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Research Article

Szeged-like topological indices and the efficacy of the cut method: The case of melem structures*

Micheal Arockiaraj[1], Shagufa Mushtaq[1], Sandi Klavžar[2,3,4], J. Celin Fiona[1], Krishnan Balasubramanian[5,†]

[1]*Department of Mathematics, Loyola College, Chennai, India*
[2]*Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia*
[3]*Faculty of Natural Sciences and Mathematics, University of Maribor, Maribor, Slovenia*
[4]*Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia*
[5]*School of Molecular Sciences, Arizona State University, Tempe, USA*

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Abstract

The Szeged index is a bond-additive topological descriptor that quantifies each bond's terminal atoms based on their closeness sets which is measured by multiplying the number of atoms in the closeness sets. Based on the high correlation between the Szeged index and physico-chemical properties of chemical compounds, Szeged-like indices have been proposed by considering closeness sets with bond counts and other mathematical operations like addition and subtraction. As there are many ways to compute the Szeged-like indices, the cut method is predominantly used due to its complexity compared to other approaches based on algorithms and interpolations. Yet, we here analyze the usefulness of the cut method in the case of melem structures and find that it is less effective when the size and shape of the cavities change in the structures.

Keywords: distance; Szeged index; cut-method; melem.

2020 Mathematics Subject Classification: 05C09, 05C12, 05C90, 05C92.

1. Introduction

Chemical graph theory is applied extensively in the field of quantitative structural activity and property relationships (QSAR/QSPR), which has great importance in modern chemistry, pharmacology, chemometrics, toxicology, and so on [4, 6, 19]. This has led to the emergence of various molecular descriptors, predominantly the topological indices, for the prediction of physicochemical properties of compounds, as research shows that the properties of compounds are intimately related to their underlying topological nature. The need to represent a molecular structure by a single number arises from the fact that most molecular properties are recorded as single numbers. Therefore, QSPR modelling reduces to a correlation between the two sets of numbers via an algebraic expression [14]. During the past decades, various topological indices have been defined and studied for their development in the study of quantitative structure-property relations [1, 4, 6, 7, 10, 11, 15, 21].

Wiener's pioneering work in predicting the boiling point of parrafin using the path number broadened the scope of QSAR/QSPR studies by predicting various correlations between the physicochemical properties of chemical compounds. Since then, many indices were introduced based on the distance, degree, and bond additive invariants of a graph. Gutman introduced the vertex variant of the Szeged index based on the bond-additive structural invariant that was used to ease the computation of the Wiener indices for trees, and since its existence, a lot of research has been devoted towards its study as a useful molecular topological descriptor. Various physicochemical properties of organic compounds such as molecular volume, boiling point, vapour pressure, molar volume, van der Waals volume, proton-ligand formation constants and so on were modelled using Szeged index (see [11]). Consequently, several variations of the Szeged index were introduced for possible applications in QSAR/QSPR studies [7, 16]. In particular, the PI index has fairly good structural selectivity and correlation ability [10], while the Mostar index provides a quantitative measure of distance nonbalancedness as well as a measure of the global peripherality of molecular structures [1, 3, 5].

To formally define the Szeged-like indices, we need to recall a few graph theoretical notions. The open neighborhood $N_G(v)$ of a simple connected graph G, consisting of a vertex set $V(G)$ and an edge set $E(G)$, is the set of vertices adjacent to v. Its cardinality is the degree of v and denoted by $d_G(v)$. For an edge $e = xy$ in $E(G)$, the weighted sum/product is based on the degree of the end-vertices and is given by $w^{\circledast}(e|G) = d_G(x) \circledast d_G(y)$ where $\circledast \in \{+, *\}$. For any two vertices $x, y \in V(G)$,

*In memory of Prof. Nenad Trinajstić, a pioneer in chemical graph theory.
†Corresponding author (baluk@asu.edu).

the distance $d_G(x,y)$ between them is the number of edges in a shortest path from the vertex x to y. The shortest distance between the vertex x and the edge $f=uv \in E(G)$ is defined as $d_G(x,f)=\min\{d_G(x,u),d_G(x,v)\}$. The cardinalities of the closeness sets of an edge $f=uv$ are defined in the following.

