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Sombor Index of Polymers

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Abstract

Let $G = (V, E)$ be a finite simple graph. The Sombor index $SO(G)$ of G is defined as $\sum_{uv\in E(G)} \sqrt{d_u^2 + d_v^2}$, where d_u is the degree of vertex u in G. Let G be a connected graph constructed from pairwise disjoint connected graphs $G_1, \ldots, G_k$ by selecting a vertex of G_1, a vertex of G_2, and identifying these two vertices. Then continue in this manner inductively. We say that G is a polymer graph, obtained by point-attaching from monomer units $G_1, ..., G_k$. In this paper, we consider some particular cases of these graphs that are of importance in chemistry and study their Sombor index.

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. Let $G = (V, E)$ be a finite, connected, simple graph. We denote the degree of a vertex v in G by d_v. A topological index of G is a real number related to G. It does not depend on the labeling or pictorial representation of a graph. The Wiener index $W(G)$ is the first distance based topological index defined as $W(G) = \sum_{\{u,v\}\subseteq G} d(u, v) = \frac{1}{2}\sum_{u,v\in V(G)} d(u, v)$ with the summation runs over all pairs of vertices of G [18]. The topological indices and graph invariants based on distances between vertices of a graph are widely used for characterizing molecular graphs, establishing relationships between structure and properties of molecules, predicting biological activity of chemical

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compounds, and making their chemical applications. The Wiener index is one of the most used topological indices with high correlation with many physical and chemical indices of molecular compounds [18]. Recently in [9] a new vertex-degree-based molecular structure descriptor was put forward, the Sombor index, defined as

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

Cruz, Gutman and Rada in [3] characterized the graphs extremal with respect to this index over the chemical graphs, chemical trees and hexagon systems (see [8]). In [5], the chemical importance of the Sombor index has investigated and it is shown that this index is useful in predicting physico-chemical properties with high accuracy compared to some well-established and often used indices. Also a sharp upper bound for the Sombor index among all molecular trees with fixed numbers of vertices has obtained, and those molecular trees achieving the extremal value has characterized. In [14] the predictive and discriminative potentials of Sombor index, reduced Sombor index, and average Sombor index examined. All three topological molecular descriptors showed good predictive potential. In [4] some novel lower and upper bounds on the Sombor index of graphs has presented by using some graph parameters, especially, maximum and minimum degree. Moreover, several relations on Sombor index with the first and second Zagreb indices of graphs obtained. The mathematical relations between the Sombor index and some other well-known degree-based descriptors investigated in [17].

In this paper, we consider the Sombor index of polymer graphs. Such graphs can be decomposed into subgraphs that we call monomer units. Blocks of graphs are particular examples of monomer units, but a monomer unit may consist of several blocks. For convenience, the definition of these kind of graphs will be given in the next section. In Section 2, the 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 Sombor index of families of graphs that are of importance in chemistry.

2 Sombor index of polymers

Let G be a connected graph constructed from pairwise disjoint connected graphs $G_1, \ldots, G_k$ 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). Usually say that G is a polymer graph, obtained by point-attaching from $G_1, \ldots, G_k$ 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 [7]).

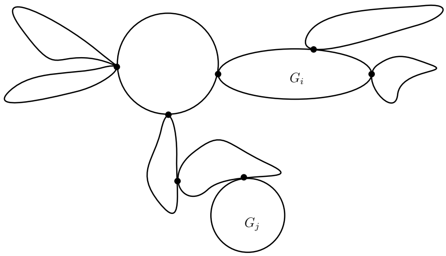

Figure 1. A polymer graph with monomer units $G_1, \ldots, G_k$.

By the definition of the Sombor index, we have the following easy result:

Proposition 2.1 *Let G be a polymer graph with composed of monomers $\{G_i\}_{i=1}^k$. Then*

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

We consider some particular cases of these graphs and study their Sombor index. As an example of point-attaching graph, consider the graph K_m and m copies of K_n. By definition, 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.

