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Mostar index and edge Mostar index of polymers

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Abstract
Let $G = (V, E)$ be a graph and $e = uv \in E$. Define $n_u(e, G)$ be the number of vertices of G closer to u than to v. The number $n_v(e, G)$ can be defined in an analogous way. The Mostar index of G is a new graph invariant defined as $Mo(G) = \sum_{uv \in E(G)} |n_u(uv, G) - n_v(uv, G)|$. The edge version of Mostar index is defined as $Mo_e(G) = \sum_{e=uv \in E(G)} |m_u(e|G) - m_v(G|e)|$, where $m_u(e|G)$ and $m_v(e|G)$ are the number of edges of G lying closer to vertex u than to vertex v and the number of edges of G lying closer to vertex v than to vertex u, respectively. Let G be a connected graph constructed from pairwise disjoint connected graphs $G_1, \ldots, G_k$ by selecting a vertex of G_1, a vertex of G_2, and identifying these two vertices. Then continue in this manner inductively. We say that G is a polymer graph, obtained by point-attaching from monomer units $G_1, \ldots, G_k$. In this paper, we consider some particular cases of these graphs that are of importance in chemistry and study their Mostar and edge Mostar indices.

Keywords Mostar index · Edge Mostar index · Polymer · Chain

Mathematics Subject Classification 05C09 · 05C92

1 Introduction

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds of a molecule. Let $G = (V, E)$ be a finite, connected, simple graph. A topological index of G is a real number related to G. It does not depend on the labeling or pictorial representation of a graph. The Wiener index $W(G)$ is the first distance-based topological index defined as $W(G) = \sum_{\{u,v\} \subseteq G} d(u, v) = \frac{1}{2} \sum_{u,v \in V(G)} d(u, v)$ with the

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summation runs over all pairs of vertices of G Wiener (1947). The topological indices and graph invariants based on distances between vertices of a graph are widely used for characterizing molecular graphs, establishing relationships between structure and properties of molecules, predicting biological activity of chemical compounds, and making their chemical applications. The Wiener index is one of the most used topological indices with high correlation with many physical and chemical indices of molecular compounds Wiener (1947). In a recent paper, Doslić et al. (2018) introduced a newbond-additive structural invariant as a quantitative refinement of the distance nonbalancedness and also a measure of peripherality in graphs. They used the name Mostar index for this invariant which is defined as $Mo(G) = \sum_{uv \in E(G)} |n_u(uv, G) - n_v(uv, G)|$, where $n_u(uv, G)$ is the number of vertices of G closer to u than to v, and similarly, $n_v(uv, G)$ is the number of vertices closer to v than to u. They determined the extremal values of this invariant and characterized extremal trees and unicyclic graphs with respect to the Mostar index. Akhter in [1] computed the Mostar index of corona product, Cartesian product, join, lexicographic product, Indu-Bala product and subdivision vertex-edge join of graphs and applied results to find the Mostar index of various classes of chemical graphs and nanostructures. The Mostar index of bicyclic graphs was studied by Tepeh (2019). A cacti graph is a graph in which any block is either a cut edge or a cycle, or equivalently, a graph in which any two cycles have at most one common vertex. Hayat and Zhou (2019) gave an upper bound for the Mostar index of cacti of order n with k cycles, and also they characterized those cacti that achieve the bound.

The edge version of Mostar index has considered in Arockiaraj et al. (2019), Liu et al. (2020) and is defined as $Mo_e(G) = \sum_{e=uv \in E(G)} |m_u(e|G) - m_v(G|e)|$, where $m_u(e|G)$ and $m_v(e|G)$ are the number of edges of G lying closer to vertex u than to vertex v and the number of edges of G lying closer to vertex v than to vertex u, respectively. Liu et al. (2020) determined the extremal values of edge Mostar index of some graphs such as trees and unicyclic graphs.

For every edge $uv \in E(G)$, since u is closer to u than v and v is closer to v than u, and they do not effect on the results by the definition of Mostar index, we do not consider them in our counting.

In this paper, we consider the Mostar index and the edge Mostar index of polymer graphs. Such graphs can be decomposed into subgraphs that we call monomer units. Blocks of graphs are particular examples of monomer units, but a monomer unit may consist of several blocks. For convenience, the definition of these kind of graphs will be given in the next section. In Sect. 2, the Mostar index of some graphs are computed from their monomer units. In Sect. 3, we obtain the Mostar index and the edge Mostar index of families of graphs that are of importance in chemistry.

2 Mostar index and edge Mostar index of polymers

Let G be a connected graph constructed from pairwise disjoint connected graphs $G_1, \ldots, G_k$ as follows. Select a vertex of G_1, a vertex of G_2, and identify these two vertices. Then continue in this manner inductively. Note that the graph G constructed in this way has a tree-like structure, the G_i's being its building stones (see Fig. 1). Usually say that G is a polymer graph, obtained by point-attaching from $G_1, \ldots, G_k$ and that G_i's are the monomer units of G. A particular case of this construction is the decomposition of a connected graph into blocks (see Alikhani and Ghanbari 2021; Emeric and Klavžar 2013).

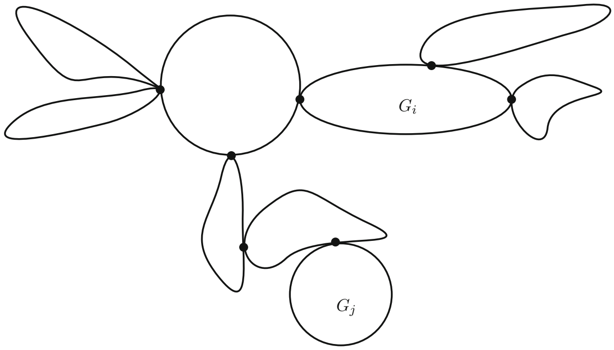


Fig. 1 A polymer graph with monomer units $G_1, \ldots, G_k$

The following theorem is easy result which obtain by the definition of Mostar index, edge Mostar index and point-attaching graph.

Theorem 2.1 *If G is a polymer graph with the monomer units $G_1, \ldots, G_k$, then $Mo(G) > \sum_{i=1}^{n} Mo(G_i)$, and $Mo_e(G) > \sum_{i=1}^{n} Mo_e(G_i)$.*

We consider some particular cases of point-attaching graphs and study their Mostar and edge Mostar index. As an example of point-attaching graph, consider the graph K_m and m copies of K_n. By definition, the graph $Q(m, n)$ is obtained by identifying each vertex of K_m with a vertex of a unique K_n. The graph $Q(5, 4)$ is shown in Fig. 2.

Theorem 2.2 *For the graph $Q(m, n)$ (see Fig. 2), we have*

(i) $Mo(Q(m, n)) = mn(m-1)(n-1)$.
(ii) $Mo_e(Q(m, n)) = \frac{m(n-1)(m-1)}{2}(n^2 - n + m)$.

Proof (i) First, consider the edge u_iu_j in K_m. There are $n-1$ vertices which are closer to u_i than u_j, and there are $n-1$ vertices closer to u_j than u_i. So $|n_{u_i}(u_iu_j, Q(m, n)) - n_{u_j}(u_ju_i, Q(m, n))| = 0$. Now consider the edge vw in the ith K_n. There is no vertices which are closer to v than w, and visa versa. So $|n_v(vw, Q(m, n)) - n_w(vw, Q(m, n))| = 0$. Finally, consider the edge u_iv in the ith K_n. There are $n(m-1)$ vertices which are closer to u_i than v, and there is no vertices closer to v than u_i. So $|n_{u_i}(u_iv, Q(m, n)) - n_v(u_iv, Q(m, n))| = n(m-1)$. Since there are $m(n-1)$ edges like u_iv in $Q(m, n)$; therefore, we have the result.

