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Elliptic Sombor Index of Graphs From Primary Subgraphs

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Abstract Suppose that G is a connected graph constructed from pairwise disjoint connected graphs $G_1, \ldots, G_t$ by selecting a vertex of G_1, a vertex of G_2, and identifying these two vertices. Then continue in this manner inductively. The graphs $G_1, \ldots, G_k$ are the primary subgraphs of G. Some particular cases of these graphs are important in chemistry which we consider them in this paper and study their elliptic Sombor index.

Keywords Sombor index · Elliptic Sombor index · Graph · Polymer

Mathematics Subject Classification (2010) 05C31

1 Introduction

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds of a molecule. Suppose that $G = (V, E)$ is a finite, connected, simple graph. As usual the degree of a vertex v in G is denoted by d_v.

The topological indices are the numerical parameters associated with the graph which are usually graph invariant. The topological index of a graph is based on the properties of graphs such as degree, distance, number of non-incident edges and so on. From this index it is possible to analyze the mathematical values and further investigate some physicochemical properties of a

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molecule. Therefore, it is also called a molecular descriptor. The first distance based topological index, is Wiener index

$$W(G) = \sum_{\{u,v\}\subseteq G} d(u,v) = \frac{1}{2}\sum_{u,v\in V(G)} d(u,v),$$

with the summation runs over all pairs of vertices of G [27]. The Wiener index is one of the most used topological indices with high correlation with many physical and chemical indices of molecular compounds [27]. The Sombor index which is a vertex-degree-based molecular structure descriptor introduced by Gutman in [16] and is defined as

$$SO(G) = \sum_{uv\in E(G)} \sqrt{d_u^2 + d_v^2}.$$

In a remarkably brief period, the Sombor index has garnered considerable attention from both mathematicians and theoretical chemists. Redžepović [23] delved into its efficacy in prognosticating alkanes' entropy as well as enthalpy of vaporization, utilizing statistical analyzing techniques. Owing to its notably enhanced predictive capabilities, the Sombor index is adopted regarding the purpose of modeling thermodynamic properties of organic molecular structures [19]. For more details and aspects on the Sombor index we refer the reader to [1,5,6,8,12,14,15,23,26].

In [17] a novel geometric method is proposed for constructing vertex-degree-based molecular structure descriptors (topological indices). The model is based on an ellipse whose focal points represent the degrees of a pair of adjacent vertices. The approach enables a geometric interpretation of several previously known topological indices, and lead to design of a few new. The area of the ellipse induces a vertex-degree-based topological index of remarkable simplicity, which is called elliptic Sombor index. In [17]), the elliptic Sombor index (ESO) of G is defined as

$$ESO(G) = \sum_{uv\in E(G)} (d_u + d_v)\sqrt{d_u^2 + d_v^2}.$$

In [10], the extremal value problem for ESO over the set of (connected) graphs with equal number of vertices has studied. Also, the elliptic Sombor energy has investigated in [2].

Suppose that G is a connected graph constructed from pairwise disjoint connected graphs $G_1, \ldots, G_t$ as follows. Select a vertex of G_1, a vertex of G_2, and identify these two vertices. Then continue in this manner inductively. Note that the graph G constructed in this way has a tree-like structure, the G_i's being its building stones (see Figure 1). The graphs $G_1, \ldots, G_k$ are the primary subgraphs of G. Usually say that G is a graph (polymer graph), obtained by point-attaching from $G_1, \ldots, G_t$ and that G_i's are the monomer units of G. A particular case of this construction is the decomposition of a connected graph into blocks (see [9]). For more details and aspects on the polymers, we refer the reader to [1,11,13]. In [1] we have studied the Sombor index of polymers.

