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Zagreb Connection Indices for Analyzing Chemical and Metallic Structures

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Abstract In the study of molecular structures, topological indices give useful information regarding connectivity, symmetry and physicochemical properties. It helps the researchers to engineer and investigate chemical and metallic structures by using graph tools and algebraic models. This study analyzes the chemical, Concealed Non-Kekulean Benzenoid Hydrocarbons (CNBH)and metallic, Face Centered Cubic Lattice (FCC) structures, by examining their different types of topological indices, including the first Zagreb connection index, second Zagreb connection index, forgotten index, redefined Zagreb index, general Randić index, and symmetric division degree index from generalized Zagreb connection index. Furthermore, the results are presented through mathematical quantities in tables and visualized using 3D plots.

1 Introduction

Graph theory can be applied to the theory of alkanes and other hydrocarbons. Any hydrocarbon with only single bond can be represented as a graph. A hydrocarbon is any organic chemical molecule that only comprises the elements carbon (C) and hydrogen (H) [1]. The carbon atoms join together to generate the compound's structure, and the hydrogen atoms unite with them in diverse ways. The structural formulas of dipolar bonded compounds are graphs and are therefore known as molecular graphs. Hydrocarbons are the primary compounds of petroleum and natural gas. They are utilised as fuels and as raw materials in the manufacture of polymers, rubber, gunpowder, and industrial chemicals [2]. The most crucial electron structures are benzenoid hydrocarbons. They have been extensively used to test different theories of molecular or biochemical behavior [3].

Face Centered Cubic (FCC) is an explanation of the sorting of atoms in crystal composition. The FCC structure contains an atom at every cube corner and an atom in the middle of every cube face [4]. These atoms are compact, meaning they may not fill any thick space, and each atom is connected to its neighboring vertices in some way. A nearby stuffed level, like that achieved by removing each eight corner particles and forming an octahedron with them, is called the Octahedral planes [5]. Therefore, the Face Centered Cube framework possesses four incites of two equivalent levels. Ultimate metals and mixtures are translucent, which means their atoms arrange themselves in an enjoined form. In particular, Face Centered Cubic metals and mixtures possess attractive plasticity. Chemical graph theory is a topology branch of numerical science that relates graph theory to the mathematical shaping of compound occurrence in order to obtain insight into the physical properties of the chemical composite [6].

Molecular structures are shown using graphs in this field of research. The vertices as well as edges on the molecular graph correspond to atoms and bonds, respectively. These mathematical networks, known as graph-theoretical descriptors or indices, reflect the physical features of molecules [7]. While it is acknowledged that the discussion of numerous polyaromatic hydrocar-

bon groups is beyond the scope of this research, it is worth considering the current identification of benzenoid hydrocarbons [8]. Chemical graph theory is an interdisciplinary field that emerged from research in both chemistry and mathematics, demonstrating the value of their relationship. Initially, chemical graphs were used to depict the intricate interplay between atoms within molecules. Alkanes have predominantly been used in the production of diesel and jet fuels, but they still pose challenges in achieving lower pour points for emerging synthetic fuels.

The topological index is a numerical coding of molecular graphs that can forecast the physicochemical, natural, microbiological, and primary qualities of synthetic mixtures associated with the molecular graphs. One such molecule is Kekulene, a donut-shaped polycyclic aromatic hydrocarbon composed of consistently displayed benzene rings. The Face Centered Cubic Lattice (FCC(n)) has recently gained significant attention due to its recognized properties, non-toxic nature, low cost, abundance, and straightforward production process.

A topological index is a real number associated with a graph, which must remain invariant under constitutional changes [9]. Several topological indices have been described, many of which have been implemented to represent chemical, medicinal, and other molecular resources [10]. The Wiener index, introduced by Harold Wiener in 1947, was the first topological index applied in chemistry to calculate physical properties of different types of alkanes, specifically paraffin [11, 12]. Consequently, topological indices have recently shown use in constructing QSAR models for various purposes, including DNA analysis, protein folding, 2D RNA frameworks, drug or toxin QSPR, protein surface data decoding, and protein association networks [13].

Degree-based topological indices, which provide important information about graphs and are particularly relevant in chemistry, are widely studied. Among them, the Zagreb indices are the most extensively researched [14, 15]. Zagreb indices are computed for different molecular structures such as oxides, hexagonal, octahedral, honeycomb, and benzenoid compounds [16]. Recent research has also focused on topological indices for the molecular structure of Pectin [17].

Recent studies have significantly expanded the applications of generalized Zagreb indices, Zagreb connection indices, entropy-based descriptors, and graph invariants in chemical graph theory. Cai et al. [18] investigated generalized Zagreb indices under graph operations and established important relationships with line graph structures, whereas Cheng and Wu [19] examined the behavior of the first general Zagreb index through line graph transformations and derived several theoretical properties. Furthermore, Rahbani et al. [20] developed new bounds for Zagreb connection indices of trees with fixed domination numbers, while Raza et al. [21] characterized graph families attaining maximal Zagreb connection index values, highlighting the importance of connection-based descriptors in extremal graph theory.

In addition, Akmal et al. [22] employed entropy measures associated with topological indices to analyze the structural complexity of rectangular bilayer germanium phosphide, demonstrating the effectiveness of graph-theoretical descriptors in advanced materials science. More recently, Yang et al. [23] investigated topological invariants of sustainable networks from the perspectives of energy efficiency and environmental impact reduction, further emphasizing the growing role of graph invariants and topological descriptors in sustainable and complex network analysis.

