Iranian J. Math. Chem. 12 (1) March (2021) 1 – 18

IRANIAN JOURNAL OF
Mathematical Chemistry
Journal homepage: ijmc.kashanu.ac.ir

Original Scientific Paper

Computing the Mostar Index in Networks with Applications to Molecular Graphs

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ARTICLE INFO

Article History:

Received: 9 October 2020
Accepted: 19 October 2020
Published online: 30 March 2021
Academic Editor: Tomislav Došlić

Keywords:
Mostar index
Cut method
Weighted graph
Tree-like polyphenyl system
Benzenoid system

ABSTRACT

Recently, a bond-additive topological descriptor, named as the Mostar index, has been introduced as a measure of peripherality in networks. For a connected graph G, the Mostar index is defined as $\mathrm{Mo}(G) = \sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|$, where for an edge $e = uv$ we denote by $n_u(e)$ the number of vertices of G that are closer to u than to v and by $n_v(e)$ the number of vertices of G that are closer to v than to u. In the present paper, we prove that the Mostar index of a weighted graph can be computed in terms of Mostar indices of weighted quotient graphs. Inspired by this result, several generalizations to other versions of the Mostar index already appeared in the literature. Furthermore, we apply the obtained method to benzenoid systems, tree-like polyphenyl systems, and to a fullerene patch. Closed-form formulas for two families of these molecular graphs are also deduced.

1. INTRODUCTION

Szeged and PI indices are some of the well known distance-based molecular descriptors defined as the sum of edge contributions. Very recently, another bond-additive topological index, named as the Mostar index, has been introduced [16]. For any connected graph G, the *Mostar index* of G, denoted as $Mo(G)$, is defined as

$$Mo(G) = \sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|,$$

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DOI: 10.22052/ijmc.2020.240316.1526

where for an edge $e = uv$ we denote by $n_u(e)$ the number of vertices of G that are closer to u than to v and by $n_v(e)$ the number of vertices of G that are closer to v than to u. This index measures peripherality of individual edges and then sums the contributions of all edges into a global measure of peripherality for a given graph. Some chemical applications of the Mostar index were reported in [3, 13], while some other results can be found in [14, 21, 25]. In [16], a simple cut method for computing the Mostar index of benzenoid systems was also presented. Note that the cut method is a very useful tool for the computation of such topological descriptors [22].

In the present paper, we first define the Mostar index for weighted graphs, which are also sometimes called networks. Later on, we prove that the Mostar index of a weighted graph can be computed as the sum of Mostar indices of weighted quotient graphs obtained by a partition of the edge set that is coarser than the Θ^*-partition. Such methods were recently developed also for other distance-based molecular descriptors (see [4, 7, 12, 23, 24]) and can be used to calculate the indices for various carbon nanostructures. Moreover, our method is used to compute the Mostar index for some benzenoid systems and for a fullerene patch. In addition, we present how the main theorem can be applied to tree-like polyphenyl systems.

Note that since the preprint of the present paper was published on arXiv in 2019 (arXiv:1904.04131), the results were already generalized to strength-weighted graphs and to other versions of the Mostar index, see [2, 3]. However, some results of this paper are essentially used in [2, 3, 6, 26] and therefore, we present the main part of the paper (Section 3) in the original form.

2. PRELIMINARIES

Unless stated otherwise, the graphs considered in this paper are simple, finite, and connected. For a graph G, we denote by $V(G)$ the set of vertices of G and by $E(G)$ the set of its edges. Moreover, $d_G(u, v)$ is the usual shortest-path distance between vertices $u, v \in V(G)$.

Let G be a graph and $e = uv$ an edge of G. Throughout the paper we will use the following notation:

$$N_u(e|G) = \{x \in V(G) \mid d_G(x, u) < d_G(x, v)\},$$
$$N_v(e|G) = \{x \in V(G) \mid d_G(x, v) < d_G(x, u)\}.$$

Let $\mathbb{R}_0^+ = [0, \infty)$. If $w: V(G) \to \mathbb{R}_0^+$ and $w': E(G) \to \mathbb{R}_0^+$ are given weights, then (G, w, w') is called a *vertex-edge-weighted graph* or shortly just a *weighted graph*. For any $e = uv \in E(G)$ we define:

$$n_u(e|(G, w)) = \sum_{x \in N_u(e|G)} w(x), \quad n_v(e|(G, w)) = \sum_{x \in N_v(e|G)} w(x).$$

We now introduce the Mostar index of (G, w, w') as $Mo(G, w, w') = \sum_{e=uv \in E(G)} w'(e)|n_u(e|(G, w)) - n_v(e|(G, w))|$. Obviously, for $w, w' \equiv 1$ this is exactly the Mostar index of G.

Let $e = xy$ and $f = ab$ be two edges of a graph G. If

$$d_G(x, a) + d_G(y, b) \neq d_G(x, b) + d_G(y, a),$$

we say that e and f are in relation Θ (also known as Djokovic′-Winkler relation) and write $e\Theta f$. Note that in some graphs this relation is not transitive (for example in odd cycles), although it is always reflexive and symmetric. As a consequence, we often consider the smallest transitive relation that contains relation Θ (i.e. the transitive closure of Θ) and denote it by Θ^*. It is known that in a *partial cube*, which is defined as an isometric subgraph of some hypercube, relation Θ is always transitive, so $\Theta = \Theta^*$. More precisely, a connected graph G is a partial cube if and only if G is bipartite and $\Theta = \Theta^*$ [20]. Moreover, the class of partial cubes contains many interesting molecular graphs (for example benzenoid systems and phenylenes). For more information on partial cubes and relation Θ, see [20].

