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# Computing Szeged Index of Certain Nanosheets Using Partition Technique*

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**Abstract**

Distance properties of molecular graphs form an important topic in chemical graph theory. The Szeged index is a molecular structure descriptor equal to the sum of products $n_{eu}(e|G) \cdot n_{ev}(e|G)$ over all edges $e = (uv)$ of the molecular graph $G$, where $n_{eu}(e|G)$ is the number of vertices whose distance to vertex $u$ is smaller than the distance to vertex $v$, and where $n_{ev}(e|G)$ is defined analogously. In this paper we compute the Szeged index of certain chemical graphs without using distance matrix.

## 1 Introduction

Graph theory has found considerable use in Chemistry, particularly in modeling chemical structures. To identify molecular structures of chemical compounds, the molecular graph invariants, called topological indices could be used too. Topological indices are designed basically by transforming a molecular graph into a number. The first use of a topological index was made in 1947 by the chemist Harold Wiener [1]. Wiener introduced the notion

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of path number of a graph as the sum of distances between any two carbon atoms in the molecules, in terms of carbon-carbon bonds. Wiener originally defined his index on trees and studied its use for correlations of physico-chemical properties of alkanes, alcohols, amines and their analogous compounds.

The Wiener index $W$ is the first topological index to be used in chemistry. In graph theoretical language, the Wiener index is equal to the count of all shortest distances in a graph [2, 3, 4]. In 1990s, a large number of other topological indices have been put forward, all being based on the distances between vertices of molecular graphs and all being closely related to $W$. The Szeged index is one of these topological indices, which is introduced by Ivan Gutma [5].

Many physicochemical properties related to organic compounds acting as drugs were modeled by using Szeged index to develop structure-property-relationships. Important physicochemical properties which were modeled using Szeged index are: molecular weight (MW), density (d), boiling point (bp), vapor pressure (VP), molar volume (MV), molar refraction (MR), parachor (PR), van der Waals volume (Vw), equalized electronegativity ($\chi_{eq}$), dipole moments ($\mu$), proton-ligand formation constants and polarizability ($\alpha$). In addition, some spectroscopic parameters, such as infrared (i.r.) group frequency, edge-shift ($\triangle$E) in the extended X-ray absorption fine structure spectroscopy, isomer shift (IS) and quadrupole splitting (QS) in Mossbauer spectroscopy, and chemical shifts ($\delta$) in Nuclear Magnetic Resonance Spectroscopy (NMR Spectroscopy) are also modeled using Szeged index [6].

In addition to the above, Szeged index has also been found useful in modeling various biological activities viz. antihypertensive, antimalarial, antituberculotic, anti HIV, CA inhibitory antagonists, Lipoxygenase inhibitory activity, lipophilicity etc [6].

In a series of papers, authors defined and computed the Szeged index of some chemical graphs [7, 8, 9, 10, 11, 12, 13, 14]. In this paper, we compute the Szeged index of certain chemical graphs.

## 2 Basic Concepts and Terminology

All graphs in this paper will be finite, simple and undirected and we will use standard graph-theoretic terminology. A graph $G$ consists of a set of vertices $V(G)$ and a set of edges $E(G)$. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds.

In this section we give the basic definitions and preliminaries which are required for the remaining study.

**Definition 2.1.** *Let $G$ be a graph and $e = uv$ an edge of $G$. Then the vertex Szeged index of $G$ is defined as*

$$Sz_v(G) = \sum_{e \in E(G)} [n_{eu}(e|G)\ n_{ev}(e|G)]$$

*where $n_{eu}(e|G)$ denotes the number of vertices lying closer to the vertex $u$ than the vertex $v$ and $n_{ev}(e|G)$ denotes the number of vertices lying closer to the vertex $v$ than the vertex $u$.*

We also define the edge Szeged index $Sz_e(G)$ of $G$ introduced by Gutman et al. [15] as follows.

**Definition 2.2.** *Let $G$ be a graph and $e = uv$ an edge of $G$. Then the edge Szeged index of $G$ is defined as*

$$Sz_e(G) = \sum_{e \in E(G)} [m_{eu}(e|G)\ m_{ev}(e|G)]$$

*where $m_{eu}(e|G)$ denotes the number of edges lying closer to the vertex $u$ than the vertex $v$ and $m_{ev}(e|G)$ denotes the number of edges lying closer to the vertex $v$ than the vertex $u$.*

**Remark 2.3.** *In both definitions, vertices equidistant from both ends of the edge $e = uv$ are not counted.*

To our knowledge, there is no unified technique to compute Wiener and Szeged index of graphs. This motivated Bojan Mohar and Tomaž Pisanski to throw an open problem, Is there an algorithm for general graphs that would calculate the Wiener index without calculating the distance matrix?. This open problem was posed in 1988 in the Journal of Mathematical Chemistry [16]. It remains unsolved until now. Our objective in this paper is to compute the Szeged index of certain nano structures without using distance matrix.

