Degree-Based Topological Indices of the Benzenoid Circumcoronene Series

Abdu Alameri (*,1)

Mohammed Alsharafi [2], **Yusuf Zeren** [2]
Abdelhafidh Modabish [3]
Mohammed El Marraki [4]

[1] Department of Biomedical Engineering, Faculty of Engineering, University of Science and Technology, Sana'a, Yemen

[2] Department of Mathematics, Faculty of Arts and Science, Yildiz Technical University, Istanbul, Turkey

[3] Department of Mathematics, Faculty of Science, Sana'a University, Sana'a, Yemen

[4] Department of Computer Sciences, Faculty of Science, University of Mohamed V, Rabat, Morocco

* Corresponding author: alameri2222@gmail.com, alsharafi205010@gmail.com, yzeren@yildiz.edu.tr, a.modabish@su.esu.ye, marraki@fsr.ac.ma

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Abstract:

This paper deals with some types of topological indices called valency-based indices or degree-Based Indices. Specifically, Multiplicative Forgotten, Multiplicative Yemen, modified Forgotten, modified Yemen, generalized modified first Zagreb, generalized modified sum connectivity, and generalized modified product connectivity indices of the benzenoid circumcoronene series are computed. Moreover, the formulas of polynomials for all these topological indices were derived.

Keywords: Topological Indices, Multiplicative Indices, Modified Indices, Molecular Graph; Benzenoid Circumcoronene Series.

المؤشرات الطوبولوجية المعتمدة على الدرجة لسلسلة بنزينويد سيركومكورونين

الملخص:

يتناول هذا البحث بعض أنواع المؤشرات الطوبولوجية التي تسمى المؤشرات المعتمدة على التكافؤ أو المؤشرات المعتمدة على الدرجة. على وجه التحديد، تم حساب المؤشر المنسي المضاعف، والمؤشر اليمني المضاعف، والمؤشر المنسي المعدل، والمؤشر اليمني المعدل، ومؤشر زغرب المعدل المعمم الأول، ومؤشر اتصال المجموع المعدل العام، ومؤشر اتصال المنتج المعدل العام لسلسلة البنزينويد سيركومكورونين. علاوة على ذلك، تم اشتقاق صيغ كثيرات الحدود لجميع هذه المؤشرات الطوبولوجية.

الكلمات المفتاحية : المؤشرات الطوبولوجية؛ المؤشرات المضاعفة، المؤشرات المعدلة، الرسم البياني الجزيئي، سلسلة بنزينويد سيركومكورونين.

1. Introduction

A graph can be recognized by a numeric number, a polynomial, a sequence of numbers or a matrix which represent the whole graph, and these representations are aimed to be uniquely defined for that graph. Topological index is a numeric quantity with a graph which characterizes the topology of the graph and is invariant under graph automorphism [19]. All graphs in this paper are finite and simple, let G be a finite simple graph on V(G)=n, vertices and E(G)=m, edges, the degree of a vertex v is the number of edges incident to v, denoted by δ_G (v) [13].

A new subject that is a combination of chemistry, information sciences, and mathematics. Topological indices are real numbers related to a graph, that must be a structural invariant. Topological indices play an important role in mathematical chemistry, especially QSAR/QSPR investigations [1, 2, 6, 8]. In practical applications, Multiplicative and Modified indices are among the best topological indices applications to recognize physical properties, chemical reactions, and biological activities. Throughout this paper, we consider a finite connected graph Γ that has no loops or multiple edges. The vertex and the edge sets of a graph Γ are denoted by $V(\Gamma)$ and $E(\Gamma)$, respectively. The degree of the vertex a is the number of edges joined with this vertex denoted by $\delta(a)$. In practical applications, Zagreb Indices are among the best applications to recognize the physical properties and chemical reactions. First Zagreb index M_1 (G), and Second Zagreb index M_2 (Γ) were first considered by I. Gutman and N. Trinajestić in 1972 [10, 19, 20, 21]. They are defined as:

$$M_1(\Gamma) = \sum_{\mu\nu\in E(\Gamma)} (\delta_\Gamma(\mu) + \delta_\Gamma(\nu)), \qquad M_2(\Gamma) = \sum_{\mu\nu\in E(\Gamma)} \delta_\Gamma(\mu)\,\delta_\Gamma(\nu).$$

These Indices were deduced within the study of the dependence of total π-electron energy on molecular structures and are measures of branching of the molecular carbon-atom skeleton. Furtula and Gutman (2015) introduced the forgotten index (F-index) [11, 14, 15] which is defined as:

$$F(\Gamma) = \sum_{\mu\nu\in E(\Gamma)} \left({\delta_\Gamma}^2(\mu) + {\delta_\Gamma}^2(\nu)\right).$$

Furtula and Gutman raised that the predictive ability of the forgotten index is almost similar to that of the first Zagreb index and for the acentric factor and entropy, and both of them obtain correlation coefficients larger than 0.95. This fact implies the reason why the forgotten index is useful for testing

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the chemical and pharmacological properties of drug molecular structures and reported that this index can reinforce the physicochemical flexibility of Zagreb indices [12, 13, 16].

