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## Research article

# Unveiling novel eccentric neighborhood forgotten indices for graphs and gaph operations: A comprehensive exploration of boiling point prediction

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Abstract: This paper marks a significant advancement in the field of chemoinformatics with the introduction of two novel topological indices: the forgotten eccentric neighborhood index (FENI) and the modified forgotten eccentric neighborhood index (MFENI). Uniquely developed for predicting the boiling points of various chemical substances, these indices offer groundbreaking tools in understanding and interpreting the thermal properties of compounds. The distinctiveness of our study lies in the in-depth exploration of the discriminative capabilities of FENI and MFENI. Unlike existing indices, they provide a nuanced capture of structural features essential for determining boiling points, a key factor in drug design and chemical analysis. Our comprehensive analyses demonstrate the superior predictive power of FENI and MFENI, highlighting their exceptional potential as innovative tools in the realms of chemoinformatics and pharmaceutical research. Furthermore, this study conducts an extensive investigation into their various properties. We present explicit results on the behavior of these indices in relation to diverse graph types and operations, including join, disjunction, composition and symmetric difference. These findings not only deepen our understanding of FENI and MFENI but also establish their practical versatility across a spectrum of chemical and pharmaceutical applications. Thus the introduction of FENI and MFENI represents a pivotal step forward in the predictive analysis of boiling points, setting a new standard in the field and opening avenues for future research advancements.

**Keywords:** eccentric neighborhood forgotten indices; modified eccentric neighborhood forgotten indices; boiling point; graph operations **Mathematics Subject Classification:** 05C12, 05C90

#### 1. Introduction

A topological index is a numerical representation derived from a graph's structural arrangement, independent of vertex labels. It remains consistent even for isomorphic graphs, indicating robustness. In mathematical chemistry, the focus is on deriving these indices for chemical graphs, correlating with intrinsic physicochemical attributes. This comes from the belief that molecular traits relate to atom valences and positions. Graph-theoretical language effectively conveys these ideas, making chemical graphs rich in real-world molecular information for precise modeling. According to Milan Randić [1], a topological index's acceptance depends on satisfying criteria: positive property correlations, structural interpretation, insightful potential, adaptability, simplicity, non-triviality, effective composition and rooted in structural abstractions. While some molecular attributes align clearly with indices, this is not uniform, leading to doubts about engineered indices and coincidental correlations. Yet. validating indices often involves understanding their relevance to molecular structure components linked to properties. Even when comprehension is elusive, dismissing outcomes hastily is unwise. Meticulous analysis might reveal overlooked physicochemical mechanisms. Given the complexity of ab initio methods for molecular treatment, topological indices remain essential tools in mathematical chemistry's landscape. Numerous distinct topological indices have undergone extensive exploration and application in QSAR/QSPR studies, yielding varying levels of effectiveness. Among the most valuable constants are those that fall into two overarching categories: distance-derived or bondadditive. The former group encompasses indices that find definition in vertex pair distances, while the latter includes indices formed by aggregating contributions across all edges. In the first category, the Wiener index and its various adaptations stand out [2], while the second category features indices such as the Randić index [3] and the Zagreb indices pair [4, 5]. The initiation of topological indices dates back to 1947, when chemist Wiener discovered the inaugural Wiener index [6]. This index was devised to predict boiling points of chemical compounds and is defined as

$$W(\zeta) = \frac{1}{2} \sum_{\{u,v\} \in V(\zeta)} d(u,v).$$
(1.1)

Building upon this initial index, a variety of new topological indices have been introduced to improve the accuracy of boiling point predictions for diverse chemical compounds. Recent advancements in this area are noteworthy. For an in-depth analysis of these developments in boiling point prediction, please consult reference [7], which highlights a pivotal discovery, i.e., the boiling point of benzenoid hydrocarbons shows a stronger correlation with the first Zagreb eccentricity index compared to the second. This crucial finding enhances our comprehension of these compounds' physical characteristics, opening new avenues for both their practical usage and theoretical exploration. In [8], the authors achieved a significant result in their Quantitative Structure-Property Relationship (QSPR) analysis: they were able to accurately predict the boiling points of these compounds using the fifth nearest neighbor (5th NN) entropy method. This finding holds significant importance due to the widespread application of benzene in diverse fields like pharmaceuticals, dyes and lubricants. We encourage interested readers to consult [9–11]. In recent scholarly discourse, there has been a notable surge of interest in the broader computational quandaries surrounding the determination of topological indices and their algebraic operations [12] presents a simplicial network's model to capture complex higher-order interactions in various systems. It examines the network's

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structure and derives the Sombor index, revealing key patterns like power-law behavior. The study underscores the model's effectiveness in understanding complex interactions. Also, [13] introduced the variable sum exdeg index was originally used for predicting the octanol-water partition coefficient of certain chemical compounds. It is a unique measure for a graph, calculated by summing up the products of the degree of each vertex raised to the power of a positive real number, with the real number being different from one. This paper, focuses on certain sub groups of tricyclic graphs. Identifying the graph that has the highest variable sum exdeg index from each subgroup ensures that all these graphs have perfect matching. This allows us to compare these graphs and determine which one in the larger collection has the highest value of this index.

In 2015, B. Furtula and I. Gutman [14] defined the forgotten index, or F-index, as follows:

$$F(\zeta) = \sum_{v \in V(\zeta)} d_{\zeta}^{3}(v) = \sum_{uv \in E(\zeta)} (d_{\zeta}^{2}(u) + d_{\zeta}^{2}(v)).$$
(1.2)

In a seminal study [15], both the forgotten topological index and the first Zagreb index played pivotal roles in computing the total  $\pi$ -electron energy. Acting as indicators, these indices enabled the assessment of the intricate branching intricacies within the molecule's carbon-atom framework. Despite an initial lack of attention, the F-index has emerged as a focus of recent research, attributed to the noteworthy investigation by Furtula and Gutman [15]. This study elucidated the F-index's underlying principles and unveiled its predictive prowess, akin to that of the first Zagreb index. Remarkably, both indices exhibited strong correlation coefficients, exceeding 0.95, when linked with entropy and acetic factor. Notably, [16] accentuated the significance of the F-index by showcasing its accurate prognostication of the logarithm of the octanol-water partition coefficient. Sufficient conditions for a graph to be  $\ell$ -connected,  $\ell$ -deficient,  $\ell$ -Hamiltonian and  $\ell$ -independent in terms of the forgotten topological index is presented in [17]. The forgotten index assumes a crucial role by upholding molecular structure symmetry, while providing a robust mathematical foundation to anticipate the physicochemical attributes of molecules. Recent strides in understanding the forgotten index and its diverse applications have been meticulously documented in contemporary works [18-21]. Motivated by this backdrop, our current study delves into unearthing a novel iteration of this index. We specifically concentrate on its potential in predicting the boiling points of primary amines. By expanding our understanding of this index's capabilities, we aim to contribute to the advancement of predictive models for molecular properties, enhancing their practical utility in various scientific and industrial contexts.

Throughout this paper, we consider only simple connected graphs. For a graph  $\zeta = (V(\zeta), E(\zeta))$ ,  $V(\zeta)$  and  $E(\zeta)$  denote the set of vertices and edges, respectively. The set  $\aleph(v)$  of all neighbors of v is called the open neighborhood of v. Thus,  $\aleph(v) = \{u \in V : uv \in E(\zeta)\}$ . The degree  $d_{\zeta}(u) = d(u)$  of a vertex u in  $\zeta$  is defined as  $d(u) = |\aleph(v)|$ . The distance  $d_{\zeta}(u, v)$  or d(u, v) [22] between two vertices in a graph  $\zeta$  is the length of the shortest path joining them. The eccentricity  $\varepsilon(u) = max_{v \in V(\zeta)}d(u, v)$ . The radius of  $\zeta$  is  $r(\zeta) = min_{v \in V(\zeta)} \varepsilon(v)$ , and the diameter of  $\zeta$  is  $D(\zeta) = max_{v \in V(\zeta)} \varepsilon(v)$ . For any graph  $\zeta$  with n vertices, we define  $V_{\omega}(\zeta) = \{v \in V(\zeta) : \varepsilon(v) = 1\}$ . In [23], Ahmed et al. introduced new degree-based topological indices known as eccentric neighborhood Zagreb indices which are defined as follows: Let  $\zeta = (V(\zeta), E(\zeta))$  be a connected simple graph and  $\delta_{en}(v) = \sum_{u \in \aleph(v)} \varepsilon(u)$  be the eccentricity neighborhood degree. Then, the first, second and third eccentric neighborhood Zagreb indices are defined as follows:

$$E_{\aleph}M_1(\zeta) = \sum_{\nu \in V(\zeta)} \delta_{en}^2(\nu), \qquad (1.3)$$

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$$E_{\aleph}M_2(\zeta) = \sum_{uv \in E(\zeta)} \delta_{en}(u)\delta_{en}(v), \qquad (1.4)$$

$$E_{\aleph}M_{3}(\zeta) = \sum_{uv \in E(\zeta)} (\delta_{en}(u) + \delta_{en}(v)).$$
(1.5)

Continuing along this research trajectory, our investigation delves into the intricate dynamics of the eccentric neighborhood forgotten index and the eccentric neighborhood modified forgotten index. We systematically analyze their behavior in response to a spectrum of graph operations. Notably, our inquiry extends to the application of these findings within the domain of molecular graphs, with a specific focus on primary amines groups. In recent scholarly discourse, there has been a notable surge of interest in the broader computational quandaries surrounding the determination of topological indices and their algebraic operations [24–30]. In this intellectual milieu, we make a significant contribution by introducing and rigorously defining the eccentric neighborhood forgotten index and the eccentric neighborhood modified forgotten index. Their precise formulations are as follows:

$$E_{\aleph}F(\zeta) = \sum_{\nu \in V(\zeta)} \delta_{en}^3(\nu), \tag{1.6}$$

$$E_{\aleph}F^{*}(\zeta) = \sum_{uv \in E(\zeta)} (\delta_{en}^{2}(u) + \delta_{en}^{2}(v)).$$
(1.7)

In this study, our presentation follows a structured and methodical progression.

Section 2 introduces preliminary findings, laying a foundational groundwork for the more intricate discussions that ensue. In Subsection 2.1, we delve into the computational methodologies associated with two distinct indices: the eccentric neighborhood forgotten index (ENFI) and its modified counterpart, the modified eccentric neighborhood forgotten index (MENFI). Our exploration will encompass their applicability across a diverse range of graph structures. An integral component of this subsection will be dedicated to the nuances of graph products, a specialized category within graph operations. As we transition further into Subsection 2.1, we provide an in-depth analysis of how these indices integrate seamlessly into the expansive domain of graph theory. Section 3 pivots our focus towards the pragmatic relevance of topological indices, emphasizing their pivotal role in predicting specific physicochemical attributes. To substantiate our assertions, we employ the robust technique of nonlinear regression analysis. Our choice of primary amines as the subject of study is motivated by their structural heterogeneity, positioning them as ideal candidates for this analytical endeavor. Within this context, we juxtapose the Wiener index with ENFI and MENFI, aiming to discern potential correlations between these indices and the boiling points intrinsic to primary amines. Finally, Section 4 contains our conclusions and reflections on the study.

## 2. Preliminaries

In this section, we present a set of preliminary results that will serve as essential foundations for the subsequent segments of the paper. These preliminary findings are integral for establishing the groundwork necessary to advance the discussion further.

**Lemma 2.1.** [5] Let  $\zeta_1$  and  $\zeta_2$  be graphs. Then,

- (a)  $d_{\zeta_1 \times \zeta_2}(u, v) = d_{\zeta_1}(u) + d_{\zeta_2}(v)$ ,
- **(b)**  $d_{\zeta_1[\zeta_2]}(u,v) = |V(\zeta_2)|d_{\zeta_1}(u) + d_{\zeta_2}(v),$
- (c)  $d_{\zeta_1+\zeta_2}(u) = \begin{cases} d_{\zeta_1}(u) + |V(\zeta_2)|, & u \in V(\zeta_1); \\ d_{\zeta_2}(u) + |V(\zeta_1)|, & u \in V(\zeta_2). \end{cases}$
- (d)  $d_{\zeta_1 \vee \zeta_2}(u, v) = |V(\zeta_2)|d_{\zeta_1}(u) + |V(\zeta_1)|d_{\zeta_2}(v) d_{\zeta_1}(u)d_{\zeta_2}(v),$
- (e)  $d_{\zeta_1 \oplus \zeta_2}(u, v) = |V(\zeta_2)|d_{\zeta_1}(u) + |V(\zeta_1)|d_{\zeta_2}(v) 2d_{\zeta_1}(u)d_{\zeta_2}(v).$
- (f)  $|V(\zeta_1 \times \zeta_2)| = |V(\zeta_1 \vee \zeta_2)| = |V(\zeta_1[\zeta_2])| = |V(\zeta_1 \oplus \zeta_2)| = |V(\zeta_1)||V(\zeta_2)|,$   $|E(\zeta_1 \times \zeta_2)| = |E(\zeta_1)||V(\zeta_2)| + |V(\zeta_1)||E(\zeta_2)|,$   $|E(\zeta_1 + \zeta_2)| = |E(\zeta_1)| + |E(\zeta_2)| + |V(\zeta_1)||V(\zeta_2)|,$   $|E(\zeta_1[\zeta_2])| = |E(\zeta_1)||V(\zeta_2)|^2 + |E(\zeta_2)||V(\zeta_1)|,$   $|E(\zeta_1 \vee \zeta_2)| = |E(\zeta_1)||V(\zeta_2)|^2 + |E(\zeta_2)||V(\zeta_1)|^2 - 2|E(\zeta_1)||E(\zeta_2)|,$  $|E(\zeta_1 \oplus \zeta_2)| = |E(\zeta_1)||V(\zeta_2)|^2 + |E(\zeta_2)||V(\zeta_1)| - 4|E(\zeta_1)||E(\zeta_2)|.$

**Lemma 2.2.** [31] Suppose  $\zeta_1$  and  $\zeta_2$  be graphs. Then,

(a) 
$$\varepsilon_{\zeta_{1}+\zeta_{2}}(u) = \begin{cases} 1, & \text{if } \varepsilon_{\zeta_{i}}(u) = 1; \\ 2, & \text{if } \varepsilon_{\zeta_{i}}(u) \ge 2, \end{cases}$$
 where  $i \in \{1, 2\}$ .  
(b)  $\varepsilon_{\zeta_{1}\vee\zeta_{2}}(u, v) = \begin{cases} 1, & \text{if } \varepsilon_{\zeta_{1}}(u) = \varepsilon_{\zeta_{2}}(v) = 1; \\ 2, & \text{if } \varepsilon_{\zeta_{1}}(u) \ge 2 \text{ or } \varepsilon_{\zeta_{2}}(v) \ge 2. \end{cases}$   
(c)  $\varepsilon_{\zeta_{1}[\zeta_{2}]}(u, v) = \begin{cases} 1, & \text{if } \varepsilon_{\zeta_{1}}(u) = \varepsilon_{\zeta_{2}}(v) = 1; \\ 2, & \text{if } \varepsilon_{\zeta_{1}}(u) = 2 \text{ or } \varepsilon_{\zeta_{2}}(v) \ge 2; \\ \varepsilon_{\zeta_{1}}(u), & \text{if } \varepsilon_{\zeta_{1}}(u) \ge 2. \end{cases}$ 

(d)  $\varepsilon_{\zeta_1\oplus\zeta_2}(u,v) = 2.$ 

Corollary 2.1. [19]

$$F(\zeta + \mathcal{F}) = F(\zeta) + F(\mathcal{F}) + 3(V(\mathcal{F})M_1(\zeta) + V(\zeta)M_1(\mathcal{F})) + 6(V(\mathcal{F})^2|E(\zeta)| + V(\zeta)^2|E(\mathcal{F})|)$$
  
+  $(V(\mathcal{F}))^3V(\zeta) + (V(\zeta))^3(\mathcal{F}).$ 

**Theorem 2.1.** [19]

$$F(\zeta[\mathcal{F}]) = (V(\mathcal{F}))^4 F(\zeta) + V(\zeta)F(\mathcal{F}) + 6(V(\mathcal{F}))^2 |E(\mathcal{F})| M_1(\zeta) + 6V(\mathcal{F})|E(\zeta)| M_1(\mathcal{F}).$$

#### **Theorem 2.2.** [19]

$$\begin{split} F(\zeta \vee \mathcal{F}) = &(V(\mathcal{F}))^4 F(\zeta) + (V(\zeta))^4 F(\mathcal{F}) - F(\zeta)F(\mathcal{F}) + 6V(\zeta)(V(\mathcal{F}))^2 |E(\mathcal{F})| M_1(\zeta) \\ &+ 6(V(\zeta))^2 V(\mathcal{F}) |E(\zeta)| M_1(\mathcal{F}) + 3V(\mathcal{F})F(\zeta) M_1(\mathcal{F}) + 3V(\zeta)F(\mathcal{F}) M_1(\zeta) \\ &- 6(V(\mathcal{F}))^2 |E(\mathcal{F})| F(\zeta) - 6(V(\zeta))^2 |E(\zeta)| F(\mathcal{F}) - 6V(\zeta)V(\mathcal{F}) M_1(\zeta) M_1(\mathcal{F}). \end{split}$$

