Zagreb Polynomials of Certain Families of Dendrimer Nanostars

Nabeel E. Arif
Department of Mathematics , College of Computer Sciences and Mathematics , Tikrit University, Tikrit, Iraq

Abstract
Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The first, second and third Zagreb polynomials of G are defined as $ZG_1(G,x)=\sum_{uv\in E(G)} x^{d_u+d_v}$, $ZG_2(G,x)=\sum_{uv\in E(G)} x^{d_u d_v}$ and $ZG_3(G,x)=\sum_{uv\in E(G)} x^{|d_u-d_v|}$. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this paper, the first, second and third Zagreb polynomials of three types of dendrimers are computed.

1. Introduction
Throughout this paper, we consider only simple connected graphs, i.e., connected graphs without loops and multiple edges. For a graph G, $V(G)$ and $E(G)$ denote the set of all vertices and edges, respectively. For a graph G, the degree of a vertex v is the number of edges incident to v and denoted by $\deg_G(v)$ or d_v.

A topological index $Top(G)$ of a graph G, is a number with this property that every graph H isomorphic to G, $Top(H) = Top(G)$. The Winer index is the first and most studied topological indices, both from theoretical point of view and applications [8,9,21].

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajestic [14] and they are defined as $ZG_1(G)=\sum_{u\in V(G)} d_u+d_v$ and $ZG_2(G)=\sum_{uv\in E(G)} d_u d_v$, where $ZG_1(G)$ and $ZG_2(G)$ denote the first and second Zagreb indices of G, respectively. We encourage the reader to consult [6,7,15,20,23-25] for historical background and mathematical properties of Zagreb indices. In 2011, Fath-Tabar [12] introduced a new graph invariant, namely, the third Zagreb index and defined as $ZG_3(G)=\sum_{uv\in E(G)}|d_u-d_v|$.

Recently, Fath-Tabar [13] has put forward the concept of the first and the second Zagreb polynomials of the graph G, defined respectively as

$$ZG_1(G,x)=\sum_{uv\in E(G)} x^{d_u+d_v} ,$$

$$ZG_2(G,x)=\sum_{uv\in E(G)} x^{d_u d_v} ,$$

where x is a dummy variable. The third Zagreb polynomial was first studied in [3] and defined as follows.

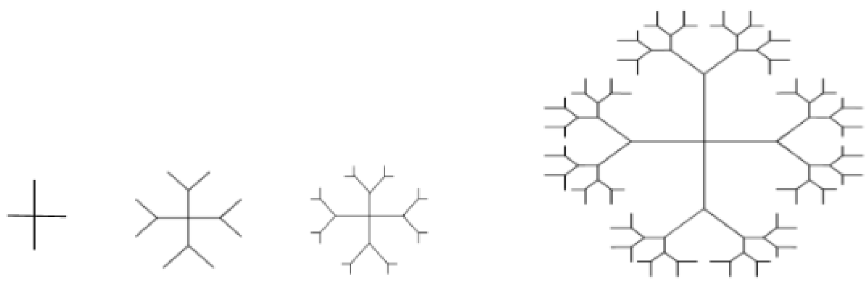
$$ZG_3(G,x)=\sum_{uv\in E(G)} x^{|d_u-d_v|}.$$

Dendrimers are a new class of polymeric materials. They are highly branched, monodisperse macromolecules. The structure of these materials has a great impact on their physical and chemical properties. As a result of their unique behavior dendrimers are suitable for a wide range of biomedical and industrial applications [17]. Recently, some researchers investigated the mathematical properties of this nano-structure in [1,2,4,5,16,19,22].

It is well-known that a graph can be described by a connection table, a sequence of numbers, a matrix, a polynomial or a derived number called a topological index. In this paper, we apply a polynomial approach to study the molecular graphs. In [3,10,11,13,18], the authors investigated the Zagreb polynomials of dendrimers, Cartesian product of graphs, thorn graphs, nanotubes and hydrocarbon structures. Motivated by these works, in this paper, we continue this program to compute a formula of Zagreb polynomials of three types of dendrimers.

2. Main results
In this section, we shall compute the first, second and third Zagreb polynomials of three types of dendrimers.

We first consider the first type of dendrimers, namely tree dendrimer $D[n]$, see [1], where n is the stage of growth in this type of dendrimer. Figure 1 shows the molecular graph $D[n]$ with stage n = 1,2,3,5.



(a) $D[1]$ (b) $D[2]$ (c) $D[3]$ (d) $D[5]$

Figure 1. Molecular graph of dendrimer $D[n]$ with stage n =1,2,3,5.

Our main results are Theorems 1 to 3.