Let $\mathcal{E} = \{E_1, \ldots, E_t\}$ be the Θ^*-partition of the edge set $E(G)$ and $\mathcal{F} = \{F_1, \ldots, F_k\}$ an arbitrary partition of $E(G)$. If every element of $\mathcal{E}$ is a subset of some element of $\mathcal{F}$, we say that $\mathcal{F}$ is *coarser* than $\mathcal{E}$. In such a case $\mathcal{F}$ will be shortly called a *c-partition*.

Suppose G is a graph and $F \subseteq E(G)$ is some subset of its edges. The *quotient graph* G/F is defined as the graph that has connected components of $G \backslash F$ as vertices; two such components X and Y being adjacent in G/F if and only if some vertex from X is adjacent to a vertex from Y in graph G. If $E = XY \in E(G/F)$ is an edge in graph G/F, then we denote by $\hat{E}$ the set of edges of G that have one end vertex in X and the other end vertex in Y, i.e. $\hat{E} = \{xy \in E(G) \mid x \in V(X), y \in V(Y)\}$.

3. COMPUTING THE MOSTAR INDEX FROM THE QUOTIENT GRAPHS

We show in this section that the Mostar index of a weighted graph can be computed from the corresponding quotient graphs.

Throughout the section, let G be a connected graph and $\{F_1, \ldots, F_k\}$ a c-partition of the set $E(G)$. Moreover, the quotient graph G/F_i will be shortly denoted as G_i for any $i \in \{1, \ldots, k\}$. In addition, we define the function $\ell_i: V(G) \to V(G_i)$ as follows: for any $u \in V(G)$, let $\ell_i(u)$ be the connected component U of the graph $G \backslash F_i$ such that $u \in V(U)$. The next lemma was obtained in [23], but the proof can be also found in [24, 27].

Lemma 3.1. [23, 24, 27] *If $u, v \in V(G)$ are two vertices, then*

$$d_G(u, v) = \sum_{i=1}^{k} d_{G_i}(\ell_i(u), \ell_i(v)).$$

The following lemma is the key to our method. The result was actually obtained in [24], but was not stated in this way. Therefore, for the sake of completeness we give the whole proof.

Lemma 3.2. *If* $e = uv \in F_i$, *where* $i \in \{1, \dots, k\}$, *then* $U = \ell_i(u)$ *and* $V = \ell_i(v)$ *are adjacent vertices in* G_i, *i.e.* $E = UV \in E(G_i)$. *Moreover,*

$$N_u(e|G) = \bigcup_{X \in N_U(E|G_i)} V(X),$$
$$N_v(e|G) = \bigcup_{X \in N_V(E|G_i)} V(X).$$

Proof. We follow the idea used inside the proof of Theorem 3.1 from [24]. Obviously, for any $j \in \{1, \dots, k\}$, $j \neq i$, it holds $\ell_j(u) = \ell_j(v)$ and therefore $d_{G_j}(\ell_j(u), \ell_j(v)) = 0$. By Lemma 3.1 we now obtain

$$d_G(u, v) = \sum_{j=1}^{k} d_{G_j}(\ell_j(u), \ell_j(v)) = d_{G_i}(\ell_i(u), \ell_i(v)),$$

which implies $d_{G_i}(\ell_i(u), \ell_i(v)) = 1$. Hence, $U = \ell_i(u)$ and $V = \ell_i(v)$ are adjacent vertices in G_i and we denote $E = UV$. Next, let $z \in V(G)$ be an arbitrary vertex in G. Again, for any $j \in \{1, \dots, k\}$, $j \neq i$, it holds $d_{G_j}(\ell_j(z), \ell_j(u)) = d_{G_j}(\ell_j(z), \ell_j(v))$. Therefore, by Lemma 3.1 we have

$$\begin{aligned} d_G(z, u) - d_G(z, v) &= \sum_{j=1}^{k} d_{G_j}(\ell_j(z), \ell_j(u)) - \sum_{j=1}^{k} d_{G_j}(\ell_j(z), \ell_j(v)) \\ &= \sum_{j=1}^{k} \left(d_{G_j}(\ell_j(z), \ell_j(u)) - d_{G_j}(\ell_j(z), \ell_j(v)) \right) \\ &= d_{G_i}(\ell_i(z), \ell_i(u)) - d_{G_i}(\ell_i(z), \ell_i(v)). \end{aligned}$$

Obviously, we can see from the obtained equality that $d_G(z, u) < d_G(z, v)$ if and only if $d_{G_i}(\ell_i(z), \ell_i(u)) < d_{G_i}(\ell_i(z), \ell_i(v))$. Hence, $z \in N_u(e|G)$ if and only if $\ell_i(z) \in N_{\ell_i(u)}(E|G_i) = N_U(E|G_i)$, which is equivalent to $z \in V(X)$ for some $X \in N_U(E|G_i)$. This proves the following equality:

$$N_u(e|G) = \bigcup_{X \in N_U(E|G_i)} V(X).$$

The remaining equality can be shown in the same way. □

Let $w: V(G) \to \mathbb{R}_0^+$, $w': E(G) \to \mathbb{R}_0^+$ be given weights and $i \in \{1, \dots, k\}$. We define $\lambda_i: V(G_i) \to \mathbb{R}_0^+$ in the following way: for any $X \in V(G_i)$, let $\lambda_i(X) = \sum_{x \in V(X)} w(x)$. So $\lambda_i(X)$ is the sum of all the weights of vertices from X.