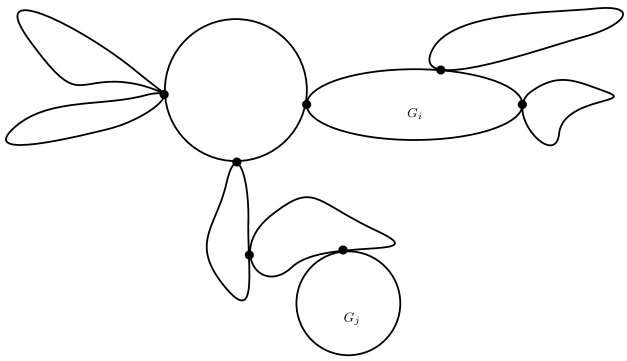

Fig. 1 A graph G obtained by point-attaching from $G_1, \ldots, G_t$.

We follow the paper [1] and since we think that the similar results for elliptic Sombor index are useful for researchers, we consider the elliptic Sombor index of graphs from primary subgraphs. In Section 2, the elliptic Sombor index of some graphs are computed from their monomer units. In Section 3, we apply the results of Section 2, in order to obtain the elliptic Sombor index of families of graphs that are of importance in chemistry.

2 Results for graph from primary subgraphs

In this section, we study the elliptic Sombor index of polymers (see [1]). By the definition of the elliptic Sombor index, we have the following easy result:

Proposition 1 *If G is a polymer graph with composed of monomers $\{G_i\}_{i=1}^k$, then*

$$ESO(G) > \sum_{i=1}^{k} ESO(G_i).$$

We consider some particular cases of these graphs and study their elliptic Sombor index. As an example of point-attaching graph, consider the graph K_m and m copies of K_n. Suppose that the graph $Q(m,n)$ is obtained by identifying each vertex of K_m with a vertex of a unique K_n. The graph $Q(5,4)$ is shown in Figure 2. The ESO index of $Q(m,n)$ is easy to compute.

Theorem 1 *For the graph $Q(m,n)$ (see Figure 2), and $n \geq 2$ we have:*

$$\begin{aligned} ESO(Q(m,n)) &= m((m+n-2)^2(m-1) + (n-1)^3(n-2))\sqrt{2} \\ &\quad + m(n-1)(m+2n-3)\sqrt{(m+n-2)^2+(n-1)^2}. \end{aligned}$$

Proof There are $\frac{m(m-1)}{2}$ edges with endpoints of degree $m+n-2$. Also there are $m(n-1)$ edges with endpoints of degree $m+n-2$ and $n-1$ and there

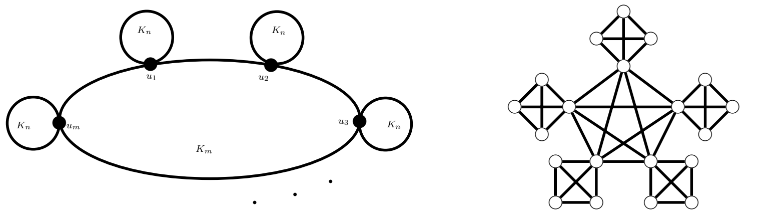

Fig. 2 The graph $Q(m,n)$ and $Q(5,4)$, respectively.

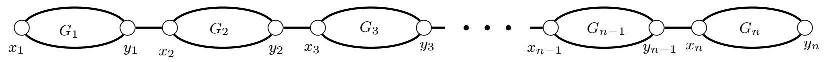

Fig. 3 Link of n graphs $G_1, G_2, \ldots, G_n$

are $m(n-1)(\frac{n}{2}-1)$ edges with endpoints of degree $n-1$. Therefore

$$\begin{aligned} ESO(Q(m,n)) &= \frac{m(m-1)(2m+2n-4)}{2}\sqrt{(m+n-2)^2+(m+n-2)^2} \\ &+ m(n-1)(m+2n-3)\sqrt{(m+n-2)^2+(n-1)^2} \\ &+ m(n-1)(2n-2)(\frac{n}{2}-1)\sqrt{(n-1)^2+(n-1)^2}, \end{aligned}$$

and so we have the result. □

To obtain more results, we need the following theorem.