Partitioning edge set of chemical graphs has been studied in [17]. We apply a specific way of partitioning the edge set $E$ of $G$, called the J-*Partition* and use embedding of graphs as a tool to establish an elegant technique to compute the Szeged index of graphs. We apply this tool to certain nano structures. We begin with the definitions of embedding parameters.

**Embedding:** Graph embedding has been known as a powerful tool for implementation of parallel algorithms or simulation of different interconnection networks. An *embedding* [18] of a guest graph $G$ into a host graph $H$ is defined by an injective function $f : V(G) \to V(H)$ together with a mapping $P_f$ which assigns to each edge $(u, v)$ of $G$ a path $P_f((u, v))$ between $f(u)$ and $f(v)$ in $H$. If $e = (u, v) \in E(G)$, then the length of $P_f((u, v))$ in $H$ is called the dilation of the edge $e$.

The dilation-sum [19] $\widetilde{D_f}(G, H)$ of an embedding $f$ of $G$ into $H$ is defined as

$$\widetilde{D_f}(G, H) = \sum_{(u,v)\in E(G)} |P_f(u, v)|$$

where $|P_f(u, v)|$ is the length of the path $P_f(u, v)$ in $H$.

Then the *dilation-sum* of $G$ into $H$ is defined as

$$\widetilde{D}(G, H) = \min_f \widetilde{D_f}(G, H),$$

where the minimum is taken over all embeddings $f$ of $G$ into $H$.

The *congestion* of an embedding $f$ of $G$ into $H$ is the maximum number of edges of the guest graph that are embedded on any single edge of the host graph. Let $C_f(G, H(e))$ denote the number of edges $(u, v)$ of $G$ such that $e$ is in the path $P_f((u, v))$. In other words,

$$C_f(G, H(e)) = |\{(u, v) \in E(G) : e \in P_f(u, v)\}|.$$

The congestion-sum [19] $\widetilde{C_f}(G, H)$ of an embedding $f$ of $G$ into $H$ is defined as

$$\widetilde{C_f}(G, H) = \sum_{e\in E(H)} C_f(G, H(e)).$$

Then the *congestion-sum* of $G$ into $H$ is defined as

$$\widetilde{C}(G, H) = \min_f \widetilde{C_f}(G, H)$$

where the minimum is taken over all embeddings $f$ of $G$ into $H$.

For $S \subseteq E(H)$, the congestion on $S$ is the sum of the congestions on the edges in $S$. That is, $C_f(G, H(S)) = \sum_{e\in S} C_f(G, H(e))$.

For any embedding, the dilation-sum and the congestion-sum are one and the same [19, 20]. It is also referred to as the wirelength of embedding $G$ into $H$ and is denoted as $W(G, H)$.

When the guest graph is the complete graph $K_n$ and is embedded on graph $G$, then the wirelength of embedding $K_n$ onto $G$ is nothing but the Wiener index of $G$ and is denoted by $W(G)$ [21]. The I-Partition and the $k$I-Partition Lemma [21] have been used as tools to compute the Wiener index of graphs.

**Definition 2.4.** [17, 21] Let $G$ be a graph on $n$ vertices. Let $\{S_1, S_2, ..., S_m\}$ be a partition of $E(G)$ such that each $S_i$ is an edge cut of $G$ and the removal of edges of $S_i$ leaves $G$ into 2 components $G_i$ and $G'_i$. Also each $S_i$ satisfies the following conditions:

(i) For any two vertices $u, v \in G_i$, a shortest path between $u$ and $v$ has no edges in $S_i$.

(ii) For any two vertices $u, v \in G'_i$, a shortest path between $u$ and $v$ has no edges in $S_i$.

(iii) For any two vertices $u \in G_i$ and $v \in G'_i$, a shortest path between $u$ and $v$ has exactly one edge in $S_i$.

Such a partition of $E(G)$ is called an I-Partition of $G$. Each member of an I-Partition is referred to as an I-edge cut.