In 2013, Shirdel et al. [18, 24] introduced degree-based of Zagreb indices named the Hyper-Zagreb index:

$$HM(\Gamma) = \sum_{\mu\nu\in E(\Gamma)} (\delta_\Gamma(\mu) + \delta_\Gamma(\nu))^2.$$

In 2016, Gao et al. [25, 28] defined a new degree-based of Zagreb indices named the second Hyper-Zagreb index as:

$$HM_2(\Gamma) = \sum_{\mu\nu\in E(\Gamma)} {\delta_\Gamma}^2(\mu)\, {\delta_\Gamma}^2(\nu).$$

In 2018, S. Ghobadi and M. Ghorbaninejad [17] introduced a new Zagreb index named Hyper Forgotten topological index:

$$HF(\Gamma) = \sum_{\mu\nu\in E(\Gamma)} \left[{\delta_\Gamma}^2(\mu) + {\delta_\Gamma}^2(\nu)\right]^2.$$

Benzenoid series is a family of molecular graphs, which are generalizations of benzene molecule C_6. We can see the first three members of benzenoid series in Fig. 1 (H_1= Benzene, H_2= circumcoronene, H3= circumcoronene). In general, the benzenoid series are shown in Fig. 2. The benzene molecule is a usual molecule in chemistry, physics, and nanosciences. This molecule is very useful to synthesize aromatic compounds [5, 7, 9, 22, 23].

Alameri et al. [2, 4, 3] (2020) defined new degree-based descriptors, denoted by the Yemen-index or (Y-index), defined as:

$$Y(\Gamma) = \sum_{\mu\in V(\Gamma)} \delta_\Gamma^4(\mu) = \sum_{\mu\nu\in E(\Gamma)} [\delta_\Gamma^3(\mu) + \delta_\Gamma^3(\nu)].$$

Let (f=H_k :k≥1) be the Benzenoid Circumcoronene series (Fig. 2), then [26]

$$M_1(\mathrm{F}) = 54k^2 - 30k, \quad {}^{m}M_1(\mathrm{F}) = \frac{2}{3}k^2 + \frac{5}{36}k, \tag{1}$$

$$M_2(\mathrm{F}) = 81k^2 - 63k + 6, \quad {}^{m}M_2(\mathrm{F}) = k^2 + \frac{1}{3}k + \frac{1}{6}, \tag{2}$$

$$F(H_k) = 162k^2\text{â€“}114k. \tag{3}$$

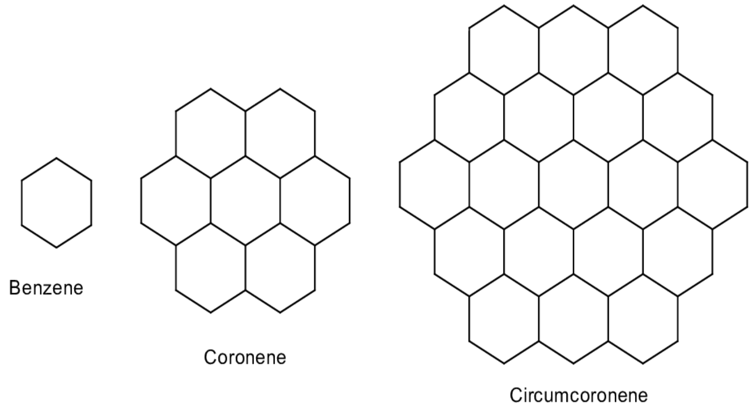

Figure 1: The edge partition of the Benzenoid Circumcoronene series H_k

The benzenoid circumcoronene series is a family of polycyclic aromatic hydrocarbons (PAHs) that are derived from circumcoronene by removing one or more adjacent benzene rings. Circumcoronene is a large PAH composed of twelve benzene rings fused together in a hexagonal pattern. The benzenoid circumcoronene series includes several important PAHs, including coronene (with six benzene rings), ovalene (with seven benzene rings), and circumovalene (with eight benzene rings). These compounds are of interest in various fields of chemistry and materials science due to their unique electronic and optical properties, as well as their potential applications in organic electronics, solar cells, and other optoelectronic devices.

In particular, circumcoronene and its derivatives have been studied for their ability to form self-assembled monolayers on various surfaces, which can be used for the development of molecular electronic devices. The benzenoid circumcoronene series is also of interest from a theoretical perspective, as it provides a useful framework for studying the relationship between molecular structure and electronic properties. Various topological indices and other mathematical descriptors have been developed to characterize the structure and properties of these compounds, and these have been used to develop predictive models for their electronic and optical behavior [26- 33].

2. Computational Results

In this section, we will provide definitions for new topological indices, which are the basis for deriving the mathematical formulas in this paper through the theorems in the same section. These formulas attract researchers and

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those interested to compare the indices and choose the most appropriate from an applied perspective. In more precise words, choosing topological indices that have a strong relationship (strong correlation coefficient) with the physical and chemical properties of some chemical compounds such as Benzenoid Circumcoronene Series.

Definition 2.1 The Multiplicative (Y-index) of a graph Γ is denoted by (PY), and defined as:

$$PY(\Gamma) = \prod_{\mu\nu\in E(\Gamma)} [\delta_\Gamma^3(\mu) + \delta_\Gamma^3(\nu)] = \prod_{\mu\in V(\Gamma)} \delta_\Gamma^4(\mu).$$

Definition 2.2 The modified (Y-index) and modified (Y-coindex) of a graph Γ are denoted by (^mY), (^{m-}Y) and defined as:

$$^mY(\Gamma) = \sum_{\mu\nu\in E(\Gamma)} \frac{1}{\delta_\Gamma^3(\mu) + \delta_\Gamma^3(\nu)} = \sum_{\mu\in V(\Gamma)} \frac{1}{\delta_\Gamma^4(\mu)}.$$

Definition 2.3 The generalized modified first Zagreb index of a graph Γ is defined as:

$$^mM_1^{\alpha+1}(\Gamma) = \sum_{\mu\nu\in E(\Gamma)} \frac{1}{\delta^\alpha(\mu) + \delta^\alpha(\nu)} = \sum_{\mu\in V(\Gamma)} \frac{1}{\delta^{\alpha+1}(\mu)}.$$

