GENERALIZED MULTIPLICATIVE INDICES OF POLYCYCLIC AROMATIC HYDROCARBONS AND BENZENIOD SYSTEMS

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ABSTRACT. Many types of topological indices such as degree-based topological indices, distance-based topological indices and counting related topological indices are explored during past recent years. Among degree based topological indices, Zagreb indices are the oldest one and studied well. In the paper, we define a generalized multiplicative version of these indices and compute exact formulas for Polycyclic Aromatic Hydrocarbons and Jagged-Rectangle Benzenoid Systems.

1. INTRODUCTION

A molecular graph is a finite simple graph, representing the carbon-atom skeleton of an organic molecule of a hydrocarbon. The vertices of a molecular graph represent the carbon atoms and its undirected edges the carbon-carbon bounds. Throughout this paper $G = (V, E)$ is a connected molecular graph with vertex set $V = V(G)$ and edge set $E = E(G)$. The degree $d(v)$ of a vertex $v$ is the number of vertices adjacent to $v$.\(^1\)

Studying molecular graphs is a constant focus in chemical graph theory; an effort to better understand molecular structure. For instance, in 1947 H. Wiener [Wie47] introduced a topological index of a molecule, now called the Wiener index. This index was originally defined as the sum of path distances between any two carbons in a saturated acyclic hydrocarbon. Since its inception this index has been generalized to a variety of structures as well as used in Quantitative structure-activity relationship (QSAR) regression models [FCH01, ME05, RPNP10, YWH04].

Some indices related to Wiener’s work are the first and second multiplicative Zagreb indices [GRTW75], respectively

\[ \mathcal{M}_1(G) = \prod_{u \in V(G)} d(u)^2 \quad \text{and} \quad \mathcal{M}_2(G) = \prod_{uv \in E(G)} d(u)d(v), \]

and the Narumi-Katayama index [NK84]

\[ NK(G) = \prod_{v \in V(G)} d(v). \]

Like the Wiener index, these types of indices are the focus of considerable research in computational chemistry [Gut11, TBC10, TC10, WW15]. For example, in 2011 I. Gutman [Gut11] characterized the multiplicative Zagreb indices for trees and determined the unique trees that obtained maximum and minimum values for $\mathcal{M}_1(G)$

\(^{1}\)For more on this notation and terminology, the readers are referred to [BM08].
and $\mathcal{M}_2(G)$, respectively. S. Wang and the last author [WW15] then extended Gutman’s result to the following index for $k$-trees,

$$W_s^k(G) = \prod_{u \in V(G)} d(u)^s.$$ 

Notice that $s = 1, 2$ is the Narumi-Katayama and Zagreb index, respectively.

Based on the successful consideration of multiplicative Zagreb indices, M. Eliasi et al [EIG12] continued to define a new multiplicative version of the first Zagreb index as

$$M^*_1(G) = \prod_{uv \in E(G)} (d(u) + d(v)).$$

Furthering the concept of indexing with the edge set, the first author introduced the first and second hyper-Zagreb indices [Kul16]. They are defined as

$$H_1(G) = \prod_{uv \in E(G)} (d(u) + d(v))^2$$

and

$$H_2(G) = \prod_{uv \in E(G)} (d(u)d(v))^2.$$ 

In this paper, we continue this generalization and define the general first and second multiplicative Zagreb indices of a graph $G$ as

$$M^a_1(G) = \prod_{uv \in E(G)} (d(u) + d(v))^a$$

and

$$M^a_2(G) = \prod_{uv \in E(G)} (d(u)d(v))^a.$$ 

In Section 2 we determine the multiplicative Zagreb and the general multiplicative Zagreb indices for Polycyclic Aromatic Hydrocarbons (PAH$_n$). Section 3 contains similar results for a jagged-rectangle Benzenoid system ($B_{m,n}$).

2. Results for Polycyclic Aromatic Hydrocarbons

In this section, we focus on the molecular graph structure of the family of Polycyclic Aromatic Hydrocarbons, denoted PAH$_n$. These graphs of hydrocarbon molecules are defined recursively as follows. The 6-cycle with leaves at each vertex is PAH$_1$ ($C_6H_6$, benzene). The next element in the family, PAH$_2$, is given by deleting the leaves of PAH$_1$ and gluing 6-cycles to each exterior edge, then adding leaves to each exterior vertex. We give the first three members of the family PAH$_n$ in Figure 1.