(ii) First consider the edge u_iu_j in K_m. There are $\frac{n(n-1)}{2}$ edges which are closer to u_i than u_j, and there are $\frac{n(n-1)}{2}$ edges closer to u_j than u_i. So $|m_{u_i}(u_iu_j, Q(m, n)) - m_{u_j}(u_ju_i, Q(m, n))| = 0$. Now consider the edge vw in the ith K_n. There is no edges which are closer to v than w, and visa versa. So $|m_v(vw, Q(m, n)) - m_w(vw, Q(m, n))| = 0$. Finally, consider the edge u_iv in the ith K_n. There are $\frac{n(n-1)(m-1)}{2} + \frac{m(m-1)}{2}$ edges which are closer to u_i than v, and there is no edges closer to v than u_i. So $|m_{u_i}(u_iv, Q(m, n)) - m_v(u_iv, Q(m, n))| = \frac{(m-1)}{2}(n^2 - n + m)$. Since there are $m(n-1)$ edges like u_iv in $Q(m, n)$, so we have the result.

□

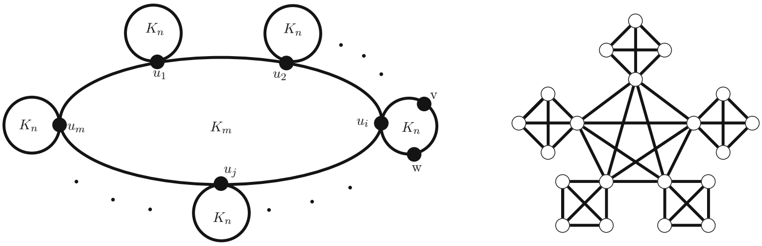


Fig. 2 The graph $Q(m, n)$ and $Q(5, 4)$, respectively

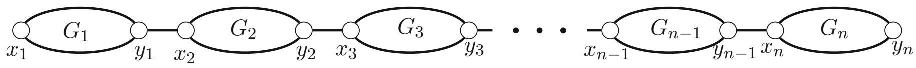


Fig. 3 Link of n graphs $G_1, G_2, \ldots, G_n$

2.1 Upper bounds for the Mostar (edge Mostar) index of polymers

In this subsection, we consider some special polymer graphs and present upper bounds for the Mostar index and edge Mostar index of them. The following theorem is about the link of graphs.

Theorem 2.3 *Let G be a polymer graph with composed of monomers $\{G_i\}_{i=1}^k$ with respect to the vertices $\{x_i, y_i\}_{i=1}^k$. Let G be the link of graphs (see Fig. 3). Then*

(i)

$$Mo(G) \leq \sum_{i=1}^{n} Mo(G_i) + \sum_{i=1}^{n} |E(G_i)|(|V(G)| - |V(G_i)|) + \sum_{i=1}^{n-1} \left| \sum_{t=1}^{i} |V(G_t)| - \sum_{t=i+1}^{n} |V(G_t)| \right|.$$

(ii)

$$Mo_e(G) \leq \sum_{i=1}^{n} Mo_e(G_i) + \sum_{i=1}^{n} |E(G_i)|(|E(G)| - |E(G_i)|) + \sum_{i=1}^{n-1} \left| \sum_{t=1}^{i} |E(G_t)| - \sum_{t=i+1}^{n} |E(G_t)| \right|.$$

Proof (i) Consider the graph G_i (Fig. 3) and let $n'_u(uv, G_i)$ be the number of vertices of G_i closer to u than v in G_i. By the definition of Mostar index, we have

$$Mo(G) = \sum_{uv \in E(G)} |n_u(uv, G) - n_v(uv, G)| = \sum_{i=1}^{n} \sum_{uv \in E(G_i)} |n_u(uv, G_i) - n_v(uv, G_i)|$$

$$+\sum_{i=1}^{n-1}\sum_{y_ix_{i+1}\in E(G)}|n_{y_i}(y_ix_{i+1},G)-n_{x_{i+1}}(y_ix_{i+1},G)|$$

$$=\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(u,y_i)<d(v,y_i)}|n_u(uv,G_i)-n_v(uv,G_i)|$$

$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(v,y_i)<d(u,y_i)}|n_u(uv,G_i)-n_v(uv,G_i)|$$

$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(u,y_i)=d(v,y_i)}|n_u(uv,G_i)-n_v(uv,G_i)|$$

$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)=d(v,x_i),d(u,y_i)<d(v,y_i)}|n_u(uv,G_i)-n_v(uv,G_i)|$$

$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)=d(v,x_i),d(u,y_i)=d(v,y_i)}|n_u(uv,G_i)-n_v(uv,G_i)|$$

$$+\sum_{i=1}^{n-1}\sum_{y_ix_{i+1}\in E(G)}|n_{y_i}(y_ix_{i+1},G)-n_{x_{i+1}}(y_ix_{i+1},G)|$$

$$=\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(u,y_i)<d(v,y_i)}$$

$$\left|n'_u(uv,G_i)+|V(G)-V(G_i)|-n'_v(uv,G_i)\right|$$

$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(v,y_i)<d(u,y_i)}$$

$$\left|n'_u(uv,G_i)+\sum_{t=1}^{i}|V(G_t)|-n'_v(uv,G_i)-\sum_{t=i+1}^{n}|V(G_t)|\right|$$

$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(u,y_i)=d(v,y_i)}\Bigg|$$

$$n'_u(uv,G_i)+\sum_{t=1}^{i}|V(G_t)|-n'_v(uv,G_i)\Bigg|$$

$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)=d(v,x_i),d(u,y_i)<d(v,y_i)}$$

$$\left|n'_u(uv,G_i)-n'_v(uv,G_i)-\sum_{t=i+1}^{n}|V(G_t)|\right|$$

$$+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)=d(v,x_i),d(u,y_i)=d(v,y_i)}|n'_u(uv,G_i)-n'_v(uv,G_i)|$$

$$
\begin{aligned}
&+\sum_{i=1}^{n-1}\Big|\sum_{t=1}^{i}|V(G_t)|-\sum_{t=i+1}^{n}|V(G_t)|\Big|\\
&\le \sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(u,y_i)<d(v,y_i)}|n'_u(uv,G_i)-n'_v(uv,G_i)|\\
&+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(u,y_i)<d(v,y_i)}|V(G)-V(G_i)|\\
&+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(v,y_i)<d(u,y_i)}|n'_u(uv,G_i)-n'_v(uv,G_i)|\\
&+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(u,y_i)<d(v,y_i)}|V(G)-V(G_i)|\\
&+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(u,y_i)=d(v,y_i)}|n'_u(uv,G_i)-n'_v(uv,G_i)|\\
&+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(u,y_i)<d(v,y_i)}|V(G)-V(G_i)|\\
&+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)=d(v,x_i),d(u,y_i)<d(v,y_i)}|n'_u(uv,G_i)-n'_v(uv,G_i)|\\
&+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i),d(u,y_i)<d(v,y_i)}|V(G)-V(G_i)|\\
&+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)=d(v,x_i),d(u,y_i)=d(v,y_i)}|n'_u(uv,G_i)-n'_v(uv,G_i)|\\
&+\sum_{i=1}^{n-1}\Big|\sum_{t=1}^{i}|V(G_t)|-\sum_{t=i+1}^{n}|V(G_t)|\Big|\\
&=\sum_{i=1}^{n}Mo(G_i)+\sum_{i=1}^{n}|E(G_i)|(|V(G)|-|V(G_i)|)\\
&+\sum_{i=1}^{n-1}\Big|\sum_{t=1}^{i}|V(G_t)|-\sum_{t=i+1}^{n}|V(G_t)|\Big|.
\end{aligned}
$$

Therefore, we have the result.

