

# Topological characterization of the full $k$ -subdivision of a family of partial cubes and their applications to $\alpha$ -types of novel graphyne and graphdiyne materials

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## Abstract

Graphene, an allotrope of carbon, has gained tremendous importance due to its novel, chemical, structural, optical and reactivity properties. A class of graphene allotropes with both  $sp^2$  and  $sp$  carbons named  $\alpha$ -types of graphyne and graphdiyne have been synthesized recently and have received considerable attention due to their novel structural and optical properties with multiple wide ranging applications in developing sensors, catalysis, chemisorption and nanomedicine. In the present study we have considered mathematical techniques for the topological characterization of these novel materials. We have extended full subdivisions of partial cubes in which transitive closure of Djoković-Winkler relation is used to compute analytical expressions for various distance-based topological indices for their deployment in chemical and medicinal applications via QSAR and QSPR studies.

**Keywords:** Partial cubes; subdivision; graphene; distance.

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# 1 Introduction

Graphyne and graphdiyne materials have received significant recent attention [1–15] due to their novel material properties, optical properties and chemical properties. The existence of a conjugated network of both carbon-carbon double and triple bonds in these materials that exist in sheet forms, nanosheet forms, nanowires, arrays of nanotubes and other forms have provided a new vista and opportunity to explore interesting chemistry in yet another dimension of carbon allotropes. These materials are also expected to exhibit very interesting chemical and optical properties due to their excitonic nature of a network of  $sp$  and  $sp^2$  hybrid orbitals analogous to polycyclic aromatic compounds [16, 17]. Furthermore, the unsaturated network of multiple bonds in these materials are likely to provide an effective platform to investigate chemical phenomena such as chemisorption, reactivities with clusters, catalysis, hydrogenation, complexation with heavy metals and ions, study of relativistic effects in such complexes, and so on [17–21]. It is anticipated that functionalization of these graphyne and graphdiyne materials would provide novel avenues for developing sensors, sequestration and complexation of inorganic metal ions, toxic heavy metal ions such as cadmium, mercury, thallium, lanthanide and actinide ions similar to the engineered functionalized mesoporous silica that have been employed for actinide sequestration [22, 23]. As medicinal chemistry has made quantum leaps into nanomedicines, these materials could find novel applications in drug discovery, efficient drug delivery and protein-protein and protein-drug interactions [24]. Such carbonaceous species with  $sp$  carbons both in chains and other forms appear to occur in circumstellar shells and carbon-rich stars [25]. The existence of conjugated networks of multiple bondings comprised of both  $sp$  and  $sp^2$  carbons make these species interesting candidates for exploration of aromaticity and super aromaticity- a topic of considerable interest over the years [26–28]. As a result of such increasingly important and novel applications of these materials, it is both useful and necessary to provide efficient mathematical and topological characterization for the structural properties of these materials. Moreover, high-level quantum computations may not always be feasible for larger networks of arrays of nanotubes comprised of graphynes and graphdienes. Therefore topological characterization of these materials could provide alternative promising approaches for quantitative characterizations of structures and reactivities of these species. Consequently, in this study we consider mathematical techniques for obtaining exact analytical expressions for several topological descriptors of these emerging novel materials.

In chemical graph theory, the structure of a molecule or a chemical compound is considered as a

graph with atoms as its vertices and the covalent bonds between them as edges of the graph. A number of practical applications such as computer-aided drug discovery, relies on efficient correlations of physico-chemical properties with molecular structures and the biological activities of molecules. These relations of molecular structures to their properties are often characterized as quantitative structure-activity, structure-property and structure-toxicity relationships (QSAR/QSPR/QSTR). Determining structural-relationships of molecules require multiple topological molecular descriptors that would correlate to different properties such as dermal penetrations, drug activities, optical properties, reactivities and physico-chemical properties.

Many topological indices have been introduced and applied in QSAR/QSPR/QSTR studies to determine the properties and biological activities of compounds for their potential applicability in several areas such as chemical reactivity studies, spectroscopy, computer-assisted structure elucidation and computer-aided drug discovery [24, 29]. The topological indices of a chemical compound depends primarily on the molecular structure and hence the underlying connectivity. Our motivation for the current study comes from the fact that the implementation of full subdivisions of partial cubes is restricted to only few classes of graphs [30, 31] and these techniques are not applicable to emerging novel materials such as graphynes and graphdiynes. In the present study we extend the previous techniques to encompass computation of topological indices for such extended molecular materials that are comprised of multiple acetylenic linkages, thus in effect large structures that contain both  $sp$  and  $sp^2$  carbons. We accomplish this by a graph theoretical expansion wherein an edge is subdivided multiple times. Consequently, we extend full subdivisions of partial cubes to full  $k$ -subdivision graphs which facilitate computations of exact analytical expressions for the distance-based topological indices of graphynes and graphdiynes.

## 1.1 Background

Throughout the paper, a graph  $G$  is considered as a simple and finite connected graph with the cardinality of its vertex and edge set being denoted as  $|V(G)|$  and  $|E(G)|$  respectively. The usual shortest path distance between any two vertices  $u, v \in V(G)$  is denoted as  $d_G(u, v)$  and the degree of any vertex  $v$  is denoted as  $d_G(v)$ . Furthermore, for an edge  $e = ab$  of  $G$ , a vertex-edge-shortest path distance  $d_G(u, e)$  is defined as  $\min\{d_G(u, a), d_G(u, b)\}$ , as a consequence of which, for any two edges  $e = ab$  and  $f = cd$  of  $G$ , an edge-edge shortest path distance  $D_G(e, f)$  is defined as  $\min\{d_G(e, c), d_G(e, d)\}$  [32]. Let  $S \subseteq E(G)$ , the quotient graph  $G/S$  is obtained by removing  $S$  from  $G$  such that  $V(G/S) = \{X : X \text{ is a connected component of } G - S\}$  and  $E(G/S) = \{XY :$

there exists a vertex  $x$  of  $X$  and a vertex  $y$  of  $Y$  such that  $xy \in S$

An  $n$ -dimensional cube or an  $n$ -cube is defined as a recursive Cartesian product of  $K_2$ ,  $Q_1 = K_2, Q_n = K_2 \square Q_{(n-1)}$  where two vertices represented as an  $n$ -dimensional boolean vectors (vectors containing binary coordinates  $\{0, 1\}^n$ ) are adjacent iff they differ by exactly one position. A subgraph  $H$  of  $G$  is said to be isometric if  $d_H(u, v)$  preserves distance equality with  $G$  for all  $u, v \in V(H)$ . Moreover, the isometric embedding of  $H$  into  $G$  is a mapping  $f : V(H) \rightarrow V(G)$  such that  $f(H)$  is an isometric subgraph of  $G$ . An isometric embedding of an  $n$ -cube is a partial cube or a binary Hamming graph which is an undirected graph whose vertices can be labeled by binary vectors in such a way that the distance between any two vertices in the graph is equal to the Hamming distance between the corresponding labels [33]. It was first introduced by Graham and Pollak [34] while they were working on communication networks and since then the variants of cubes have been a topic of discussion for an extensive variety of mathematical systems.

Partial cubes have several applications in computational biology [35, 36], media theory [37], psychology [38] and most particularly in mathematical chemistry [39]. These classes of graphs were well understood and characterized in [40–42]. Djoković [42] and Winkler [40] characterized them in terms of equivalence relation to edges with the relation that for any two edges  $e = ab$  and  $f = cd$ ,  $d_G(a, c) + d_G(b, d) \neq d_G(a, d) + d_G(b, c)$ . This relation is known as  $\Theta$  and has become an effective tool in the cut method [39, 43] for partitioning the edges as it eases the computation process of topological indices.

The concept of strength-weighted graph was initially introduced in [44] as a triple  $G_{sw} = (G, SW_V, SW_E)$  where  $G$  is a simple graph and  $SW_V$  is the pair  $(w_v, s_v)$  where  $w_v$  is the vertex-weight and  $s_v$  is the vertex-strength such that  $(w_v, s_v) : V(G_{sw}) \rightarrow \mathbb{R}_0^+$ , and  $SW_E$  is the pair  $(w_e, s_e)$  where  $w_e$  is the edge-weight and  $s_e$  is the edge-strength such that  $(w_e, s_e) : E(G_{sw}) \rightarrow \mathbb{R}_0^+$ . For our context of study we consider  $w_e = 1$  for every edge  $e \in G_{sw}$  and henceforth  $G_{sw} = (G, (w_v, s_v), s_e)$ . We now compare certain terminologies of a simple graph  $G$  and a strength-weighted graph  $G_{sw}$  which is required for our further study.

1. The distance between vertex-vertex, vertex-edge and edge-edge in  $G_{sw}$  is the same as in  $G$ .
2. For a vertex  $u$ , its neighborhood in  $G$  and  $G_{sw}$  are equal and defined as  $N_G(u) = N_{G_{sw}}(u) = \{v \in V(G) : d_G(u, v) = 1\}$ .
3. The degree of a vertex  $u$  in  $G$  is defined as  $d_G(u) = |N_G(u)|$  while in  $G_{sw}$  as  $d_{G_{sw}}(u) = 2s_v(u) + \sum_{x \in N_{G_{sw}}(u)} s_e(ux)$ .

4. The closeness sets for an edge  $e = uv$ ,

- $N_u(e|G) = \{x \in V(G) : d_G(u, x) < d_G(v, x)\} = N_u(e|G_{sw})$  with its cardinality for  $G$  as  $n_u(e|G) = |N_u(e|G)|$  and for  $G_{sw}$  as  $n_u(e|G_{sw}) = \sum_{x \in N_u(e|G_{sw})} w_v(x)$ .
- $M_u(e|G) = \{f \in E(G) : d_G(u, f) < d_G(v, f)\} = M_u(e|G_{sw})$  with its cardinality for  $G$  as  $m_u(e|G) = |M_u(e|G)|$  and for  $G_{sw}$  as  $m_u(e|G_{sw}) = \sum_{x \in N_u(e|G_{sw})} s_v(x) + \sum_{f \in M_u(e|G_{sw})} s_e(f)$ .
- The other quantities  $n_v(e|G)$ ,  $n_v(e|G_{sw})$ ,  $m_v(e|G)$  and  $m_v(e|G_{sw})$  are defined analogously.

## 1.2 Topological indices

The computation process of topological indices is closely related to graph theoretical methods because the structural formula of a compound is equivalent to a molecular graph. Since the advent of the well-known Wiener index [45], there are many other distance-based topological indices introduced to determine the structural properties of compounds.

In this section, we define the topological indices ( $TI$ ) such as Wiener ( $W$ ), edge-Wiener ( $W_e$ ), vertex-edge-Wiener ( $W_{ve}$ ), vertex-Szeged ( $Sz_v$ ), edge-Szeged ( $Sz_e$ ), edge-vertex-Szeged ( $Sz_{ev}$ ), total Szeged ( $Sz_t$ ), Padmakar-Ivan ( $PI$ ), Schultz ( $S$ ) and Gutman ( $Gut$ ) of the strength-weighted graph  $G_{sw}$ . Moreover, it is easy to notice that if  $w_v = s_e = 1$  and  $s_v = 0$ , then  $TI(G_{sw}) = TI(G)$ .