(i) $n_u(f|G)=|N_u(f|G)|=|\{z\in V(G):\ d_G(u,z)<d_G(v,z)\}|$.

(ii) $m_u(f|G)=|M_u(f|G)|=|\{h\in E(G):\ d_G(u,h)<d_G(v,h)\}|$.

(iii) $n_v(f|G)$ and $m_v(f|G)$ are analogous to (i)-(ii).

Based on the above notations, we now define the Szeged-like topological indices in the following form [3, 18],

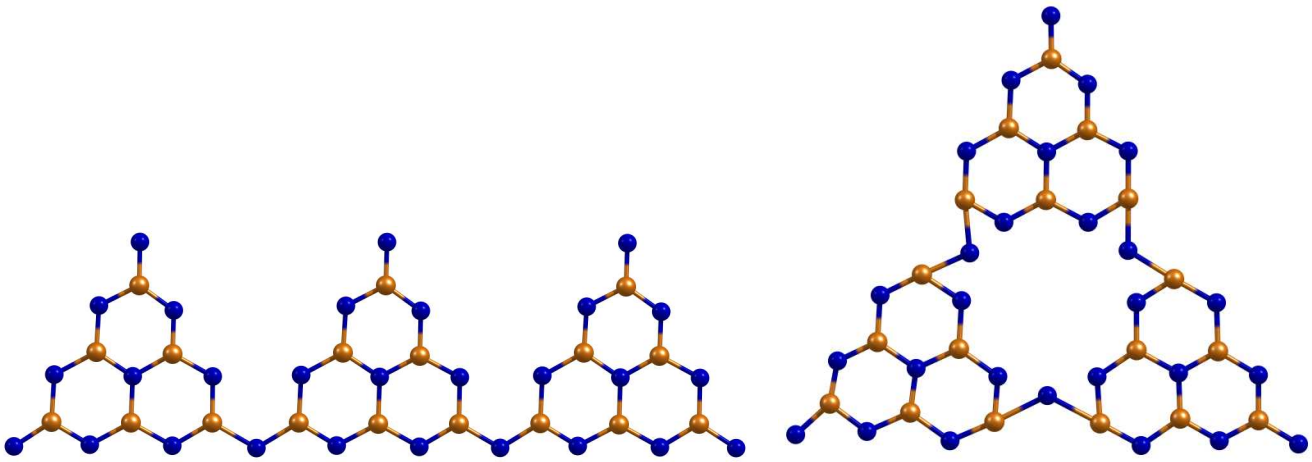
$$wSz_k^{\circ}(G) \ = \sum_{f=uv\in E(G)} w(f|G)\ |p_u(f|G)\circ p_v(f|G)|$$

whereas the reductions can be accomplished by assigning appropriate values to k, w, p and employing mathematical operations at $\circ$.

1. vertex Szeged $Sz_v(G)$: $k=v, w=1, p=n, \circ=*$
2. edge Szeged $Sz_e(G)$: $k=e, w=1, p=m, \circ=*$
3. vertex PI $PI_v(G)$: $k=v, w=1, p=n, \circ=+$
4. edge PI $PI_e(G)$: $k=e, w=1, p=m, \circ=+$
5. vertex Mostar $Mo_v(G)$: $k=v, w=1, p=n, \circ=-$
6. edge Mostar $Mo_e(G)$: $k=e, w=1, p=m, \circ=-$
7. weighted-plus vertex Szeged $w^+Sz_v(G)$: $k=v, w=w^+, p=n, \circ=*$
8. weighted-plus edge Szeged $w^+Sz_e(G)$: $k=e, w=w^+, p=m, \circ=*$
9. weighted-plus vertex PI $w^+PI_v(G)$: $k=v, w=w^+, p=n, \circ=+$
10. weighted-plus edge PI $w^+PI_e(G)$: $k=e, w=w^+, p=m, \circ=+$
11. weighted-plus vertex Mostar $w^+Mo_v(G)$: $k=v, w=w^+, p=n, \circ=-$
12. weighted-plus edge Mostar $w^+Mo_e(G)$: $k=e, w=w^+, p=m, \circ=-$
13. weighted-product vertex Szeged $w^*Sz_v(G)$: $k=v, w=w^*, p=n, \circ=*$
14. weighted-product edge Szeged $w^*Sz_e(G)$: $k=e, w=w^*, p=m, \circ=*$
15. weighted-product vertex PI $w^*PI_v(G)$: $k=v, w=w^*, p=n, \circ=+$
16. weighted-product edge PI $w^*PI_e(G)$: $k=e, w=w^*, p=m, \circ=+$
17. weighted-product vertex Mostar $w^*Mo_v(G)$: $k=v, w=w^*, p=n, \circ=-$
18. weighted-product edge Mostar $w^*Mo_e(G)$: $k=e, w=w^*, p=m, \circ=-$