Theorem 2 *Suppose that $G=(V,E)$ is a graph and $e=uv\in E$. If d_w is the degree of vertex w in G, then,*

$$ESO(G-e) < ESO(G) - \frac{|d_u^2-d_v^2|}{\sqrt{2}}.$$

Proof First we remove edge e and find $ESO(G-e)$. Obviously, by adding edge e to $G-e$ and $(d_u+d_v)\sqrt{d_u^2+d_v^2}$ to $SO(G-e)$, the $ESO(G)$ is greater than $ESO(G-e)$. Since $\sqrt{a^2+b^2}\geq\frac{|a-b|}{\sqrt{2}}$, so

$$ESO(G) > ESO(G-e)+(d_u+d_v)\sqrt{d_u^2+d_v^2} \geq ESO(G-e)+\frac{(d_u+d_v)|d_u-d_v|}{\sqrt{2}},$$

and therefore we have the result. □

In the following we study the elliptic Sombor index for links of graphs, circuits of graphs, chains of graphs, and bouquets of graphs.

Theorem 3 *Suppose that G is a polymer graph with composed of monomers $\{G_i\}_{i=1}^k$ with respect to the vertices $\{x_i,y_i\}_{i=1}^k$. If G is the link of graphs (see Figure 3), then,*

$$ESO(G) > \sum_{i=1}^{k} ESO(G_i) + \sum_{i=1}^{k-1}\frac{|d_{x_{i+1}}^2-d_{y_i}^2|}{\sqrt{2}}.$$

Proof First we remove edge y_1x_2 (Figure 3). By Proposition 2, we have

$$ESO(G) > ESO(G - y_1x_2) + \frac{|d_{y_1}^2 - d_{x_2}^2|}{\sqrt{2}}.$$

If G' is the link graph related to graphs $\{G_i\}_{i=2}^k$ with respect to the vertices $\{x_i, y_i\}_{i=2}^k$, then,

$$ESO(G - y_1x_2) = ESO(G_1) + ESO(G'),$$

and so,

$$ESO(G) > ESO(G_1) + ESO(G') + \frac{|d_{y_1}^2 - d_{x_2}^2|}{\sqrt{2}}.$$

By continuing this process, we have the result. □

Theorem 4 *Let $G_1, G_2, \ldots, G_k$ be a finite sequence of pairwise disjoint connected graphs and let $x_i \in V(G_i)$. Suppose that G is the circuit of graphs $\{G_i\}_{i=1}^k$ with respect to the vertices $\{x_i\}_{i=1}^k$ and obtained by identifying the vertex x_i of the graph G_i with the i-th vertex of the cycle graph C_k (Figure 4). Then,*

$$ESO(G) > \frac{|d_{x_1}^2 - d_{x_n}^2|}{\sqrt{2}} + \sum_{i=1}^{k} ESO(G_i) + \sum_{i=1}^{k-1} \frac{|d_{x_i}^2 - d_{x_{i+1}}^2|}{\sqrt{2}}.$$

Proof First we remove edge x_nx_1 (Figure 4). By Proposition 2, we have

$$ESO(G) > ESO(G - x_nx_1) + \frac{|d_{x_n}^2 - d_{x_1}^2|}{\sqrt{2}}.$$

Now we remove edge x_1x_2. So,

$$ESO(G) > ESO(G - \{x_nx_1, x_1x_2\}) + \frac{|d_{x_n}^2 - d_{x_1}^2|}{\sqrt{2}} + \frac{|d_{x_2}^2 - d_{x_1}^2|}{\sqrt{2}}.$$

Suppose that G' is the graph related to circuit graph with $\{G_i\}_{i=2}^k$ with respect to the vertices $\{x_i\}_{i=2}^k$ and removing the edge x_nx_1. Then we have,

$$ESO(G - \{x_nx_1, x_1x_2\}) = ESO(G_1) + ESO(G'),$$

and therefore,

$$ESO(G) > ESO(G_1) + ESO(G') + \frac{|d_{x_n}^2 - d_{x_1}^2|}{\sqrt{2}} + \frac{|d_{x_2}^2 - d_{x_1}^2|}{\sqrt{2}}.$$

By continuing this process, we have the result. □

In the following theorem we present another lower bound for the elliptic Sombor index of the circuit of graphs.

