Topological indices of the subdivision of a family of partial cubes and computation of SiO_2 related structures

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Abstract

The aim of this paper is to apply the Djoković-Winkler relation to subdivisions of partial cubes and then to derive closed formulae for computing the topological indices of the subdivision graphs, provided the indices of its associated partial cubes are known. We have applied the obtained formulae to the subdivisions of circumcoronenes to compute the exact analytical expressions of its distance and degree-distance based indices. We have also obtained distance-based and degree-distance based indices of silicate graphs such as pruned quartz. Such silicate molecular structures have potential applications in nanomedicine for drug delivery systems, as these materials could serve as molecular belts for efficient drug delivery.

Keywords: Subdivision graph; topological indices; circumcoronene; cut method; quotient graph.

1 Introduction

Graph theory has become an important and integral part in drug discovery and predictive toxicology, as it plays a key role in the analysis of structure-property and structure-activity relationships. That is, various properties of molecules depend on their structures and consequently, quantitative structure-activity-property-toxicity relationships (QSAR/QSPR/QSTR) research has emerged as a prolific area of research in in-silico characterization of physico-chemical properties, pharmocologic

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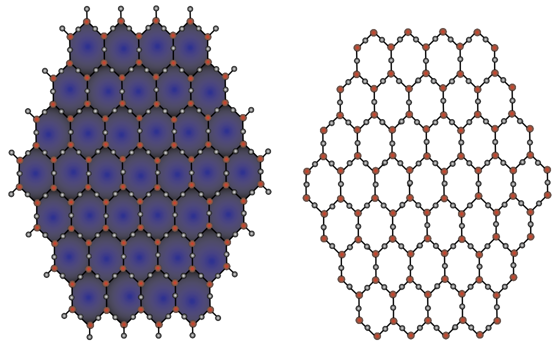
and biological activities of chemical compounds and materials. These studies have been extensively applied to chemometrics, pharmacodynamics, pharma-cokinetics, toxicology and so on [24].

Topological indices are molecular structural descriptors which theoretically and computationally characterize the underlying connectivity of chemical compounds and nanomaterials and hence facilitate faster techniques to analyze their properties and activities. The molecular graphs are to a great extent related to the topological approach of graph theory which replaces the traditional additive scheme. Such applications of combinatorics and graph theory to chemical and drug research have been the topic of several studies over the years [4, 6, 7]. Topological indices are usually based on underlying connectivity as characterized by degrees, distances or degree-distances. In our present investigation, we focus on deriving results for the distance-based and degree-distance-based descriptors using the cut method that serves as an efficient method in the computation of these indices for SiO_2 molecular belts.

Silicon dioxide, also widely known as quartz, is a naturally occurring compound of silicon and oxygen. Silica has three main crystalline varieties: tridymite, cristobalite and quartz. Quartz is the most common polymorph of crystalline silica and is the single most abundant mineral in the earth's crust, while cristobalite and tridymite are formed at a high temperature from quartz. The structure of quartz and its related structure are shown in Figures 1(a) and 1(b), respectively. Since the topological indices of tridymite and cristobalite have been studied [3, 11, 14, 16, 25], we focus on deriving exact analytical expressions of topological indices of pruned quartz and its related structure. It is noted that the pruned quartz with the removal of pendant bonds constitute an interesting bridge for studies on silicon clusters [5, 31] through laser vaporization techniques.

The hypercube structure is one of the most powerful graph-theoretical structured which is used in different fields of research. Isometric subgraphs of hypercubes are known as partial cubes. Djoković characterized these graphs in terms of the convexity of subgraphs called half spaces [8]. This characterization contains the seed of the relation Θ for bipartite graphs. It took a decade, however, before Winkler explicitly defined the relation in [29]. Moreover, his definition does apply to all graphs which turned out to be the milestone for numerous developments since then. In this paper, we have developed closed formulae for the efficient computation of the subdivision of families of partial cubes by applying the key concept of cut method [18, 20] to the edges and joining the decomposed graphs to form strength-weighted graphs [2, 3].



(a) (b)

Figure 1: SiO_2 structures (a) Quartz, (b) Quartz without pendant vertices

2 Graph theoretical terminologies

Let G be a simple, finite, connected graph with $|V(G)|$ and $|E(G)|$ to represent the number of vertices and edges, respectively. The degree of a vertex $v \in V(G)$ is the number of edges incident to v, denoted by $d_G(v)$, and the minimum number of edges in a shortest u,v-path between the vertices $u, v \in V(G)$ is denoted by $d_G(u,v)$. The distance between an edge $e = ab \in E(G)$ and a vertex v is defined as $d_G(e,v) = \min\{d_G(a,v), d_G(b,v)\}$ and for any two edges $e = ab, f = xy$, the distance between them is defined by $D_G(e,f) = \min\{d_G(e,x), d_G(e,y)\}$. This definition is from [30]. The function D_G is not a distance function in the sense of the theory of metric spaces because for adjacent edges e and f, $e \neq f$, we have $D_G(e,f) = 0$. Independently from [30], the way how a distance between two edges can be defined was carefully examined in [13]. As pointed out, if the distance between two edges of G is defined as the distance between the corresponding vertices in the line graph of G one gets a metric space. So one can define the edge-Wiener index of a graph using one of these two definitions. Luckily, this is only a technical matter because, as shown in [13, Corollary 8], the two indices differ exactly by the factor $\binom{m}{2}$, where m is the number of edges of the graph in question.

Recently, a strength-weighted graph [2] has been introduced as the generalization of weighted-graph. A strength-weighted graph is a triple $G_{sw} = (G, SW_V, SW_E)$ where G is a simple graph and SW_V, SW_E are the strength-weighted functions defined on vertices and edges of G respectively as follows:

- $SW_V = \{(w_v, s_v) : \quad w_v, s_v : V(G_{sw}) \to \mathbb{R}_0^+\}$,
- $SW_E = \{(w_e, s_e) : \; w_e, s_e : E(G_{sw}) \to \mathbb{R}_0^+\}$.

