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VERTEX-ECCENTRICITY DESCRIPTORS IN DENDRIMERS

MAHDIEH AZARI[a]*, ALI IRANMANESH[b] AND MIRCEA V. DIUDEA[c]*

ABSTRACT. In this paper, we present graph theoretical methods to compute several vertex-eccentricity-based molecular descriptors such as the eccentric connectivity index, total eccentricity, average eccentricity and first and second Zagreb eccentricity indices for the generalized and ordinary Bethe trees and some dendrimer graphs. Also, we study the behavior of these descriptors under the rooted product of graphs and apply our results to compute these indices for some classes of molecular graphs, designed by attaching copies of ordinary Bethe trees to paths and cycles.

Keywords: *Vertex eccentricity, Molecular descriptor**,** Molecular graph**,** Bethe tree, Dendrimer, Rooted product of graphs.*

INTRODUCTION

Chemical graph theory is a branch of mathematical chemistry dealing with the study of chemical graphs [1]. Chemical graphs, particularly molecular graphs, are models of molecules in which atoms are represented by vertices and chemical bonds by edges of a graph. Physico-chemical or biological properties of molecules can be predicted by using the information encoded in the molecular graphs, eventually translated in the adjacency or connectivity matrix associated to these graphs. This paradigm is achieved by considering various graph theoretical invariants of molecular graphs (also known as topological indices, molecular descriptors, etc.) and evaluating how strongly are they correlated with various molecular properties. In this way, chemical

[a] *Department of Mathematics, Kazerun Branch, Islamic Azad University, P. O. Box: 73135-168, Kazerun, Iran, azari@kau.ac.ir*
[b] *Department of Pure Mathematics, Faculty of Mathematical Sciences, Tarbiat Modares University, P. O. Box: 14115-137, Tehran, Iran, iranmanesh@modares.ac.ir*
[c] *Department of Chemistry, Faculty of Chemistry and Chemical Engineering, "Babes-Bolyai" University, Arany Janos 11, 400028, Cluj, Romania, Diudea@gmail.com*
* *Corresponding authors: azari@kau.ac.ir, Diudea@gmail.com*

graph theory plays an important role in mathematical foundation of QSAR and QSPR research. A graph invariant is any function calculated on a molecular graph, irrespective of the labeling of its vertices. Many invariants have been proposed and employed to date with various degrees of success in QSAR/QSPR studies. We refer the reader to consult the monographs [1,2].

In the recent years, some invariants based on vertex eccentricity such as eccentric connectivity index [3], total eccentricity, average eccentricity [4], and first and second Zagreb eccentricity indices [5] have attracted much attention in chemistry. These invariants are successfully used for mathematical modeling of biological activity of diverse nature [6-8]. They were also proposed as a measure of branching in alkanes [9].

Dendrimers are highly ordered hyper-branched molecular structures [10-12] reaching the nano-dimensions. The end-groups (the pendant groups reaching the outer periphery) can be functionalized, thus modifying their physico-chemical or biological properties. Dendrimers have gained a wide range of applications in supra-molecular chemistry, particularly in catalysis, host-guest reactions, and self-assembly processes [13,14]. Promising applications come to cancer therapy [15] but their applications are unlimited.

In this paper, we present graph theoretical methods to compute these descriptors for generalized and ordinary Bethe trees and several classes of molecular graphs and dendrimers derived from them.

DEFINITIONS AND PRELIMINARIES

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex $u \in V(G)$ is the number of first neighbors of u in G. The (topological) distance $d_G(u,v)$ between the vertices $u,v \in V(G)$ is defined as the length of any shortest path in G connecting u and v. The eccentricity $\varepsilon_G(u)$ of a vertex u is the largest distance between u and any other vertex v of G, $\varepsilon_G(u)=\max\{d_G(u,v); v \in V(G)\}$.

The best known and widely used topological index is the Wiener index, W, introduced in 1947 by Wiener [16], who used it for modeling the thermodynamic properties of alkanes. The Wiener index of a molecular graph G represents the sum of topological distances between all pairs of atoms/vertices of G. Details on the Wiener index can be found in [17-20].