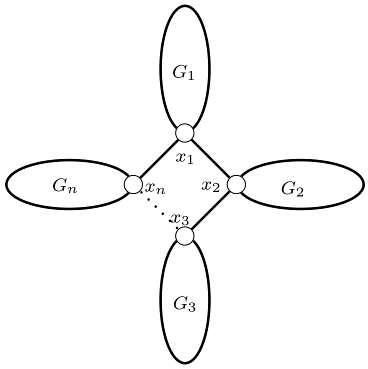

Fig. 4 Circuit of n graphs $G_1, G_2, \ldots, G_n$

Theorem 5 *Let $G_1, G_2, \ldots, G_k$ be a finite sequence of pairwise disjoint connected graphs and let $x_i \in V(G_i)$. Suppose that G is the circuit of graphs $\{G_i\}_{i=1}^k$ with respect to the vertices $\{x_i\}_{i=1}^k$ and obtained by identifying the vertex x_i of the graph G_i with the i-th vertex of the cycle graph C_k (Figure 4). Then,*

$$ESO(G) \geq 8k\sqrt{2} + \sum_{i=1}^{k} ESO(G_i).$$

The equality holds if and only if for every $1 \leq i \leq k$, $G_i = K_1$.

Proof Let d_i be the degree of the vertex x_i before creating G. Since $d(x_i) = d_i + 2$, we have:

$$\begin{aligned}
ESO(G) &= (d_k + 2 + d_1 + 2)\sqrt{(d_k + 2)^2 + (d_1 + 2)^2} \\
&\quad + \sum_{i=1}^{k-1} (d_i + 2 + d_{i+1} + 2)\sqrt{(d_i + 2)^2 + (d_{i+1} + 2)^2} \\
&\quad + \sum_{i=1}^{k} \Big(\sum_{uv \in E(G_i - x_i)} (d_u + d_v)\sqrt{d_u^2 + d_v^2} + \sum_{x_i \sim u \in G_i} (d_i + 2 + d_u)\sqrt{(d_i + 2)^2 + d_u^2} \Big) \\
&\geq 4\sqrt{4+4} + \sum_{i=1}^{k-1} 4\sqrt{4+4} \\
&\quad + \sum_{i=1}^{k} \Big(\sum_{uv \in E(G_i - x_i)} (d_u + d_v)\sqrt{d_u^2 + d_v^2} + \sum_{x_i \sim u \in G_i} (d_i + 2 + d_u)\sqrt{(d_i + 2)^2 + d_u^2} \Big) \\
&= 8k\sqrt{2} + \sum_{i=1}^{k} SO(G_i).
\end{aligned}$$

If G_i has at least one edge then the equality does not hold and so we have the result. □

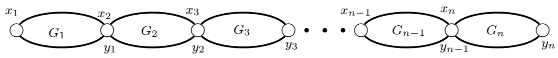

Fig. 5 Chain of n graphs $G_1, G_2, \ldots, G_n$

Theorem 6 *Let $G_1, G_2, \ldots, G_n$ be a finite sequence of pairwise disjoint connected graphs and let $x_i, y_i \in V(G_i)$. Suppose that $C(G_1, \ldots, G_n)$ is the chain of graphs $\{G_i\}_{i=1}^n$ with respect to the vertices $\{x_i, y_i\}_{i=1}^k$ which obtained by identifying the vertex y_i with the vertex x_{i+1} for $i = 1, 2, \ldots, n-1$ (Figure 5). Then,*

(i)

$$ESO(C(G_1, \ldots, G_n)) > ESO(C(G_1, \ldots, G_{n-1}) + ESO(G_n - y_{n-1}) + \sum_{\substack{u \sim y_{n-1} \\ u \in V(G_n)}} \frac{|d_u^2 - d_{y_{n-1}}^2|}{\sqrt{2}}.$$

(ii)

$$ESO(C(G_1, \ldots, G_n)) > ESO(C(G_1)) + \sum_{i=2}^{n} ESO(G_i - y_{i-1}) + \sum_{i=1}^{n-1} \sum_{\substack{u \sim y_i \\ u \in V(G_{i+1})}} \frac{|d_u^2 - d_{y_i}^2|}{\sqrt{2}}.$$

Proof (i) Consider $C(G_1, \ldots, G_n)$ in Figure 5. Using inductively Theorem 2 for all edges in G_n which one of the their end vertices is y_{n-1} we have the result.