Table 1: Topological indices of a strength-weighted graph  $G_{sw}$

$TI$	$TI(G_{sw})$
$W$	$\sum_{\{u,v\} \subseteq V(G_{sw})} w_v(u) w_v(v) d_{G_{sw}}(u, v)$
$W_e$	$\sum_{\{u,v\} \subseteq V(G_{sw})} s_v(u) s_v(v) d_{G_{sw}}(u, v) + \sum_{\{e,f\} \subseteq E(G_{sw})} s_e(e) s_e(f) D_{G_{sw}}(e, f)$ $+ \sum_{u \in V(G_{sw})} \sum_{f \in E(G_{sw})} s_v(u) s_e(f) d_{G_{sw}}(u, f)$
$W_{ve}$	$\frac{1}{2} \left( \sum_{\{u,v\} \subseteq V(G_{sw})} \{w_v(u) s_v(v) + w_v(v) s_v(u)\} d_{G_{sw}}(u, v) \right.$ $\left. + \sum_{u \in V(G_{sw})} \sum_{f \in E(G_{sw})} w_v(u) s_e(f) d_{G_{sw}}(u, f) \right)$
$Sz_v$	$\sum_{e=uv \in E(G_{sw})} s_e(e) n_u(e G_{sw}) n_v(e G_{sw})$
$Sz_e$	$\sum_{e=uv \in E(G_{sw})} s_e(e) m_u(e G_{sw}) m_v(e G_{sw})$
$Sz_{ev}$	$\frac{1}{2} \sum_{e=uv \in E(G_{sw})} s_e(e) \left[ n_u(e G_{sw}) m_v(e G_{sw}) + n_v(e G_{sw}) m_u(e G_{sw}) \right]$
$Sz_t$	$Sz_v(G_{sw}) + Sz_e(G_{sw}) + 2 Sz_{ev}(G_{sw})$

$PI$	$\sum_{e=uv \in E(G_{sw})} s_e(e) \left[ m_u(e G_{sw}) + m_v(e G_{sw}) \right]$
$S$	$\sum_{\{u,v\} \subseteq V(G_{sw})} \left[ w_v(v) d_{G_{sw}}(u) + w_v(u) d_{G_{sw}}(v) \right] d_{G_{sw}}(u,v)$
$Gut$	$\sum_{\{u,v\} \subseteq V(G_{sw})} d_{G_{sw}}(u) d_{G_{sw}}(v) d_{G_{sw}}(u,v)$

## 2 Computational tools

The cut method serves as an efficient tool in the investigation of topological indices. If  $G$  is a partial cube then the cut method states that the Djoković-Winkler relation  $\Theta$  partitions the edge set of  $G$  into equivalence classes  $\{F_1, \dots, F_r\}$  such that the graph  $G - F_i$ ,  $1 \leq i \leq r$  consists of exactly two connected components  $\{C_i^1, C_i^2\}$  and for each pair of vertices  $u, v \in V(C_i^j)$ ,  $j = 1, 2$ , the shortest path between them lies within  $C_i^j$ .

**Theorem 1.** *Let  $\mathcal{F}(G) = \{F_1, \dots, F_r\}$  be the  $\Theta$ -partition of a partial cube  $G$ . Let  $n_1(F_i)$ ,  $n_2(F_i)$  be the orders and  $m_1(F_i)$ ,  $m_2(F_i)$  the sizes of the two components of  $G - F_i$ , respectively. Then*

- (i) [39]  $W(G) = \sum_{i=1}^r n_1(F_i) n_2(F_i)$ .
- (ii) [32]  $W_e(G) = \sum_{i=1}^r m_1(F_i) m_2(F_i)$ .
- (iii) [46]  $W_{ve}(G) = \frac{1}{2} \sum_{i=1}^r [n_1(F_i) m_2(F_i) + n_2(F_i) m_1(F_i)]$ .
- (iv) [47]  $Sz_v(G) = \sum_{i=1}^r |F_i| n_1(F_i) n_2(F_i)$ .
- (v) [32]  $Sz_e(G) = \sum_{i=1}^r |F_i| m_1(F_i) m_2(F_i)$ .
- (vi) [48]  $Sz_{ev}(G) = \frac{1}{2} \sum_{i=1}^r |F_i| \{n_1(F_i) m_2(F_i) + n_2(F_i) m_1(F_i)\}$ .
- (vii) [49]  $PI(G) = |E(G)|^2 - \sum_{i=1}^r |F_i|^2$ .
- (viii) [50]  $S(G) = |E(G)||V(G)| + 2 \sum_{i=1}^r [n_1(F_i) m_2(F_i) + n_2(F_i) m_1(F_i)]$ .
- (ix) [50]  $Gut(G) = 2|E(G)|^2 + \sum_{i=1}^r [4m_1(F_i) m_2(F_i) - |F_i|^2]$ .

However,  $\Theta$  is an equivalence relation on partial cubes but in general graphs it might not satisfy the transitive property of the equivalence relation. The transitive closure  $\Theta^*$  forms an equivalence relation on  $E(G)$  and partitions the edge set into  $\Theta^*$ -classes that disconnect the graph into multiple components. If  $\mathcal{F}(G) = \{F_1, \dots, F_k\}$  denotes the  $\Theta^*$ -partition of  $E(G)$ , then  $\mathcal{E}(G) = \{E_1, \dots, E_p\}$ , where each  $E_i$  is the union of one or more  $\Theta^*$ -classes, is a partition coarser than the partition  $\mathcal{F}(G)$  and denoted by  $\Theta^{c*}$ -partition. We now conclude this section by stating general theorem for a strength-weighted graph.

**Theorem 2.** [31, 44] *Let  $G_{sw} = (G, (w_v, s_v), s_e)$  be a strength-weighted graph. Let  $\mathcal{E}(G) = \{E_1, \dots, E_p\}$  be a  $\Theta^{c*}$ -partition of  $E(G)$ , and let  $TI \in \{W, W_e, W_{ve}, Sz_v, Sz_e, Sz_{ev}, PI, S, Gut\}$ . Then,*

$$TI(G_{sw}) = \sum_{i=1}^p TI(G/E_i, (w_v^i, s_v^i), s_e^i),$$

where

- $w_v^i : V(G_{sw}/E_i) \rightarrow \mathbb{R}^+$ ,  $w_v^i(X) = \sum_{x \in V(X)} w_v(x)$ ,  $\forall X \in V(G_{sw}/E_i)$ ,
- $s_v^i : V(G_{sw}/E_i) \rightarrow \mathbb{R}_0^+$ ,  $s_v^i(X) = \sum_{xy \in E(X)} s_e(xy) + \sum_{x \in V(X)} s_v(x)$ ,  $\forall X \in V(G_{sw}/E_i)$ ,
- $s_e^i : E(G_{sw}/E_i) \rightarrow \mathbb{R}^+$ ,  $s_e^i(XY) = \sum_{\substack{xy \in E_i \\ x \in V(X), y \in V(Y)}} s_e(xy)$ ,  $\forall XY \in E(G_{sw}/E_i)$ .

### 3 Full $k$ -subdivision of partial cubes

In this section, we apply Theorem 2 to full  $k$ -subdivision of partial cubes and thereby derive the closed formulae for the indices  $\{W, W_e, W_{ve}, Sz_v, Sz_e, Sz_{ev}, PI, S, Gut\}$  based on the  $\Theta$ -partition of partial cubes, but some preparation is necessary.

For  $k \geq 1$ , and  $l \geq 3$ , a uniform theta graph  $\theta(l; k)$  is constructed from a pair of end vertices, called North pole (N) and South pole (S), by joining  $l$  internal disjoint paths of equal length with  $k$  internal vertices. Suppose we allow  $l \geq 1$ , then the uniform theta graph can be treated as parallel composition of paths [51] and denoted by  $P(l; k)$ , see Figure 1.

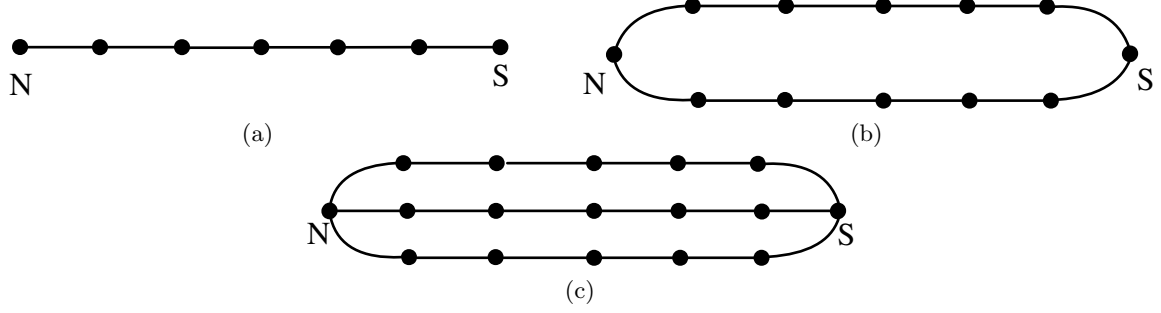


Figure 1: Parallel composition of paths (a)  $P(1;5)$  (b)  $P(2;5)$  (c)  $P(3;5)$

We now study the number of  $\Theta^*$ -classes of  $P(l;k)$  and interestingly, it is based on  $k$ . For  $1 \leq i \leq \lceil \frac{k}{2} \rceil$ , let  $F_i = \{e \in E(P(l;k)) : d_{P(l;k)}(N, e) = i - 1\} \cup \{f \in E(P(l;k)) : d_{P(l;k)}(S, f) = i - 1\}$ . When  $k$  is even, set in addition  $F_{\frac{k}{2}+1} = \{e \in E(P(l;k)) : d_{P(l;k)}(N, e) = d_{P(l;k)}(S, e) = \frac{k}{2}\}$ . Clearly,  $\{F_i : 1 \leq i \leq \lceil \frac{k}{2} \rceil\}$  and  $\{F_i : 1 \leq i \leq \frac{k}{2} + 1\}$  are the  $\Theta^*$ -partitions of  $P(l;k)$  respectively when  $k$  is odd and even, see Figure 2. Moreover,  $P(l;k) - F_i$ ,  $1 \leq i \leq \lceil \frac{k}{2} \rceil$ , results a quotient graph, which is a complete bipartite graph  $K_{2,l}$ , and in addition,  $P(l;k) - F_{\frac{k}{2}+1}$ ,  $k$  even, results a quotient graph  $K_2$ .

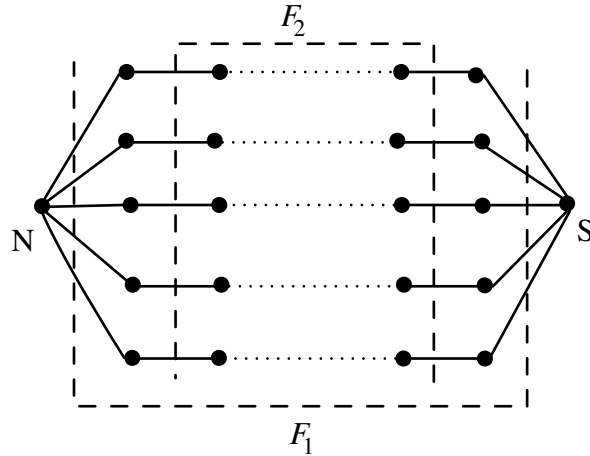


Figure 2:  $\Theta^*$ -partition of  $P(l;k)$

If  $G$  is a graph, then the full  $k$ -subdivision ( $k \geq 1$ ) graph  $S^k(G)$  of  $G$  is the graph obtained from  $G$  by replacing every edge  $uv$  of  $G$  with  $k$  new vertices  $x_{uv}^1, x_{uv}^2, \dots, x_{uv}^k$  which are connected to each other by a path along with the first vertex  $x_{uv}^1$  and the  $k^{th}$  vertex  $x_{uv}^k$  being connected to  $u$  and  $v$  respectively. Therefore, the cardinality of the vertex set and edge set in  $S^k(G)$  becomes  $|V(G)| + k|E(G)|$  and  $(k + 1)|E(G)|$  respectively.