Theorem 1. Let $D[n]$ be the tree dendrimer with n is the stage of growth and $n = \{1,2,\dots\}$. Then we have

$$ZG_1(D[n],x) = \begin{cases} 4x^5 & n = 1 \\ 4x^7 + (8(2^{n-2}) - 8)x^6 + (8(2^{n-2}))x^4 & n \geq 2 \end{cases};$$

$$ZG_2(D[n],x) = \begin{cases} 4x^4 & n = 1 \\ 4x^{12} + (8(2^{n-2}) - 8)x^9 + (8(2^{n-2}))x^3 & n \geq 2 \end{cases};$$

$$ZG_3(D[n],x) = \begin{cases} 4x^3 & n = 1 \\ (8(2^{n-1}))x^2 + 4x + (8(2^{n-2}) - 8) & n \geq 2 \end{cases}.$$

Proof. It is easy to see that the graph $D[n]$, where $n \geq 2$, has three types of edges, with degrees 3 and 4 (or simply (3,4)), degrees 3 and 3 (or simply (3,3)), degrees 1 and 3 (or simply (1,3)). There is only one type of edges with degree (1,4) of subgraph $D[1]$(Figure 1(a)) and two types of edges with degrees (3,4) and (1,3) of subgraph $D[2]$ (Figure 1(b)).

By using the definition of the first Zagreb polynomial, we have $ZG_1(D[1],x) = 4x^5$, and by induction on n, we obtain

$$ZG_1(D[n],x) = 4x^7 + (8(2^{n-2}) - 8)x^6 + (8(2^{n-2}))x^4$$

where $n \geq 2$.

Similarly, by using the definition of the second and third Zagreb polynomial, we obtain

$$ZG_2(D[n],x) = \begin{cases} 4x^4 & n = 1 \\ 4x^{12} + (8(2^{n-2}) - 8)x^9 + (8(2^{n-2}))x^3 & n \geq 2 \end{cases};$$

$$ZG_3(D[n],x) = \begin{cases} 4x^3 & n = 1 \\ (8(2^{n-1}))x^2 + 4x + (8(2^{n-2}) - 8) & n \geq 2 \end{cases}.$$

This completes the proof of Theorem 1. □

We now consider the polyphenylene dendrimer with n stage of growth, denoted by $D_4[n]$ (see [4]). Figure 2 shows polyphenylene dendrimer $D_4[n]$ with two growth stages.

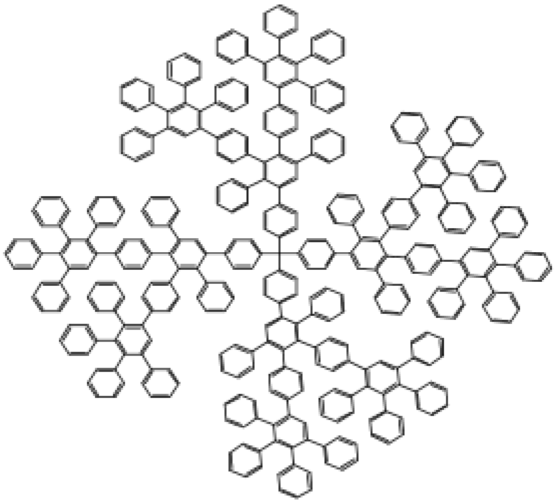


Figure 2. Polyphenylene dendrimer with two growth stages, $D_4[2]$

Theorem 2. Let $D_4[n]$ be the polyphenylene dendrimer with n stage of growth and $n = \{0,1,2,\dots\}$. Then, we have

$ZG_1(D_4[n],x) = 4x^7 + (36(2^n) - 36)x^6 + (48(2^n) - 40)x^5 + (56(2^n) - 40)x^4$;

$ZG_2(D_4[n],x) = 4x^{12} + (36(2^n) - 36)x^9 + (48(2^n) - 40)x^6 + (56(2^n) - 40)x^4$;

$ZG_3(D_4[n],x) = (48(2^n) - 36)x + 92(2^n) - 76$.

Proof. Note that the core of this dendrimer represents the graph $D_4[0]$ of stage $n = 0$. The graph $D_4[n]$ has four types of edges, with degrees (3,4), (3,3), (2,3) and (2,2). There are three types of edges with degrees (3,4), (2,3) and (2,2) in graph $D_4[0]$ (Fig. 3) and four types of edges with degrees (3,4), (3,3), (2,3) and (2,2) in the other stages. So in general we can see there are 4 edges of type (3,4), $36(2^n) - 36$ of type (3,3), $48(2^n) - 40$ of type (2,3), and $56(2^n) - 40$ of type (2,2).