For our purpose of study, we assume that $w_e = 1$ for every edge $e \in G_{sw}$, and henceforth $G_{sw} =$

$(G, (w_v, s_v), s_e)$. A few basic terminologies related to G and G_{sw} are presented in Table 1. Collecting these terms, the definitions of the distance-based and degree-distance-based topological indices for a simple graph and strength-weighted graph are presented in Tables 2 and 3, respectively. If $w_v = s_e = 1$ and $s_v = 0$, then the topological indices of strength-weighted graphs yield $TI(G_{sw}) = TI(G)$.

Table 1: Basic terminologies of G and G_{sw}

Terms	**Simple Graph** G	**Strength-weighted graph** G_{sw}
Distance	$d_G(u,v) = d_{G_{sw}}(u,v)$	
Neighborhood	$N_G(u) = \{v \in V(G) :\ d_G(u,v) = 1\} = N_{G_{sw}}(u)$	
Degree	$d_G(u) = \|N_G(u)\|$	$d_{G_{sw}}(u) = 2s_v(u) + \sum\limits_{x \in N_{G_{sw}}(u)} s_e(ux)$
Counting sets for $e = uv$	$N_u(e\|G) = \{x \in V(G) :\ d_G(u,x) < d_G(v,x)\} = N_u(e\|G_{sw})$ $M_u(e\|G) = \{f \in E(G) :\ d_G(u,f) < d_G(v,f)\} = M_u(e\|G_{sw})$	
$n_u(e)$	$n_u(e\|G) = \|N_u(e\|G)\|$	$n_u(e\|G_{sw}) = \sum\limits_{x \in N_u(e\|G_{sw})} w_v(x)$
$m_u(e)$	$m_u(e\|G) = \|M_u(e\|G)\|$	$m_u(e\|G_{sw}) = \sum\limits_{x \in N_u(e\|G_{sw})} s_v(x) + \sum\limits_{f \in M_u(e\|G_{sw})} s_e(f)$

The n-dimensional cube or a hypercube Q_n, $n \geq 1$, is a recursive Cartesian product of n factors of K_2, in other words, $V(Q_n) = \{0,1\}^n$ and two vertices are adjacent if they differ exactly in one position. If $d_H(u,v) = d_G(u,v)$ for all $u, v \in V(H)$ where $H \subseteq G$, then the subgraph H of G is said to be isometric. A mapping $f : V(H) \to V(G)$ is an isometric embedding if $f(H)$ is an isometric subgraph of G. As already said, partial cubes are graphs that admit isometric embeddings into hypercubes. Since $V(Q_n) = \{0,1\}^n$, this can be rephrased by saying that a graph G is a partial cube if and only if its vertices u can be labeled with binary strings $\ell(u)$ of fixed length, such that $d_G(u,v) = H(\ell(u), \ell(v))$ for any vertices $u, v \in V(G)$, where H is the Hamming distance of the strings, cf. [22]. (The Hamming distance between two strings is the number of positions in which the strings differ.) Hypercubes, even cycles, trees, median graphs, benzenoid graphs, phenylenes, and Cartesian products of partial cubes are all partial cubes and partial cubes are bipartite graphs [19]. A subgraph H of a graph G is said to be convex in G if every shortest path in H is a shortest path in G.

Computing topological indices based on distance for larger families of partial cubes become a tedious process, whereas the cut method serves as one of the most useful methods for calculating the distance-based topological indices of families of partial cubes without actually calculating their

Table 2: Topological indices of a simple graph G

Topological indices	**Mathematical expressions**
Wiener	$W(G) = \sum\limits_{\{u,v\}\subseteq V(G)} d_G(u,v)$
Edge-Wiener	$W_e(G) = \sum\limits_{\{e,f\}\subseteq E(G)} D_G(e,f)$
Vertex-edge-Wiener	$W_{ve}(G) = \frac{1}{2} \sum\limits_{u\in V(G)} \sum\limits_{f\in E(G)} d_G(u,f)$
Vertex-Szeged	$Sz_v(G) = \sum\limits_{e=uv\in E(G)} n_u(e\|G)\ n_v(e\|G)$
Edge-Szeged	$Sz_e(G) = \sum\limits_{e=uv\in E(G)} m_u(e\|G)\ m_v(e\|G)$
Edge-vertex-Szeged	$Sz_{ev}(G) = \frac{1}{2} \sum\limits_{e=uv\in E(G)} \Big[n_u(e\|G)\ m_v(e\|G) + n_v(e\|G)\ m_u(e\|G)\Big]$
Total-Szeged	$Sz_t(G) = Sz_v(G) + Sz_e(G) + 2\ Sz_{ev}(G)$
Padmakar-Ivan	$PI(G) = \sum\limits_{e=uv\in E(G)} \Big[m_u(e\|G) + m_v(e\|G)\Big]$
Schultz	$S(G) = \sum\limits_{\{u,v\}\subseteq V(G)} \Big[d_G(u) + d_G(v)\Big]\ d_G(u,v)$
Gutman	$Gut(G) = \sum\limits_{\{u,v\}\subseteq V(G)} d_G(u)\ d_G(v)\ d_G(u,v)$

distance and by means of Djoković-Winkler relation. The Djoković-Winkler relation Θ [8, 29] is defined on $E(G)$ as follows: if $e = ab \in E(G)$ and $f = cd \in E(G)$, then $e\Theta f$ if $d_G(a,c) + d_G(b,d) \neq d_G(a,d) + d_G(b,c)$. The relation Θ is reflexive and symmetric, but not transitive in general. If G is bipartite, then Θ is transitive if and only if G is a partial cube. Consequently, if G is a partial cube, then Θ yields a Θ-partition $\mathcal{F}(G) = \{F_1, \ldots, F_k\}$ of $E(G)$. Moreover, for any Θ-class F_i, the graph $G - F_i$ consists of exactly two components, cf. [20]. On the other hand, the transitive closure Θ^* forms an equivalence relation on any graph G and partitions $E(G)$ into Θ^*-classes $\mathcal{F}'(G) = \{F'_1, \ldots, F'_k\}$. If $F'_i \in \mathcal{F}'(G)$, then the quotient graph G/F'_i has the components of $G - F_i$ as vertices, two components being adjacent if there exists an edge from F'_i with one end-vertex in one component and the other end-vertex in the other component.