**Definition 2.5.** [17, 22] Let $G$ be a graph on $n$ vertices and $m$ edges. Let $\{S_1, S_2, ..., S_p\}$ be a partition of $E(G)$ such that each $S_i$ is an edge cut of $G$ and the removal of edges of $S_i$ leaves $G$ into 2 components $G_i$ and $G'_i$ satisfying the following conditions:

(i) For any edge $e = uv$ in $S_i, 1 \leq i \leq p$ and a vertex $x$ in $G_i$, $d(x, u) < d(x, v)$

(ii) For any edge $e = uv$ in $S_i, 1 \leq i \leq p$ and a vertex $y$ in $G'_i$, $d(y, v) < d(y, u)$.

Such a partition of $E(G)$ is called a J-Partition of $G$. Each member of a J-Partition is referred to as a J-edge cut.

**Remark 2.6.** In the literature, the edge cuts defined above are also referred to as orthogonal cuts [23].

**Theorem 2.7.** [22] Let $G$ ba a graph. Then every J-edge cut of $G$ is an I-edge cut of $G$.

**Remark 2.8.** [22] Let $G$ be a graph. Not every I-edge cut of $G$ is a J-edge cut of $G$.

However when $G$ is bipartite, we have the following result.

**Theorem 2.9.** [22] Let $G$ be bipartite. Then every I-edge cut of $G$ is a J-edge cut of $G$.

**Theorem 2.10.** [22] Let $G$ ba a graph and $S$ ba an edge cut of $G$. Then $S$ is a J-edge cut if and only if $S$ is an I-edge cut.

**Theorem 2.11.** [22] Let $G$ ba a bipartite graph. Let $S$ be a J-edge cut of $G$ which partitions $G$ into $G'$ and $G''$. Then for any edge $e'$ in $G'$ and an edge $e = (u, v)$ in $S$, $e'$ is closer to $u$ than $v$.

**Theorem 2.12.** [22] Let $G$ be a bipartite graph and $\{S_1, S_2, \cdots, S_p\}$ be an I-Partition of $G$. Let $S_i = \{e_i^1, e_i^2, \cdots, e_i^{|S_i|}\}$, $1 \leq i \leq p$, $e_j^i = (u_{ij}, v_{ij})$, $k'_{ij}$ be the number of edges in $S_i$ closer to $u_{ij}$ than $v_{ij}$ and $k''_{ij}$ be the number of edges in $S_i$ closer to $v_{ij}$ than $u_{ij}$, $1 \leq j \leq |S_i|$, $1 \leq i \leq p$. Then

$$Sz_v(G) = \sum_{i=1}^{p} |S_i| \; [|V(G'_i)| \, (n - |V(G'_i)|)] \quad and$$

$$Sz_e(G) = \sum_{i=1}^{p} |S_i| \sum_{j=1}^{|S_i|} (|E(G'_i)| + k'_{ij}) \; (|E(G''_i)| + k''_{ij}).$$

# 3 Computing Szeged index

Even though there is an extensive literature available on the computation of Szeged index, there is no known method to solve the Szeged index of general graphs. In this paper, we describe an efficient method of computing Szeged index of certain hexagonal and octagonal nano structures such as $C_4C_8(S)$ Nanosheet and $H$-Naphtalenic Nanosheet.

## 3.1 $C_4C_8(S)$ Nanosheets of Type I and II

A $C_4C_8(S)$ Nonosheet is a trivalent decoration made by alternating squares $C_4$ and octagons $C_8$. The arrangement of $C_4$ and $C_8$ determine two types of nanosheets which we refer to as Type I and Type II. See Figure 1(a) and (b). Throughout this paper the Type I and Type II $C_4C_8(S)$ Nanosheets are denoted by $T^1[2p, 2q]$ and $T^2[2p, 2q]$ respectively. The number of vertices in $T^1[2p, 2q]$ and $T^2[2p, 2q]$ is $8pq$ and $4(p+1)(q+1)$ respectively [21].

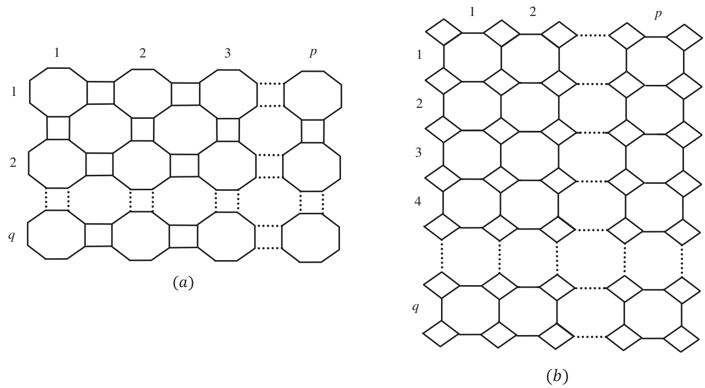



Figure 1: (a) Type I-$C_4C_8(S)$ Nanosheet $T^1[2p, 2q]$ (b) Type II-$C_4C_8(S)$ Nanosheet $T^2[2p, 2q]$