Definition 2.4 The generalized modified sum connectivity index of a graph Γ is defined as:

$$^mSM_1^\alpha(\Gamma) = \sum_{\mu\nu\in E(\Gamma)} \frac{1}{[\delta(\mu) + \delta(\nu)]^\alpha}.$$

Definition 2.5 The generalized modified product connectivity index of a graph Γ is defined as:

$$^mM_2^\alpha(\Gamma) = \sum_{\mu\nu\in E(\Gamma)} \frac{1}{[\delta(\mu) \cdot \delta(\nu)]^\alpha}.$$

Definition 2.6 The modified (Y-polynomail) of a graph Γ is defined as:

$$^mY(\Gamma, x) = \sum_{\mu\nu\in E(\Gamma)} x^{\frac{1}{\delta^3(\mu)+\delta^3(\nu)}}.$$

Theorem 2.1 Suppose that f=H_k is the circumcoronene series of Benzenoid (See Fig. 2), then,

$$(i) \quad PY(\mathrm{F}) = 16^6 \times 35^{12(k-1)} \times 54^{(9k^2-15k+6)},$$

$$(ii) \quad PF(\mathrm{F}) = 8^6 \times 13^{12(k-1)} \times 18^{(9k^2-15k+6)},$$

$$(iii) \quad Y(\mathrm{F}) = 486k^2 - 390k,$$

$$(iv) \quad ^mY(\mathrm{F}) = \frac{1}{6}k^2 + \frac{41}{630}k + \frac{361}{2520},$$

$$(v) \quad ^mF(\mathrm{F}) = \frac{1}{2}k^2 + \frac{7}{78}k + \frac{25}{156},$$

$(vi)\quad {}^{m}M_1^{\alpha+1}(\mathrm{F}) = \frac{3}{2^\alpha} + \frac{12}{2^\alpha+3^\alpha}(k-1) + \frac{1}{2\times 3^\alpha}(9k^2-15k+6),$

$(vii)\quad {}^{m}SM_1^{\alpha}(\mathrm{F}) = \frac{6}{4^\alpha} + \frac{12}{5^\alpha}(k-1) + \frac{1}{6^\alpha}(9k^2-15k+6),$

$(viii)\quad {}^{m}M_2^{\alpha}(\mathrm{F}) = \frac{6}{4^\alpha} + \frac{12}{6^\alpha}(k-1) + \frac{1}{9^\alpha}(9k^2-15k+6).$

Proof. The vertex and edge sets of f=H_k are divided into two vertex partitions and three edges partitions based on the degree of the end vertices, respectively, shown as:

$V_1(\mathrm{F}) = \{\mu \in V(\mathrm{F}): \delta(\mu) = 2\}, V_2(\mathrm{F}) = \{\nu \in V(\mathrm{F}): \delta(\nu) = 3\},$
$E_4(\mathrm{F}) = E_4^* = \{e = \mu\nu \in E(\mathrm{F}): \delta(\mu) = \delta(\nu) = 2, \delta^3(\mu) + \delta^3(\nu) = 16\},$ $E_5(\mathrm{F}) = E_6^* = \{e = \mu\nu \in E(\mathrm{F}): \delta(\mu) = 2, \delta(\nu) = 3, \delta^3(\mu) + \delta^3(\nu) = 35\},$ $E_6(\mathrm{F}) = E_9^* = \{e = \mu\nu \in E(\mathrm{F}): \delta(\mu) = \delta(\nu) = 3, \delta^3(\mu) + \delta^3(\nu) = 54\}.$

The partitions of the vertex set and edge set V(f) & E(f) are given in (Tables 1,2)

Table 1: The vertex partitions of circumcoronene series of Benzenoid H_k

Vertex partition	**V_2**	**V_3**
Cardinality	6k	6k(k-1)

Table 2: The edge partitions of circumcoronene series of Benzenoid H_k

Edge partition	**$E_4=E_4^*$**	**$E_5=E_6^*$**	**$E_6=E_9^*$**
Cardinality	6	12(k-1)	$9.k^2$-15k+6

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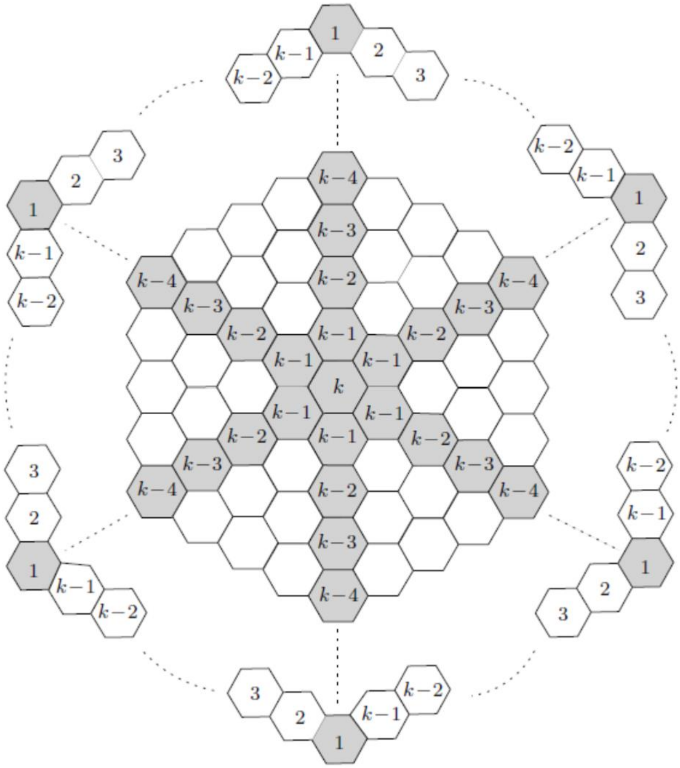