Moreover, we define $\lambda'_i: E(G_i) \to \mathbb{R}_0^+$ as follows: for any $E = XY \in E(G_i)$, let $\lambda'_i(E) = \sum_{e \in \hat{E}} w'(e)$. Therefore, $\lambda'_i(E)$ is the sum of weights of edges that have one end vertex in X and the other end vertex in Y.

The following lemma will be needed as well. For a special case the result of this lemma can be found inside the proof of Theorem 3.1 from [24].

Lemma 3.3. *Let $e = uv \in F_i$, where $i \in \{1, \dots, k\}$, and $U = \ell_i(u)$, $V = \ell_i(v)$. If $E = UV \in E(G_i)$, then*

$$n_u(e|(G,w)) = n_U(E|(G_i,\lambda_i)),$$
$$n_v(e|(G,w)) = n_V(E|(G_i,\lambda_i)).$$

Proof. By Lemma 3.2 we calculate

$$\begin{aligned} n_u(e|(G,w)) &= \sum_{x\in N_u(e|G)} w(x) \\ &= \sum_{X\in N_U(E|G_i)} \left(\sum_{x\in V(X)} w(x)\right) \\ &= \sum_{X\in N_U(E|G_i)} \lambda_i(X) \\ &= n_U(E|(G_i,\lambda_i)), \end{aligned}$$

which proves the first equality. The other equality can be shown in the same way. □

Now we can state the main theorem. Based on the proof of this result, generalization to strength-weighted graphs and to other versions of the Mostar index was already published in [2] (see also [3, 6]). However, we include the proof anyway.

Theorem 3.4. *If (G,w,w') is a weighted connected graph and $\{F_1, \dots, F_k\}$ is a c-partition of the set $E(G)$, then*

$$Mo(G,w,w') = \sum_{i=1}^{k} Mo(G_i,\lambda_i,\lambda'_i).$$

Proof. Obviously, it holds $E(G) = \bigcup_{i=1}^{k} F_i$. Moreover, for all $i \in \{1, \dots, k\}$ we have (by Lemma 3.2)

$$F_i = \bigcup_{E\in E(G_i)} \hat{E}.$$

In the rest of the proof, we will write just Mo instead of $Mo(G,w,w')$. Therefore, one can compute

$$\begin{aligned} Mo &= \sum_{e=uv\in E(G)} w'(e)|n_u(e|(G,w)) - n_v(e|(G,w))| \\ &= \sum_{i=1}^{k} \left(\sum_{e=uv\in F_i} w'(e)|n_u(e|(G,w)) - n_v(e|(G,w))|\right) \\ &= \sum_{i=1}^{k} \left(\sum_{E=UV\in E(G_i)} \left[\sum_{e=uv\in \hat{E}} w'(e)|n_u(e|(G,w)) - n_v(e|(G,w))|\right]\right). \end{aligned}$$

If $E = UV$ is an edge in G_i and $e = uv$ is an arbitrary edge from $\hat{E}$, then by Lemma 3.3 we have

$$|n_u(e|(G,w)) - n_v(e|(G,w))| = |n_U(E|(G_i,\lambda_i)) - n_V(E|(G_i,\lambda_i))|.$$

Finally,

$$\begin{aligned} Mo &= \sum_{i=1}^{k} \left(\sum_{E=UV\in E(G_i)} \left[\sum_{e\in \hat{E}} w'(e)|n_U(E|(G_i,\lambda_i)) - n_V(E|(G_i,\lambda_i))|\right]\right) \\ &= \sum_{i=1}^{k} \left(\sum_{E=UV\in E(G_i)} |n_U(E|(G_i,\lambda_i)) - n_V(E|(G_i,\lambda_i))|\left[\sum_{e\in \hat{E}} w'(e)\right]\right) \\ &= \sum_{i=1}^{k} \left(\sum_{E=UV\in E(G_i)} \lambda'_i(E)|n_U(E|(G_i,\lambda_i)) - n_V(E|(G_i,\lambda_i))|\right) \\ &= \sum_{i=1}^{k} Mo(G_i,\lambda_i,\lambda'_i), \end{aligned}$$

which is what we wanted to prove. □

If $w(u) = 1$ for any $u \in V(G)$ and $w'(e) = 1$ for any $e \in E(G)$, then $Mo(G, w, w') = Mo(G)$, which leads to the next corollary.

Corollary 3.5. *If G is a connected graph and $\{F_1, \dots, F_k\}$ a c-partition of the set $E(G)$, then*

$$Mo(G) = \sum_{i=1}^{k} Mo(G_i, \lambda_i, \lambda'_i),$$

where $\lambda_i : V(G/F_i) \to \mathbb{R}_0^+$, $\lambda'_i : E(G/F_i) \to \mathbb{R}_0^+$ are defined as follows: $\lambda_i(X)$ is the number of vertices in the connected component X of $G \backslash F_i$ and $\lambda'_i(XY)$ is the number of edges in the set $\widehat{XY}$ (the number of edges between X and Y).

4. APPLICATIONS TO MOLECULAR GRAPHS

We apply the main result of the paper to some important molecular graphs. In particular, we consider benzenoid systems, polyphenyl systems, and a fullerene patch.

4.1 BENZENOID SYSTEMS

In this subsection, we show on two examples how the obtained method can be used to efficiently calculate the Mostar index of a benzenoid system (see also [3] for closely related topics). Note that such a computation can be done even by hand.