With respect to the property of being a partial cube, the investigation of  $S^1(G)$  was initiated



in [52] where it was proved that if  $G$  is a connected graph, then  $S^1(G)$  is a partial cube if and only if every block of  $G$  is either a cycle or a complete graph. So not many graphs  $S^1(G)$  are partial cubes and consequently one is interested in the structure of the  $\Theta^*$ -classes of  $S^1(G)$ . These classes have been explicitly described in [30] for partial cubes  $G$ . Afterwards, the problem of determining the  $\Theta^*$ -classes of  $S^1(G)$  for an arbitrary graph  $G$  has been investigated in [53]. To describe these classes in general appears a very difficult problem, nevertheless some general properties have been developed and applied to describe the  $\Theta^*$ -classes of  $S^1(G)$  when  $G$  is a fullerene, a plane triangulation, or a chordal graph. In this paper we are interested in  $S^k(G)$  for an arbitrary  $k$ , and for our purposes the following fact is very important.

**Lemma 3.** *Let  $G$  be a partial cube and let  $k \geq 1$ . If the edges  $uv$  and  $wz$  of  $G$  are not in relation  $\Theta$ , then for an arbitrary edge  $e \in E(S^k(G)) \cap \{ux_{uv}^1, x_{uv}^1x_{uv}^2, \dots, x_{uv}^k v\}$  and an arbitrary edge  $f \in E(S^k(G)) \cap \{wx_{wz}^1, x_{wz}^1x_{wz}^2, \dots, x_{wz}^k z\}$ , the edge  $e$  is not in relation  $\Theta$  with the edge  $f$ .*

*Proof.* Since  $uv$  is not in relation  $\Theta$  with  $wz$ , we may assume without loss of generality that  $d_G(w, u) < d_G(w, v)$  and  $d_G(z, u) < d_G(z, v)$ . As partial cubes are bipartite graphs, we thus infer that there exists a shortest  $v, z$  path  $P$  in  $G$  which is of the form  $v \rightarrow u \rightarrow P' \rightarrow w \rightarrow z$ , where  $P'$  is a shortest  $u, w$ -path. But then, by the structure of  $S^k(G)$ , there exists a shortest  $v, z$ -path in  $S^k(G)$  that contains all the edges from  $\{ux_{uv}^1, x_{uv}^1x_{uv}^2, \dots, x_{uv}^k v\} \cup \{wx_{wz}^1, x_{wz}^1x_{wz}^2, \dots, x_{wz}^k z\}$ . Since no two edges of a shortest path are in relation  $\Theta$ , the assertion follows.  $\square$

The key message of Lemma 3 is that if  $G$  is a partial cube and  $F'$  is a  $\Theta^*$ -class of the graph  $S^k(G)$ , then there exists a  $\Theta$ -class  $F$  of  $G$  such that  $F'$  is a subset of the set of edges that are obtained by replacing the edges of  $F$  with paths of length  $k + 1$ .

**Theorem 4.** *Let  $\mathcal{F}(G) = \{F_1, \dots, F_r\}$  be the  $\Theta$ -partition of a partial cube  $G$ . If  $F_i = \{u_1v_1, \dots, u_s v_s\}$ ,  $1 \leq i \leq r$ , and let  $F'_i = \bigcup_{j=1}^s \{u_j x_{u_j v_j}^1, x_{u_j v_j}^1 x_{u_j v_j}^2, \dots, x_{u_j v_j}^k v_j\}$ , then  $\mathcal{F}'(S^k(G)) = \{F'_1, \dots, F'_r\}$  is the  $\Theta^{c*}$ -partition of  $S^k(G)$ . If  $TI \in \{W, W_e, W_{ve}, Sz_v, Sz_e, Sz_{ev}, PI, S, Gut\}$ , then*

$$TI(S^k(G)) = \sum_{i=1}^r \left[ \sum_{j=1}^{\lceil \frac{k}{2} \rceil} TI(K_{2, |F_i|^j}, (w_v^i, s_v^i), s_e^i) + \frac{1 + (-1)^k}{2} TI(K_2, (w_v^i, s_v^i), s_e^i) \right].$$

Furthermore,

$$(i) \quad W(S^k(G)) = (k + 1) \left\{ W(G) + 2kW_{ve}(G) + k^2W_e(G) + k|E(G)| \left( \frac{1}{2}|V(G)| + \frac{(2k+1)}{6}|E(G)| - \frac{(k+2)}{6} \right) + \frac{k(k-1)}{6}PI(G) \right\}.$$

$$(ii) \quad W_e(S^k(G)) = (k+1) \left\{ (k+1)^2 W_e(G) + \frac{k(k+2)}{6} PI(G) + k|E(G)| \left( \frac{2k+1}{6} |E(G)| - \frac{k+2}{6} \right) \right\}.$$

$$(iii) \quad W_{ve}(S^k(G)) = (k+1) \left\{ (k+1) W_{ve}(G) + k(k+1) W_e(G) + k|E(G)| \left( \frac{(2k+1)}{6} |E(G)| + \frac{1}{4} |V(G)| - \frac{k+2}{6} \right) + \frac{k(2k+1)}{12} PI(G) \right\}.$$

$$(iv) \quad Sz_v(S^k(G)) = (k+1) \left\{ Sz_v(G) + 2k Sz_{ev}(G) + k^2 Sz_e(G) + k(|E(G)|^2 - PI(G)) \left( \frac{k+1}{2} |V(G)| + \frac{k(k+1)}{2} |E(G)| + \frac{(k+2)}{3} \right) - \frac{k(k+2)}{3} |E(G)| - \frac{k(2k+1)}{6} \sum_{i=1}^r |F_i|^3 \right\}.$$

$$(v) \quad Sz_e(S^k(G)) = (k+1) \left\{ (k+1)^2 Sz_e(G) - \frac{k(k+2)}{3} |E(G)| + k(|E(G)|^2 - PI(G)) \left( \frac{(k+1)}{2} |E(G)| + \frac{(k+2)}{3} \right) - \frac{k(k+2)}{3} \sum_{i=1}^r |F_i|^3 \right\}.$$

$$(vi) \quad Sz_{ev}(S^k(G)) = (k+1) \left\{ (k+1) Sz_{ev}(G) + k(k+1) Sz_e(G) - \frac{k(k+2)}{3} |E(G)| + \left( \frac{k}{4} |V(G)| + \frac{k(2k+1)}{4} |E(G)| + \frac{k(k+2)}{3} \right) (|E(G)|^2 - PI(G)) - \frac{k(4k+5)}{12} \sum_{i=1}^k |F_i|^3 \right\}.$$

$$(vii) \quad PI(S^k(G)) = (k+1) \left\{ k|E(G)|^2 + PI(G) \right\}.$$

$$(viii) \quad S(S^k(G)) = (k+1) \left\{ 4(k+1) W_{ve}(G) + 4k(k+1) W_e(G) + |E(G)| \left( (k+1) |V(G)| - \frac{2k(k+2)}{3} \right) + \frac{k(4k+5)}{3} |E(G)|^2 + \frac{k(2k+1)}{3} PI(G) \right\}.$$

$$(ix) \quad Gut(S^k(G)) = (k+1) \left\{ 4(k+1)^2 W_e(G) + \left( \frac{(2k+1)(2k+3)}{3} \right) |E(G)|^2 - \frac{2k(k+2)}{3} |E(G)| + \frac{2k^2+4k+3}{3} PI(G) \right\}.$$

*Proof.* It is well-known that removing a  $\Theta$ -class  $F_i$  of a partial cube  $G$  dissects the original graph into exactly two components, resulting in a quotient graph  $K_2$  with edge-strength value  $|F_i|$  and vertex-strength-weighted values  $(n_1(F_i), m_1(F_i))$  and  $(n_2(F_i), m_2(F_i))$ . If  $F_i = \{u_j v_j : 1 \leq j \leq s\}$ , then it follows from Lemma 3 (see also the remark after its proof) that  $F'_i$  is a union of some  $\Theta^*$ -classes of  $S^k(G)$ . Moreover, a removal of  $F'_i$  from  $S^k(G)$  dissects  $S^k(G)$  into  $k|F_i| + 2$  components resulting in a quotient graph of parallel composition of paths  $P(|F_i|; k)$  with vertex-strength-weighted values of North and South poles respectively  $(a_i(F'_i), b_i(F'_i))$  and  $(c_i(F'_i), d_i(F'_i))$  where  $a_i(F'_i) = n_1(F_i) + km_1(F_i)$ ,  $b_i(F'_i) = (k+1)m_1(F_i)$ ,  $c_i(F'_i) = n_2(F_i) + km_2(F_i)$ , and  $d_i(F'_i) = (k+1)m_2(F_i)$ , and all the internal vertices with  $(1,0)$  and edge strength for all the edges to 1. As we have mentioned

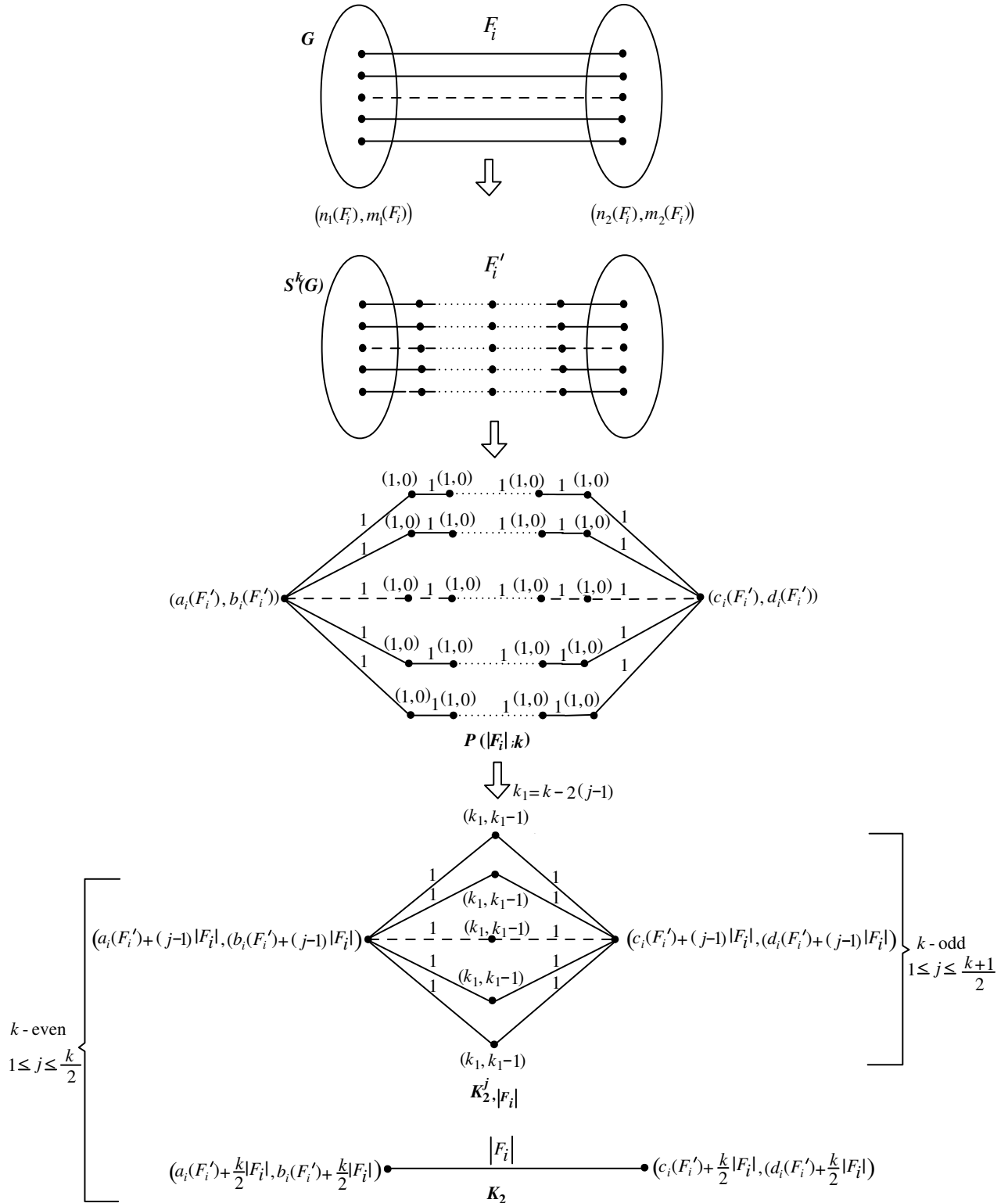


Figure 3: Construction of quotient graphs from full  $k$ -subdivision of partial cubes