A partition $\mathcal{E}(G) = \{E_1, \ldots, E_p\}$ of $E(G)$ is said to be coarser than the partition $\mathcal{F}(G)$, if each

Table 3: Topological indices for strength-weighted graph G_{sw}

Topological index	Mathematical expressions
Wiener	$W(G_{sw}) = \sum_{\{u,v\}\subseteq V(G_{sw})} w_v(u)\ w_v(v)\ d_{G_{sw}}(u,v)$
Vertex-Szeged	$Sz_v(G_{sw}) = \sum_{e=uv\in E(G_{sw})} s_e(e)\ n_u(e\|G_{sw})\ n_v(e\|G_{sw})$
Edge-Szeged	$Sz_e(G_{sw}) = \sum_{e=uv\in E(G_{sw})} s_e(e)\ m_u(e\|G_{sw})\ m_v(e\|G_{sw})$
Edge-vertex-Szeged	$Sz_{ev}(G_{sw}) = \frac{1}{2} \sum_{e=uv\in E(G_{sw})} s_e(e)\ \Big[n_u(e\|G_{sw})\ m_v(e\|G_{sw}) + n_v(e\|G_{sw})\ m_u(e\|G_{sw})\Big]$
Total-Szeged	$Sz_t(G_{sw}) = Sz_v(G_{sw}) + Sz_e(G_{sw}) + 2\ Sz_{ev}(G_{sw})$
Padmakar-Ivan	$PI(G_{sw}) = \sum_{e=uv\in E(G_{sw})} s_e(e)\ \Big[m_u(e\|G_{sw}) + m_v(e\|G_{sw})\Big]$
Schultz	$S(G_{sw}) = \sum_{\{u,v\}\subseteq V(G_{sw})} \Big[w_v(v)d_{G_{sw}}(u) + w_v(u)d_{G_{sw}}(v)\Big]\ d_{G_{sw}}(u,v)$
Gutman	$Gut(G_{sw}) = \sum_{\{u,v\}\subseteq V(G_{sw})} d_{G_{sw}}(u)\ d_{G_{sw}}(v)\ d_{G_{sw}}(u,v)$

set E_i is the union of one or more Θ^*-classes of G. We now conclude this section by stating two key-theorems on the cut method for our further study.

Theorem 1. *Let $\mathcal{F}(G) = \{F_1, \ldots, F_k\}$ be the Θ-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) [20] $W(G) = \sum_{i=1}^{k} n_1(F_i)\ n_2(F_i)$,

(ii) [30] $W_e(G) = \sum_{i=1}^{k} m_1(F_i)\ m_2(F_i)$,

(iii) [1] $W_{ve}(G) = \frac{1}{2} \sum_{i=1}^{k} [n_1(F_i)\ m_2(F_i) + n_2(F_i)\ m_1(F_i)]$,

(iv) [10] $Sz_v(G) = \sum_{i=1}^{k} |F_i|\ n_1(F_i)\ n_2(F_i)$,

(v) [30] $Sz_e(G) = \sum_{i=1}^{k} |F_i|\ m_1(F_i)\ m_2(F_i)$,

(vi) *[26]* $Sz_{ev}(G) = \frac{1}{2}\sum_{i=1}^{k} |F_i| \{n_1(F_i)\ m_2(F_i) + n_2(F_i)\ m_1(F_i)\}$,

(vii) *[15]* $PI(G) = |E(G)|^2 - \sum_{i=1}^{k} |F_i|^2$,

$(viii)$ *[17]* $S(G) = |E(G)||V(G)| + 2\sum_{i=1}^{k}[n_1(F_i)\ m_2(F_i) + n_2(F_i)\ m_1(F_i)]$,

(ix) *[17]* $Gut(G) = 2|E(G)|^2 + \sum_{i=1}^{k}[4m_1(F_i)\ m_2(F_i) - |F_i|^2]$.

It is interesting to observe from the above theorem that if G is a partial cube, then

- $S(G) = |E(G)||V(G)| + W_{ve}(G)$, and
- $Gut(G) = |E(G)|^2 + PI(G) + 4W_e(G)$.

Theorem 2. *[2] Let $G_{sw} = \big(G, (w_v, s_v), s_e\big)$ be a strength-weighted graph, let $\mathcal{E}(G) = \{E_1, \ldots, E_p\}$ be a partition of $E(G)$ coarser than $\mathcal{F}(G)$, and let $TI \in \{W, Sz_v, Sz_e, Sz_{ev}, PI, S, Gut\}$. Then,*

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

where

- $w_v^i : V(G/E_i) \to \mathbb{R}^+$ *is defined by* $w_v^i(C) = \sum_{x\in C} w_v(x)$, $\forall\ C \in G/E_i$,
- $s_v^i : V(G/E_i) \to \mathbb{R}^+$ *is defined by* $s_v^i(C) = \sum_{xy\in C} s_e(xy) + \sum_{x\in C} s_v(x)$, $\forall\ C \in G/E_i$,
- $s_e^i : E(G/E_i) \to \mathbb{R}^+$ *is defined by* $s_e^i(CD) = \sum_{\substack{xy\in E_i\\ x\in C, y\in D}} s_e(xy)$, *for any two connected components C and D of G/E_i.*