The novelty of the present study lies in the development of generalized Zagreb connection index formulations for two important molecular structures, namely Concealed Non-Kekulean Benzenoid Hydrocarbons and Face-Centered Cubic lattices. The derived generalized expressions provide a unified framework that simultaneously produces several classical connection-based topological indices as special cases. Consequently, the proposed methodology reduces repetitive computations and offers a systematic approach for investigating structural characteristics of both chemical and metallic networks.

Several connection-based topological indices have been extensively studied in chemical graph theory due to their ability to characterize molecular structures through graph invariants. Among these descriptors, Zagreb indices and Zagreb connection indices have attracted significant attention because of their applications in molecular characterization, QSAR/QSPR studies, and structural analysis. Recent investigations have focused on generalized Zagreb indices, connection indices, and related graph descriptors for various chemical and lattice networks.

Despite the growing literature on Zagreb connection indices, generalized formulations for several important chemical and metallic structures remain unexplored. In particular, Concealed Non-Kekulean Benzenoid Hydrocarbons and Face-Centered Cubic lattices possess distinct topo-

logical characteristics that make them suitable candidates for comparative investigation. This motivates the development of closed-form generalized Zagreb connection index expressions for these graph families.

The main contributions of this work are summarized as follows:

- We derive generalized Zagreb connection index formulas for CNBH(n) and FCC(n) structures.
- We obtain several classical connection-based topological indices as special cases of the generalized formulation.
- We establish closed-form analytical expressions for arbitrary values of the structural parameter n.
- We provide numerical and asymptotic comparisons between chemical and metallic graph families.
- We analyze the structural implications of the obtained descriptors through tabular and graphical representations.

In this article, we have expanded on two distinct molecular frameworks, considering the varying number of successive copies (n) and their chemical and metal composition. Additionally, we have determined the generalized Zagreb connection index for these structures. Furthermore, we have acquired diverse additional indices and connection indices using the offered generalised version. Ultimately, we provide an analysis of these distinct indices by using quantitative values and their three-dimensional visualization.

Section 2 discusses the fundamental concepts and methodology commonly used in the central conclusion. In sections 3 as well as 4, we evaluate the generalized Zagreb connection index for concealed non-kekulean benzenoid hydrocarbons and the face-centered cubic lattice. Furthermore, using these generalized Zagreb connection indices, we compute many additional Zagreb connection indices. Section 5 provides some applications of topological indices, while section 6 summarizes the findings and concludes the study.

The present work focuses on the case $j = 2$ because the corresponding parameter $\tau_2(v)$ represents the connection number of a vertex. Consequently, the generalized Zagreb connection index provides information beyond ordinary vertex degrees by incorporating second-neighborhood interactions. Owing to its importance in chemical graph theory and molecular characterization, the case $j = 2$ has received considerable attention in the literature and is therefore adopted in this study.

2 Application of Topological Indices

2.1 Studies on QSAR-QSPR

It is well accepted that a compound's chemical characteristics extend beyond the arrangement of its components. Two important areas of chemical analysis, namely Quantitative Structure-Activity Relationship (QSAR) analysis and Quantitative Structure-Property Relationship (QSPR) studies, focus on understanding these dependencies. These quantitative approaches involve mathematical models that link various variables, such as boiling point, taste threshold, antiviral activity, or specific attributes like sweetness or toxicity, to structural parameters [36]. Regression analysis and pattern recognition techniques are commonly employed in these models.

There have been several articles published on QSAR as well as QSPR investigations, indicating the wide applicability and benefits of these approaches. Notable journals that have featured such research include Journal of Pharmaceutical Science, Basics of Applied Pharmacology, Analytical Chemistry, Environmental Health Perspectives, Drug Information Journal, IEC Method Design and Development, Chemical Senses and Journal of Medicinal Chemistry. Additionally, QSAR was introduced and reviewed in 1982. Graph theory has shown its usefulness in QSAR and QSPR investigations [37]. Trinajstic and colleagues have recently stated that there are thirty-nine topological indices that are already documented in the existing literature [38]. In the following sections, we shall examine many significant topological indices and provide documented instances of their use [39].

The present work focuses on the theoretical computation of generalized Zagreb connection indices and related descriptors for CNBH and FCC structures. Although no explicit QSAR/QSPR model is developed herein, the obtained descriptors can serve as useful structural parameters for future predictive studies involving chemical and material properties.

2.2 Topological Indices in Material Science

Topological indices have diverse applications in material science and mechanical engineering. They can be utilized in various areas, including nano-scale studies of material structures and characteristics. These indices provide valuable insights into mechanical properties, such as intensity, tensile strength, and dimensional stability, by defining the connectivity between atoms.

In structural analysis, topological indices offer valuable data for examining the behavior of complex mechanical systems. For example, when analyzing truss structures, the appropriate indices can quantify the topological characteristics of truss connections. This information helps determine load paths, optimize structural configurations, and evaluate the stability and reliability of the system.

Topological indices including the Chern number and the winding number, may be used to globally understand the geometric properties of certain systems. These indices are particularly useful in odd and even dimensions and are related to the bulk-edge correspondence [40]. The application of topological characterization extends beyond nano-photonics to classical wave problems, and even macroscopic elastic waves [41]. In classical wave systems, related concepts like adiabatic evolution and geometrical phase are also applicable [42]. Furthermore, the author of a recent study [43] presents a general method for defining topological indices in mechanical systems that accounts for nonlinear effects without resorting to any approximations.