Theorem 2.2 *For the graph $Q(m, n)$ (see Figure 2), and $n \geq 2$ we have:*

$$SO(Q(m,n)) = m(\frac{(m+n-2)(m-1)}{2} + (n-1)^2(\frac{n}{2}-1))\sqrt{2}$$
$$+ m(n-1)\sqrt{(m+n-2)^2+(n-1)^2}.$$

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

$$SO(Q(m,n)) = \frac{m(m-1)}{2}\sqrt{(m+n-2)^2+(m+n-2)^2}$$
$$+ m(n-1)\sqrt{(m+n-2)^2+(n-1)^2}$$
$$+ m(n-1)(\frac{n}{2}-1)\sqrt{(n-1)^2+(n-1)^2},$$

and we have the result. ■

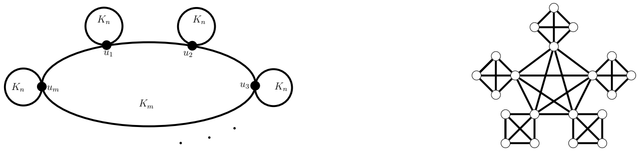

Figure 2. The graph $Q(m,n)$ and $Q(5,4)$, respectively.

To obtain more results, we need the following theorem:

Theorem 2.3 [8] *Let $G=(V,E)$ be a graph and $e=uv \in E$. Also let d_w be the degree of vertex w in G. Then,*

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

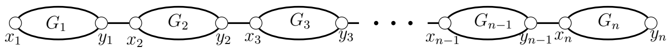

Figure 3. Link of n graphs $G_1, G_2, \ldots, G_n$

Here we study the Sombor index for links of graphs, circuits of graphs, chains of graphs, and bouquets of graphs.

Theorem 2.4 *Let G be a polymer graph with composed of monomers $\{G_i\}_{i=1}^k$ with respect to the vertices $\{x_i, y_i\}_{i=1}^k$. Let G be the link of graphs (see Figure 3). Then,*

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

Proof. First we remove edge y_1x_2 (Figure 3). By Proposition 2.3, we have

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

Let G' be the link graph related to graphs $\{G_i\}_{i=2}^k$ with respect to the vertices $\{x_i, y_i\}_{i=2}^k$. Then we have,

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

and therefore,

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

By continuing this process, we have the result. ■

Theorem 2.5 *Let $G_1, G_2, \ldots, G_k$ be a finite sequence of pairwise disjoint connected graphs and let $x_i \in V(G_i)$. Let G be 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,*

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

Proof. First we remove edge $x_n x_1$ (Figure 4). By Proposition 2.3, we have

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

Now we remove edge $x_1 x_2$. Then,

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

Let G' be 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 $x_n x_1$. Then we have,

$$SO(G - \{x_n x_1, x_1 x_2\}) = SO(G_1) + SO(G'),$$

and therefore,

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

By continuing this process, we have the result. ■

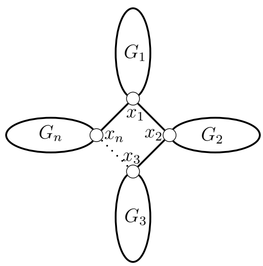

Figure 4. Circuit of n graphs $G_1, G_2, \ldots, G_n$

The following theorem is another lower bound for the Sombor index of the circuit of graphs.

Theorem 2.6 *Let $G_1, G_2, \ldots, G_k$ be a finite sequence of pairwise disjoint connected graphs and let $x_i \in V(G_i)$. Let G be 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,*

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

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:

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

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

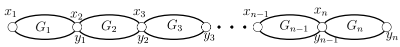

Figure 5. Chain of n graphs $G_1, G_2, \ldots, G_n$

Theorem 2.7 *Let $G_1, G_2, \ldots, G_n$ be a finite sequence of pairwise disjoint connected graphs and let $x_i, y_i \in V(G_i)$. Let $C(G_1, ..., G_n)$ be 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)

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

(ii)

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

Proof.

(i) Consider $C(G_1,...,G_n)$ in Figure 5. By using inductively Theorem 2.3 for all edges in G_n which one of the their end vertices is y_{n-1} we have the result.

(ii) The result follows by applying Part (i) inductively. ■

Similar to the Theorem 2.7 we have:

Theorem 2.8 *Let $G_1, G_2, \dots, G_n$ be a finite sequence of pairwise disjoint connected graphs and let $x_i \in V(G_i)$. Let $B(G_1,...,G_n)$ 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,*

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

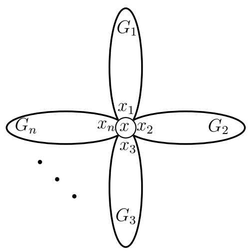

Figure 6. Bouquet of n graphs $G_1, G_2, \dots, G_n$ and $x_1 = x_2 = \dots = x_n = x$

3 Chemical applications

In this section, we apply our previous results in order to obtain the Sombor index of families of graphs that are of importance in chemistry.