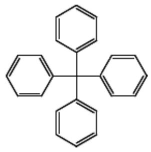


Figure 3. The core of polyphenylene dendrimer, $D_4[0]$

Thus by definition of Zagreb polynomial, we can compute the result for first Zagreb polynomials of $D_4[n]$ as follows:

$ZG_1(D_4[n],x) = 4x^7 + (36(2^n) - 36)x^6 + (48(2^n) - 40)x^5 + (56(2^n) - 40)x^4$;

By the same way we compute the results for second and third Zagreb polynomials of $D_4[n]$ as follows:

$ZG_2(D_4[n],x) = 4x^{12} + (36(2^n) - 36)x^9 + (48(2^n) - 40)x^6 + (56(2^n) - 40)x^4$;

$ZG_3(D_4[n],x) = (48(2^n) - 36)x + 92(2^n) - 76$.

This completes the proof of Theorem 2. □

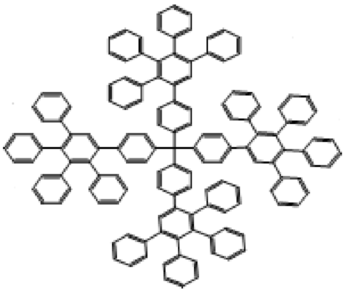


Figure 4. Polyphenylene dendrimer, $D_4[1]$

Finally, we consider the second type of polyphenylene dendrimers, denoted by $D_2[n]$. Figure 5 shows polyphenylene dendrimer $D_2[n]$ with three growth stages.

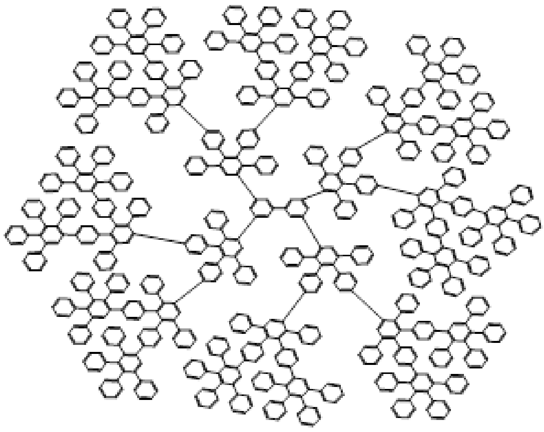


Figure 5. Polyphenylene dendrimer with 3 growth stages, $D_2[3]$

Theorem 3. Let $D_2[n]$ be the polyphenylene dendrimer with n stage of growth and $n = \{0,1,2,...\}$. Then, we have

$ZG_1(D_2[n],x) = (36(2^n) - 35)x^6 + (48(2^n) - 44)x^5 + (56(2^n) - 48)x^4$;

$ZG_2(D_2[n],x) = (36(2^n) - 35)x^9 + (48(2^n) - 44)x^6 + (56(2^n) - 48)x^4$;

$ZG_3(D_2[n],x) = (48(2^n) - 44)x + 92(2^n) - 83$.

Proof. We can see that the graph $D_2[n]$ has three types of edges, with degrees (3,3), (2,3) and (2,2). So in general there are $36(2^n) - 35$ of type (3,3), $48(2^n) - 44$ of type (2,3), and $56(2^n) - 48$ of type (2,2).

Similarly, by using the definition of Zagreb polynomial, we can compute the first, second and third Zagreb polynomials of $D_2[n]$ as follows:

$ZG_1(D_2[n],x) = (36(2^n) - 35)x^6 + (48(2^n) - 44)x^5 + (56(2^n) - 48)x^4$;

$ZG_2(D_2[n],x) = (36(2^n) - 35)x^9 + (48(2^n) - 44)x^6 + (56(2^n) - 48)x^4$;

$ZG_3(D_2[n],x) = (48(2^n) - 44)x + 92(2^n) - 83$.