Melem is a trimer of melamine with excellent photocatalytic and photoresponsive properties that have great potential for several applications as they posses high stability, low cell toxicity and high efficiency. It is a new, efficient and metal-free ecofriendly blue emitting material composed of carbon, nitrogen, and hydrogen with the molecular formula $C_6N_7(NH_2)_3$ [8, 17, 20]. Each melem unit cell consists of three hexagons arranged in a triangular manner which is called a heptazine. The melem chain and ring structures are displayed in Figures 1a and 1b, which are obtained by assembling melem unit cells in linear and circular forms. The melem chain with s units is denoted by MC[s] while the melem ring is denoted by MR[s].

In this paper, we discuss the cut method based on the Djoković-Winkler relation and analyze its efficacy in the computation of the Szeged-like topological indices in melem chain and ring structures.



(a) (b)

Figure 1: Melem structure with three units (a) Chain form (b) Ring form.

2. The cut method

The cut method was introduced in order to simplify the computation of topological indices and to derive closed formulas for chemically important families of graphs. The method is based on the Djoković-Winkler relation Θ which is defined as follows. Two bonds $b_1 = c_1d_1$ and $b_2 = c_2d_2$ are in relation Θ if $d_G(c_1, c_2) + d_G(d_1, d_2) \neq d_G(c_1, d_2) + d_G(c_2, d_1)$. The relation Θ is reflexive and symmetric, but not transitive in general whereas the transitive closure Θ^* forms an equivalence relation thereby enabling the Θ^*-partition of the edge set $E(G)$ as $E_1, \ldots, E_p$. These classes split each of the graphs $G - E_i$ into two or more smaller components. The quotient graph G/E_i is defined as a graph in which the vertices are the connected components of $G - E_i$, and two components A_1 and A_2 are linked by an edge if there exists an edge $xy \in E_i$ such that $x \in A_1$ and $y \in A_2$. To ease the computational process we make use of the recently developed concept where these quotient graphs are reduced to a strenght-weighted graph with vertex and edge sets consisting of their corresponding strenght-weighted parameters.

A graph G with strength-weighted functions (SW_V, SW_E) assigned to the vertex set $V(G)$ and edge set $E(G)$ is a strength-weighted graph [2] $G_{sw} = (G, SW_V, SW_E)$, where SW_V is the pair (w_v, s_v) of a vertex weight function $w_v : V(G) \to \mathbb{R}_0^+$ and a strength function $s_v : V(G) \to \mathbb{R}_0^+$, while SW_E is the pair (w_e, s_e) of an edge weight function $w_e : E(G) \to \mathbb{R}_0^+$ and a strength function $s_e : E(G) \to \mathbb{R}_0^+$. The distance function of the strength-weighted graph G_{sw} remains the same as in the graph G, while the degree and the bond closeness set parameters of a vertex u and an edge $f = uv$ are defined as follows.

(i) $d_{G_{sw}}(u) = \sum_{x \in N_{G_{sw}}(u)} s_e(ux)$.

(ii) $n_u(f|G_{sw}) = \sum_{x \in N_u(f|G_{sw})} w_v(x)$.

(iii) $m_u(f|G_{sw}) = \sum_{x \in N_u(f|G_{sw})} s_v(x) + \sum_{h \in M_u(f|G_{sw})} s_e(h)$.