### **Theorem 2.3.** [19]

$$F(\zeta \oplus \mathcal{F}) = (V(\mathcal{F}))^4 F(\zeta) + (V(\zeta))^4 F(\mathcal{F}) - 8F(\zeta)F(\mathcal{F}) + 6V(\zeta)(V(\mathcal{F}))^2 |E(\mathcal{F})| M_1(\zeta) + 6(V(\zeta))^2 V(\mathcal{F}) |E(\zeta)| M_1(\mathcal{F}) + 12V(\mathcal{F})F(\zeta) M_1(\mathcal{F}) + 12V(\zeta)F(\mathcal{F}) M_1(\zeta) - 12(V(\mathcal{F}))^2 |E(\mathcal{F})| F(\zeta) - 12(V(\zeta))^2 |E(\zeta)| F(\mathcal{F}) - 12V(\zeta)V(\mathcal{F}) M_1(\zeta) M_1(\mathcal{F}).$$

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**Theorem 2.4.** [19]

$$F(\zeta \times \mathcal{F}) = V(\mathcal{F})F(\zeta) + V(\zeta)F(\mathcal{F}) + 6|E(\mathcal{F})|M_1(\zeta) + 6|E(\zeta)|M_1(\mathcal{F})$$

Lemma 2.3. [23]

(1) If  $\zeta \cong S_r$  is a star graph with r + 1 vertices, then

$$\delta_{en}(v) = \begin{cases} 1, & \text{if } v \text{ is pendent vertex;} \\ 2r, & \text{if } v \text{ is the center.} \end{cases}$$

(2) If  $\zeta \cong S_{r,s}$  is the double star with r + s + 2 vertices, then

$$\delta_{en}(v) = \begin{cases} 2, & \text{if } v \text{ is pendent vertex;} \\ 3r + 2, & \text{if } v \text{ is the center in first star;} \\ 3s + 2, & \text{if } v \text{ is the center in second star.} \end{cases}$$

(3) If  $\zeta \cong C_n$  with  $n \ge 4$ , then

$$\delta_{en}(v) = \begin{cases} n, & \text{if } n \text{ is even;} \\ n-1, & \text{if } n \text{ is odd.} \end{cases}$$

(4) If  $\zeta \cong W_n$  is the wheel graph with  $n \ge 5$  vertices, then

$$\delta_{en}(v) = \begin{cases} 2n-2, & \text{if } v \text{ is the center vertex;} \\ 5, & \text{otherwise.} \end{cases}$$

**Proposition 2.1.** [23] Let  $\zeta$  be a graph with  $D(\zeta) = r(\zeta) = t$ . Then,

$$E_{\aleph}M_1(\zeta) = t^2 M_1(\zeta), \quad E_{\aleph}M_2(\zeta) = t^2 M_2(\zeta), \quad E_{\aleph}M_3(\zeta) = t M_1(\zeta).$$

2.1. Computing ENFI and MENFI of graphs and graph operations

Within this section, we provide explicit formulas detailing the computation of ENFI and MENFI for various graph classes. Additionally, we explore graph operations stemming from binary graph operations, specifically recognized as graph products.

**Proposition 2.2.** (1) For star graph  $S_r$  with r+1 vertices, we have  $E_{\aleph}F(S_r) = 8r^3 + r$  and  $E_{\aleph}F^*(S_r) = 4r^3 + r$ .

(2) If  $\zeta \cong S_{r,s}$  with r + s + 2 vertices, then

$$E_{\aleph}F(S_{r,s}) = 27(r^3 + s^3) + 54(r^2 + s^2) + 44(r + s) + 16,$$
  
$$E_{\aleph}F^*(S_{r,s}) = 9(r^* + s^3) + 21(r^2 + s^2) + 20(r + s) + 8.$$

(3) Suppose  $\zeta \cong C_n$ ,  $n \ge 4$ . Then,

$$E_{\aleph}F(C_n) = \begin{cases} n^4, & \text{if } n \text{ is even;} \\ n(n-1)^3, & \text{if } n \text{ is odd.} \end{cases}$$
$$E_{\aleph}F^*(C_n) = \begin{cases} 2n^3, & \text{if } n \text{ is even;} \\ 2n^3 - 4n + 2n, & \text{if } n \text{ is odd.} \end{cases}$$

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(4) If  $\zeta \cong W_n$  is the wheel graph with  $n \ge 5$  vertices, then

$$E_{\aleph}F(W_n) = 8n^3 - 24n^2 + 149n - 133,$$
  
$$E_{\aleph}F^*(W_n) = 4n^3 - 12n^2 + 87n - 79.$$

A banana tree of type (r, s), denoted as  $B_{r,s}$  according to the definition by Chan et al. [32], is a graph formed by linking a single leaf from each of r instances of an *s*-star graph with a unique root vertex that is separate from all the *s*-stars.

**Lemma 2.4.** [23] Let  $\zeta \cong B_{r,s}$  with  $r \ge 2$  and  $s \ge 3$  and w as the root vertex. Then,

$$\delta_{en}(v) = \begin{cases} 5, & \text{if } v \text{ is pendent vertex;} \\ 4r, & \text{if } v = w; \\ 6s - 8, & \text{if } v \text{ is the center vertex;} \\ 8, & \text{if } v \in \{v : vw \in E(B_{r,s})\}. \end{cases}$$

**Proposition 2.3.** If  $\zeta \cong B_{r,s}$  with  $r \ge 2$  and  $s \ge 3$ , then

$$E_{\aleph}F(B_{r,s}) = 64r^3 + 216s^3r - 864s^2r + 1277sr - 250r,$$
$$E_{\aleph}F^*(B_{r,s}) = 16r^3 + 14r + 36s^3r - 132s^2r + 185sr.$$

*Proof.* Suppose  $\zeta \cong B_{r,s}$  with  $r \ge 2$  and  $s \ge 3$ . One can define the edge partitions of  $\zeta$  as following:  $E_1 = \{uv \in E(\zeta) : \delta_{en}(u) = 4r, \delta_{en}(v) = 8\}, E_2 = \{uv \in E(\zeta) : \delta_{en}(u) = 8, \delta_{en}(v) = 6s - 8\}$  and  $E_3 = \{uv \in E(\zeta) : \delta_{en}(u) = 6s - 8, \delta_{en}(v) = 5\}$ . Note that  $|E_1| = |E_2| = r$  and  $|E_3| = r(s - 2)$ . Hence, by applying Eqs (1.6) and (1.7) we get the required result.

**Proposition 2.4.** If  $\delta_{en}(u) \leq Dd(u)$  and  $rd(u) \leq \delta_{en}(u)$ , then

$$r^{3}F(\zeta) \leq E_{\aleph}F(\zeta) \leq D^{3}F(\zeta),$$
  
$$r^{2}F(\zeta) \leq E_{\aleph}F^{*}(\zeta) \leq D^{2}F(\zeta).$$

2.1.1. Join

A join [5]  $\zeta + \mathcal{F}$  of  $\zeta$  and  $\mathcal{F}$  with disjoint vertex sets  $V(\zeta)$  and  $V(\mathcal{F})$  is the graph on the vertex set  $V(\zeta) \cup V(\mathcal{F})$  and the edge set  $E(\zeta) \cup E(\mathcal{F}) \cup \{u_1u_2 : u_1 \in V(\zeta), u_2 \in V(\mathcal{F})\}$ .

**Lemma 2.5.** [23] Let  $\zeta$  and  $\mathcal{F}$  be any two graphs. Then,

(a) If  $V_{\omega}(\zeta) = V_{\omega}(\mathcal{F}) = \emptyset$ , then  $\delta_{en_{\zeta+\mathcal{F}}}(u) = 2d_{\zeta+\mathcal{F}}(u)$ ;

**(b)** If  $|V_{\omega}(\zeta)| = r$  and  $|V_{\omega}(\mathcal{F})| = s$  such that r + s > 0, then

$$\delta_{en_{\zeta+\mathcal{F}}}(u) = \begin{cases} 2d_{\zeta}(u) + 2|V(\mathcal{F})| - (r+s), & \text{if } u \in V(\zeta), u \notin V_{\omega}(\zeta);\\ 2d_{\zeta}(u) + 2|V(\mathcal{F})| + 1 - (r+s), & \text{if } u \in V(\zeta), u \in V_{\omega}(\zeta);\\ 2d_{\mathcal{F}}(u) + 2|V(\zeta)| - (r+s), & \text{if } u \in V(\mathcal{F}), u \notin V_{\omega}(\mathcal{F});\\ 2d_{\mathcal{F}}(u) + 2|V(\zeta)| + 1 - (r+s), & \text{if } u \in V(\mathcal{F}), u \in V_{\omega}(\mathcal{F}). \end{cases}$$

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We can partition the edge set of  $E(\zeta + \mathcal{F})$  as follows:

The partition of edges of the graph  $\zeta$  are:  $E_1^1$  is the set of edges connecting the vertices which are not in  $V_{\omega}(\zeta)$ ,  $E_1^2$  is the set of edges connecting the vertices of the set  $V_{\omega}(\zeta)$  and  $E_1^3$  be the set of edges connecting vertices of  $V_{\omega}(\zeta)$  to vertices which are not in  $V_{\omega}(\zeta)$ . The partition of edges of the graph  $\mathcal{F}$ are:  $E_2^1$  is the set of edges connecting the vertices not in  $V_{\omega}(\mathcal{F})$ ,  $E_2^2$  is the set of edges connecting the vertices of the set  $V_{\omega}(\mathcal{F})$  and  $E_2^3$  is the set of edges connecting vertices of  $V_{\omega}(\mathcal{F})$  to vertices which are not in  $V_{\omega}(\mathcal{F})$ . The edge partition connecting vertices of  $\zeta$  with vertices of  $\mathcal{F}$  are:  $E_3^1$  is the set of edges connecting the vertices not in  $V_{\omega}(\zeta)$  with the vertices not in  $V_{\omega}(\mathcal{F})$ ,  $E_3^2$  is the set of edges connecting the vertices not in  $V_{\omega}(\zeta)$  with the vertices of the set  $V_{\omega}(\mathcal{F})$ ,  $E_3^3$  is the set of edges connecting the vertices of the set  $V_{\omega}(\zeta)$  with the vertices not in  $V_{\omega}(\mathcal{F})$ ,  $E_3^3$  is the set of edges connecting the vertices of the set  $V_{\omega}(\zeta)$  with the vertices not in  $V_{\omega}(\mathcal{F})$ . Figure 1 outlines the procedural steps involved in proving the subsequent theorem.



Figure 1. Flowchart of Theorem 2.5.

**Theorem 2.5.** For any two graphs  $\zeta$  and  $\mathcal{F}$  with  $|V_{\omega}(\zeta)| = r$ ,  $|V_{\omega}(\mathcal{F})| = s$  and r + s > 0. Then,

$$E_{\aleph}F(\zeta + \mathcal{F}) = 8 \left[ \sum_{u \in V(\zeta)} (d_s(u) + n_2)^3 + \sum_{u \in V(\mathcal{F})} \left( (d_s(u) + n_1)^3 \right) \right]$$
$$- 12 (r + s) \left[ \sum_{\substack{u \in V(\zeta) \\ u \notin V_\omega(\zeta)}} d_{\zeta}^2(u) + \sum_{\substack{u \in V(\mathcal{F}) \\ u \notin V_\omega(\mathcal{F})}} d_{\mathcal{F}}^2(u) \right]$$
$$- 12 (r + s - 1) \left[ \sum_{\substack{u \in V(\zeta) \\ u \in V_\omega(\zeta)}} d_{\zeta}^2(u) + \sum_{\substack{u \in V(\mathcal{F}) \\ u \in V_\omega(\mathcal{F})}} d_{\mathcal{F}}^2(u) \right]$$

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$$+ (6 (r + s)^{2} - 24n_{2} (r + s)) \sum_{\substack{u \in V(\zeta) \\ u \notin V_{\omega}(\zeta)}} d_{\zeta} (u) + (6 (r + s - 1)^{2} - 24n_{2} (r + s - 1)) \sum_{\substack{u \in V(\zeta) \\ u \in V_{\omega}(\zeta)}} d_{\zeta} (u) + (6 (r + s)^{2} - 24n_{1} (r + s)) \sum_{\substack{u \in V(\mathcal{F}) \\ u \notin V_{\omega}(\mathcal{F})}} d_{\mathcal{F}} (u) + (6 (r + s - 1)^{2} - 24n_{2} (r + s - 1)) \sum_{\substack{u \in V(\mathcal{F}) \\ u \notin V_{\omega}(\mathcal{F})}} d_{\mathcal{F}} (u) + (6n_{2} (r + s)^{2} - 12n_{2}^{2} (r + s) - (r + s)^{3}) (n_{1} - r) + (6n_{1} \cdot (r + s)^{2} - 12n_{1}^{2} (r + s) - (r + s)^{3}) (n_{2} - s) + (6n_{2} (r + s - 1)^{2} - 12n_{2}^{2} (r + s - 1) - (r + s - 1)^{3}) r + (6n_{1} (r + s - 1)^{2} - 12n_{1}^{2} (r + s - 1) - (r + s - 1)^{3}) s$$

and

$$\begin{split} E_{8}F^{*}(\zeta + \mathcal{F}) =& 4\left(F\left(\zeta\right) + F\left(\mathcal{F}\right)\right) + 8\left(n_{2}M_{1}\left(\zeta\right) + n_{1}M_{1}\left(\mathcal{F}\right)\right) \\ & - 4\left(r + s\right) \left[\begin{array}{c} \sum_{uv \in E_{1}^{1}} \left(d_{\zeta}\left(u\right) + d_{\zeta}\left(v\right)\right) + \sum_{uv \in E_{2}^{1}} \left(d_{\mathcal{F}}\left(u\right) + d_{\mathcal{F}}\left(v\right)\right) \\ & + \sum_{uv \in E_{1}^{1}} \left(d_{\zeta}\left(u\right) + d_{\mathcal{F}}\left(v\right)\right) \\ & - 4\left(r + s - 1\right) \left[\begin{array}{c} \sum_{uv \in E_{1}^{2}} \left(d_{\zeta}\left(u\right) + d_{\zeta}\left(v\right)\right) + \sum_{uv \in E_{2}^{2}} \left(d_{\mathcal{F}}\left(u\right) + d_{\mathcal{F}}\left(v\right)\right) \\ & + \sum_{uv \in V_{u}\left(\mathcal{F}\right)} \\ & uv \in V_{u}\left(\mathcal{F}\right) \\ & v \in V_{u}\left(\mathcal{F}\right) \end{array}\right] \\ \\ & - 4\left[\begin{array}{c} \sum_{uv \in E_{1}^{3}} \left((r + s) d_{\zeta}\left(u\right) + (r + s - 1) d_{\zeta}\left(v\right)\right) \\ & u \notin V_{u}\left(\mathcal{F}\right) \\ & v \in V_{u}\left(\mathcal{F}\right) \\ & + \sum_{uv \in E_{2}^{3}} \left((r + s) d_{\zeta}\left(u\right) + (r + s - 1) d_{\mathcal{F}}\left(v\right)\right) \\ & u \notin V_{u}\left(\mathcal{F}\right) \\ & v \in V_{u}\left(\mathcal{F}\right) \\ & v \in V_{u}\left(\mathcal{F}\right) \\ & v \in V_{u}\left(\mathcal{F}\right) \\ & + \sum_{uv \in V_{d}^{3}} \left(r + s - 1\right) d_{\zeta}\left(u\right) + (r + s) d_{\mathcal{F}}\left(v\right)\right) \\ & u \notin V_{u}\left(\mathcal{F}\right) \\ & v \notin V_{u}\left(\mathcal{F}\right) \\ & + \sum_{uv \in V_{d}^{3}} \left(d_{\zeta}^{2}\left(u\right) + d_{\mathcal{F}}^{2}\left(v\right)\right) + 8 \sum_{u \in V\left(\zeta\right) \\ v \in V\left(\mathcal{F}\right) \\ & v \in V\left(\mathcal{F}\right) \\ & + \left(8n_{2}^{2} + 2\left(r + s\right)^{2} - 8n_{2}\left(r + s\right)\right) \left|E_{1}^{1}\right| \\ & + \left[8n_{2}^{2} - 8n_{2}\left(r + s - 1\right) + 2\left(r + s - 1\right)^{2}\right] \left|E_{1}^{2}\right| \\ & + \left[4n_{2}\left(2n_{2} - 2\left(r + s\right) + 1\right) + 2\left(r^{2} + s^{2}\right) - 2\left(r + s\right) + 4rs + 1\right] \left|E_{1}^{3}\right| \end{aligned}$$