(ii) The proof is similar to Part (i). □

By the same argument similar to the proof of Theorem 2.3, we have

Theorem 2.4 *Let $G_1, G_2, \ldots, G_n$ be a finite sequence of pairwise disjoint connected graphs and let $x_i, y_i \in V(G_i)$. Let $C(G_1, ..., G_n)$ be the chain of graphs $\{G_i\}_{i=1}^n$ with respect to the vertices $\{x_i, y_i\}_{i=1}^k$ which obtained by identifying the vertex y_i with the vertex x_{i+1} for $i = 1, 2, \ldots, n-1$ (Fig. 4). Then*

(i) $Mo(C(G_1, ..., G_n)) \le \sum_{i=1}^n Mo(G_i) + \sum_{i=1}^n |E(G_i)|(|V(G)| - |V(G_i)|)$.

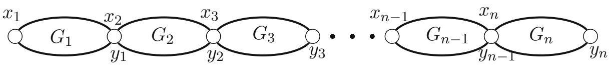


Fig. 4 Chain of n graphs $G_1, G_2, \ldots, G_n$

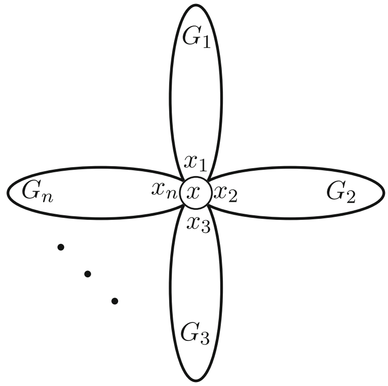


Fig. 5 Bouquet of n graphs $G_1, G_2, \ldots, G_n$ and $x_1 = x_2 = \ldots = x_n = x$

(ii) $Mo_e(C(G_1, ..., G_n)) \leq \sum_{i=1}^{n} Mo_e(G_i) + \sum_{i=1}^{n} |E(G_i)|(|E(G)| - |E(G_i)|)$.

With similar argument to the proof of Theorem 2.3, we have

Theorem 2.5 *Let $G_1, G_2, \ldots, G_n$ be a finite sequence of pairwise disjoint connected graphs and let $x_i \in V(G_i)$. Let $B(G_1, ..., G_n)$ be the bouquet of graphs $\{G_i\}_{i=1}^n$ with respect to the vertices $\{x_i\}_{i=1}^n$ and obtained by identifying the vertex x_i of the graph G_i with x (see Fig. 5). Then*

(i)

$$Mo(B(G_1, ..., G_n)) \leq \sum_{i=1}^{n} Mo(G_i) + \sum_{i=1}^{n} |E(G_i)|(|V(G)| - |V(G_i)|).$$

(ii)

$$Mo_e(B(G_1, ..., G_n)) \leq \sum_{i=1}^{n} Mo_e(G_i) + \sum_{i=1}^{n} |E(G_i)|(|E(G)| - |E(G_i)|).$$

Theorem 2.6 *Let $G_1, G_2, \ldots, G_n$ be a finite sequence of pairwise disjoint connected graphs and let $x_i \in V(G_i)$. Let G be the circuit of graphs $\{G_i\}_{i=1}^n$ with respect to the vertices $\{x_i\}_{i=1}^n$ and obtained by identifying the vertex x_i of the graph G_i with the ith vertex of the cycle graph C_n (Fig. 6). Then*

$$Mo(G) \leq \sum_{i=1}^{n} Mo(G_i) + \sum_{i=1}^{n} |E(G_i)|(|V(G)| - |V(G_i)|) + \begin{cases} n \sum_{i=1}^{t} \Big| |V(G_i)| - |V(G_{t+i})| \Big| & \text{if } n = 2t, \\ (n-1)|V(G)| & \text{if } n = 2t-1. \end{cases}$$

Proof First consider the edge x_1x_n. There are two cases, n is even or odd. If $n = 2t$ for some $t \in \mathbb{N}$, then, the vertices in the graphs $G_1, G_2, G_3, \ldots, G_t$ are closer to x_1 than x_n, and the rest are closer to x_n than x_1. So

$$\begin{aligned}|n_{x_1}(x_1x_n, G) - n_{x_n}(x_1x_n, G)| &= \left|\sum_{i=1}^{t} |V(G_i)| - \sum_{i=1}^{t} |V(G_{t+i})|\right| \\ &\le \sum_{i=1}^{t}\Big||V(G_i)| - |V(G_{t+i})|\Big|.\end{aligned}$$

It is easy to check that the same happens for x_ix_{i+1} for all $1 \le i \le n-1$.

If $n = 2t-1$ for some $t \in \mathbb{N}$, then, the vertices in the graphs $G_1, G_2, G_3, \ldots, G_{t-1}$ are closer to x_1 than x_n, and the vertices in the graphs $G_{t+1}, G_{t+2}, G_{t+3}, \ldots, G_n$ are closer to x_n than x_1. The vertices in the graph G_t have the same distance to x_1 and x_n. So

$$\begin{aligned}|n_{x_1}(x_1x_n, G) - n_{x_n}(x_1x_n, G)| &= \left|\sum_{i=1}^{t-1} |V(G_i)| - \sum_{i=1}^{t-1} |V(G_{t+i})|\right| \\ &\le |V(G_1)| + |V(G_2)| + \cdots + |V(G_{t-1})| \\ &\quad + |V(G_{t+1})| + |V(G_{t+2})| + \cdots + |V(G_n)| \\ &= |V(G)| - |V(G_t)|.\end{aligned}$$

It is easy to check that $|n_{x_1}(x_1x_2, G) - n_{x_2}(x_1x_2, G)| \le |V(G)| - |V(G_{t+1})|$, and this continues. Now we consider the edge $uv \in G_i$. There are two cases, first u is closer to x_i than v, and second they have the same distance to x_i. Let $n'_u(uv, G_i)$ be the number of vertices of G_i closer to u than v in G_i. Then by the definition of Mostar index, we have

$$\begin{aligned}Mo(G) &= \sum_{uv\in E(G)} |n_u(uv, G) - n_v(uv, G)| \\ &= \sum_{i=1}^{n} \sum_{uv\in E(G_i)} |n_u(uv, G_i) - n_v(uv, G_i)| \\ &\quad + \sum_{i=1}^{n-1} \sum_{x_ix_{i+1}\in E(G)} |n_{x_i}(x_ix_{i+1}, G) - n_{x_{i+1}}(x_ix_{i+1}, G)| \\ &\quad + |n_{x_1}(x_1x_n, G) - n_{x_n}(x_1x_n, G)| \\ &= \sum_{i=1}^{n} \sum_{uv\in E(G_i), d(u,x_i)<d(v,x_i)} |n_u(uv, G_i) - n_v(uv, G_i)| \\ &\quad + \sum_{i=1}^{n} \sum_{uv\in E(G_i), d(u,x_i)=d(v,x_i)} |n_u(uv, G_i) - n_v(uv, G_i)| \\ &\quad + \sum_{i=1}^{n-1} \sum_{x_ix_{i+1}\in E(G)} |n_{x_i}(x_ix_{i+1}, G) - n_{x_{i+1}}(x_ix_{i+1}, G)| \\ &\quad + |n_{x_1}(x_1x_n, G) - n_{x_n}(x_1x_n, G)| \\ &= \sum_{i=1}^{n} \sum_{uv\in E(G_i), d(u,x_i)<d(v,x_i)} \Big|n'_u(uv, G_i) + |V(G) - V(G_i)| - n'_v(uv, G_i)\Big|\end{aligned}$$