Hence, the Szeged-like indices of G_{sw} can be in the form

$$wSz_k^\circ(G_{sw}) = \sum_{f=uv \in E(G_{sw})} w(f|G_{sw})\, |p_u(f|G_{sw}) \circ p_v(f|G_{sw})|$$

such that simple Szeged, PI and Mostar will take weighted measure as the edge strength value s_e and $wSz_k^\circ(G) = wSz_k^\circ(G_{sw})$ whenever $w_v = 1, s_v = 0, s_e = 1$.

The seminal paper [12] developed the cut method for the Wiener index and for the case when Θ is transitive. In [13], the method was extened to general graphs, that is, to compute the Wiener index of an arbitrary graph no matter whether Θ is transitive or not. Here we consider the currently most general set-up of the cut method in terms of strength weighted graphs as recently proposed in [2] as follows. Let G be a molecular graph with the Θ^*-partition $\mathcal{E}(G) = \{E_1, \ldots, E_p\}$. Then

$$wSz_k^\circ(G) = \sum_{i=1}^{p} wSz_k^\circ(G/E_i, (w_v^i, s_v^i), (w_e^i, s_e^i)),$$

where

(*i*) $w_v^i : V(G/E_i) \to \mathbb{R}_0^+$, $w_v^i(X) = \sum_{x \in V(X)} w_v(x), \forall\, X \in V(G/E_i)$,

(*ii*) $s_v^i : V(G/E_i) \to \mathbb{R}_0^+$, $s_v^i(X) = \sum_{xy \in E(X)} s_e(xy) + \sum_{x \in V(X)} s_v(x), \forall\, X \in V(G/E_i)$,

(*iii*) $w_e^i : E(G/E_i) \to \mathbb{R}_0^+$, $w_e^i(XY) = \sum_{\substack{xy \in E_i \\ x \in V(X),\, y \in V(Y)}} w_e(xy), \forall\, XY \in E(G/E_i)$,

and in particular,

- for weighted-plus, $w_e^i(XY) = w_e^{+i}(XY) = \sum_{\substack{xy \in E_i \\ x \in V(X), y \in V(Y)}} (d_G(x) + d_G(y)), \forall\, XY \in E(G/E_i)$,
- for weighted-product, $w_e^i(XY) = w_e^{*i}(XY) = \sum_{\substack{xy \in E_i \\ x \in V(X),\, y \in V(Y)}} d_G(x) * d_G(y), \forall\, XY \in E(G/E_i)$.

(*iv*) $s_e^i : E(G/E_i) \to \mathbb{R}_0^+$, $s_e^i(XY) = \sum_{\substack{xy \in E_i \\ x \in V(X),\, y \in V(Y)}} s_e(xy), \forall\, XY \in E(G/E_i)$.

3. Szeged-like indices of melem structures

Theorem 3.1. *Let* MC[s] *be a melem chain of dimension* s *where* $s \geq 2$.

1. $Sz_v(\text{MC}[s]) = 90s(5s^2 + 7s - 2)$.
2. $Sz_e(\text{MC}[s]) = 18s(36s^2 + 19s - 15)$.
3. $PI_v(\text{MC}[s]) = 18s(15s + 1)$.
4. $PI_e(\text{MC}[s]) = 6s(54s - 7)$.
5. $Mo_v(\text{MC}[s]) = 3(60s^2 - 22s - 3 + 3(-1)^s)$.
6. $Mo_e(\text{MC}[s]) = 8(27s^2 - 10s - 1 + (-1)^s)$.
7. $w^+Sz_v(\text{MC}[s]) = 3s(775s^2 + 1095s - 322)$.
8. $w^+Sz_e(\text{MC}[s]) = 18s(186s^2 + 101s - 78)$.
9. $w^+PI_v(\text{MC}[s]) = 2(46s - 1)(15s + 1)$.
10. $w^+PI_e(\text{MC}[s]) = 2(828s^2 - 127s + 1)$.
11. $w^+Mo_v(\text{MC}[s]) = \frac{1}{2}(1830s^2 - 752s - 97 + 101(-1)^s)$.
12. $w^+Mo_e(\text{MC}[s]) = 2(549s^2 - 228s - 22 + 23(-1)^s)$.
13. $w^*Sz_v(\text{MC}[s]) = 9s(325s^2 + 465s - 142)$.
14. $w^*Sz_e(\text{MC}[s]) = 54s(78s^2 + 44s - 33)$.
15. $w^*PI_v(\text{MC}[s]) = 6(19s - 1)(15s + 1)$.
16. $w^*PI_e(\text{MC}[s]) = 6(342s^2 - 64s + 1)$.
17. $w^*Mo_v(\text{MC}[s]) = \frac{3}{2}(750s^2 - 356s - 43 + 47(-1)^s)$.
18. $w^*Mo_e(\text{MC}[s]) = 6(225s^2 - 108s - 10 + 11(-1)^s)$.