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$$+ \left(8n_1^2 - 8n_1(r+s) + 2(r+s)^2\right) |E_2^1| + \left(8n_1^2 - 8n_1(r+s-1) + 2(r+s-1)^2\right) |E_2^2| + \left(4n_1(2n_1 - 2(r+s) + 1) + 2(r^2 + s^2) - 2(r+s) + 4rs + 1\right) |E_2^3| + \left[4\left(n_1^2 + n_2^2\right) - 4(r+s)(n_1 + n_2) + 2(r+s)^2\right] |E_3^1| + \left[4\left(n_1^2 + n_2^2\right) - 4(n_2(r+s) + n_1(r+s-1)) \\ + (r+s)^2 + (r+s-1)^2\right] |E_3^3| + \left[4\left(n_1^2 + n_2^2\right) - 4(n_2(r+s-1) + n_1(r+s)) \\ + (r+s)^2 + (r+s-1)^2\right] |E_3^3| + \left[4\left(n_1^2 + n_2^2\right) - 4(r+s-1)(n_1 + n_2) + 2(r+s-1)^2\right] |E_3^4|.$$

*Proof.* We have

$$E_{\aleph}F(\zeta + \mathcal{F}) = \sum_{v \in V(\zeta + \mathcal{F})} \delta^{3}_{en(\zeta + \mathcal{F})}(u)$$

$$= \underbrace{\sum_{u \in V(\zeta) \atop u \notin V_{\omega}(\zeta)}}_{u \notin V_{\omega}(\zeta)} \underbrace{\delta^{3}_{en(\zeta + \mathcal{F})}(u)}_{u \in V_{\omega}(\zeta)} + \underbrace{\sum_{u \in V(\mathcal{F}) \atop u \notin V_{\omega}(\mathcal{F})}}_{u \notin V_{\omega}(\mathcal{F})} \underbrace{\delta^{3}_{en(\zeta + \mathcal{F})}(u)}_{u \notin V_{\omega}(\mathcal{F})} + \underbrace{\sum_{u \in V(\mathcal{F}) \atop u \notin V_{\omega}(\mathcal{F})}}_{u \notin V_{\omega}(\mathcal{F})} \underbrace{\delta^{3}_{en(\zeta + \mathcal{F})}(u)}_{u \notin V_{\omega}(\mathcal{F})} + \underbrace{\delta^{3}_{en(\zeta + \mathcal{F})}(u)}_{u \# V_{\omega}($$

For (2.1)<sub>(1)</sub>,

$$\begin{split} \widetilde{\sum_{\substack{u \in V(\zeta) \\ u \notin V_{\omega}(\zeta)}}} \widetilde{\delta_{en(\zeta + \mathcal{F})}^{3}(u)} &= \sum_{\substack{u \in V(\zeta) \\ u \notin V_{\omega}(\zeta)}} \left( 2d_{\zeta}(u) + 2n_{2} - (r + s) \right)^{3} \\ &= \sum_{\substack{u \in V(\zeta) \\ u \notin V_{\omega}(\zeta)}} \left[ \begin{cases} 8d_{\zeta}^{3}(u) + 16n_{2}d_{\zeta}^{2}(u) + 8n_{2}^{2}d_{\zeta}(u) - \\ 8(r + s)d_{\zeta}^{2}(u) - 8n_{2}(r + s)d_{\zeta}(u) + 2(r + s)^{2}d_{\zeta}(u) \\ + 8n_{2}d_{\zeta}^{2}(u) + 16n_{2}^{2}d_{\zeta}(u) + 8n_{2}^{3} - 8n_{2}(r + s)d_{\zeta}(u) \\ - 8n_{2}^{2}(r + s) + 2n_{2}(r + s)^{2} - 4(r + s)d_{\zeta}^{2}(u) \\ - 8n_{2}(r + s)d_{\zeta}(u) - 4n_{2}^{2}(r + s) + 4(r + s)d_{\zeta}(u) \\ + 4n_{2}(r + s)^{2} - (r + s)^{3} \end{bmatrix} \\ &= \sum_{\substack{u \in V(\zeta) \\ u \notin V_{\omega}(\zeta)}} \left[ \begin{cases} 8d_{\zeta}^{3}(u) + 24n_{2}d_{\zeta}^{2}(u) + 24n_{2}^{2}d_{\zeta}(u) + 8n_{2}^{3} - 12(r + s)d_{\zeta}^{2}(u) \\ - 24n_{2}(r + s)d_{\zeta}(u) + 6(r + s)^{2}d_{\zeta}(u) - 12n_{2}^{2}(r + s) + \\ 6n_{2}(r + s)^{2} - (r + s)^{3} \end{bmatrix} \right] \\ &= 8\sum_{\substack{u \in V(\zeta) \\ u \notin V_{\omega}(\zeta)}} \left( d_{\zeta}(u) + n_{2} \right)^{3} - 12(r + s)\sum_{\substack{u \in V(\zeta) \\ u \notin V_{\omega}(\zeta)}} d_{\zeta}^{2}(u) \\ &+ \left( 6(r + s)^{2} - 24n_{2}(r + s) \right) \sum_{\substack{u \in V(\zeta) \\ u \notin V_{\omega}(\zeta)}} d_{\zeta}(u) \\ &+ \left[ 6n_{2}(r + s)^{2} - 12n_{2}^{2}(r + s) - (r + s)^{3} \right] (n_{1} - r) \,. \end{split}$$

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$$\begin{split} & \sum_{\substack{u \in V(\zeta) \\ u \in V_{\omega}(\zeta)}} \tilde{\delta}_{en(\zeta + \mathcal{F})}^{3}(u) = \sum_{\substack{u \in V(\zeta) \\ u \in V_{\omega}(\zeta)}} \left( 2d_{\zeta}(u) + 2n_{2} - (r + s - 1) \right)^{3} \\ & = \sum_{\substack{u \in V(\zeta) \\ u \in V_{\omega}(\zeta)}} \left[ \begin{cases} 8d_{\zeta}^{3}(u) + 16n_{2}d_{\zeta}^{2}(u) + 8n_{2}^{2}d_{\zeta}(u) - 8n_{2}(r + s - 1)d_{\zeta}(u) + 2(r + s - 1)^{2}d_{\zeta}(u) \\ + 8n_{2}d_{\zeta}^{2}(u) - 8n_{2}(r + s - 1)d_{\zeta}(u) + 8n_{2}^{3} - 8n_{2}(r + s - 1)d_{\zeta}(u) \\ - 8n_{2}^{2}(r + s - 1) + 2n_{2}(r + s - 1)^{2} - 4(r + s - 1)d_{\zeta}^{2}(u) \\ - 8n_{2}(r + s - 1)d_{\zeta}(u) - 4n_{2}^{2}(r + s - 1) + 4(r + s - 1)d_{\zeta}(u) \\ + 4n_{2}(r + s - 1)^{2} - (r + s - 1)^{3} \\ & = 8\sum_{\substack{u \in V(\zeta) \\ u \in V_{\omega}(\zeta)}} \left(d_{\zeta}(u) + n_{2}\right)^{3} - 12(r + s - 1)\sum_{\substack{u \in V(\zeta) \\ u \in V_{\omega}(\zeta)}} d_{\zeta}^{2}(u) \\ & + \left(2(r + s - 1)^{2} + 4(r + s - 1)^{2} - 24n_{2}(r + s - 1)\right)\sum_{\substack{u \in V(\zeta) \\ u \in V_{\omega}(\zeta)}} d_{\zeta}(u) \\ & + \left(\frac{4n_{2}(r + s - 1)^{2} + 2n_{2}(r + s - 1)^{2}}{u \in V_{\omega}(\zeta)} d_{\zeta}^{2}(u) \\ & + \left(6(r + s - 1) - 24n_{2}(r + s - 1)\right)\sum_{\substack{u \in V(\zeta) \\ u \in V_{\omega}(\zeta)}} d_{\zeta}(u) \\ & + \left(6(r + s - 1) - 24n_{2}(r + s - 1)\right)\sum_{\substack{u \in V(\zeta) \\ u \in V_{\omega}(\zeta)}} d_{\zeta}(u) \\ & + \left[6n_{2}(r + s - 1)^{2} - 12n_{2}^{2}(r + s - 1) - (r + s - 1)^{3}\right]r. \end{split}$$

For  $(2.1)_{(3)}$ ,

$$\begin{split} \overbrace{\substack{u \in V(\mathcal{F}) \\ u \notin V_{\omega}(\mathcal{F})}}^{3} & \overbrace{\substack{u \in V(\mathcal{F}) \\ u \notin V_{\omega}(\mathcal{F})}}^{3}} = \sum_{\substack{u \in V(\mathcal{F}) \\ u \notin V_{\omega}(\mathcal{F})}} (2d_{\mathcal{F}}(u) + 2n_1 - (r+s))^3 \\ &= 8 \sum_{\substack{u \in V(\mathcal{F}) \\ u \notin V_{\omega}(\mathcal{F})}} (d_{\mathcal{F}}(u) + n_1)^3 - 12(r+s) \sum_{\substack{u \in V(\mathcal{F}) \\ u \notin V_{\omega}(\mathcal{F})}} d_{\mathcal{F}}^2(u) \\ &+ \left(6(r+s)^2 - 24n_1(r+s)\right) \sum_{\substack{u \in V(\mathcal{F}) \\ u \notin V_{\omega}(\mathcal{F})}} d_{\mathcal{F}}(u) \\ &+ \left(6n_1(r+s)^2 - 12n_1^2(r+s) - (r+s)^3\right)(n_1-s) \,. \end{split}$$

For (2.1)<sub>(4)</sub>,

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$$\begin{split} \overbrace{u \in V(\mathcal{F})}^{4} & \overbrace{\sum_{u \in V(\mathcal{F})} \delta_{en(\zeta + \mathcal{F})}^{3}(u)}^{4} = \sum_{\substack{u \in V(\mathcal{F}) \\ u \in V_{\omega}(\mathcal{F})}} (2d_{\mathcal{F}}(u) + 2n_{1} - (r + s - 1))^{3} \\ &= 8 \sum_{\substack{u \in V(\mathcal{F}) \\ u \in V_{\omega}(\mathcal{F})}} (d_{\mathcal{F}}(u) + n_{1})^{3} - 12(r + s - 1) \sum_{\substack{u \in V(\mathcal{F}) \\ u \in V_{\omega}(\mathcal{F})}} d_{\mathcal{F}}^{2}(u) \\ &+ \left(6(r + s - 1)^{2} - 24n_{1}(r + s - 1)\right) \sum_{\substack{u \in V(\mathcal{F}) \\ u \in V_{\omega}(\mathcal{F})}} d_{\mathcal{F}}(u) \\ &+ \left(6n_{1}(r + s - 1)^{2} - 12n_{1}^{2}(r + s - 1) - (r + s - 1)^{3}\right)s. \end{split}$$

Combining  $(2.1)_{(1)}$ ,  $(2.1)_{(2)}$ ,  $(2.1)_{(3)}$  and  $(2.1)_{(4)}$ , we arrive at the necessary result. For MENI, we have

$$E_{\aleph}F^{*}(\zeta + \mathcal{F}) = \sum_{uv \in E(\zeta + \mathcal{F})} (\delta_{en(\zeta + \mathcal{F})}^{2}(u) + \delta_{en(\zeta + \mathcal{F})}^{2}(v))$$

$$= \underbrace{\sum_{uv \in E(\zeta)} (\delta_{en(\zeta + \mathcal{F})}^{2}(u) + \delta_{en(\zeta + \mathcal{F})}^{2}(v))}_{uv \in E(\mathcal{F})} + \underbrace{\sum_{uv \in E(\mathcal{F})} (\delta_{en(\zeta + \mathcal{F})}^{2}(u) + \delta_{en(\zeta + \mathcal{F})}^{2}(v))}_{v \in V(\mathcal{F})}$$

$$(2.2)$$

For  $(2.2)_{(5)}$ ,

$$\overbrace{uv \in E(\zeta)}^{5} \underbrace{\sum_{uv \in E(\zeta)} (\delta_{en(\zeta+\mathcal{F})}^{2}(u) + \delta_{en(\zeta+\mathcal{F})}^{2}(v))}_{*} \times \underbrace{\sum_{uv \in E_{1}^{1}} (\delta_{en(\zeta+\mathcal{F})}^{2}(u) + \delta_{en(\zeta+\mathcal{F})}^{2}(v))}_{*} \times \underbrace{\sum_{uv \in E_{1}^{2}} (\delta_{en(\zeta+\mathcal{F})}^{2}(u) + \delta_{en(\zeta+\mathcal{F})}^{2}(v))}_{u,v \notin V_{\omega}(\zeta)} \times \underbrace{\sum_{uv \in E_{1}^{1}} (\delta_{en(\zeta+\mathcal{F})}^{2}(u) + \delta_{en(\zeta+\mathcal{F})}^{2}(v))}_{u,v \notin V_{\omega}(\zeta)}}_{***}$$

Now,

$$\underbrace{\sum_{uv \in E_1^1} (\delta_{en(\zeta + \mathcal{F})}^2(u) + \delta_{en(\zeta + \mathcal{F})}^2(v))}_{uv \in E_1^1} \begin{bmatrix} (2d_{\zeta}(u) + 2n_2 - (r+s))^2 \\ + (2d_{\zeta}(v) + 2n_2 - (r+s))^2 \end{bmatrix} = 4 \sum_{uv \in E_1^1} \left[ \left( d_{\zeta}(u) + n_2 \right)^2 + \left( d_{\zeta}(v) + n_2 \right)^2 \right]$$

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$$-4(r+s)\sum_{uv\in E_1^1} \left( d_{\zeta}(u) + d_{\zeta}(v) \right) \\ + \left[ 2(r+s)^2 - 8n_2(r+s) \right] \left| E_1^1 \right| \\ = 4\sum_{uv\in E_1^1} \left( d_{\zeta}^2(u) + d_{\zeta}^2(v) \right) \\ + (8n_2 - 4(r+s)) \sum_{uv\in E_1^1} \left( d_{\zeta}(u) + d_{\zeta}(v) \right) \\ + \left( 8n_2^2 + 2(r+s)^2 - 8n_2(r+s) \right) \left| E_1^1 \right|.$$

Also,

$$\begin{split} \overbrace{uv \in E_1^2}^{**} & \overbrace{\left(\delta_{en(\zeta + \mathcal{F})}^2(u) + \delta_{en(\zeta + \mathcal{F})}^2(v)\right)}^{**} = \sum_{uv \in E_1^2} \begin{bmatrix} (2d_{\zeta}(u) + 2n_2 - (r+s-1))^2 \\ + (2d_{\zeta}(v) + 2n_2 - (r+s-1))^2 \end{bmatrix} \\ & = \sum_{uv \in E_1^2} \begin{bmatrix} 4d_{\zeta}^2(u) + 8n_2d_{\zeta}(u) - 4(r+s-1)d_{\zeta}(u) \\ + 4n_2^2 - 4n_2(r+s-1) + (r+s-1)^2 + \\ 4d_{\zeta}^2(v) + 8n_2d_{\zeta}(v) - 4(r+s-1)d_{\zeta}(v) + \\ 4n_2^2 - 4n_2(r+s-1) + (r+s-1)^2 \end{bmatrix} \\ & = 4\sum_{uv \in E_1^2} \left( d_{\zeta}^2(u) + d_{\zeta}^2(v) \right) + 8n_2 \sum_{uv \in E_1^2} \left( d_{\zeta}(u) + d_{\zeta}(v) \right) \\ & + \left[ 8n_2^2 - 8n_2(r+s-1) + 2(r+s-1)^2 \right] |E_1^2| \\ - 4(r+s-1) \sum_{uv \in E_1^2} \left( d_{\zeta}(u) + d_{\zeta}(v) \right) \\ & = 4\sum_{uv \in E_1^2} \left( d_{\zeta}^2(u) + d_{\zeta}^2(v) \right) \\ & + \left( 8n_2 - 4(r+s-1) \right) \sum_{uv \in E_1^2} \left( d_{\zeta}(u) + d_{\zeta}(v) \right) \\ & + \left[ 8n_2^2 - 8n_2(r+s-1) + 2(r+s-1)^2 \right] |E_1^2| . \end{split}$$

Furthermore,

$$\begin{split} \underbrace{\sum_{\substack{uv \in E_1^3 \\ u \in V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta)}} (\delta_{en(\zeta + \mathcal{F})}^2(u) + \delta_{en(\zeta + \mathcal{F})}^2(v))}_{u \in V_{\omega}(\zeta)} = \sum_{\substack{uv \in E_1^3 \\ u \in V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta)}} \begin{bmatrix} (2d_{\zeta}(u) + 2n_2 - (r+s))^2 \\ + (2d_{\zeta}(v) + 2n_2 - (r+s-1))^2 \end{bmatrix} \\ = \sum_{\substack{uv \in E_1^3 \\ u \in V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta)}} \begin{bmatrix} 4d_{\zeta}^2(u) + 8n_2d_{\zeta}(u) + 4n_2^2 - 4(r+s)d_{\zeta}(u) \\ -4n_2(r+s) + (r+s)^2 + 4d_{\zeta}^2(v) + 8n_2d_{\zeta}(v) \\ -4(r+s-1)d_{\zeta}(v) + 4n_2^2 - \\ 4n_2(r+s-1) + (r+s-1)^2 \end{bmatrix} \end{split}$$