**Lemma 2.1.** Let $G = $ PAH$_n$ be the molecular graph in the family of Polycyclic Aromatic Hydrocarbons. Then

$$|V(G)| = 6n^2 + 6n,$$

$$|E(G)| = 9n^2 + 3n.$$ 

**Proof.** We first need to show that $G$ has $6n$ leaves; we do this by induction on $n$. The result is clear for $n = 1, 2$ and we assume PAH$_{n-1}$ has $6(n-1)$ leaves. To construct PAH$_n$ from PAH$_{n-1}$, we attached $n - 1$ hexagons; one between each pair of neighboring leaves. As six of these hexagons contribute two leaves to PAH$_n$ (and the rest contribute one), we see that PAH$_n$ has $6 + 6(n - 1) = 6n$ leaves.

We are now able to find $|V(G)|$ and $|E(G)|$. Notice that each leaf in $G$ contributes 2 vertices. Removing these vertices from PAH$_n$ yields PAH$_{n-1}$. Hence, by induction,

$$|V(G)| = 2(6n) + (6(n-1)^2 + 6(n-1)) = 6n^2 + 6n.$$
Similarly, the leaves of PAH\(_n\) contribute \(3(6n) - 6\) extra edges over PAH\(_{n-1}\) (subtracting 6 accounts for the six hexagons contributing two leaves). Once again by induction,

\[ |E(G)| = (3(6n) - 6) + (9(n - 1)^2 + 3(n - 1)) = 9n^2 + 3n. \]

\(\square\)

We are now ready to compute the general indices of the molecular graph PAH\(_n\).

**Theorem 2.2.** Let \(G = \text{PAH}_n\) be the molecular graph in the family of Polycyclic Aromatic Hydrocarbons. Then

1. \(\mathcal{M}_1^1(G) = 4^{6an} \times 6^{(9n^2 - 3n)a}\);
2. \(\mathcal{M}_2^2(G) = 3^{18an^2}\);
3. \(\mathcal{W}_1(G) = 3^{6sn^2}\).

**Proof.** According to Lemma 2.1, \(G\) has \(6n^2 - 6n\) vertices and \(6n\) of those vertices are on leaves. With this information, we are able to partition of the vertex set of \(G\) into two sets, one containing the vertices on leaves, and the other containing the rest of the vertices in the graph. We define them as

\[ V_1 = \{v \in V(G) \mid d(v) = 1\}, \quad |V_1| = 6n; \]
\[ V_3 = \{v \in V(G) \mid d(v) = 3\}, \quad |V_3| = 6n^2. \]

Likewise, we obtain two partitions of the \(9n^2 + 3n\) edges of \(G\) as

\[ E_1 = \{uv \in E(G) \mid d(u) = 1, d(v) = 3\}, \quad |E_1| = 6n; \]
\[ E_3 = \{uv \in E(G) \mid d(u) = d(v) = 3\}, \quad |E_2| = 9n^2 - 3n. \]
Thus we are able to factor the products along these partitions. In particular,

$$M_1^a(G) = \prod_{uv \in E(G)} (d(u) + d(v))^a$$

$$= \prod_{uv \in E_1} (d(u) + d(v))^a \times \prod_{uv \in E_3} (d(u) + d(v))^a$$

$$= [(1 + 3)^a]^{6n} \times [(3 + 3)^a]^{9n^2 - 3n}$$

$$= 4^{6n^2} \times (6)^{(9n^2-3n)a}.$$  

Similarly we have

$$M_2^a(G) = \prod_{uv \in E(G)} (d(u)d(v))^a$$

$$= \prod_{uv \in E_1} (d(u)d(v))^a \times \prod_{uv \in E_3} (d(u)d(v))^a$$

$$= [(1 \times 3)^a]^{6n} \times [(3 \times 3)^a]^{9n^2 - 3n}$$

$$= 3^{18n^2}.$$  

To see the last result we use the partitions of the vertex set to obtain

$$W_s^a(G) = \prod_{u \in V(G)} d(u)^s$$

$$= \prod_{u \in V_1} d(u)^s \times \prod_{u \in V_3} d(u)^s$$

$$= (1^s)^{6n} \times (3^s)^{6n^2}$$

$$= 3^{6sn^2}.$$  

With this result we are able to calculate the remaining indices.