Proof. There are $s + 2$ pendant bonds in MC[s], each of them forming a separate Θ-class P_i, $1 \leq i \leq s + 2$. The quotient graph MC[s]$/P_i$ is the complete bipartite graph $K_{1,1}$ with partite sets $\{A_i^p\}$ and $\{B_i^p\}$ with vertex weights $w_v^i(A_i^p) = 1$, $w_v^i(B_i^p) = 15s$, vertex strengths $s_v^i(A_i^p) = 0$, $s_v^i(B_i^p) = 18s - 1$, edge weights $w_e^{+i}(A_i^pB_i^p) = 4$, $w_e^{*i}(A_i^pB_i^p) = 3$, and edge strength $s_e^i(A_i^pB_i^p) = 1$. There are two bridging bonds between two consecutive heptazines, we shall denote them FB_i and SB_i, $1 \leq i \leq s - 1$. Due to chain arrangement, the graph theoretical measures of FB_i are equivalent to those of SB_{s-i} and hence, we restrict our computation to only FB_i. As before, the quotient graph MC[s]$/FB_i$ has partite set $\{A_i^b\}$ and

$\{B_i^b\}$ with weighted graph theoretical measures $w_v^i(A_i^b) = 15i$, $w_v^i(B_i^b) = 15(s-i)+1$, $s_v^i(A_i^d) = 18i-1$, $s_v^i(B_i^b) = 18(s-i)$, $w_e^{+i}(A_i^bB_i^b) = 5$, $w_e^{*i}(A_i^bB_i^b) = 6$, and $s_e^i(A_i^bB_i^b) = 1$.

We now reckon the bonds of heptazines based on the horizontal and slanting types. For $1 \leq i \leq s$, let FH_i and SH_i be the Θ-classes constructed from the first and second layers horizontal bonds of i^{th} heptazine. The quotient graphs produced by FH_i and SH_i are also $K_{1,1}$, but the vertex weights, vertex strengths, edge weights, edge strength for FH_i and SH_i are $4, 15s-3, 3, 18s-5, 10, 12, 2$ and $9, 15s-8, 9, 18s-12, 16, 21, 3$ respectively. As we did for horizontal bonds, let FO_i and SO_i ($1 \leq i \leq s$) be the Θ-classes constructed from the first and second layers' obtuse bonds of i^{th} heptazine. Then the weighted measures for the quotient graphs $K_{1,1}$ produced by FO_i and SO_i are respectively $15i-11, 15(s-i)+12, 18i-15, 18(s-i)+13, 10, 12, 2$ and $15i-6, 15(s-i)+7, 18i-9, 18(s-i)+6, 16, 21, 3$. Finally, let FA_i and SA_i ($1 \leq i \leq s$) be the Θ-classes constructed from the acute bonds and the graph theoretical quantities of the i^{th} obtuse Θ-class are equivalent to $(s-i+1)^{th}$ acute Θ-class due to their symmetrical nature. Therefore, the computation of all forms of Szeged-like indices can be done from the following equation.

