Research Article

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Expressions for Mostar and weighted Mostar invariants in a chemical structure

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Abstract: The bond-additive topological invariants are largely employed to recognize the characteristics of chemical graphs. They provide quantitative measures of peripheral shapes of molecules and attract considerable attention, both in the context of complex networks and in more classical applications of chemical graph theory. In this article, we compute exact analytical expressions of Mostar and weighted Mostar invariants for a chemical structure.

Keywords: Mostar, weighted Mostar invariants, distance, molecular graph

1 Introduction

Chemical graph theory is a branch of mathematical chemistry in which tools of graph theory are utilized to model chemical occurrence mathematically. Cheminformatics is a brand-new discipline that combines chemistry, mathematics, and information science. It investigates the quantitative structure–property relations (QSPR) and quantitative structure–activity relations (QSAR), both of which are used to predict the bioactivity and physiochemical characteristics of chemical compounds. The assessment and exploration of topological invariants of molecular structures are current research topics with significant implications in nanotechnology and theoretical chemistry (Javaid et al., 2017, Liu et al., 2019).

Let $G = (V, E)$ be a molecular graph with vertex set $V(G)$ and edge set $E(G)$. For an edge xy, we call x and y the end vertices of xy. For a vertex $x \in V(G)$, the open neighborhood of x is the set $N(x) = \{y \in V(G): xy \in E(G)\}$, and the closed neighborhood of x is $N[x] = N(x) \cup \{x\}$. The degree of a vertex $x \in V(G)$, denoted by $\delta(x)$, is $|N(x)|$. The distance between two vertices x and y, denoted $d(x, y)$, is the length of a shortest $x - y$ path in G. For any two edges $e_1 = xy$ and $e_2 = uv$ of G, define $d(x, e_2) = \min\{d(x, u), d(x, v)\}$ and the distance between edges as $D(e_1, e_2) = \min\{d(x, e_2), d(y, e_2)\} = \min\{d(u, e_1), d(v, e_1)\}$.

For an edge $e_1 = xy$, the values $n_x(e_1)$ and $m_x(e_1)$ are defined to be the number of vertices and edges of G, respectively, whose distance to the vertex x is smaller than the distance to the vertex y. Similarly, $n_y(e_1)$ and $m_y(e_1)$ are defined to be the number of vertices and edges of G, respectively, whose distance to the vertex y is smaller than the distance to the vertex x. Furthermore, $t_x(e_1)$ is the number of vertices and edges of G whose distance to the vertex x is smaller than the distance to the vertex y. Similarly, $t_y(e_1)$ is the number of vertices and edges of G whose distance to the vertex y is smaller than the distance to the vertex x. Mathematically:

- $n_x(e_1) = |\{a \in V(G) : d(x, a) < d(y, a)\}|$
- $n_y(e_1) = |\{a \in V(G) : d(y, a) < d(x, a)\}|$
- $m_x(e_1) = |\{e_2 \in E(G) : d(x, e_2) < d(y, e_2)\}|$
- $m_y(e_1) = |\{e_2 \in E(G) : d(y, e_2) < d(x, e_2)\}|$
- $t_x(e_1) = n_x(e_1) + m_x(e_1)$
- $t_y(e_1) = n_y(e_1) + m_y(e_1)$

The bond-additive topological invariants are extensively used to recognize the characteristics of chemical graphs. A notable bond-additive invariant is the Wiener index (Wiener, 1947). Inspired by the miscellaneous productive invariants, such as Zagreb (Gutman and Trinajstić, 1972), irregularity (Albertson, 1997), Szeged (Gutman, 1994), Padmakar-Ivan (Khadikar et al., 2001), and revised-Szeged (Klavžar et al., 2018; Li and Zhang, 2017; Pisanski and Randić, 2010); recently, Došlić et al. (2018) proposed a

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new bond-additive invariant, which they named the Mostar invariant. This index provides information related to the peripherality of individual bonds and then sums up each bond's inputs into a global measure of peripherality of the underline graph. Mostar index is also seem to provide quantitative measures of peripheral shapes of molecules. For any simple connected graph G, the Mostar index is represented as

$$Mo_v(G) = \sum_{e_1=xy\in E(G)} |n_x(e_1) - n_y(e_1)|$$

Deng and Li (2020) determined the Mostar invariant of benzenoid system. For trees and unicyclic graphs, they found the extremal Mostar invariant. Later, the expression for the Mostar invariant of bicyclic graphs was derived in Solé and Valverde (2014). Tratnik (2021) proved that the Mostar invariant of the weighted graph can be deduced in the form of the Mostar invariant of quotient graphs. Arockiaraj et al. (2019) recently presented other versions of the Mostar invariant, dubbed edge Mostar, and total Mostar invariants. These invariants are reported for G as follows:

$$Mo_e(G) = \sum_{e_1=xy\in E(G)} |m_x(e_1) - m_y(e_1)|$$

$$Mo_t(G) = \sum_{e_1=xy\in E(G)} |t_x(e_1) - t_y(e_1)|$$

For an edge $e_1 = xy \in E(G)$, the two types of weight based on the degree of end vertices are as follows:

$$\begin{aligned} w^+(e_1 = xy) &= \delta(x) + \delta(y), \\ w^\star(e_1 = xy) &= \delta(x) \times \delta(y) \end{aligned} \tag{1}$$