earlier, we apply the  $\Theta^*$ -partition of  $P(|F_i|; k)$  to obtain a quotient graph  $K_{2,|F_i|}^j$  with the edge-strength 1 for all the edges and the vertex-strength-weighted values for first partite vertices as  $(a_i(F'_i) + (j-1)|F_i|, b_i(F'_i) + (j-1)|F_i|)$  and  $(c_i(F'_i) + (j-1)|F_i|, d_i(F'_i) + (j-1)|F_i|)$ , and the other each partite vertex as  $(k - 2(j-1), k - 2j + 1)$ , where  $1 \leq j \leq \frac{k+1}{2}$  and  $k$  is odd. When  $k$  is even, we have quotient graphs as above  $K_{2,|F_i|}^j$ ,  $1 \leq j \leq \frac{k}{2}$ , and in addition, there is a unique  $\Theta^*$ -class producing a quotient graph  $K_2$  with edge-strength value  $|F_i|$  and vertex-strength-weighted values as  $(a_i(F'_i) + \frac{k}{2}|F_i|, b_i(F'_i) + \frac{k}{2}|F_i|)$  and  $(c_i(F'_i) + \frac{k}{2}|F_i|, d_i(F'_i) + \frac{k}{2}|F_i|)$ , see Figure 3. Hence the main formula of the theorem follows from Theorem 2. Applying the same theorem we obtain the closed formulae as follows:

$$\begin{aligned}
(ii) \quad W(K_{2,|F_i|}^j, (w_v^i, s_v^i), s_e^i) &= 2(a_i(F'_i) + (j-1)|F_i|)(c_i(F'_i) + (j-1)|F_i|) + (k - 2(j-1))|F_i| \\
&\quad (a_i(F'_i) + (j-1)|F_i| + c_i(F'_i) + (j-1)|F_i|) + (k - 2(j-1))^2|F_i|(|F_i| - 1) \\
&= 2(n_1(F_i) + km_1(F_i) + (j-1)|F_i|)(n_2(F_i) + km_2(F_i) + (j-1)|F_i|) \\
&\quad + (k - 2(j-1))|F_i|(n_1(F_i) + km_1(F_i) + (j-1)|F_i| + n_2(F_i) + km_2(F_i) \\
&\quad + (j-1)|F_i|) + (k - 2(j-1))^2|F_i|(|F_i| - 1) \\
&= 8|F_i|j - 4|F_i| - 4|F_i|k + 2n_1(F_i)n_2(F_i) - 4|F_i|j^2 - 4|F_i|^2j - |F_i|k^2 \\
&\quad + 2|F_i|^2k + 2|F_i|^2 + 2|F_i|^2j^2 + |F_i|^2k^2 + 2k^2m_1(F_i)m_2(F_i) \\
&\quad + 4|F_i|jk + |F_i|kn_1(F_i) + |F_i|kn_2(F_i) + 2km_1(F_i)n_2(F_i) \\
&\quad + 2km_2(F_i)n_1(F_i) - 2|F_i|^2jk + |F_i|k^2m_1(F_i) + |F_i|k^2m_2(F_i).
\end{aligned}$$

$$\begin{aligned}
W(K_2, (w_v^i, s_v^i), s_e^i) &= (a_i(F'_i) + \frac{k}{2}|F_i|)(c_i(F'_i) + \frac{k}{2}|F_i|) \\
&= (n_1(F_i) + km_1(F_i) + \frac{k}{2}|F_i|)(n_2(F_i) + km_2(F_i) + \frac{k}{2}|F_i|).
\end{aligned}$$

$$\begin{aligned}
W(S^k(G)) &= \sum_{i=1}^r \left[ \sum_{j=1}^{\lceil \frac{k}{2} \rceil} W(K_{2,|F_i|}^j, (w_v^i, s_v^i), s_e^i) + \frac{1 + (-1)^k}{2} W(K_2, (w_v^i, s_v^i), s_e^i) \right] \\
&= (k+1) \left\{ W(G) + 2kW_{ve}(G) + k^2W_e(G) + k|E(G)| \left( \frac{1}{2}|V(G)| \right. \right. \\
&\quad \left. \left. + \frac{(2k+1)}{6}|E(G)| - \frac{(k+2)}{6} \right) + \frac{k(k-1)}{6}PI(G) \right\}.
\end{aligned}$$

$$\begin{aligned}
(ii) \quad W_e(K_{2,|F_i|}^j, (w_v^i, s_v^i), s_e^i) &= 2(b_i(F'_i) + (j-1)|F_i|)(d_i(F'_i) + (j-1)|F_i|) + ((k - 2j + 1) + 1) \\
&\quad |F_i|[(b_i(F'_i) + (j-1)|F_i|) + (d_i(F'_i) + (j-1)|F_i|)] + \\
&\quad ((k - 2j + 1) + 1)^2|F_i|(|F_i| - 1)
\end{aligned}$$

$$\begin{aligned}
&= 2((k+1)m_1(F_i) + (j-1)|F_i|)((k+1)m_2 + (j-1)|F_i|) + \\
&\quad (k-2(j-1))|F_i|((k+1)m_1(F_i) + (j-1)|F_i| + (k+1)m_2(F_i) \\
&\quad + (j-1)|F_i|) + (k-2(j-1))^2|F_i|(|F_i| - 1) \\
&= 8|F_i|j - 4|F_i| - 4|F_i|k + 2m_1(F_i)m_2(F_i) \\
&\quad - 4|F_i|j^2 - 4|F_i|^2j - |F_i|k^2 + 2|F_i|^2k + 2|F_i|^2 + 2|F_i|^2j^2 \\
&\quad + |F_i|^2k^2 + 2k^2m_1(F_i)m_2(F_i) + 4|F_i|jk + |F_i|km_1(F_i) \\
&\quad + |F_i|km_2(F_i) + 4km_1(F_i)m_2(F_i) - 2|F_i|^2jk \\
&\quad + |F_i|k^2m_1(F_i) + |F_i|k^2m_2(F_i).
\end{aligned}$$

$$\begin{aligned}
W_e(K_2, (w_v^i, s_v^i), s_e^i) &= (b_i(F_i') + \frac{k}{2}|F_i|)(d_i(F_i') + \frac{k}{2}|F_i|) \\
&= ((k+1)m_1(F_i) + \frac{k}{2}|F_i|)((k+1)m_2(F_i) + \frac{k}{2}|F_i|).
\end{aligned}$$

$$\begin{aligned}
W_e(S^k(G)) &= \sum_{i=1}^r \left[ \sum_{j=1}^{\lfloor \frac{k}{2} \rfloor} W_e(K_{2,|F_i|^j}^j, (w_v^i, s_v^i), s_e^i) + \frac{1+(-1)^k}{2} W_e(K_2, (w_v^i, s_v^i), s_e^i) \right] \\
&= (k+1) \left\{ (k+1)^2 W_e(G) + \frac{k(k+2)}{6} PI(G) \right. \\
&\quad \left. + k|E(G)| \left( \frac{2k+1}{6} |E(G)| - \frac{(k+2)}{6} \right) \right\}.
\end{aligned}$$

$$\begin{aligned}
(iii) \quad W_{ve}(K_{2,|F_i|^j}^j, (w_v^i, s_v^i), s_e^i) &= 2((a_i(F_i') + (j-1)|F_i|)(d_i(F_i') + (j-1)|F_i|) + (b_i(F_i') + (j-1)|F_i|) \\
&\quad (c_i(F_i') + (j-1)|F_i|)) + (k-2(j-1))|F_i|((b_i(F_i') + (j-1)|F_i|) \\
&\quad + (d_i(F_i') + (j-1)|F_i|)) + (k-2j+1)|F_i|(a_i + (j-1)|F_i| + c_i(F_i') \\
&\quad + (j-1)|F_i|) + |F_i|(a_i(F_i') + (j-1)|F_i| + c_i(F_i') + (j-1)|F_i| \\
&\quad + 2(k-2(j-1))(F-1)) + 2(k-2j+1)(k-2(j-1))|F_i|(|F_i| - 1) \\
&= 2((n_1(F_i) + km_1(F_i) + (j-1)|F_i|)((k+1)m_1(F_i) + (j-1)|F_i|) \\
&\quad + (n_2(F_i) + km_2(F_i) + (j-1)|F_i|)((k+1)m_2(F_i) + (j-1)|F_i|)) \\
&\quad + (k-2(j-1))|F_i|(((k+1)m_1(F_i) + (j-1)|F_i|) + ((k+1)m_2(F_i) \\
&\quad + (j-1)|F_i|)) + (k-2j+1)|F_i|(n_1(F_i) + km_1(F_i) + (j-1)|F_i| \\
&\quad + n_2(F_i) + km_2(F_i) + (j-1)|F_i|) + |F_i|(n_1(F_i) + km_1(F_i) \\
&\quad + (j-1)|F_i| + n_2(F_i) + km_2(F_i) + (j-1)|F_i| + 2(k-2(j-1)) \\
&\quad (|F_i| - 1)) + 2(k-2j+1)(k-2(j-1))|F_i|(|F_i| - 1)
\end{aligned}$$

$$\begin{aligned}
&= 16|F_i|j - 8|F_i| - 8|F_i|k + 2m_1(F_i)n_2(F_i) + 2m_2(F_i)n_1(F_i) - 8|F_i|j^2 \\
&\quad - 8|F_i|^2j - 2|F_i|k^2 + 4|F_i|^2k + 4|F_i|^2 + 4|F_i|^2j^2 + 2|F_i|^2k^2 + \\
&\quad 4k^2m_1(F_i)m_2(F_i) + 8|F_i|jk + |F_i|km_1(F_i) + |F_i|km_2(F_i) \\
&\quad + |F_i|kn_1(F_i) + |F_i|kn_2(F_i) + 4km_1(F_i)m_2(F_i) + 2km_1(F_i)n_2(F_i) \\
&\quad + 2km_2(F_i)n_1(F_i) - 4|F_i|^2jk + 2|F_i|k^2m_1(F_i) + 2|F_i|k^2m_2(F_i).
\end{aligned}$$

$$\begin{aligned}
W_{ve}(K_2, (w_v^i, s_v^i), s_e^i) &= (b_i(F_i') + \frac{k}{2}|F_i|)(d_i(F_i') + \frac{k}{2}|F_i|) \\
&= ((k+1)m_1(F_i) + \frac{k}{2}|F_i|)((k+1)m_2(F_i) + \frac{k}{2}|F_i|).
\end{aligned}$$

$$\begin{aligned}
W_{ve}(S^k(G)) &= \sum_{i=1}^r \left[ \sum_{j=1}^{\lceil \frac{k}{2} \rceil} W_{ve}(K_{2,|F_i|^j}^j, (w_v^i, s_v^i), s_e^i) + \frac{1+(-1)^k}{2} W_{ve}(K_2, (w_v^i, s_v^i), s_e^i) \right] \\
&= (k+1) \left\{ (k+1)W_{ve}(G) + k(k+1)W_e(G) + k|E(G)| \left( \frac{(2k+1)}{6}|E(G)| \right. \right. \\
&\quad \left. \left. + \frac{1}{4}|V(G)| - \frac{k+2}{6} \right) + \frac{k(2k+1)}{12}PI(G) \right\}.
\end{aligned}$$