Figure 2: Generalized Benzenoid Circumcoronene series

Then, by the concept of the Multiplicative (Y-index), Multiplicative F-index, Y-index, the modified (Y-index), modified (F-index), the generalized modified first Zagreb index, the generalized modified sum connectivity index, and the generalized modified product connectivity index we have

$$(i)\quad PY(\mathrm{F}) = \prod_{\mu\nu\in E(\mathrm{F})} [\delta_{\mathrm{F}}^3(\mu) + \delta_{\mathrm{F}}^3(\nu)]$$

$$= \prod_{\mu\nu\in E_4^*(\mathrm{F})} [\delta_{\mathrm{F}}^3(\mu) + \delta_{\mathrm{F}}^3(\nu)] \times \prod_{\mu\nu\in E_6^*(\mathrm{F})} [\delta_{\mathrm{F}}^3(\mu) + \delta_{\mathrm{F}}^3(\nu)]$$

$$\times \prod_{\mu\nu\in E_9^*(\mathrm{F})} [\delta_{\mathrm{F}}^3(\mu) + \delta_{\mathrm{F}}^3(\nu)] = 16^{|E_4^*(\mathrm{F})|} \times 35^{|E_6^*(\mathrm{F})|} \times 54^{|E_9^*(\mathrm{F})|}. \quad \square$$

$$(ii)\quad PF(\mathrm{F}) = \prod_{\mu\nu\in E(\mathrm{F})} [\delta_{\mathrm{F}}^2(\mu) + \delta_{\mathrm{F}}^2(\nu)]$$

$$= \prod_{\mu\nu\in E_4^*(\mathrm{F})} [\delta_{\mathrm{F}}^2(\mu) + \delta_{\mathrm{F}}^2(\nu)] \times \prod_{\mu\nu\in E_6^*(\mathrm{F})} [\delta_{\mathrm{F}}^2(\mu) + \delta_{\mathrm{F}}^2(\nu)]$$

$$\times \prod_{\mu\nu\in E_9^*(\mathrm{F})} [\delta_{\mathrm{F}}^2(\mu) + \delta_{\mathrm{F}}^2(\nu)] = 8^{|E_4^*(\mathrm{F})|} \times 13^{|E_6^*(\mathrm{F})|} \times 18^{|E_9^*(\mathrm{F})|}. \quad \square$$

$$(iii)\quad Y(\mathrm{F})=\sum_{\mu\nu\in E(\mathrm{F})}[\delta_{\mathrm{F}}^{3}(\mu)+\delta_{\mathrm{F}}^{3}(\nu)]$$

$$=\sum_{\mu\nu\in E_4^*(\mathrm{F})}[\delta_{\mathrm{F}}^{3}(\mu)+\delta_{\mathrm{F}}^{3}(\nu)]+\sum_{\mu\nu\in E_6^*(\mathrm{F})}[\delta_{\mathrm{F}}^{3}(\mu)+\delta_{\mathrm{F}}^{3}(\nu)]$$

$$+\sum_{\mu\nu\in E_9^*(\mathrm{F})}[\delta_{\mathrm{F}}^{3}(\mu)+\delta_{\mathrm{F}}^{3}(\nu)]=16|E_4^*(\mathrm{F})|+35|E_6^*(\mathrm{F})|+54|E_9^*(\mathrm{F})|$$

$$=96+420(k-1)+54(9k^2-15k+6).\quad\square$$

$$(iv)\quad {}^{m}Y(\mathrm{F})=\sum_{\mu\nu\in E(\mathrm{F})}\frac{1}{\delta_{\mathrm{F}}^{3}(\mu)+\delta_{\mathrm{F}}^{3}(\nu)}=\sum_{\mu\nu\in E_4^*(\mathrm{F})}\frac{1}{\delta_{\mathrm{F}}^{3}(\mu)+\delta_{\mathrm{F}}^{3}(\nu)}+\sum_{\mu\nu\in E_6^*(\mathrm{F})}\frac{1}{\delta_{\mathrm{F}}^{3}(\mu)+\delta_{\mathrm{F}}^{3}(\nu)}$$

$$+\sum_{\mu\nu\in E_9^*(\mathrm{F})}\frac{1}{\delta_{\mathrm{F}}^{3}(\mu)+\delta_{\mathrm{F}}^{3}(\nu)}=\frac{1}{16}|E_4^*(\mathrm{F})|+\frac{1}{35}|E_6^*(\mathrm{F})|+\frac{1}{54}|E_9^*(\mathrm{F})|$$

$$=\frac{6}{16}+\frac{12}{35}(k-1)+\frac{1}{54}(9k^2-15k+6).$$

$$(v)\quad {}^{m}F(\mathrm{F})=\sum_{\mu\nu\in E(\mathrm{F})}\frac{1}{\delta_{\mathrm{F}}^{2}(\mu)+\delta_{\mathrm{F}}^{2}(\nu)}=\sum_{\mu\nu\in E_4^*(\mathrm{F})}\frac{1}{\delta_{\mathrm{F}}^{2}(\mu)+\delta_{\mathrm{F}}^{2}(\nu)}+\sum_{\mu\nu\in E_6^*(\mathrm{F})}\frac{1}{\delta_{\mathrm{F}}^{2}(\mu)+\delta_{\mathrm{F}}^{2}(\nu)}$$

