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Calculating Sombor Index of Certain Networks

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Abstract

Recently I. Gutman [5] have put forward a novel topological index viz., Sombor index of molecular graph G. In this paper, we compute the Sombor index of certain chemical networks like hexagonal parallogram, tringular benzoid, zig-zag edge coronoid and dominating networks of three kinds.

Keywords: Sombor index, nanostructures, chemical network.

$\mathcal{AMS}$ **Subject Classification:** 05C90; 05C35; 05C12.

1 Introduction

In mathematical chemistry, topological indices plays vital role in prediction of physical properties. Topological indices are technically relevent tools for QSPR / QSAR studies. Basically, topological index is just a positive integer to indicate the structural property of a molecule. Various novel topological indices have been studied so far, such as Zagreb indices [4], forgotten index [2] etc., for more details on topological indices refer [7-14].

Sombor index was put forward in [5] which is defined as follows:

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

2 Chemical Structures

R In this section we consider the chemical structures like hexagonal parallelogram $P(m,n)$-nanotube, triangular benzenoid G_n, zigzag-edge coronoid fused with starphene nanotubes $ZCS(k,l,m)$ and dominating derived networks D_1, D_2, D_3.

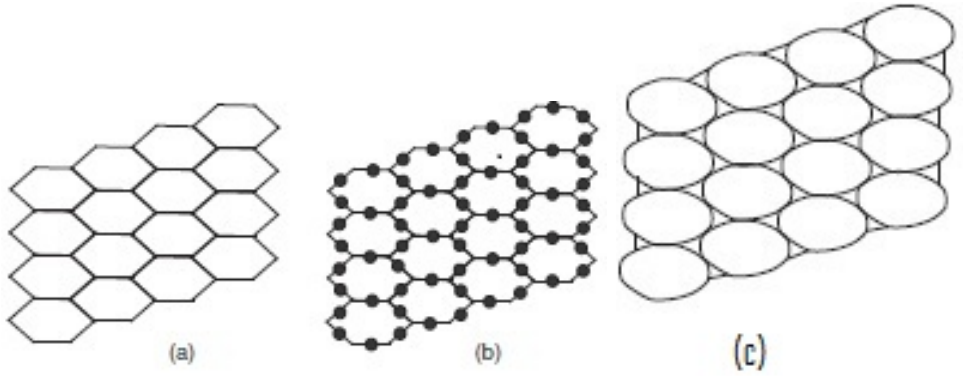

Figure 1: (a)$P(4,4)$ (b) $S(P(4,4))$ (c) $L(S(P(4,4)))$

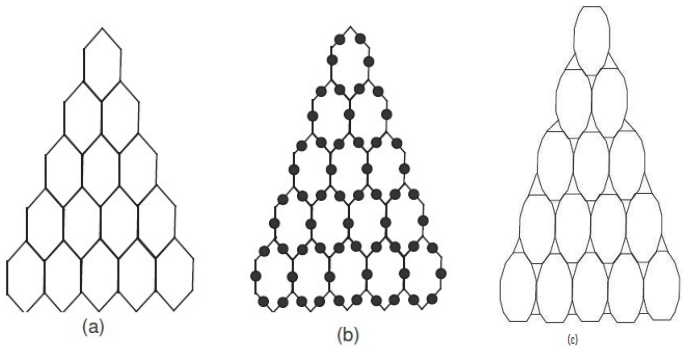

Figure 2: (a) G_n for $n = 5$(b) $S(G_n)$ (c) $L(S(G_n))$

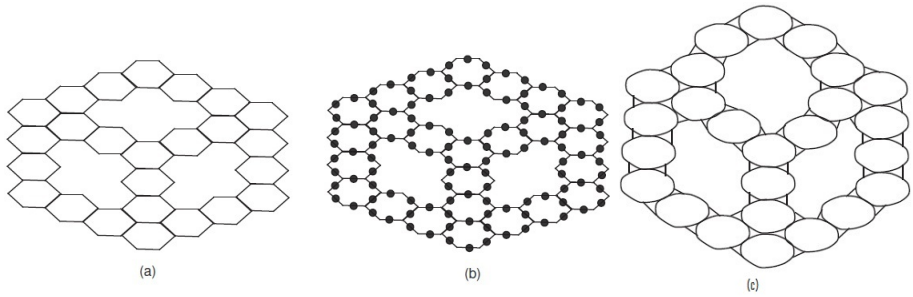

Figure 3: (a) $ZCS(k,l,m)$ for $k = l = m = 4$ (b) $S(ZCS(k,l,m))$ (c) $L(S(ZCS(k,l,m)))$