Let H be the hexagonal (graphite) lattice and let Z be a cycle on it. A *benzenoid system* is the graph induced by the vertices and edges of H, lying on Z or in its interior. The benzenoid systems defined in this way are sometimes called *simple* [15]. In the figures, we usually do not use dots to denote the vertices of benzenoid systems. For an example of a benzenoid system see Figure 1 or Figure 3. More information on these molecular graphs can be found in [18].

An *elementary cut* of a benzenoid system G is a line segment that starts at the center of a peripheral edge of a benzenoid system, goes orthogonal to it and ends at the first next peripheral edge of G. The main insight for our consideration is that every Θ-class of a benzenoid system G coincides with exactly one of its elementary cuts. Therefore, we can easily see that benzenoid systems are partial cubes [20]. As a consequence, by removing all the edges that correspond to an elementary cut of a benzenoid system, the obtained graph has exactly two connected components.

The edge set of a benzenoid system G can be naturally partitioned into sets F_1, F_2, and F_3 of edges of the same direction. Obviously, the partition $\{F_1, F_2, F_3\}$ is a c-partition of the set $E(G)$. For $i \in \{1, 2, 3\}$, let $T_i = G/F_i$ be the corresponding quotient graph. It is well known that T_1, T_2, and T_3 are trees [10].

Next, we define the weights $\lambda_i: V(T_i) \to \mathbb{R}_0^+$ and $\lambda'_i: E(T_i) \to \mathbb{R}_0^+$ as in Corollary 3.5:

1. for $X \in V(T_i)$, let $\lambda_i(X)$ be the number of vertices in the component X of $G \backslash F_i$;
2. for $E = XY \in E(T_i)$, let $\lambda'_i(E)$ be the number of edges between components X and Y (the number of edges in the set $\hat{E}$).

By Corollary 3.5 we immediately arrive to the following theorem.

Theorem 4.1. [3] *If G is a benzenoid system, then*

$$Mo(G) = Mo(T_1, \lambda_1, \lambda'_1) + Mo(T_2, \lambda_2, \lambda'_2) + Mo(T_3, \lambda_3, \lambda'_3).$$

The following lemma will be also needed. The proof is based on the standard BFS (breadth-first search) algorithm and is almost the same as the proof of Proposition 4.4 in [12].

Lemma 4.2. [3] *If (T, w, w') is a weighted tree with n vertices, then the index $Mo(T, w, w')$ can be computed in $O(n)$ time.*

In [10] it was shown that for each $i \in \{1,2,3\}$ the quotient tree T_i can be computed in linear time with respect to the number of vertices in a benzenoid system (calculation of the corresponding weights λ_i, λ'_i can be done within the same time complexity). Therefore, by Lemma 4.2 and Theorem 4.1, the Mostar index of a benzenoid system G can be computed in linear time $O(|V(G)|)$ [3]. However, by following the idea from [11], the Mostar index can be computed even faster, i.e. in sub-linear time (see [3] for more details). The proof of this fact uses a special construction of weighted trees $(T_i, \lambda_i, \lambda'_i)$, $i \in \{1,2,3\}$, that depends only on the boundary cycle of a benzenoid system (actually it relies on Chazelle's algorithm [8] for computing all vertex-edge visible pairs of edges of a simple finite polygon in linear time).

In the rest of the subsection, we apply Theorem 4.1 to some benzenoid systems. As the first example, we calculate the Mostar index for an infinite family of molecular graphs called *coronenes*, which was already done in Theorem 14 of [16]. However, we now show how the same result can be achieved by using our method. In particular, coronene G_1 is just a single hexagon, and G_h is obtained from G_{h-1} by adding a ring of hexagons around it. Coronene G_3 is depicted in Figure 1.

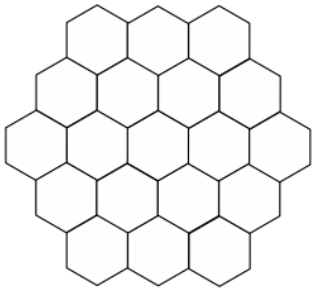

Figure 1: Coronene G_3.

Firstly, we determine the weighted quotient tree $(T_i, \lambda_i, \lambda'_i)$ for every $i \in \{1,2,3\}$. Because of the symmetry, all the weighted trees are equal. Let F_1 be the set of all the vertical edges in G_h, $h \geq 1$. For the graph G_3 these edges and the corresponding elementary cuts are shown in Figure 2 (a). Moreover, the weighted quotient tree $(T_1, \lambda_1, \lambda'_1)$ can be seen in Figure 2 (b).

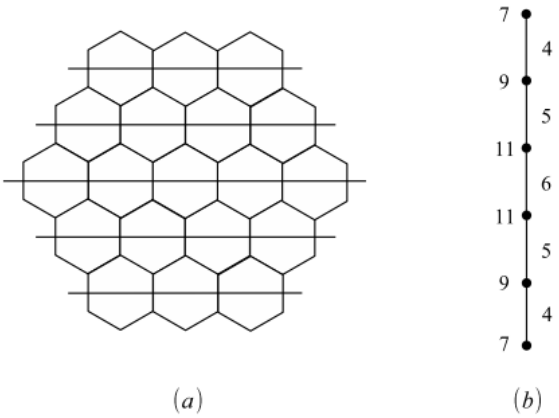

Figure 2: (a) Horizontal elementary cuts for coronene G_3 and (b) the weighted tree $(T_1, \lambda_1, \lambda'_1)$.

However, we can easily generalize the above example to coronene G_h and obtain that the quotient tree T_1 is isomorphic to the path on $2h$ vertices. Moreover, the weighted tree $(T_1, \lambda_1, \lambda'_1)$ is depicted in Figure 3.