$$
\begin{aligned}
&+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)=d(v,x_i)}|n'_u(uv,G_i)-n'_v(uv,G_i)|\\
&+\sum_{i=1}^{n-1}\sum_{x_ix_{i+1}\in E(G)}|n_{x_i}(x_ix_{i+1},G)-n_{x_{i+1}}(x_ix_{i+1},G)|\\
&+|n_{x_1}(x_1x_n,G)-n_{x_n}(x_1x_n,G)|\\
\le&\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i)}|n'_u(uv,G_i)-n'_v(uv,G_i)|\\
&+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)<d(v,x_i)}|V(G)-V(G_i)|\\
&+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)=d(v,x_i)}|n'_u(uv,G_i)-n'_v(uv,G_i)|\\
&+\sum_{i=1}^{n}\sum_{uv\in E(G_i),d(u,x_i)=d(v,x_i)}|V(G)-V(G_i)|\\
&+\begin{cases} n\sum_{i=1}^{t}\Big||V(G_i)|-|V(G_{t+i})|\Big| & \text{if } n=2t,\\ (n-1)|V(G)| & \text{if } n=2t-1,\end{cases}\\
=&\sum_{i=1}^{n}Mo(G_i)+\sum_{i=1}^{n}|E(G_i)|(|V(G)|-|V(G_i)|)\\
&+\begin{cases} n\sum_{i=1}^{t}\Big||V(G_i)|-|V(G_{t+i})|\Big| & \text{if } n=2t,\\ (n-1)|V(G)| & \text{if } n=2t-1.\end{cases}
\end{aligned}
$$

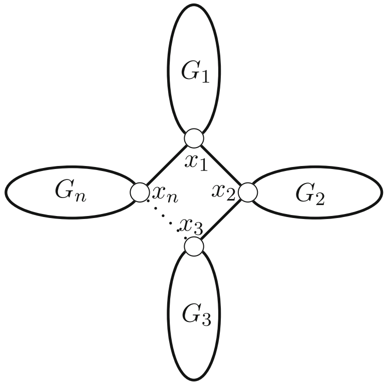
Therefore, we have the result. □

Similarly, we have the following result for the edge Mostar index of circuit of graphs:

Theorem 2.7 *Let $G_1, G_2, \ldots, G_n$ be a finite sequence of pairwise disjoint connected graphs and let $x_i \in V(G_i)$. Let G be the circuit of graphs $\{G_i\}_{i=1}^n$ with respect to the vertices $\{x_i\}_{i=1}^n$ and obtained by identifying the vertex x_i of the graph G_i with the ith vertex of the cycle graph C_n (Fig. 6). Then*

$$
\begin{aligned}
Mo_e(G)\le&\sum_{i=1}^{n}Mo_e(G_i)+\sum_{i=1}^{n}|E(G_i)|(|E(G)|-|E(G_i)|)\\
&+\begin{cases} n\sum_{i=1}^{t}\Big||E(G_i)|-|E(G_{t+i})|\Big| & \textit{if } n=2t,\\ (n-1)|E(G)| & \textit{if } n=2t-1.\end{cases}
\end{aligned}
$$

Fig. 6 Circuit of n graphs $G_1, G_2, \ldots, G_n$



2.2 Lower bounds for the Mostar (edge Mostar) index of polymers

In this subsection, we consider some special polymer graphs and present lower bounds for the Mostar index and the edge Mostar index of them.

Theorem 2.8 *Let G be a link of two graphs G_1 and G_2 with respect to the vertices x, y. Then*

(i) $MO(G) > MO(G_1) + MO(G_2) + \Big||V(G_1)| - |V(G_2)|\Big|$.

(ii) $MO_e(G) > MO_e(G_1) + MO_e(G_2) + \Big||E(G_1)| - |E(G_2)|\Big|$.

Proof (i) Let $n'_u(uv, G_i)$ be the number of vertices of G_i closer to u than v in G_i for $i = 1, 2$. By the definition of Mostar index, we have

$$\begin{aligned} Mo(G) &= \sum_{uv\in E(G)} |n_u(uv, G) - n_v(uv, G)| \\ &= \sum_{uv\in E(G_1)} |n_u(uv, G) - n_v(uv, G)| \\ &\quad + \sum_{uv\in E(G_2)} |n_u(uv, G) - n_v(uv, G)| \\ &\quad + |n_x(xy, G) - n_y(xy, G)| \\ &= \sum_{uv\in E(G_1), d(u,x)<d(v,x)} |n_u(uv, G) - n_v(uv, G)| \\ &\quad + \sum_{uv\in E(G_1), d(u,x)=d(v,x)} |n_u(uv, G) - n_v(uv, G)| \\ &\quad + \sum_{uv\in E(G_2), d(u,x)<d(v,x)} |n_u(uv, G) - n_v(uv, G)| \\ &\quad + \sum_{uv\in E(G_2), d(u,x)=d(v,x)} |n_u(uv, G) - n_v(uv, G)| \\ &\quad + |n_x(xy, G) - n_y(xy, G)| \end{aligned}$$

$$
\begin{aligned}
&= \sum_{uv\in E(G_1),d(u,x)<d(v,x)} \left| n'_u(uv, G_1) + |V(G_2)| - n'_v(uv, G-1) \right| \\
&\quad + \sum_{uv\in E(G_1),d(u,x)=d(v,x)} |n'_u(uv, G_1) - n'_v(uv, G_1)| \\
&\quad + \sum_{uv\in E(G_2),d(u,x)<d(v,x)} \left| n'_u(uv, G_2) + |V(G_1)| - n'_v(uv, G_2) \right| \\
&\quad + \sum_{uv\in E(G_2),d(u,x)=d(v,x)} |n'_u(uv, G_2) - n'_v(uv, G_2)| \\
&\quad + \left| |V(G_1)| - |V(G_2)| \right| \\
&> \sum_{uv\in E(G_1),d(u,x)<d(v,x)} |n'_u(uv, G_1) - n'_v(uv, G_1)| \\
&\quad + \sum_{uv\in E(G_1),d(u,x)=d(v,x)} |n'_u(uv, G_1) - n'_v(uv, G_1)| \\
&\quad + \sum_{uv\in E(G_2),d(u,x)<d(v,x)} |n'_u(uv, G_2) - n'_v(uv, G_2)| \\
&\quad + \sum_{uv\in E(G_2),d(u,x)=d(v,x)} |n'_u(uv, G_2) - n'_v(uv, G_2)| \\
&\quad + \left| |V(G_1)| - |V(G_2)| \right| \\
&= MO(G_1) + MO(G_2) + \left| |V(G_1)| - |V(G_2)| \right|.
\end{aligned}
$$

(ii) The proof is similar to the proof of Part (i). □

As an immediate result of Theorem 2.8, we have

Theorem 2.9 *Let G be a polymer graph with composed of monomers $\{G_i\}_{i=1}^k$ with respect to the vertices $\{x_i, y_i\}_{i=1}^k$. Let G be the link of graphs (see Fig. 3). Then*

(i)

$$
Mo(G) > \sum_{i=1}^{n} Mo(G_i) + \sum_{t=1}^{n-1} \left| |V(G) - \bigcup_{i=1}^{t} V(G_i)| - |V(G_t)| \right|.
$$

(ii)

$$
Mo_e(G) > \sum_{i=1}^{n} Mo_e(G_i) + \sum_{t=1}^{n-1} \left| |E(G) - \bigcup_{i=1}^{t} E(G_i)| - |E(G_t)| \right|.
$$

3 Chemical applications

In this section, we obtain the Mostar index and the edge-Mostar index of families of graphs that are of importance in chemistry.