Theorem 1. *Let G denotes the line graph of subdivision graph of the hexagonal parallelogram, then*

$$SO(G) \quad = \quad 2\sqrt{2}(\alpha+\beta+4)+4\sqrt{13}(\alpha+\beta-2)+3\sqrt{2}(9\alpha\beta-2\alpha+2\beta-5)$$

Proof. Let G denotes the line graph of the hexagonal parallelogram $P(m,n); m,n \in \mathbb{Z}^+$. Then the order and size of $P(m,n)$ and G are given by:

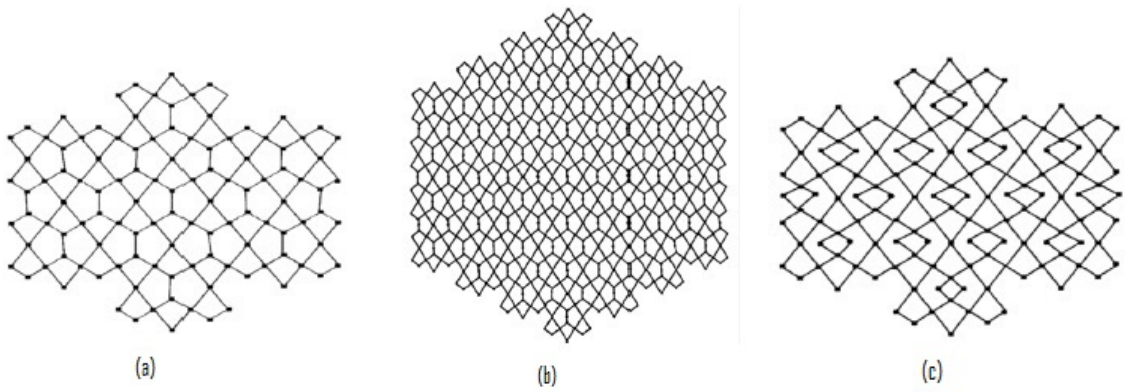

Figure 4: (a) $D_1(2)$ (b) $D_2(4)$ (c) $D_3(n)$

Table 1.

Graph	Order	Size
$P(m,n)$	$2(\alpha+\beta+\alpha\beta)$	$3\alpha\beta+2\alpha+2\beta+1$
$G=L(P(m,n))$	$2(3\alpha\beta+2\alpha+2\beta+1)$	$9\alpha\beta+4\alpha+4\beta+5$

The edge set of $L(P(m,n))$ can be partitioned into three disjoint sets $E_{2,2}, E_{2,3}$ and $E_{3,3}$, where $E(G)=E_{2,2}\cup E_{2,3}\cup E_{3,3}$. By algebraic method the edge partition of G is calculated as:

Table 2.

$uv\in E(G)$	$(2,2)$	$(2,3)$	$(3,3)$
Number of edges	$2(\alpha+\beta+4)$	$4(\alpha+\beta-2)$	$9\alpha\beta-2m-2n-5$

Thus, using the information in Table 2, we have

$$\begin{aligned}
SO(G) &= \sum_{uv\in E(G)}\sqrt{d_G(u)^2+d_G(v)^2}\\
&= \sum_{uv\in E_{2,2}(G)}\sqrt{d_G(u)^2+d_G(v)^2}+\sum_{uv\in E_{2,3}(G)}\sqrt{d_G(u)^2+d_G(v)^2}\\
&+ \sum_{uv\in E_{3,3}(G)}\sqrt{d_G(u)^2+d_G(v)^2}\\
&= (\sqrt{2^2+2^2})2(\alpha+\beta+4)+\sqrt{2^2+3^2}(4(\alpha+\beta-2))+\sqrt{3^2+3^2}(9\alpha\beta-2m-2n-5).
\end{aligned}$$

as desired. □

Theorem 2. *Let $G=L(S(G_n))$ denotes the line graph of subdivision graph of the hexagonal parallelogram, then*

$$SO(L(S(G_n))) = 6\sqrt{2}(n+3)+6\sqrt{13}(n-1)+\frac{9}{\sqrt{2}}(3\alpha^2+n-4)$$

Proof. Let G denotes the line graph of the hexagonal parallelogram G_n. Then the order and size of $P(m,n)$ and G are given by:

Table 3.

Graph	Order	Size
G_n	α^2+4n+1	$\frac{3}{2}n(n+3)$
$G=L(S(G_n))$	$3n(n+3)$	$\frac{3(3\alpha^2+7n+2)}{2}$

The edge set of $L(S(G_n))$ can be partitioned into three disjoint sets $E_{2,2}, E_{2,3}$ and $E_{3,3}$, where $E(L(S(G_n))) = E_{2,2} \cup E_{2,3} \cup E_{3,3}$. By algebraic method the edge partition of G is calculated as:

Table 4.