This completes the proof of Theorem 2. □

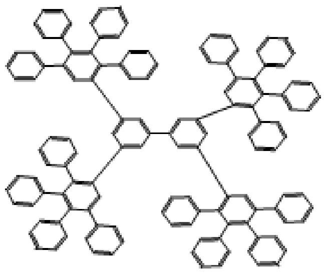


Figure 6. Polyphenylene dendrimer, $D_2[1]$

References

1. M.B. Ahmadi, M. Sadeghimehr, Second order connectivity index of an infinite class of dendrimer nanostars, Dig. J. Nanomater. Bios. 4 (2009), 639-643.
2. S. Alikhani, M.A. Iranmanesh, Chromatic polynomials of some dendrimers, J. Comput. Theor. Nanosci. 7 (2010), 2314-2316.
3. A. Astaneh-Asl, G. Fath-Tabar, Computing the first and third Zagreb polynomials of Cartesian product of graphs, Iranian J. Math. Chem 2(2) (2011), 73-78.
4. N.E. Arif, R. Hasni, S. Alikhani, Chromatic polynomials of certain families of dendrimer nanostars, Dig. J. Nano. Biostr. 6 (2011), 1551-1556.
5. A.R. Ashrafi, M. Mirzargar, PI Szeged and edge Szeged indices of an infinite family of nanostar dendrimers, Indian J. Chem. 47A (2008), 538-541.
6. N. Dorosti, A. Iranmanesh. M.V. Diudea, Computing the Cluj index of dendrimer nanostars, MATCH Commun. Math. Comput. Chem. 62 (2009), 389-395.
7. J. Braun, A. Kerber, M. Meringer, C. Rucker, Similarity of molecular descriptors: the equivalence of Zagreb indices and walk counts, MATCH Commun. Math. Comput. Chem. 54 (2005), 163-176.
8. K.C. Das, I. Gutman, Some properties of the second Zagreb index, MATCH Commun. Math. Comput. Chem. 52 (2004), 103-112.
9. A.A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, Acta Appl. Math. 66 (2001), 211-249.
10. A.A. Dobrynin, I. Gutman, S. Klavzar, P. Zigert, Wiener index of hexagonal systems, Acta Appl. Math. 72 (2002), 247-294
11. M.R. Farahani, First and second Zagreb polynomials of VC5C7[p,q] and HC5C7[p,q] nanotubes, Int. Lett. Chem. Phsy. Astr. 12 (2014), 56-62.
12. M.R. Farahani, Zagreb indices and Zagreb polynomials of Polycyclic Aromatic Hydrocarbons PAHs, J. Chem. Acta 2 (2013), 70-72.
13. G.H. Fath-Tabar, Old and new Zagreb indices of graphs, MATCH Commun. Math. Comput. Chem. 65 (2011), 79-84.
14. G.H. Fath-Tabar, Zagreb polynomials and PI indices of some nano-structures, Dig. J. Nanomater. Bios. 4 (2009), 189-191.
15. I. Gutman, N. Trinajstic, Graph theory and molecular orbitals, Total π electron energy of

alternant hydrocarbons, Chem. Phys. Lett. 17 (1972), 535-538.
16. I. Gutman, K.C. Das, The first Zagreb index 30 years after, MATCH Commun. Math. Comput. Chem. 50 (2004), 83-92.
17. A. Iranmanesh, N.A. Gholami, Computing the Szeged index of styrylbenzene dendrimer and triarylamine dendrimer of generation 1-3, MATCH Commun. Math. Comput. Chem. 62 (2009), 371-379.
18. B. Klajnert, M. Bryszewska, Dendrimers: properties and applications, Acta Biochim. Polonica 48 (2001), 199-208.
19. S. Li, Zagreb polynomials of thorn graphs, Kragujevac J. Sci. 33 (2011), 33-38.
20. M. Mirzagar, PI, Szeged and edge Szeged polynomials of a dendrimer nanostar, MATCH Commun. Math. Comput. Chem. 62 (2009), 363-370.
21. S. Nikolic, G. Kovacevic, A. Milicevic, N. Trinajstic, The Zagreb indices 30 years after, Croat. Chem. Acta 76 (2003), 113-124.
22. H. Wiener, Structural determination of the paraffin boiling points, J. Am. Chem. Soc. 69 (1947), 17-20.
23. H. Yousefi-Azari, A.R. Ashrafi, A. Bahrami, Y. Yazdani, Computing topological indices of some types of benzenoid systems and nanostars, Asian J. Chem. 20 (2008), 15-20.
24. B. Zhou, I. Gutman, Relations between Wiener, hyper-Wiener and Zagreb indices, Chem. Phys. Lett. 394 (2004), 93-95.
25. B. Zhou, Zagreb indices, MATCH Commun. Math. Comput. Chem. 52 (2004), 113-118.
26. B. Zhou, I. Gutman, Further properties of Zagreb indices, MATCH Commun. Math. Comput. Chem. 54 (2005), 233-239.

متعددات حدود زغرب لبعض عوائل الديندراميرات النانوية

نبيل عزالدين عارف

قسم الرياضيات ، كلية علوم الحاسوب والرياضيات ، جامعة تكريت ، تكريت ، العراق

nabarif@yahoo.com

الملخص

البيان المتصل البسيط G هو المتكون من مجموعة الرؤوس V(G) ومجموعة الحافات E(G). متعددة حدود زغرب من الصنف الاول والثاني والثالث للبيان G معرفة بالشكل

$ZG_1(G,x) = \sum_{uv\in E(G)} x^{d_u+d_v}$, $ZG_2(G,x) = \sum_{uv\in E(G)} x^{d_u d_v}$ and $ZG_3(G,x) = \sum_{uv\in E(G)} x^{|d_u-d_v|}$.

الديندرايمر النانوي هو جزيئات تم تصنيعها وتوليفها من خلال التفاعل الكيمياوي وتكون بشكل متراكم من وحدات متفرعة تسمى المونومرات. في هذا البحث تم احتساب متعددة حدود زغرب للاصناف الثلاثة المذكورة لبعض عوائل الديندراميرات النانوية.