Zagreb indices are among the oldest topological indices, and were introduced in 1972 by Gutman and Trinajstić [21] within the study about the dependence of total π-electron energy of molecular structures. The first and the second Zagreb indices of a graph G, $M_1(G)$ and $M_2(G)$, respectively, are defined as:

$$M_1(G)=\sum_{u\in V(G)} d_G(u)^2 \quad \text{and} \quad M_2(G)=\sum_{uv\in E(G)} d_G(u)d_G(v).$$

The eccentric connectivity index $\xi(G)$ was introduced by Sharma *et al*. [3] in 1997; it is defined as:

$$\xi(G)=\sum_{u\in V(G)} d_G(u)\varepsilon_G(u).$$

It is sometimes interesting to consider the sum of eccentricities of all vertices of a given graph G. This quantity is called the total eccentricity of G and denoted by $\zeta(G)$.

The average eccentricity [4] of G is denoted by $\eta(G)$ and defined as:

$$\eta(G)=\frac{\zeta(G)}{|V(G)|}.$$

The Zagreb eccentricity indices were introduced by Vukičević and Graovac [5] in 2010. They are defined, analogously to the Zagreb indices, by replacing the vertex degree with the vertex eccentricity, as:

$$\xi_1(G)=\sum_{u\in V(G)} \varepsilon_G(u)^2,\ \xi_2(G)=\sum_{uv\in E(G)} \varepsilon_G(u)\varepsilon_G(v).$$

RESULTS AND DISCUSSION

Let us compute some vertex-eccentricity-based invariants for path and cycle. The results follow easily by direct calculations, so the proofs are omitted.

Lemma 1. Let P_n and C_n denote the n-vertex path and cycle, respectively.

(i) If n is even, then

$$\xi(P_n)=\frac{3n^2-6n+4}{2},\ \zeta(P_n)=\frac{n(3n-2)}{4},\ \eta(P_n)=\frac{3n-2}{4},$$

$$\xi_1(P_n)=\frac{n(n-1)(7n-2)}{12},\ \xi_2(P_n)=\frac{n(7n^2-21n+20)}{12},$$

and if n is odd, we have

$$\xi(P_n)=\frac{3(n-1)^2}{2},\ \zeta(P_n)=\frac{(n-1)(3n+1)}{4},\ \eta(P_n)=\frac{(n-1)(3n+1)}{4n},$$

$$\xi_1(P_n)=\frac{(n-1)(7n^2-2n-3)}{12},\ \xi_2(P_n)=\frac{(n-1)(7n^2-14n+3)}{12}.$$

(ii) For every $n \geq 3$,

$$\xi(C_n) = 2n\left\lfloor \frac{n}{2} \right\rfloor,\ \zeta(C_n) = n\left\lfloor \frac{n}{2} \right\rfloor,\ \eta(C_n) = \left\lfloor \frac{n}{2} \right\rfloor,\ \xi_1(C_n) = \xi_2(C_n) = n\left\lfloor \frac{n}{2} \right\rfloor^2.$$

A generalized Bethe tree [22] of k levels, $k>1$, is a rooted tree in which vertices lying at the same level have the same degree (Figure 1). The level of a vertex in a rooted tree equals its distance from the root vertex plus one.

Let B_k be a generalized Bethe tree of k levels. For i=1,2,..,k, let d_{k-i+1} and n_{k-i+1} denote the degree of the vertices at the level i of B_k and their number, respectively. Also, suppose $e_k = d_k$ and $e_i = d_i - 1$ for I =1,2,…,k-1.

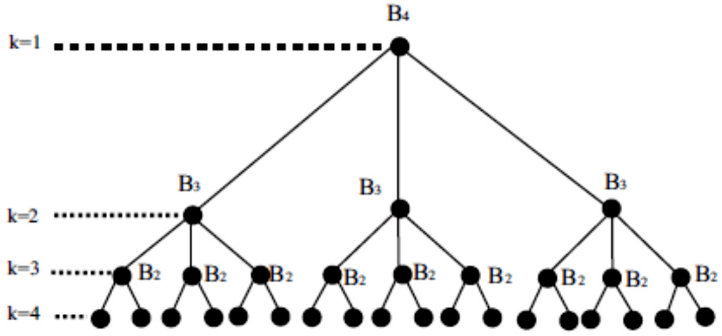

Figure 1. A generalized Bethe tree of 4 levels.