$$+\sum_{\mu\nu\in E_9^*(\mathrm{F})}\frac{1}{\delta_{\mathrm{F}}^{2}(\mu)+\delta_{\mathrm{F}}^{2}(\nu)}=\frac{1}{8}|E_4^*(\mathrm{F})|+\frac{1}{13}|E_6^*(\mathrm{F})|+\frac{1}{18}|E_9^*(\mathrm{F})|$$

$$=\frac{6}{8}+\frac{12}{13}(k-1)+\frac{1}{18}(9k^2-15k+6).$$

$$(vi)\quad {}^{m}M_1^{\alpha+1}(\mathrm{F})=\sum_{\mu\nu\in E(\mathrm{F})}\frac{1}{\delta^{\alpha}(\mu)+\delta^{\alpha}(\nu)}=\sum_{\mu\nu\in E_4^*(\mathrm{F})}\frac{1}{\delta^{\alpha}(\mu)+\delta^{\alpha}(\nu)}$$

$$+\sum_{\mu\nu\in E_6^*(\mathrm{F})}\frac{1}{\delta^{\alpha}(\mu)+\delta^{\alpha}(\nu)}+\sum_{\mu\nu\in E_9^*(\mathrm{F})}\frac{1}{\delta^{\alpha}(\mu)+\delta^{\alpha}(\nu)}$$

$$=\frac{1}{2^{\alpha}+2^{\alpha}}|E_4^*(\mathrm{F})|+\frac{1}{2^{\alpha}+3^{\alpha}}|E_6^*(\mathrm{F})|+\frac{1}{3^{\alpha}+3^{\alpha}}|E_9^*(\mathrm{F})|.$$

$$(vii)\quad {}^{m}SM_1^{\alpha}(\mathrm{F})=\sum_{\mu\nu\in E(\mathrm{F})}\frac{1}{[\delta(\mu)+\delta(\nu)]^{\alpha}}=\sum_{\mu\nu\in E_4^*(\mathrm{F})}\frac{1}{[\delta(\mu)+\delta(\nu)]^{\alpha}}$$

$$+\sum_{\mu\nu\in E_6^*(\mathrm{F})}\frac{1}{[\delta(\mu)+\delta(\nu)]^{\alpha}}+\sum_{\mu\nu\in E_9^*(\mathrm{F})}\frac{1}{[\delta(\mu)+\delta(\nu)]^{\alpha}}$$

$$=\frac{1}{[2+2]^{\alpha}}|E_4^*(\mathrm{F})|+\frac{1}{[2+3]^{\alpha}}|E_6^*(\mathrm{F})|+\frac{1}{[3+3]^{\alpha}}|E_9^*(\mathrm{F})|.$$

$$(viii)\quad {}^{m}M_2^{\alpha}(\mathrm{F}) = \sum_{\mu\nu\in E(\mathrm{F})} \frac{1}{[\delta(\mu)\cdot\delta(\nu)]^{\alpha}} = \sum_{\mu\nu\in E_4^*(\mathrm{F})} \frac{1}{[\delta(\mu)\cdot\delta(\nu)]^{\alpha}}$$
$$+ \sum_{\mu\nu\in E_6^*(\mathrm{F})} \frac{1}{[\delta(\mu)\cdot\delta(\nu)]^{\alpha}} + \sum_{\mu\nu\in E_9^*(\mathrm{F})} \frac{1}{[\delta(\mu)\cdot\delta(\nu)]^{\alpha}}$$
$$= \frac{1}{[2\cdot 2]^{\alpha}}|E_4^*(\mathrm{F})| + \frac{1}{[2\cdot 3]^{\alpha}}|E_6^*(\mathrm{F})| + \frac{1}{[3\cdot 3]^{\alpha}}|E_9^*(\mathrm{F})|. \quad \square$$

Corollary 2.1 Suppose that S_r is the n[th] level in chain of Benzenoid System. Then the multiplicative polynomials of S_r for the indices mentioned in (Theorem 3.3) are given as follows:

$$(i)\quad PY(\mathrm{F},x) = x^{486k^2-390k},$$
$$(ii)\quad PF(\mathrm{F},x) = x^{162k^2-114k},$$
$$(iii)\quad Y(\mathrm{F},x) = 6x^{16} + 12(k-1)x^{35} + (9k^2-15k+6)x^{54},$$
$$(iv)\quad {}^{m}Y(\mathrm{F},x) = 6x^{\frac{1}{16}} + 12(k-1)x^{\frac{1}{35}} + (9k^2-15k+6)x^{\frac{1}{54}},$$
$$(v)\quad F(\mathrm{F},x) = 6x^{8} + 12(k-1)x^{13} + (9k^2-15k+6)x^{18},$$
$$(vi)\quad {}^{m}F(\mathrm{F},x) = 6x^{\frac{1}{8}} + 12(k-1)x^{\frac{1}{13}} + (9k^2-15k+6)x^{\frac{1}{18}},$$
$$(vii)\quad {}^{m}M_1^{\alpha+1}(\mathrm{F},x) = 6x^{\frac{1}{2^{\alpha+1}}} + 12(k-1)x^{\frac{1}{2^{\alpha}+3^{\alpha}}} + (9k^2-15k+6)x^{\frac{1}{2\times 3^{\alpha}}}$$
$$(viii)\quad {}^{m}SM_1^{\alpha}(\mathrm{F},x) = 6x^{\frac{1}{4^{\alpha}}} + 12(k-1)x^{\frac{1}{5^{\alpha}}} + (9k^2-15k+6)x^{\frac{1}{6^{\alpha}}},$$
$$(ix)\quad {}^{m}M_2^{\alpha}(\mathrm{F},x) = 6x^{\frac{1}{4^{\alpha}}} + 12(k-1)x^{\frac{1}{6^{\alpha}}} + (9k^2-15k+6)x^{\frac{1}{9^{\alpha}}}.$$