Using the edge weights (Eq. 1), the Mostar invariants for G are classified into two types, weighted plus Mostar invariants and weighted product Mostar invariants and defined (Arockiaraj et al., 2020) as follows:

$$w^+Mo_v(G) = \sum_{e_1=xy\in E(G)} w^+(e_1)|n_x(e_1) - n_y(e_1)|$$

$$w^\star Mo_v(G) = \sum_{e_1=xy\in E(G)} w^\star(e_1)|n_x(e_1) - n_y(e_1)|$$

$$w^+Mo_e(G) = \sum_{e_1=xy\in E(G)} w^+(e_1)|\, m_x(e_1) - m_y(e_1)|$$

$$w^\star Mo_e(G) = \sum_{e_1=xy\in E(G)} w^\star(e_1)|\, m_x(e_1) - m_y(e_1)|$$

$$w^+Mo_t(G) = \sum_{e_1=xy\in E(G)} w^+(e_1)|\, t_x(e_1) - t_y(e_1)|$$

$$w^\star Mo_t(G) = \sum_{e_1=xy\in E(G)} w^\star(e_1)|\, t_x(e_1) - t_y(e_1)|$$

2 Computational technique

The cut method in a general form reads as follows (Klavžar, 2008). For a given (molecular) graph G:

1. partition the edge set of G into classes F_1, F_2 ... F_r, call them cuts, such that each of the graphs $G - F_i$, $i = 1, 2 \ldots r$, consists of two (or more) connected components; and
2. use properties (of the components) of the graphs $G - F_i$ to derive a required property of G.

The cut method demonstrated its usefulness, especially for those topological indices that are based on the distances in the molecular graphs; the common name for such indices is distance-based topological indices. The power of the cut method stems from the fact that in a way it enables to obtain distance-based topological indices of families of chemical graphs without actually calculating the distances between pairs of vertices.

A subgraph H of a graph G is convex if, for any two vertices u, v of H, any shortest path in G between u and v lies completely in H, and H is an isometric subgraph of G if $d_H(u, v) = d_G(u, v)$ holds for any two vertices u, v of H. Clearly, a convex subgraph is isometric but not the other way around. The class of graphs that consists of all isometric subgraphs of hypercubes are called partial cubes. A few well-known partial cubes are hypercubes, even cycles, trees, median graphs, benzenoid graphs, phenylenes, and Cartesian products of partial cubes. The edges $e_1 = xy$ and $e_2 = uv$ are in the Djoković–Winkler relation Θ if $d_G(x, u) + d_G(y, v) \neq d_G(x, v) + d_G(y, u)$. The relation Θ is always reflexive, symmetric, and transitive on partial cubes. Therefore, Θ partitions the edge set of a partial cube G into equivalence classes F_1, F_2 ... F_r, called Θ-classes or cuts.

Theorem 1. *Let G be a partial cube and let $F_1, F_2 \ldots F_r$ be its Θ-classes. Let $n_1(F_i)$ and $n_2(F_i)$ be the number of vertices in the two connected components of $G - F_i$. Let $m_1(F_i)$ and $m_2(F_i)$ be the number of edges in the two connected components of $G - F_i$. Let $t_1(F_i) = n_1(F_i) + m_1(F_i)$, $t_2(F_i) = n_2(F_i) + m_2(F_i)$, $w^+(F_i) = \sum_{f\in F_i} w^+(f)$ and $w^\star(F_i) = \sum_{f\in F_i} w^\star(f)$. Then:*

1. $Mo_v(G) = \sum_{i=1}^{r} |F_i||n_1(F_i) - n_2(F_i)|$ (Doslić et al., 2018).
2. $Mo_e(G) = \sum_{i=1}^{r} |F_i||m_1(F_i) - m_2(F_i)|$ (Arockiaraj et al., 2019).
3. $Mo_t(G) = \sum_{i=1}^{r} |F_i||t_1(F_i) - t_2(F_i)|$ (Arockiaraj et al., 2019).
4. $w^+Mo_v(G) = \sum_{i=1}^{r} w^+(F_i)|\, n_1(F_i) - n_2(F_i)|$ (Arockiaraj et al., 2020).
5. $w^\star Mo_v(G) = \sum_{i=1}^{r} w^\star(F_i)|\, n_1(F_i) - n_2(F_i)|$ (Arockiaraj et al., 2020).