In the following theorem, some vertex-eccentricity-based invariants of the generalized Bethe tree B_k are computed.

Theorem 2. Let B_k be a generalized Bethe tree whose root vertex has degree $d_k>1$. Then

(i) $\xi(B_k) = \sum_{i=1}^{k} d_i (2k-1-i) \prod_{j=i+1}^{k} e_j$,

(ii) $\zeta(B_k) = \sum_{i=1}^{k} (2k-1-i) \prod_{j=i+1}^{k} e_j$,

(iii) $\eta(B_k) = \dfrac{\sum_{i=1}^{k} (2k-1-i) \prod_{j=i+1}^{k} e_j}{\sum_{i=1}^{k} \prod_{j=i+1}^{k} e_j}$,

(iv) $\xi_1(B_k)=\sum_{i=1}^{k}(2k-1-i)^2\prod_{j=i+1}^{k}e_j$,

(v) $\xi_2(B_k)=\sum_{i=2}^{k}(2k-1-i)(2k-i)\prod_{j=i}^{k}e_j$.

Proof. We just prove parts (i) and (v); other parts can be proven similarly. To prove part (i), let v be an arbitrary vertex of the level k-i+1 of B_k, where $1 \le i \le k$. It is easy to see that, $\varepsilon_{Bk}(v)=(k-i)+(k-1)=2k-1-i$. So,

$$\xi(B_k)=\sum_{i=1}^{k}n_i d_i(2k-1-i) . \qquad (1)$$

On the other hand, the number of vertices of the level k-i+1 is equal to $n_i=n_{i+1}e_{i+1}$, $1 \le i \le k-1$. Thus,

$$n_i=n_{i+1}e_{i+1}=(n_{i+2}e_{i+2})e_{i+1}=((n_{i+3}e_{i+3})e_{i+2})e_{i+1}=...=n_k e_k e_{k-1}...e_{i+1}=\prod_{j=i+1}^{k}e_j .$$

Now using (1), we can get the formula for $\xi(B_k)$. To prove part (v), let E_{k-i+1}, $2 \le i \le k$, denote the set of all edges of B_k which connect vertices of the level k-i+1 and level k-i+2 of B_k. It is easy to see that,

$$\left|E_{k-i+1}\right|=n_i e_i=e_i\prod_{j=i}^{k}e_j=\prod_{j=i}^{k}e_j ,$$

and if $uv \in E_{k-i+1}$, then $\varepsilon_{Bk}(u)\varepsilon_{Bk}(v)=(2k-1-i)(2k-i)$. Now, by definition of the second Zagreb eccentricity index, we can get the formula for $\xi_2(B_k)$.

The ordinary Bethe tree $B_{d,k}$ is a rooted tree of k levels whose root vertex has degree d, the vertices from levels 2 to k-1 have degree d+1 and the vertices at level k have degree 1 (Figure 2). Note that $B_{1,k}=P_k$ and $B_{d,2}=S_{d+1}$.

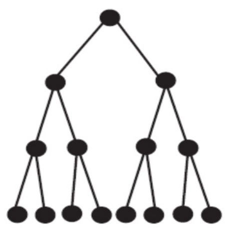

Figure 2. The ordinary Bethe tree $B_{2,4}$.

Using Theorem 2, we easily arrive at:

Corollary 3. For the ordinary Bethe tree $B_{d,k}$ with d>1, we have:

(i) $\xi(B_{d,k})=d(k-1)(2d^{k-2}+1)+(d+1)\sum_{i=1}^{k-2}(k-1+i)d^i$,

(ii) $\zeta(B_{d,k})=\sum_{i=0}^{k-1}(k-1+i)d^i$,

(iii) $\eta(B_{d,k})=\dfrac{\sum_{i=0}^{k-1}(k-1+i)d^i}{\sum_{i=0}^{k-1}d^i}$,

(iv) $\xi_1(B_{d,k})=\sum_{i=0}^{k-1}(k-1+i)^2 d^i$,

(v) $\xi_2(B_{d,k})=\sum_{i=1}^{k-1}(k-2+i)(k-1+i)d^i$.