$$\begin{aligned}
(iv) \ Sz_v(K_{2,|F_i|^j}^j, (w_v^i, s_v^i), s_e^i) &= |F_i| \left( (a_i(F_i') + (j-1)|F_i| + (k-2(j-1))(|F_i|-1) + c_i(F_i') + (j-1)|F_i| \right. \\
&\quad \left. + k-2(j-1)) + (c_i(F_i') + (j-1)|F_i| + (k-2(j-1))(|F_i|-1) + a_i(F_i') \right. \\
&\quad \left. + (j-1)|F_i| + k-2(j-1)) \right) \\
&= |F_i| \left( (n_1(F_i) + km_1(F_i) + (j-1)|F_i| + (k-2(j-1))(|F_i|-1) + n_2(F_i) + \right. \\
&\quad \left. km_2(F_i) + (j-1)|F_i| + k-2(j-1)) + (n_2(F_i) + km_2(F_i) + (j-1)|F_i| + \right. \\
&\quad \left. (k-2(j-1))(|F_i|-1) + n_1(F_i) + km_1(F_i) + (j-1)|F_i| + k-2(j-1)) \right) \\
&= -|F_i|(8k - 16j - 8|F_i| + 16|F_i|j - 8|F_i|k - 8jk - 2n_1(F_i)n_2(F_i) \\
&\quad - 8|F_i|j^2 - 4|F_i|^2j - 2|F_i|k^2 + 2|F_i|^2k + 2|F_i|^2 + 8j^2 + 2k^2 + 2|F_i|^2j^2 \\
&\quad - 2k^2m_1(F_i)m_2(F_i) + 8|F_i|jk - |F_i|kn_1(F_i) - |F_i|kn_2(F_i) \\
&\quad - 2km_1(F_i)n_2(F_i) - 2km_2(F_i)n_1(F_i) - 2|F_i|^2jk - |F_i|k^2m_1(F_i) \\
&\quad - |F_i|k^2m_2(F_i) + 8).
\end{aligned}$$

$$\begin{aligned}
Sz_v(K_2, (w_v^i, s_v^i), s_e^i) &= (a_i(F_i') + \frac{k}{2}|F_i|)(c_i(F_i') + \frac{k}{2}|F_i|) \\
&= (n_1(F_i) + km_1(F_i) + \frac{k}{2}|F_i|)(n_2(F_i) + km_2(F_i) + \frac{k}{2}|F_i|).
\end{aligned}$$

$$\begin{aligned}
Sz_v(S^k(G)) &= \sum_{i=1}^r \left[ \sum_{j=1}^{\lfloor \frac{k}{2} \rfloor} Sz_v(K_{2,|F_i|^j}^j, (w_v^i, s_v^i), s_e^i) + \frac{1+(-1)^k}{2} Sz_v(K_2, (w_v^i, s_v^i), s_e^i) \right] \\
&= (k+1) \left\{ Sz_v(G) + 2k Sz_{ev}(G) + k^2 Sz_e(G) + k(|E(G)|^2 - PI(G)) \right. \\
&\quad \left( \frac{k+1}{2} |V(G)| + \frac{k(k+1)}{2} |E(G)| + \frac{(k+2)}{3} \right) - \frac{k(k+2)}{3} |E(G)| \\
&\quad \left. - \frac{k(2k+1)}{6} \sum_{i=1}^r |F_i|^3 \right\}.
\end{aligned}$$

$$\begin{aligned}
(v) \quad Sz_e(K_{2,|F_i|^j}^j, (w_v^i, s_v^i), s_e^i) &= |F_i| \left( (b_i(F_i') + (j-1)|F_i| + (k-2j+1)(|F_i|-1) + |F_i|-1) \right. \\
&\quad (d_i(F_i') + (j-1)|F_i| + k-2j+2) + (d_i(F_i') + (j-1)|F_i| + \\
&\quad \left. (k-2j+1)(|F_i|-1) + |F_i|-1)(b_i(F_i') + (j-1)|F_i| + k-2j+2) \right) \\
&= |F_i| \left( ((k+1)m_1 + (j-1)|F_i| + (k-2j+1)(|F_i|-1) + |F_i|-1) \right. \\
&\quad ((k+1)m_2 + (j-1)|F_i| + k-2j+2) + ((k+1)m_2 + (j-1)|F_i| + \\
&\quad \left. (k-2j+1)(|F_i|-1)((k+1)m_1 + (j-1)|F_i| + k-2(j-1)+2) \right) \\
&= -|F_i|(8k-16j-8|F_i|+16|F_i|j-8|F_i|k-8jk-2m_1(F_i)m_2(F_i) \\
&\quad -8|F_i|j^2-4|F_i|^2j-2|F_i|k^2+2|F_i|^2k+2|F_i|^2+8j^2+2k^2+2|F_i|^2j^2 \\
&\quad -2k^2m_1(F_i)m_2(F_i)+8|F_i|jk-|F_i|km_1(F_i)-|F_i|km_2(F_i) \\
&\quad -4km_1(F_i)m_2(F_i)-2|F_i|^2jk-|F_i|k^2m_1(F_i)-|F_i|k^2m_2(F_i)+8).
\end{aligned}$$

$$\begin{aligned}
Sz_e(K_2, (w_v^i, s_v^i), s_e^i) &= (b_i(F_i') + \frac{k}{2}|F_i|)(d_i(F_i') + \frac{k}{2}|F_i|) \\
&= ((k+1)m_1(F_i) + \frac{k}{2}|F_i|)((k+1)m_2(F_i) + \frac{k}{2}|F_i|).
\end{aligned}$$

$$\begin{aligned}
Sz_e(S^k(G)) &= \sum_{i=1}^r \left[ \sum_{j=1}^{\lfloor \frac{k}{2} \rfloor} Sz_e(K_{2,|F_i|^j}^j, (w_v^i, s_v^i), s_e^i) + \frac{1+(-1)^k}{2} Sz_e(K_2, (w_v^i, s_v^i), s_e^i) \right] \\
&= (k+1) \left\{ (k+1)^2 Sz_e(G) - \frac{k(k+2)}{3} |E(G)| + k(|E(G)|^2 - PI(G)) \right. \\
&\quad \left. \left( \frac{(k+1)}{2} |E(G)| + \frac{(k+2)}{3} \right) - \frac{k(k+2)}{3} \sum_{i=1}^r |F_i|^3 \right\}.
\end{aligned}$$

$$(vi) \quad Sz_{ev}(K_{2,|F_i|^j}^j, (w_v^i, s_v^i), s_e^i) = |F_i| \left( (a_i(F_i') + (j-1)|F_i| + (k-2(j-1))(|F_i|-1))(d_i(F_i')
\right.$$

$$\begin{aligned}
& + (j-1)|F_i| + k - 2j + 2)) + ((c_i(F'_i) + (j-1)|F_i| + (k-2(j-1))) \\
& (b_i(F'_i) + (j-1)|F_i| + (k-2j+1)(|F_i|-1) + |F_i|-1))(c_i(F'_i) \\
& + (j-1)|F_i| + (k-2(j-1))(|F_i|-1))(b_i(F'_i) + (j-1)|F_i| \\
& + k - 2j + 2)) + ((a_i(F'_i) + (j-1)|F_i| + (k-2(j-1)))(d_i(F'_i) \\
& + (j-1)|F_i| + (k-2j+1)(|F_i|-1) + |F_i|-1))) \\
= & |F_i| \left( (n_1(F_i) + km_1(F_i) + (j-1)|F_i| + (k-2(j-1))(|F_i|-1)) \right. \\
& ((k+1)m_2(F_i) + (j-1)|F_i| + k - 2j + 2)) + ((n_2(F_i) + km_2(F_i) \\
& + (k-2(j-1)))(k+1)m_1(F_i) + (j-1)|F_i| + (k-2j+1)(|F_i|-1) \\
& + |F_i|-1))(n_2(F_i) + km_2(F_i) + (j-1)|F_i| + (k-2(j-1))(|F_i|-1)) \\
& ((k+1)m_1(F_i) + (j-1)|F_i| + k - 2j + 2)) + ((n_1(F_i) + km_1(F_i) \\
& + (j-1)|F_i| + (k-2(j-1)))(k+1)m_2(F_i) + (j-1)|F_i| \\
& \left. + (k-2j+1)(|F_i|-1) + |F_i|-1) \right) \\
= & - |F_i|(16k - 32j - 16|F_i| + 32|F_i|j - 16|F_i|k - 16jk - 2m_1(F_i)n_2(F_i) \\
& - 2m_2(F_i)n_1(F_i) - 16|F_i|j^2 - 8|F_i|^2j - 4|F_i|k^2 + 4F^2k + 4|F_i|^2 + 16j^2 \\
& + 4k^2 + 4|F_i|^2j^2 - 4k^2m_1(F_i)m_2(F_i) + 16|F_i|jk - |F_i|km_1(F_i) \\
& - |F_i|km_2(F_i) - |F_i|kn_1(F_i) - |F_i|kn_2(F_i) - 4km_1(F_i)m_2(F_i) \\
& - 2km_1(F_i)n_2(F_i) - 2km_2(F_i)n_1(F_i) - 4|F_i|^2jk - 2|F_i|k^2m_1(F_i) \\
& - 2|F_i|k^2m_2(F_i) + 16). \\
Sz_{ev}(K_2, (w_v^i, s_v^i), s_e^i) = & (a_i(F'_i) + \frac{k}{2}|F_i|)(d_i(F'_i) + \frac{k}{2}|F_i|) + (c_i(F'_i) + \frac{k}{2}|F_i|)(b_i(F'_i) + \frac{k}{2}|F_i|) \\
= & (n_1(F_i) + km_1(F_i) + \frac{k}{2}|F_i|)((k+1)m_2(F_i) + \frac{k}{2}|F_i|) + (n_2(F_i) \\
& + km_2(F_i) + \frac{k}{2}|F_i|)((k+1)m_1(F_i) + \frac{k}{2}|F_i|). \\
Sz_{ev}(S^k(G)) = & \sum_{i=1}^r \left[ \sum_{j=1}^{\lfloor \frac{k}{2} \rfloor} Sz_{ev}(K_{2,|F_i|^j}^j, (w_v^i, s_v^i), s_e^i) + \frac{1+(-1)^k}{2} Sz_{ev}(K_2, (w_v^i, s_v^i), s_e^i) \right] \\
= & (k+1) \left\{ (k+1)Sz_{ev}(G) + k(k+1)Sz_e(G) - \frac{k(k+2)}{3}|E(G)| + \left( \frac{k}{4}|V(G)| \right. \right. \\
& \left. \left. + \frac{k(2k+1)}{4}|E(G)| + \frac{k(k+2)}{3} \right) (|E(G)|^2 - PI(G)) - \frac{k(4k+5)}{12} \sum_{i=1}^k |F_i|^3 \right\}
\end{aligned}$$



$$\begin{aligned}
(vii) \quad PI(K_{2,|F_i|}^j, (w_v^i, s_v^i), s_e^i) &= |F_i| \left( (b_i(F'_i) + (j-1)|F_i| + (k-2j+1)(|F_i|-1) + |F_i|-1) \right. \\
&\quad + (d_i(F'_i) + (j-1)|F_i| + k-2j+2) + (d_i(F'_i) + (j-1)|F_i| \\
&\quad \left. + (k-2j+1)(|F_i|-1) + |F_i|-1) + (b_i(F'_i) + (j-1)|F_i| + k-2j+2) \right) \\
&= |F_i| \left( ((k+1)m_1 + (j-1)|F_i| + (k-2j+1)(|F_i|-1) + |F_i|-1) \right. \\
&\quad + ((k+1)m_2 + (j-1)|F_i| + k-2j+2) + ((k+1)m_2 + (j-1)|F_i| \\
&\quad \left. + (k-2j+1)(|F_i|-1) + ((k+1)m_1 + (j-1)|F_i| + k-2(j-1)+2) \right) \\
&= |F_i|(k+1)(m_1(F_i) + m_2(F_i) + |F_i|k + km_1(F_i) + km_2(F_i)) \\
PI(K_2, (w_v^i, s_v^i), s_e^i) &= (b_i(F'_i) + \frac{k}{2}|F_i|) + (d_i(F'_i) + \frac{k}{2}|F_i|) \\
&= ((k+1)m_1(F_i) + \frac{k}{2}|F_i|) + ((k+1)m_2(F_i) + \frac{k}{2}|F_i|). \\
PI(S^k(G)) &= \sum_{i=1}^r \left[ \sum_{j=1}^{\lfloor \frac{k}{2} \rfloor} PI(K_{2,|F_i|}^j, (w_v^i, s_v^i), s_e^i) + \frac{1+(-1)^k}{2} PI(K_2, (w_v^i, s_v^i), s_e^i) \right] \\
&= (k+1) \left\{ k|E(G)|^2 + PI(G) \right\}.
\end{aligned}$$