3 Subdivisions of partial cubes

If G is a graph, then the subdivision graph $Sub(G)$ of G is the graph obtained from G by replacing every edge uv of G with a new vertex x_{uv} and connecting x_{uv} with u and v. The cardinalities of the vertices and the edges of $Sub(G)$ become $|V(G)| + |E(G)|$ and $2|E(G)|$, respectively. As we have already mentioned that every Θ-class of a partial cube G decomposes the graph into exactly two components resulting in quotient graph K_2 with edge-strength value $|F_i|$ and vertex-strength-weighted values $(n_1(F_i), m_1(F_i))$ and $(n_2(F_i), m_2(F_i))$ as shown in Figure 2. It has been proved in [3] that any Θ-class $F_i = \{u_jv_j : 1 \leq j \leq s\}$ of a partial cube G with $|F_i| \geq 3$ yields a Θ^*-class $F_i' = \{u_jx_j, x_jv_j : 1 \leq j \leq s\}$ in $Sub(G)$. Clearly, F_i' decomposes $Sub(G)$ into $|F_i| + 2$ components resulting in the quotient graph $K_{2,|F_i|}$ with the edge-strength 1 for all the edges and the vertex-strength-weighted values for one partite vertices as $(a_i(F_i'), b_i(F_i'))$ and $(c_i(F_i'), d_i(F_i'))$ and the other partite vertices $(1, 0)$, see Figure 2. In the case of $|F_i| \leq 2$, i.e. $s = 1$ or 2, we assume that $F_i' = \{u_jx_j, x_jv_j : 1 \leq j \leq s\}$ which is a union of two Θ^*-classes in $Sub(G)$ [3] and the above arguments hold.

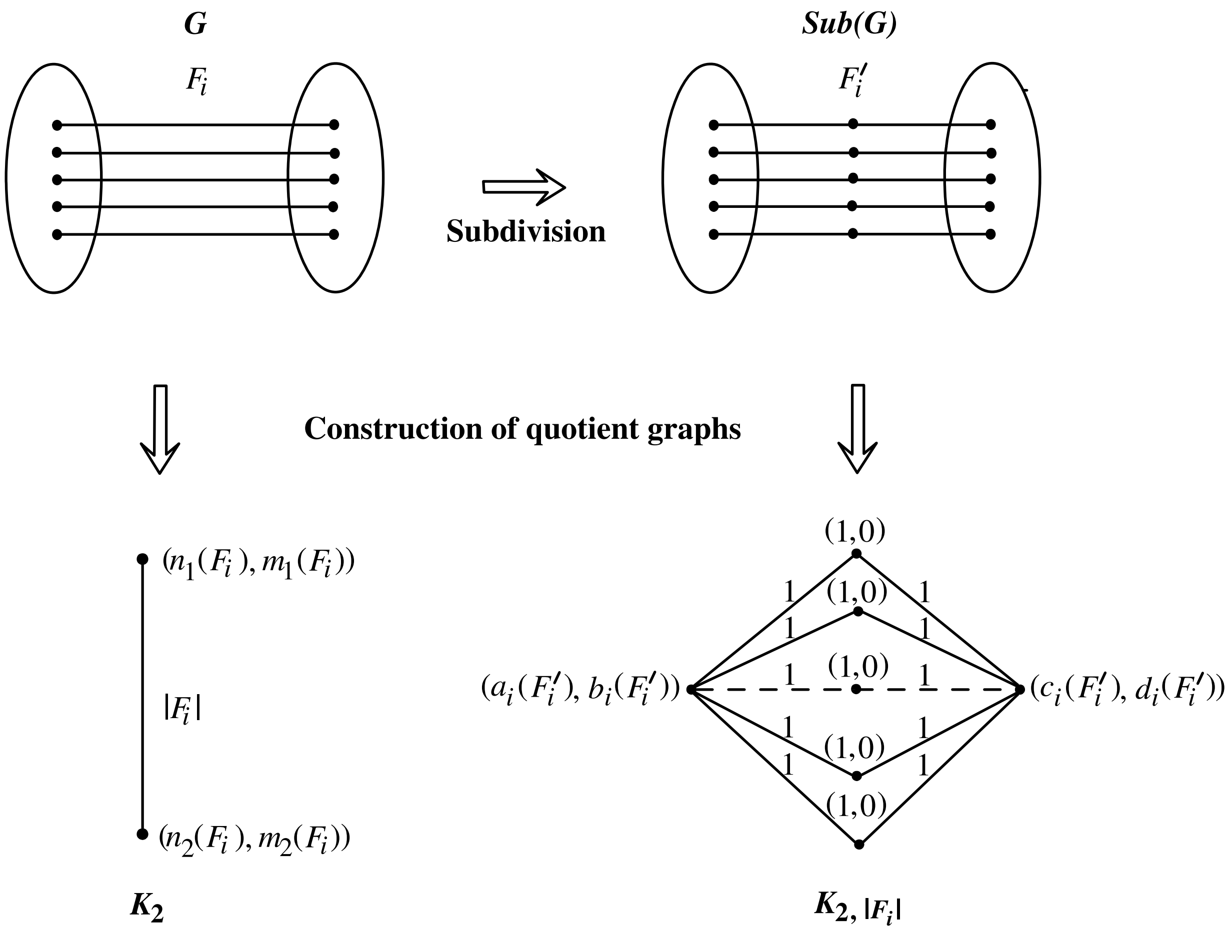


Figure 2: Construction of quotient graphs G/F_i and $Sub(G)/F_i'$

Theorem 3. *Let* $\mathcal{F}(G) = \{F_1, \ldots, F_k\}$ *be the* Θ*-partition of a partial cube* G *and* $\mathcal{F}'\big(Sub(G)\big) = \{F_1', \ldots, F_k'\}$ *the* Θ^**-partition of* $Sub(G)$*. If* $TI \in \{W, Sz_v, Sz_e, Sz_{ev}, PI, S, Gut\}$*, then*

$$TI\big(Sub(G)\big) = \sum_{i=1}^{k} TI\big(K_{2,|F_i|}, (w_v^i, s_v^i), s_e^i\big) .$$