Proof. By the concept of the PY-polynomial, F-polynomial, PF-polynomial, Y-polynomial, the modified Y-polynomial, modified F-polynomial, the generalized modified first Zagreb polynomial, the generalized modified sum connectivity polynomial, and the generalized modified product connectivity polynomial, we have

$$(i)\quad PY(\mathrm{F},x) = \prod_{\mu\nu\in E(\mathrm{F}} x^{[\delta_{\mathrm{F}}^3(\mu)+\delta_{\mathrm{F}}^3(\nu)]} = \prod_{\mu\nu\in E_4^*(\mathrm{F})} x^{[\delta_{\mathrm{F}}^3(\mu)+\delta_{\mathrm{F}}^3(\nu)]} \times \prod_{\mu\nu\in E_6^*(\mathrm{F})} x^{[\delta_{\mathrm{F}}^3(\mu)+\delta_{\mathrm{F}}^3(\nu)]}$$
$$\times \prod_{\mu\nu\in E_9^*(\mathrm{F})} x^{[\delta_{\mathrm{F}}^3(\mu)+\delta_{\mathrm{F}}^3(\nu)]}$$
$$= [x^{16}]^{|E_4^*(\mathrm{F})|} \times [x^{35}]^{|E_6^*(\mathrm{F})|} \times [x^{54}]^{|E_9^*(\mathrm{F})|}.$$

$$(ii)\quad PF(\mathrm{F},x)=\prod_{\mu\nu\in E(\mathrm{F})} x^{[\delta_{\mathrm{F}}^{2}(\mu)+\delta_{\mathrm{F}}^{2}(\nu)]}=\prod_{\mu\nu\in E_4^*(\mathrm{F})} x^{[\delta_{\mathrm{F}}^{2}(\mu)+\delta_{\mathrm{F}}^{2}(\nu)]}\times\prod_{\mu\nu\in E_6^*(\mathrm{F})} x^{[\delta_{\mathrm{F}}^{2}(\mu)+\delta_{\mathrm{F}}^{2}(\nu)]}$$
$$\times\prod_{\mu\nu\in E_9^*(\mathrm{F})} x^{[\delta_{\mathrm{F}}^{2}(\mu)+\delta_{\mathrm{F}}^{2}(\nu)]}$$
$$=[x^{8}]^{|E_4^*(\mathrm{F})|}\times[x^{13}]^{|E_6^*(\mathrm{F})|}\times[x^{18}]^{|E_9^*(\mathrm{F})|}.$$

$$(iii)\quad Y(\mathrm{F},x)=\sum_{\mu\nu\in E(\mathrm{F}} x^{[\delta^{3}(\mu)+\delta^{3}(\nu)]}=\sum_{\mu\nu\in E_4^*(\mathrm{F})} x^{[\delta^{3}(\mu)+\delta^{3}(\nu)]}+\sum_{\mu\nu\in E_6^*(\mathrm{F})} x^{[\delta^{3}(\mu)+\delta^{3}(\nu)]}$$
$$+\sum_{\mu\nu\in E_6^*(\mathrm{F})} x^{[\delta^{3}(\mu)+\delta^{3}(\nu)]}$$
$$=|E_4^*(\mathrm{F})|x^{16}+|E_6^*(\mathrm{F})|x^{35}+|E_9^*(\mathrm{F})|x^{54}.$$

$$(iv)\quad {}^{m}Y(\mathrm{F},x)=\sum_{\mu\nu\in E(\mathrm{F})} x^{\frac{1}{\delta^{3}(\mu)+\delta^{3}(\nu)}}=\sum_{\mu\nu\in E_4^*(\mathrm{F})} x^{\frac{1}{\delta^{3}(\mu)+\delta^{3}(\nu)}}+\sum_{\mu\nu\in E_6^*(\mathrm{F})} x^{\frac{1}{\delta^{3}(\mu)+\delta^{3}(\nu)}}$$
$$+\sum_{\mu\nu\in E_9^*(\mathrm{F})} x^{\frac{1}{\delta^{3}(\mu)+\delta^{3}(\nu)}}=|E_4^*(\mathrm{F})|x^{\frac{1}{16}}+|E_6^*(\mathrm{F})|x^{\frac{1}{35}}+|E_9^*(\mathrm{F})|x^{\frac{1}{54}}.$$

$$(v)\quad F(\mathrm{F},x)=\sum_{\mu\nu\in E(\mathrm{F}} x^{[\delta^{2}(\mu)+\delta^{2}(\nu)]}=\sum_{\mu\nu\in E_4^*(\mathrm{F})} x^{[\delta^{2}(\mu)+\delta^{2}(\nu)]}+\sum_{\mu\nu\in E_6^*(\mathrm{F})} x^{[\delta^{2}(\mu)+\delta^{2}(\nu)]}$$
$$+\sum_{\mu\nu\in E_6^*(\mathrm{F})} x^{[\delta^{2}(\mu)+\delta^{2}(\nu)]}$$
$$=|E_4^*(\mathrm{F})|x^{8}+|E_6^*(\mathrm{F})|x^{13}+|E_9^*(\mathrm{F})|x^{18}.$$