$$\begin{aligned}
(viii) \quad S(K_{2,|F_i|}^j, (w_v^i, s_v^i), s_e^i) &= 2((a_i(F'_i) + (j-1)|F_i|)((2d_i(F'_i) + (j-1)|F_i|) + |F_i|) + \\
&\quad (c_i(F'_i) + (j-1)|F_i|)(2(b_i(F'_i) + (j-1)|F_i|) + |F_i|)) + \\
&\quad |F_i|(k-2(j-1))(2(a_i(F'_i) + (j-1)|F_i|) + 2(c_i(F'_i) + (j-1)|F_i|) \\
&\quad + (2(b_i(F'_i) + (j-1)|F_i|) + |F_i|) + (2(d_i(F'_i) + (j-1)|F_i|) + |F_i|)) \\
&\quad + 2(((k-2(j-1))^2)|F_i|(|F_i|-1)) \\
&= 2((n_1(F_i) + km_1(F_i) + (j-1)|F_i|)((2(k+1)m_2 + (j-1)|F_i|) + |F_i|) + \\
&\quad (n_2(F_i) + km_2(F_i) + (j-1)|F_i|)(2((k+1)m_1 + (j-1)|F_i|) + |F_i|)) + \\
&\quad |F_i|(k-2(j-1))(2(n_1(F_i) + km_1(F_i) + (j-1)|F_i|) + 2(n_2(F_i) + km_2(F_i) \\
&\quad + (j-1)|F_i|) + (2((k+1)m_1 + (j-1)|F_i|) + |F_i|) + (2((k+1)m_2 \\
&\quad + (j-1)|F_i|) + |F_i|)) + 2(((k-2(j-1))^2)|F_i|(|F_i|-1)) \\
&= 2(16|F_i|j - 8|F_i| - 8|F_i|k + |F_i|n_1(F_i) + |F_i|n_2(F_i) + 2m_1(F_i)n_2(F_i) \\
&\quad + 2m_2(F_i)n_1(F_i) - 8|F_i|j^2 - 8|F_i|^2j - 2|F_i|k^2 + 5|F_i|^2k + 4|F_i|^2 + \\
&\quad 4|F_i|^2j^2 + 2|F_i|^2k^2 + 4k^2m_1(F_i)m_2(F_i) + 8|F_i|jk + 2|F_i|km_1(F_i)
\end{aligned}$$

$$\begin{aligned}
& + 2|F_i|km_2(F_i) + |F_i|kn_1(F_i) + |F_i|kn_2(F_i) + 4km_1(F_i)m_2(F_i) \\
& + 2km_1(F_i)n_2(F_i) + 2km_2(F_i)n_1(F_i) - 4|F_i|^2jk + 2|F_i|k^2m_1(F_i) \\
& + 2|F_i|k^2m_2(F_i)).
\end{aligned}$$

$$\begin{aligned}
S(K_2, (w_v^i, s_v^i), s_e^i) &= ((2(d_i(F_i') + \frac{k}{2}|F_i|) + |F_i|)(a_i(F_i') + \frac{k}{2}|F_i|)) \\
&+ ((2(b_i(F_i') + \frac{k}{2}|F_i|) + |F_i|)(c_i(F_i') + \frac{k}{2}|F_i|)) \\
&= ((2((k+1)m_2(F_i) + \frac{k}{2}|F_i|) + |F_i|)(n_1(F_i) + km_1(F_i) + \frac{k}{2}|F_i|)) \\
&+ ((2((k+1)m_1(F_i) + \frac{k}{2}|F_i|) + |F_i|)(n_2(F_i) + km_2(F_i) + \frac{k}{2}|F_i|)).
\end{aligned}$$

$$\begin{aligned}
S(S^k(G)) &= \sum_{i=1}^r \left[ \sum_{j=1}^{\lceil \frac{k}{2} \rceil} S(K_{2,|F_i|^j}, (w_v^i, s_v^i), s_e^i) + \frac{1+(-1)^k}{2} S(K_2, (w_v^i, s_v^i), s_e^i) \right] \\
&= (k+1) \left\{ 4(k+1)W_{ve}(G) + 4k(k+1)W_e(G) + |E(G)| \left( (k+1)|V(G)| - \frac{2k(k+2)}{3} \right) \right. \\
&\quad \left. + \frac{k(4k+5)}{3}|E(G)|^2 + \frac{k(2k+1)}{3}PI(G) \right\}.
\end{aligned}$$

$$\begin{aligned}
(ix) \text{ Gut}(K_{2,|F_i|^j}^j, (w_v^i, s_v^i), s_e^i) &= 2((2(b_i(F_i') + (j-1)|F_i|) + |F_i|)(2(d_i(F_i') + (j-1)|F_i|) + |F_i|)) \\
&+ |F_i|2(k-2(j-1))((2(b_i(F_i') + (j-1)|F_i|) + |F_i|) + (2(b_i(F_i') \\
&+ (j-1)|F_i|) + |F_i|)) + 4(k-2(j-1))^2|F_i|(|F_i|-1) \\
&= 2((2((k+1)m_1(F_i) + (j-1)|F_i|) + |F_i|)(2((k+1)m_2(F_i) \\
&+ (j-1)|F_i|) + |F_i|)) + |F_i|2(k-2(j-1))((2((k+1)m_1(F_i) \\
&+ (j-1)|F_i|) + |F_i|) + (2((k+1)m_2(F_i) + (j-1)|F_i|) + |F_i|)) \\
&+ 4(k-2(j-1))^2|F_i|(|F_i|-1) \\
&= 2(16|F_i|j - 8|F_i| - 8|F_i|k + 2|F_i|m_1(F_i) + 2|F_i|m_2(F_i) + 4m_1(F_i)m_2(F_i) \\
&\quad - 8|F_i|j^2 - 8|F_i|^2j - 2|F_i|k^2 + 6|F_i|^2k + 5|F_i|^2 + 4|F_i|^2j^2 + 2|F_i|^2k^2 \\
&\quad + 4k^2m_1(F_i)m_2(F_i) + 8|F_i|jk + 4|F_i|km_1(F_i) + 4|F_i|km_2(F_i) + \\
&\quad 8|F_i|m_1(F_i)m_2(F_i) - 4|F_i|^2jk + 2|F_i|k^2m_1(F_i) + 2|F_i|k^2m_2(F_i)).
\end{aligned}$$

$$\begin{aligned}
\text{Gut}(K_2, (w_v^i, s_v^i), s_e^i) &= ((2(d_i(F_i') + \frac{k}{2}|F_i|) + |F_i|)(2(b_i(F_i') + \frac{k}{2}|F_i|) + |F_i|)) \\
&= ((2((k+1)m_1(F_i) + \frac{k}{2}|F_i|) + |F_i|)(2((k+1)m_2(F_i) + \frac{k}{2}|F_i|))).
\end{aligned}$$

$$\text{Gut}(S^k(G)) = \sum_{i=1}^r \left[ \sum_{j=1}^{\lceil \frac{k}{2} \rceil} \text{Gut}(K_{2,|F_i|^j}^j, (w_v^i, s_v^i), s_e^i) + \frac{1+(-1)^k}{2} \text{Gut}(K_2, (w_v^i, s_v^i), s_e^i) \right]$$

$$\begin{aligned}
&= (k+1) \left\{ 4(k+1)^2 W_e(G) + \left( \frac{(2k+1)(2k+3)}{3} \right) |E(G)|^2 \right. \\
&\quad \left. - \frac{2k(k+2)}{3} |E(G)| + \frac{2k^2+4k+3}{3} PI(G) \right\}.
\end{aligned}$$

□

## 4 Implementation of full $k$ -subdivision on graphene

In this section, we implement Theorem 4 on full  $k$ -subdivision of graphene to obtain the indices of the variants of graphene.

### 4.1 Graphene

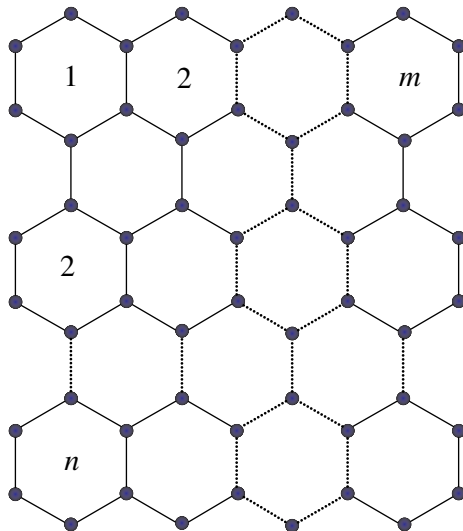


Figure 4: Structure of graphene nanoribbon  $GN(m, n)$

Carbon has various hybridized states ( $sp$ ,  $sp^2$ ,  $sp^3$ ) and can form diverse bonding, with the ability to bind to itself and to nearly all elements [9]. Since the advent of fullerenes [54], an allotrope of carbon, many carbon nanomaterials have been extracted such as carbon nanotube [4] in 1991 and graphene which was proposed in [15] and broadly studied in [7]. Graphene is arranged as a two-dimensional layer of carbon atoms with  $sp^2$  hybridization that are packed in a honeycomb lattice structure as shown in the Figure 4 of dimension  $(m, n)$ . It has attracted considerable attention with its peculiar properties in fundamental and applied research as it is the thinnest and strongest known material due to its excellent electrical, thermal, mechanical, electronic, and optical properties. It has a high specific surface area, high chemical stability, high optical transmittance, high elasticity,

high porosity, biocompatibility, tunable band gap, and ease of chemical functionalization which actually helps in tuning its properties [10, 55]. Due to its unique properties and nontoxic nature, graphene sheets are extensively studied and applied as drug carriers by chemists in the field of nanobiomedicine, and thus QSAR, QSPR and QSTR studies of such structures have become very vital to determine their structural properties and biological activities. Various degree and distance-based topological indices for graphene nanoribbon have been computed in [46]. We now state the distance-based topological indices of graphene nanoribbon which are essential for our further theorems.