3 Preliminaries

In the molecular graph $\Upsilon = (K(\Upsilon), E(\Upsilon))$, $K(\Upsilon) = q_1, q_2, \ldots, q_n$ represents the set of vertices, and $E(\Upsilon)$ represents the set of edges. These sets specify the connections between chemical and organic substances or between two molecular substances. The order of Υ, denoted as $|K(\Upsilon)| = s$, represents the number of vertices, and the size of Υ, denoted as $|E(\Upsilon)| = e$, indicates the number of edges. A graph is considered connected if there exists a trail between any two vertices. The distance between two vertices, t and w, is referred to as their interval, denoted as $d(\iota, \kappa)$. For a vertex $w \in K(\Upsilon)$ and a positive integer j, the extended j-parts of κ in the graph Υ are interpreted as $N_j(\kappa)$, which can be defined as $N_j(\kappa) = \kappa \in K(\Upsilon) : d(\iota, \kappa) = j$. The j-distance degree of a vertex κ in Υ is defined as $d_j(\kappa) = |N_j(\kappa)|$.

In Table 1, we introduce several indices based on j-distance for any integral value of $j \geq 2$. These indices include the j-distance second Zagreb index $(C^{(j)}2(\Upsilon))$, the j-distance forgotten index $(F^{(j)}(\Upsilon))$, the j-distance Redefined Zagreb index $(ReZC^{(j)}(\Upsilon))$, the j-distance general first Zagreb index $(C_1^{(j)\alpha}(\Upsilon))$, the j-distance general Randić index $(R^{(j)}\alpha(\Upsilon))$, and the j-distance symmetric division deg index $(SDD^{(j)}(\Upsilon))$.

For a vertex $v \in V(\Upsilon)$, the quantity

$$\tau_j(v) = |N_j(v)|$$

denotes the number of vertices at distance exactly j from v. In particular, when $j = 2$, $\tau_2(v)$ represents the connection number of the vertex v.

Definition 2.1: For $p, q \in Z^+$ and $j \geq 1$, the j-distance generalized Zagreb index is defined as:

$$C_{p,q}^{(j)}(\Upsilon) = \sum_{\iota\kappa \in E(\Upsilon)} [\tau(\iota)^p \tau(\kappa)^q + \tau(\kappa)^p \tau(\iota)^q]. \tag{3.1}$$

More precisely, the term "generalised Zagreb index" is used when $j = 1$, whereas the term "generalised Zagreb Connection index" is used when $j = 2$.

For $j = 1$, the Zagreb indices, also known as the 1-distance Zagreb indices, can be referred to as the general Randić index, first Zagreb index, Redefined Zagreb index, second Zagreb index, general first Zagreb index, forgotten index [24]. Additionally, the symmetric division degree

Table 1. Zagreb connection indices

Indices	Values
$C_1^{(2)}(\Upsilon)$	$\sum_{\iota\kappa\in E(\Upsilon)}[\tau_j(\iota)+\tau_j(\kappa)]$
$C_2^{(2)}(\Upsilon)$	$\sum_{\iota\kappa\in E(\Upsilon)}[\tau_j(\iota)\times\tau_j(\kappa)]$
$F^{(2)}(\Upsilon)$	$\sum_{\iota\kappa\in E(\Upsilon)}[\tau_j(\iota)^2+\tau_j(\kappa)^2]$
$ReZC^{(2)}(\Upsilon)$	$\sum_{\iota\kappa\in E(\Upsilon)}\tau_j(\iota)\tau_j(\kappa)[\tau_j(\iota)+\tau_j(\kappa)]$
$C_1^{(2)\alpha}(\Upsilon)$	$\sum_{\iota\in Q(\Upsilon)}[\tau_j(\iota)]^\alpha$
$R_\alpha^{(2)}(\Upsilon)$	$\sum_{\iota\kappa\in E(\Upsilon)}[\tau_j(\iota)\times\tau_j(\kappa)]^\alpha$
$SDD^{(2)}(\Upsilon)$	$\sum_{\iota\kappa\in E(\Upsilon)}[\frac{\tau_j(\iota)}{\tau_j(\kappa)}+\frac{\tau_j(\kappa)}{\tau_j(\iota)}]$

Table 2. Zagreb connection indices in terms of generalized Zagreb connection index

Indices	Values from Eq. 3.1
$C_1^{(2)}(\Upsilon)$	$C_{1,0}^{(2)}(\Upsilon)$
$C_2^{(2)}(\Upsilon)$	$\frac{1}{2}C_{1,1}^{(2)}(\Upsilon)$
$F^{(2)}(\Upsilon)$	$C_{2,0}^{(2)}(\Upsilon)$
$ReZC^{(2)}(\Upsilon)$	$C_{2,1}^{(2)}(\Upsilon)$
$C^{(2)\alpha}(\Upsilon)$	$C_{\alpha-1,0}^{(2)}(\Upsilon)$
$R_\alpha^{(2)}(\Upsilon)$	$\frac{1}{2}C_{\alpha,\alpha}^{(2)}(\Upsilon)$
$SDD^{(2)}(\Upsilon)$	$C_{1,-1}^{(2)}(\Upsilon)$

index as well as generalized Zagreb index are explained by [25, 26, 27, 28, 29, 30, 31], respectively. For $j=2$, the 2-distance Zagreb indices, or Zagreb connection indices, for instance, the first Zagreb connection index and second Zagreb connection index, are defined by [32, 33, 34]. In [35], degree-based topological indices like the Sanskruti index for the web graph are calculated. We also cite the Chemical Framework (ChF), which represents the configuration of a chemical substance, as shown in Figure 1.