Furthermore,

(i) $W\big(Sub(G)\big) = 2W(G) + 4W_{ve}(G) + 2W_e(G) + |E(G)|(|V(G)| + |E(G)| - 1)$,

(ii) $Sz_v\big(Sub(G)\big) = 2Sz_v(G) + 4Sz_{ev}(G) + 2Sz_e(G) + (|E(G)|^2 - PI(G))(|V(G)| + |E(G)| + 2) - 2|E(G)| - \sum_{i=1}^{k} |F_i|^3$,

(iii) $Sz_e\big(Sub(G)\big) = 8Sz_e(G) - 2|E(G)| + 2(|E(G)|^2 - PI(G))(|E(G)| + 1) - 2\sum_{i=1}^{k} |F_i|^3$,

(iv) $Sz_{ev}\big(Sub(G)\big) = \frac{1}{2}\big[8Sz_{ev}(G) + 8Sz_e(G) + (|V(G)| + 3|E(G)| + 4)(|E(G)|^2 - PI(G)) - 4|E(G)| - 3\sum_{i=1}^{k} |F_i|^3\big]$,

(v) $Sz_t\big(Sub(G)\big) = 2\big[9Sz_e(G) + 6Sz_{ev}(G) + Sz_v(G) + (|V(G)| + 3|E(G)| + 4)(|E(G)|^2 - PI(G)) - 4|E(G)| - 3\sum_{i=1}^{k} |F_i|^3\big]$,

(vi) $PI\big(Sub(G)\big) = 2\big(|E(G)|^2 + PI(G)\big)$,

(vii) $S\big(Sub(G)\big) = 16W_{ve}(G) + 16W_e(G) + 4|E(G)|(|V(G)| - 1) + 6|E(G)|^2 + 2PI(G)$,

(viii) $G\big(Sub(G)\big) = 32W_e(G) + 10|E(G)|^2 - 4|E(G)| + 6PI(G)$.

Proof. As noted above, the Θ^*-classes of $Sub(G)$ yield the quotient graphs $K_{2,|F_i|}$ with strengths and weights as given in Figure 2. Hence the first formula of the theorem follows from Theorem 2. Applying the same theorem, we can compute as follows.

$$
\begin{aligned}
(i)\ W(Sub(G)) &= \sum_{i=1}^{k} W\big(K_{2,|F_i|}, (w_v^i, s_v^i), s_e^i\big) \\
&= \sum_{i=1}^{k} \Big[2a_i(F_i')c_i(F_i') + |F_i|\big[a_i(F_i') + c_i(F_i')\big] + |F_i|(|F_i| - 1)\Big] \\
&= \sum_{i=1}^{k} \Big[2n_1(F_i)n_2(F_i) + 2\big[n_1(F_i)m_2(F_i) + m_1(F_i)n_2(F_i)\big] + \\
&\quad 2m_1(F_i)m_2(F_i) + |F_i|\big[n_1(F_i) + n_2(F_i) + m_1(F_i) + m_2(F_i) + |F_i| - 1\big]\Big] \\
&= 2W(G) + 4W_{ve}(G) + 2W_e(G) + |E(G)|(|V(G)| + |E(G)| - 1).
\end{aligned}
$$

$$(ii)\ Sz_v(Sub(G)) = \sum_{i=1}^{k} Sz_v\big(K_{2,|F_i|}, (w_v^i, s_v^i), s_e^i\big)$$

$$= \sum_{i=1}^{k} |F_i| \Big[(a_i(F_i') + |F_i| - 1)(c_i(F_i') + 1) + (c_i(F_i') + |F_i| - 1)$$

$$(a_i(F_i') + 1) \Big]$$

$$= \sum_{i=1}^{k} |F_i| \Big[2a_i(F_i')c_i(F_i') + |F_i| \big[c_i(F_i') + a_i(F_i') + 2 \big] - 2 \Big]$$

$$= \sum_{i=1}^{k} |F_i| \Big[2n_1(F_i)n_2(F_i) + 2\big[n_1(F_i)m_2(F_i) + m_1(F_i)n_2(F_i) \big] +$$

$$2m_1(F_i)m_2(F_i) + |F_i| \big[n_1(F_i) + n_2(F_i) + m_1(F_i) + m_2(F_i) + |F_i| + 2 \big] -$$

$$|F_i|^2 - 2 \Big]$$

$$= 2Sz_v(G) + 4Sz_{ev}(G) + 2Sz_e(G) + (|E(G)|^2 - PI(G))(|V(G)| +$$

$$|E(G)| + 2) - 2|E(G)| - \sum_{i=1}^{k} |F_i|^3.$$

$$(iii)\ Sz_e(Sub(G)) = \sum_{i=1}^{k} Sz_e\big(K_{2,|F_i|}, (w_v^i, s_v^i), s_e^i\big)$$

$$= \sum_{i=1}^{k} |F_i| \Big[(b_i(F_i') + |F_i| - 1)(d_i(F_i') + 1) + (d_i(F_i') + |F_i| - 1)$$

$$(b_i(F_i') + 1) \Big]$$

$$= \sum_{i=1}^{k} |F_i| \Big[2b_i(F_i')d_i(F_i') + |F_i| \big[b_i(F_i') + d_i(F_i') + 2 \big] - 2 \Big]$$

$$= \sum_{i=1}^{k} |F_i| \Big[8m_1(F_i)m_2(F_i) + 2|F_i| \big[m_1(F_i) + m_2(F_i) + |F_i| + 1 \big] -$$

$$2|F_i|^2 - 2 \Big]$$

$$= 8Sz_e(G) - 2|E(G)| + 2(|E(G)|^2 - PI(G))(|E(G)| + 1) - 2\sum_{i=1}^{k} |F_i|^3.$$