$$\begin{aligned}
wSz_k^\circ(\mathbf{MC}[s]) &= \sum_{i=1}^{s+2} wSz_k^\circ(\mathbf{MC}[s]/P_i) + \sum_{i=1}^{s-1}\{wSz_k^\circ(\mathbf{MC}[s]/FB_i) + wSz_k^\circ(\mathbf{MC}[s]/SB_i)\} \\
&\quad + \sum_{i=1}^{s}\{wSz_k^\circ(\mathbf{MC}[s]/FH_i) + wSz_k^\circ(\mathbf{MC}[s]/SH_i)\} + \sum_{i=1}^{s}\{wSz_k^\circ(\mathbf{MC}[s]/FO_i) + wSz_k^\circ(\mathbf{MC}[s]/SO_i)\} \\
&\quad + \sum_{i=1}^{s}\{wSz_k^\circ(\mathbf{MC}[s]/FA_i) + wSz_k^\circ(\mathbf{MC}[s]/SA_i)\} \\
&= (s+2)Mo(\mathbf{MC}[s]/P_i) + 2\sum_{i=1}^{s-1} wSz_k^\circ(\mathbf{MC}[s]/FB_i) + \sum_{i=1}^{s}\{wSz_k^\circ(\mathbf{MC}[s]/FH_i) + wSz_k^\circ(\mathbf{MC}[s]/SH_i)\} \\
&\quad + 2\sum_{i=1}^{s}\{wSz_k^\circ(\mathbf{MC}[s]/FO_i) + wSz_k^\circ(\mathbf{MC}[s]/SO_i)\}.
\end{aligned}$$

□

Theorem 3.2. *Let* $\mathrm{MR}[s]$ *be a melem chain of dimension* $s \geq 2$.

1. $Sz_v(\mathbf{MR}[s]) = \frac{1}{2}s(9(150s^2+120s-73) - (-1)^s 19)$.
2. $Sz_e(\mathbf{MR}[s]) = 2s(486s^2+63s-187-(-1)^s(18s-1))$.
3. $PI_v(\mathbf{MR}[s]) = 270s^2$.
4. $PI_e(\mathbf{MR}[s]) = 2s(3(54s-11) - 2(-1)^s)$.
5. $Mo_v(\mathbf{MR}[s]) = 2s(15(3s-1) + (-1)^s)$.
6. $Mo_e(\mathbf{MR}[s]) = 4s(27s-7)$.
7. $w^+Sz_v(\mathbf{MR}[s]) = \frac{s}{4}(5(2790s^2+2256s-1379) - 193(-1)^s)$.
8. $w^+Sz_e(\mathbf{MR}[s]) = s(5022s^2+702s-1967-(-1)^s(198s-15))$.
9. $w^+PI_v(\mathbf{MR}[s]) = 1380s^2$.
10. $w^+PI_e(\mathbf{MR}[s]) = 2s(9(92s-19) - 11(-1)^s)$.
11. $w^+Mo_v(\mathbf{MR}[s]) = s(450s-163+11(-1)^s)$.
12. $w^+Mo_e(\mathbf{MR}[s]) = 12s(45s-13)$.
13. $w^*Sz_v(\mathbf{MR}[s]) = \frac{3s}{4}(5850s^2+4800s-2953-79(-1)^s)$.
14. $w^*Sz_e(\mathbf{MR}[s]) = 3s(2106s^2+324s-845-(-1)^s(90s-9))$.
15. $w^*PI_v(\mathbf{MR}[s]) = 1710s^2$.
16. $w^*PI_e(\mathbf{MR}[s]) = 6s(18(19s-4) - 5(-1)^s)$.
17. $w^*Mo_v(\mathbf{MR}[s]) = s(540s-219+15(-1)^s)$
18. $w^*Mo_e(\mathbf{MR}[s]) = 216s(3s-1)$.

Proof. We use two different cases to compute the Szeged-like indices of melem rings based on the odd and even number of melem units. In the case of even s, we identify the appropriate Θ^*-classes and then use a strength-weighted quotient graph to obtain the necessary results. But if s is odd, the strength-weighted quotient graph is more complex, and hence we partition the bonds of corresponding quotient graph based on the cardinalities of the closeness sets of terminal vertices.

Case 1 (s even): For $1 \leq i \leq s$, let PP_i be a Θ-class that contains the peripheral pendant bond of MR[s]. The quotient graph MR[s]/PP_i is the complete bipartite graph $K_{1,1}$ with partite sets $\{A_i^p\}$ and $\{B_i^p\}$ with strength and weighted quantities $w_v^i(A_i^p) = 1$, $w_v^i(B_i^p) = 15s - 1$, $s_v^i(A_i^p) = 0$, $s_v^i(B_i^p) = 18s - 1$, $w_e^{+i}(A_i^p B_i^p) = 4$, $w_e^{*i}(A_i^p B_i^p) = 3$, and $s_e^i(A_i^p B_i^p) = 1$. Two diametrically-opposite bridging bonds exist between two melem units of interval $s/2$, denoted as FD_i and SD_i, respectively where $1 \leq i \leq s$. The graph theoretical measures of FD_i are equivalent to SD_i due to ring arrangement, and in addition the vertex strength-weighted values are equal for the quotient graph $K_{1,1}$ arising from MR[s]/FD_i. The vertex strength and vertex weight of MR[s]/FD_i are $15s/2$ and $9s-1$ respectively, while edge weight and edge strength are $\{10, 12\}$ and 2.