6. $w^{+}Mo_e(G) = \sum_{i=1}^{r} w^{+}(F_i)|\, m_1(F_i) - m_2(F_i)|$ (Arockiaraj et al., 2020).
7. $w^{\star}Mo_e(G) = \sum_{i=1}^{r} w^{\star}(F_i)|\, m_1(F_i) - m_2(F_i)|$ (Arockiaraj et al., 2020).
8. $w^{+}Mo_t(G) = \sum_{i=1}^{r} w^{+}(F_i)|\, t_1(F_i) - t_2(F_i)|$ (Arockiaraj et al., 2020).
9. $w^{\star}Mo_t(G) = \sum_{i=1}^{r} w^{\star}(F_i)|\, t_1(F_i) - t_2(F_i)|$ (Arockiaraj et al., 2020).

3 Polyphenylene superhoneycomb networks

Polyphenylenes are macromolecules which comprise benzenoid aromatic nuclei directly joined to one another by C–C bonds. These materials have been known for many years. They attract great interest, particularly as active materials for electronic devices such as light-emitting diodes, photovoltaic cells, and field-effect transistors. The polyphenylene superhoneycomb network, often known as porous graphene, is one of the most important and well-studied two-dimensional materials (Figure 1).

Bieri et al. (2009) reported the observation by scanning tunneling microscopy spectroscopy of a polyphenylene superhoneycomb network, which is a graphene lattice with holes (the authors called porous graphene). The polyphenylene superhoneycomb is obtained starting with a precursor (hexaiodo-substituted macrocycle cyclohexa-*m*-phenylene, named CHP) that is polymerized at the Ag(111) surface by the silver-promoted aryl–aryl coupling of iodobenzene to biphenyl. The polyphenylene network belongs to a class of covalently linked hydrocarbon superhoneycomb networks, which present large potentialities by tuning the electronic properties through the size of the holes.

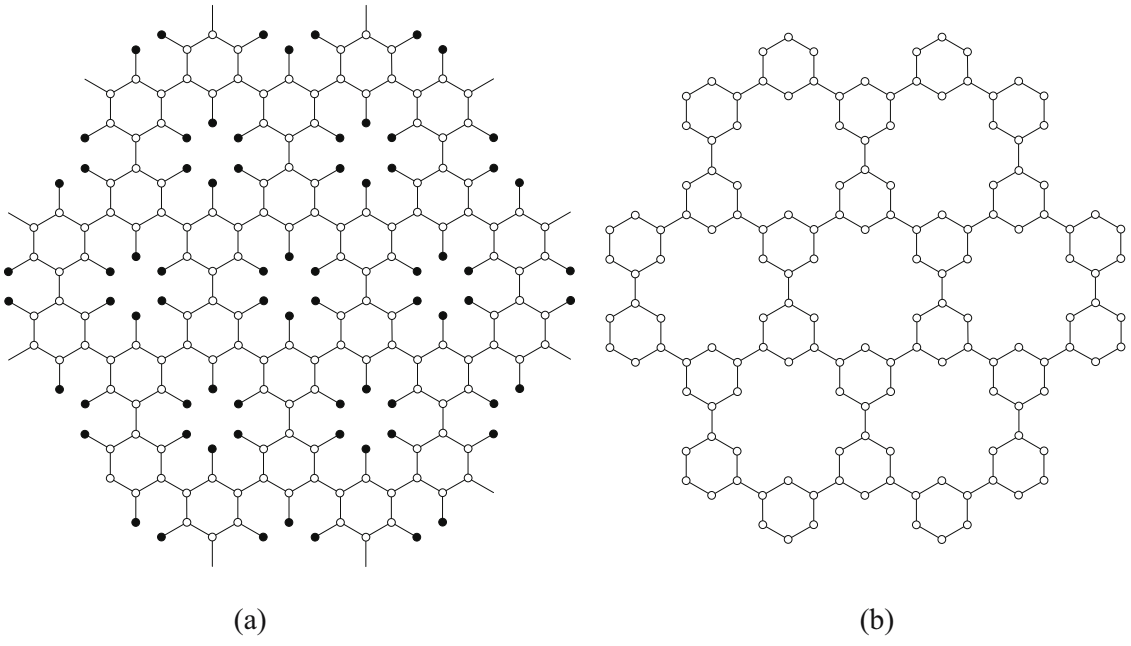
Polyphenylene superhoneycomb network can be constructed in different ways. The construction of a polyphenylene superhoneycomb network from a honeycomb network is described in Krishnan and Rajan (2022).

Theorem 2. (*Krishnan and Rajan, 2022*)

Let G be the polyphenylene superhoneycomb network of dimension n. Then, the number of vertices and edges of G are $36n^2$ *and* $45n^2 - 3n$*, respectively.*

Consider three directions, say X, Y, and Z, all of which are mutually inclined at an angle of 120°. We begin with the X direction and define cuts made up of edges perpendicular to the X direction. The cuts X_i, $-(n-1) \le i \le n-1$ are depicted in Figure 2.