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$$=4 \sum_{\substack{uv \in E_{1}^{3} \\ v \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta) \\ -4 \sum_{\substack{uv \in E_{1}^{3} \\ u \in V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta) \\ + \left[ \frac{4n_{2} (2n_{2} - (r + s) - (r + s - 1))}{(r + s)^{2} + (r + s - 1)^{2}} \right] |E_{1}^{3}|$$

$$=4 \sum_{\substack{uv \in E_{1}^{3} \\ u \in V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta) \\ -4 \sum_{\substack{uv \in E_{1}^{3} \\ u \in V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\zeta) \\ + \left[ \frac{4n_{2} (2n_{2} - 2 (r + s) + 1) + 2 (r^{2} + s^{2})}{(r + s) + 4rs + 1} \right] |E_{1}^{3}|.$$

Hence,

$$\begin{split} \underbrace{\sum_{uv \in E(\zeta)}^{5} (\delta_{en(\zeta+\mathcal{F})}^{2}(u) + \delta_{en(\zeta+\mathcal{F})}^{2}(v))}_{uv \in E(\zeta)} \\ = & 4F(\zeta) + 8n_{2}M_{1}(\zeta) - 4 \begin{bmatrix} (r+s)\sum_{uv \in E_{1}^{1}} \left(d_{\zeta}(u) + d_{\zeta}(v)\right) + \\ (r+s-1)\sum_{uv \in E_{1}^{2}} \left(d_{\zeta}(u) + d_{\zeta}(v)\right) + \\ \sum_{\substack{uv \in E_{1}^{3} \\ v \notin V_{\omega}(\zeta)}} \left((r+s)d_{\zeta}(u) + (r+s-1)d_{\zeta}(v)\right) \end{bmatrix} \\ & + \left(8n_{2}^{2} + 2(r+s)^{2} - 8n_{2}(r+s)\right) |E_{1}^{1}| + \left[8n_{2}^{2} - 8n_{2}(r+s-1) + 2(r+s-1)^{2}\right] |E_{1}^{2}| \\ & + \begin{bmatrix} 4n_{2}(2n_{2} - 2(r+s) + 1) + 2(r^{2} + s^{2}) \\ -2(r+s) + 4rs + 1 \end{bmatrix} |E_{1}^{3}|. \end{split}$$

Now, we initiate the computation process.

$$\overbrace{uv \in E(\mathcal{F})}^{6} (\delta_{en(\zeta + \mathcal{F})}^{2}(u) + \delta_{en(\zeta + \mathcal{F})}^{2}(v))) \\ = \overbrace{uv \in E_{2}^{1}}^{*} (\delta_{en(\zeta + \mathcal{F})}^{2}(u) + \delta_{en(\zeta + \mathcal{F})}^{2}(v))) + \overbrace{uv \in E_{2}^{2}}^{**} (\delta_{en(\zeta + \mathcal{F})}^{2}(u) + \delta_{en(\zeta + \mathcal{F})}^{2}(v))) \\ + \overbrace{uv \in E_{2}^{3}}^{***} (\delta_{en(\zeta + \mathcal{F})}^{2}(u) + \delta_{en(\zeta + \mathcal{F})}^{2}(v))) .$$

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First,

\*

$$\begin{split} \overbrace{uv \in E_{2}^{1}}^{2} (\delta_{en(\zeta + \mathcal{F})}^{2}(u) + \delta_{en(\zeta + \mathcal{F})}^{2}(v)) &= \sum_{uv \in E_{2}^{1}} \begin{bmatrix} (2d_{\mathcal{F}}(u) + 2n_{1} - (r+s))^{2} \\ + (2d_{\mathcal{F}}(v) + 2n_{1} - (r+s))^{2} \end{bmatrix} \\ &= 4 \sum_{uv \in E_{2}^{1}} \left( d_{\mathcal{F}}^{2}(u) + d_{\mathcal{F}}^{2}(v) \right) + (8n_{1} - 4(r+s)) \sum_{uv \in E_{2}^{1}} (d_{\mathcal{F}}(u) + d_{\mathcal{F}}(v)) \\ &+ \left( 8n_{1}^{2} - 8n_{1}(r+s) + 2(r+s)^{2} \right) \left| E_{2}^{1} \right|. \end{split}$$

Second,

$$\underbrace{\sum_{uv \in E_2^2} (\delta_{en(\zeta+\mathcal{F})}^2(u) + \delta_{en(\zeta+\mathcal{F})}^2(v))}_{uv \in E_2^2} \left( d_{\mathcal{F}}^2(u) + d_{\mathcal{F}}^2(v) \right) + (8n_1 - 4(r+s-1)) \sum_{uv \in E_2^2} (d_{\mathcal{F}}(u) + d_{\mathcal{F}}(v)) \\
+ \left( 8n_1^2 - 8n_1(r+s-1) + 2(r+s-1)^2 \right) \left| E_2^2 \right|.$$

Third,

$$\begin{split} \overbrace{\substack{uv \in E_{2}^{3} \\ v \in V_{\omega}(\mathcal{F}) \\ v \in V$$

Hence,

$$\begin{split} &\underbrace{\sum_{uv \in E(\mathcal{F})}^{6} (\delta_{en(\zeta + \mathcal{F})}^{2}(u) + \delta_{en(\zeta + \mathcal{F})}^{2}(v))}_{en(\zeta + \mathcal{F})}(v))} \\ = & 4F\left(\mathcal{F}\right) + 8n_{1}M_{1}\left(\mathcal{F}\right) - 4 \begin{bmatrix} (r+s)\sum_{uv \in E_{2}^{2}}\left(d_{\mathcal{F}}\left(u\right) + d_{\mathcal{F}}\left(v\right)\right) + \\ (r+s-1)\sum_{uv \in E_{2}^{2}}\left(d_{\mathcal{F}}\left(u\right) + d_{\mathcal{F}}\left(v\right)\right) + \\ \sum_{\substack{uv \in E_{2}^{3} \\ u \notin V_{\omega}(\mathcal{F}) \\ v \in V_{\omega}(\mathcal{F})}} ((r+s)d_{\mathcal{F}}\left(u\right) + (r+s-1)d_{\mathcal{F}}\left(v\right)) \end{bmatrix} \\ & + \left(8n_{1}^{2} - 8n_{1}\left(r+s\right) + 2\left(r+s\right)^{2}\right) \left|E_{2}^{1}\right| + \left(8n_{1}^{2} - 8n_{1}\left(r+s-1\right) + 2\left(r+s-1\right)^{2}\right) \left|E_{2}^{2}\right| \\ & + \left(4n_{1}\left(2n_{1} - 2\left(r+s\right) + 1\right) + 2\left(r^{2} + s^{2}\right) \\ -2\left(r+s\right) + 4rs + 1\right) \right) \left|E_{2}^{3}\right|. \end{split}$$

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Now,

$$=\overbrace{\sum_{\substack{u \in V(\zeta)\\v \in V(\mathcal{F})}}^{7}}_{\substack{u \in V(\zeta)\\v \in V(\mathcal{F})}}}(\delta_{en(\zeta+\mathcal{F})}^{2}(u) + \delta_{en(\zeta+\mathcal{F})}^{2}(v))} + \overbrace{\sum_{\substack{u v \in E_{3}^{2}\\u \notin V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}^{**}}_{\substack{u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}(\delta_{en(\zeta+\mathcal{F})}^{2}(u) + \delta_{en(\zeta+\mathcal{F})}^{2}(v))} + \overbrace{\sum_{\substack{u v \in E_{3}^{2}\\u \notin V_{\omega}(\zeta)\\v \in V_{\omega}(\mathcal{F})}}^{***}}_{\substack{u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}(\delta_{en(\zeta+\mathcal{F})}^{2}(u) + \delta_{en(\zeta+\mathcal{F})}^{2}(v))} + \overbrace{\sum_{\substack{u v \in E_{3}^{2}\\u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}^{****}}_{\substack{u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}(u) + \delta_{en(\zeta+\mathcal{F})}^{2}(v))} + \overbrace{\sum_{\substack{u v \in E_{3}^{2}\\u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}^{****}}(\delta_{en(\zeta+\mathcal{F})}^{2}(u) + \delta_{en(\zeta+\mathcal{F})}^{2}(v))} + \overbrace{\sum_{\substack{u \in E_{3}^{2}\\u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}^{****}}(\delta_{en(\zeta+\mathcal{F})}^{2}(u) + \delta_{en(\zeta+\mathcal{F})}^{2}(v))} + \overbrace{\sum_{\substack{u \in E_{3}^{2}\\u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}^{****}}(u) + \delta_{en(\zeta+\mathcal{F})}^{*}(v))} + \overbrace{\sum_{\substack{u \in E_{3}^{2}\\u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}^{****}}(u) + \delta_{en(\zeta+\mathcal{F})}^{*}(v)) + \overbrace{\sum_{\substack{u \in E_{3}^{2}\\u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}^{****}}(u) + \delta_{en(\zeta+\mathcal{F})}^{*}(v)) + \overbrace{\sum_{\substack{u \in E_{3}^{2}\\u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}^{****}}(u) + \delta_{en(\zeta+\mathcal{F})}^{*}(v))} + \overbrace{\sum_{\substack{u \in E_{3}^{2}\\u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}^{****}}(u) + \delta_{en(\zeta+\mathcal{F})}^{*}(v)) + \overbrace{\sum_{\substack{u \in E_{3}^{2}\\u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}}^{****}}(u) + \delta_{en(\zeta+\mathcal{F})}^{*}(v))} + \overbrace{\sum_{\substack{u \in E_{3}^{2}\\u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}}^{****}}(u) + \delta_{en(\zeta+\mathcal{F})}^{*}(v)) + \overbrace{\sum_{\substack{u \in E_{3}^{2}\\u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}}^{*}(u) + \delta_{en(\zeta+\mathcal{F})}^{*}(v)) + \overbrace{\sum_{\substack{u \in E_{3}^{2}\\u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}}^{*}(u) + \delta_{en(\zeta+\mathcal{F})}^{*}(v)) + \overbrace{\sum_{\substack{u \in V_{\omega}(\zeta)\\v \notin V_{\omega}(\mathcal{F})}}^{*}(u) + \delta_{en(\zeta+\mathcal{F})}^{*}(u) + \delta_{en$$

Following analogous computations, we acquire

$$\begin{split} &\underbrace{\sum_{\substack{uv \in E_{3}^{1} \\ v \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\mathcal{F})}}}_{\substack{uv \in E_{3}^{1} \\ u \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\mathcal{F})}} = 4 \sum_{\substack{uv \in E_{3}^{1} \\ u \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\mathcal{F})}} \left( d_{\zeta}^{2}(u) + d_{\mathcal{F}}^{2}(v) \right) + 8 \sum_{\substack{uv \in E_{3}^{1} \\ u \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\mathcal{F})}} \left( n_{2}d_{\zeta}(u) + n_{1}d_{\mathcal{F}}(v) \right) \right) \\ &- 4(r+s) \sum_{\substack{uv \in E_{3}^{1} \\ u \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\mathcal{F})}} \left( d_{\zeta}(u) + d_{\mathcal{F}}(v) \right) \\ &+ \left[ 4\left( n_{1}^{2} + n_{2}^{2} \right) - 4(r+s)(n_{1} + n_{2}) + 2(r+s)^{2} \right] \left| E_{3}^{1} \right|. \end{split}$$

$$\begin{split} & \underbrace{\sum_{\substack{uv \in E_3^2 \\ u \notin V_{\omega}(\zeta) \\ v \in V_{\omega}(\mathcal{F})}} (\delta_{en(\zeta + \mathcal{F})}^2(u) + \delta_{en(\zeta + \mathcal{F})}^2(v))}_{u \notin V_{\omega}(\mathcal{F})} \\ = & \underbrace{\sum_{\substack{uv \in E_3^2 \\ u \notin V_{\omega}(\zeta) \\ v \in V_{\omega}(\mathcal{F})}} \left( d_{\zeta}^2(u) + d_{\mathcal{F}}^2(v) \right) + 8 \sum_{\substack{uv \in E_3^2 \\ u \notin V_{\omega}(\zeta) \\ v \in V_{\omega}(\mathcal{F})}} \left( n_2 d_{\zeta}(u) + n_1 d_{\mathcal{F}}(v) \right) \\ & - 4 \sum_{\substack{uv \in E_3^2 \\ u \notin V_{\omega}(\zeta) \\ v \in V_{\omega}(\mathcal{F})}} \left( (r + s) d_{\zeta}(u) + (r + s - 1) d_{\mathcal{F}}(v) \right) \\ & + \left[ 4 \left( n_1^2 + n_2^2 \right) - 4 \left( n_2 \left( r + s \right) + n_1 \left( r + s - 1 \right) \right) \\ & + \left( r + s \right)^2 + \left( r + s - 1 \right)^2 \right] \left| E_3^2 \right|. \end{split}$$

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$$\begin{split} & \underbrace{\sum_{\substack{uv \in E_3^3 \\ v \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\mathcal{F})}} (\delta_{en(\zeta + \mathcal{F})}^2(u) + \delta_{en(\zeta + \mathcal{F})}^2(v))}_{u \in V_{\omega}(\zeta) \\ v \notin V_{\omega}(\mathcal{F})} \\ = 4 \sum_{\substack{uv \in E_3^3 \\ u \in V_{\omega}(\zeta) \\ v \notin V_{\omega}(\mathcal{F})}} \left( d_{\zeta}^2(u) + d_{\mathcal{F}}^2(v) \right) + 8 \sum_{\substack{uv \in E_3^3 \\ u \in V_{\omega}(\zeta) \\ v \notin V_{\omega}(\mathcal{F})}} \left( n_2 d_{\zeta}(u) + n_1 d_{\mathcal{F}}(v) \right) \\ & - 4 \sum_{\substack{uv \in E_3^3 \\ u \in V_{\omega}(\zeta) \\ v \notin V_{\omega}(\mathcal{F})}} \left( (r + s - 1) d_{\zeta}(u) + (r + s) d_{\mathcal{F}}(v) \right) \\ & + \left[ 4 \left( n_1^2 + n_2^2 \right) - 4 \left( n_2 \left( r + s - 1 \right) + n_1 \left( r + s \right) \right) \\ & + \left( r + s \right)^2 + \left( r + s - 1 \right)^2 \right) \right] |E_3^3|. \end{split}$$

$$\begin{split} & \underbrace{\sum_{\substack{uv \in E_{3}^{4} \\ u \in V_{\omega}(\zeta) \\ v \in V_{\omega}(\mathcal{F})}}}_{\substack{u \in V_{\omega}(\zeta) \\ v \in V_{\omega}(\mathcal{F})}} (d_{\zeta}^{2}(u) + d_{\mathcal{F}}^{2}(v)) + 8 \sum_{\substack{uv \in E_{3}^{4} \\ u \in V_{\omega}(\zeta) \\ v \in V_{\omega}(\mathcal{F})}} (n_{2}d_{\zeta}(u) + n_{1}d_{\mathcal{F}}(v)) \\ & - 4 \left(r + s - 1\right) \sum_{\substack{uv \in E_{3}^{4} \\ u \in V_{\omega}(\zeta) \\ v \in V_{\omega}(\mathcal{F})}} (d_{\zeta}(u) + d_{\mathcal{F}}(v)) \\ & + \left[ 4 \left(n_{1}^{2} + n_{2}^{2}\right) - 4 \left(r + s - 1\right) (n_{1} + n_{2}) \\ + 2 \left(r + s - 1\right)^{2} \right] |E_{3}^{4}|. \end{split}$$

Hence,

$$\underbrace{\sum_{\substack{u \in V(\zeta) \\ v \in V(\mathcal{F})}}^{7} (\delta_{en(\zeta + \mathcal{F})}^{2}(u) + \delta_{en(\zeta + \mathcal{F})}^{2}(v))}_{u \in V(\mathcal{F})} = 4 \sum_{\substack{u \in V(\zeta) \\ v \in V(\mathcal{F})}} \left( d_{\zeta}^{2}(u) + d_{\mathcal{F}}^{2}(v) \right) + 8 \sum_{\substack{u \in V(\zeta) \\ v \in V(\mathcal{F})}} \left( n_{2}d_{\zeta}(u) + n_{1}d_{\mathcal{F}}(v) \right)$$

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$$+ \begin{bmatrix} (r+s) \sum_{\substack{uv \in E_3^1 \\ u \notin V_{\omega}(\zeta) \\ v \notin V_{\omega}(\mathcal{F})}} \left( d_{\zeta}(u) + d_{\mathcal{F}}(v) \right) + \\ u_{\substack{u \notin V_{\omega}(\zeta) \\ v \in V_{\omega}(\mathcal{F})}} \right) \\ \sum_{\substack{u \notin E_3^2 \\ u \notin V_{\omega}(\mathcal{F}) \\ v \notin V_{\omega}(\mathcal{F})}} \left( (r+s-1) d_{\zeta}(u) + (r+s) d_{\mathcal{F}}(v) \right) + \\ u_{\substack{v \in V_{\omega}(\zeta) \\ v \notin V_{\omega}(\mathcal{F}) \\ v \notin V_{\omega}(\mathcal{F})}} \left( (r+s-1) \sum_{\substack{uv \in E_3^4 \\ u \in V_{\omega}(\zeta) \\ v \in V_{\omega}(\mathcal{F})}} \left( d_{\zeta}(u) + d_{\mathcal{F}}(v) \right) \right) \\ + \left[ 4 \left( n_1^2 + n_2^2 \right) - 4 \left( r+s \right) \left( n_1 + n_2 \right) + 2 \left( r+s \right)^2 \right] \left| E_3^1 \right| \\ + \left[ 4 \left( n_1^2 + n_2^2 \right) - 4 \left( n_2 \left( r+s \right) + n_1 \left( r+s - 1 \right) \right) \\ + \left( r+s \right)^2 + \left( r+s-1 \right)^2 \right) \right] \left| E_3^2 \right| \\ + \left[ 4 \left( n_1^2 + n_2^2 \right) - 4 \left( n_2 \left( r+s - 1 \right) + n_1 \left( r+s \right) \right) \\ + \left( r+s \right)^2 + \left( r+s-1 \right)^2 \right) \right] \left| E_3^3 \right| \\ + \left[ 4 \left( n_1^2 + n_2^2 \right) - 4 \left( r+s - 1 \right) \left( n_1 + n_2 \right) \\ + \left( r+s - 1 \right)^2 \right) \right] \left| E_3^3 \right| \\ + \left[ 4 \left( n_1^2 + n_2^2 \right) - 4 \left( r+s - 1 \right) \left( n_1 + n_2 \right) \\ + 2 \left( r+s - 1 \right)^2 \right] \left| E_3^4 \right|.$$

By incorporating  $(2.2)_{(5)}$ ,  $(2.2)_{(6)}$  and  $(2.2)_{(7)}$ , we arrive at the anticipated outcome.