**Corollary 2.3.** Let $G = \text{PAH}_n$ be the molecular graph in the family of Polycyclic Aromatic Hydrocarbons. Then

1. $M_1(G) = 3^{12n^2};$
2. $M_2(G) = 3^{18n^2};$
3. $N_K(G) = 3^{6n^2};$
4. $M_1^*(G) = 4^{6n \times 6^{9n^2-3n}};$
5. $H_1(G) = 4^{12n \times 6^{18n^2-6n}};$
6. $H_2(G) = 3^{36n^2}.$
Proof. Each of the above indices are special cases of the general indices in Theorem 2.2. In particular we have,
\[ M_1(G) = \mathcal{W}_1^2(G) = 3^{12n^2}; \]
\[ M_2(G) = M_1^2(G) = 3^{18n^2}; \]
\[ NK(G) = W_1^1(G) = 3^{6n^2}; \]
\[ M_1^*(G) = M_1^1(G) = 4^{6n} \times 6^{9n^2-3n}; \]
\[ H_1(G) = M_2^1(G) = 4^{12n} \times 6^{18n^2-6n}; \]
\[ H_2(G) = M_2^2(G) = 3^{36n^2}. \]

3. RESULTS FOR BENZENOID SYSTEMS

We now focus on the molecular graph structure of a jagged-rectangle Benzenoid system, denoted \( B_{m,n} \) for all \( m, n \in \mathbb{N} \). As can be seen in Figure 2 the rectangles \( B_{m,n} \) are constructed by gluing \( n+1 \) chains of \( m-1 \) hexagons (or \( C_6 \)) to \( n \) chains of \( m \) hexagons, alternating by starting with a \( m-1 \)-chain of hexagons. This family of graphs was defined in [LLZNQLQ05]. In this section we will calculate the generalized multiplicative indices for these types of molecular graphs.

As to the general indices for this system, we have the following result.

**Theorem 3.1.** Let \( G = B_{m,n} \) be a molecular graph of a jagged-rectangle Benzenoid system. Then

\begin{align*}
(1) \quad & M_1(G) = 4^a(2n+4) \times 5^a(4m+4n-4) \times 6^a(6mn+m-5n-4); \\
(2) \quad & M_2(G) = 4^a(2n+4) \times 6^a(4m+4n-4) \times 9^a(6mn+m-5n-4); \\
(3) \quad & W_1^a(G) = 2^{(2m+4n+2)s} \times 3^{(4mn+2m-2n-4)s}. 
\end{align*}

**Proof.** We first calculate the number of vertices and edges of \( G \). To do this notice that the number of vertices in the top row of \( m-1 \) hexagons (oriented according to Figure 2) is \( 4m-2 \). As there are \( n+1 \) rows containing \( m-1 \) hexagons in the graph, we have counted \( (4m-2)(n+1) = 4mn - 2n + 4m - 2 \) vertices so far. The only remaining vertices are on the left and right ends of the \( n \) rows containing \( m \) hexagons; there are \( 4n \) of these. Hence we get

\[ |V(G)| = (4mn - 2n + 4m - 2) + (4n) = 4mn + 4m + 2n - 2. \]
To find the number of edges, we partition $V(G)$ into two sets, vertices of degree 2 and 3 respectively,

\[ V_2 = \{ v \in V(G) \mid d(v) = 2 \}, \quad |V_2| = 2m + 4n + 2; \]
\[ V_3 = \{ v \in V(G) \mid d(v) = 3 \}, \quad |V_3| = 4mn + 2m - 2n - 4. \]

As the total degree of the graph is equal to twice the number of edges, we know that

\[ |E(G)| = \frac{1}{2} [2(2m + 4n + 2) + 3(4mn + 2m - 2n - 4)] = 6mn + 5m + n - 4. \]