For the sake of consistency, the notation

$$C_{p,q}^{(2)}(\Upsilon)$$

will be used throughout the manuscript to denote the generalized Zagreb connection index. The associated topological descriptors are expressed according to the notation given in Table (2). Furthermore, the generalized Zagreb index corresponds to the case $j=1$, whereas the generalized Zagreb connection index corresponds to $j=2$.

The larger node represents a water softener alkali chemical, while the smaller vertex represents an organic substance. The edges represent bonds between the chemical and the organic substance. A structure is simply a connected graph that has multiple edges and is formed when there is at least one edge connecting a certain number of nodes.

Remark:
The generalized Zagreb connection index represents a parametric extension of several classical connection-based topological indices. By selecting appropriate values of p and q, numerous descriptors such as the First Zagreb Connection Index, Second Zagreb Connection Index, Forgotten Index, Redefined Zagreb Connection Index, General Randić Index, and Symmetric Division Degree Index can be obtained directly. Hence, the generalized model provides a comprehensive framework for studying multiple topological characteristics using a single mathematical expression.

4 Topological Indices for the Concealed Non-Kekulean Benzenoid Hydrocarbon

In this section, we explore the topological indices for the structure of benzenoid hydrocarbons. Theorem 4.1, introduces a topological index based on the connection number of the vertices. From corollary 4.2, we determine the First and Second Zagreb indices, the forgotten topological index, the redefined Zagreb index, the general first Zagreb index, the general Randić index, and the symmetric division degree index using the j-generalized Zagreb index of the chemical structure.

For $j = 2$, we examine the division of the set of vertices CK as well as the collection of edges CE of $CNBH(n)$ w.r.t the degrees of adjacent vertices at a two-interval in $CChF(n)$. Consequently, for 2-distance $\iota k \in CE$, the resulting Table 3 is presented below.

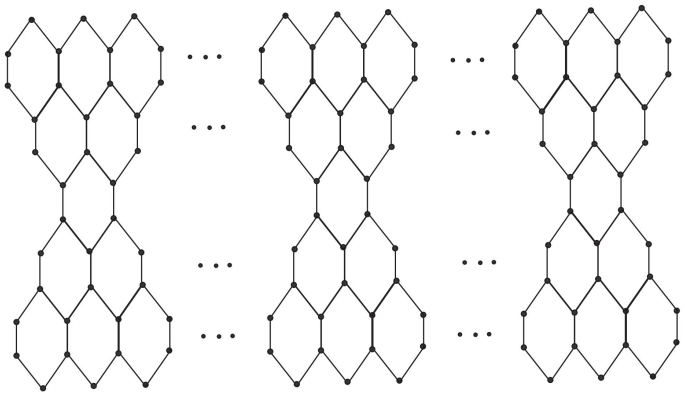


Figure 1. Concealed Non-Kekulean Benzenoid Hydrocarbon

Table 3. The edge division in $CNBH(n)$

$CE_{\{\tau(\iota),\tau(\kappa)\}}$	$\lvert CE_{\{\tau(\iota),\tau(\kappa)\}}\rvert$
(3,2)	8
(3,4)	8
(4,4)	$4n$
(4,5)	4
(4,6)	$2n+4$
(5,5)	2
(5,6)	4
(6,6)	$11n-16$

Theorem 4.1. *Suppose $\Upsilon \cong CNBH(n)$ is a chemical structure with a capacity of n for $n \geq 2$. Then, the generalized Zagreb connection index, denoted as $C^2_{p,q}(CNBH(n))$, is defined as follows:*

$$\begin{aligned} C^2_{p,q}(CNBH(n)) =& 2[4(3^p2^q + 2^p3^q) + 4(3^p4^q + 4^p3^q) + 2(4^p5^q + 5^p4^q) + 2(4^p6^q + 6^p4^q) \\ &+ (5^p5^q + 5^p5^q) + 2(5^p6^q + 6^p5^q) - 8(6^p6^q + 6^p6^q)] \\ &+ 4n(4^p4^q + 4^p4^q) + 2n(4^p6^q + 4^p6^q) + 11n(6^p6^q + 6^p6^q). \end{aligned}$$

Proof. From Table 3 and the method evaluated in Section 3, we aim to compute the required result as demonstrated below.