$$
\begin{aligned}
(iv)\ Sz_{ev}(Sub(G)) &= \sum_{i=1}^{k} Sz_{ev}\big(K_{2,|F_i|},(w_v^i,s_v^i),s_e^i\big)\\
&= \frac{1}{2}\sum_{i=1}^{k}|F_i|\Big[(a_i(F_i')+|F_i|-1)(d_i(F_i')+1)+(d_i(F_i')+|F_i|-1)\\
&\quad (a_i(F_i')+1)+(b_i(F_i')+|F_i|-1)(c_i(F_i')+1)+(c_i(F_i')+|F_i|-1)\\
&\quad (b_i(F_i')+1)\Big]\\
&= \frac{1}{2}\sum_{i=1}^{k}|F_i|\Big[2\big[a_i(F_i')d_i(F_i')+b_i(F_i')c_i(F_i')\big]+|F_i|\big[a_i(F_i')+d_i(F_i')\\
&\quad +b_i(F_i')+d_i(F_i')+4\big]-4\Big]\\
&= \frac{1}{2}\sum_{i=1}^{k}|F_i|\Big[4[n_1(F_i)m_2(F_i)+m_1(F_i)n_2(F_i)]+8m_1(F_i)m_2(F_i)+\\
&\quad |F_i|[n_1(F_i)+n_2(F_i)+3m_1(F_i)+3m_2(F_i)+3|F_i|+4]-3|F_i|^2-4\Big]\\
&= \frac{1}{2}\Big[8Sz_{ev}(G)+8Sz_e(G)+(|V(G)|+3|E(G)|+4)(|E(G)|^2-PI(G))-\\
&\quad 4|E(G)|-3\sum_{i=1}^{k}|F_i|^3\Big].
\end{aligned}
$$

$$
\begin{aligned}
(v)\ Sz_t(Sub(G)) &= \sum_{i=1}^{k} Sz_t\big(K_{2,|F_i|},(w_v^i,s_v^i),s_e^i\big)\\
&= Sz_v(Sub(G))+Sz_e(Sub(G))+2Sz_{ev}(Sub(G)).
\end{aligned}
$$

$$
\begin{aligned}
(vi)\ PI(Sub(G)) &= \sum_{i=1}^{k} PI\big(K_{2,|F_i|},(w_v^i,s_v^i),s_e^i\big)\\
&= \sum_{i=1}^{k}|F_i|\Big[b_i(F_i')+|F_i|-1+d_i(F_i')+1+d_i(F_i')+|F_i|-1\\
&\quad +b_i(F_i')+1\Big]\\
&= 2\sum_{i=1}^{k}|F_i|\Big[b_i(F_i')+d_i(F_i')+|F_i|\Big]\\
&= 2\sum_{i=1}^{k}|F_i|\Big[2m_1(F_i)+2m_2(F_i)+2|F_i|-|F_i|\Big]\\
&= 2\big(|E(G)|^2+PI(G)\big).
\end{aligned}
$$

$$
\begin{aligned}
(vii)\ S(Sub(G)) &= \sum_{i=1}^{k} S\big(K_{2,|F_i|}, (w_v^i, s_v^i), s_e^i\big) \\
&= \sum_{i=1}^{k} \Big[2\big[a_i(F_i')(2d_i(F_i') + |F_i|) + c_i(F_i')(2b_i(F_i') + |F_i|)\big] + |F_i|\big[2b_i(F_i') + \\
&\quad 2d_i(F_i') + 2a_i(F_i') + 2c_i(F_i') + 2|F_i|\big] + 4|F_i|(|F_i| - 1)\Big] \\
&= \sum_{i=1}^{k} \Big[4\big[a_i(F_i')d_i(F_i') + c_i(F_i')b_i(F_i')\big] + 2|F_i|\big[2a_i(F_i') + 2c_i(F_i') + \\
&\quad b_i(F_i') + d_i(F_i') + 3|F_i| - 2\big]\Big] \\
&= \sum_{i=1}^{k} \Big[8\big[n_1(F_i)m_2(F_i) + n_2(F_i)m_1(F_i)\big] + 16m_1(F_i)m_2(F_i) + \\
&\quad 2|F_i|\big[2n_1(F_i) + 2n_2(F_i) + 4m_1(F_i) + 4m_2(F_i) + 3|F_i| - 2\big]\Big] \\
&= 16W_{ve}(G) + 16W_e(G) + 4|E(G)|(|V(G)| - 1) + 6|E(G)|^2 + 2PI(G).
\end{aligned}
$$

$$
\begin{aligned}
(viii)\ G(Sub(G)) &= \sum_{i=1}^{k} G\big(K_{2,|F_i|}, (w_v^i, s_v^i), s_e^i\big) \\
&= \sum_{i=1}^{k} \Big[2\big[(2b_i(F_i') + |F_i|)(2d_i(F_i') + |F_i|)\big] + |F_i|\big[2(2b_i(F_i') + |F_i|) + \\
&\quad 2(2d_i(F_i') + |F_i|)\big] + 4|F_i|^2 - 4|F_i|\Big] \\
&= \sum_{i=1}^{k} \Big[8b_i(F_i')d_i(F_i') + |F_i|\big[8b_i(F_i') + 8d_i(F_i') + 10|F_i| - 4\big]\Big] \\
&= \sum_{i=1}^{k} \Big[32m_1(F_i)m_2(F_i) + 16|F_i|\big[m_1(F_i) + m_2(F_i)\big] + 10|F_i|^2 - 4|F_i|\Big] \\
&= 32W_e(G) + 10|E(G)|^2 - 4|E(G)| + 6PI(G).
\end{aligned}
$$

□

We now show an application of Theorem 3 to the subdivisions of circumcoronenes. For the circumcoronene series depicted in Figure 3, the cuts are shown in Table 4. Due to the symmetry of the circumcoronene H_n, the cuts are symmetric to each other and clearly $|H_{\pm i}| = |A_{\pm i}| = |O_{\pm i}|$.

