Mostar index and edge Mostar index of polymers

Nima Ghanbari  Saeid Alikhani *

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Department of Informatics, University of Bergen, P.O. Box 7803, 5020 Bergen, Norway
Department of Mathematics, Yazd University, 89195-741, Yazd, Iran
Nima.ghanbari@uib.no, alikhani@yazd.ac.ir

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 $Mo_e(G) = \sum_{e=uv \in E(G)} |m_u(e|G) - m_v(e|G)|$, 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.

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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 summation runs over all pairs of vertices of $G$ [12]. The topological indices and graph invariants based on distances between vertices of a graph

*Corresponding author
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 \[12\]. In a recent paper, Došlić et al. \[4\] introduced a newbond-additive structural invariant as a quantitative refinement of the distance non-balancedness 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. S. 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 \[11\]. 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 in \[7\] 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 \[3, 9\] and is defined as \(Me(G) = \sum_{e=uv \in E(G)} |m_u(e|G) - m_v(e|G)|\), 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, in \[9\] determined the extremal values of edge Mostar index of some graphs such as trees and unicyclic graphs.

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 Section 2, the Mostar index of some graphs are computed from their monomer units. In Section 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 Figure 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 \[2, 5\]).

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 Figure 2.

**Theorem 2.2** For the graph $Q(m, n)$ (see Figure 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 $u_i u_j$ 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 $|n_{u_i}(u_i u_j, Q(m, n)) - n_{u_j}(u_j u_i, Q(m, n))| = 0$. Now consider the edge $vw$ in the $i$-th $K_n$. There is no vertex which is 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 $u_i v$ in the $i$-th $K_n$. 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 $|n_{u_i}(u_i v, Q(m, n)) - n_v(u_i v, Q(m, n))| = n(m-1)$. Since there are $m(n-1)$ edges like $u_i v$ in $Q(m, n)$, therefore we have the result.

(ii) First consider the edge $u_i u_j$ 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 $|m_{u_i}(u_i u_j, Q(m, n)) - m_{u_j}(u_j u_i, Q(m, n))| = 0$. Now consider the edge $vw$ in the $i$-th $K_n$. There is no edges which are closer to $v$ than $w$, and visa versa. So $|m_v(vw, Q(m, n)) -
Proof. Theorem 2.3 on the link of graphs. For the Mostar index and edge Mostar index of them. The following theorem is about 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 Mosoar 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 Figure 3). Then,

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

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

**Proof.**

(i) Consider the graph $G_i$ (Figure 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:

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

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

Figure 2: The graph $Q(m, n)$ and $Q(5, 4)$, respectively.
\[+ \sum_{i=1}^{n-1} \sum_{y_i, y_{i+1} \in E(G)} |n_{y_i}(y_i, y_{i+1}, G) - n_{y_{i+1}}(y_i, y_{i+1}, G)|
\]

\[= \sum_{i=1}^{n} \sum_{uv \in E(G_i), d(u, v), d(u, y_i), d(v, y_i), <d(v, y_i) - \sum_{i=1}^{n} \sum_{y_i, y_{i+1} \in E(G)} |n_{y_i}(y_i, y_{i+1}, G) - n_{y_{i+1}}(y_i, y_{i+1}, G)|
\]

\[\leq \sum_{i=1}^{n} \sum_{uv \in E(G_i), d(u, v), d(u, y_i), d(v, y_i), <d(v, y_i) - \sum_{i=1}^{n} \sum_{y_i, y_{i+1} \in E(G)} |n_{y_i}(y_i, y_{i+1}, G) - n_{y_{i+1}}(y_i, y_{i+1}, G)|
\]
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 $C(G_1, \ldots, G_n)$ be the chain of graphs $\{G_i\}_{i=1}^n$ with $x_i \rightarrow y_i$ in $G_i$. Then

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

Therefore, we have the result.