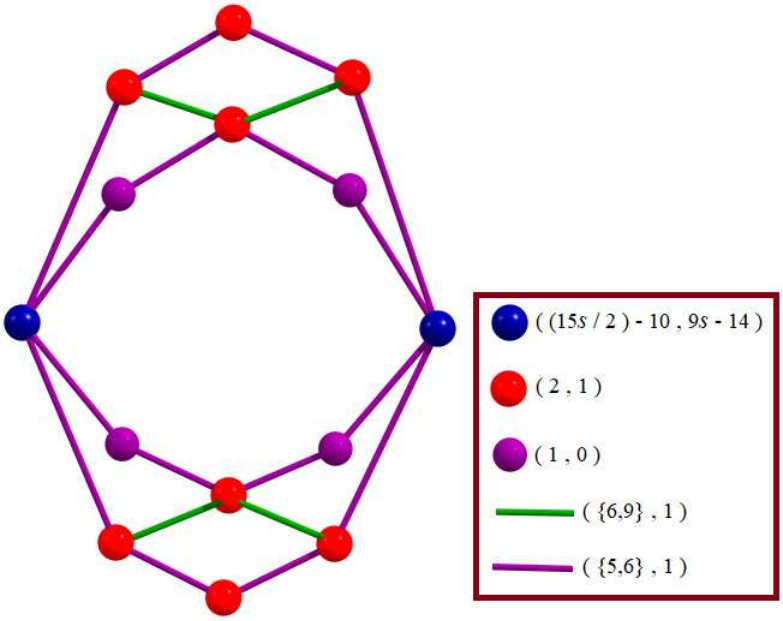


Figure 2: Quotient graph corresponds to the slanting bonds of two diametrically-opposite melem units.

For $1 \leq i \leq s/2$, let DS_i be a Θ^*-class encompassing the slanting bonds of two diametrically-opposite melem units of MR[s]. The vertex and edge strength-weighted quotient graph MR[s]/DS_i is shown in Figure 2. As we constructed for MC[s], let FH_i and SH_i be the Θ-classes for horizontal bonds for MR[s]. Here FH_i and SH_i generate an identical quotient graph $K_{1,1}$, but the vertex weights, vertex strengths, edge weights, edge strength for FH_i and SH_i are $4, 15s-4, 3, 18s-5, 10, 12, 2$ and $9, 15s-9, 9, 18s-12, 16, 21, 3$ respectively. We compute the required indices by simplifying the following equation.

$$wSz_k^\circ(\text{MR}[s]) = \sum_{i=1}^{s} wSz_k^\circ(\text{MR}[s]/PP_i) + \sum_{i=1}^{s}\{wSz_k^\circ(\text{MR}[s]/FD_i) + wSz_k^\circ(\text{MR}[s]/SD_i)\} + \sum_{i=1}^{s/2} wSz_k^\circ(\text{MR}[s]/DS_i)$$
$$+ \sum_{i=1}^{s}\{wSz_k^\circ(\text{MR}[s]/FH_i) + wSz_k^\circ(\text{MR}[s]/SH_i)\}.$$

Case 2 (s odd): In this case, we use the Θ-classes PP_i, FH_i and SH_i, where $1 \leq i \leq s$ as in Case 1. It is important to note that all the slanting and bridging bonds belong to the single Θ^*-class SB and the corresponding quotient graph is displayed in Figure 3. We now classify the bonds of the quotient graph by considering the cardinalities of closeness sets in which the graph theoretical quantities are given in Table 1. Hence, the Szeged-like indices are derived from the following equation.