$$C^2_{p,q}(CNBH(n)) = \sum_{\iota\kappa \in E(CNBH(n))} (\tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q)$$

$$
\begin{aligned}
&= \sum_{\iota\kappa\in E_{\{3,2\}}} (\tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q) \\
&\quad + \sum_{\iota\kappa\in E_{\{3,4\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q) + \sum_{\iota\kappa\in E_{\{4,4\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q) \\
&\quad + \sum_{\iota\kappa\in E_{\{4,5\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q) + \sum_{\iota\kappa\in E_{\{4,6\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q) \\
&\quad + \sum_{\iota\kappa\in E_{\{5,5\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q) + \sum_{\iota\kappa\in E_{\{5,6\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q) \\
&\quad + \sum_{\iota\kappa\in E_{\{6,6\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q), \\
&= 8(3^p2^q + 2^p3^q) + 8(3^p4^q + 4^p3^q) + 4n(4^p4^q + 4^p4^q) + 4(4^p5^q + 5^p4^q) \\
&\quad + (2n+4)(4^p6^q + 6^p4^q) + 2(5^p5^q + 5^p5^q) + 4(5^p6^q + 6^p5^q) \\
&\quad + (11n-16)(6^p6^q + 6^p6^q), \\
&= 2[4(3^p2^q + 2^p3^q) + 4(3^p4^q + 4^p3^q) + 2(4^p5^q + 5^p4^q) + 2(4^p6^q + 6^p4^q) \\
&\quad + (5^p5^q + 5^p5^q) + 2(5^p6^q + 6^p5^q) - 8(6^p6^q + 6^p6^q)] + 4n(4^p4^q + 4^p4^q) \\
&\quad + 2n(4^p6^q + 4^p6^q) + 11n(6^p6^q + 6^p6^q).
\end{aligned}
$$

□

Corollary 4.2. *We could derive the following findings for different topological indices from the equation at the top of the generalised Zagreb connection index.*

(i) $C_1^2(CNBH(n)) = Z_{1,0}(CNBH(n)) = 1$,

(ii) $C_2^2(CNBH(n)) = \frac{1}{2}Z_{1,1}(CNBH(n)) = 508n - 86$,

(iii) $F^2(CNBH(n)) = Z_{2,0}(CNBH(n)) = 1024n - 132$,

(iv) $ReZC^2(CNBH(n)) = Z_{2,1}(CNBH(n)) = 5744n - 2500$,

(v) $C^{2\alpha}(CNBH(n)) = Z_{\alpha-1,0}(CNBH(n)) = 2[4(3^{\alpha-1}+2^{\alpha-1})+4(3^{\alpha-1}+4^{\alpha-1})+2(4^{\alpha-1}+5^{\alpha-1})+2(4^{\alpha-1}+6^{\alpha-1})+2(5^{\alpha-1})+2(5^{\alpha-1}+6^{\alpha-1})-16(6^{\alpha-1})]+8n(4^{\alpha-1})+2n(4^{\alpha-1}+6^{\alpha-1})+22n(6^{\alpha-1})$,

(vi) $R_\alpha^2(CNBH(n)) = \frac{1}{2}Z_{\alpha,\alpha}(CNBH(n)) = 4(3^\alpha2^\alpha+2^\alpha3^\alpha)+4(3^\alpha4^\alpha+4^\alpha3^\alpha)+2(4^\alpha5^\alpha+5^\alpha4^\alpha)+2(4^\alpha6^\alpha+6^\alpha4^\alpha)+2(5)^\alpha+2(5^\alpha6^\alpha+6^\alpha5^\alpha)-16(6)^\alpha+4n(4)^\alpha+n(4^\alpha6^\alpha+6^\alpha4^\alpha)+11n(6)^\alpha$,

(vii) $SDD^2(CNBH(n)) = Z_{1,-1}(CNBH(n)) = 34.333n + 31$.

5 Topological Indices for the Face Centered Cubic Lattice

In this section, we aim to define the topological indices for the FCC structure. In Theorem 5.1, we introduce the j-generalized Zagreb connection index, which is based on the 2-distance end vertices. In addition, we present the first along with second Zagreb indices, the forgotten topological index, the general first Zagreb index, the general Randić index, the redefined Zagreb index, and the Symmetric division degree index in Corollary 5.2.These indices are produced using the Metallic framework's j-generalized Zagreb connection index.

The partition of the set of nodes CK and the set of edges CE of FCC could be defined for the scenario when $j = 2$. You can use this division to get the degrees of neighbours who are 2-distances away from the vertices of $CFCC(n)$. Hence, we present the Table 4, which shows the values at the 2-distance $\iota k \in CE$.

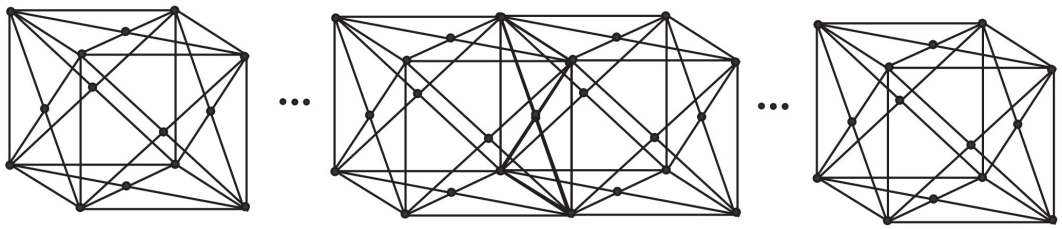


Figure 2. Face Centered Cubic Lattice

Table 4. The edge division in $FCC(n)$

$CE_{\{\tau(\iota),\tau(\kappa)\}}$	$\lvert CE_{\{\tau(\iota),\tau(\kappa)\}}\rvert$
(15,12)	8
(15,15)	8
(15,17)	16
(15,23)	8
(17,23)	16
(20,23)	8
(20,26)	$4n-12$
(22,23)	16
(22,26)	$16n-48$
(23,23)	8
(23,26)	8
(26,26)	$8n-28$