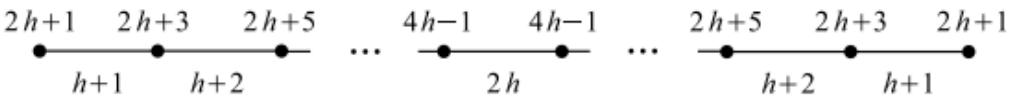

Figure 3: Weighted quotient tree $(T_1, \lambda_1, \lambda'_1)$ for graph G_h.

Therefore, it is easy to compute

$$Mo(T_1, \lambda_1, \lambda'_1) = 2\sum_{i=h+1}^{2h-1} \left(2i \sum_{j=i}^{2h-1} (2j+1)\right)$$
$$= 9h^4 - 6h^3 - 3h^2.$$

Finally, by Theorem 4.1 we have

$$Mo(G_h) = Mo(T_1, \lambda_1, \lambda'_1) + Mo(T_2, \lambda_2, \lambda'_2) + Mo(T_3, \lambda_3, \lambda'_3)$$
$$= 3Mo(T_1, \lambda_1, \lambda'_1)$$
$$= 27h^4 - 18h^3 - 9h^2,$$

which coincides with the result from [16].

As the second example, we compute the Mostar index for a branched benzenoid system G from Figure 4.

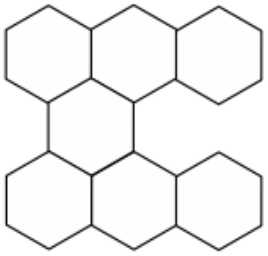

Figure 4: Benzenoid system G.

Again, let F_1 be the set of all vertical edges of G and let F_2, F_3 be the edges in the other two directions. Then, the weighted quotient trees are shown in Figure 4.

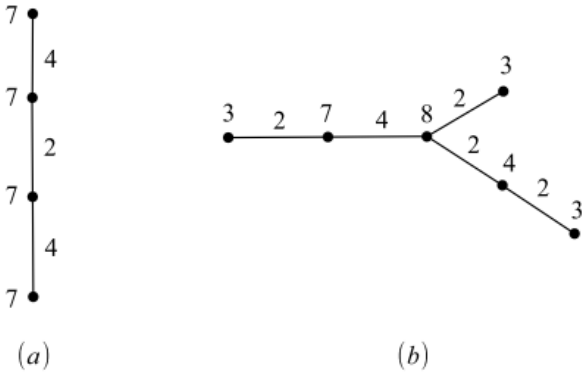

Figure 5: Weighted quotient trees (a) $(T_1, \lambda_1, \lambda'_1)$ and (b) $(T_2, \lambda_2, \lambda'_2) = (T_3, \lambda_3, \lambda'_3)$ for graph G.

Hence, we can compute

$$Mo(T_1, \lambda_1, \lambda'_1) = 4 \cdot 14 + 4 \cdot 14 = 112,$$
$$Mo(T_2, \lambda_2, \lambda'_2) = Mo(T_2, \lambda_2, \lambda'_2)$$
$$= 2 \cdot 22 + 4 \cdot 8 + 2 \cdot 22 + 2 \cdot 14 + 2 \cdot 22 = 192.$$

Finally, by Theorem 4.1 one can calculate

$$\begin{aligned} Mo(G) &= Mo(T_1, \lambda_1, \lambda'_1) + Mo(T_2, \lambda_2, \lambda'_2) + Mo(T_3, \lambda_3, \lambda'_3) \\ &= 112 + 192 + 192 \\ &= 496. \end{aligned}$$

We should mention that by using our method, analogous results can be deduced for some other families of interesting molecular graphs and networks, in particular for phenylenes [7] and C_4C_8 systems [12]. Another application to tree-like polyphenyl systems is considered in the following subsection.

4.2 TREE–LIKE POLYPHENYL SYSTEMS

Polyphenyls are conjugated hydrocarbons consisting of benzene rings that are connected by some bonds. In graph theory, molecular graphs of polyphenyls belong to the family of polyphenyl systems. In this subsection, we develop a method for computing the Mostar index of tree-like polyphenyl systems. Note that by using our procedure, various other distance-based topological indices of these graphs can be efficiently computed (for example the Wiener index, the edge-Wiener index, the Szeged indices, etc.). Some research on tree-like polyphenyl systems can be found in [5, 9, 19]. Next, we formally define polyphenyl systems in the language of graph theory.

A connected graph G is called a *polyphenyl system* if the following conditions hold true:

i. every vertex of G belongs to exactly one 6-cycle (also called *hexagon*), which means that G is constructed by a certain number of disjoint hexagons;
ii. every edge of G which does not belong to a hexagon has the end vertices in two distinct hexagons (in such a case, we say that the edge *connects* these two hexagons);
iii. for any two distinct hexagons there is at most one edge that connects them.

Two distinct hexagons H_1 and H_2 of a polyphenyl system are *adjacent* if there exists an edge with one end vertex in H_1 and another end vertex in H_2. The graph obtained by contracting every hexagon of a polyphenyl system G into a vertex is called the *squeeze* of G. Moreover, G is called *tree-like* if the squeeze of G is a tree, see Figure 6. Obviously, in a tree-like polyphenyl system with h hexagons there are exactly $h-1$ edges with the end vertices in two distinct hexagons and those edges must be bridges. Note that in [19] tree-like polyphenyl systems were called just polyphenyls.