(ii) It follows by induction and Part (i). □

Similar to the Theorem 6 we have:

Theorem 7 *Let $G_1, G_2, \ldots, G_n$ be a finite sequence of pairwise disjoint connected graphs and let $x_i \in V(G_i)$. Let $B(G_1, \ldots, G_n)$ be the bouquet of graphs $\{G_i\}_{i=1}^n$ with respect to the vertices $\{x_i\}_{i=1}^n$ and obtained by identifying the vertex x_i of the graph G_i with x (see Figure 6). Then,*

$$ESO(B(G_1, \ldots, G_n)) > ESO(G_1) + \sum_{i=2}^{n} ESO(G_i - x_i) + \sum_{i=1}^{n-1} \sum_{\substack{u \sim x_{i+1} \\ u \in V(G_{i+1})}} \frac{|d_u^2 - d_{x_{i+1}}^2|}{\sqrt{2}}.$$

3 Chemical applications

In this section, using results of Section 2 to obtain the elliptic Sombor index of families of graphs that are of importance in chemistry.

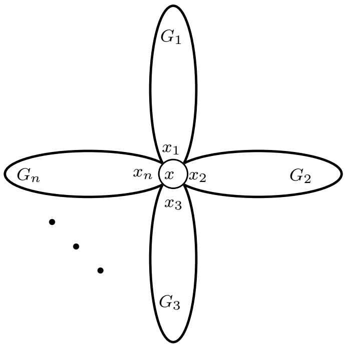

Fig. 6 Bouquet of n graphs $G_1, G_2, \ldots, G_n$ and $x_1 = x_2 = \ldots = x_n = x$

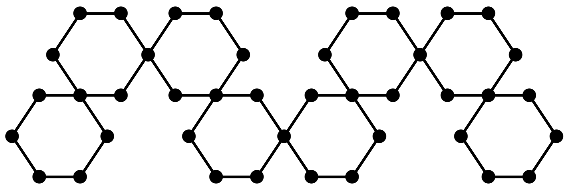

Fig. 7 The graph $S_{6,2,8}$

3.1 Spiro-chains

Spiro-chains are defined in [7]. Using the concept of chain of graphs, a spiro-chain can be defined as a chain of cycles. We denote by $S_{q,h,k}$ the chain of k cycles C_q in which the distance between two consecutive contact vertices is h (see $S_{6,2,8}$ in Figure 7).

Theorem 8 *ESO index of the graph $S_{q,h,k}$, for $h \geq 2$ is:*

$$ESO(S_{q,h,k}) = (8qk - 32k + 32)\sqrt{2} + (24k - 24)\sqrt{5}.$$

Proof There are $4(k-1)$ edges with endpoints of degree 2 and 4. Also there are $qk - 4(k-1)$ edges with endpoints of degree 2. So, we have the result. □

Theorem 9 *The ESO index of the graph $S_{q,1,k}$ is:*

$$ESO(S_{q,1,k}) = (8qk + 8k - 48)\sqrt{2} + 48k\sqrt{5}.$$

Proof There are $k-2$ edges with endpoints of degree 4. Also there are $2k$ edges with endpoints of degree 4 and 2, and there are $qk - 3k + 2$ edges with endpoints of degree 2. Therefore we have the result. □

Cactus graphs were first known as Husimi tree, are a class of simple linear polymers. They appeared in the scientific literature some sixty years ago in