(ii) The proof is similar to Part (i). \qed

By the same argument similar to the proof of the 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 $C(G_1, \ldots, G_n)$ be the chain of graphs $\{G_i\}_{i=1}^n$ with

Figure 3: Link of $n$ graphs $G_1, G_2, \ldots, G_n$
Figure 4: Chain of $n$ graphs $G_1, G_2, \ldots, G_n$

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

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 $i = 1, 2, \ldots, n - 1$ (Figure 4). Then,

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

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

With similar argument to the proof of the 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 $B(G_1, \ldots, G_n)$ 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 Figure 5). Then,

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

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

**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 \( i \)-th vertex of the cycle graph \( C_n \) (Figure 6). Then,

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

**Proof.** First consider the edge \( x_1 x_n \). 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

\[
|n_{x_1}(x_1 x_n, G) - n_{x_n}(x_1 x_n, G)| = \left| \sum_{i=1}^{t} |V(G_i)| - \sum_{i=1}^{t} |V(G_{t+i})| \right| \\
\leq \sum_{i=1}^{t} |V(G_i)| - |V(G_{t+i})|.
\]

It is easy to check that the same happens for \( x_i x_{i+1} \) for all \( 1 \leq i \leq n - 1 \).

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

\[
|n_{x_1}(x_1 x_n, G) - n_{x_n}(x_1 x_n, G)| = \left| \sum_{i=1}^{t-1} |V(G_i)| - \sum_{i=1}^{t-1} |V(G_{t+i})| \right| \\
\leq |V(G_1)| + |V(G_2)| + \ldots + |V(G_{t-1})| \\
+ |V(G_{t+1})| + |V(G_{t+2})| + \ldots + |V(G_n)| \\
= |V(G)| - |V(G_t)|.
\]

It is easy to check that \( |n_{x_1}(x_1 x_2, G) - n_{x_2}(x_1 x_2, G)| \leq |V(G)| - |V(G_{t+1})| \), 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:

\[
Mo(G) = \sum_{uv \in E(G)} |n_u(uv, G) - n_v(uv, G)| \\
= \sum_{i=1}^{n} \sum_{uv \in E(G_i)} |n_u(uv, G_i) - n_v(uv, G_i)|
\]
\[
+ \sum_{i=1}^{n-1} \sum_{x_i, x_{i+1} \in E(G)} \left| n_{x_i}(x_i x_{i+1}, G) - n_{x_{i+1}}(x_i x_{i+1}, G) \right| \\
+ \left| n_{x_1}(x_1 x_n, G) - n_{x_n}(x_1 x_n, G) \right| \\
= \sum_{i=1}^{n} \sum_{u \in E(G_i), d(u, x_i) < d(v, x_i)} \left| n_u(\ uv, G_i) - n_v(\ uv, G_i) \right| \\
+ \sum_{i=1}^{n} \sum_{u \in E(G_i), d(u, x_i) = d(v, x_i)} \left| n_u(\ uv, G_i) - n_v(\ uv, G_i) \right| \\
+ \sum_{i=1}^{n-1} \sum_{x_i, x_{i+1} \in E(G)} \left| n_{x_i}(x_i x_{i+1}, G) - n_{x_{i+1}}(x_i x_{i+1}, G) \right| \\
+ \left| n_{x_1}(x_1 x_n, G) - n_{x_n}(x_1 x_n, G) \right| \\
\leq \sum_{i=1}^{n} \sum_{u \in E(G_i), d(u, x_i) < d(v, x_i)} \left| n'_u(\ uv, G_i) - n'_v(\ uv, G_i) \right| \\
+ \sum_{i=1}^{n} \sum_{u \in E(G_i), d(u, x_i) < d(v, x_i)} |V(G) - V(G_i)| \\
+ \sum_{i=1}^{n} \sum_{u \in E(G_i), d(u, x_i) = d(v, x_i)} \left| n'_u(\ uv, G_i) - n'_v(\ uv, G_i) \right| \\
+ \sum_{i=1}^{n} \sum_{u \in E(G_i), d(u, x_i) = d(v, x_i)} |V(G) - V(G_i)| \\
+ \begin{cases} 
  n \sum_{i=1}^{t} |V(G_i)| - |V(G_{i+t})| & \text{if } n = 2t, \\
  (n-1)|V(G)| & \text{if } n = 2t-1,
\end{cases}
\]
\[= \sum_{i=1}^{n} Mo(G_i) + \sum_{i=1}^{n} |E(G_i)||(|V(G)| - |V(G_i)|)\]

\[+ \left\{ \begin{array}{ll}
n \sum_{i=1}^{t} |V(G_i)| - |V(G_{t+i})| & \text{if } n = 2t, \\
(n-1)|V(G)| & \text{if } n = 2t - 1. \end{array} \right.\]

Therefore, we have the result. \(\square\)

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 \(i\)-th vertex of the cycle graph \(C_n\) (Figure 6). Then,

\[Mo_e(G) \leq \sum_{i=1}^{n} Mo_e(G_i) + \sum_{i=1}^{n} |E(G_i)||(|E(G)| - |E(G_i)|)\]

\[+ \left\{ \begin{array}{ll}
n \sum_{i=1}^{t} |E(G_i)| - |E(G_{t+i})| & \text{if } n = 2t, \\
(n-1)|E(G)| & \text{if } n = 2t - 1. \end{array} \right.\]

### 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) $MO(G) > MO(G_1) + MO(G_2) + |V(G_1)| - |V(G_2)|$.

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

Proof.