For each X_i, $-(n-1) \le i \le n-1$, we associate two sets of cuts parallel to the X direction called X_i^T and X_i^B (Figure 3).



(a) (b)

Figure 1: (a) Polyphenylene superhoneycomb network with carbon and hydrogen atoms depicted by hollow circle and dark circle bullets, respectively. (b) Hydrogen-depleted structure of polyphenylene superhoneycomb network.

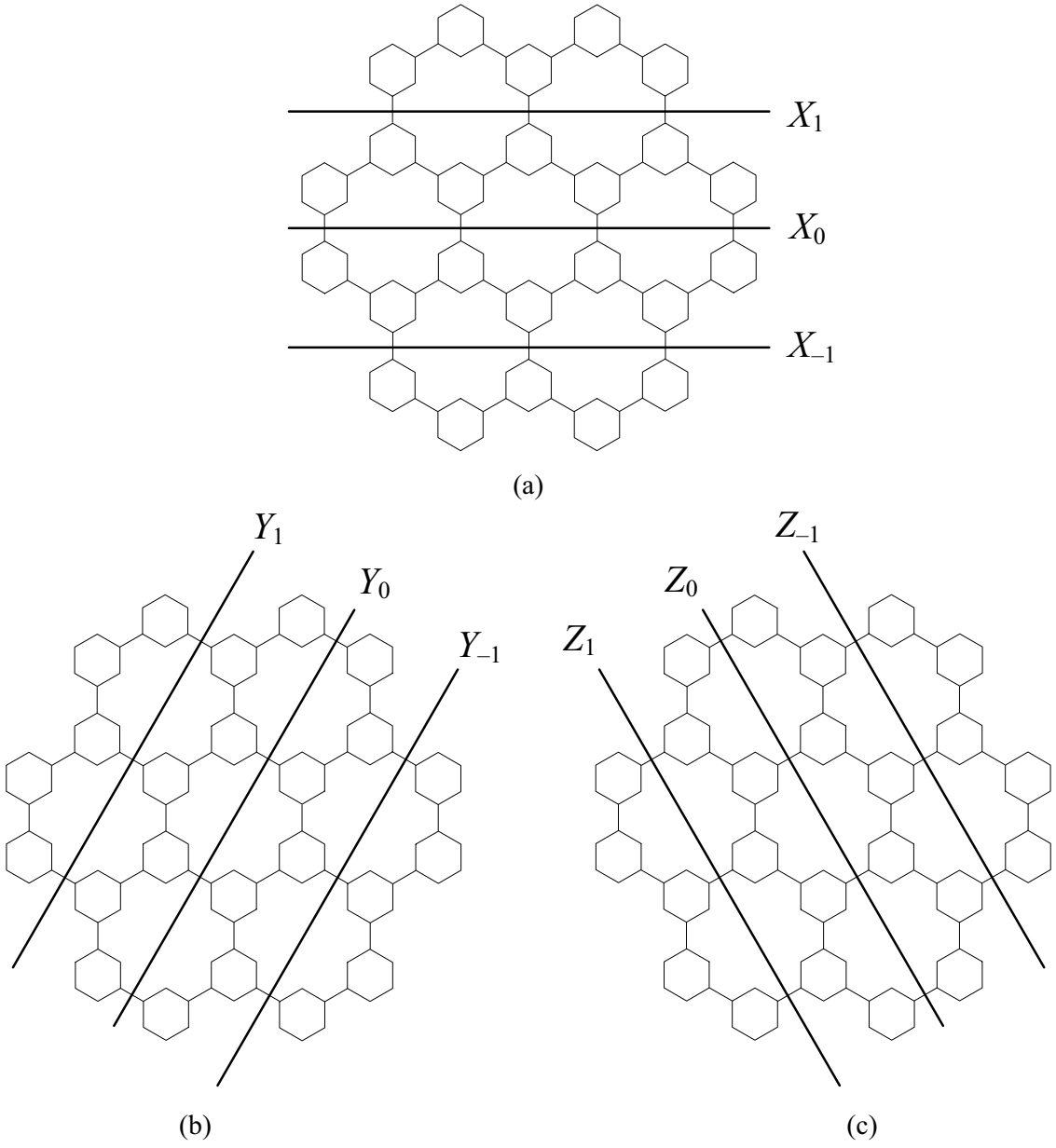


Figure 2: Edge cuts made up of edges perpendicular to (a) *X* direction, (b) *Y* direction, and (c) *Z* direction.

Let $\{X_n^j : 1 \le j \le n\}$ be the cuts as shown in Figure 3. Similar terminology is applied to *Y* and *Z* directions.