**Theorem 5.** *Let  $G$  be a graphene nanoribbon  $GN(m, n)$ ,  $1 \leq n \leq m$ .*

1. [46]  $W(G) = \frac{n}{15}(-8n^4 + 40n^3m + 20n^3 + 80n^2m^2 + 80n^2m + 30n^2 + 80nm^3 + 120nm^2 + 30nm - 20n - 20m^2 - 20m - 7)$ .
2. [46]  $W_e(G) = \frac{-1}{30}(36n^5 - 180n^4m - 60n^4 - 360n^3m^2 + 20n^3 - 360n^2m^3 + 540n^2m^2 + 120n^2m + 75n^2 + 120nm^3 - 180nm^2 - 90nm - 71n - 10m^3 + 30m^2 + 10m)$ .
3. [46]  $W_{ev}(G) = \frac{-n}{30}(24n^4 - 120n^3m - 50n^3 - 240n^2m^2 - 120n^2m - 20n^2 - 240nm^3 + 120nm + 65n + 40m^3 + 30m^2 - 10m - 19)$ .
4. [46]  $Sz_v(G) = \frac{n}{15}(24n^4 - 80n^3m - 50n^3 + 240n^2m^3 + 360n^2m^2 + 200n^2m - 30n^2 + 80nm + 50n - 20m^3 + 15m + 21)$ .
5. [46]  $Sz_e(G) = \frac{1}{6}(12n^5 + 12n^4m - 44n^4 + 216n^3m^3 - 12n^3m^2 + 90n^3m - 11n^3 - 120n^2m^3 - 54n^2m^2 - 63n^2m + 41n^2 + 34nm^3 + 30nm^2 + 17nm + 2n - 6m^3)$ .
6. [46]  $Sz_{ev}(G) = \frac{n}{30}(56n^4 - 100n^3m - 100n^3 + 720n^2m^3 + 520n^2m^2 + 300n^2m - 70n^2 - 200nm^3 - 210nm^2 - 15nm + 85n + 50m^2 + 15m + 29)$ .
7. [46]  $SZ_t(G) = \frac{1}{6}(44m^5 - 60m^4n - 104m^4 + 600m^3n^3 + 340m^3n^2 + 290m^3n - 51m^3 - 200m^2n^3 - 138m^2n^2 - 37m^2n + 95m^2 + 26mn^3 + 50mn^2 + 29mn + 22m - 6n^3)$ .
8. [56]  $PI(G) = \frac{1}{3}(8n^3 + 108n^2m^2 + 12n^2m + 3n^2 - 42nm^2 - 12nm - 11n + 6m^2)$ .
9. [46]  $S(G) = 2n(2m + 1)(n - m + 6nm) + 4W_{ev}(G)$ .
10. [46]  $Gut(G) = (n - m + 6nm)^2 + 4W_e(G) + PI(G)$ .

## 4.2 $\alpha$ -graphyne

Gaphyne was first proposed in [14], is an allotrope of carbon arranged in a crystal lattice as depicted in the Figure 5. It is a variation of graphene which is built by inserting an acetylenic linkage  $-C\equiv C-$  between two bonded carbon atoms in the hexagonal lattice of graphene. In mathematical terms, graphyne nanoribbon is formed from graphene nanoribbon by full 2-subdivision on each edge. The topological indices of  $\alpha$ -graphyne are derived in the following as a consequence of Theorems 4 and 5 along with a minor computation that if  $\{F_1, F_2, \dots, F_r\}$  is the  $\Theta$ -partition [46] of graphyne, then

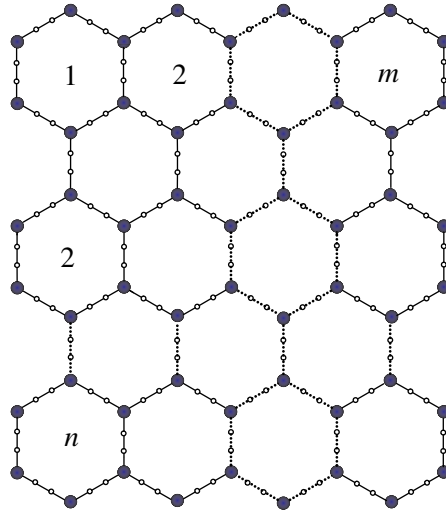
$$\sum_{i=1}^r |F_i|^3 = 2m^3n + 16mn^3 - 8n^4 - m^3 + 3m^2n + 3mn + 8n^2 + n.$$


Figure 5: Structure of  $\alpha$ -graphyne nanoribbon  $\alpha$ -GyN( $m, n$ )

**Theorem 6.** *If  $G$  is an  $\alpha$ -graphyne nanoribbon  $\alpha$ -GyN( $m, n$ ),  $1 \leq n \leq m$ , then*

1.  $W(G) = \frac{1}{15}(3840m^3n^2 - 960m^3n + 60m^3 + 3840m^2n^3 + 1440m^2n^2 - 450m^2n - 75m^2 + 1920mn^4 + 960mn^3 + 330mn^2 - 120mn - 384n^5 + 720n^4 + 130n^3 - 720n^2 + 404n),$
2.  $W_e(G) = \frac{1}{30}(9720m^3n^2 - 3240m^3n + 270m^3 + 9720m^2n^3 - 4860m^2n^2 + 1380m^2n - 420m^2 + 4860mn^4 - 960mn^2 + 930mn - 150m - 972n^5 + 1620n^4 - 220n^3 - 1755n^2 + 1357n),$
3.  $W_{ve}(G) = \frac{1}{15}(4320m^3n^2 - 1260m^3n + 90m^3 + 4320m^2n^3 - 270m^2n^2 - 30m^2n - 120m^2 + 2160mn^4 + 540mn^3 - 210mn^2 + 150mn - 30m - 432n^5 + 765n^4 + 10n^3 - 810n^2 + 527n),$
4.  $S_{z_v}(G) = \frac{1}{15}(11520m^3n^3 - 3360m^3n^2 - 90m^3n - 15m^3 + 9600m^2n^3 - 1800m^2n^2 + 855m^2n - 120m^2 - 2400mn^4 + 5580mn^3 + 2220mn^2 - 390mn + 120m + 768n^5 - 1950n^4 - 1160n^3 + 1950n^2 + 542n),$

5.  $Sz_e(G) = \frac{1}{6}(5832m^3n^3 - 2592m^3n^2 + 390m^3n - 60m^3 + 2268m^2n^3 - 1134m^2n^2 + 600m^2n - 48m^2 - 540mn^4 + 2238mn^3 - 21mn^2 - 75mn + 48m + 324n^5 - 948n^4 - 425n^3 + 921n^2 + 134n)$ ,
6.  $Sz_{ev}(G) = \frac{1}{30}(25920m^3n^3 - 9540m^3n^2 + 690m^3n - 120m^3 + 15840m^2n^3 - 4860m^2n^2 + 2280m^2n - 240m^2 - 3900mn^4 + 10800mn^3 + 2355mn^2 - 705mn + 240m + 1584n^5 - 4140n^4 - 2260n^3 + 4050n^2 + 886n)$ ,
7.  $Sz_t(G) = \frac{1}{30}(104040m^3n^3 - 38760m^3n^2 + 3150m^3n - 570m^3 + 62220m^2n^3 - 18990m^2n^2 + 9270m^2n - 960m^2 - 15300mn^4 + 43950mn^3 + 9045mn^2 - 2565mn + 960m + 6324n^5 - 16920n^4 - 8965n^3 + 16605n^2 + 3526n)$ ,
8.  $PI(G) = 324m^2n^2 - 114m^2n + 12m^2 + 84mn^2 - 24mn + 8n^3 + 9n^2 - 11n$ ,
9.  $S(G) = \frac{-2}{15}(8640m^3n^2 - 2520m^3n + 180m^3 + 8640m^2n^3 + 1620m^2n^2 - 690m^2n - 195m^2 + 4320mn^4 + 1080mn^3 + 480mn^2 + 165mn - 60m - 864n^5 + 1530n^4 + 20n^3 - 1530n^2 + 1054n)$ ,
10.  $Gut(G) = \frac{1}{15}(19440m^3n^2 - 6480m^3n + 540m^3 + 19440m^2n^3 - 570m^2n - 525m^2 + 9720mn^4 + 960mn^2 + 1230mn - 300m - 1944n^5 + 3240n^4 - 320n^3 - 3240n^2 + 2549n)$ .

### 4.3 $\alpha$ -graphdiyne

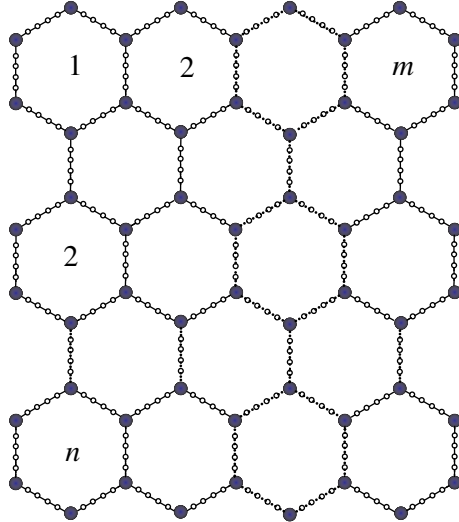


Figure 6: Structure of  $\alpha$ -graphdiyne nanoribbon  $\alpha$ -GdN( $m, n$ )

Graphdiyne initially synthesized and proposed in [3], is a variant of graphene with two acetylenic linkage rather than one as given in the Figure 6. The two acetylenic linkages double the length of the carbon chains connecting the hexagonal rings. In the following theorem, we have determined

the distance-based topological indices for  $\alpha$ -graphdiyne nanoribbon to be applied in the study of QSAR/QSPR/QSTR studies.

**Theorem 7.** *If  $G$  is an  $\alpha$ -graphdiyne nanoribbon  $\alpha$ -GdN( $m, n$ ),  $1 \leq n \leq m$ , then*

1.  $W(G) = \frac{1}{3}(3920m^3n^2 - 1120m^3n + 80m^3 + 3920m^2n^3 + 840m^2n^2 - 320m^2n - 90m^2 + 1960mn^4 + 560mn^3 + 270mn^2 + 20mn - 20m - 392n^5 + 700n^4 + 30n^3 - 700n^2 + 467n)$ ,
2.  $W_e(G) = \frac{5}{6}(1800m^3n^2 - 600m^3n + 50m^3 + 1800m^2n^3 - 540m^2n^2 + 132m^2n - 66m^2 + 900mn^4 - 72mn^2 + 138mn - 26m - 180n^5 + 300n^4 - 36n^3 - 315n^2 + 243n)$ ,
3.  $W_{ve}(G) = \frac{5}{6}(1680m^3n^2 - 520m^3n + 40m^3 + 1680m^2n^3 - 72m^2n^2 - 18m^2n - 48m^2 + 840mn^4 + 120mn^3 + 70mn - 16m - 168n^5 + 290n^4 - 12n^3 - 299n^2 + 213n)$ ,
4.  $Sz_v(G) = \frac{1}{3}(11760m^3n^3 - 3920m^3n^2 + 80m^3n - 30m^3 + 8680m^2n^3 - 1920m^2n^2 + 950m^2n - 120m^2 - 2240mn^4 + 5320mn^3 + 1900mn^2 - 435mn + 120m + 728n^5 - 1970n^4 - 1070n^3 + 1970n^2 + 447n)$ ,
5.  $Sz_e(G) = \frac{5}{6}(5400m^3n^3 - 2280m^3n^2 + 274m^3n - 42m^3 + 2580m^2n^3 - 990m^2n^2 + 522m^2n - 48m^2 - 660mn^4 + 2122mn^3 + 249mn^2 - 131mn + 48m + 300n^5 - 876n^4 - 403n^3 + 861n^2 + 130n)$ ,
6.  $Sz_{ev}(G) = \frac{5}{6}(5040m^3n^3 - 1904m^3n^2 + 140m^3n - 24m^3 + 3064m^2n^3 - 894m^2n^2 + 446m^2n - 48m^2 - 788mn^4 + 2100mn^3 + 517mn^2 - 161mn + 48m + 296n^5 - 820n^4 - 418n^3 + 811n^2 + 155n)$ ,
7.  $Sz_t(G) = \frac{1}{6}(100920m^3n^3 - 38280m^3n^2 + 2930m^3n - 510m^3 + 60900m^2n^3 - 17730m^2n^2 + 8970m^2n - 960m^2 - 15660mn^4 + 42250mn^3 + 10215mn^2 - 3135mn + 960m + 5916n^5 - 16520n^4 - 8335n^3 + 16355n^2 + 3094n)$ ,
8.  $PI(G) = \frac{5}{3}(540m^2n^2 - 186m^2n + 18m^2 + 156mn^2 - 36mn + 8n^3 + 15n^2 - 11n)$
9.  $S(G) = \frac{10}{3}(1680m^3n^2 - 520m^3n + 40m^3 + 1680m^2n^3 + 180m^2n^2 - 96m^2n - 42m^2 + 840mn^4 + 120mn^3 + 96mn^2 + 55mn - 16m - 168n^5 + 290n^4 - 12n^3 - 290n^2 + 213n)$ ,
10.  $Gut(G) = \frac{5}{3}(3600m^3n^2 - 1200m^3n + 100m^3 + 3600m^2n^3 - 102m^2n - 99m^2 + 1800mn^4 + 192mn^2 + 210mn - 52m - 360n^5 + 600n^4 - 64n^3 - 600n^2 + 475n)$ .