**Szeged Index Algorithm A**

**Input :** The Nanosheet $T^1[2p, 2q]$, $p, q \geq 1$.

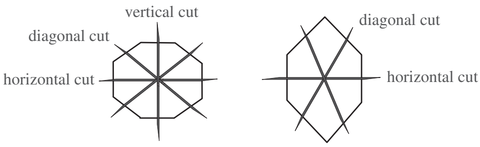
**Output :** Szeged index of the nanosheet $T^1[2p, 2q]$.

**Proof of correctness :** We use vertical, horizontal and diagonal cuts as shown in Figure 2(a) that yield an J-Partition of the edge set of $T^1[2p, 2q]$.

Now let $\{S_i : 1 \leq i \leq 2p-1\}, \{S'_i : 1 \leq i \leq 2q-1\}, \{S_i^j : 1 \leq i \leq 2, 1 \leq j \leq p+q-1\}$ as shown in Figure 3 be the vertical, horizontal and diagonal cuts in $T^1[2p, 2q]$ respectively. We observe that $\{S_i : 1 \leq i \leq 2p-1\}, \{S'_i : 1 \leq i \leq 2q-1\}$ and $\{S_i^j : 1 \leq i \leq 2, 1 \leq j \leq p+q-1\}$ form an J-Partition of $E(T^1[2p, 2q])$.

For $1 \leq i \leq 2p-1$, the removal of $S_i$ leaves $T^1[2p, 2q]$ into two components $G_{S_i}$ and $G'_{S_i}$ where $|V(G_{S_i})| = 4iq$ and $|V(G'_{S_i})| = 8pq - 4iq$. For $1 \leq i \leq 2q-1$, the removal of $S'_i$ leaves $T^1[2p, 2q]$ into two components $G_{S'_i}$ and $G'_{S'_i}$ where $|V(G_{S'_i})| = 4ip$ and $|V(G'_{S'_i})| = 8pq - 4ip$.

By the symmetry of $T^1[2p, 2q]$, we consider only the case when $p > q$. For $i = 1$, $1 \leq j \leq q-1$, the removal of $S_i^j$ leaves $T^1[2p, 2q]$ into two components $G_{S_i^j}$ and $G'_{S_i^j}$ where $|V(G_{S_i^j})| = 4j^2$ and $|V(G'_{S_i^j})| = 8pq - 4j^2$. For $i = 1$, $0 \leq j \leq p-q$, the removal of $S_i^{j'}$ leaves $T^1[2p, 2q]$ into two components $G_{S_i^{j'}}$ and $G'_{S_i^{j'}}$ where $|V(G_{S_i^{j'}})| = 4q^2 + 4jq$ and $|V(G'_{S_i^{j'}})| = 8pq - (4q^2 + 4jq)$. Similar results hold good when $i = 2$.




$(a)$ $(b)$

Figure 2: (a) The edge cut of octagonal structure (b) The edge cut of hexagonal structure

Hence the edge cuts $\{S_i : 1 \leq i \leq 2p-1\}, \{S'_i : 1 \leq i \leq 2q-1\}, \{S_i^j : 1 \leq i \leq 2, 1 \leq j \leq p+q-1\}$, satisfy conditions (i)-(ii) of J-Partition Lemma. Also, for $1 \leq i \leq 2p-1$, $|S_i| = 2q$, for $1 \leq i \leq 2q-1$, $|S'_i| = 2p$ and for $i = 1, 2$ and when $1 \leq j \leq q-1$, $|S_i^j| = 2j$ and when $0 \leq j \leq p-q$, $|S_i^j| = 2q$.