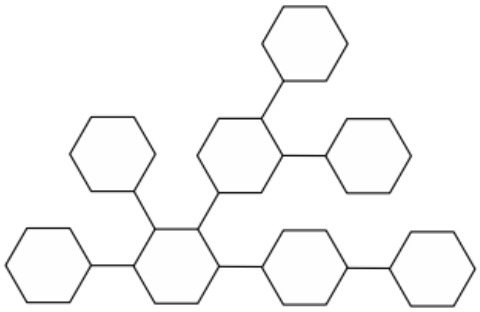

Figure 6: A tree-like polyphenyl system.

In this paper, we always assume that polyphenyl systems contain only regular hexagons and that all the hexagons are identically oriented, i.e. any two hexagons have three pairs of parallel edges. As a consequence, the edges of hexagons of a tree-like polyphenyl system G can be naturally partitioned into sets F_1, F_2, and F_3 of edges of the same direction. Moreover, let F_4 be the set of all the other edges of G (those that do not belong to a hexagon). We can prove the following lemma.

Lemma 4.3. *If G is a tree-like polyphenyl system, then the partition $\{F_1, F_2, F_3, F_4\}$ is a c-partition of the set $E(G)$. Moreover, G is a partial cube.*

Proof. Let e and f be two distinct edges of G. If e and f are not opposite edges of a hexagon, then there exists a shortest path in G that contains e and f. As a consequence, e and f are not in relation Θ (see Lemma 11.1 in [20]). On the other hand, if e and f are opposite edges of a hexagon, then they are in relation Θ. We now see that relation Θ is transitive and that any Θ-class of G either contains two opposite edges of a hexagon or consists of a single edge connecting two distinct hexagons. Therefore, $\{F_1, F_2, F_3, F_4\}$ obviously is a c-partition of the set $E(G)$.

We next show that G is bipartite. It is enough to prove that the vertices of G can be colored with two colors such that adjacent vertices get different colors. We first color the vertices of the hexagon H_0 that is chosen as a root of the squeeze T of G. Then, we continue with coloring the vertices of hexagons according to the breadth-first search order (BFS) on T. In this way, we can color all the vertices of G such that adjacent vertices receive different colors. Therefore, since G is bipartite and relation Θ is transitive, G is a partial cube (see Theorem 11.8 in [20]). □

However, the fact that tree-like polyphenyl systems are partial cubes is already well known. More precisely, in [9] it was observed that if G is a tree-like polyphenyl system, then it admits a partition of the edge set $E(G)$ into convex cuts, and therefore, by

Proposition 2.1 from [23] it follows that G is a partial cube. Moreover, the convex cuts used in [9] coincide with Θ-classes of G (but unification of different Θ-classes to obtain a c-partition was not considered).

Based on the c-partition $\{F_1, F_2, F_3, F_4\}$ described above Lemma 4.3, we now consider quotient graphs. Hence, for $i \in \{1, 2, 3, 4\}$ the corresponding quotient graph G/F_i will be denoted by T_i . Obviously, the graph T_4 is exactly the squeeze of G.

Lemma 4.4. *If G is a tree-like polyphenyl system, then the quotient graphs T_1, T_2, T_3, T_4 are trees.*

Proof. Since T_4 is the squeeze of G, it must be a tree. Next, we show that T_i, $i \in \{1,2,3\}$, is a tree by performing some transformations on the squeeze $T = T_4$ of G:

i. Choose a vertex H of T and replace it by two vertices, H_1 and H_2, which correspond to the two parts of the hexagon H after removing the edges from the set F_i. Then, for every neighbour H' of H in T either add an edge between H' and H_1 (if some vertex in H_1 is adjacent in graph G to a vertex of H') or add an edge between H' and H_2 (if some vertex in H_2 is adjacent in graph G to a vertex of H'). These new edges will be called *thin* edges. Finally, add an edge between H_1 and H_2, which is called a *thick* edge). Obviously, after performing this transformation the obtained graph, still denoted by T, is a tree.

ii. Apply transformation (i) also on every remaining vertex (that represents a hexagon) of T. The final tree obtained by following this procedure is denoted as T'.

iii. Choose a thin edge of T' and contract it into one vertex (i.e. identify the end vertices of this edge). The obtained graph, which is again denoted by T', is obviously a tree.

iv. Apply transformation (iii) for every remaining thin edge of T'. We denote the tree obtained after this procedure by T''.

It is easy to see that tree T'' is isomorphic to T_i, which proves that T_i is a tree. □

Let $i \in \{1, 2, 3, 4\}$. We define the weights $\lambda_i: V(T_i) \to \mathbb{R}_0^+$ and $\lambda'_i: E(T_i) \to \mathbb{R}_0^+$ as in Corollary 3.5, so in the same way as in the previous subsection. Therefore, by using the mentioned corollary, we arrive to the following theorem.

Theorem 4.5. *If G is a tree-like polyphenyl system, then*

$$Mo(G) = Mo(T_1, \lambda_1, \lambda'_1) + Mo(T_2, \lambda_2, \lambda'_2) + Mo(T_3, \lambda_3, \lambda'_3) + Mo(T_4, \lambda_4, \lambda'_4).$$

Similarly as for the benzenoid systems [10] it can be shown that every quotient tree T_i, $i \in \{1,2,3,4\}$, of a tree-like polyphenyl system can be computed in linear time with respect to the number of vertices. It is also straightforward to determine the corresponding weights. Therefore, by Lemma 4.2 and Theorem 4.5 we obtain the following result.

Proposition 4.6. *If G is a tree-like polyphenyl system on n vertices, then the Mostar index $Mo(G)$ can be computed in $O(n)$ time.*

To conclude this subsection, we present how Theorem 4.5 can be used to calculate the closed-form formula for the Mostar index of an infinite family of polyphenyl chains. Some additional definitions are firstly needed.