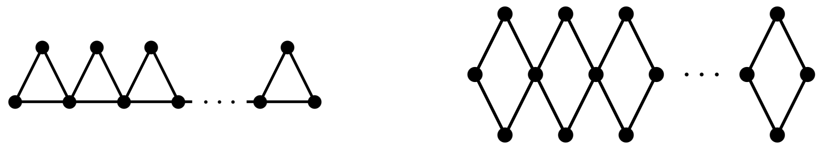

Fig. 8 Chain triangular cactus T_n and para-chain square cactus Q_n

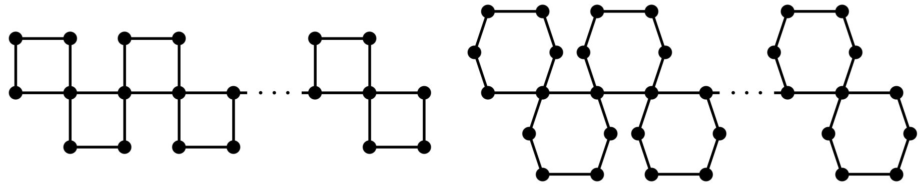

Fig. 9 Para-chain square cactus O_n and ortho-chain graph O_n^h

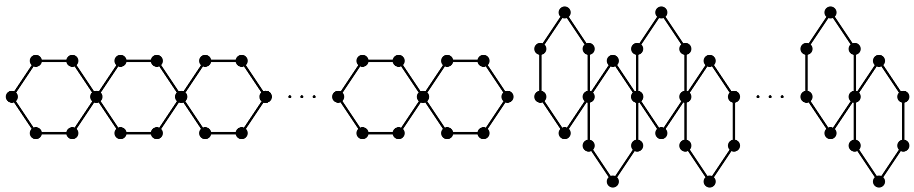

Fig. 10 Para-chain L_n and Meta-chain M_n

papers by Husimi and Riddell [18,20,24]. For some aspects of parameters of cactus graphs, refer to [4,22,25] .

As an immediate result of Theorems 8 and 9 we have the following results for cactus chains:

Corollary 1 *(i) If T_n is the chain triangular graph (see Figure 8) of order n, then for every $n \geq 2$, $ESO(T_n) = (32n-48)\sqrt{2} + 32n\sqrt{5}$.*

(ii) If Q_n is the para-chain square cactus graph (see Figure 8) of order n, then for every $n \geq 2$, $ESO(Q_n) = 32\sqrt{2} + (48n-48)\sqrt{5}$.

(iii) If O_n is the para-chain square cactus (see Figure 9) graph of order n, then for every $n \geq 2$, $ESO(O_n) = (40n-48)\sqrt{2} + 24n\sqrt{5}$.

(iv) If O_n^h is the Ortho-chain graph (see Figure 9) of order n, then for every $n \geq 2$, $ESO(O_n^h) = (56n-48)\sqrt{2} + 24n\sqrt{5}$.

(v) If L_n is the para-chain hexagonal cactus graph (see Figure 10) of order n, then for every $n \geq 2$, $ESO(L_n) = (16n+32)\sqrt{2} + (48n-48)\sqrt{5}$.

(vi) If M_n is the Meta-chain hexagonal cactus graph (see Figure 10) of order n, then for every $n \geq 2$, $ESO(M_n) = (16n+32)\sqrt{2} + (48n-48)\sqrt{5}$.

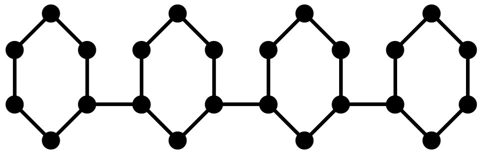

Fig. 11 The graph $L_{6,2,4}$

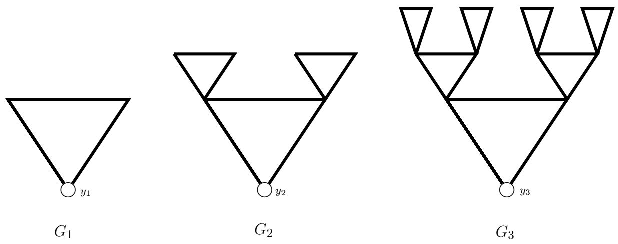

Fig. 12 Graphs G_1, G_2 and G_3

3.2 Polyphenylenes

Similar to the definition of the spiro-chain $S_{q,h,k}$, we can define the graph $L_{q,h,k}$ as the link of k cycles C_q in which the distance between the two contact vertices in the same cycle is h (see $L_{6,2,4}$ in Figure 11).