(i) Let $n'_u(\cdot, G_i)$ 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:

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

$= \sum_{uv \in E(G_1)} |n_u(\cdot, G) - n_v(\cdot, G)|$

$+ \sum_{uv \in E(G_2)} |n_u(\cdot, G) - n_v(\cdot, G)|$

$+ |n_x(x, G) - n_y(x, G)|$

$= \sum_{uv \in E(G_1), d(u, x) < d(v, x)} |n_u(\cdot, G) - n_v(\cdot, G)|$

$+ \sum_{uv \in E(G_1), d(u, x) = d(v, x)} |n_u(\cdot, G) - n_v(\cdot, G)|$

$+ \sum_{uv \in E(G_2), d(u, x) < d(v, x)} |n_u(\cdot, G) - n_v(\cdot, G)|$

$+ \sum_{uv \in E(G_2), d(u, x) = d(v, x)} |n_u(\cdot, G) - n_v(\cdot, G)|$

$+ |n_x(x, G) - n_y(x, G)|$

$= \sum_{uv \in E(G_1), d(u, x) < d(v, x)} |n'_u(\cdot, G_1) + |V(G_2)| - n'_v(\cdot, G - 1)|$

$+ \sum_{uv \in E(G_1), d(u, x) = d(v, x)} |n'_u(\cdot, G_1) - n'_v(\cdot, G_1)|$

$+ \sum_{uv \in E(G_2), d(u, x) < d(v, x)} |n'_u(\cdot, G_2) + |V(G_1)| - n'_v(\cdot, G_2)|$

$+ \sum_{uv \in E(G_2), d(u, x) = d(v, x)} |n'_u(\cdot, G_2) - n'_v(\cdot, G_2)|$
\[ + \left| V(G_1) - V(G_2) \right| \]
\[ > \sum_{uv \in E(G_1), d(u, x) < d(v, x)} |n'_{u}(uv, G_1) - n'_{v}(uv, G_1)| \]
\[ + \sum_{uv \in E(G_1), d(u, x) = d(v, x)} |n'_{u}(uv, G_1) - n'_{v}(uv, G_1)| \]
\[ + \sum_{uv \in E(G_2), d(u, x) < d(v, x)} |n'_{u}(uv, G_2) - n'_{v}(uv, G_2)| \]
\[ + \sum_{uv \in E(G_2), d(u, x) = d(v, x)} |n'_{u}(uv, G_2) - n'_{v}(uv, G_2)| \]
\[ + \left| V(G_1) - V(G_2) \right| \]
\[ = MO(G_1) + MO(G_2) + \left| V(G_1) - V(G_2) \right|. \]

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

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 Figure 3). Then,

(i)

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

(ii)

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

### 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.

**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:
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 Figure 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 $u_i u_i$ 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:

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

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

Figure 7: Chain triangular cactus $T_{2k}$
Case 2. Suppose that

\[(\text{ii}) \text{ The proof is similar to proof of Part (i).} \]

\[\square\]

Therefore, we have the result.

Finally, consider the middle triangle. For the edge \(ab\) red one, then by our argument, we have:

\[Mo(T_{2k}) = 2 \left( \sum_{i=1}^{k} 2(i-1) + \sum_{i=1}^{k} 2(2k - i) + \sum_{i=1}^{k} 2(2k - 2i + 1) \right) \]

\[= 12k^2 - 4k.\]

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 Figure [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 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 \(w_i v_i\) and \(w_{2k-i+2} v_{2k-i+2}\), and also for \(w_i u_i\) 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 \(u_i v_i\) 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,

\[|n_u(\{u_i v_i, T_{2k+1}\}) - n_v(\{u_i v_i, T_{2k+1}\})| = 2(i-1).\]

Now consider the green edge \(u_i w_i\) 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,

\[|n_u(\{u_i w_i, T_{2k+1}\}) - n_v(\{u_i w_i, T_{2k+1}\})| = 2(2k - i + 1).\]

Now consider the red edge \(v_i w_i\) 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,

\[|n_v(\{v_i w_i, T_{2k+1}\}) - n_u(\{v_i w_i, T_{2k+1}\})| = 4(k - i + 1).\]

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:

\[Mo(T_{2k+1}) = 2 \left( \sum_{i=1}^{k} 2(i-1) + \sum_{i=1}^{k} 2(2k - i + 1) + \sum_{i=1}^{k} 4(k - i + 1) \right) + 4k\]

\[= 12k^2 + 8k.\]

Therefore, we have the result.