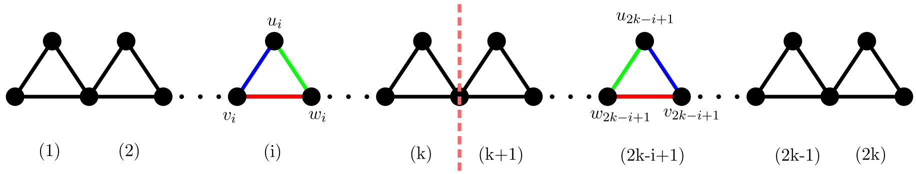


Fig. 7 Chain triangular cactus T_{2k}

Theorem 3.1 *Let T_n be the chain triangular graph of order n. Then for every $n \geq 2$, and $k \geq 1$, we have*

(i)

$$Mo(T_n) = \begin{cases} 12k^2 - 4k & if n = 2k, \\ 12k^2 + 8k & if n = 2k + 1. \end{cases}$$

(ii)

$$Mo_e(T_n) = \begin{cases} 18k^2 - 6k & if n = 2k, \\ 18k^2 + 12k & if n = 2k + 1. \end{cases}$$

Proof (i) We consider the following cases:

Case 1. Suppose that n is even, and $n = 2k$ for some $k \in \mathbb{N}$. Consider the T_{2k} as shown in Fig. 7. One can easily check that whatever happens to computation of Mostar index related to the edge $u_i v_i$ in the (i)th triangle in T_{2k}, is the same as computation of Mostar index related to the edge $u_{2k-i+1}v_{2k-i+1}$ in the $(2k - i + 1)$th triangle. The same goes for $w_i v_i$ and $w_{2k-i+1}v_{2k-i+1}$, and also for $w_i u_i$ and $w_{2k-i+1}u_{2k-i+1}$. So for computing Mostar index, it suffices to compute the $|n_u(uv, T_{2k}) - n_v(uv, T_{2k})|$ for every $uv \in E(T_{2k})$ in the first k triangles and then multiple that by 2. So from now, we only consider the first k triangles.
Consider the blue edge $u_i v_i$ in the (i)th triangle. There are $2(i-1)$ vertices which are closer to v_i than u_i, but there are no vertices closer to u_i than v_i. So, $|n_{u_i}(u_i v_i, T_{2k}) - n_{v_i}(u_i v_i, T_{2k})| = 2(i - 1)$.
Now consider the green edge $u_i w_i$ in the (i)th triangle. There are $2(2k - i)$ vertices which are closer to w_i than u_i, but there are no vertices closer to u_i than w_i. So, $|n_{u_i}(u_i w_i, T_{2k}) - n_{w_i}(u_i w_i, T_{2k})| = 2(2k - i)$.
Finally, consider the red edge $v_i w_i$ in the (i)th triangle. There are $2(2k - i)$ vertices which are closer to w_i than v_i, and there are $2(i - 1)$ vertices closer to v_i than w_i. So, $|n_{v_i}(v_i w_i, T_{2k}) - n_{w_i}(v_i w_i, T_{2k})| = 2(2k - 2i + 1)$.
Since we have k edges like blue one, k edges like green one and k edges like red one, then by our argument, we have

$$\begin{aligned} Mo(T_{2k}) &= 2\left(\sum_{i=1}^{k} 2(i-1) + \sum_{i=1}^{k} 2(2k-i) + \sum_{i=1}^{k} 2(2k-2i+1)\right) \\ &= 12k^2 - 4k. \end{aligned}$$

Case 2. Suppose that n is odd and $n = 2k + 1$ for some $k \in \mathbb{N}$. Now consider the T_{2k+1} as shown in Fig. 8. One can easily check that whatever happens to computation of Mostar index related to the edge $u_i v_i$ in the (i)th triangle in T_{2k+1}, is the same

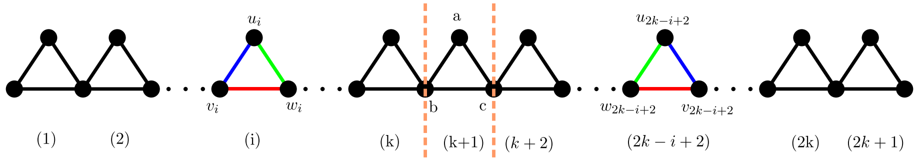


Fig. 8 Chain triangular cactus T_{2k+1}

as computation of Mostar index related to the edge $u_{2k-i+2}v_{2k-i+2}$ in the $(2k-i+2)$th triangle. The same goes for w_iv_i and $w_{2k-i+2}v_{2k-i+2}$, and also for w_iu_i and $w_{2k-i+2}u_{2k-i+2}$. So for computing Mostar index, it suffices to compute the $|n_u(uv, T_{2k+1}) - n_v(uv, T_{2k+1})|$ for every $uv \in E(T_{2k+1})$ in the first k triangles and then multiple that by 2 and add it to $\sum_{uv\in A} |n_u(uv, T_{2k+1}) - n_v(uv, T_{2k+1})|$, where $A = \{ab, bc, ac\}$. So from now, we only consider the first k triangles and the middle one.

Consider the blue edge u_iv_i in the (i)th triangle. There are $2(i-1)$ vertices which are closer to v_i than u_i, but there are no vertices closer to u_i than v_i. So, $|n_{u_i}(u_iv_i, T_{2k+1}) - n_{v_i}(u_iv_i, T_{2k+1})| = 2(i-1)$.

Now consider the green edge u_iw_i in the (i)th triangle. There are $4k-2i+2$ vertices which are closer to w_i than u_i, but there are no vertices closer to u_i than w_i. So, $|n_{u_i}(u_iw_i, T_{2k+1}) - n_{w_i}(u_iw_i, T_{2k+1})| = 2(2k-i+1)$.

Now consider the red edge v_iw_i in the (i)th triangle. There are $2(2k-i+1)$ vertices which are closer to w_i than v_i, and there are $2(i-1)$ vertices closer to v_i than w_i. So, $|n_{v_i}(v_iw_i, T_{2k+1}) - n_{w_i}(v_iw_i, T_{2k+1})| = 4(k-i+1)$.

Finally, consider the middle triangle. For the edge ab, there are $2k$ vertices which are closer to b than a, but there are no vertices closer to a than b. Also for the edge ac, there are $2k$ vertices which are closer to c than a, but there are no vertices closer to a than c and for the edge bc, there are $2k$ vertices which are closer to b than c, and there are $2k$ vertices closer to c than b. Hence, $\sum_{uv\in A} |n_u(uv, T_{2k+1}) - n_v(uv, T_{2k+1})| = 4k$, where $A = \{ab, bc, ac\}$.

Since we have k edges like blue one, k edges like green one and k edges like red one, then by our argument, we have

$$\begin{aligned} Mo(T_{2k+1}) &= 2\left(\sum_{i=1}^{k} 2(i-1) + \sum_{i=1}^{k} 2(2k-i+1) + \sum_{i=1}^{k} 4(k-i+1)\right) + 4k \\ &= 12k^2 + 8k. \end{aligned}$$

Therefore, we have the result.