Theorem 10 *The ESO index of the graph $L_{q,h,k}$, for $h \geq 2$ is:*

$$ESO(L_{q,h,k}) = (8qk - 14k + 14)\sqrt{2} + (20k - 20)\sqrt{13}.$$

Proof There are $k-1$ edges with endpoints of degree 3. Also there are $4(k-1)$ edges with endpoints of degree 3 and 2, and there are $qk - 4(k-1)$ edges with endpoints of degree 2. Therefore we have the result. □

Theorem 11 *The ESO index of the graph $L_{q,1,k}$ is:*

$$ESO(L_{q,1,k}) = (8qk + 12k - 38)\sqrt{2} + 10k\sqrt{13}.$$

Proof There are $2k - 3$ edges with endpoints of degree 3. Also there are $2k$ edges with endpoints of degree 3 and 2, and there are $qk - 3k + 2$ edges with endpoints of degree 2. Therefore we have the result. □

3.3 Triangulanes

We want to obtain the elliptic Sombor index of the triangulane T_k defined pictorially in [21]. The triangulane T_k is defined recursively in a manner that is useful in our approach. First define recursively an auxiliary family of triangulanes G_k ($k \geq 1$). Let G_1 be a triangle and denote one of its vertices by y_1.

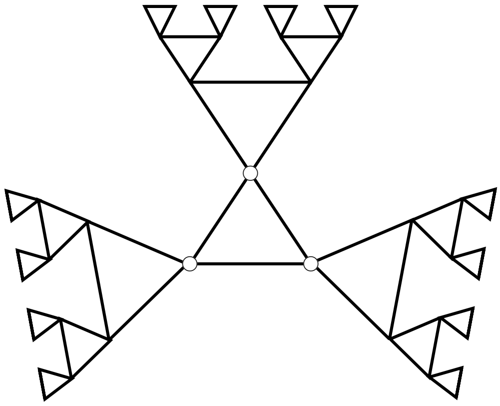

Fig. 13 Graphs T_3

Define G_k $(k \geq 2)$ as the circuit of the graphs G_{k-1}, G_{k-1}, and K_1 and denote by y_k the vertex where K_1 has been placed. The graphs G_1, G_2 and G_3 are shown in Figure 12.

Theorem 12 *The ESO index of the graph T_k (see T_3 in Figure 13) is:*

$$ESO(T_k) = \big(288(2^{k-1} - 1) + 24(2^{k-1}) + 96\big)\sqrt{2} + 36(2^k)\sqrt{5}.$$

Proof By recursive structure of the graph T_k, observe that there are $3 + 3\sum_{n=0}^{k-2} 3(2^n)$ edges with endpoints of degree 4. Also there are $3(2^k)$ edges with endpoints of degree 4 and 2, and there are $3(2^{k-1})$ edges with endpoints of degree 2. Therefore

$$ESO(T_k) = (3 + 9\sum_{n=0}^{k-2} 2^n)(8)\sqrt{16+16} + 3(2^k)(6)\sqrt{16+4} + 3(2^{k-1})(4)\sqrt{4+4},$$

and so we have the result. □

3.4 Nanostar dendrimers

In this subsection, we want to compute the elliptic Sombor index of the nanostar dendrimer D_k defined in [3]. In order to define D_k, we follow [9]. First we define recursively an auxiliary family of rooted dendrimers G_k $(k \geq 1)$. We need a fixed graph F defined in Figure 14, we consider one of its endpoint to be the root of F.

The graph G_1 is defined in Figure 14, the leaf being its root. Now we define G_k $(k \geq 2)$ the bouquet of the following three graphs: G_{k-1}, G_{k-1}, and F with respect to their roots; the root of G_k is taken to be its unique leaf (see G_2 and G_3 in Figure 15). Finally, we define D_k $(k \geq 1)$ as the bouquet of three copies of G_k with respect to their roots (D_2 is shown in Figure 16, where the circles represent hexagons).