Thus, for each $i$, $1 \leq i \leq 2p-1$, $C_f(K_n, G(S_i)) = 8iq^2(8pq - 4iq)$, for $1 \leq i \leq 2q-1$, $C_f(K_n, G(S'_i)) = 8ip^2(8pq - 4ip)$, for $i = 1, 2, 1 \leq j \leq q-1$, $C_f(K_n, G(S_i^j)) = 8j^3(8pq - 4j^2)$ and for $i = 1, 2, 0 \leq j \leq p-q$, $C_f(K_n, G(S_i^{j'})) = 2q(4q^2 + 4jq)[8pq - (4q^2 + 4jq)]$. Hence

$$\begin{aligned} Sz_v(T^1[2p, 2q]) &= 16\sum_{i=1}^{2p-1}(2q)iq(2pq - iq) + 16\sum_{i=1}^{2q-1}(2p)ip(2pq - ip) + 64\sum_{j=1}^{q-1}(2j)j^2(2pq - j^2) \\ &\quad +32\sum_{j=0}^{p-q}2q(q^2 + qj)(2pq - (q^2 + qj)) \\ &= \frac{8}{3}q[6q^5 - 6(3p+1)q^4 + (12p-1)q^3 + 2p(24p^2 + 6p - 1)q^2 + q - 4p^3]. \end{aligned}$$

From Szeged Index Algorithm A, we have the following result.

**Theorem 3.1.** *The Szeged index of the nanosheet* $T^1[2p, 2q]$ *is given by*

$$Sz_v(T^1[2p, 2q]) = \frac{8}{3}q[6q^5 - 6(3p+1)q^4 + (12p-1)q^3 + 2p(24p^2 + 6p - 1)q^2 + q - 4p^3].$$

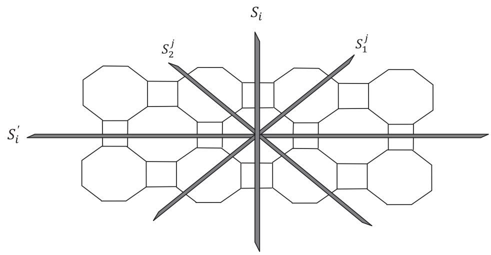



Figure 3: The edge cut of $T^1[8, 4]$

**Szeged Index Algorithm B**

**Input :** The Nanosheet $T^2[2p, 2q]$, $p, q \geq 1$.

**Output :** Szeged index of the nanosheet $T^2[2p, 2q]$.

**Proof of correctness :** We use vertical, horizontal and diagonal cuts as shown in Figure 2(a) that yield an J-Partition of the edge set of $T^2[2p, 2q]$.

Now let $\{S_i : 1 \leq i \leq p\}, \{S'_i : 1 \leq i \leq q\}, \{S^j_i : 1 \leq i \leq 2, 1 \leq j \leq p+q+1\}$ as shown in Figure 4 be the vertical, horizontal and diagonal cuts in $T^2[2p, 2q]$ respectively. We observe that $\{S_i : 1 \leq i \leq p\}, \{S'_i : 1 \leq i \leq q\}$ and $\{S^j_i : 1 \leq i \leq 2, 1 \leq j \leq p+q+1\}$ form an J-Partition of $E(T^2[2p, 2q])$.

For $1 \leq i \leq p$, the removal of $S_i$ leaves $T^2[2p, 2q]$ into two components $G_{S_i}$ and $G'_{S_i}$ where $|V(G_{S_i})| = 4i(q+1)$ and $|V(G'_{S_i})| = 4(p+1)(q+1) - 4i(q+1)$. For $1 \leq i \leq q$, the removal of $S'_i$ leaves $T^2[2p, 2q]$ into two components $G_{S'_i}$ and $G'_{S'_i}$ where $|V(G_{S'_i})| = 4i(p+1)$ and $|V(G'_{S'_i})| = 4(p+1)(q+1) - 4i(p+1)$.

By the symmetry of $T^2[2p, 2q]$, we consider only the case when $p > q$. For $i = 1$, $1 \leq j \leq q-1$, the removal of $S^j_i$ leaves $T^2[2p, 2q]$ into two components $G_{S^j_i}$ and $G'_{S^j_i}$ where $|V(G_{S^j_i})| = 2j^2$ and $|V(G'_{S^j_i})| = 4(p+1)(q+1) - 2j^2$. For $i = 1$, $0 \leq j \leq p-q$, the removal of $S^{j'}_i$ leaves $T^2[2p, 2q]$ into two components $G_{S^{j'}_i}$ and $G'_{S^{j'}_i}$ where $|V(G_{S^{j'}_i})| = 2q^2 + 2jq$ and $|V(G'_{S^{j'}_i})| = 4(p+1)(q+1) - (2q^2 + 2jq)$. Similar results hold good when $i = 2$.