A dendrimer tree $T_{d,k}$ [23] is a rooted tree having the degree of its non-pendent vertices equal to d and the distance between the root (central) vertex and the pendent vertices equal to k (Figure 3). Thus, $T_{d,k}$ can be seen as a generalized Bethe tree with k+1 levels and the non-pendent vertices have the same degree. Note that $T_{2,k}$ = P_{2k+1} and $T_{d,1}$ = S_{d+1}.

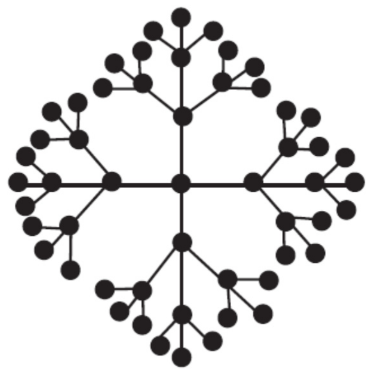

Figure 3. The dendrimer tree $T_{4,3}$.

Using Theorem 2, we easily arrive at:

Corollary 4. For the dendrimer tree $T_{d,k}$ with d>1, we have:

(i) $\xi(T_{d,k})=kd(2(d-1)^{k-1}+1)+d^2\sum_{i=0}^{k-2}(k+1+i)(d-1)^i$,

(ii) $\zeta(T_{d,k})=k+d\sum_{i=0}^{k-1}(k+1+i)(d-1)^i$,

(iii) $\eta(T_{d,k}) = \dfrac{k + d\sum_{i=0}^{k-1}(k+1+i)(d-1)^i}{1 + d\sum_{i=0}^{k-1}(d-1)^i}$,

(iv) $\xi_1(T_{d,k}) = k^2 + d\sum_{i=0}^{k-1}(k+1+i)^2(d-1)^i$,

(v) $\xi_2(T_{d,k}) = d\sum_{i=0}^{k-1}(k+i)(k+1+i)(d-1)^i$.

The formula of part (i) of Corollary 4 has also been obtained in [24].

Now, we introduce a class of dendrimers constructed from copies of ordinary Bethe trees. This molecular structure can be encountered in real chemistry, e.g. in some tertiary phosphine dendrimers. Let D_0 be the graph depicted in Figure 4. For $d,k>0$, let $D_{d,k}$ be a series of dendrimers obtained by attaching d pendent vertices to each pendent vertex of $D_{d,k-1}$ and let $D_{d,0}=D_0$. Some examples of these graphs are shown in Figure 5.

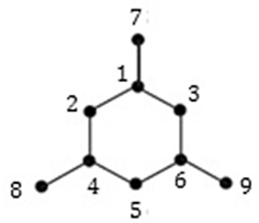

Figure 4. The dendrimer graph D_0 with a numbering for its vertices.

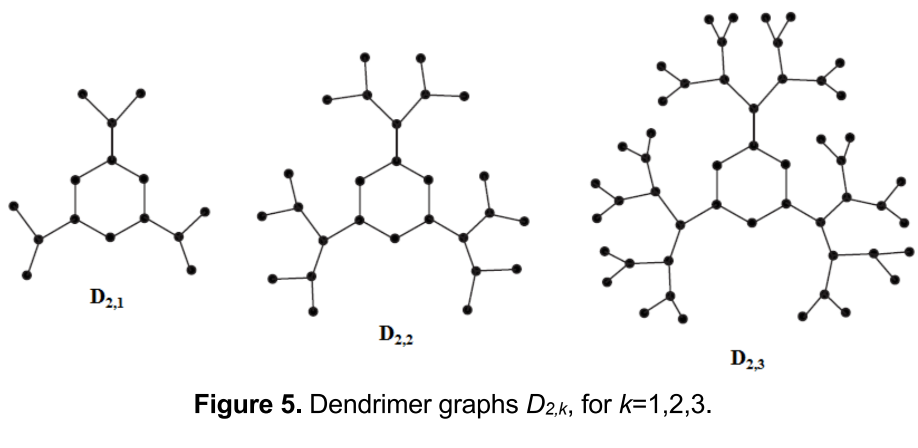

Figure 5. Dendrimer graphs $D_{2,k}$, for k=1,2,3.