Theorem 5.1. *Let $\Upsilon \cong FCC(n)$ be a Metallic framework of size n for $n \geq 2$. Then, the generalized Zagreb connection index $C^2_{p,q}(FCC(n))$ is determined as follows:*

$$\begin{aligned}C^2_{p,q}(FCC(n)) = 4n[&(20^p26^q + 26^p20^q) + 4(22^p26^q + 26^p22^q) + 2(26^p26^q + 26^p26^q)]\\ &+4[2(15^p12^q + 12^p15^q) + 2(15^p15^q + 15^p15^q) + 4(15^p17^q + 17^p15^q)\\ &+2(15^p23^q + 23^p15^q) + 4(17^p23^q + 23^p17^q) + 2(20^p23^q + 23^p20^q)\\ &-3(20^p26^q + 26^p20^q) + 4(22^p23^q + 23^p22^q) - 12(22^p26^q + 26^p22^q)\\ &+2(23^p23^q + 23^p23^q) + 2(23^p26^q + 26^p23^q) - 7(26^p26^q + 26^p26^q)].\end{aligned}$$

Proof. By utilizing Table 4 along with the techniques discussed in the Section 3, we aim to evaluate the desired results as presented below.

$$C^2_{p,q}(FCC(n)) = \sum_{\iota\kappa\in E(FCC(n))} (\tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q)$$

$$\begin{aligned}=&\sum_{\iota\kappa\in E_{\{15,12\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q + \sum_{\iota\kappa\in E_{\{15,15\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q\\ &+\sum_{\iota\kappa\in E_{\{15,17\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q + \sum_{\iota\kappa\in E_{\{15,23\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q\\ &+\sum_{\iota\kappa\in E_{\{17,23\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q + \sum_{\iota\kappa\in E_{\{20,23\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q\\ &+\sum_{\iota\kappa\in E_{\{20,26\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q + \sum_{\iota\kappa\in E_{\{22,23\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q\\ &+\sum_{\iota\kappa\in E_{\{22,26\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q + \sum_{\iota\kappa\in E_{\{23,23\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q\end{aligned}$$

$$
\begin{aligned}
&+ \sum_{\iota\kappa\in E_{\{23,26\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q + \sum_{\iota\kappa\in E_{\{26,26\}}} \tau(\iota)^p\tau(\kappa)^q + \tau(\kappa)^p\tau(\iota)^q,\\
&= 8(15^p12^q + 12^p15^q) + 8(15^p15^q + 15^p15^q) + 16(15^p17^q + 17^p15^q) + 8(15^p23^q + 23^p15^q)\\
&\quad + 16(17^p23^q + 23^p17^q) + 8(20^p23^q + 23^p20^q) + (4n-12)(20^p26^q + 26^p20^q)\\
&\quad + 16(22^p23^q + 23^p22^q) + (16n-48)(22^p26^q + 26^p22^q) + 8(23^p23^q + 23^p23^q)\\
&\quad + 8(23^p26^q + 26^p23^q) + (8n-28)(26^p26^q + 26^p26^q),\\
&= 4n[(20^p26^q + 26^p20^q) + 4(22^p26^q + 26^p22^q) + 2(26^p26^q + 26^p26^q)]\\
&\quad + 4[2(15^p12^q + 12^p15^q) + 2(15^p15^q + 15^p15^q) + 4(15^p17^q + 17^p15^q)\\
&\quad + 2(15^p23^q + 23^p15^q) + 4(17^p23^q + 23^p17^q) + 2(20^p23^q + 23^p20^q)\\
&\quad - 3(20^p26^q + 26^p20^q) + 4(22^p23^q + 23^p22^q) - 12(22^p26^q + 26^p22^q)\\
&\quad + 2(23^p23^q + 23^p23^q) + 2(23^p26^q + 26^p23^q) - 7(26^p26^q + 26^p26^q)].
\end{aligned}
$$

□

Corollary 5.2. *The equation for the generalized Zagreb connection index allows us to evaluate the following outcomes of various topological indices:*

(i) $C_1^2(FCC(n)) = Z_{1,0}(FCC(n)) = 1368n - 576,$

(ii) $C_2^2(FCC(n)) = \frac{1}{2}Z_{1,1}(FCC(n)) = 16640n - 15496,$

(iii) $F^2(FCC(n)) = Z_{2,0}(FCC(n)) = 33680n - 30808,$

(iv) $ReZC^2(FCC(n)) = Z_{2,1}(FCC(n)) = 816192n - 1058976,$

(v) $C^\alpha(FCC(n)) = Z_{\alpha-1,0}(FCC(n)) = 8(15^{\alpha-1}+12^{\alpha-1})+8(15^{\alpha-1}+15^{\alpha-1})+16(15^{\alpha-1}+17^{\alpha-1}) + 8(15^{\alpha-1}+23^{\alpha-1}) + 16(17^{\alpha-1}+23^{\alpha-1}) + 8(20^{\alpha-1}+23^{\alpha-1}) + 4n(20^{\alpha-1}+26^{\alpha-1}) - 12(20^{\alpha-1}+26^{\alpha-1}) + 16(22^{\alpha-1}+23^{\alpha-1}) + 16n(22^{\alpha-1}+26^{\alpha-1}) - 48(22^{\alpha-1}+26^{\alpha-1}) + 8(23^{\alpha-1}+23^{\alpha-1}) + 8(23^{\alpha-1}+26^{\alpha-1}) + 8n(26^{\alpha-1}+26^{\alpha-1}) - 28(26^{\alpha-1}+26^{\alpha-1}),$