Hence the edge cuts $\{S_i : 1 \leq i \leq p\}, \{S'_i : 1 \leq i \leq q\}, \{S^j_i : 1 \leq i \leq 2, 1 \leq j \leq p+q+1\}$, satisfy conditions (i)-(ii) of J-Partition Lemma. Also, for $1 \leq i \leq p$, $|S_i| = q+1$, for $1 \leq i \leq q$, $|S'_i| = p+1$ and for $i = 1, 2$ and when $1 \leq j \leq q-1$, $|S^j_i| = 2j$ and when $0 \leq j \leq p-q$, $|S^j_i| = 2q$.

Thus, for each $i$, $1 \leq i \leq p$, $C_f(K_n, G(S_i)) = 16i(q+1)^2((p+1)(q+1) - i(q+1))$, for $1 \leq i \leq q$, $C_f(K_n, G(S'_i)) = 16i(p+1)^2((p+1)(q+1) - i(p+1))$, for $i = 1, 2, 1 \leq j \leq q-1$, $C_f(K_n, G(S^j_i)) = 8j^3(2(p+1)(q+1) - j^2)$ and for $i = 1, 2, 0 \leq j \leq p-q$, $C_f(K_n, G(S^{j'}_i)) = 8q(q^2 + jq)[2(p+1)(q+1) - (q^2 + jq)]$. Hence

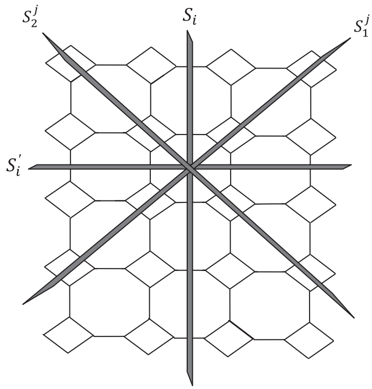



Figure 4: The edge cut of $T^2[6,8]$

$$
\begin{aligned}
Sz_v(T^2[2p,2q]) &= 16\sum_{i=1}^{p} i(q+1)^2((p+1)(q+1)-i(q+1)) \\
&+ 16\sum_{i=1}^{q} i(p+1)^2((p+1)(q+1)-i(p+1)) \\
&+ 32\sum_{j=1}^{q-1} j^3(2(p+1)(q+1)-j^2) \\
&+ 16q\sum_{j=0}^{p-q}(q^2+jq)[2(p+1)(q+1)-(q^2+jq)] \\
&= \frac{8}{3}(p+1)(q+1)[p(p+2)(q+1)^2+q(q+2)(p+1)^2] \\
&+ \frac{8}{3}q^2[(q-1)^2(-2q^2+6pq+8q+6p+7)+(p-q+1) \\
&\quad (4p^2q+6p^2+11pq+6p+4pq^2+6p-2q^3+7q^2)]\ .
\end{aligned}
$$

From Szeged Index Algorithm B, we have the following result.

**Theorem 3.2.** *The Szeged index of the nanosheet $T^2[2p,2q]$ is given by*

$$
\begin{aligned}
Sz_v(T^2[2p,2q]) &= \frac{8}{3}(p+1)(q+1)[p(p+2)(q+1)^2+q(q+2)(p+1)^2] \\
&+ \frac{8}{3}q^2[(q-1)^2(-2q^2+6pq+8q+6p+7)+(p-q+1) \\
&\quad (4p^2q+6p^2+11pq+6p+4pq^2+6p-2q^3+7q^2)]\ .
\end{aligned}
$$

## 3.2 *H*-Naphtalenic Nanosheet$(2n, 2m)$

Carbon nanotubes (CNTs) are peri-condensed Benzenoids, which are ordered in graphite-like, hexagonal pattern. They may be derived from graphite by rolling up the rectangular sheets along certain vectors. All benzenoids, including graphite and CNTs are aromatic structures [21].

A $H$-Naphtalenic Nanosheet$(2n, 2m)$ is made by alternating hexagons $C_6$, squares $C_4$ and octagons $C_8$. See Figure 5. The number of vertices in $H$-Naphtalenic Nanosheet$(2n, 2m)$ is $10nm$ [21].

In this section, we compute the vertex Szeged index of $H$-Naphtalenic Nanosheet$(2n, 2m)$, where $n, m \geq 1$.

**Szeged Index Algorithm C**

**Input :** The $H$-Naphtalenic Nanosheet$(2n, 2m)$, $n, m \geq 1$.

**Output :** Szeged index of the $H$-Naphtalenic Nanosheet$(2n, 2m)$, $n, m \geq 1$.

**Proof of correctness :** We use vertical, horizontal and diagonal cuts, that yield an J-Partition of the edge set of $G$.