We can also introduce the dendrimer graph $D_{d,k}$ as the graph obtained by identifying the root vertex of the ordinary Bethe tree $B_{d,k+1}$ with all three pendant vertices of the graph D_0. In the following theorem, some vertex-eccentricity-based invariants of the dendrimer graph $D_{d,k}$ are calculated.

Theorem 5. For the dendrimer graph $D_{d,k}$ with $k \geq 0$, we have:

(i) $\xi(D_{d,k}) = 15k + 51 + 6(k+2)d^k + 3(d+1)\sum_{i=0}^{k-1}(k+4+i)d^i$,

(ii) $\zeta(D_{d,k}) = 6k + 21 + 3\sum_{i=0}^{k}(k+4+i)d^i$,

(iii) $\eta(D_{d,k}) = \dfrac{6k + 21 + 3\sum_{i=0}^{k}(k+4+i)d^i}{6 + 3\sum_{i=0}^{k}d^i}$,

(iv) $\xi_1(D_{d,k}) = 3(2k^2 + 14k + 25) + 3\sum_{i=0}^{k}(k+4+i)^2 d^i$,

(v) $\xi_2(D_{d,k}) = 9(k+3)(k+4) + 3\sum_{i=1}^{k}(k+3+i)(k+4+i)d^i$.

Proof. Consider a subgraph of $D_{d,k}$ isomorphic to the graph D_0 and choose a numbering for its vertices as shown in Figure 4. It is easy to see that:

$$\varepsilon_{D_{d,k}}(1) = \varepsilon_{D_{d,k}}(4) = \varepsilon_{D_{d,k}}(6) = k+3 , \ \varepsilon_{D_{d,k}}(2) = \varepsilon_{D_{d,k}}(3) = \varepsilon_{D_{d,k}}(5) = k+4 .$$

Now, let G be a subgraph of $D_{d,k}$ isomorphic to the ordinary Bethe tree $B_{d,k+1}$ and let v be an arbitrary vertex of the level i, $1 \leq i \leq k+1$ of G. Then

$$\varepsilon_{D_{d,k}}(v) = (i-1) + 4 + k = k + 3 + i ,$$

and the number of vertices of this level is equal to d^{i-1}. Next, using the definition of the eccentric connectivity index, total eccentricity, average eccentricity, and Zagreb eccentricity indices, the proof is obvious.

Let now consider two other molecular graphs constructed from copies of the ordinary Bethe tree $B_{d,k}$ and compute some of their vertex-eccentricity-based invariants. Recall that the rooted product $G_1\{G_2\}$ of simple connected graphs G_1 and G_2 is the graph obtained by taking one copy of G_1 and $|V(G_1)|$ copies of the rooted graph G_2, and identifying the root vertex of the i-th copy of G_2 with the i-th vertex of G_1, for $i=1,2,\ldots, |V(G_1)|$. More about topological indices of rooted product of graphs can be found in [25-29]. In what follows, we denote the root vertex of G_2 by w, and the copy of G_2 whose root is identified with the vertex $u \in V(G_1)$ by $G_{2,u}$. The degree of a vertex x of $G_1\{G_2\}$ is calculated as:

$$d_{G_1\{G_2\}}(x)=\begin{cases} d_{G_2}(x) & x\in V(G_{2,u})-\{w\} \\ d_{G_1}(u)+\mathrm{d}_{G_2}(w) & x=w\in V(G_{2,u}) \end{cases}.$$

Also, if x∈$V(G_{2,u})$ then the eccentricity of the vertex x is:

$$\varepsilon_{G_1\{G_2\}}(x)=d_{G_2}(x,w)+\varepsilon_{G_1}(u)+\varepsilon_{G_2}(w).$$

Let G be a simple connected graph and $u\in V(G)$. In order to express our next formulas in more compact forms, we introduce some quantities related to graph G as follows:

$$D_G(u)=\sum_{x\in V(G)-\{u\}} d_G(x,u),\ D_G^2(u)=\sum_{x\in V(G)-\{u\}} d_G(x,u)^2,$$

$$DD_G(u)=\sum_{x\in V(G)-\{u\}} \deg_G(x)d_G(x,u),\ DD_G^*(u)=\sum_{xy\in E(G)} d_G(x,u)d_G(y,u).$$

In the following lemma, we compute the above quantities in case G is the ordinary Bethe tree $B_{d,k}$ and u is its root vertex. The proof follows immediately from definitions, so is omitted.