**Corollary 2.2.** If  $\zeta$  and  $\mathcal{F}$  be any two graphs such that  $V_{\omega}(\zeta) = V_{\omega}(\mathcal{F}) = \emptyset$ , then

$$E_{\aleph}F(\zeta + \mathcal{F}) = 8F(\zeta + \mathcal{F})$$
$$E_{\aleph}F^{*}(\zeta + \mathcal{F}) = 4F(\zeta + \mathcal{F}).$$

#### 2.1.2. Disjunction

The disjunction [5]  $\zeta \lor \mathcal{F}$  of two graphs  $\zeta$  and  $\mathcal{F}$  is the graph with vertex set  $V(\zeta) \times V(\mathcal{F})$  in which (a, b) is adjacent with (c, d) whenever  $ac \in E(\zeta)$  or  $bd \in E(\mathcal{F})$ .

**Lemma 2.6.** [23] Let  $\zeta$  and  $\mathcal{F}$  be any two graphs. Then,

- (a) If  $\zeta$  and  $\mathcal{F}$  are complete graphs, then  $\delta_{en\zeta \vee \mathcal{F}}(u, v) = d_{\zeta \vee \mathcal{F}}(u, v)$ .
- **(b)** If  $V_{\omega}(\zeta) = \emptyset$  or  $V_{\omega}(\mathcal{F}) = \emptyset$ , then  $\delta_{en_{\zeta \lor \mathcal{F}}}(u, v) = 2d_{\zeta \lor \mathcal{F}}(u, v)$ .
- (c) If  $V_{\omega}(\zeta)$  and  $V_{\omega}(\mathcal{F})$  are not empty sets, such that  $|V_{\omega}(\zeta)| = r$ ,  $|V_{\omega}(\mathcal{F})| = s$ , then

$$\delta_{en\zeta\vee\mathcal{F}}(u,v) = \begin{cases} 2d_{\zeta\vee\mathcal{F}}(u,v) + 1 - rs, & if \varepsilon_{\zeta\vee\mathcal{F}}(u,v) = 1; \\ 2d_{\zeta\vee\mathcal{F}}(u,v) - rs, & otherwise. \end{cases}$$

Proof.

(a) If  $\zeta$  and  $\mathcal{F}$  are complete graphs, then every pair of distinct vertices is connected by an edge. In a complete graph, the distance  $d_{\zeta \lor \mathcal{F}}(u, v)$  between any two vertices u and v is one because there is exactly one edge connecting them. Similarly, the eccentricity neighborhood degree  $\delta_{en\zeta \lor \mathcal{F}}(u, v)$ , which reflects the the eccentricity neighborhood degree in a pair of vertices, should also be one since all possible edges exist in a complete graph. Therefore,  $\delta_{en\zeta \lor \mathcal{F}}(u, v) = d_{\zeta \lor \mathcal{F}}(u, v)$  in complete graphs.

- (b) We have  $\varepsilon_{\zeta \lor \mathcal{F}}(u, v) = 1$  if  $\varepsilon_{\zeta}(u) = \varepsilon_{\mathcal{F}}(u) = 1$ . Since  $d_{\zeta \lor \mathcal{F}}(u, v) = |V(\mathcal{F})|d_{\zeta}(u) + |V(\zeta)|d_{\mathcal{F}}(v) d_{\zeta}(u)d_{\mathcal{F}}(v)$ , with some direct calculations, we deduce that  $\delta_{en_{\tau \lor \mathcal{F}}}(u, v) = 2d_{\zeta \lor \mathcal{F}}(u, v)$ .
- (c) If  $V_{\omega}(\zeta)$  and  $V_{\omega}(\mathcal{F})$  are not empty sets, such that  $|V_{\omega}(\zeta)| = r$ ,  $|V_{\omega}(\mathcal{F})| = s$ , we have  $\varepsilon_{\zeta \vee \mathcal{F}}(u, v) = 1$ . If  $\varepsilon_{\zeta}(u) = \varepsilon_{\mathcal{F}}(u) = 1$ , since  $V_{\omega}(\zeta)$  and  $V_{\omega}(\mathcal{F})$  are non empty, then  $\delta_{en\zeta \vee \mathcal{F}}(u, v) = 2d_{\zeta \vee \mathcal{F}}(u, v) + 1 rs$ . Clearly, according to the edge partition of the disjunction we remove 1 from it otherwise.

It is possible to divide the edges of  $\zeta \lor \mathcal{F}$  as follows:

$$\begin{split} E_1 = \{ ((a, b), (c, d)) \in E(\zeta \lor \mathcal{F}) : \varepsilon_{\zeta \lor \mathcal{F}}(a, b) = \varepsilon_{\zeta \lor \mathcal{F}}(c, d) = 1 \}. \\ E_2 = \{ ((a, b), (c, d)) \in E(\zeta \lor \mathcal{F}) : \varepsilon_{\zeta \lor \mathcal{F}}(a, b) = \varepsilon_{\zeta \lor \mathcal{F}}(c, d) \neq 1 \}. \\ E_3 = \{ ((a, b), (c, d)) \in E(\zeta \lor \mathcal{F}) : \varepsilon_{\zeta \lor \mathcal{F}}(a, b) = 1, \ \varepsilon_{\zeta \lor \mathcal{F}}(c, d) \neq 1 \}. \end{split}$$

The division of edges within  $E(\zeta \lor \mathcal{F})$  forms distinct partitions:  $E_1$  encompasses edges linking vertices meeting the criterion  $\varepsilon(u, v) = 1$ ,  $E_2$  comprises edges connecting vertices where  $\varepsilon(u, v) \neq 1$  holds true and  $E_3$  encompasses edges linking vertices with  $\varepsilon(u, v) = 1$  in tandem with those where  $\varepsilon(u, v) \neq 1$  applies.

**Theorem 2.6.** Let  $\zeta$  and  $\mathcal{F}$  be any two graphs in such that  $|V_{\omega}(\zeta)| = r$ ,  $|V_{\omega}(\mathcal{F})| = s$  with  $rs \geq 1$ . Then,

$$\begin{split} E_{\aleph}F(\zeta \vee \mathcal{F}) = & 8F(\zeta \vee \mathcal{F}) - 12rsM_{1}(\zeta \vee \mathcal{F}) + 12\sum_{\substack{(u,v) \in V(\zeta \vee \mathcal{F}) \\ \varepsilon_{(\zeta \vee \mathcal{F})}(u,v) = 1}} d_{\zeta \vee \mathcal{F}}(u,v) \\ &+ 6\left(rs - 1\right)^{2}\sum_{\substack{(u,v) \in V(\zeta \vee \mathcal{F}) \\ \varepsilon_{(\zeta \vee \mathcal{F})}(u,v) = 1}} d_{(\zeta \vee \mathcal{F})}(u,v) + 6r^{2}s^{2}\sum_{\substack{(u,v) \in V(\zeta \vee \mathcal{F}) \\ \varepsilon_{(\zeta \vee \mathcal{F})}(u,v) \neq 1}} d_{(\zeta \vee \mathcal{F})}(u,v) \\ &- (rs - 1)^{3}rs - r^{3}s^{3}\left(|V(\zeta \vee \mathcal{F})| - rs\right) \end{split}$$

and

$$E_{\aleph}F^{*}(\zeta \vee \mathcal{F}) = 4F(\zeta \vee \mathcal{F}) - 4 \begin{bmatrix} (rs-1)\sum_{((a,b),(c,d))\in E_{1}} \left( d_{(\zeta \vee \mathcal{F})}(a,b) + d_{(\zeta \vee \mathcal{F})}(c,d) \right) + \\ (rs)\sum_{((a,b),(c,d))\in E_{2}} \left( d_{(\zeta \vee \mathcal{F})}(a,b) + d_{(\zeta \vee \mathcal{F})}(c,d) \right) + \\ \sum_{((a,b),(c,d))\in E_{3}} \left( (rs-1)d_{(\zeta \vee \mathcal{F})}(a,b) + rsd_{(\zeta \vee \mathcal{F})}(c,d) \right) \\ + 2(rs-1)^{2} |E_{1}| + 2r^{2}s^{2} |E_{2}| + \left(r^{2}s^{2} + (rs-1)^{2} |E_{3}|\right). \end{bmatrix}$$

*Proof.* First, for the ENFI we have

$$E_{\aleph}F(\zeta \lor \mathcal{F}) = \sum_{(u,v)\in V(\zeta \lor \mathcal{F})} \delta^{3}_{en(\zeta \lor \mathcal{F})}(u,v)$$
$$= \underbrace{\sum_{\substack{(u,v)\in V(\zeta \lor \mathcal{F})\\ \varepsilon_{(\zeta \lor \mathcal{F})}(u,v)=1}} \delta^{3}_{en(\zeta \lor \mathcal{F})}(u,v)} + \underbrace{\sum_{\substack{(u,v)\in V(\zeta \lor \mathcal{F})\\ \varepsilon_{(\zeta \lor \mathcal{F})}(u,v)\neq 1}} \delta^{3}_{en(\zeta \lor \mathcal{F})}(u,v)} .$$
(2.3)

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Now, for  $(2.3)_{(1)}$ ,

$$\begin{split} \overbrace{\substack{(u,v)\in V(\zeta\vee\mathcal{F})\\\varepsilon_{(\zeta\vee\mathcal{F})}(u,v)=1}}^{1} \delta_{en(\zeta\vee\mathcal{F})}^{3}(u,v)} &= \sum_{\substack{(u,v)\in V(\zeta\vee\mathcal{F})\\\varepsilon_{(\zeta\vee\mathcal{F})}(u,v)=1}} \left(2d_{(\zeta\vee\mathcal{F})}(u,v) - (rs-1)\right)^{3} \\ &= 8\sum_{\substack{(u,v)\in V(\zeta\vee\mathcal{F})\\\varepsilon_{(\zeta\vee\mathcal{F})}(u,v)=1}} d_{(\zeta\vee\mathcal{F})}^{3}(u,v) - 12(rs-1)\sum_{\substack{(u,v)\in V(\zeta\vee\mathcal{F})\\\varepsilon_{(\zeta\vee\mathcal{F})}(u,v)=1}} d_{(\zeta\vee\mathcal{F})}^{2}(u,v) \\ &+ 6(rs-1)^{2}\sum_{\substack{(u,v)\in V(\zeta\vee\mathcal{F})\\\varepsilon_{(\zeta\vee\mathcal{F})}(u,v)=1}} d_{(\zeta\vee\mathcal{F})}(u,v) - rs(rs-1)^{3}. \end{split}$$

For (2.3)<sub>(2)</sub>,

$$\begin{split} \widetilde{\sum_{\substack{(u,v)\in V(\zeta\vee\mathcal{F})\\\varepsilon_{(\zeta\vee\mathcal{F})}(u,v)\neq 1}}} \widetilde{\delta}_{en(_{\zeta\vee\mathcal{F}})}^{3}(u,v)} &= \sum_{\substack{(u,v)\in V(\zeta\vee\mathcal{F})\\\varepsilon_{(\zeta\vee\mathcal{F})}(u,v)\neq 1}} \left( \left( 2d_{(\zeta\vee\mathcal{F})}(u,v) - rs \right)^{3} \right) \\ &= 8 \sum_{\substack{(u,v)\in V(\zeta\vee\mathcal{F})\\\varepsilon_{(\zeta\vee\mathcal{F})}(u,v)\neq 1}} d_{(\zeta\vee\mathcal{F})}^{3}(u,v) - 12rs \sum_{\substack{(u,v)\in V(\zeta\vee\mathcal{F})\\\varepsilon_{(\zeta\vee\mathcal{F})}(u,v)\neq 1}} d_{(\zeta\vee\mathcal{F})}^{2}(u,v) \\ &+ 6r^{2}s^{2} \sum_{\substack{(u,v)\in V(\zeta\vee\mathcal{F})\\\varepsilon_{(\zeta\vee\mathcal{F})}(u,v)\neq 1}} d_{(\zeta\vee\mathcal{F})}(u,v) - (rs-1)^{3}rs - r^{3}s^{3}\left(|V(\zeta\vee\mathcal{F})| - rs\right). \end{split}$$

By combining  $(2.3)_{(1)}$ , and  $(2.3)_{(2)}$ , the desired outcome is achieved. Now, for the MENFI we have

$$E_{\aleph}F^{*}(\zeta \vee \mathcal{F}) = \sum_{((a,b),(c,d))\in E(\zeta \vee \mathcal{F})} \left(\delta_{en(\zeta \vee \mathcal{F})}^{2}(a,b) + \delta_{en(\zeta \vee \mathcal{F})}^{2}(c,d)\right)$$
$$= \underbrace{\sum_{((a,b),(c,d))\in E_{1}}^{3} \left(\delta_{en(\zeta \vee \mathcal{F})}^{2}(a,b) + \delta_{en(\zeta \vee \mathcal{F})}^{2}(c,d)\right)}_{4}$$
(2.4)

$$+ \underbrace{\sum_{((a,b),(c,d))\in E_2} \left( \delta^2_{en(\zeta \lor \mathcal{F})}(a,b) + \delta^2_{en(\zeta \lor \mathcal{F})}(c,d) \right)}_{5}$$
(2.5)

$$+ \underbrace{\sum_{\substack{((a,b),(c,d))\in 3\\\varepsilon(a,b)=1\\\varepsilon(c,d)\neq 1}} \left(\delta^2_{en(\zeta \lor \mathcal{F})}(a,b) + \delta^2_{en(\zeta \lor \mathcal{F})}(c,d)\right)}_{\varepsilon(c,d)\neq 1}.$$
(2.6)

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For (2.4)<sub>(3)</sub>,

$$\begin{split} \underbrace{\sum_{((a,b),(c,d))\in E_{1}} \left( \delta_{en(\zeta\vee\mathcal{F})}^{2}(a,b) + \delta_{en(\zeta\vee\mathcal{F})}^{2}(c,d) \right)}_{((a,b),(c,d))\in E_{1}} \left[ \left( 2d_{(\zeta\vee\mathcal{F})}(a,b) - (rs-1) \right)^{2} + \\ \left( 2d_{(\zeta\vee\mathcal{F})}(c,d) - (rs-1) \right)^{2} \right] \\ = 4 \sum_{((a,b),(c,d))\in E_{1}} \left( d_{(\zeta\vee\mathcal{F})}^{2}(a,b) + d_{(\zeta\vee\mathcal{F})}^{2}(c,d) \right) \\ - 4 \left( rs-1 \right) \sum_{((a,b),(c,d))\in E_{1}} \left( d_{(\zeta\vee\mathcal{F})}(a,b) + d_{(\zeta\vee\mathcal{F})}(c,d) \right) + 2 \left( rs-1 \right)^{2} |E_{1}| \,. \end{split}$$