Fig. 14 Graphs F and G_1, respectively.

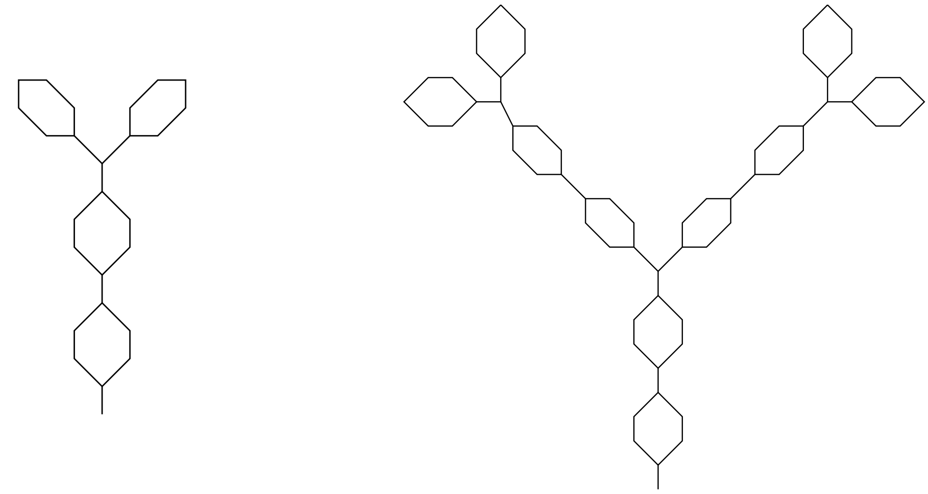

Fig. 15 Graphs G_2 and G_3, respectively.

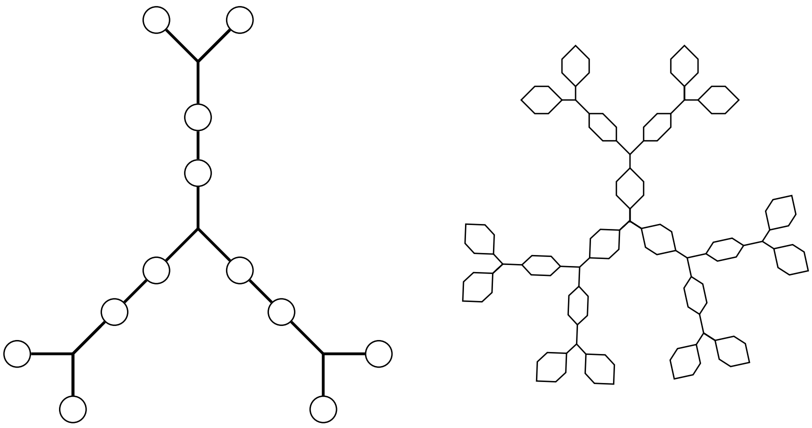

Fig. 16 Nanostar D_2 and $D_3[2]$, respectively.

Theorem 13 *The ESO index of the dendrimer* $D_3[n]$ *(see* $D_3[2]$ *in Figure 16) is:*

$$ESO(D_3[n]) = (468 \times 2^n + 204)\sqrt{2} + (90 \times 2^n + 30)\sqrt{13}.$$

Proof There are $3+9\sum_{k=0}^{n-1}2^k$ edges with endpoints of degree 3. Also there are $6+18\sum_{k=0}^{n-1}2^k$ edges with endpoints of degree 3 and 2, and there are $12+18\sum_{k=0}^{n-1}2^k$ edges with endpoints of degree 2. Therefore

$$ESO(D_3[n]) = (3+9\sum_{k=0}^{n-1}2^k)(6)\sqrt{9+9} + (6+18\sum_{k=0}^{n-1}2^k)(5)\sqrt{9+4} + (12+18\sum_{k=0}^{n-1}2^k)(4)\sqrt{4+4},$$

and we have the result. □

Disclosure and data availability statements.

The authors report there are no competing interests to declare. Also there is no data set associated with the paper.

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