Lemma 6. Let w denote the root vertex of $B_{d,k}$. Then

(i) $D_{B_{d,k}}(w)=\sum_{i=1}^{k-1} id^i$,

(ii) $D^2_{B_{d,k}}(w)=\sum_{i=1}^{k-1} i^2d^i$,

(iii) $DD_{B_{d,k}}(w)=(d+1)\sum_{i=1}^{k-2} id^i+(k-1)d^{k-1}$,

(iv) $DD^*_{B_{d,k}}(w)=\sum_{i=1}^{k-1} i^2d^i-\sum_{i=1}^{k-1} id^i$.

In the following theorem, some vertex-eccentricity-based invariants of the rooted product $G_1\{G_2\}$ are computed.

Theorem 7. Let G_1 and G_2 be simple connected graphs with $|V(G_i)|=n_i$, $|E(G_i)|=m_i$, $1\le i\le 2$, and let the copies of G_2 used in the construction of $G_1\{G_2\}$ be rooted in w. Then

(i) $\xi(G_1\{G_2\})=\xi(G_1)+2m_2\zeta(G_1)+2(m_1+n_1m_2)\varepsilon_{G_2}(w)+n_1DD_{G_2}(w)$,

(ii) $\zeta(G_1\{G_2\})=n_2\zeta(G_1)+n_1D_{G_2}(w)+n_1n_2\varepsilon_{G_2}(w)$,

(iii) $\eta(G_1\{G_2\})=\eta(G_1)+\frac{1}{n_2}D_{G_2}(w)+\varepsilon_{G_2}(w)$,

(iv) $\xi_1(G_1\{G_2\})=n_2\xi_1(G_1)+2(D_{G_2}(w)+n_2\varepsilon_{G_2}(w))\zeta(G_1)+n_1D^2_{G_2}(w)$
$+n_1n_2\varepsilon_{G_2}(w)^2+2n_1\varepsilon_{G_2}(w)D_{G_2}(w)$,

(v) $\xi_2(G_1\{G_2\}) = \xi_2(G_1) + m_2\xi_1(G_1) + \varepsilon_{G_2}(w)\xi(G_1) + 2m_2\varepsilon_{G_2}(w)\zeta(G_1)$
$+ (m_1 + n_1m_2)\varepsilon_{G_2}(w)^2 + (n_1\varepsilon_{G_2}(w) + \zeta(G_1))DD_{G_2}(w) + n_1DD^*_{G_2}(w)$.

Proof. We prove part (i); other parts can be proven similarly.

$$\xi(G_1\{G_2\}) = \sum_{x\in V(G_1\{G_2\})} d_{G_1\{G_2\}}(x)\varepsilon_{G_1\{G_2\}}(x)$$
$$= \sum_{u\in V(G_1)} \sum_{x\in V(G_{2,u})-\{w\}} d_{G_2}(x)[d_{G_2}(x,w)+\varepsilon_{G_1}(u)+\varepsilon_{G_2}(w)]$$
$$+ \sum_{u\in V(G_1)}[d_{G_1}(u)+d_{G_2}(w)][\varepsilon_{G_1}(u)+\varepsilon_{G_2}(w)]$$
$$= [n_1DD_{G_2}(w) + (2m_2 - d_{G_2}(w))\zeta(G_1) + n_1(2m_2 - d_{G_2}(w))\varepsilon_{G_2}(w)]$$
$$+ [\xi(G_1) + 2m_1\varepsilon_{G_2}(w) + d_{G_2}(w)\zeta(G_1) + n_1d_{G_2}(w)\varepsilon_{G_2}(w)]$$
$$= \xi(G_1) + 2m_2\zeta(G_1) + 2(m_1+n_1m_2)\varepsilon_{G_2}(w) + n_1DD_{G_2}(w).$$

Denote by $P(d,k,n)$, the tree obtained by attaching the root vertex of $B_{d,k}$ to the vertices of P_n (Figure 6 and ref. [30]).