We conclude this section with a graphical comparative analysis of topological indices for graphene,  $\alpha$ -graphyne and  $\alpha$ -graphdiyne.

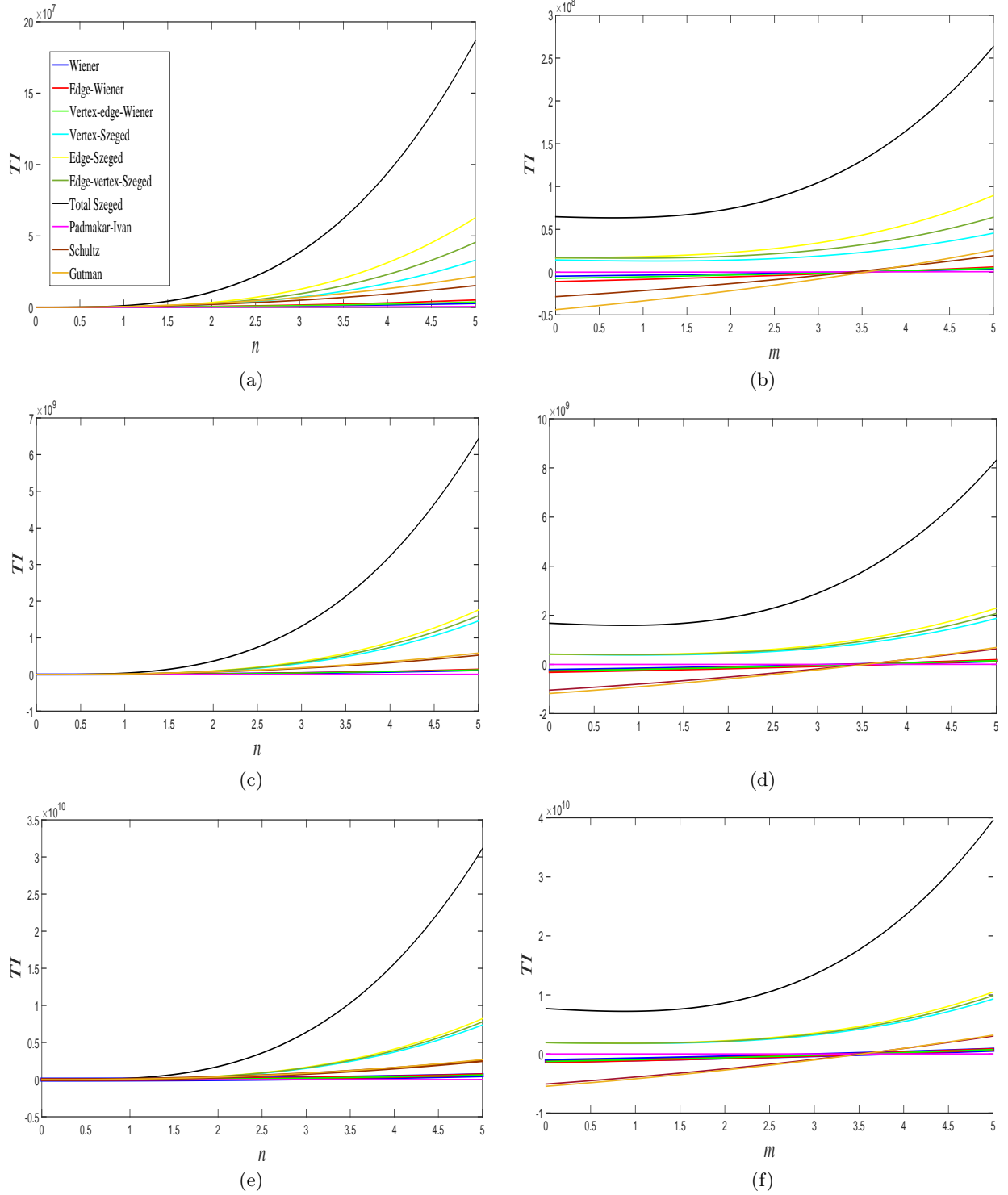


Figure 7: Comparative analysis of (a)  $GN(25, n)$  (b)  $GN(m, 25)$  (c)  $\alpha-GyN(25, n)$  (d)  $\alpha-GyN(m, 25)$  (e)  $\alpha-GdN(25, n)$  (f)  $\alpha-GdN(m, 25)$



## 5 Applications

In this section we outline several potential applications of the derived topological indices for the prediction of physicochemical properties and drug/biological activities of these novel materials. This is especially important and useful for derivative compounds of graphdiyne as these are emerging novel materials [57]. Among several observable physicochemical properties, a combination of edge-based topological indices such as the vertex-Szeged, edge-Szeged, total Szeged and edge-Wiener indices, have been quite useful in the statistical correlation of the observable properties such as proton-ligand binding affinities, vapor pressures, molar volumes, chromatographic retention indices, dermal penetration, etc. Other properties such as melting points and boiling points have been correlated quite well with both vertex or distance-degree based indices such as the Wiener Index, Schultz index, etc. Szeged indices have had reasonable success in predicting drug activities and toxicity parameters, for example, anti-inflammatory, anti-HIV, anti-tuberculosic activities, anti-malarial activities for phenyl-analogs, etc., most of which on the derivatives of polycyclic aromatic compounds [29]. Thus it is anticipated that the Szeged indices should have reasonable predictive power in correlating with various activity parameters of related graphene and graphdiyne for properties such as  $pK$ ,  $pIC_{50}$  and other toxicity parameters such as NOAEL, LOAEL, LD<sub>50</sub>, etc., of various related compounds.

In the case of graphdienes, it has been shown [14] that the fragment based approach similar to the ones generated from the cut methods have had reasonable success in predicting enthalpies of formation for a number of layered structures of varied complexities derived from the graphdiyne structures. That is, the heats of formations of large structures have been correlated with a linear combination of the heats of formations of various fragments generated from the cleavage of parent structures. This is especially important as *ab initio* based quantum chemical techniques such as the Gaussian-2 based theory for heats of formations are extremely cumbersome, for a series of layered compounds and nanoribbons such as the ones considered here containing a large number of carbon atoms. We believe that for such systems fragment based techniques such as the cut method considered here would have greater predictive power and efficacy.

Next we demonstrate the types of numerical correlations of physical properties that are feasible with our computed topological indices. Table 2 shows the numerical values of some of the indices that we have computed for the special cases of the structures considered here with appropriate substitutions. Typically, the Szeged index  $Sz$  correlates with the negative logarithms of observed equilibrium constants for first and second protonation, which we denote by  $pK_1^H$  and  $pK_2^H$ . Proto-

nation has been attributed as one of the key mechanisms for the graphdiyne containing molecules as an efficient drug delivery vehicles for Pentasa and Hyoscyamine drugs [58]. Due to the existence of  $sp^2$  and  $sp$  carbon atoms in the graphdiyne and graphene structures, we anticipate these compounds to exhibit favorable proton affinities. Consequently, using the numbers shown in Table 2 simple statistical correlations of the type shown below can be obtained:

$$pK_1^H = aSz + b$$

and

$$pK_2^H = cSz + d$$

where  $a, b, c, d$  are numerical constants obtained by fitting the results with the observed  $pK_1^H$  and  $pK_2^H$  values for known compounds.

Table 2: Indices for specific values of  $GyN(m, n)$  and  $GdN(m, n)$

<b><i>TI</i></b>	<b><i>GyN(3, 2)</i></b>	<b><i>GyN(6, 4)</i></b>	<b><i>GdN(3, 2)</i></b>	<b><i>GdN(6, 4)</i></b>
<i>W</i>	53379	1679996	259600	8361860
<i>W<sub>e</sub></i>	54668	1912664	262420	9016500
<i>W<sub>ve</sub></i>	54126	1793432	261685	8688150
<i>Sz<sub>v</sub></i>	186483	11191232	908290	55777820
<i>Sz<sub>e</sub></i>	192507	12812864	925470	60389760
<i>Sz<sub>ev</sub></i>	189597	11977040	917050	58042110
<i>Sz<sub>t</sub></i>	758184	47958176	3667860	232251800
<i>S</i>	226794	7339016	1076140	35229720

Once such an equation is obtained for QSAR, one can make predictions for the unknown structures. However at present experimental data are not yet available for the protonation equilibrium constants for the relatively newer structures that we have considered. Moreover a better correlation can also be obtained using the linear regression methods, and principal component analysis using several of the indices that have been computed and shown in Table 2. The PCA method would show which of the indices shown in Table 2 would have better correlation and predictive power.

Another important property pertinent to these species of biological relevance is the epoxidation potential and hydrolysis propensity following epoxide formation at unsaturated  $sp^2$  and  $sp$  carbons, as these properties measure the carcinogenic propensities of these species [59]. Again more sophisticated higher level *ab initio* quantum chemical studies of the energetics of various metabolic products formed and the rate constants of metabolic reactions would be quite cumbersome, especially for a series of larger compounds of the kinds studied here. Once there are experimental results available for a few of the smaller compounds studied here, one can seek statistical correlations for the larger compounds where the computed indices would have predictive powers within reasonable accuracies. Likewise hydrophobicities and lipophilicities ( $\log P$ , octanol-water partition coefficients) of these compounds can be correlated with good accuracy using Szeged indices. For example, previous studies [29] have shown that these properties can be correlated quite well with  $Sz$  with the following expressions for polyacenes which are structurally related to the structures considered here:

$$\log P(L_h) = 1.0875 \times 10^{-4} Sz + 9.210, \text{ with an } R \text{ value of } 0.9258.$$

We note that the ratios of  $Sz_v$  in Table 2 are 60 and 61 for graphene and graphdiyne respectively. Likewise for the two structures the ratios of  $Sz_e$  are 63 and 65, respectively whereas the ratios for  $Sz_{ev}$  and  $Sz_t$  are all close to 63, where we have rounded up the ratios to the nearest integers. Evidently, the nearly constant ratios suggest that any of the Szeged indices should work well with linear regression expression for  $\log P$  and other properties. Similar expressions should work reasonably well for the structure-property correlations for the various compounds derived from these structures such as oxides, fluoro-graphdienes, chloro-graphdienes and so on [57]. At the present time, available experimental data are somewhat limited, especially for the larger structures considered in the present study. Once more data is available one should be able to use the mathematical expressions obtained here to compute the numerical values for the various indices which can be effectively used to obtain QSAR correlation relations from the observed results for smaller structures. Subsequently, such QSAR relation can be used for the larger homologs in the series considered here. Hence our derived mathematical expressions can be of considerable use in future computations and experiments on obtaining physicochemical properties and biological activities of the compounds considered here.

## 6 Conclusion

The rise of graphene with unique properties has given way to other allotropes such as graphyne and graphdiyne which have been studied in recent years to determine their properties. In this paper, we have presented a technique to compute topological indices of molecular structures that have both sp and sp<sup>2</sup> hybridization, wherein one or more acetylenic linkage is added to each bond in the molecular structure. Mathematically, the technique involves the extension to full  $k$ -subdivisions of partial cube and thereby compute their distance, degree-distance and bond-additive topological indices. The results obtained can be applied to any number of subdivision of edges when the indices of their associated partial cubes with  $\Theta$ -classes are known. We have implemented the results obtained on  $\alpha$ -graphyne and  $\alpha$ -graphdiyne and presented a comparative analysis to examine the behaviors of their topological indices. The computed expressions provide a promising avenue for further exploration and correlation of structure-activity properties of these novel materials of considerable interest from the standpoint of interesting chemical, medicinal and spectroscopic applications.

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