We now compute exact analytical expressions of $Mo_v(G)$, $Mo_e(G)$, $Mo_t(G)$, $w^+Mo_v(G)$, $w^*Mo_v(G)$, $w^+Mo_e(G)$, $w^*Mo_e(G)$, $w^+Mo_t(G)$, and $w^*Mo_t(G)$ for the graph of polyphenylene superhoneycomb networks.

Theorem 3. *Let G be the polyphenylene superhoneycomb network of dimension n. Then:*

(i) $Mo_v(G) = 810n^4 - 108n^3 + 18n^2 - 72n$.

(ii) $Mo_e(G) = \frac{1}{2}[2025n^4 - 350n^3 - 15n^2 + 124n]$.

(iii) $Mo_t(G) = \frac{1}{2}[3645n^4 - 566n^3 + 21n^2 - 268n]$.

(iv) $w^+Mo_v(G) = 4212n^4 - 888n^3 + 144n^2 - 372n$.

(v) $w^*Mo_v(G) = 5346n^4 - 1452n^3 + 162n^2 - 456n$.

(vi) $w^+Mo_e(G) = 5265n^4 - 1318n^3 + 57n^2 - 332n$.

(vii) $w^*Mo_e(G) = \frac{3}{2}[4455n^4 - 1386n^3 - 137n^2 - 244n]$.

(viii) $w^+Mo_t(G) = 9477n^4 - 2206n^3 + 201n^2 - 704n$.

(ix) $w^*Mo_t(G) = \frac{3}{2}[8019n^4 - 2354n^3 + 163n^2 - 580n]$.

Proof. Removal of the edges in X_0 leaves *G* into two components say G_{X_0} and G'_{X_0} with $|X_0| = 2n$, $n_1(X_0) = 18n^2$,

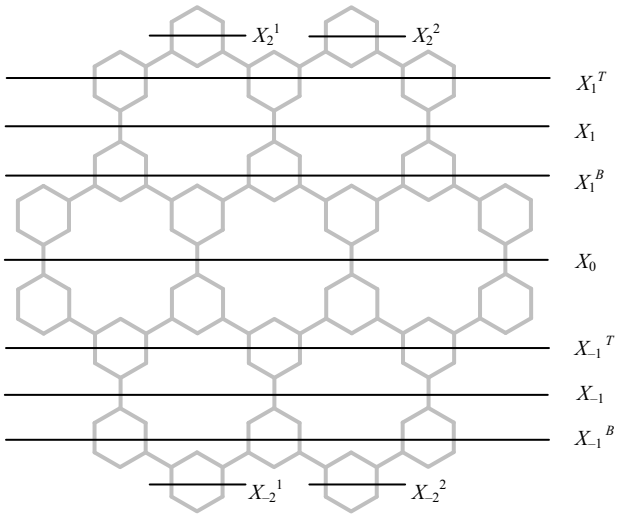


Figure 3: Various edge cuts made up of edges perpendicular to X direction.

$n_2(X_0) = 18n^2, m_1(X_0) = \frac{1}{2}(45n^2 - 5n), m_2(X_0) = \frac{1}{2}(45n^2 - 5n)$, $t_1(X_0) = \frac{1}{2}(81n^2 - 5n)$, and $t_2(X_0) = \frac{1}{2}(81n^2 - 5n)$.

For $1 \le k \le n-1$, removal of the edges in X_k leaves G into two components say G_{X_k} and G'_{X_k} with $|X_k| = 2n - k$, $n_1(X_k) = 18n^2 - 24nk + 6k^2, n_2(X_k) = 18n^2 + 24nk - 6k^2$, $m_1(X_k) = \frac{1}{2}(45n^2 - 60nk + 15k^2 - 5n + 3k)$, $m_2(X_k) = \frac{1}{2}(45n^2 + 60nk - 15k^2 - 5n - k)$, $t_1(X_k) = \frac{1}{2}(81n^2 - 108nk + 27k^2 - 5n + 3k)$, and $t_2(X_k) = \frac{1}{2}(81n^2 + 108nk - 27k^2 - 5n - k)$. The argument is similar for $X_{-k}, 1 \le k \le n-1$.

Removal of the edges in X_k^T, $1 \le k \le n-1$ leaves G into two components say $G_{X_k^T}$ and $G'_{X_k^T}$ with $|X_k^T| = 4n - 2k$, $n_1(X_k^T) = 18n^2 - 24nk + 6k^2 - 6n + 3k$, $n_2(X_k^T) = 18n^2 + 24nk - 6k^2 + 6n - 3k$, $m_1(X_k^T) = \frac{1}{2}(45n^2 - 60nk + 15k^2 - 21n + 11k)$, $m_2(X_k^T) = \frac{1}{2}(45n^2 + 60nk - 15k^2 + 7n - 7k)$, $t_1(X_k^T) = \frac{1}{2}(81n^2 - 108nk + 27k^2 - 33n + 17k)$, and $t_2(X_k^T) = \frac{1}{2}(81n^2 + 108nk - 27k^2 + 19n - 13k)$. A similar argument holds for $X_{-k}^T, 1 \le k \le n-1$.

