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 $\text{deg}_G(v)$ 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 Wiener 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 Trinajstic [14] and they are defined as $ZG_1(G) = \sum_{uv \in V(G)} d_u + d_v$ 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 $n = 1,2,3,5$.

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 $n \in \{1,2,\ldots\}$. Then we have

\[
\begin{align*}
ZG_1(D[n], x) &= \begin{cases} 
4x^5 & n = 1 ;
4x^7 + (8(2^{n-2}) - 8)x^6 + (8(2^{n-2}))x^4 & n \geq 2 ;
\end{cases} \\
ZG_2(D[n], x) &= \begin{cases} 
4x^4 & n = 1 ;
4x^{12} + (8(2^{n-2}) - 8)x^9 + (8(2^{n-2}))x^3 & n \geq 2 ;
\end{cases} \\
ZG_3(D[n], x) &= \begin{cases} 
(6(2^{n-1}))x^2 + 4x + (8(2^{n-2}) - 8) & n \geq 2.
\end{cases}
\]

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

\[
ZG_2(D[n], x) = \begin{cases} 
4x^4 & n = 1 ;
4x^{12} + (8(2^{n-2}) - 8)x^9 + (8(2^{n-2}))x^3 & n \geq 2 ;
\end{cases} \\
ZG_3(D[n], x) = \begin{cases} 
(6(2^{n-1}))x^2 + 4x + (8(2^{n-2}) - 8) & n \geq 2.
\end{cases}
\]

This completes the proof of Theorem 1.

We now consider the polyphenylene dendrimer with $n$ stage of growth, denoted by $D_{n}[n]$ (see [4]). Figure 2 shows polyphenylene dendrimer $D_{1}[n]$ with two growth stages.

![Figure 2. Polyphenylene dendrimer with two growth stages, $D_{1}[2]$](image)

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

\[
\begin{align*}
ZG_1(D_{n}[n], x) &= 4x^7 + (36(2^n) - 36)x^6 + (48(2^n) - 40)x^5 + (56(2^n) - 40)x^4 ; \\
ZG_2(D_{n}[n], x) &= 4x^{12} + (36(2^n) - 36)x^9 + (48(2^n) - 40)x^6 + (56(2^n) - 40)x^4 ; \\
ZG_3(D_{n}[n], x) &= (48(2^n) - 36)x + 92(2^n) - 76.
\]

Proof. Note that the core of this dendrimer represents the graph $D_{0}[0]$ of stage $n = 0$. The graph $D_{0}[0]$ 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 $D_{0}[0]$ (Fig. 3) and four types of edges with degrees (3,3), (3,4), (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).

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

\[
ZG_1(D_{n}[n], x) = 4x^7 + (36(2^n) - 36)x^6 + (48(2^n) - 40)x^5 + (56(2^n) - 40)x^4 ;
\]

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

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

\[
ZG_3(D_{n}[n], x) = (48(2^n) - 36)x + 92(2^n) - 76.
\]

This completes the proof of Theorem 2. □
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.

**References**

15. I. Gutman, N. Trinajstic, Graph theory and molecular orbitals, Total π electron energy of


متعددات حدود زغرب لبعض عوائل الديندراميرات النانوية
نيل عزالدين عارف
قسم الرياضيات، كلية علوم الحاسوب والرياضيات، جامعة تكريت، تكريت، العراق
nabarif@yahoo.com

الملخص
البيان المتكون من مجموعة الرؤوس V(G) والحدود E(G) هو المكون من مجموعة الدرجات الأولى والثاني والثالث للبيان G وعرف بـ 

\[ ZG_1(G, x) = \sum_{u \in E(G)} x^{d_u + d_v}, \quad ZG_2(G, x) = \sum_{u \in E(G)} x^{d_u + d_v} \quad \text{and} \quad ZG_3(G, x) = \sum_{u \in E(G)} x^{d_u - d_v}. \]

الديندرامير النانوي هو جزيئات تم تصنيعها وتوليفها من خلال التفاعل الكيميائي وتكون بشكل متراكم من وحدات متفرعة تسمى المونومرات. في هذا البحث تم احتساب متعددات حدود زغرب لالسلاسل الثلاثة المذكورة لبعض عوائل الديندراميرات النانوية.