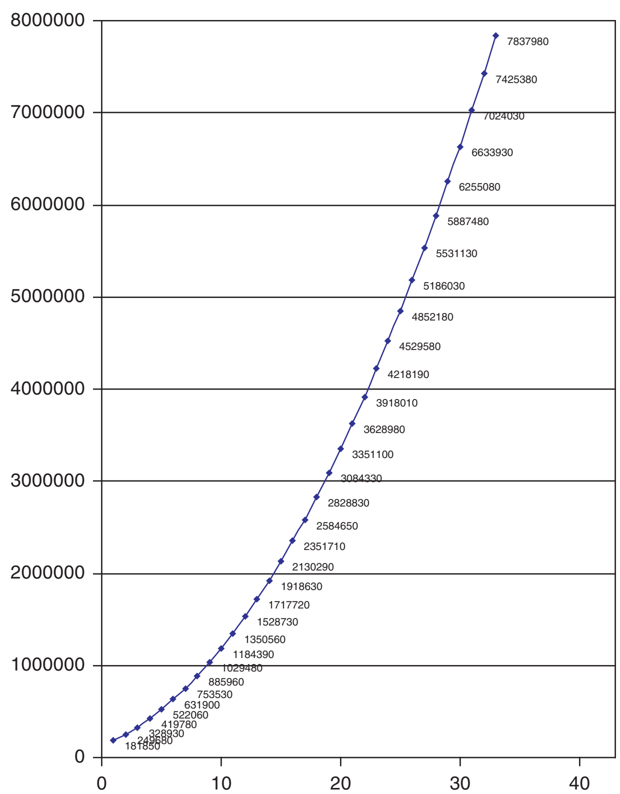

Fig. 5. Diagram of PI index of the fullerenes $C_{50m+250}$.

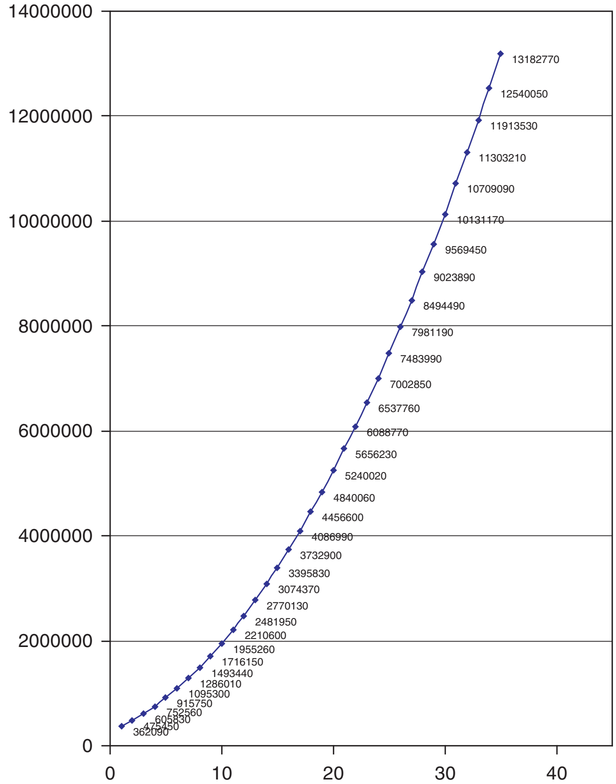

Fig. 6. Diagram of PI index of the fullerenes $C_{60m+360}$.