For $1 \le k \le n-1$, removal of the edges in X_k^B leaves G into two components say $G_{X_k^B}$ and $G'_{X_k^B}$ with $|X_k^B| = 4n - 2k$, $n_1(X_k^B) = 18n^2 - 24nk + 6k^2 + 6n - 3k$, $n_2(X_k^B) = 18n^2 + 24nk - 6k^2 - 6n + 3k$, $m_1(X_k^B) = \frac{1}{2}(45n^2 - 60nk + 15k^2 + 7n - 3k), m_2(X_k^B) = \frac{1}{2}(45n^2 + 60nk - 15k^2 - 21n + 7k)$, $t_1(X_k^B) = \frac{1}{2}(81n^2 - 108nk + 27k^2 + 19n - 9k)$, and $t_2(X_k^B) = \frac{1}{2}(81n^2 + 108nk - 27k^2 - 33n + 13k)$. The argument is similar for $X_{-k}^B, 1 \le k \le n-1$.

For $k = 0$, the removal of the edges in X_0^T leaves G into two components $G_{X_0^T}$ and $G'_{X_0^T}$ where $|X_0^T| = 4n$, $n_1(X_0^T) = 18n^2 - 6n$, $n_2(X_0^T) = 18n^2 + 6n$, $m_1(X_0^T) = \frac{1}{2}(45n^2 - 21n)$, $m_2(X_0^T) = \frac{1}{2}(45n^2 + 7n)$, $t_1(X_0^T) = \frac{1}{2}(81n^2 - 33n)$, and $t_2(X_0^T) = \frac{1}{2}(81n^2 + 19n)$.

Similarly, for $k = 0$, the removal of the edges in X_0^B leaves G into two components $G_{X_0^B}$ and $G'_{X_0^B}$ where $|X_0^B| = 4n$, $n_1(X_0^B) = 18n^2 + 6n$, $n_2(X_0^B) = 18n^2 - 6n$, $m_1(X_0^B) = \frac{1}{2}(45n^2 + 7n)$, $m_2(X_0^B) = \frac{1}{2}(45n^2 - 21n)$, $t_1(X_0^B) = \frac{1}{2}(81n^2 + 19n)$, and $t_2(X_0^B) = \frac{1}{2}(81n^2 - 33n)$.

For $1 \le j \le n$, the removal of the edges in X_n^j leaves G into two components say $G_{X_n^j}$ and $G'_{X_n^j}$ with $|X_n^j| = 2$, $n_1(X_n^j) = 3$, $n_2(X_n^j) = 36n^2 - 3$, $m_1(X_n^j) = 2$, $m_2(X_n^j) = 45n^2 - 3n - 4$, $t_1(X_n^j) = 5$, and $t_2(X_n^j) = 81n^2 - 3n - 7$. The argument is similar for $X_{-n}^j, 1 \le j \le n$. Then:

(i) $Mo_v(G) = 3[(2n)|(18n^2) - (18n^2)| + 2\sum_{k=1}^{n-1}(2n-k)|(18n^2 - 24nk + 6k^2) - (18n^2 + 24nk - 6k^2)| + 2\sum_{k=1}^{n-1}(4n-2k)|(18n^2 - 24nk + 6k^2 - 6n + 3k) - (18n^2 + 24nk - 6k^2 + 6n - 3k)| + 2\sum_{k=1}^{n-1}(4n-2k)|(18n^2 - 24nk + 6k^2 + 6n - 3k) - (18n^2 + 24nk - 6k^2 - 6n + 3k)| + 2(4n)|(18n^2 - 6n) - (18n^2 + 6n)| + 2n(2)|3 - (36n^2 - 3)|]$.

(ii) $Mo_e(G) = 3[(2n)|\frac{1}{2}(45n^2 - 5n) - \frac{1}{2}(45n^2 - 5n)| + 2\sum_{k=1}^{n-1}(2n-k)|\frac{1}{2}(45n^2 - 60nk + 15k^2 - 5n + 3k) - \frac{1}{2}(45n^2 + 60nk - 15k^2 - 5n - k)| + 2\sum_{k=1}^{n-1}(4n-2k)|\frac{1}{2}(45n^2 - 60nk + 15k^2 - 21n + 11k) - \frac{1}{2}(45n^2 + 60nk - 15k^2 + 7n - 7k)| + 2\sum_{k=1}^{n-1}(4n-2k)|\frac{1}{2}(45n^2 - 60nk + 15k^2 + 7n - 3k) - \frac{1}{2}(45n^2 + 60nk - 15k^2 - 21n + 7k)| + (2)(4n)|\frac{1}{2}(45n^2 - 21n) - \frac{1}{2}(45n^2 + 7n)| + 2n(2)|(45n^2 - 3n - 4) - 2|]$.