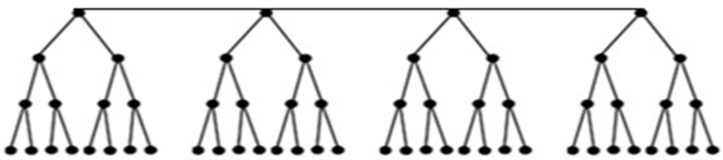

Figure 6. The chemical tree $P(2,4,4)$.

The graph $P(d,k,n)$ can be considered as the rooted product of P_n and $B_{d,k}$. So, we can apply Theorem 7 and Lemmas 1 and 6 to get the formulas for the eccentric connectivity index, total eccentricity, average eccentricity, and Zagreb eccentricity indices of $P(d,k,n)$.

Corollary 8. For the tree $P(d,k,n)$ with $d>1$, the following hold:

(i) If n is even, then

$$\xi(P(d,k,n)) = n(d+1)\sum_{i=1}^{k-2} id^i + n[\frac{3n-2}{2} + 2(k-1)]\sum_{i=1}^{k-1} d^i$$
$$+ [2(n-1) + nd^{k-1}](k-1) + \frac{3n^2-6n+4}{2},$$

and if n is odd, then

$$\xi(P(d,k,n)) = n(d+1)\sum_{i=1}^{k-2} id^i + [\frac{(n-1)(3n+1)}{2} + 2n(k-1)]\sum_{i=1}^{k-1} d^i$$
$$+ [2(n-1) + nd^{k-1}](k-1) + \frac{3(n-1)^2}{2},$$

(ii) If n is even, then

$$\zeta(P(d,k,n)) = n\sum_{i=1}^{k-1} id^i + n[\frac{3n-2}{4} + k - 1]\sum_{i=0}^{k-1} d^i \ ,$$

and if n is odd, then

$$\zeta(P(d,k,n)) = n\sum_{i=1}^{k-1} id^i + [\frac{(n-1)(3n+1)}{4} + n(k-1)]\sum_{i=0}^{k-1} d^i \ .$$

(iii) If n is even, then

$$\eta(P(d,k,n)) = \frac{\sum_{i=1}^{k-1} id^i}{\sum_{i=0}^{k-1} d^i} + \frac{3n-2}{4} + k - 1,$$

and if n is odd, then

$$\eta(P(d,k,n)) = \frac{\sum_{i=1}^{k-1} id^i}{\sum_{i=0}^{k-1} d^i} + \frac{(n-1)(3n+1)}{4n} + k - 1.$$

(iv) If n is even, then

$$\xi_1(P(d,k,n)) = n\sum_{i=1}^{k-1} i^2 d^i + n[\frac{3n-2}{2} + 2(k-1)]\sum_{i=1}^{k-1} id^i$$
$$+ n[\frac{(n-1)(7n-2)}{12} + \frac{(k-1)(3n-2)}{2} + (k-1)^2]\sum_{i=0}^{k-1} d^i \ ,$$

and if n is odd, then

$$\xi_1(P(d,k,n)) = n\sum_{i=1}^{k-1} i^2 d^i + [\frac{(n-1)(3n+1)}{2} + 2n(k-1)]\sum_{i=1}^{k-1} id^i$$
$$+ [\frac{(n-1)(7n^2-2n-3)}{12} + \frac{(k-1)(n-1)(3n+1)}{2} + n(k-1)^2]\sum_{i=0}^{k-1} d^i \ .$$

(v) If n is even, then

$$\xi_2(P(d,k,n)) = n\sum_{i=1}^{k-1} i^2 d^i + n[(d+1)(\frac{3n-2}{4} + k - 1) - 1]\sum_{i=1}^{k-2} id^i$$
$$+ n[\frac{(n-1)(7n-2)}{12} + \frac{(k-1)(3n-2)}{2} + (k-1)^2]\sum_{i=1}^{k-1} d^i$$
$$+ n(k-1)d^{k-1}(\frac{3n-2}{4} + k - 2) + \frac{n(7n^2-21n+20)}{12}$$
$$+ \frac{(k-1)(3n^2-6n+4)}{2} + (n-1)(k-1)^2,$$