3.1 Spiro-chains

Spiro-chains are defined in [6]. Making use of 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 3.1 *For the graph $S_{q,h,k}$, when $h \geq 2$, we have:*

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

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. Therefore

$$SO(S_{q,h,k}) = 4(k-1)\sqrt{4+16} + (qk - 4(k-1))\sqrt{4+4},$$

and we have the result. ■

Theorem 3.2 *For the graph $S_{q,1,k}$, we have:*

$$SO(S_{q,1,k}) = (2qk - 2k - 4)\sqrt{2} + 4k\sqrt{5}.$$

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

$$SO(S_{q,1,k}) = (k-2)\sqrt{16+16} + 2k\sqrt{16+4} + (qk - 3k + 2)\sqrt{4+4},$$

and we have the result. ■

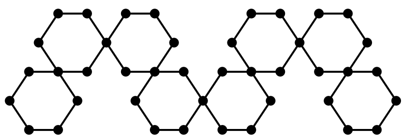

Figure 7. The graph $S_{6,2,8}$

Cactus graphs which are a class of simple linear polymers, were first known as Husimi tree, they appeared in the scientific literature some sixty years ago in papers by Husimi and Riddell concerned with cluster integrals in the theory of condensation in statistical mechanics [10, 11, 15]. We refer the reader to papers [2, 13, 16] for some aspects of parameters of cactus graphs.

As an immediate result of Theorems 3.1 and 3.2 we have the following results for cactus chains (see [8]):

Corollary 3.3 [8]

(i) Let T_n be the chain triangular graph (see Figure 8) of order n. Then for every $n \geq 2$, $SO(T_n) = (4n-4)\sqrt{2} + 4n\sqrt{5}$.

(ii) Let Q_n be the para-chain square cactus graph (see Figure 8) of order n. Then for every $n \geq 2$, $SO(Q_n) = 8\sqrt{2} + (8n-8)\sqrt{5}$.

(iii) Let O_n be the para-chain square cactus (see Figure 9) graph of order n. Then for every $n \geq 2$, $SO(O_n) = (6n-4)\sqrt{2} + 4n\sqrt{5}$.

(iv) Let O_n^h be the Ortho-chain graph (see Figure 9) of order n. Then for every $n \geq 2$, $SO(O_n^h) = (10n-4)\sqrt{2} + 4n\sqrt{5}$.

(v) Let L_n be the para-chain hexagonal cactus graph (see Figure 10) of order n. Then for every $n \geq 2$, $SO(L_n) = (4n+8)\sqrt{2} + (8n-8)\sqrt{5}$.

(vi) Let M_n be the Meta-chain hexagonal cactus graph (see Figure 10) of order n. Then for every $n \geq 2$, $SO(M_n) = (4n+8)\sqrt{2} + (8n-8)\sqrt{5}$.

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

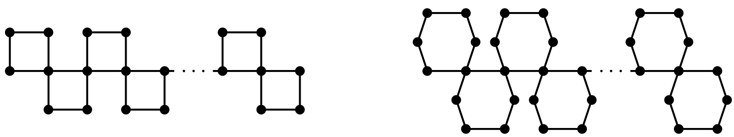

Figure 9. Para-chain square cactus O_n and ortho-chain graph O_n^h

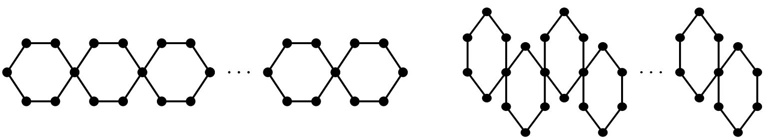

Figure 10. Para-chain L_n and Meta-chain M_n

3.2 Polyphenylenes

Similarly to the above 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 3.4 *For the graph $L_{q,h,k}$, when $h \geq 2$, we have:*

$$SO(L_{q,h,k}) = (2qk - 5k + 5)\sqrt{2} + (4k - 4)\sqrt{13}.$$

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

$$SO(L_{q,h,k}) = (k - 1)\sqrt{9 + 9} + 4(k - 1)\sqrt{9 + 4} + (qk - 4(k - 1))\sqrt{4 + 4},$$