(ii) The proof is similar to proof of Part (i). □

Theorem 3.2 *Let Q_n be the para-chain square cactus graph of order n. Then for every $n \geq 1$, and $k \geq 1$, we have*

(i)

$$Mo(Q_n) = \begin{cases} 24k^2 & if n = 2k, \\ 24k^2 + 24k & if\, n = 2k+1, \end{cases}$$

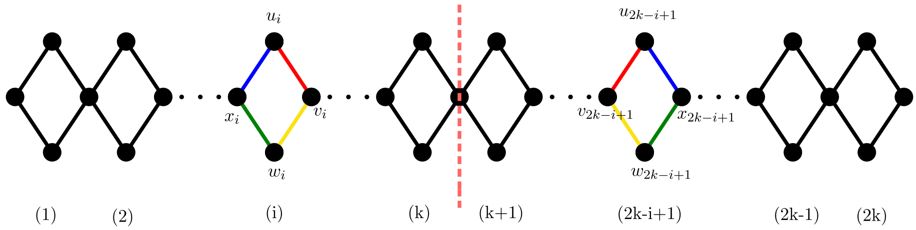


Fig. 9 Para-chain square cactus Q_{2k}

(ii)

$$Mo_e(Q_n) = \begin{cases} 32k^2 & if\, n = 2k, \\ 32k^2 + 32k & if\, n = 2k+1, \end{cases}$$

Proof (i) We consider the following cases:

Case 1. Suppose that n is even and $n = 2k$ for some $k \in \mathbb{N}$. Now consider the Q_{2k} as shown in Fig. 9. One can easily check that whatever happens to computation of Mostar index related to the edge $u_i v_i$ in the (i)th rhombus in Q_{2k}, is the same as computation of Mostar index related to the edge $u_{2k-i+1}v_{2k-i+1}$ in the $(2k-i+1)$th rhombus. The same goes for $w_i v_i$ and $w_{2k-i+1}v_{2k-i+1}$, for $w_i x_i$ and $w_{2k-i+1}x_{2k-i+1}$, and also for $x_i u_i$ and $x_{2k-i+1}u_{2k-i+1}$. So for computing Mostar index, it suffices to compute the $|n_u(uv, Q_{2k}) - n_v(uv, Q_{2k})|$ for every $uv \in E(Q_{2k})$ in the first k rhombus and then multiple that by 2. So from now, we only consider the first k rhombus.
Consider the red edge $u_i v_i$ in the (i)th rhombus. There are $3k + 3(k-i) + 1$ vertices which are closer to v_i than u_i, and there are $3i - 2$ vertices closer to u_i than v_i. So, $|n_{u_i}(u_i v_i, Q_{2k}) - n_{v_i}(u_i v_i, Q_{2k})| = 6k - 6i + 3$.
One can easily check that the edges $w_i v_i$, $w_i x_i$ and $x_i u_i$ have the same attitude as $u_i v_i$. Since we have k edges like blue one, k edges like green one, k edges like yellow one and k edges like red one, then by our argument, we have

$$Mo(Q_{2k}) = 2\left(4\sum_{i=1}^{k} 3(2k - 2i + 1)\right) = 24k^2.$$

Case 2. Suppose that n is odd and $n = 2k+1$ for some $k \in \mathbb{N}$. Now consider the Q_{2k+1} as shown in Figure 10. One can easily check that whatever happens to computation of Mostar index related to the edge $u_i v_i$ in the (i)th rhombus in Q_{2k+1}, is the same as computation of Mostar index related to the edge $u_{2k-i+2}v_{2k-i+2}$ in the $(2k-i+2)$th rhombus. The same goes for $w_i v_i$ and $w_{2k-i+2}v_{2k-i+2}$, for $w_i x_i$ and $w_{2k-i+2}x_{2k-i+2}$, and also for $x_i u_i$ and $x_{2k-i+2}u_{2k-i+2}$. So for computing Mostar index, it suffices to compute the $|n_u(uv, Q_{2k+1}) - n_v(uv, Q_{2k+1})|$ for every $uv \in E(Q_{2k+1})$ in the first k rhombus and then multiple that by 2 and add it to $\sum_{uv\in A} |n_u(uv, Q_{2k+1}) - n_v(uv, Q_{2k+1})|$, where $A = \{ab, bc, cd, da\}$. So from now, we only consider the first $k+1$ rhombus.
Consider the red edge $u_i v_i$ in the (i)th rhombus. There are $3(k+1) + 3(k-i) + 1$ vertices which are closer to v_i than u_i, and there are $3i - 2$ vertices closer to u_i than v_i. So, $|n_{u_i}(u_i v_i, Q_{2k+1}) - n_{v_i}(u_i v_i, Q_{2k+1})| = 6k - 6i + 6$.

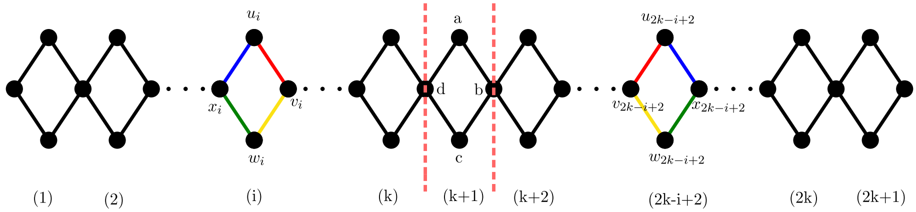


Fig. 10 Para-chain square cactus Q_{2k+1}

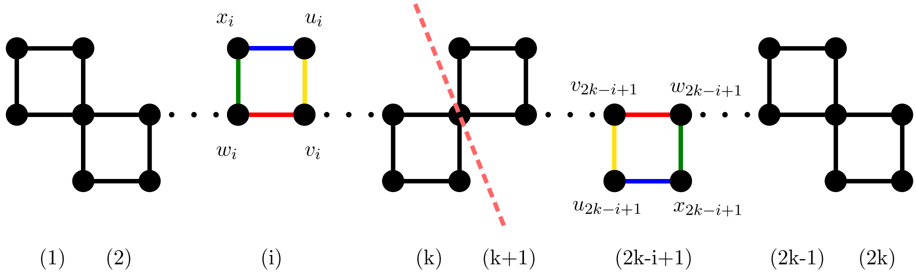


Fig. 11 Para-chain square cactus O_{2k}

One can easily check that the edges w_iv_i, w_ix_i and x_iu_i have the same attitude as u_iv_i.

Now consider the middle rhombus. For the edge ab, there are $3k+1$ vertices which are closer to b than a, and there are $3k+1$ vertices closer to a than b. the edges bc, cd and da have the same attitude as ab. Hence, $\sum_{uv\in A} |n_u(uv, Q_{2k+1}) - n_v(uv, Q_{2k+1})| = 0$, where $A = \{ab, bc, cd, da\}$.

Since we have k edges like blue one, k edges like green one, k edges like yellow one and k edges like red one, then by our argument, we have

$$Mo(Q_{2k+1}) = 2\left(4\sum_{i=1}^{k} 6(k-i+1)\right) = 24k^2 + 24k.$$

Therefore, we have the result.

(ii) The proof is similar to the proof of Part (i). □

Theorem 3.3 *Let O_n be the para-chain square cactus graph of order n. Then for every $n \geq 1$, and $k \geq 1$, we have*

(i)

$$Mo(O_n) = \begin{cases} 36k^2 - 12k & if n = 2k, \\ 36k^2 + 24k & if n = 2k+1. \end{cases}$$

(ii)

$$Mo_e(O_n) = \begin{cases} 48k^2 - 16k & if n = 2k, \\ 48k^2 + 32k & if n = 2k+1. \end{cases}$$

Proof (i) We consider the following cases:

Case 1. Suppose that n is even and $n = 2k$ for some $k \in \mathbb{N}$. Now consider the O_{2k} as shown in Figure 11. One can easily check that whatever happens to computation of Mostar index related to the edge $u_i v_i$ in the (i)th square in O_{2k}, is the same as computation of Mostar index related to the edge $u_{2k-i+1}v_{2k-i+1}$ in the $(2k-i+1)$th square. The same goes for $w_i v_i$ and $w_{2k-i+1}v_{2k-i+1}$, for $w_i x_i$ and $w_{2k-i+1}x_{2k-i+1}$, and also for $x_i u_i$ and $x_{2k-i+1}u_{2k-i+1}$. So for computing Mostar index, it suffices to compute the $|n_u(uv, O_{2k}) - n_v(uv, O_{2k})|$ for every $uv \in E(O_{2k})$ in the first k squares and then multiple that by 2. So from now, we only consider the first k squares.