$uv \in E(G)$	$(2,2)$	$(2,3)$	$(3,3)$
Number of edges	$3(n+3)$	$6(n-1)$	$\frac{3(3\alpha^2+7n+2)}{2}$

Thus, using the information in Table 4, we have

$$\begin{aligned} SO(G) &= \sum_{uv\in E(G)} \sqrt{d_G(u)^2+d_G(v)^2} \\ &= \sum_{uv\in E_{2,2}(G)} \sqrt{d_G(u)^2+d_G(v)^2} + \sum_{uv\in E_{2,3}(G)} \sqrt{d_G(u)^2+d_G(v)^2} \\ &+ \sum_{uv\in E_{3,3}(G)} \sqrt{d_G(u)^2+d_G(v)^2} \\ &= (\sqrt{2^2+2^2})3(n+3) + \sqrt{2^2+3^2}(6(n-1)) + \sqrt{3^2+3^2}(\frac{3(3\alpha^2+7n+2)}{2}). \end{aligned}$$

as desired. □

Theorem 3. *Let $G = L(S(I))$ be the line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k,l,m)$ for $k=l=m=4$. Then*

$$SO(G) = 12\sqrt{2}(k+l+m-5) + 24\sqrt{2}(k+l+m-7) + 63\sqrt{2}(k+l+m) - 118\sqrt{2}.$$

Proof. Let G denotes the line graph of the hexagonal parallelogram G_n. Then the order and size of $P(m,n)$ and G are given by:

Table 5.

Graph	Order	Size
$ZCS(k,l,m)$	$36k+54$	$15(k+l+m)-63$
$G=L(S(G_n))$	$30(k+l+m126)$	$39(k+l+m)+153$

The edge set of $G = L(S(I))$ can be partitioned into three disjoint sets $E_{2,2}, E_{2,3}$ and $E_{3,3}$, where $E(L(S(I))) = E_{2,2} \cup E_{2,3} \cup E_{3,3}$. By algebraic method the edge partition of G is calculated as:

Table 6.

$uv \in E(G)$	$(2,2)$	$(2,3)$	$(3,3)$
Number of edges	$6(k+l+m-5)$	$12(k+l+m-7)$	$21(k+l+m)-39$

Thus, using the information in Table 4, we have

$$\begin{aligned} SO(G) &= \sum_{uv\in E(G)} \sqrt{d_G(u)^2+d_G(v)^2} \\ &= \sum_{uv\in E_{2,2}(G)} \sqrt{d_G(u)^2+d_G(v)^2} + \sum_{uv\in E_{2,3}(G)} \sqrt{d_G(u)^2+d_G(v)^2} \\ &+ \sum_{uv\in E_{3,3}(G)} \sqrt{d_G(u)^2+d_G(v)^2} \\ &= (\sqrt{2^2+2^2})6(k+l+m-5)+\sqrt{2^2+3^2}12(k+l+m-7)+\sqrt{3^2+3^2}(21(k+l+m)-39). \end{aligned}$$

as asserted. □

Theorem 4. *Let $D_1(n)$ be the dominating derived network of 1st type. Then*

$$\begin{aligned} SO(D_1(n)) &= 8\sqrt{2}n+\sqrt{13}(4n-4)+\sqrt{20}(28n-16)+3\sqrt{2}(9\alpha^2-13n+5) \\ &+ 5(36\alpha^2-56n+24)+4\sqrt{2}(36\alpha^2-56n+20). \end{aligned}$$

Proof. Let $D_1(n)$ be the dominating derived network of 1st type. The edge set of $D_1(n)$ can be partitioned into six disjoint sets $E_{2,2}, E_{2,3}, E_{2,4}, E_{3,3}, E_{3,4}$ and $E_{4,4}$, where $E(D_1(n)) = E_{2,2}\cup E_{2,3}\cup E_{2,4}\cup E_{3,3}\cup E_{3,4}\cup E_{4,4}$. By algebraic method the edge partition of G is calculated as:

Table 7.