A *polyphenyl chain* is a tree-like polyphenyl system in which every hexagon is adjacent to at most two other hexagons. Moreover, every hexagon adjacent to exactly two other hexagons is called *internal*.

Let H_0 be an internal hexagon of a polyphenyl chain and let u, v be the vertices of H_0 incident to the two edges that connect H_0 with the other two hexagons. If the distance between u and v equals 3, then H_0 is a *para-hexagon* [5]. A polyphenyl chain with h hexagons is a *para-polyphenyl chain*, denoted as PPC_h, if every internal hexagon is a para-hexagon. See Figure 7.

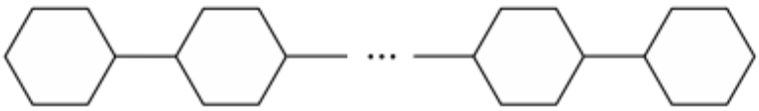

Figure 7: Para-polyphenyl chain with h hexagons, PPC_h.

In the next proposition, we deduce the closed-form formula for an arbitrary para-polyphenyl chain with h hexagons.

Proposition 4.7. *If PPC_h is a para-polyphenyl chain with h hexagons, then*

$$Mo(PPC_h) = \begin{cases} 21h^2 - 6h - 15; & h \text{ is odd}, \\ 21h^2 - 6h; & h \text{ is even}. \end{cases}$$

Proof. In order to apply Theorem 4.5, we have to determine the weighted quotient trees. In Figure 8 we can see the edges in the set F_1 and weighted quotient tree $(T_1, \lambda_1, \lambda'_1)$. It is easy to observe that for the edges (on hexagons) of other two directions, F_2 and F_3, we obtain the same weighted quotient trees. On the other hand, the edges in the set F_4, together with the weighted quotient tree $(T_4, \lambda_4, \lambda'_4)$, are shown in Figure 9.

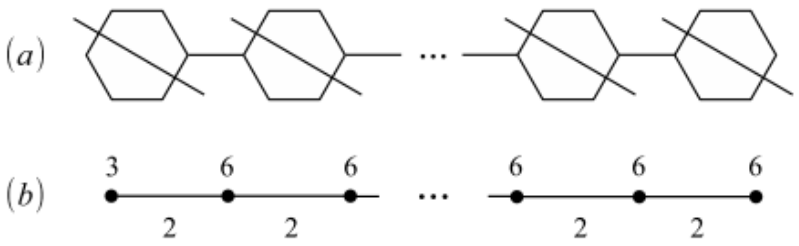

Figure 8: (a) The edges in the set F_1 and (b) the weighted quotient tree $(T_1, \lambda_1, \lambda'_1)$ on $h+1$ vertices for graph PPC_h.

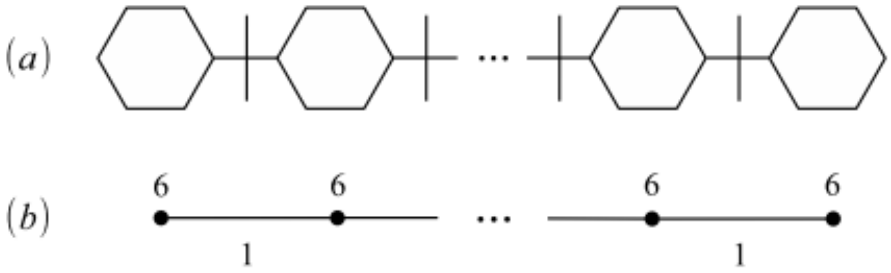

Figure 9: (a) The edges in the set F_4 and (b) the weighted quotient tree $(T_4, \lambda_4, \lambda'_4)$ on h vertices for graph PPC_h.

Firstly, assume that h is an even number. We can now compute

$$Mo(T_1, \lambda_1, \lambda'_1) = 2\sum_{i=1}^{\frac{h}{2}} 2 \cdot (6h - 6i + 3 - 6i + 3) = 6h^2,$$
$$Mo(T_4, \lambda_4, \lambda'_4) = 2\sum_{i=1}^{\frac{h-2}{2}} (6h - 6i - 6i) = 3h^2 - 6h.$$

Therefore, by Theorem 4.5 we have

$$Mo(PPC_h) = 3Mo(T_1, \lambda_1, \lambda'_1) + Mo(T_4, \lambda_4, \lambda'_4) = 21h^2 - 6h.$$

Finally, let h be an odd number. By using a similar procedure as above, one can deduce

$$Mo(T_1, \lambda_1, \lambda'_1) = 2\sum_{i=1}^{\frac{h-1}{2}} 2 \cdot (6h - 6i + 3 - 6i + 3) = 6h^2 - 6,$$
$$Mo(T_4, \lambda_4, \lambda'_4) = 2\sum_{i=1}^{\frac{h-1}{2}} (6h - 6i - 6i) = 3h^2 - 6h + 3,$$

which finally leads to

$$Mo(PPC_h) = 3Mo(T_1, \lambda_1, \lambda'_1) + Mo(T_4, \lambda_4, \lambda'_4) = 21h^2 - 6h - 15.$$

Therefore, the proof is complete. □

Note that polyphenyl systems from Figures 6 and 7 can be embedded into the regular hexagonal lattice without overlapping hexagons. However, it is important to point out that according to Theorem 4.5, our method can be applied also to tree-like polyphenyl systems that cannot be embedded into the regular hexagonal lattice.