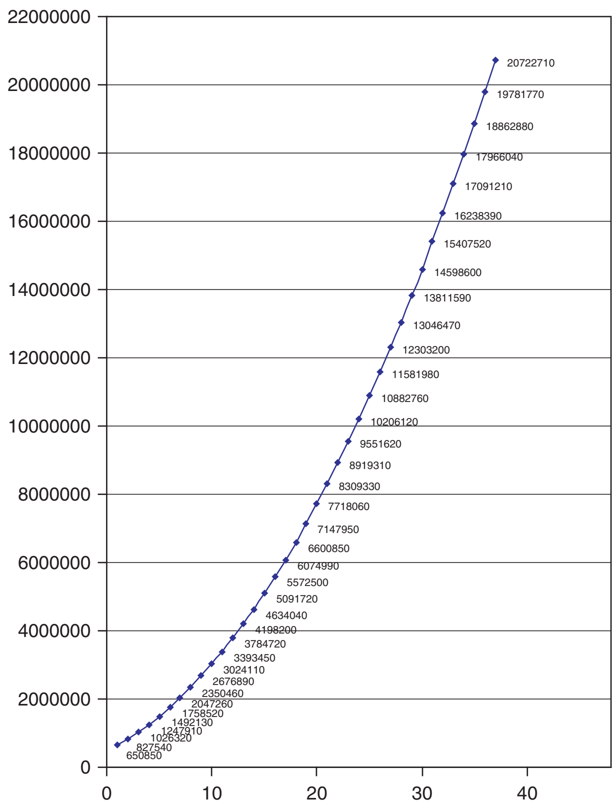

Fig. 7. Diagram of PI index of the fullerenes $C_{70m+490}$.

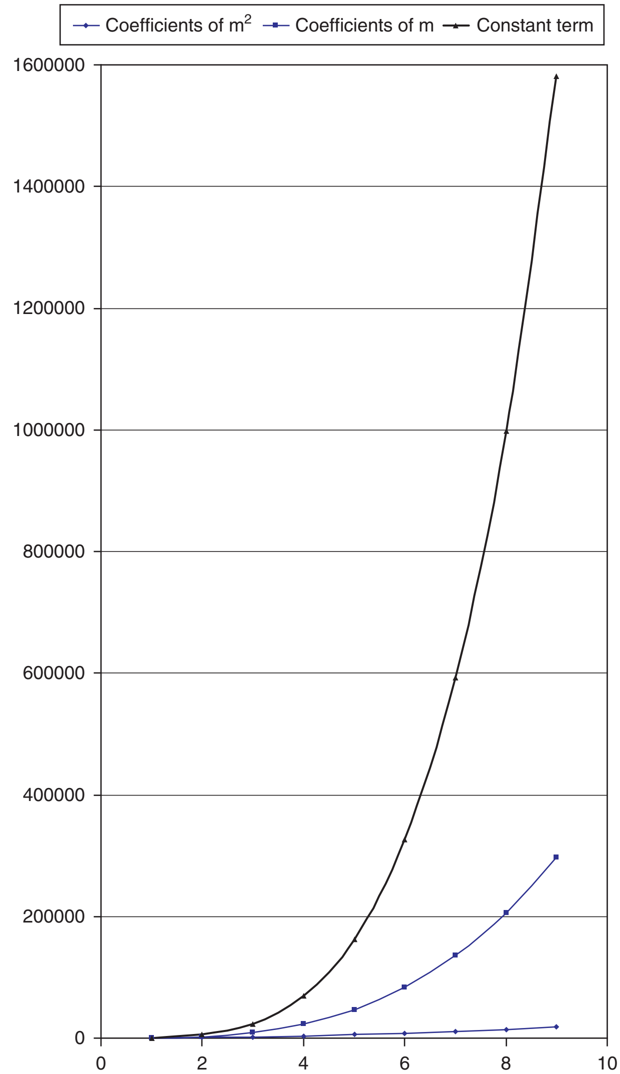

Fig. 8. The relationship between coefficients of m^2, m and constant term.

other hand, one can see that

$$\begin{aligned} PI(G[m,n]) &= \sum_{e=uv\in E(G[m,n])} [m_u(e)+m_v(e)] \\ &\le \sum_{e=uv\in E(G[m,n])} [3/2(10n(m+n))-1] \\ &= [225n^2]m^2+[225n^3-15n]m \\ &\quad +[225n^4-15n^2] \end{aligned}$$

This shows that the PI index of $G[m,n]$ has degree 2 in terms of m. In Figures 2–7, the diagrams of PI index in terms of m are depicted. The Figure 8, shows the relationship between the coefficients of m^2, m and constant term in terms of n.

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