Consider the yellow edge $u_i v_i$ in the (i)th square. There are $3(2k) - 2$ vertices which are closer to v_i than u_i, and there is only 1 vertex closer to u_i than v_i which is x_i. So, $|n_{u_i}(u_i v_i, O_{2k}) - n_{v_i}(u_i v_i, O_{2k})| = 6k - 3$. By the same argument, the same happens to the edge $x_i w_i$.

Now consider the blue edge $u_i x_i$ in the (i)th square. There are $3i - 2$ vertices which are closer to x_i than u_i, and there are $3k + 3(k - i) + 1$ vertices closer to u_i than x_i. So, $|n_{u_i}(u_i x_i, O_{2k}) - n_{x_i}(u_i x_i, O_{2k})| = 6k - 6i + 3$. By the same argument, the same happens to the edge $v_i w_i$.

Since we have k edges like blue one, k edges like green one, k edges like yellow one and k edges like red one, then by our argument, we have

$$Mo(O_{2k}) = 2\left(2\sum_{i=1}^{k} 3(2k - 2i + 1) + 2\sum_{i=1}^{k} 3(2k - 1)\right) = 36k^2 - 12k.$$

Case 2. Suppose that n is odd and $n = 2k + 1$ for some $k \in \mathbb{N}$. Now consider the O_{2k+1} as shown in Figure 12. One can easily check that whatever happens to computation of Mostar index related to the edge $u_i v_i$ in the (i)th square in O_{2k+1}, is the same as computation of Mostar index related to the edge $u_{2k-i+2}v_{2k-i+2}$ in the $(2k-i+2)$th square. The same goes for $w_i v_i$ and $w_{2k-i+2}v_{2k-i+2}$, for $w_i x_i$ and $w_{2k-i+2}x_{2k-i+2}$, and also for $x_i u_i$ and $x_{2k-i+2}u_{2k-i+2}$. So for computing Mostar index, it suffices to compute the $|n_u(uv, O_{2k+1}) - n_v(uv, O_{2k+1})|$ for every $uv \in E(O_{2k+1})$ in the first k squares and then multiple that by 2 and add it to $\sum_{uv \in A} |n_u(uv, O_{2k+1}) - n_v(uv, O_{2k+1})|$, where $A = \{ab, bc, cd, da\}$. So from now, we only consider the first $k + 1$ squares.

Consider the yellow edge $u_i v_i$ in the (i)th square. There are $3(2k + 1) - 2$ vertices which are closer to v_i than u_i, and there is only 1 vertex closer to u_i than v_i which is x_i. So, $|n_{u_i}(u_i v_i, O_{2k}) - n_{v_i}(u_i v_i, O_{2k})| = 6k$. By the same argument, the same happens to the edge $x_i w_i$.

Now consider the blue edge $u_i x_i$ in the (i)th square. There are $3i - 2$ vertices which are closer to x_i than u_i, and there are $3(k + 1) + 3(k - i) + 1$ vertices closer to u_i than x_i. So, $|n_{u_i}(u_i x_i, O_{2k}) - n_{x_i}(u_i x_i, O_{2k})| = 6k - 6i + 6$. By the same argument, the same happens to the edge $v_i w_i$.

Now consider the middle square. For the edge ab, there are $3k + 1$ vertices which are closer to b than a, and there are $3k + 1$ vertices closer to a than b. the edge cd has the same attitude as ab. But for the edge ad, there are $3(2k + 1) - 2$ vertices which are closer to d than a, and there is only 1 vertex closer to a than d which is b, and the edge bc has the same attitude as ad. Hence, $\sum_{uv \in A} |n_u(uv, O_{2k+1}) - n_v(uv, O_{2k+1})| = 12k$, where $A = \{ab, bc, cd, da\}$.

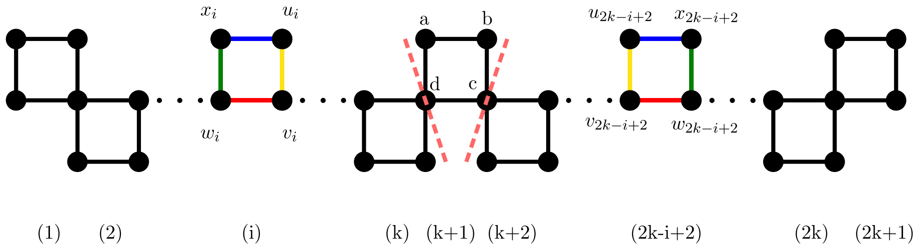
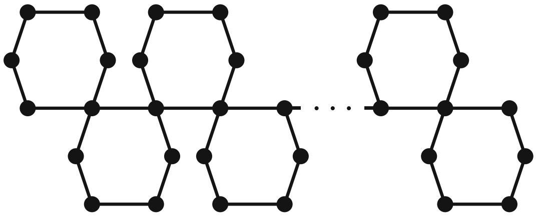


Fig. 12 Para-chain square cactus O_{2k+1}

Fig. 13 Ortho-chain graph O_n^h



Since we have k edges like blue one, k edges like green one, k edges like yellow one and k edges like red one, then by our argument, we have

$$Mo(O_{2k+1}) = 2\left(2\sum_{i=1}^{k} 6(k-i+1) + 2\sum_{i=1}^{k} 6k\right) + 12k = 36k^2 + 24k.$$

Therefore, we have the result.

(ii) The proof is similar to the proof of Part (i). □

By the same argument as the proof of Theorem 3.3, we have

Theorem 3.4 *Let O_n^h be the ortho-chain graph of order n (See Fig. 13). Then for every $n \geq 1$, and $k \geq 1$, we have*

(i)

$$Mo(O_n^h) = \begin{cases} 100k^2 - 40k & \text{if } n = 2k, \\ 100k^2 + 60k & \text{if } n = 2k+1. \end{cases}$$

(ii)

$$Mo_e(O_n^h) = \begin{cases} 72k^2 & \text{if } n = 2k, \\ 72k^2 + 72k & \text{if } n = 2k+1. \end{cases}$$

By the same argument as the proof of Theorem 3.2, we have

Theorem 3.5 *Let L_n be the para-chain hexagonal graph of order n (See Fig. 14). Then for every $n \geq 1$, and $k \geq 1$, we have*

(i)

$$Mo(L_n) = \begin{cases} 60k^2 & \text{if } n = 2k, \\ 60k^2 + 60k & \text{if } n = 2k+1. \end{cases}$$

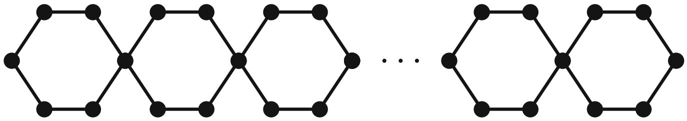
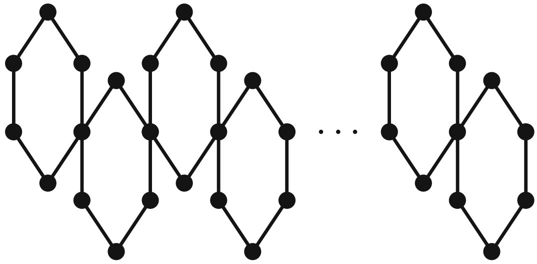


Fig. 14 Para-chain hexagonal graph L_n

Fig. 15 Meta-chain hexagonal graph M_n



(ii)

$$Mo_e(L_n) = \begin{cases} 72k^2 & \text{if } n = 2k, \\ 72k^2 + 72k & \text{if } n = 2k + 1. \end{cases}$$

By the same argument as the proof of Theorem 3.3, we have

Theorem 3.6 *Let M_n be the meta-chain hexagonal of order n (See Fig. 15). Then for every $n \geq 1$, and $k \geq 1$, we have*

(i)

$$Mo(M_n) = \begin{cases} 80k^2 - 20k & \text{if } n = 2k, \\ 80k^2 + 60k & \text{if } n = 2k + 1. \end{cases}$$

(ii)

$$Mo_e(M_n) = \begin{cases} 72k^2 & \text{if } n = 2k, \\ 72k^2 + 72k & \text{if } n = 2k + 1. \end{cases}$$

We intend to derive the Mostar index and edge Mostar index of the triangulane T_k defined pictorially in Khalifeh et al. (2008). We define T_k recursively in a manner that will be useful in our approach. First, we define recursively an auxiliary family of triangulanes G_k ($k \geq 1$). Let G_1 be a triangle and denote one of its vertices by y_1. We define G_k ($k \geq 2$) as the circuit of the graphs G_{k-1}, G_{k-1}, and K_1 and denote by y_k the vertex where K_1 has been placed The graphs G_1, G_2 and G_3 are shown in Fig. 16.