$$(vi)\quad {}^{m}F(\mathrm{F},x)=\sum_{\mu\nu\in E(\mathrm{F})} x^{\frac{1}{\delta^{2}(\mu)+\delta^{2}(\nu)}}=\sum_{\mu\nu\in E_4^*(\mathrm{F})} x^{\frac{1}{\delta^{2}(\mu)+\delta^{2}(\nu)}}+\sum_{\mu\nu\in E_6^*(\mathrm{F})} x^{\frac{1}{\delta^{2}(\mu)+\delta^{2}(\nu)}}$$
$$+\sum_{\mu\nu\in E_9^*(\mathrm{F})} x^{\frac{1}{\delta^{2}(\mu)+\delta^{2}(\nu)}}=|E_4^*(\mathrm{F})|x^{\frac{1}{8}}+|E_6^*(\mathrm{F})|x^{\frac{1}{13}}+|E_9^*(\mathrm{F})|x^{\frac{1}{18}}.$$

$$(vii)\quad {}^{m}M_1^{\alpha+1}(\mathrm{F},x)=\sum_{\mu\nu\in E(\mathrm{F})} x^{\frac{1}{\delta^{\alpha}(\mu)+\delta^{\alpha}(\nu)}}=\sum_{\mu\nu\in E_4^*(\mathrm{F})} x^{\frac{1}{\delta^{\alpha}(\mu)+\delta^{\alpha}(\nu)}}+\sum_{\mu\nu\in E_6^*(\mathrm{F})} x^{\frac{1}{\delta^{\alpha}(\mu)+\delta^{\alpha}(\nu)}}$$
$$+\sum_{\mu\nu\in E_9^*(\mathrm{F})} x^{\frac{1}{\delta^{\alpha}(\mu)+\delta^{\alpha}(\nu)}}=x^{\frac{1}{2^{\alpha}+2^{\alpha}}}|E_4^*(\mathrm{F})|+x^{\frac{1}{2^{\alpha}+3^{\alpha}}}|E_6^*(\mathrm{F})|+x^{\frac{1}{3^{\alpha}+3^{\alpha}}}|E_9^*(\mathrm{F})|.$$

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$$(viii)\quad {}^{m}SM_1^{\alpha}(\mathrm{F},x)=\sum_{\mu\nu\in E(\mathrm{F})} x^{\frac{1}{[\delta(\mu)+\delta(\nu)]^{\alpha}}}$$

$$=\sum_{\mu\nu\in E_4^*(\mathrm{F})} x^{\frac{1}{[\delta(\mu)+\delta(\nu)]^{\alpha}}}+\sum_{\mu\nu\in E_6^*(\mathrm{F})} x^{\frac{1}{[\delta(\mu)+\delta(\nu)]^{\alpha}}}$$

$$+\sum_{\mu\nu\in E_9^*(\mathrm{F})} x^{\frac{1}{[\delta(\mu)+\delta(\nu)]^{\alpha}}}=|E_4^*(\mathrm{F})|x^{\frac{1}{[2+2]^{\alpha}}}+|E_6^*(\mathrm{F})|x^{\frac{1}{[2+3]^{\alpha}}}+|E_9^*(\mathrm{F})|x^{\frac{1}{[3+3]^{\alpha}}}.$$

$$(ix)\quad {}^{m}M_2^{\alpha}(\mathrm{F},x)=\sum_{\mu\nu\in E(\mathrm{F})} x^{\frac{1}{[\delta(\mu)\cdot\delta(\nu)]^{\alpha}}}=\sum_{\mu\nu\in E_4^*(\mathrm{F})} x^{\frac{1}{[\delta(\mu)\cdot\delta(\nu)]^{\alpha}}}+\sum_{\mu\nu\in E_6^*(\mathrm{F})} x^{\frac{1}{[\delta(\mu)\cdot\delta(\nu)]^{\alpha}}}$$

$$+\sum_{\mu\nu\in E_9^*(\mathrm{F})} x^{\frac{1}{[\delta(\mu)\cdot\delta(\nu)]^{\alpha}}}=|E_4^*(\mathrm{F})|x^{\frac{1}{[2\cdot 2]^{\alpha}}}+|E_6^*(\mathrm{F})|x^{\frac{1}{[2\cdot 3]^{\alpha}}}+|E_9^*(\mathrm{F})|x^{\frac{1}{[3\cdot 3]^{\alpha}}}.$$

3. Conclusion

The purpose of this paper is to study some well-known indices of a molecular structure H_k. Here, we studied Multiplicative Forgotten, Multiplicative Yemen, Yemen, modified Yemen, modified Forgotten, generalized modified first Zagreb, general modified sum connectivity, and general modified product connectivity indices. Furthermore, polynomials of the Benzenoid Circumcoronene Series have been computed. In future, these formulas attract researchers and those interested to compare the indices and choose the most appropriate from an applied perspective.

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Data Availability

The data used to support the findings of this work are cited at relevant places within the text as references.

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Conflicts of Interest

The authors declare that they have no conflicts of interest.

References

[1] V. Andova, *Some Distance and Degree Graph Invariants and Fullerene Structures*, Doctoral Thesis. 2013.

[2] A. Alameria, N. Al-Naggara, M. Alromaimah, M. Alsharafi, *Y-index of some graph operations*, International Journal of Applied Engineering Research (IJAER). 15 (2), (2020): 173-179.

[3] A. Ayache, A. Alameri, M. Alsharafi, H. Ahmed, *The Second Hyper-Zagreb Coindex of Chemical Graphs and Some Applications*, Journal of Chemistry, 2021, (2021): 3687533.

[4] A. Alameri, M. Al-Rumaima, M. Almazah, *Y-coindex of graph operations and its applications of molecular descriptors*, Journal of Molecular Structure (2020): 128754.