$$wSz_k^\circ(\text{MR}[s]) = \sum_{i=1}^{s} wSz_k^\circ(\text{MR}[s]/PP_i) + wSz_k^\circ(\text{MR}[s]/SB) + \sum_{i=1}^{s}\{wSz_k^\circ(\text{MR}[s]/FH_i) + wSz_k^\circ(\text{MR}[s]/SH_i)\}.$$

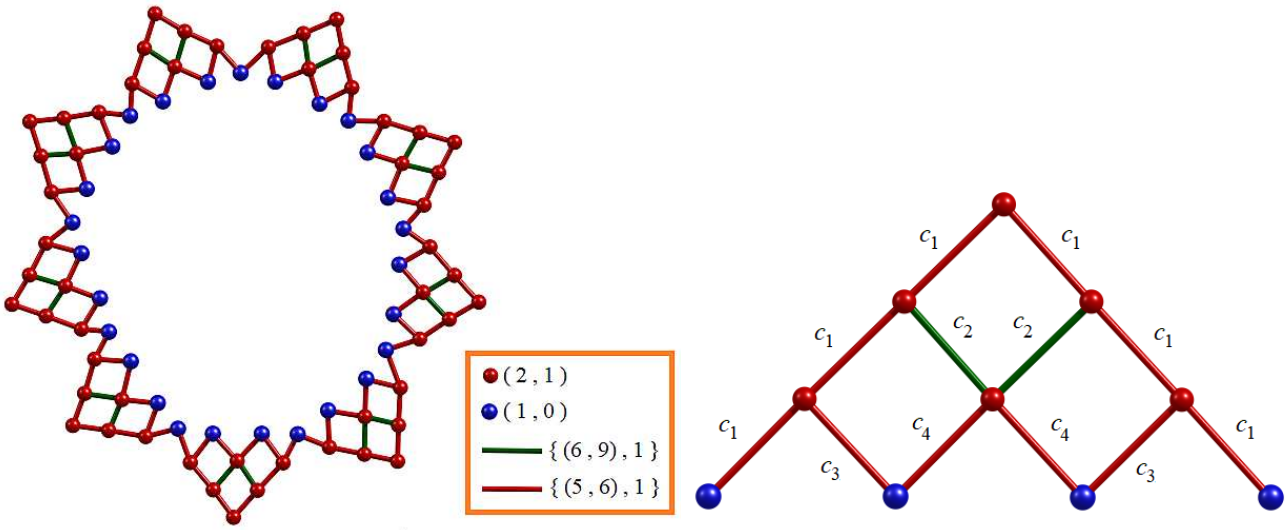


Figure 3: (a) Quotient graph corresponds to all slanting and bridging bonds of MR[9] (b) A fragment of the figure based on the closeness sets classification.

Table 1: Graph theoretical quantities of MR[s]/SB based on the cardinality of the closeness sets of end-vertices.

Class	$\lvert c_i\rvert$	$e_{ij} = u_{ij}v_{ij} \in c_i$					
		$n_{u_{ij}}$	$n_{v_{ij}}$	$m_{u_{ij}}$	$m_{v_{ij}}$	$w^+(e_{ij})$	$w^*(e_{ij})$
c_1	$6s$	s_1+9	s_1+6	s_2+9	s_2+5	5	6
c_2	$2s$	s_1+8	s_1+7	s_2+8	s_2+6	6	9
c_3	$2s$	s_1+9	s_1+6	s_2+8	s_2+5	5	6
c_4	$2s$	s_1+11	s_1+4	s_2+12	s_2+3	5	6
$s_1 = 15(s-1)/2, s_2 = 18(s-1)/2$							

□

4. Concluding remarks

It is evident that the cut method is effective in the case of melem chain, but when applied to melem ring, it is weak and requires some other methods to compute the Szeged-like indices successfully. Topological indices developed here are expected to find applications in the characterization of melems and melem chains which act as a bridge between molecular states and graphitic carbon nitrides of importance in low dimensional materials [8]. Furthermore, as demonstrated in the previous work [9], the edge equivalence classes obtained through the cut method can also be useful in the efficient computation of enthalpies of formations of large periodic networks containing melem chains in terms of the bond enthalpies of each representative in the edge equivalance classes.

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