(iii) $Mo_t(G) = 3[(2n)|\frac{1}{2}(81n^2 - 5n) - \frac{1}{2}(81n^2 - 5n)| + 2\sum_{k=1}^{n-1}(2n-k)|\frac{1}{2}(81n^2 - 108nk + 27k^2 - 5n + 3k) - \frac{1}{2}(81n^2 + 108nk - 27k^2 - 5n - k)| + 2\sum_{k=1}^{n-1}(4n-2k)|\frac{1}{2}(81n^2 - 108nk + 27k^2 - 33n + 17k) - \frac{1}{2}(81n^2 + 108nk - 27k^2 + 19n - 13k)| + 2\sum_{k=1}^{n-1}(4n-2k)|\frac{1}{2}(81n^2 - 108nk + 27k^2 + 19n - 9k) - \frac{1}{2}(81n^2 + 108nk - 27k^2 - 33n + 13k)| + (2)(4n)|\frac{1}{2}(81n^2 - 33n) - \frac{1}{2}(81n^2 + 19n)| + 2n(2)|(81n^2 - 3n - 7) - 5|]$.

(iv) $w^+Mo_v(G) = 3[(3+3)(2n)|(18n^2) - (18n^2)| + 2\sum_{k=1}^{n-1}(3+3)(2n-k)|(18n^2 - 24nk + 6k^2) - (18n^2 + 24nk$

$-6k^2)| + 2\sum_{k=1}^{n-1}[(3+2)(4n-2k-2)+(2+2)(2)]|(18n^2-24nk+6k^2-6n+3k)-(18n^2+24nk-6k^2+6n-3k)| + 2\sum_{k=1}^{n-1}[(3+2)(4n-2k)]|(18n^2-24nk+6k^2+6n-3k)-(18n^2+24nk-6k^2-6n+3k)| + 2[(3+2)(4n-2)+(2+2)(2)]|(18n^2-6n)-(18n^2+6n)| + 2n(3+2)(2)|3-(36n^2-3)|]$.

(v) $w^{*}Mo_v(G) = 3[(3)(3)(2n)|(18n^2)-(18n^2)| + 2\sum_{k=1}^{n-1}(3)(3)(2n-k)|(18n^2-24nk+6k^2)-(18n^2+24nk-6k^2)| + 2\sum_{k=1}^{n-1}[(3)(2)(4n-2k-2)+(2)(2)(2)]|(18n^2-24nk+6k^2-6n+3k)-(18n^2+24nk-6k^2+6n-3k)| + 2\sum_{k=1}^{n-1}(3)(2)(4n-2k)|(18n^2-24nk+6k^2+6n-3k)-(18n^2+24nk-6k^2-6n+3k)| + 2[(3)(2)(4n-2)+(2)(2)(2)]|(18n^2-6n)-(18n^2+6n)| + 2n(3)(2)(2)|3-(36n^2-3)|]$.

(vi) $w^{+}Mo_e(G) = 3[(3+3)(2n)|\frac{1}{2}(45n^2-5n)-\frac{1}{2}(45n^2-5n)| + 2\sum_{k=1}^{n-1}(3+3)(2n-k)|\frac{1}{2}(45n^2-60nk+15k^2-5n+3k)-\frac{1}{2}(45n^2+60nk-15k^2-5n-k)| + 2\sum_{k=1}^{n-1}[(3+2)(4n-2k-2)+(2+2)(2)]|\frac{1}{2}(45n^2-60nk+15k^2-21n+11k)-\frac{1}{2}(45n^2+60nk-15k^2+7n-7k)| + 2\sum_{k=1}^{n-1}[(3+2)(4n-2k)]|\frac{1}{2}(45n^2-60nk+15k^2+7n-3k)-\frac{1}{2}(45n^2+60nk-15k^2-21n+7k)| + (2)[(3+2)(4n-2)+(2+2)(2)]|\frac{1}{2}(45n^2-21n)-\frac{1}{2}(45n^2+7n)| + 2n(3+2)(2)|(45n^2-3n-4)-2|]$.

(vii) $w^{*}Mo_e(G) = 3[(3)(3)(2n)|\frac{1}{2}(45n^2-5n)-\frac{1}{2}(45n^2-5n)| + 2\sum_{k=1}^{n-1}(3)(3)(2n-k)|\frac{1}{2}(45n^2-60nk+15k^2-5n+3k)-\frac{1}{2}(45n^2+60nk-15k^2-5n-k)| + 2\sum_{k=1}^{n-1}[(3)(2)(4n-2k-2)+(2)(2)(2)]|\frac{1}{2}(45n^2-60nk+15k^2-21n+11k)-\frac{1}{2}(45n^2+60nk-15k^2+7n-7k)| + 2\sum_{k=1}^{n-1}[(3)(2)(4n-2k)]|\frac{1}{2}(45n^2-60nk+15k^2+7n-3k)-\frac{1}{2}(45n^2+60nk-15k^2-21n+7k)| + (2)[(3)(2)(4n-2)+(2)(2)(2)]|\frac{1}{2}(45n^2-21n)-\frac{1}{2}(45n^2+7n)| + 2n(3)(2)(2)|(45n^2-3n-4)-2|]$.