Now let $\{S_i : 1 \leq i \leq n-1\}, \{S'_i : 1 \leq i \leq 2m-1\}, \{S_i^j : 1 \leq i \leq 2, 1 \leq j \leq n+m+3\}$ be the vertical, horizontal and diagonal cuts in $G$ respectively. We observe that $\{S_i : 1 \leq i \leq n-1\}, \{S'_i : 1 \leq i \leq 2m-1\}$ and $\{S_i^j : 1 \leq i \leq 2, 1 \leq j \leq n+m+3\}$ form an J-Partition of $E(G)$.

For $1 \leq i \leq n-1$, the removal of $S_i$ leaves $G$ into two components $G_{S_i}$ and $G'_{S_i}$ where $|V(G_{S_i})| = 10mi$ and $|V(G'_{S_i})| = 10nm - 10mi$. For $1 \leq i \leq 2m-1$, the removal of $S'_i$ leaves $G$ into two components $G_{S'_i}$ and $G'_{S_i}$ where $|V(G_{S_i})| = 5ni$ and $|V(G'_{S_i})| = 10nm - 5ni$.

For $i = 1$, $1 \leq j \leq m$, the removal of $S_i^j$ leaves $G$ into two components $G_{S_i^j}$ and $G'_{S_i^j}$ where $|V(G_{S_i^j})| = \sum\limits_{k=1}^{j}[(4k-1) + 2\lfloor\frac{k-1}{2}\rfloor]$ and $|V(G'_{S_i^j})| = 10nm - \sum\limits_{k=1}^{j}[(4k-1) + 2\lfloor\frac{k-1}{2}\rfloor]$. Similar results hold good when $i = 2$.

For $i = 1$, $1 \leq j \leq 2n - (m+1)$, the diagonal cuts are categorized as follows.

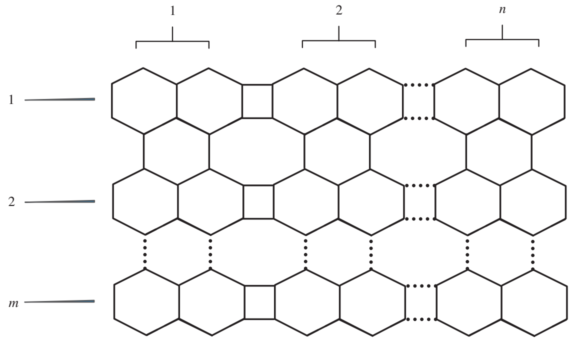



Figure 5: $H$-Naphtalenic Nanosheet$(2n, 2m)$

**Case 1** ($m$ even): The removal of $S_i^{j'}$ leaves $G$ into two components $G_{S_i^{j'}}$ and $G'_{S_i^{j'}}$ where

$$|V(G_{S_i^{j'}})| = \sum_{k=1}^{m}[(4k-1)+2\left\lfloor\frac{k-1}{2}\right\rfloor] + j\left\{4m+2+2\left\lfloor\frac{m-1}{2}\right\rfloor\right\}$$

and

$$|V(G'_{S_i^{j}})| = 10mn - \left[\sum_{k=1}^{m}[(4k-1)+2\left\lfloor\frac{k-1}{2}\right\rfloor] + j\left\{4m+2+2\left\lfloor\frac{m-1}{2}\right\rfloor\right\}\right].$$

**Case 2** ($m$ odd):

**Subcase 1** ($j$ odd): The removal of $S_i^{j'}$ leaves $G$ into two components $G_{S_i^{j'}}$ and $G'_{S_i^{j'}}$ where $|V(G_{S_i^{j'}})| = \sum\limits_{k=1}^{m}[(4k-1)+2\lfloor\frac{k-1}{2}\rfloor] + j\{4m+2\lfloor\frac{m-1}{2}\rfloor\} + j - 1$ and $|V(G'_{S_i^{j}})| = 10mn - [\sum\limits_{k=1}^{m}[(4k-1)+2\lfloor\frac{k-1}{2}\rfloor] + j\{4m+2\lfloor\frac{m-1}{2}\rfloor\} + j - 1]$.

**Subcase 1** ($j$ even): The removal of $S_i^{j'}$ leaves $G$ into two components $G_{S_i^{j'}}$ and $G'_{S_i^{j'}}$ where $|V(G_{S_i^{j'}})| = \sum\limits_{k=1}^{m}[(4k-1)+2\lfloor\frac{k-1}{2}\rfloor] + j\{4m+2+2\lfloor\frac{m-1}{2}\rfloor\} - j$ and $|V(G'_{S_i^{j}})| = 10mn - [\sum\limits_{k=1}^{m}[(4k-1)+2\lfloor\frac{k-1}{2}\rfloor] + j\{4m+2+2\lfloor\frac{m-1}{2}\rfloor\} - j]$.