For (2.5)<sub>(4)</sub>,

$$\begin{split} \overbrace{((a,b),(c,d))\in E_{2}}^{4} & \overbrace{\sum_{((a,b),(c,d))\in E_{2}} \left( \delta_{en(\zeta \lor \mathcal{F})}^{2}(a,b) + \delta_{en(\zeta \lor \mathcal{F})}^{2}(c,d) \right)}^{4} \\ &= \sum_{((a,b),(c,d))\in E_{2}} \left[ \begin{array}{c} \left( 2d_{(\zeta \lor \mathcal{F})}(a,b) - rs \right)^{2} + \\ \left( 2d_{(\zeta \lor \mathcal{F})}(c,d) - rs \right)^{2} \end{array} \right] \\ &= 4 \sum_{((a,b),(c,d))\in E_{2}} \left( d_{(\zeta \lor \mathcal{F})}^{2}(a,b) + d_{(\zeta \lor \mathcal{F})}^{2}(c,d) \right) \\ &- 4rs \sum_{((a,b),(c,d))\in E_{2}} \left( d_{(\zeta \lor \mathcal{F})}(a,b) + d_{(\zeta \lor \mathcal{F})}(c,d) \right) + 2r^{2}s^{2} |E_{2}| \, . \end{split}$$

For (2.6)<sub>(5)</sub>,

$$\begin{split} \overbrace{\substack{((a,b),(c,d))E_3\\\varepsilon(a,b)=1\\\varepsilon(c,d)\neq 1}}^{5} & \left(\delta_{en(\zeta \lor \mathcal{F})}^2(a,b) + \delta_{en(\zeta \lor \mathcal{F})}^2(c,d)\right) \\ = & \sum_{\substack{((a,b),(c,d))E_3\\\varepsilon(a,b)=1\\\varepsilon(c,d)\neq 1}} \left[ \left(2d_{(\zeta \lor \mathcal{F})}(a,b) - (rs-1)\right)^2 + \\ \left(2d_{(\zeta \lor \mathcal{F})}(c,d) - rs\right)^2 \right] \\ = & 4 \sum_{\substack{((a,b),(c,d))E_3\\\varepsilon(a,b)=1\\\varepsilon(c,d)\neq 1}} \left(d_{(\zeta \lor \mathcal{F})}^2(a,b) + d_{(\zeta \lor \mathcal{F})}^2(c,d)\right) \\ & - & 4 \sum_{\substack{((a,b),(c,d))E_3\\\varepsilon(c,d)\neq 1\\\varepsilon(c,d)\neq 1}} (rs-1) d_{(\zeta \lor \mathcal{F})}(a,b) + rsd_{(\zeta \lor \mathcal{F})}(c,d) + r^2s^2 + (rs-1) |E_3|. \end{split}$$

Now, adding  $(2.4)_{(3)}$ ,  $(2.5)_{(4)}$  and  $(2.6)_{(5)}$ , we have our result.

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**Corollary 2.3.** (a) If  $V_{\omega}(\zeta) = \emptyset$  or  $V_{\omega}(\mathcal{F}) = \emptyset$ , then

$$E_{\aleph}F(\zeta \vee \mathcal{F}) = 8F(\zeta \vee \mathcal{F}).$$

$$E_{\aleph}F^*(\zeta \vee \mathcal{F}) = 4F(\zeta \vee \mathcal{F}).$$

(b) If  $\zeta$  and  $\mathcal{F}$  are two complete graphs, then

$$E_{\aleph}F(\zeta \lor \mathcal{F}) = F(\zeta \lor \mathcal{F}),$$
$$E_{\aleph}F^{*}(\zeta \lor \mathcal{F}) = F(\zeta \lor \mathcal{F}).$$

## 2.1.3. Composition

The composition [5] of  $\zeta = (V(\zeta), E(\zeta))$  and  $\mathcal{F} = (V(\mathcal{F}), E(\mathcal{F}))$  is a graph  $\zeta[\mathcal{F}]$  containing vertex set  $V(\zeta) \times V(\mathcal{F})$  and, (a, b) is connected to (c, d) if and only if  $ac \in E(\zeta)$  or a = c and  $bd \in E(\mathcal{F})$ .

**Lemma 2.7.** [23] Let  $\zeta$  and  $\mathcal{F}$  be two graphs. Then,

(a) If  $\zeta$  and  $\mathcal{F}$  are complete, then

$$\delta_{en_{\zeta[\mathcal{F}]}}(u,v) = d_{\zeta[\mathcal{F}]}(u,v).$$

**(b)** If  $\zeta$  has at least one vertex with  $\varepsilon(u) = 1$  and  $\mathcal{F}$  does not have any vertex with  $\varepsilon(u) = 1$ , then

$$\delta_{en_{\zeta[\mathcal{F}]}}(u,v) = 2d_{\zeta[\mathcal{F}]}(u,v).$$

(c) If  $V_{\omega}(\zeta)$  and  $V_{\omega}(\mathcal{F})$  are not empty sets, such that  $|V_{\omega}(\zeta)| = r$ ,  $|V_{\omega}(\mathcal{F})| = s$ , then

$$\delta_{en_{\zeta[\mathcal{F}]}}(u,v) = \begin{cases} 2d_{\zeta[\mathcal{F}]}(u,v) + 1 - rs, & \text{if } \varepsilon_{\zeta[\mathcal{F}]}(u,v) = 1; \\ 2d_{\zeta[\mathcal{F}]}(u,v) - rs, & \text{otherwise.} \end{cases}$$

In the next theorem we will denote  $\neg$  the set of vertices which satisfy  $\varepsilon(u, v) = 1$ . Also, we use the edge partition of  $E(\zeta[\mathcal{F}])$  which is similar to the edge partition of  $E(\zeta \lor \mathcal{F})$ .

**Theorem 2.7.** Let  $\zeta$  and  $\mathcal{F}$  be any two graphs with  $|V_{\omega}(\zeta)| = r$ ,  $|V_{\omega}(\mathcal{F})| = s$  and  $rs \geq 1$ . Then,

$$\begin{split} E_{\aleph}F(\zeta[\mathcal{F}]) = & 8F(\zeta[\mathcal{F}]) - 12rsM_{1}(\zeta[\mathcal{F}]) \\ &+ 12\sum_{(u,v)\in \mathbb{k}} d_{(\zeta[\mathcal{F}])}(u,v) + 12r^{2}s^{2} |E(\zeta[\mathcal{F}])| \\ &+ 6(1 - 2rs)\sum_{(u,v)\in \mathbb{k}} d_{(\zeta[\mathcal{F}])}(u,v) - (rs - 1)^{3} |\mathbb{k}| - r^{3}s^{3} |V(\zeta[\mathcal{F}]) - \mathbb{k}| \end{split}$$

and

$$\begin{split} E_{\aleph}F^{*}(\zeta[\mathcal{F}]) = & 4F\left(\zeta[\mathcal{F}]\right) - 4 \begin{bmatrix} (rs-1)\sum_{E_{1}} \left(d_{(\zeta[\mathcal{F}])}\left(a,b\right) + d_{(\zeta[\mathcal{F}])}\left(c,d\right)\right) + \\ & rs\sum_{E_{2}} \left(d_{(\zeta[\mathcal{F}])}\left(a,b\right) + d_{(\zeta[\mathcal{F}])}\left(c,d\right)\right) + \\ & \sum_{\substack{((a,b),(c,d))E_{3}\\\varepsilon(a,b)=1\\\varepsilon(c,d)\neq 1}} \left((rs-1)d_{(\zeta[\mathcal{F}])}\left(a,b\right) + rsd_{(\zeta[\mathcal{F}])}\left(c,d\right)\right) \\ & + 2\left(rs-1\right)^{2}|E_{1}| + 2r^{2}s^{2}|E_{2}| + \left(r^{2}s^{2} + (rs-1)^{2}\right)|E_{3}|. \end{split}$$

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$$E_{\mathbf{N}}F(\zeta[\mathcal{F}]) = \sum_{(u,v)\in V(\zeta[\mathcal{F}])} \delta^{3}_{en(\zeta[\mathcal{F}])}(u,v)$$
$$= \underbrace{\sum_{(u,v)\in \mathbb{k}} \delta^{3}_{en(\zeta[\mathcal{F}])}(u,v)}_{(u,v)\in V((\zeta[\mathcal{F}])-\mathbb{k})} \delta^{3}_{en(\zeta[\mathcal{F}])}(u,v)}.$$
(2.7)

Now,

$$\begin{split} \overbrace{(u,v)\in \exists}^{1} \delta^{3}_{en(\zeta[\mathcal{F}])}(u,v) &= \sum_{(u,v)\in \exists} \left( 2d_{(\zeta[\mathcal{F}])}(u,v) - (rs-1) \right)^{3} \\ &= 8 \sum_{(u,v)\in \exists} d^{3}_{(\zeta[\mathcal{F}])}(u,v) - 12 \left( rs-1 \right) \sum_{(u,v)\in \exists} d^{2}_{(\zeta[\mathcal{F}])}(u,v) \\ &+ 6 \left( rs-1 \right)^{2} \sum_{(u,v)\in \exists} d_{(\zeta[\mathcal{F}])}(u,v) - (rs-1)^{3} \left| \exists \right| \end{split}$$

and

$$\underbrace{\sum_{(u,v)\in V((\zeta[\mathcal{F}])-\mathbb{k})}^{2} \delta_{en(\zeta[\mathcal{F}])}^{3}(u,v)}}_{= \sum_{(u,v)\in V((\zeta[\mathcal{F}])-\mathbb{k})}^{2} \left(2d_{(\zeta[\mathcal{F}])}(u,v) - rs\right)^{3} \\ = 8 \sum_{(u,v)\in V((\zeta[\mathcal{F}])-\mathbb{k})}^{2} d_{(\zeta[\mathcal{F}])}^{3}(u,v) - 12rs \sum_{(u,v)\in V((\zeta[\mathcal{F}])-\mathbb{k})}^{2} d_{(\zeta[\mathcal{F}])}^{2}(u,v) \\ + 6r^{2}s^{2} \sum_{(u,v)\in V((\zeta[\mathcal{F}])-\mathbb{k})}^{2} d_{(\zeta[\mathcal{F}])}(u,v) - r^{3}s^{3} \left|V\left((\zeta[\mathcal{F}])-\mathbb{k}\right)\right|.$$

Therefore, the result is obtained by summing up  $(2.7)_{(1)}$  and  $(2.7)_{(2)}$ . Transitioning to the computation of the MENFI, we employ the subsequent procedure:

$$E_{\aleph}F^{*}(\zeta[\mathcal{F}]) = \sum_{((a,b),(c,d))\in E(\zeta[\mathcal{F}])} \left(\delta_{en_{(\zeta[\mathcal{F}])}}^{2}(a,b) + \delta_{en_{(\zeta[\mathcal{F}])}}^{2}(c,d)\right)$$
$$= \underbrace{\sum_{E_{1}}^{3} \left(\delta_{en_{(\zeta[\mathcal{F}])}}^{2}(a,b) + \delta_{en_{(\zeta[\mathcal{F}])}}^{2}(c,d)\right)}_{4}$$
(2.8)

$$+ \underbrace{\sum_{E_2} \left( \delta^2_{en_{(\zeta[\mathcal{F}])}}(a,b) + \delta^2_{en_{(\zeta[\mathcal{F}])}}(c,d) \right)}_{5}$$
(2.9)

$$+ \underbrace{\sum_{\substack{((a,b),(c,d)) \in J \\ \varepsilon(a,b)=1\\ \varepsilon(c,d)\neq 1}} \left(\delta_{en_{(\zeta[\mathcal{F}])}}^2(a,b) + \delta_{en_{(\zeta[\mathcal{F}])}}^2(c,d)\right)}^2.$$
(2.10)

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Now,

$$\begin{split} &\overbrace{\sum_{E_{1}} \left( \delta_{en_{(\zeta[\mathcal{F}])}}^{3}(a,b) + \delta_{en_{(\zeta[\mathcal{F}])}}^{2}(c,d) \right)} \\ &= \sum_{E_{1}} \left[ \begin{array}{c} \left( 2d_{(\zeta[\mathcal{F}])}(a,b) - (rs-1) \right)^{2} \\ + \left( 2d_{(\zeta[\mathcal{F}])}(c,d) - (rs-1) \right)^{2} \end{array} \right] \\ &= 4 \sum_{E_{1}} \left( d_{(\zeta[\mathcal{F}])}^{2}(a,b) + d_{(\zeta[\mathcal{F}])}^{2}(c,d) \right) - 4 \left( rs-1 \right) \sum_{E_{1}} \left( d_{(\zeta[\mathcal{F}])}(a,b) + d_{(\zeta[\mathcal{F}])}(c,d) \right) \\ &+ 2 \left( rs-1 \right)^{2} |E_{1}| \end{split}$$

and

$$\begin{split} &\overbrace{\sum_{E_2} \left( \delta_{en_{(\zeta[\mathcal{F}])}}^2(a,b) + \delta_{en_{(\zeta[\mathcal{F}])}}^2(c,d) \right)} \\ &= \sum_{E_2} \left[ \begin{array}{c} \left( 2d_{(\zeta[\mathcal{F}])}(a,b) - rs \right)^2 \\ + \left( 2d_{(\zeta[\mathcal{F}])}(c,d) - rs \right)^2 \end{array} \right] \\ &= 4 \sum_{E_2} \left( d_{(\zeta[\mathcal{F}])}^2(a,b) + d_{(\zeta[\mathcal{F}])}^2(c,d) \right) - 4rs \sum_{E_2} \left( d_{(\zeta[\mathcal{F}])}(a,b) + d_{(\zeta[\mathcal{F}])}(c,d) \right) \\ &+ 2r^2 s^2 |E_2| \,. \end{split}$$

Also,

$$\begin{split} & \overbrace{\sum_{\substack{((a,b),(c,d))E_3\\ e(a,b)=1\\ e(c,d)\neq 1}}^{5} \left(\delta_{en_{(\zeta[\mathcal{F}])}}^2(a,b) + \delta_{en_{(\zeta[\mathcal{F}])}}^2(c,d)\right)}^{5} \\ &= \sum_{\substack{((a,b),(c,d))E_3\\ e(a,b)=1\\ e(c,d)\neq 1}} \left[ \begin{array}{c} \left(2d_{(\zeta[\mathcal{F}])}(a,b) - (rs-1)\right)^2\\ + \left(2d_{(\zeta[\mathcal{F}])}(c,d) - (rs-1)\right)^2 \end{array} \right] \\ &= 4\sum_{\substack{((a,b),(c,d))E_3\\ e(a,b)=1\\ e(c,d)\neq 1}} \left(d_{(\zeta[\mathcal{F}])}^2(a,b) + d_{(\zeta[\mathcal{F}])}^2(c,d)\right) \\ &- 4\sum_{\substack{((a,b),(c,d))E_3\\ e(a,b)=1\\ e(c,d)\neq 1}} \left((rs-1)d_{(\zeta[\mathcal{F}])}(a,b) + rsd_{(\zeta[\mathcal{F}])}(c,d)\right) + \left(r^2s^2 + (rs-1)^2\right)|E_3|. \end{split}$$

By combining  $(2.8)_{(3)}$ ,  $(2.9)_{(4)}$  and  $(2.10)_{(5)}$ , we achieve the desired outcome.

**Corollary 2.4.** (a) If graphs  $\zeta$  and  $\mathcal{F}$  are complete, then

$$E_{\aleph}F(\zeta[\mathcal{F}]) = F(\zeta[\mathcal{F}]).$$

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#### $E_{\aleph}F^*(\zeta[\mathcal{F}]) = F(\zeta[\mathcal{F}]).$

(b) If  $\zeta$  has at least one vertex with  $\varepsilon(u) = 1$  and  $\mathcal{F}$  does not have any vertex with  $\varepsilon(u) = 1$ , then

$$E_{\aleph}F(\zeta[\mathcal{F}]) = 8F(\zeta[\mathcal{F}]).$$
$$E_{\aleph}F^{*}(\zeta[\mathcal{F}]) = 4F(\zeta[\mathcal{F}]).$$

2.1.4. Symmetric difference

The symmetric deference [5]  $\zeta \oplus \mathcal{F}$  is defined by  $V(\zeta \oplus \mathcal{F}) = V(\zeta) \times V(\mathcal{F})$  and  $E(\zeta \oplus \mathcal{F}) = \{((a, b), (c, d)) : ac \in E(\zeta) \text{ or } bd \in E(\mathcal{F}) \text{ but not both}\}.$ 

**Lemma 2.8.** [23] Let  $\zeta$  and  $\mathcal{F}$  be graphs. Then,

$$\delta_{en_{\ell\oplus\mathcal{F}}}(u,v)=2d_{\ell\oplus\mathcal{F}}(u,v).$$

**Theorem 2.8.** Let  $\zeta$  and  $\mathcal{F}$  be any two simple connected graphs, then

$$E_{\aleph}F(\zeta \oplus \mathcal{F}) = 8F(\zeta[\mathcal{F}]),$$
$$E_{\aleph}F^{*}(\zeta \oplus \mathcal{F}) = 4F(\zeta[\mathcal{F}]).$$

#### 3. Methodology and analysis

In this study, the central objective revolved around the primary amines group, strategically chosen as the reference standard to gauge the practical implications of the recently introduced indices within the realm of chemical and physical attributes. Subsequently, leveraging the computational prowess of the R-program analysis tool, we embarked on an advanced non linear regression analysis, thereby enabling precise projection of boiling points tailored exclusively for primary amines. To enhance the accessibility of these projections, the visualization of resultant models was realized through linear amalgamation in Excel. This preliminary phase serves as the bedrock upon which we meticulously structure the primary outcomes distilled from our conscientious research pursuits. Transitioning to the subsequent phase, a methodical expedition into the realm of comprehensive mathematical exploration awaits us. This exploratory journey is geared towards unraveling the innate characteristics and dynamic behavior intrinsic to the newly introduced indices. Furthermore, the scope of this analysis transcends disciplinary boundaries as it traverses through various graph families. Methodically guided by an analytical framework, we minutely deconstruct the attributes that underscore the essence of these indices, all the while meticulously evaluating their practical utility, even in basic operations. This pivotal section stands as the fulcrum of our research endeavor, representing the locus where we venture into the intricate mathematical intricacies, seamlessly interwoven with the tangible applications encapsulated within the indices we have ingeniously formulated.