(viii) $w^{+}Mo_t(G) = 3[(3+3)(2n)|\frac{1}{2}(81n^2-5n)-\frac{1}{2}(81n^2-5n)| + 2\sum_{k=1}^{n-1}(3+3)(2n-k)|\frac{1}{2}(81n^2-108nk+27k^2-5n+3k)-\frac{1}{2}(81n^2+108nk-27k^2-5n-k)| + 2\sum_{k=1}^{n-1}[(3+2)(4n-2k-2)+(2+2)(2)]|\frac{1}{2}(81n^2-108nk+27k^2-33n+17k)-\frac{1}{2}(81n^2+108nk-27k^2+19n-13k)| + 2\sum_{k=1}^{n-1}[(3+2)(4n-2k)]|\frac{1}{2}(81n^2-108nk+27k^2+19n-9k)-\frac{1}{2}(81n^2+108nk-27k^2-33n+13k)| + (2)[(3+2)(4n-2)+(2+2)(2)]|\frac{1}{2}(81n^2-33n)-\frac{1}{2}(81n^2+19n)| + 2n(3+2)(2)|(81n^2-3n-7)-5|]$.

(ix) $w^{*}Mo_t(G) = 3[(3)(3)(2n)|\frac{1}{2}(81n^2-5n)-\frac{1}{2}(81n^2-5n)| + 2\sum_{k=1}^{n-1}(3)(3)(2n-k)|\frac{1}{2}(81n^2-108nk+27k^2-5n+3k)-\frac{1}{2}(81n^2+108nk-27k^2-5n-k)| + 2\sum_{k=1}^{n-1}[(3)(2)(4n-2k-2)+(2)(2)(2)]|\frac{1}{2}(81n^2-108nk+27k^2-33n+17k)-\frac{1}{2}(81n^2+108nk-27k^2+19n-13k)| + 2\sum_{k=1}^{n-1}[(3)(2)(4n-2k)]|\frac{1}{2}(81n^2-108nk+27k^2+19n-9k)-\frac{1}{2}(81n^2+108nk-27k^2-33n+13k)| + (2)[(3)(2)(4n-2)+(2)(2)(2)]|\frac{1}{2}(81n^2-33n)-\frac{1}{2}(81n^2+19n)| + 2n(3)(2)(2)|(81n^2-3n-7)-5|]$.

We have obtained the above results using MATLAB interface.

4 Graphical comparison

Graph-theoretical methods are often used to interpret chemical structures as molecular graphs. The analytical expressions are represented as a two-dimensional (2D) graph against variable n to analyze the relationship and behavioral pattern of the computed invariants. Figure 4 shows a 2D graph of Theorem 3. The invariants vary based on the chemical structure, as seen in the graph.

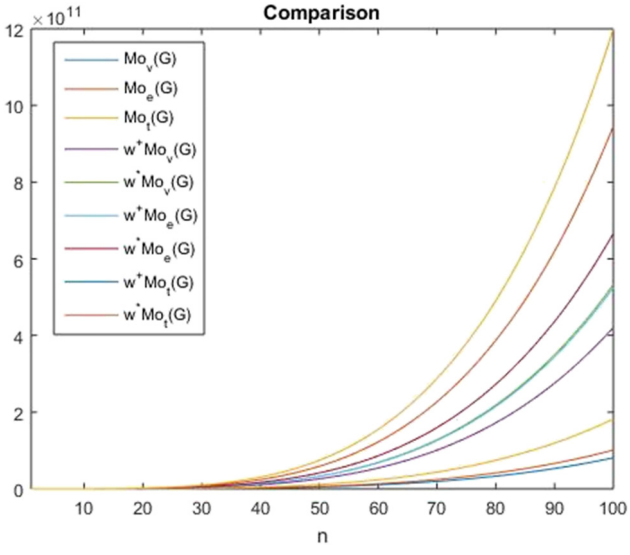


Figure 4: 2D plot for Theorem 3.

5 Conclusion

The bond-additive topological invariants considered in this article have been extensively investigated for many classes of graphs, which encouraged us to investigate these invariants for polyphenylene superhoneycomb networks. We have obtained exact analytical expressions of different versions of weighted Mostar invariants for the molecular structure of polyphenylene superhoneycomb networks by applying the cut method. Our results could be useful in determining the characteristics of these molecular structures using models of QSPR/QSAR relationships. The degree-based topological indices for the graph of polyphenylene superhoneycomb network are under investigation.

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