Hence the edge cuts $\{S_i : 1 \le i \le n-1\}, \{S'_i : 1 \le i \le 2m-1\}, \{S_i^j : 1 \le i \le 2, 1 \le j \le n+m+3\}$, satisfy conditions (i)-(ii) of J-Partition Lemma. Also, for $1 \le i \le n-1$, $|S_i| = 2m$ for $1 \le i \le 2m-1$, $|S'_i| = 2n$ or $3n$ with respect to $i$ is even or odd. And for $i = 1, 2$ and when $1 \le j \le m$, $|S_i^j| = 2j$ and when $1 \le j \le 2n-(m+1)$, $|S_i^j| = 2m$.

The proof of the following result is an easy consequence of Szeged Index Algorithm C.

**Theorem 3.3.** *Let $G$ be the H-Naphtalenic Nanosheet$(2n, 2m)$, $n, m \geq 1$. Then the Szeged index of $G$ is given by*

*1. If $m$ is even,*

$$\begin{aligned} Sz_v(G) &= \frac{25}{3}nm(14m^2n^2 - 4m^2 - n^2) + 8\sum_{j=1}^{m} j(\sum_{k=1}^{j}((4k-1) \\ &\quad +2\lfloor\frac{k-1}{2}\rfloor))(10nm - \sum_{i=1}^{j}((4k-1) + 2\lfloor\frac{k-1}{2}\rfloor)) \\ &\quad +4m\sum_{j=1}^{2n-m-1}(\sum_{k=1}^{m}((4k-1) + 2\lfloor\frac{k-1}{2}\rfloor) + j(4m+2+2\lfloor\frac{m-1}{2}\rfloor)) \\ &\quad (10nm - (\sum_{k=1}^{m}((4k-1) + 2\lfloor\frac{k-1}{2}\rfloor) + j(4m+2+2\lfloor\frac{m-1}{2}\rfloor))) \end{aligned}$$

*2. If $m$ is odd,*

$$Sz_v(G) = \begin{cases} \frac{25}{3}nm(14m^2n^2 - 4m^2 - n^2) + 8\sum_{j=1}^{m} j(\sum_{k=1}^{j}((4k-1) \\ +2\lfloor\frac{k-1}{2}\rfloor))(10nm - \sum_{i=1}^{j}((4k-1) + 2\lfloor\frac{k-1}{2}\rfloor)) \\ +4m\sum_{j=1}^{2n-m-1}(\sum_{k=1}^{m}((4k-1) + 2\lfloor\frac{k-1}{2}\rfloor) + j(4m+2\lfloor\frac{m-1}{2}\rfloor) + j - 1) \\ (10nm - (\sum_{k=1}^{m}((4k-1) + 2\lfloor\frac{k-1}{2}\rfloor) + j(4m+2\lfloor\frac{m-1}{2}\rfloor) + j - 1)), & \text{if } j \text{ odd;} \\ \\ \frac{25}{3}nm(14m^2n^2 - 4m^2 - n^2) + 8\sum_{j=1}^{m} j(\sum_{k=1}^{j}((4k-1) + 2\lfloor\frac{k-1}{2}\rfloor)) \\ (10nm - \sum_{i=1}^{j}((4k-1) + 2\lfloor\frac{k-1}{2}\rfloor)) \\ +4m\sum_{j=1}^{2n-m-1}(\sum_{k=1}^{m}((4k-1) + 2\lfloor\frac{k-1}{2}\rfloor) + j(4m+1+2\lfloor\frac{m-1}{2}\rfloor)) \\ (10nm - (\sum_{k=1}^{m}((4k-1) + 2\lfloor\frac{k-1}{2}\rfloor) + j(4m+1+2\lfloor\frac{m-1}{2}\rfloor))), & \text{if } j \text{ even;} \end{cases}$$

# 4 Concluding Remarks

In this paper, we compute the vertex Szeged index of certain chemical graphs such as $C_4C_8(S)$ Nanosheet and $H$-Naphtalenic Nanosheet. Finding tools to compute the edge Szeged index for the chemical graphs considered in this paper are under investigation. The application of the $k$J-Partition Lemma to compute the Szeged index of certain other chemical structures are also under investigation.

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