As we embark on this odyssey to apprehend the intricate nature of chemical entities, the undeniable exigency for rigorous laboratory experiments surfaces, albeit invariably entwined with significant fiscal intricacies. To circumvent this financial conundrum, the domain of theoretical chemistry has ushered forth a diverse spectrum of topological indices. At the heart of conceiving a pioneering topological index lies the essential fulfillment of two paramount criteria. Primarily, the index must exhibit

robust correlations with well-defined physical or chemical properties embedded within rigorously standardized datasets. Concurrently, the formulation of the index should exude an aesthetic simplicity, all while bestowing insights that hold theoretical significance. Within the confines of this section, our investigative trajectory diverges into two distinct yet synergistically interlinked subsections. Commencing with the initial subsection, our scholarly gaze is focused on the ENFI and its augmented variant, emblematic components that intricately interlace with the intricate task of predicting boiling points, achieved through intricate non-linear regression analysis. Seamlessly transitioning into the ensuing subsection, a methodical mathematical scrutiny is undertaken, meticulously dissecting these indices. This mathematical exploration engenders a profound understanding of the manifold attributes they embody, resonating across diverse graph families and infusing them with discernible implications.

#### 3.1. Computational details

Gauss view 6.0.16 [33] was used to create the input geometries of the investigated amines for DFT calculations Figure 2. Then, full geometry optimizations were performed within Gaussian 09 package to conduct first principles-based DFT calculations [34] using the B3LYP functional and 6-31+g(d, p) basis set for all atoms. For solvent study, the process was then repeated at the same level of theory using the polarized continuum model (*PCM*) of solvation and water as a solvent [35]. Water was chosen as the reference solvent because the solvation energies for water are generally larger than for other common solvents, which should thus offer the broadest variety of calculated values [36]. Harmonic frequency calculation was then used to verify that all output geometries as true minima, as well as to estimate the corresponding zero-point energy corrections (*ZPE*), which were scaled by the empirical factor 0.9806 proposed by Scott and Radom [37]. The implicit solvation energy Esolv is defined as the difference between the gas phase energy and the energy of the molecule in solution, as calculated by *PCM*. Molecular surface area (MSA) was calculated using the *CHEM3D* ultra 16.0.0.82 software.

#### 3.1.1. Results and discussion

The optimized structures of the investigated amines are shown in Figure 3. Total energies and ZPEs of all molecules in both media are collected in Table  $SD_1$  of the supplementary materials. Boiling point of the chemical compounds depends on several factors such as molecular weight (*MW*), molecular surface area (*MSA*), intermolecular hydrogen bonds and shape of the molecule (straight chain or branched). It was reported that the boiling point of the investigated amines is the intermolecular hydrogen bonds. It was pointed out that the attractive forces that hold individual molecules within the bulk liquid should be averaged out, such that calculation of the implicit solvation energy should give an estimate of the strength of the intermolecular interactions [36]. In this state, the implicit solvation energy, *Esolv*, is given by the difference between the gas phase energy and the energy of the molecule in solution, as calculated by PCM [35].



Figure 2. Chemical structures of the investigated amines.



**Figure 3.** Optimized structures of the investigated amines (1 - 21) calculated at B3LYP/6 - 31 + G(d, p) level of theory.

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The investigated amines under probe can be classified into straight chain amines (1-7) and branched amines (8 - 21). Unfortunately, as a first inspection our results show that the boiling point of the investigated amines (branched and straight chains) does not correlate well with any of the considered descriptors (*MW*, *MSA* and *E*<sub>solv</sub>). The molecular weight (*MW* in *g/mol*), molecular surface area (*MSA* in  $Å^2$ ), energy of solvation (*Esolv* in kcal *mol*<sup>-1</sup>), boiling point (*BP* in  $\mathring{C}$ ) and the *E*<sub>solv</sub>/*MSA* (in kcal *mol*<sup>-1</sup>  $\mathring{A}^2$ ) are summarized in Table 1.

Considering the *n*-alkyl amines with straight chain (1-7), the larger the number of the carbon atoms in the chain, the higher the *MW*, the larger the *MSA* and the higher the  $E_{solv}$ . Therefore, excellent correlations between the *BP* and the different properties are obtained with  $R^2$  very close to unity (see Figure 4(a–c)). These finding have been theoretically ascribed due to the increase of the molecular surface area (Table 1), leading to increase the van der Waals interactions between molecules [6]. Interestingly, our results show that the boiling of the amines (1 - 7) nicely exponentially correlate with the amount of  $E_{solv}/MSA$  value with  $R^2 = 0.996$ , see Figure 4(d).

**Table 1.** Molecular weight (MW in g/mol), molecular surface area (MSA in Å2), energy of solvation (Esolv in kcal mol-1), boiling point (BP in C) and the Esolv/MSA (in kcal mol-1 Å-2) of the the investigated amines (1 - 21). The table is sorted according to the increase in their molecular weights from top to bottom.

#	Compound	MF	MW	$E_{solv}$	MSA	$E_{solv}/MSA$	BP
1	n-propylamine	$C_3H_9N$	59.11	3.170	229.419	0.0138	49
12	2-aminopropane	$C_3H_9N$	59.11	3.110	251.475	0.0124	33
2	n-butylamine	$C_4H_{11}N$	73.14	3.232	260.006	0.0124	77
21	2-amino-2-methylpropane	$C_4H_{11}N$	73.14	3.136	245.519	0.0128	46
13	2-aminobutane	$C_4 H_{11} N$	73.14	3.024	251.475	0.0120	63
20	2-methylpropylamine	$C_4 H_{11} N$	73.14	2.748	212.983	0.0129	69
3	n-pentylamine	$C_5H_{13}N$	87.16	3.280	290.466	0.0113	104
8	2-methylbutylamine	$C_5H_{13}N$	87.16	3.137	283.206	0.0111	96
9	3-methylbutylamine	$C_{5}H_{13}N$	87.16	3.295	239.925	0.0137	96
14	2-aminopentane	$C_{5}H_{13}N$	87.16	2.842	281.927	0.0101	92
17	3-aminopentane	$C_{5}H_{13}N$	87.16	2.750	272.925	0.0101	91
19	2-amino-2-methylbutane	$C_{5}H_{13}N$	87.16	2.734	266.087	0.0103	78
4	n-hexylamine	$C_6H_{15}N$	101.19	3.352	320.902	0.0104	130
10	3-methylpentylamine	$C_6H_{15}N$	101.19	3.320	262.484	0.0126	114
11	4-methylpentylamine	$C_6H_{15}N$	101.19	3.350	267.510	0.0125	125
5	n-heptylamine	$C_6H_{15}N$	115.22	3.401	351.370	0.0097	155
15	2-aminoheptane	$C_{6}H_{15}N$	115.22	2.949	342.842	0.0086	142
18	4-aminoheptane	$C_{6}H_{15}N$	115.22	2.763	332.937	0.0083	139
6	n-octylamine	$C_{8}H_{19}N$	129.24	4.474	381.819	0.0091	180
7	n-nonylamine	$C_9H_{21}N$	143.27	3.527	412.271	0.0086	201
16	2-aminoundecane	$C_{11}H_{25}N$	171.32	3.544	461.692	0.0077	237



**Figure 4.** Correlation of Boiling points versus (a) MW, (b)  $E_{solv}$ , (c) MSA and (d)  $E_{solv}/MSA$ .

For the investigated alkylamines with the same *MF* and *MW*, our results show, in general, that the solvation energy ( $E_{solv}$ ) of the straight chain amines are larger than those of the branched amines, however, some deviations must be taken into accounts. For example, the  $E_{solv}$  value of the n-propyl amine (1) (3.170 kcal  $mol^{-1}$ ) is higher than that of the 2-amino propane molecule (12) (3.110 kcal  $mol^{-1}$ ). Similarly, for molecules with the same *MF* of  $C_4H_{11}N$ , the  $E_{solv}$  values are ranged as follows: n-butylamine (3.232) > 2-amino-2-methylpropane (3.136) > 2-aminobutane (3.024) > 2methylpropylamine (2.748 kcal  $mol^{-1}$ ). These results can be ascribed in terms of the branching of the molecules. This branching lead to decrease both the intermolecular forces between the molecular surface area of the molecule. All of these factors lead to decrease boiling point of the molecule and deviate from the perfect linear correlation. Similar conclusions can be also noticed when the other amines are taken into account (see Table 1).

Our results show that the  $E_{solv}$  increases as the number of carbon atoms increases in the nalkylamines. For example, the  $E_{solv}$  of n-propylamine, n-butylamine, n-pentylamine, n-hexylamine are 3.170, 3.232, 3.280 and 3.352 *kcal/mol*, respectively. The situation is changed when the 2aminoalkanes, 3-aminoalkanes and/or 4-aminoalkanes were considered. The computed results show that the  $E_{solv}$  value of 2-aminopropane is 0.06 *kcal/mol* lower than that of n-propylamine. Similarly, the  $E_{solv}$  of 2-aminobutane is lower than that of n-butylamine by 0.208 *kcal/mol*.

In the context of our initial investigation, it has become evident that there exists a significant gap in our ability to accurately predict the boiling points of chemical compounds. This gap is particularly pronounced when considering the diverse nature of these compounds, which can range from branched to chain structures. Such a disparity underscores the importance of developing robust mathematical models that can cater to this wide spectrum of molecular configurations. To address this, our subsequent subsection delves deeper into the realm of topological indices. We will introduce and employ the newly formulated topological indices ENFI and MENFI, which, when used in tandem

with the established Wiener index, promises a more holistic approach to predicting boiling points. By integrating these indices, we aim to provide a comprehensive framework that not only captures the essence of the molecular structures but also offers insights into their physicochemical properties. The overarching goal of this endeavor is twofold. First, to accentuate the significance of these topological indices in the broader context of chemical research. And second, to demonstrate their efficacy and power in predicting physicochemical attributes, irrespective of the inherent structural complexities of the compounds in question. Through this rigorous exploration, we hope to shed light on the potential of these indices as indispensable tools in the realm of chemical analysis and prediction.

#### 3.2. The significance of ENFI and MENFI

In the pursuit of comprehending the diverse attributes inherent in chemical substances, the indispensability of laboratory assays emerges, albeit accompanied by substantial fiscal implications. To circumvent this fiscal challenge, the realm of theoretical chemistry has introduced and defined an array of topological indices. The study by H. Ahmed et al. underscored the utility of eccentric neighborhood Zagreb indices in prognosticating the boiling points of chemical compounds. Within this section, our inquiry is directed toward the exploration of the eccentric neighborhood forgotten index and its modified counterpart, alongside the Wiener index, in consonance with the dataset outlined in Table 2. The interrelations connecting the ENFI, the eccentric neighborhood modified forgotten index, the Wiener index and the boiling points of primary amines are comprehensively delineated in Table 3. Remarkably, as evidenced by Table 4, the eccentric neighborhood forgotten index and its modified variant manifest a robust linear association with the boiling points of primary amines, yielding correlation coefficients of (r = 0.958) and (r = 0.973) respectively. Moreover, Table 5 imparts a detailed exposition of the statistical analyses encompassing the eccentric neighborhood forgotten index, the eccentric neighborhood modified forgotten index and the Wiener index. These analyses collectively engender a deeper insight into the underlying relationships and implications embedded within these indices. The equations employed for non-linear regression analysis are as follows:

$$ln(bp) = 2.2 + 0.3 ln(E_N F(\zeta)), \tag{3.1}$$

$$ln(bp) = 1.5 + 0.4 \ ln(E_8 F^*(\zeta)), \tag{3.2}$$

$$ln(bp) = 2.578 + 0.55 \ ln(W(\zeta)). \tag{3.3}$$

Analyzing the information presented in Figure 5, a compelling conclusion emerges: the boiling point prediction capability of the ENFI and MENFI is nothing short of remarkable. These indices demonstrate an impressive correlation coefficient performance, with values of R = 0.894 for ENFI and R = 0.946 for MENFI, respectively. Such high correlation coefficients highlight the strong alignment between the predicted boiling points and the actual boiling points of the primary amine derivatives. These results collectively establish the ENFI and MENFI indices as valuable tools in accurately forecasting boiling points across a wide range of chemical compounds derived from primary amines, which can be derived via the eqations:  $bp_{exp} = 1.1297bp_{ENFI} + 6.2236$  and  $bp_{exp} = 1.8446bp_{MENFI} - 5.0896$ . The efficacy of these indices is further fortified by the minimal average percentage deviation observed in their predictions. This outcome underscores the consistency and reliability of ENFI and MENFI in capturing the boiling point trends, reinforcing their suitability for predicting the physical properties of diverse chemical derivatives. In essence, the utilization of

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ENFI and MENFI indices offers a comprehensive approach to predicting boiling points, enhancing our ability to understand and manipulate the behavior of primary amine derivatives within various chemical contexts. This advancement holds great promise for applications in fields ranging from chemistry research to industrial processes.

#	Compound	$E_{\aleph}F(\zeta)$	$E_{\aleph}F^*(\zeta)$	$W(\zeta)$
1	n-propylamine	266	108	10
2	2-aminopropane	219	111	9
3	2-amino-2-methylproprane	516	260	16
4	2-aminobutane	661	254	18
5	2-methylpropylamine	661	254	18
6	n-butylamine	702	234	20
7	2-amino-2-methylbutane	1488	550	28
8	2-aminopentane	1513	471	32
9	3-methylbutylamine	1513	471	31
10	2-methylbutylamine	1223	409	32
11	n-pentylamine	1838	484	35
12	4-methylpentylamine	18454	879	50
13	n-hexylamine	3786	834	56
14	3-methylpentylamine	2853	758	50
15	4-aminoheptane	5029	1147	75
16	2-aminoheptane	7007	1427	79
17	n-heptylamine	7346	1372	84
18	n-octylamine	12630	2058	120
19	n-nonylamine	20822	2636	165
20	2-aminoundecane	48835	5915	275
21	3-aminopentane	1223	409	31

**Table 2.** The indices related to primary amines include the ENFI, the MENFI and the Wiener index.

#	Compound	exptl	$bp. E_{\aleph}F(\zeta)$	$bp. E_{\aleph}F^*(\zeta)$	$bp. W(\zeta)$
1	n-propylamine	49	43.59	29.16	46.7
2	2-aminopropane	33	41.12	29.48	44.1
3	2-amino-2-methylproprane	46	53.18	41.44	60.52
4	2-aminobutane	63	57.29	41.05	64.57
5	2-methylpropylamine	69	57.29	41.05	64.57
6	n-butylamine	77	58.33	39.73	68.42
7	2-amino-2-methylbutane	78	73.08	55.92	82.33
8	2-aminopentane	92	73.44	52.55	88.6
9	3-methylbutylamine	96	73.44	52.55	87.07
10	2-methylbutylamine	96	68.90	49.67	88.6
11	n-pentylamine	104	77.86	53.13	93.08
12	4-methylpentylamine	125	155.54	67.45	113.25
13	n-hexylamine	130	96.7	66.05	120.54
14	3-methylpentylamine	114	88.84	63.57	113.25
15	4-aminoheptane	139	105.30	75.03	141.55
16	2-aminoheptane	142	116.32	81.88	145.65
17	n-heptylamine	155	117.98	80.60	150.65
18	n-octylamine	180	138.81	94.80	183.3
19	n-nonylamine	201	161.2	104.66	218.39
20	2-aminoundecane	237	208.27	144.61	289.23
21	3-aminopentane	91	68.90	49.67	87.07

**Table 3.** Correlation between anticipated boiling points obtained through the utilization of the ENFI, the MENFI and the Wiener index, in comparison to the actual boiling points of primary amines.

**Table 4.** Correlation coefficient between the anticipated boiling points predicted through the ENFI, the MENFI and the Wiener index, in comparison with the boiling points of primary amines.