The cardinality of $|H_i|$ has been computed in [10]:

$$|H_i| = \begin{cases} n+i & : 1 \leq i \leq n-1 \\ 2n & : i = n \end{cases}$$

Table 4: Elementary cuts of the circumcoronene H_n

Elementary cuts	**Notation**	**Direction towards centre**
Horizontal	$\{H_i : \ 1 \leq i \leq n\}$	North
	$\{H_{-i} : \ 1 \leq i \leq n-1\}$	South
Acute	$\{A_i : \ 1 \leq i \leq n\}$	North-West
	$\{A_{-i} : \ 1 \leq i \leq n-1\}$	South-East
Obtuse	$\{O_i : \ 1 \leq i \leq n\}$	North-East
	$\{O_{-i} : \ 1 \leq i \leq n-1\}$	South-West

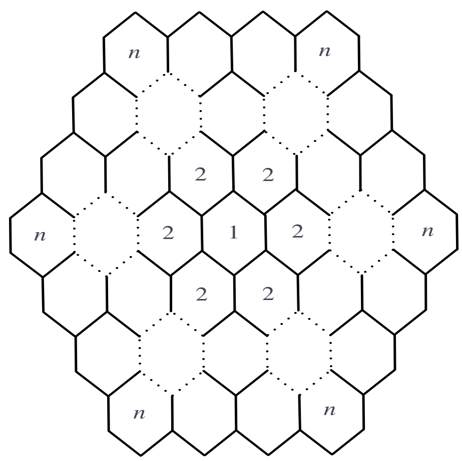


Figure 3: The structure of circumcoronene H_n

Let $\mathcal{F}$ be the set of cuts of H_n. Then $\sum\limits_{F \in \mathcal{F}} |F|^3 = 6 \sum\limits_{i=1}^{n-1} (n+i)^3 + 3(2n)^3 = \frac{3n^2(15n^2-2n+3)}{2}$. In addition to this computation, we now recall the results related to H_n in order to compute the topological indices of the subdivision of H_n.

Theorem 4. *If $n \geq 1$, then the following hold.*

1. *[21]* $W(H_n) = \frac{1}{5}(164n^5 - 30n^3 + n)$,

2. *[30]* $W_e(H_n) = \frac{3}{10}(246n^5 - 340n^4 + 140n^3 - 5n^2 - n)$,

3. *[1]* $W_{ve}(H_n) = \frac{1}{10}(492n^5 - 340n^4 + 25n^2 + 3n)$,

4. *[10]* $Sz_v(H_n) = \frac{3}{2}(36n^6 - n^4 + n^2)$,

5. *[9]* $Sz_e(H_n) = \frac{1}{10}(1215n^6 - 1599n^5 + 680n^4 - 105n^3 + 55n^2 - 6n)$,

6. *[1]* $Sz_{ev}(H_n) = \frac{1}{20}(1620n^6 - 1066n^5 + 135n^4 - 10n^3 + 45n^2 - 4n)$,

7. *[1]* $Sz_t(H_n) = \frac{1}{2}(675n^6 - 533n^5 + 160n^4 - 23n^3 + 23n^2 - 2n)$,

8. *[1]* $PI(H_n) = 81n^4 - 68n^3 + 12n^2 - n$,

9. *[12]* $S(H_n) = \frac{2}{5}(492n^5 - 205n^4 - 45n^3 + 25n^2 + 3n)$,

10. *[1]* $Gut(H_n) = \frac{1}{5}(1476n^5 - 1230n^4 + 230n^3 + 75n^2 - 11n)$.

Table 5: Asymptotic behaviors of H_n and $Sub(H_n)$

Topological index	N	Asymptotic Behavior	
		H_n	$Sub(H_n)$
Wiener	$\frac{164}{5}n^5$	N	$12.5N$
Vertex-Szeged	$54n^6$	N	$12.5N$
Edge-Szeged	$\frac{243}{2}n^6$	N	$8N$
Edge-vertex-Szeged	$81n^6$	N	$10N$
Total-Szeged	$\frac{675}{2}n^6$	N	$9.68N$
Padmakar-Ivan	$81n^4$	N	$4N$
Schultz	$\frac{984}{5}n^5$	N	$10N$
Gutman	$\frac{1476}{5}n^5$	N	$8N$

Theorem 5. *If $n \geq 1$, then the following hold.*

1. $W(Sub(H_n)) = 410n^5 - 205n^4 + 7n^2 + 4n$,

2. $SZ_v(Sub(H_n)) = \frac{1}{2}(1350n^6 - 646n^5 + 101n^4 + 64n^3 - 17n^2 + 12n)$,

3. $SZ_e(Sub(H_n)) = \frac{1}{5}(4860n^6 - 5136n^5 + 1805n^4 - 70n^3 + 25n^2 + 16n)$,

4. $SZ_{ev}(Sub(H_n)) = \frac{1}{20}(16200n^6 - 12436n^5 + 3055n^4 + 370n^3 - 85n^2 + 96n)$,

5. $SZ_t(Sub(H_n)) = \frac{1}{5}(16335n^6 - 12969n^5 + 3585n^4 + 275n^3 - 60n^2 + 94n)$,

6. $PI(Sub(H_n)) = 324n^4 - 244n^3 + 42n^2 - 2n$,

7. $S(Sub(H_n)) = 1968n^5 - 1312n^4 + 140n^3 + 58n^2 + 10n$,

8. $Gut(Sub(H_n)) = \frac{6}{5}(1968n^5 - 1640n^4 + 330n^3 + 65n^2 - 3n)$.

The exact analytical expressions of the indices presented in Theorems 4 and 5 are univariate polynomials with degree 6 for the four variants of the Szeged indices, degree 4 for the PI index and degree 5 for the Wiener, Schultz and Gutman indices. As n increases indefinitely, the asymptotic behaviors of the Szeged indices being the highest degree polynomial dominates the other indices in H_n and $Sub(H_n)$.

4 Topological indices of SiO_2 quartz

The structure of SiO_2 quartz of dimension n is shown in Figure 4. The only difference between the subdivision of circumcoronene and SiO_2 quartz is that the additional $6n$ pendant vertices. In this section, we compute various distance and degree-distance based topological indices of SiO_2 quartz.