Similar to the proof of Theorem 2.2, we will calculate the indices by factoring along partitions of the vertex and edge sets. To see the last result we use the partitions of the vertex set to obtain

\[
W_1^n(G) = \prod_{u \in V(G)} d(u)^s = \prod_{u \in V_2} d(u)^s \times \prod_{u \in V_3} d(u)^s = (2^s)^{2m+4n+2} \times (2^s)^{4mn+2m-2n-4} = 2^{(2m+4n+2)s} \times 3^{(4mn+2m-2n-4)s}.
\]

For the remaining results, we create three partitions of the edge set of the molecular graph $G$.

\[ E_2 = \{ uv \in E(G) \mid d(u) = d(v) = 2 \}, \quad |E_2| = 2n + 4; \]
\[ E_{2,3} = \{ uv \in E(G) \mid d(u) = 3, d(v) = 2 \}, \quad |E_{2,3}| = 4m + 4n - 4; \]
\[ E_3 = \{ uv \in E(G) \mid d(u) = d(v) = 3 \}, \quad |E_3| = 6mn + m - 5n - 4. \]

It is not hard to see that $|E_2| = 2n + 4$. To see the number of elements in $E_{2,3}$, notice that there are $4n + 8$ vertices of degree 2 with a unique adjacent vertex of degree 3. Further, there are $2m - 6$ vertices with two distinct adjacent vertices of degree 3. Hence $|E_{2,3}| = 4n + 8 + 2(2m - 6) = 4m + 4n - 4$. Subtracting these values from $|E(G)|$ yields $|E_3|$.

Using this edge partition, we are able to calculate $M_1^n(G)$ as

\[
M_1^n(G) = \prod_{uv \in E(G)} (d(u) + d(v))^a = \prod_{uv \in E_2} (d(u) + d(v))^a \times \prod_{uv \in E_{2,3}} (d(u) + d(v))^a \times \prod_{uv \in E_3} (d(u) + d(v))^a = [(2 + 2)^a]^{2n+4} \times [(3 + 2)^a]^{4m+4n-4} \times [(3 + 3)^a]^{6mn+m-5n-4} = 4^a(2n+4) \times 6^a(4m+4n-4) \times 6^a(6mn+m-5n-4).
\]

To see the second result, we have

\[
M_2^n(G) = \prod_{uv \in E(G)} (d(u)d(v))^a = \prod_{uv \in E_2} (d(u)d(v))^a \times \prod_{uv \in E_{2,3}} (d(u)d(v))^a \times \prod_{uv \in E_3} (d(u)d(v))^a = 4^a(2n+4) \times 6^a(4m+4n-4) \times 9^a(6mn+m-5n-4).
\]
As an immediate corollary all other indices in this paper are obtained.

**Corollary 3.2.** Let $G = B_{m,n}$ be a molecular graph of a jagged-rectangle Benzenoid system. Then

1. $M_1(G) = 4^{2m+4n+2} \times 9^{4mn+2m-2n-4}$,
2. $M_2(G) = 4^{2n+4} \times 6^{4m+4n-4} \times 9^{6mn+m-5n-4}$,
3. $NK(G) = 2^{2m+4n+2} \times 3^{4mn+2m-2n-4}$,
4. $M_1^*(G) = 4^{2n+4} \times 5^{4m+4n-4} \times 6^{6mn+m-5n-4}$,
5. $\mathcal{H}_1(G) = 4^{2(2n+4)} \times 5^{2(4m+4n-4)} \times 6^{2(6mn+m-5n-4)}$,
6. $\mathcal{H}_2(G) = 4^{2(2n+4)} \times 5^{2(4m+4n-4)} \times 6^{2(6mn+m-5n-4)}$.