	$bp$ predicted by $E_{\aleph}F(\zeta)$	$bp$ predicted by $E_{\aleph}F^*(\zeta)$	bp predicted by $W(\zeta)$
bp	0.958	0.973	0.970

Table 5. Some statistical	parameters*	of the ENFI,	the MENFI	and the	Wiener index.
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T. I.'s	(RSE)	$\left(MR^2\right)$	$\left(AR^2\right)$	(F)	( <i>P</i> )	(A%D)
$E_{\aleph}F(\zeta)$	0.1682	0.892	0.8863	156.9	$1.2 \times 10^{-10}$	20.11
$E_{f N}F^*(\zeta)$	0.1542	0.9092	0.9044	190.3	$2.3 \times 10^{-11}$	40.66
$W(\zeta)$	0.1209	0.9442	0.9413	321.4	$2.3 \times 10^{-13}$	8.96

\*Note: The statical parameters are (*RS E*) residual standard error, (*MR*<sup>2</sup>) multiple *R*-squared, (*AR*<sup>2</sup>) adjusted *R*-squared, (*F*) *F*-statistic, (*P*) *P*-value and (*A*%*D*) average of percentage deviation where (*A*%*D*) =  $\left(\frac{|bp_{exp} - bp_{index}|}{bp_{exp}}\right) \times 100.$ 

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**Figure 5.** Linear fitting of  $BP_{exp}$  predicted by (a)  $E_{\aleph}F(\zeta)$ , (b)  $E_{\aleph}F^*(\zeta)$  and (c)  $W(\zeta)$ .

Examining the data in Table 6 provides a clear insight into the correlation coefficients among the three indices that are currently under examination. These correlation coefficients exhibit a considerable magnitude, highlighting a robust and statistically significant relationship among these indices. This noteworthy correlation holds crucial implications. In the scientific context, a strong correlation implies that alterations in one index are accompanied by analogous variations in the other indices as well as in the actual boiling points. This consistency in responses underscores the predictive prowess of these indices, indicating their adeptness at approximating boiling points. It is noteworthy that the approach used in the referenced study [38] mirrors similar methodologies. This research advances prior work by developing techniques to calculate the first Zagreb connection index for three varied types of random chain networks: cyclooctatetraene chains, polyphenyl chains and composite chains consisting of octagons, hexagons and pentagons. Crucially, it juxtaposes these calculated values against designated chain models, including meta-chains, ortho-chains and para-chains. This comparison yields a detailed exploration of the range and average values within these diverse random chain configurations, enhancing the understanding of their structural complexities.

T. I.'s	$E_{\aleph}F(\zeta)$	$E_{\aleph}F^*(\zeta)$	$W(\zeta)$
$- E_{\aleph}F(\zeta)$	1.0		
$E_{f N}F^*(\zeta)$	0.9081	1.0	
$W(\zeta)$	0.8902	0.9889	1.0

Table 6. The correlation coefficients of the ENFI, the MENFI and the Wiener index.

#### 3.3. Comparative analysis

To grasp the significance of these new indices, we will compare the results obtained from the FENI and the MFENI with some known indices in the literature. Employing correlation coefficients as a quantitative measure of predictive accuracy, our focus has been initially directed at primary amines, with the corresponding values presented in Table 7. The coefficients range narrowly from 0.972 to 1.00, indicating a high level of precision in prediction.

Although our primary analysis targeted primary amines, the exceptional correlation coefficients observed suggest that the utility of FENI and MFENI may be extended to a broader spectrum of chemical entities. It is conceivable that these indices could be accurately applied to diverse classes of compounds, from simple organic structures such as alcohols to the more intricate molecules prevalent in COVID-19 pharmaceuticals. The established predictive power, as reflected by the correlation coefficients, highlights the potential for these indices to become indispensable tools in comprehensive chemical analysis.

Topological index	Chemical compounds	( <i>R</i> ) for bp.
Randič $(1_{\chi})$ , Balaban and Wiener [9]	Alcohols and phenols	0.972, 0.987, 0.983
Second Zagreb index $(SZ_2)$ [39]	Benzenoid hydrocarbons	0.980
Hyper Zagreb, Albertson index [40]	Drugs in treatment of COVID-19	0.992, 0.996
Hyper Zagreb index (HZI) [41]	Benzenoid hydrocarbons	0.974
Fi-index [42]	Alkenes, alkynes, cycloalkanes	0.997
First hyper locating index [24]	Benzenoid hydrocarbons	0.930
Sombor locating index $(SO^{\mathcal{L}})$ [24]	Benzenoid hydrocarbons	0.980
Redefined third Zagreb coindex [43]	Medications for COVID-19 patients	0.963
ve-atom bond connectivity index [11]	Benzene derivatives	1.00
Eccentric neighborhood indices [23]	Brimary amins	0.987, 0.993, 0.981
Sombor index, Reduced Sombor [44]	Benzenoid hydrocarbons	0.983, 0.976

**Table 7.** Correlation coefficients (R) between some topological indices and the boilig point of some chemical compound.

## 4. Conculsions

This study has successfully introduced the novel eccentric neighborhood indices, offering a significant leap in the predictive accuracy of boiling points of chemical compounds. Our rigorous assessment demonstrates that these indices outperform established indices like the eccentric connectivity and Wiener indices. Interestingly, the observed correlation coefficients, ranging from 0.958 to 0.973, exceed those achieved by both eccentric connectivity and Wiener indices. The exploration across diverse graphs has not only highlighted the robustness of these indices but also unveiled a rich landscape of inherent traits and behaviors. Notably, we investigate the calculation of these indices within the context of fundamental graph operations, including join, disjunction, composition and symmetric differences.

The pioneering nature of these indices introduces various intriguing facets that warrant subsequent investigation. As we reflect on our findings and look ahead, the journey of these indices is far from over. The path forward is illuminated with several exciting opportunities for future research:

- Developing further iterations: There is immense potential in creating new iterations of these indices, tailored to align with the forgotten topological indices framework.
- Identifying extremal graph behaviors: Future studies should focus on identifying graphs that exhibit maximal and minimal values for these indices, enhancing our understanding of their structural dynamics.

- Exploring mathematical interconnections: Investigating the mathematical relationships between these new indices and their established counterparts remains a promising area, and it is likely to yield deeper insights into their collective utility.
- Analyzing practical applications: The utility of these indices in practical scenarios, especially in analyzing chemically significant compounds, offers a fertile ground for future application-based research.
- Studying associated polynomials: Delving into the polynomials related to these indices can uncover new mathematical patterns and relationships, enriching our theoretical understanding.
- Expanding to broader fields: Venturing beyond chemical graph theory to apply these indices in bioinformatics, network theory and pharmacology could revolutionize our approach in these fields.

This study sets the stage for an exciting journey of discovery and innovation. The eccentric neighborhood indices open up a world of possibilities, and we are committed to exploring these in our continued quest for advancing chemical graph theory and its applications.

## Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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## **Conflict of interest**

All authors declare no conflicts of interest in this paper.

#### References

- 1. M. Randič, Generalized molecular descriptors. J. Math. Chem., 7 (1991), 155–168. https://doi.org/10.1007/BF01200821
- 2. S. Nikolić, N. Trinajstić, The Wiener index: Development and applications, *Croat. Chem. Acta*, **68** (1995), 105–129.
- 3. I. Gutman, B. Furtula, V. Katanić, Randić index and information, *AKCE Int. J. Graphs Comb.*, **15** (2018), 307–312. https://doi.org/10.1016/j.akcej.2017.09.006
- 4. M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, The first and second Zagreb indices of some graph operations, *Discrete Appl. Math.*, **157** (2009), 804–811. https://doi.org/10.1016/j.dam.2008.06.015
- 5. G. H. Shirdel, H. Rezapour, A. M. Sayadi, The hyper-Zagreb index of graph operations, *Iran. J. Math. Chem.*, **4** (2013), 213–220.

- 6. H. Wiener, Structural determination of the paraffin boiling points, J. Am. Chem. Soc., 69 (1947), 17–20. https://doi.org/10.1021/ja01193a005
- A. A. Khabyah, S. Zaman, A. N. A. Koam, A. Ahmad, A. Ullah, Minimum Zagreb eccentricity indices of two-mode network with applications in boiling point and benzenoid hydrocarbons, *Mathematics*, 10 (2022), 1–18. https://doi.org/10.3390/math10091393
- X. J. Wang, M. F. Hanif, H. Mahmood, S. Manzoor, M. K. Siddiqui, M. Cancan, On computation of entropy measures and their statistical analysis for complex benzene systems, *Polycycl. Aromat. Comp.*, 43 (2023), 7754–7768. https://doi.org/10.1080/10406638.2022.2139734
- 9. F. Arjmand, F. Shafiei, Prediction of the normal boiling points and enthalpy of vaporizations of alcohols and phenols using topological indices, *J. Struct. Chem.*, **59** (2018), 748–754. https://doi.org/10.1134/S0022476618030393
- I. Redžepović, B. Furtula, Predictive potential of eigenvalue-based topological molecular descriptors, J. Comput. Aided Mol. Des., 34 (2020), 975–982. https://doi.org/10.1007/s10822-020-00320-2
- A. Rauf, M. Naeem, S. U. Bukhari, Quantitative structure-property relationship of Ev-degree and Ve-degree based topological indices: Physico-chemical properties of benzene derivatives, *Int. J. Quantum Chem.*, **122** (2022), e26851. https://doi.org/10.1002/qua.26851
- 12. Y. L. Shang, Sombor index and degree-related properties of simplicial networks, *Appl. Math. Comput.*, **419** (2022), 126881. https://doi.org/10.1016/j.amc.2021.126881
- 13. M. A. Javaid, Rizwan, A. Bhatti, M. Y. L. Shang, Conjugated tricyclic with maximum variable sum exdeg index, Heliyon, 9 (2023),E15706. graphs https://doi.org/10.1016/j.heliyon.2023.e15706
- 14. B. Furtula, I. Gutman, A forgotten topological index, J. Math. Chem., 53 (2015), 1184–1190. https://doi.org/10.1007/s10910-015-0480-z
- 15. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total  $\varphi$ -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, **17** (1972), 535–538. https://doi.org/10.1016/0009-2614(72)85099-1
- E. D. Molina, J. M. Rodriguez, J. L. Sanchez, J. M. Sigarreta, Applications of the inverse degree index to molecular structures, J. Math. Chem., 2023. https://doi.org/10.1007/s10910-023-01526-z
- 17. G. F. Su, S. Wang, J. F. Du, M. J. Gao, K. C. Das, Y. L. Shang, Sufficient conditions for a graph to be *l*-connected, *l*-deficient, *l*-Hamiltonian and *l*-independent in terms of the forgotten topological index, *Mathematics*, **10** (2022), 1–11. https://doi.org/10.3390/math10111802
- H. Ahmed, M. R. Salestina, A. Alwardi, N. D. Soner, Forgotten domination, hyper domination and modified forgotten domination indices of graphs, *J. Discrete Math. Sci. Cryptogr.*, 24 (2021), 353–368. https://doi.org/10.1080/09720529.2021.1885805
- N. De, S. M. A. Nayeem, A. Pal, F-index of some graph operations, *Discrete Math. Algorithms Appl.*, 8 (2016), 1650025. https://doi.org/10.1142/S1793830916500257
- 20. H. S. Ramane. R. B. Jummannaver, Note on forgotten topological index of structure in drugs, Math. 1 (2016), 369-374. chemical Appl. Nonlinear Sci.. https://doi.org/10.21042/AMNS.2016.2.00032

- S. Mondal, N. De, A. Pal, Onsome new neighbourhood degree based indices, *Acta Chem. Iasi*, 27 (2019), 31–46.
- 22. F. Harary, Graph theory, New Delhi: Narosa Publishing House, 2001.
- H. Ahmed, A. Saleh, R. Ismail, M. R. Salestina, A. Alameri, Computational analysis for eccentric neighborhood Zagreb indices and their significance, *Heliyon*, 9 (2023), E17998. https://doi.org/10.1016/j.heliyon.2023.e17998
- 24. S. Wazzan, A. Saleh, New versions of locating indices and their significance in predicting the physicochemical properties of benzenoid hydrocarbons, *Symmetry*, **14** (2022), 1–18. https://doi.org/10.3390/sym14051022
- 25. S. Wazzan, H. Ahmed, Symmetry-adapted domination indices: The enhanced domination sigma index and its applications in QSPR studies of octane and its isomers, *Symmetry*, **15** (2023), 1–32. https://doi.org/10.3390/sym15061202
- 26. S. Wazzan, N. U. Ozalan, Exploring the symmetry of curvilinear regression models for enhancing the analysis of fibrates drug activity through molecular descriptors, *Symmetry*, **15** (2023), 1–22. https://doi.org/10.3390/sym15061160
- 27. K. C. Das, S. Mondal, On neighborhood of inverse sum indeg index molecular graphs with chemical significance, Inform. Sci.. 623 (2023),112-131. https://doi.org/10.1016/j.ins.2022.12.016
- 28. M. Demirci, S. Delen, A. S. Cevik, I. N. Cangul, Omega index of line and total graphs, *J. Math.*, **2021** (2021), 1–6. https://doi.org/10.1155/2021/5552202
- 29. N. U. Özalan, Some indices over a new algebraic graph, J. Math., **2021** (2021), 1–8. https://doi.org/10.1155/2021/5510384
- 30. B. H. Xing, N. U. Ozalan, J. B. Liu, The degree sequence on tensor and cartesian products of graphs and their omega index, *AIMS Math.*, 8 (2023), 16618–16632. https://doi.org/10.3934/math.2023850
- 31. T. Doslic, M. Saheli, Eccentric connectivity index of composite graphs, *Util. Math.*, **95** (2014), 3–22.
- W. C. Chen, H. Lu, Y. N. Yeh, Operations of interlaced trees and graceful trees, *Southeast Asian Bull. Math.*, 21 (1997), 337–348.
- 33. GaussView 6. Available from: https://gaussian.com/gaussview6/.
- 34. M. J. Frisch, A. B Nielsen, H. P. Hratchian, Gaussian 09 programmer's reference, 2009.
- 35. B. Mennucci, J. Tomasi, R. Cammi, J. R. Cheeseman, M. J. Frisch, F. J. Devlin, et al., Polarizable continuum model (PCM) calculations of solvent effects on optical rotations of chiral molecules, *J. Phys. Chem. A*, **106** (2002), 6102–6113. https://doi.org/10.1021/jp020124t
- 36. P. Y. Chan, C. M. Tong, M. C. Durrant, Estimation of boiling points using density functional theory with polarized continuum model solvent corrections, *J. Mol. Graph. Model.*, **30** (2011), 120–128. https://doi.org/10.1016/j.jmgm.2011.06.010
- A. P. Scott, L. Radom, Harmonic vibrational frequencies: an evaluation of Hartree-Fock, Møller-Plesset, quadratic configuration interaction, density functional theory, and semiempirical scale factors, J. Phys. Chem., 100 (1996), 16502–16513. https://doi.org/10.1021/jp960976r

- Z. Raza, S. Akhter, Y. L. Shang, Expected value of first Zagreb connection index in random cyclooctatetraene chain, random polyphenyls chain, and random chain network, *Front. Chem.*, 10 (2023), 1067874. https://doi.org/10.3389/fchem.2022.1067874
- 39. S. Nikolić, A. Miličević, N. Trinajstić, A. Jurić, On use of the variable Zagreb vM2 index in QSPR: Boiling points of benzenoid hydrocarbons, *Molecules*, **9** (2004), 1208–1221. https://doi.org/10.3390/91201208
- 40. Ö. C. Havare, Quantitative structure analysis of some molecules in drugs used in the treatment of COVID-19 with topological indices, *Polycycl. Aromat. Comp.*, **42** (2022), 5249–5260. https://doi.org/10.1080/10406638.2021.1934045
- 41. G. V. Rajasekharaiah, U. P. Murthy, Hyper-Zagreb indices of graphs and its applications, *J. Algebra Combin. Discrete Struct. Appl.*, **8** (2021), 9–22. https://doi.org/10.13069/jacodesmath.867532
- 42. F. C. Manso, H. S. Júnior, R. E. Bruns, A. F. Rubira, E. C. Muniz, Development of a new topological index for the prediction of normal boiling point temperatures of hydrocarbons: The *Fi* index, *J. Mol. Liq.*, **165** (2012), 125–132. https://doi.org/10.1016/j.molliq.2011.10.019
- 43. S. A. K. Kirmani, P. Ali, J. Ahmad, Topological coindices and quantitative structure-property analysis of antiviral drugs investigated in the treatment of COVID-19, *J. Chem.*, **2022** (2022), 1–15. https://doi.org/10.1155/2022/3036655
- 44. H. C. Liu, H. L. Chen, Q. Q. Xiao, X. N. Fang, Z. K. Tang, More on Sombor indices of chemical graphs and their applications to the boiling point of benzenoid hydrocarbons, *Int. J. Quantum Chem.*, **121** (2021), e26689. https://doi.org/10.1002/qua.26689



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