[5] A. Alameri, M, Alsharafi, E. Ali, M. S. Gumaan, *A note on Topological indices and coindices of disjunction and symmetric difference of graphs*, Discrete Applied Mathematics, 304, (2021): 230-235.

[6] A. Ashrafi, T. Doslic, A. Hamzeh, *The Zagreb coindices of graph operations*, Discrete applied mathematics 158.15 (2010): 1571-1578.

[7] M. Alsharafi, M. Shubatah, A. Alameri, *On the Hyper-Zagreb coindex of some Graphs*, J. Math. Comput.Sci. 10, (2020): 1875-1890.

[8] M. Alsharafi, A. Alameri, *The F-index and coindex of V-Phenylenic Nanotubes and Nanotorus and their molecular complement graphs*, Nanosystems Physics Chemistry Mathematics, 12, (2021): 263-270.

[9] A. Behmaram, H. Yousefi-Azari, A. Ashrafi, *Some New Results on Distance-Based Polynomials*, Commun. Math. Comput. Chem. 65(2011) 39-50.

[10] K. Chendrasekharan, S. Pattabiraman, and M. Nagarajan, *Zagreb Indices And Coindices Of Product Graphs*, Journal Of Prime Research In Mathematics 10 (2015): 80-91.

[11] N. De, S. Nayeem and A. Pal, *The F-index of some graph operations*, Discrete Mathematics, Algorithms and Applications 8.02 (2016): 1650025.

[12] N. De, S. Nayeem and A. Pal, *The F-coindex of some graph operations*, SpringerPlus 5.1 (2016): 221.

[13] N. De, *Computing F-Index of Different Corona Products of Graphs*, Bulletin of Mathematical Sciences and Applications Vol 19 (2017): 25.

[14] N. De, *F-index and coindex of some derived graphs*, arXiv:1610.02175 (2016).

https://doi.org/10.59222/ustjet.2.1.2

[15] B. Furtula, I. Gutman, *A forgotten topological index*, Journal of Mathematical Chemistry 53.4 (2015): 1184-1190.

[16] W. Gao, M. K. Siddiqui, M. Imran, M. Jamil, M. R. Farahani, *Forgotten topological index of chemical structure in drugs*, Saudi Pharmaceutical Journal 24.3 (2016): 258-264.

[17] S. Ghobadi, M. Ghorbaninejad, *On F-polynomial, multiple and hyper F-index of some molecular graphs*, Bulletin of Mathematical Sciences and Applications 20 (2018): 36-43.

[18] I. Gutman, *On Hyper-Zagreb index and coindex*, Bulletin T. CL de lâ€™AcadÂ´emie serbe des sciences et des arts 42 (2017): 1-8.

[19] I. Gutman, N. Trinajstic, *Graph theory and molecular orbitals*, Total electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972) 535-538.

[20] R. Jummannaver, I. Gutman, and R. Mundewadi, *On Zagreb Indices And Coindices Of Cluster Graphs*, Journal of the International Mathematical Virtual Institute Vol. 8(2018), 477-485

[21] M. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, *The first and second Zagreb indices of some graph operations*, Discrete applied mathematics 157.4 (2009): 804-811.

[22] R. Kumar, D. Nandappa, M. Kanna, P. Bettampady, *Redefined zagreb, Randic, Harmonic, GA indices of graphene*, Int. J. Math. Anal 11.10 (2017): 493-502.

[23] P. Ranjini, V. Lokesha, and A. Usha, *Relation between phenylene and hexagonal squeeze using harmonic index*, International Journal of Graph Theory 1.4 (2013): 116-121.

[24] G. Shirdel, A. M. Sayadi, *The hyper-Zagreb index of graph operations*, Iranian Journal of Mathematical Chemistry 4.2 (2013): 213-220.

[25] G. Wei, et al., *On the First and Second Zagreb and First and Second Hyper-Zagreb Indices of Carbon Nanocones CNC k* [n], Journal of Computational and Theoretical Nanoscience 13.10 (2016): 7475-7482.

[26] V.R. Kulli, *General topological indices of circumcoronene series of benzenoid*, International Research Journal of Pure Algebra 7.5 (2017), 748-753.

[27] Y. Zeren, A. Alameri, M. Alsharafi, A. Ayache, M. K. Jamil, *Degree-Based Molecular Descriptors of Chain Biphenylene*, Biointerface Research in Applied Chemistry, 13.5, (2023): 496.

[28] A. Modabish, A. Alameri, M. S. Gumaan, M. Alsharafi, *The second Hyper-Zagreb index of graph operations*, J. Math. Comput. Sci., 11 (2021): 1455-1469

[29] V.R.Kulli, *General topological indices of circumcoronene series of benzenoid*, International Research Journal of Pure Algebra,7.5, (2017), 748-753.

[30] M. S. Sardar et al. *Computation of Topological Indices of Double and Strong Double Graphs of Circumcoronene Series of Benzenoi*d, Journal of Mathematics, Vol. 2022, (2022): 5956802.

[31] A. Subhashini, J. Baskar Babujee, *Computing Degree-Based Topological Indices for Molecular Graphs*, Appl. Math. Inf. Sci. 13.S1, (2019): 31-37.

[32] J. Konsalraj et al. *Topological Analysis of PAHs using Irregularity based Indices*, Biointerface Research in Applied Chemistry, 12.3, (2022): 2970 - 2987.

[33] M. Alsharafi et al., *Degree-Based Topological Descriptors of Hexaphenylbenzene Molecule Graphs*, Polycyclic Aromatic Compounds, (2023) : 1- 20. https://doi.org/10.1080/10406638.2023.2190133