Theorem 3.7 *For the graph T_n (see T_3 in Fig. 17), we have*

$$Mo(T_n) = 6(2^{n+2} - 2^n) + \sum_{i=2}^{n} 3(2^i) \left((2^{n+2} + \sum_{t=0}^{i-2} 2^{n-t}) - 2^{n-i+1} \right).$$

Proof Consider the graph T_n in Fig. 18. First we consider the edge x_0x_1. There are $2(2^{n+1} - 1)$ vertices which are closer to x_o than x_1, and there are $2^n - 2$ vertices closer to x_1 than x_o. So, $|n_{x_o}(x_0x_1, T_n) - n_{x_1}(x_0x_1, T_n)| = 2^{n+2} - 2^n$. The edge ax_0 has the same attitude as the blue

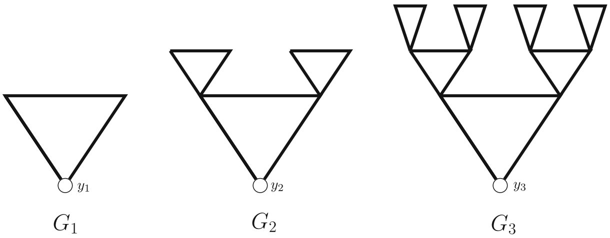
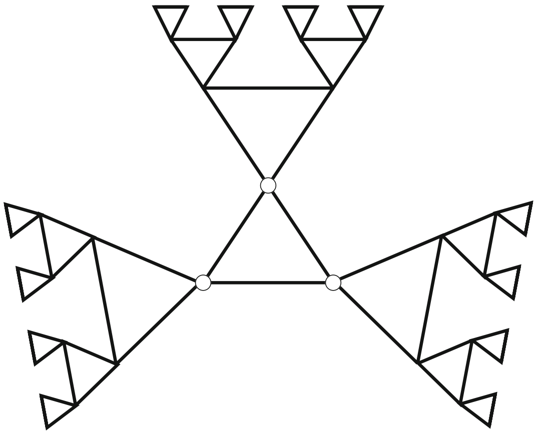


Fig. 16 Graphs G_1, G_2 and G_3

Fig. 17 Graph T_3



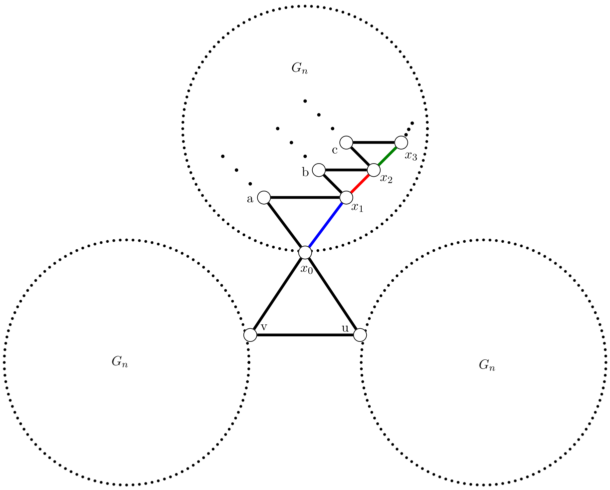


Fig. 18 Graph T_n

edge x_0x_1. In total there are 6 edges with this value related to Mostar index. The number of vertices closer to vertex a is the same as the number of vertices closer to vertex x_1, and in total, we have 3 edges like this one.

Now consider the edge x_1x_2. There are $2(2^{n+1}-1)+2^n$ vertices which are closer to x_1 than x_2, and there are $2^{n-1}-2$ vertices closer to x_2 than x_1. So, $|n_{x_o}(x_0x_1, T_n) - n_{x_1}(x_0x_1, T_n)| =$

$2^{n+2} + 2^{n+1} - 2^{n-1}$. The edge bx_1 has the same attitude as the red edge x_1x_2. In total there are 12 edges with this value related to Mostar index. The number of vertices closer to vertex b is the same as the number of vertices closer to vertex x_2, and in total, we have 6 edges like this one.

By continuing this process in the ith level, we have

$$|n_{x_{i-1}}(x_{i-1}x_i, T_n) - n_{x_i}(x_{i-1}x_i, T_n)| = (2^{n+2} + \sum_{t=0}^{i-2} 2^{n-t}) - 2^{n-i+1}.$$

We have $3(2^i)$ edges like this one. The number of vertices closer to vertex x_i is the same as the number of vertices closer to its neighbour in horizontal edge with one endpoint x_i, and in total, we have $3(2^{i-1})$ edges like this one.

Finally, the number of vertices closer to vertex x_0 is the same as the number of vertices closer to vertex u, the number of vertices closer to vertex x_0 is the same as the number of vertices closer to vertex v, and the number of vertices closer to vertex v is the same as the number of vertices closer to vertex u.

So by the definition of the Mostar index and our argument, we have

$$Mo(T_n) = 6(2^{n+2} - 2^n) + \sum_{i=2}^{n} 3(2^i)\left((2^{n+2} + \sum_{t=0}^{i-2} 2^{n-t}) - 2^{n-i+1}\right),$$

and, therefore, we have the result. □

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References

Akhter SH, Iqbal Z, Aslam A, Gao W (2021) Computation of Mostar index for some graph operations. Int J Quant Chem. https://doi.org/10.1002/qua.26674

Alikhani S, Ghanbari N (2021) Sombor index of polymers. MATCH Commun Math Comput Chem 86(3):715–728

Arockiaraj M, Clement J, Tratnik N (2019) Mostar indices of carbon nanostructures and circumscribed donut benzenoid systems. Int J Quant Chem 119:26043

Doslić T, Martinjak I, Škrekovski R, Tipurić Spužević S, Zubac I (2018) Mostar index. J Math Chem 56:2995–3013

Emeric D, Klavžar S (2013) Computing Hosoya polynomials of graphs from primary subgraphs. MATCH Commun Math Comput Chem 70:627–644

Harary F, Uhlenbeck B (1953) On the number of Husimi trees, I. Proc Nat Acad Sci 39:315–322

Hayata F, Zhou B (2019) On cacti with large Mostar index. Filomat 33(15):4865–4873

Khalifeh MH, Yousefi-Azari H, Ashrafi AR (2008) Computing Wiener and Kirchhoff indices of a triangulane. Indian J Chem 47A:1503–1507

Liu H, Song L, Xiao Q, Tang Z (2020) On edge Mostar index of graphs. Iranian J Math Chem 11(2):95–106
Sadeghieh A, Ghanbari N, Alikhani S (2018) Computation of Gutman index of some cactus chains. Elect J Graph Theory Appl 6(1):138–151
Tepeh A (2019) Extremal bicyclic graphs with respect to Mostar index. Appl Math Comput 355:319–324
Wiener H (1947) Structural determination of the Paraffin Boiling Points. J Am Chem Soc 69:17–20