(vi) $R_\alpha^2(FCC(n)) = \frac{1}{2}Z_{\alpha,\alpha}(FCC(n)) = 2n[(20^\alpha26^\alpha + 26^\alpha20^\alpha) + 4(22^\alpha26^\alpha + 26^\alpha22^\alpha) + 2(26^\alpha26^\alpha + 26^\alpha26^\alpha)] + 2[2(15^\alpha12^\alpha + 12^\alpha15^\alpha) + 4(15^\alpha15^\alpha + 15^\alpha15^\alpha) + 4(15^\alpha17^\alpha + 17^\alpha15^\alpha) + 2(15^\alpha23^\alpha + 23^\alpha15^\alpha) + 4(17^\alpha23^\alpha + 23^\alpha17^\alpha) + 2(20^\alpha23^\alpha + 23^\alpha20^\alpha) - 3(20^\alpha26^\alpha + 26^\alpha20^\alpha) + 4(22^\alpha23^\alpha + 23^\alpha22^\alpha) - 12(22^\alpha26^\alpha + 26^\alpha22^\alpha) + 2(23^\alpha23^\alpha + 23^\alpha23^\alpha) + 2(23^\alpha26^\alpha + 26^\alpha23^\alpha) - 7(26^\alpha26^\alpha + 26^\alpha26^\alpha)],$

(vii) $CSDD^2(FCC(n)) = Z_{1,-1}(FCC(n)) = 56.7245n + 17.7433.$

Finally, we present a comparison between concealed non-kekulean benzenoid hydrocarbons and the face-centered cube lattice in terms of Zagreb connection indices, including the first Zagreb connection index, second Zagreb connection index, Forgotten index, Redefined Zagreb index, general Randić index, and Symmetric division degree index. This analysis is supported by a 3-D plot and numerical values provided in Tables 5 and 6.

In conclusion, the results from Table 7 clearly indicate that the FCC(n) yields superior results compared to CNBH(n) in terms of Zagreb connection indices, as n, the number of copies, grows. Furthermore, the 3-D graph visually confirms the superiority of the FCC structures over the benzenoid structure.

5.1 Discussion of Numerical Results

The numerical results presented in Tables (5)-(7) reveal that all investigated Zagreb connection indices of FCC(n) are consistently greater than those of CNBH(n). This behavior can be attributed to the highly compact and densely connected structure of the FCC lattice (as shown mathematically in (6.1)). In comparison with CNBH(n), the FCC framework possesses larger connection numbers and a greater frequency of distance-two interactions among vertices. Consequently, the contributions of adjacent vertex pairs to the generalized Zagreb connection index and its derived descriptors become significantly larger.

Table 5. Numerical Values of CNBH

n	$C_1^{(2)}(CNBH)$	$C_2^{(2)}(CNBH)$	$F^{(2)}(CNBH)$	$ReZC^{(2)}(CNBH)$	$SDD^{(2)}(CNBH)$
2	412	930	1916	8988	99.666
3	596	1438	2940	14732	133.999
4	780	1946	3964	20476	168.332
5	964	2454	4988	26220	202.665
6	1148	2962	6012	31964	236.998
7	1332	3470	7036	37708	271.331
8	1516	3978	8060	43452	305.664
9	1700	4486	9084	49196	339.997
10	1884	4994	10108	54940	374.33

Table 6. Numerical Values of FCC

n	$C_1^{(2)}(FCC)$	$C_2^{(2)}(FCC)$	$F^{(2)}(FCC)$	$ReZC^{(2)}(FCC)$	$SDD^{(2)}(FCC)$
2	2160	17784	36552	573408	131.1923
3	3528	34424	70232	1389600	187.9168
4	4896	51064	103912	2205792	244.6413
5	6264	67704	137592	3021984	301.3658
6	7632	84344	171272	3838176	358.0903
7	9000	100984	204952	4654368	414.8148
8	10368	117624	238632	5470560	471.5393
9	11736	134264	272312	6286752	528.2638
10	13104	150904	305992	7102944	584.9883

Table 7. Comparison of CNBH and FCC

Topological Indices	$FCC(n) - CNBH(n)$	$Results$
First Zegrab Index	1184n - 620	FCC $>$ CNBH
Second Zegrab Index	16132n - 15410	FCC $>$ CNBH
Forgotten Index	32656n - 30676	FCC $>$ CNBH
Redefined Index	810448n - 1056476	FCC $>$ CNBH
Symmetric Division Degree Index	22.391n + 13.2567	FCC $>$ CNBH