(ii) The proof is similar to proof of Part (i). \(\square\)
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) $$Mo(Q_n) = \begin{cases} 24k^2 & \text{if } n = 2k, \\ 24k^2 + 24k & \text{if } n = 2k + 1, \end{cases}$$

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

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 Figure 9. One can easily check that whatever happens to computation of Mostar index related to the edge $u_iv_i$ 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 $w_iv_i$ and $w_{2k-i+1}v_{2k-i+1}$, for $u_ix_i$ and $u_{2k-i+1}x_{2k-i+1}$, and also for $x_iu_i$ and $x_{2k-i+1}u_{2k-i+1}$. So for computing Mostar index, it suffices to compute the
|\(n(uv, Q_{2k}) - n_v(uv, Q_{2k})|\) 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 \(u_iv_i\) 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, \(|n_{u_i}(u_iv_i, Q_{2k}) - n_v(u_iv_i, Q_{2k})| = 6k - 6i + 3\).

One can easily check that the edges \(w_iv_i\), \(w_ix_i\) and \(x_iu_i\) have the same attitude as \(u_iv_i\). 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.\(^{10}\) One can easily check that whatever happens to computation of Mostar index related to the edge \(u_iv_i\) 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 \(w_iv_i\) and \(w_{2k-i+2}v_{2k-i+2}\), for \(w_ix_i\) and \(w_{2k-i+2}x_{2k-i+2}\), and also for \(x_iu_i\) 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 \(u_iv_i\) 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, \(|n_{u_i}(u_iv_i, Q_{2k+1}) - n_v(u_iv_i, Q_{2k+1})| = 6k - 6i + 6\).

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

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

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 $u_iv_i$ 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 $w_iv_i$ and $w_{2k-i+1}v_{2k-i+1}$, for
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, $|n_{v_i}(u_i v_i, O_{2k}) - n_{u_i}(u_i v_i, O_{2k})| = 6k - 3$. 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:

$$Mo(O_{2k}) = 2 \left( \sum_{i=1}^{k} 3(2k - 2i + 1) + 2 \sum_{i=1}^{k} 3(2k - 1) \right) = 36k^2 - 12k.$$
as \( ad \). Hence, 
\[
\sum_{uv \in A} |n_u(uv, O_{2k+1}) - n_v(uv, O_{2k+1})| = 12k,
\]
where \( A = \{ab, bc, cd, da\} \).

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). \( \square \)

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

**Theorem 3.4** Let \( O^h_n \) be the Ortho-chain graph of order \( n \) (See Figure 13). Then for every \( n \geq 1 \), and \( k \geq 1 \), we have:

(i) 
\[
Mo(O^h_n) = \begin{cases} 
100k^2 - 40k & \text{if } n = 2k, \\
100k^2 + 60k & \text{if } n = 2k + 1.
\end{cases}
\]

(ii) 
\[
Mo_e(O^h_n) = \begin{cases} 
72k^2 & \text{if } n = 2k, \\
72k^2 + 72k & \text{if } n = 2k + 1.
\end{cases}
\]

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

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

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Figure 13: Ortho-chain graph $O^h_n$

Figure 14: Para-chain hexagonal graph $L_n$

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

(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 Figure 15). Then for every $n \geq 1$, and $k \geq 1$, we have:

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

Figure 15: Meta-chain hexagonal graph $M_n$
(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 [8]. 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 Figure 16.

\[ Mo(T_n) = 6(2^{n+2} - 2^n) + \sum_{i=2}^{n} 3(2^i) \left( (2^{n+2} + \sum_{t=0}^{i-2} 2^{n-t}) - 2^{n-i+1} \right). \]
Proof. Consider the graph $T_n$ in Figure 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 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 6 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 $i$-th 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. \(\square\)

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