and we have the result. ■

Theorem 3.5 *For the graph $L_{q,1,k}$, we have:*

$$SO(L_{q,1,k}) = (2qk - 5)\sqrt{2} + 2k\sqrt{13}.$$

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

$$SO(L_{q,1,k}) = (2k - 3)\sqrt{9 + 9} + 2k\sqrt{9 + 4} + (qk - 3k + 2)\sqrt{4 + 4},$$

and we have the result. ■

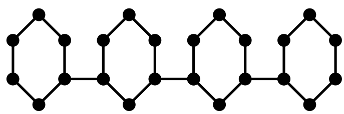

Figure 11. The graph $L_{6,2,4}$

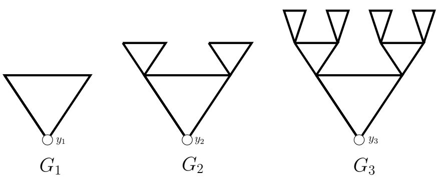

Figure 12. Graphs G_1, G_2 and G_3

3.3 Triangulanes

We intend to derive the Sombor index of the triangulane T_k defined pictorially in [12]. We define T_k recursively in a manner that will be useful in our approach. First we 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. We 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.

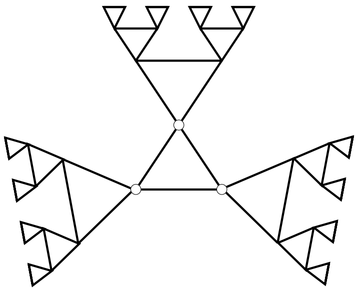

Figure 13. Graphs T_3

Theorem 3.6 *For the graph T_k (see T_3 in Figure 13), we have:*

$$SO(T_k) = \big(36(2^{k-1} - 1) + 6(2^{k-1}) + 12\big)\sqrt{2} + 6(2^k)\sqrt{5}.$$

Proof. Since creating such a graph is recursive, then 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

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

and we have the result. ■

3.4 Nanostar dendrimers

We want to compute the Sombor index of the nanostar dendrimer D_k defined in [1]. In order to define D_k, we follow [7]. 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 3 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 3 copies of G_k with respect to their roots (D_2 is shown in Figure 16, where the circles represent hexagons).

Figure 14. Graphs F and G_1, respectively.

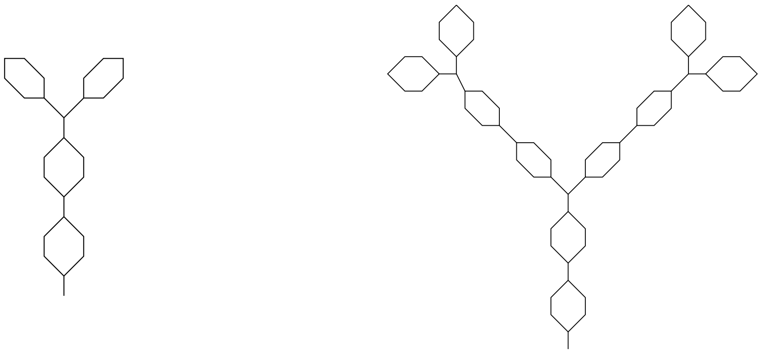

Figure 15. Graphs G_2 and G_3, respectively.

Theorem 3.7 *For the dendrimer $D_3[n]$ (see $D_3[2]$ in Figure 16) we have:*

$$SO(D_3[n]) = (63 \times 2^n - 30)\sqrt{2} + (18 \times 2^n - 12)\sqrt{13}.$$

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

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

and we have the result. ∎

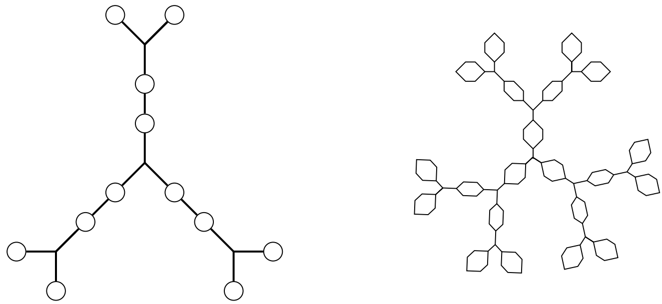

Figure 16. Nanostar D_2 and $D_3[2]$, respectively.

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