**Proof.** Each of the above indices are special cases of the general indices in Theorem 3.1. In particular we have,

\[
M_1(G) = M_1^*(G) = 4^{2m+4n+2} \times 9^{4mn+2m-2n-4},
\]
\[
M_2(G) = M_2^*(G) = 4^{2n+4} \times 6^{4m+4n-4} \times 9^{6mn+m-5n-4},
\]
\[
NK(G) = W_1^*(G) = 2^{2m+4n+2} \times 3^{4mn+2m-2n-4},
\]
\[
M_1^*(G) = M_1^*(G) = 4^{2n+4} \times 5^{4m+4n-4} \times 6^{6mn+m-5n-4},
\]
\[
\mathcal{H}_1(G) = \mathcal{M}_1^*(G) = 4^{2(2n+4)} \times 5^{2(4m+4n-4)} \times 6^{2(6mn+m-5n-4)},
\]
\[
\mathcal{H}_2(G) = \mathcal{M}_2^*(G) = 4^{2(2n+4)} \times 5^{2(4m+4n-4)} \times 6^{2(6mn+m-5n-4)}.
\]

\[
\square
\]

**References**

[BM08] J. A. Bondy and U. S. R. Murty. *Graph theory*, volume 244 of *Graduate Texts in Mathematics*. Springer, New York, 2008.

[EIG12] Mehdi Eliasi, Ali Iranmanesh, and Ivan Gutman. Multiplicative versions of first Zagreb index. *MATCH Commun. Math. Comput. Chem.*, 68(1):217–230, 2012.

[FCH01] P. W. Fowler, G. Caporossi, and P. Hansen. Distance matrices, wiener indices, and related invariants of fullerene. *The Journal of Physical Chemistry A*, 105(25):6232–6242, 2001.

[GRTW75] I. Gutman, B. Rušičć, N. Trinajstić, and C. F. Wilcox. Graph theory and molecular orbitals. xii. acyclic polyenes. *The Journal of Chemical Physics*, 62(9), 1975.

[Gut11] Ivan Gutman. Multiplicative Zagreb indices of trees. *Bull. Inst. Math. Virtual Inst.*, 1:13–19, 2011.

[Kul16] V. R. Kulli. Multiplicative hyper-Zagreb indices and coindices of graphs. *Int. Research J. of Pure Alg.*, 6(7):342–347, 2016.

[LLZNLQ05] Shui Ling-Ling, Wang Zhi-Ning, and Zheng Li-Qiang. Rheological properties of cubic liquid crystals formed from monoglyceride/H2O systems. *Chinese Journal of Chemistry*, 23(3):245–250, 2005.

[ME05] Adelio R. Matamala and Ernesto Estrada. Simplex optimization of generalized topological index (GTI-simplex): a unified approach to optimize qspr models. *The Journal of Physical Chemistry A*, 109(43):9890–9895, 2005. PMID: 16833305.

[NK84] Hideyuki Narumi and Meiseki Katayama. Simple topological index : A newly devised index characterizing the topological nature of structural isomers of saturated hydrocarbons. *Memoirs of the Faculty of Engineering, Hokkaido University*, 16(3):209–214, 1984.

[RPNP10] Milan Randi, Toma Pisanski, Marjana Novi, and Dejan Plavi. Novel graph distance matrix. *Journal of Computational Chemistry*, 31(9):1832–1841, 2010.

[TBC10] R. Todeschini, D. Ballabio, and V. Consonni. Novel molecular descriptors based on functions of new vertex degrees. In *Novel molecular structure descriptors - Theory*
and applications I, volume 8 of Mathematical Chemistry Monographs, pages 73–100. University of Kragujevac and Faculty of Science Kragujevac, 2010.

[TC10] Roberto Todeschini and Viviana Consonni. New local vertex invariants and molecular descriptors based on functions of the vertex degrees. MATCH Commun. Math. Comput. Chem., 64(2):359–372, 2010.

[Wie47] Harry Wiener. Structural determination of paraffin boiling points. Journal of the American Chemical Society, 69(1):17–20, 1947.

[WW15] Shaohui Wang and Bing Wei. Multiplicative Zagreb indices of $k$-trees. Discrete Appl. Math., 180:168–175, 2015.

[YWH04] Feng Yang, Zhen-Dong Wang, and Yun-Ping Huang. Modification of the wiener index 4. Journal of Computational Chemistry, 25(6):881–887, 2004.

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