and if n is odd, then

$$\xi_2(P(d,k,n)) = n\sum_{i=1}^{k-1} i^2 d^i + [(d+1)(\frac{(n-1)(3n+1)}{4} + n(k-1)) - n]\sum_{i=1}^{k-2} id^i$$
$$+[\frac{(n-1)(7n^2-2n-3)}{12} + \frac{(k-1)(n-1)(3n+1)}{2} + n(k-1)^2]\sum_{i=1}^{k-1} d^i$$
$$+(k-1)d^{k-1}[\frac{(n-1)(3n+1)}{4} + n(k-2)] + \frac{(n-1)(7n^2-14n+3)}{12}$$
$$+\frac{3(k-1)(n-1)^2}{2} + (n-1)(k-1)^2.$$

Denote by $C(d,k,n)$, the dendrimer graph obtained by attaching the root vertex of $B_{d,k}$ to the vertices of C_n (Figure 7 and ref. [22]). It is easy to see that, $C(d,k,n)$ is the rooted product of C_n and $B_{d,k}$. So, using Theorem 7, and Lemmas 1 and 6, we get the following results for $C(d,k,n)$.

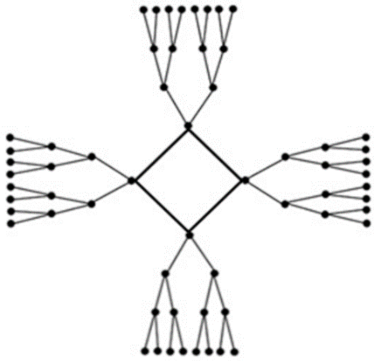

Figure 7. The dendrimer graph $C(2,4,4)$.

Corollary 9. For the dendrimer graph $C(d,k,n)$ with $d>1$, we have:

(i) $\xi(C(d,k,n)) = n(d+1)\sum_{i=1}^{k-2} id^i + 2n[\left\lfloor \frac{n}{2} \right\rfloor + k - 1](\sum_{i=1}^{k-1} d^i + 1) + n(k-1)d^{k-1}$,

(ii) $\zeta(C(d,k,n)) = n\sum_{i=1}^{k-1} id^i + n[\left\lfloor \frac{n}{2} \right\rfloor + k - 1]\sum_{i=0}^{k-1} d^i$,

(iii) $\eta(C(d,k,n)) = \frac{\sum_{i=1}^{k-1} id^i}{\sum_{i=0}^{k-1} d^i} + \left\lfloor \frac{n}{2} \right\rfloor + k - 1$,

(iv) $$\xi_1(C(d,k,n)) = n\sum_{i=1}^{k-1} i^2 d^i + 2n[\left\lfloor \frac{n}{2} \right\rfloor + k - 1]\sum_{i=1}^{k-1} id^i + n[\left\lfloor \frac{n}{2} \right\rfloor^2 + 2\left\lfloor \frac{n}{2} \right\rfloor + (k-1)^2]\sum_{i=0}^{k-1} d^i + n[\left\lfloor \frac{n}{2} \right\rfloor^2 + 2\left\lfloor \frac{n}{2} \right\rfloor + (k-1)^2]\sum_{i=0}^{k-1} d^i ,$$

(v) $$\xi_2(C(d,k,n)) = n\sum_{i=1}^{k-1} i^2 d^i + n[(d+1)(\left\lfloor \frac{n}{2} \right\rfloor + k - 1) - 1]\sum_{i=1}^{k-2} id^i + n[\left\lfloor \frac{n}{2} \right\rfloor^2 + 2(k-1)\left\lfloor \frac{n}{2} \right\rfloor + (k-1)^2](\sum_{i=1}^{k-1} d^i + 1) + n(k-1)d^{k-1}[\left\lfloor \frac{n}{2} \right\rfloor + k - 2] .$$

CONCLUSIONS

In this paper, we performed a topological study on several molecular graphs constructed from copies of Bethe trees, by applying graph theoretical methods, to obtain explicit formulas for calculation of the eccentric connectivity index, total eccentricity, average eccentricity, and first and second Zagreb eccentricity indices of these structures. These descriptors can be used in topological analysis of enzymes (in general, proteins) to identify structural similarities and ways of reactions.

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