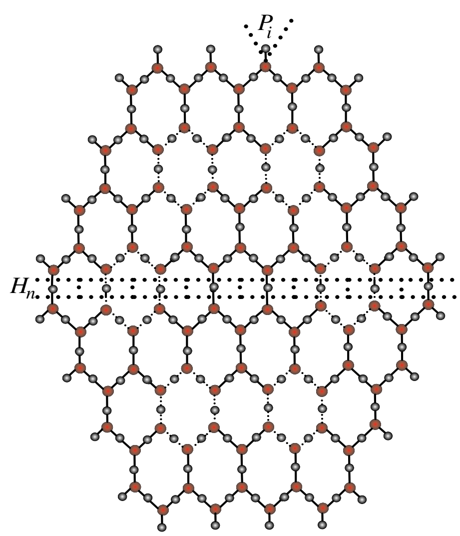


Figure 4: Elementary cuts on the structure of SiO_2 quartz

Theorem 6. *If G is the n-dimensional ($n \geq 2$) SiO_2 quartz structure, then the following holds.*

1. $W(G) = \frac{1}{6}(4460n^5 + 4745n^4 + 2748n^3 - 677n^2 + 64n)$,

2. $Sz_v(G) = \frac{1}{2}(2170n^6 + 1306n^5 - 773n^4 + 808n^3 + 7n^2 + 22n)$,

3. $Sz_e(G) = \frac{1}{5}(6910n^6 + 181n^5 - 1100n^4 + 2515n^3 - 230n^2 + 64n)$,

4. $Sz_{ev}(G) = \frac{1}{10}(13020n^6 + 3398n^5 - 3925n^4 + 4760n^3 - 305n^2 + 122n)$,

5. $Sz_t(G) = \frac{1}{10}(50710n^6 + 13688n^5 - 13915n^4 + 18590n^3 - 1035n^2 + 482n)$,

6. $PI(G) = 540n^4 - 172n^3 + 18n^2 + 4n$,

7. $S(G) = \frac{1}{3}(5352n^5 + 11057n^4 + 166n^3 + 265n^2 + 80n)$,

8. $Gut(G) = \frac{2}{5}(2676n^4 + 6455n^3 + 5875n^2 - 680n + 29)$.

Proof. We have $|V(G)| = |V(Sub(H_n))| + 6n$ and $|E(G)| = |E(Sub(H_n))| + 6n$. To proceed the computation of indices, we first identify the Θ^*-classes on the edges of G. The horizontal, acute and obtuse cuts are similar to that of the subdivision of circumcoronene, along with $6n$ pendant cuts P_i on the boundary of SiO_2 quartz structure as shown in Figure 4.

Case 1: $\{H_i : \ 1 \leq i \leq n\}$

On applying the cut H_i, the quotient graph obtained is $K_{2,|F_i|}$ which is similar to that of the quotient graph of the subdivision of a partial cube shown in the Figure 2. The edge-strength value is 1 each and the vertex-strength-weighted values $(a_i(F_i'), b_i(F_i'))$ and $(c_i(F_i'), d_i(F_i'))$ are as follows: For $1 \leq i \leq n-1$,

$$a_i(F_i') = \frac{1}{2}\{5i^2 + 10in + i\}, \qquad b_i(F_i') = 3i^2 + 6in - i - n,$$
$$c_i(F_i') = \frac{1}{2}\{30n^2 - 10in - 5i^2 + 4n - 3i\}, \quad d_i(F_i') = 18n^2 - 3i^2 - 6in - n - i.$$

We denote,

$$TI(G_1) = TI(G/H_i, (w_v^i, s_v^i), s_e^i)\,. \tag{1}$$

For $i = n$,

$$a_i(F_i') = c_i(F_i') = \frac{1}{2}\{15n^2 + n\}, \quad b_i(F_i') = d_i(F_i') = 9n^2 - 2n.$$

$$TI(G_2) = TI(G/H_i, (w_v^i, s_v^i), s_e^i)\,. \tag{2}$$

Case 2: $\{P_i : \ 1 \leq i \leq 6n\}$

Since there are $6n$ pendant vertices along the boundary of SiO_2 quartz, we observe that each pendant edge-cut forms its own Θ^*-class. The quotient graph obtained is a K_2 graph with edge-strength 1 and vertex-strength-weighted values as follows:

$$a(F_i') = 1, \qquad b(F_i') = 0,$$
$$c(F_i') = |V(G)| - 1, \quad d(F_i') = |E(G)| - 1.$$

Set

$$TI(G_3) = TI(G/P_i, (w_v^i, s_v^i), s_e^i)\,. \tag{3}$$

From Eqs. (1)-(3), we obtain

$$TI(G) = 6\sum_{i=1}^{n-1} TI(G_1) + 3TI(G_2) + 6nTI(G_3)\,.$$

Using a straightforward computation by a MATLAB interface, we get the required expressions. □

5 Conclusion

In this paper, we have shown the connection between partial cubes and its subdivision graph with respect to distance and degree-distance based topological indices. The results obtained in this paper can be used in the efficient computation of the subdivision of any member of the family of partial cubes. We have applied these formulae to compute the indices of the subdivision of a circumcoronene. The analysis of asymptotic behaviors indicated that the variants of the Szeged indices of the circumcoronene and its subdivision dominates the other indices.

In Theorems 3, 5, and 6 the edge-Wiener index and the vertex-edge-Wiener index are not included because they lead to certain technical problems. The method of computing these indices for a strength-weighted graph and application of it to the subdivision graphs of partial cubes are under investigation though. In addition, it is interesting to note that the results in Theorem 3 can be extended to more than one subdivision of an edge and applied on variants of graphyne and graphydyine such as α-, β-, and γ-graphyne, and α-, β-, and γ-graphdyine that are respectively obtained [23,27,28] by inserting one acetylenic linkage -C $\equiv$ C- and two acetylenic linkage between two bonded carbon atoms in graphene.

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