4.3. A FULLERENE PATCH

A *fullerene* F is a 3-regular plane graph with only pentagonal and hexagonal faces. If C is an elementary cycle in F, then C partitions the plane into two open regions. A *patch* of F is defined as the graph obtained from F by deleting all vertices (and edges) in the interior of one of the two regions [17].

In this subsection, we apply our method to compute the Mostar index of a patch that is obtained from the well known buckminsterfullerene C_{60}. Therefore, let G be the graph shown in Figure 10 (a). However, graph G also belongs to another family of important chemical structures called *nanocones*. Generally speaking, nanocones are planar graphs where the inner faces are mostly hexagons, but there can be also some non-hexagonal inner faces, most commonly pentagons.

Firstly, we have to determine the Θ^*-classes of G, which are denoted by E_1, E_2, E_3, E_4, E_5, E_6 and shown in Figure 10 (b). Note that the Θ^*-classes of G were already obtained in [24], where the revised edge-Szeged index was computed for this graph. For an infinite family of nanocones, the Θ^*-classes were also considered in [2]. However, here we will use another partition of the set $E(G)$ and therefore obtain different quotient graphs. It turns out that for graph G relation Θ is not transitive and hence, G is not a partial cube.

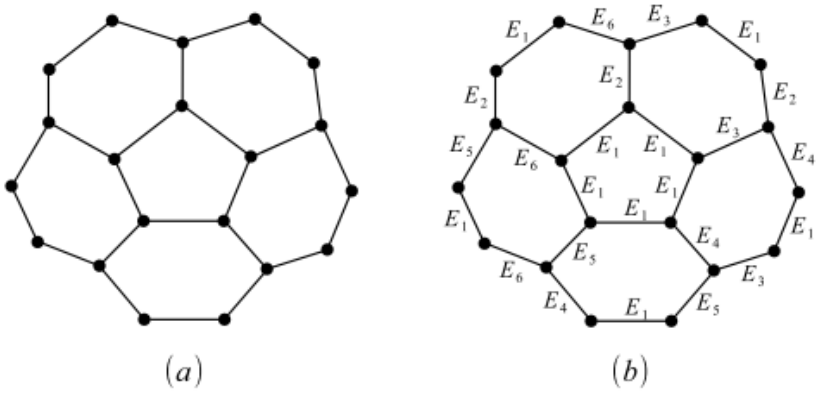

Figure 10: (a) Graph G and (b) the Θ^*-classes of G.

Let $F_1 = E_1$ and $F_2 = E_2 \cup E_3 \cup E_4 \cup E_5 \cup E_6$. Obviously, $\{F_1, F_2\}$ is a c-partition of $E(G)$. Next, the weighted quotient graphs $(G_1, \lambda_1, \lambda'_1)$ and $(G_2, \lambda_2, \lambda'_2)$ can be easily determined, see Figure 11. As in Section 3, the graph G_i denotes the quotient graph G/F_i for $i \in \{1,2\}$. Moreover, the weights are calculated as in Corollary 3.5.

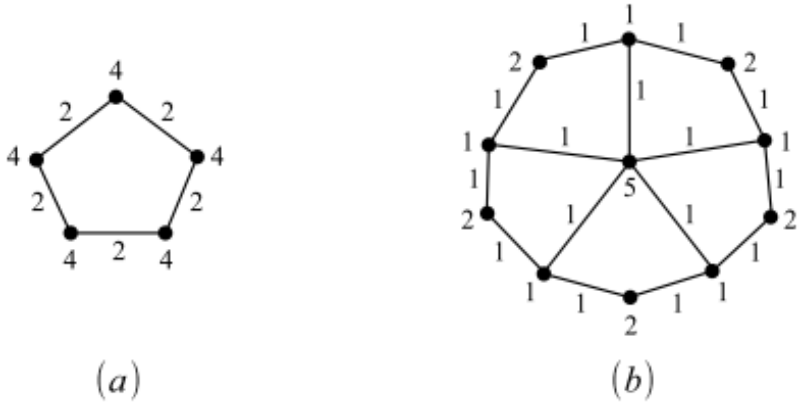

Figure 11: Weighted quotient graphs: (a) $(G_1, \lambda_1, \lambda'_1)$ and (b) $(G_2, \lambda_2, \lambda'_2)$.

It is obvious that $Mo(G_1, \lambda_1, \lambda'_1) = 0$. Moreover, to calculate $Mo(G_2, \lambda_2, \lambda'_2)$, we consider just two types of edges, i.e. the five edges that have the central vertex for an end-vertex and the remaining ten edges. Therefore, by Corollary 3.5 the calculation of the Mostar index becomes trivial:

$$\begin{aligned} Mo(G) &= Mo(G_1, \lambda_1, \lambda'_1) + Mo(G_2, \lambda_2, \lambda'_2) \\ &= Mo(G_2, \lambda_2, \lambda'_2) \\ &= 5 \cdot 1 \cdot |15 - 5| + 10 \cdot 1 \cdot |15 - 5| \\ &= 150. \end{aligned}$$

It is also interesting to consider a wider family of nanocones that were, for example, investigated in [1]. More precisely, a *single-defect m-gonal nanocone*, denoted as $CNC_m(n)$, is obtained by taking a cycle on m vertices and surrounding it by n concentric layers of hexagons. By using the cut method, Mostar indices of these graphs were already calculated in [2].

ACKNOWLEDGEMENT. The author Niko Tratnik acknowledge the financial support from the Slovenian Research Agency (research core funding No. P1-0297 and J1-9109).

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