$uv \in E(G)$	$(2,2)$	$(2,3)$	$(2,4)$	$(3,3)$	$(3,4)$	$(4,4)$
Number of edges	$4n$	$4n-4$	$28n-16$	$9\alpha^2-13n+5$	$36\alpha^2-56n+24$	$36\alpha^2-52n+20$

Thus, using the information in Table 7, we have

$$\begin{aligned} SO(G) &= \sum_{uv\in E(G)} \sqrt{d_G(u)^2+d_G(v)^2} \\ &= \sum_{uv\in E_{2,2}(G)} \sqrt{d_G(u)^2+d_G(v)^2} + \sum_{uv\in E_{2,3}(G)} \sqrt{d_G(u)^2+d_G(v)^2} \\ &+ \sum_{uv\in E_{2,4}(G)} \sqrt{d_G(u)^2+d_G(v)^2} + \sum_{uv\in E_{3,3}(G)} \sqrt{d_G(u)^2+d_G(v)^2} \\ &+ \sum_{uv\in E_{3,4}(G)} \sqrt{d_G(u)^2+d_G(v)^2} + \sum_{uv\in E_{4,4}(G)} \sqrt{d_G(u)^2+d_G(v)^2} \\ &= (\sqrt{2^2+2^2})4n+(\sqrt{2^2+3^2})4n-4+(\sqrt{2^2+4^2})(28n-16) \\ &+ (\sqrt{3^2+3^2})(9\alpha^2-13n+5)+(\sqrt{3^2+4^2})(36\alpha^2-56n+24) \end{aligned}$$

$$+ \quad (\sqrt{4^2+4^2})(36\alpha^2 - 52n + 20).$$

as desired. □

Theorem 5. *Let $D_2(n)$ be the dominating derived network of 2nd type. Then*

$$\begin{aligned} S_2(D_2(n)) &= 8\sqrt{2}n + 2\sqrt{13}(9\alpha^2 - 11n + 3) + 8\sqrt{5}(7n - 6) + 20(9\alpha^2 - 14n + 6) \\ &+ 16\sqrt{2}(9\alpha^2 - 13n + 5). \end{aligned}$$

Proof. Let $D_2(n)$ be the dominating derived network of 2nd type. The edge set of $D_1(n)$ can be partitioned into five disjoint sets $E_{2,2}, E_{2,3}, E_{2,4}, E_{3,4}$ and $E_{4,4}$, where $E(D_2(n)) = E_{2,2} \cup E_{2,3} \cup E_{2,4} \cup E_{3,4} \cup E_{4,4}$. By algebraic method the edge partition of G is calculated as:

Table 8.

$uv \in E(G)$	$(2,2)$	$(2,3)$	$(2,4)$	$(3,4)$	$(4,4)$
Number of edges	$4n$	$18\alpha^2 - 22n + 6$	$28n - 16$	$36\alpha^2 - 56n + 24$	$36\alpha^2 - 52n + 20$

Thus, using the information in Table 8, we have

$$\begin{aligned} SO(G) &= \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \\ &= \sum_{uv \in E_{2,2}(G)} \sqrt{d_G(u)^2 + d_G(v)^2} + \sum_{uv \in E_{2,3}(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \\ &+ \sum_{uv \in E_{2,4}(G)} \sqrt{d_G(u)^2 + d_G(v)^2} + \sum_{uv \in E_{3,4}(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \\ &+ \sum_{uv \in E_{4,4}(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \\ &= (\sqrt{2^2+2^2})4n + (\sqrt{2^2+3^2})(18\alpha^2 - 22n + 6) + (\sqrt{2^2+4^2})(28n - 16) \\ &+ (\sqrt{3^2+4^2})(36\alpha^2 - 56n + 24) + (\sqrt{4^2+4^2})(36\alpha^2 - 52n + 20). \end{aligned}$$

as asserted. □

Theorem 6. *Let $D_3(n)$ be the dominating derived network of 3rd type. Then*

$$S_2(D_3(n)) = 8\sqrt{2}n + 8\sqrt{5}(9\alpha^2 - 5n) + 4\sqrt{2}(72\alpha^2 - 108n + 44).$$

Proof. Let $D_3(n)$ be the dominating derived network of 3rd type. The edge set of $D_1(n)$ can be partitioned into three disjoint sets $E_{2,2}, E_{2,4}$ and $E_{4,4}$ By algebraic method the edge partition of G is calculated as:

Table 9.

$uv \in E(G)$	$(2,2)$	$(2,4)$	$(4,4)$
Number of edges	$4n$	$36\alpha^2 - 20n$	$72\alpha^2 - 108n + 44$

Thus, using the information in Table 9, we have

$$\begin{aligned} SO(G) &= \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \\ &= \sum_{uv \in E_{2,2}(G)} \sqrt{d_G(u)^2 + d_G(v)^2} + \sum_{uv \in E_{2,4}(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \\ &+ \sum_{uv \in E_{4,4}(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \\ &= (\sqrt{2^2+2^2})4n + (\sqrt{2^2+4^2})(36\alpha^2 - 20n) + (\sqrt{4^2+4^2})(72\alpha^2 - 108n + 44) \end{aligned}$$

as asserted. □

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