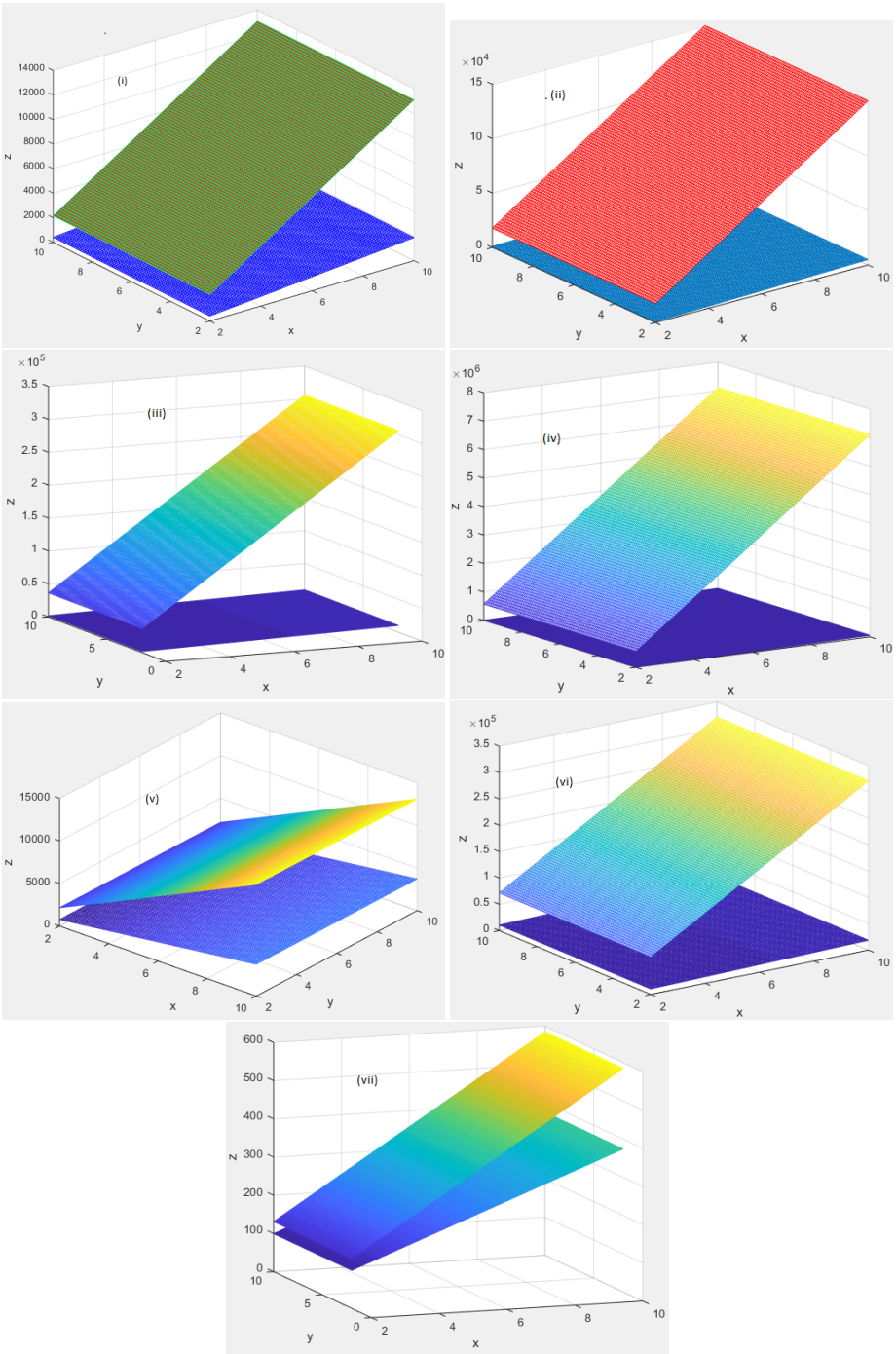


Figure 3. (i) $3D$ plot of $C_1^2(CNBH)$ and $C_1^2(FCC)$; (ii) $3D$ plot of $C_2^2(CNBH)$ and $C_2^2(FCC)$; (iii) $3D$ plot of $FC^2(CNBH)$ and $FC^2(FCC)$; (iv) $3D$ plot of $ReZC^2(CNBH)$ and $ReZC^2(FCC)$; (v) $3D$ plot of $C_1^{2\alpha}(CNBH)$ and $C_1^{2\alpha}(FCC)$ if $\alpha = 2$; (vi) $3D$ plot of $RC_\alpha(CNBH)$ and $RC_\alpha(FCC)$ if $\alpha = 2$; (vii) $3D$ plot of $SDDC^2(CNBH)$ and $SDDC^2(FCC)$

From a chemical and structural perspective, larger connection-based indices indicate a higher level of local and secondary connectivity within the underlying molecular network. Since Zagreb connection indices depend on connection numbers, larger values suggest that a greater number of vertices participate in distance-two interactions. Therefore, FCC structures exhibit stronger topological interconnectedness than CNBH structures. Such descriptors may be useful in future investigations involving structure-property relationships and molecular characterization.

The observed differences between FCC(n) and CNBH(n) are not merely numerical but also structurally significant. The FCC lattice is characterized by a highly organized and closely packed arrangement of vertices, whereas CNBH structures possess comparatively lower connectivity. As the size parameter n increases, this distinction becomes increasingly pronounced, leading to larger growth rates for all considered connection descriptors. This demonstrates that the investigated indices effectively capture fundamental structural differences between chemical and metallic frameworks.

6 New Mathematical Insights

6.1 Structural Properties of the Generalized Zagreb Connection Index

A noteworthy structural property of the obtained generalized Zagreb connection indices is that all derived expressions are linear functions of the parameter n. Consequently, the asymptotic behavior of the considered graph families is completely determined by the coefficients of n. This reveals a predictable growth pattern of the associated connection descriptors and facilitates direct comparison between different molecular structures.

6.2 Inequalities and Bounds

From Corollaries (4.2) and (5.2), it follows that

$$C_1^{(2)}(\text{FCC}) > C_1^{(2)}(\text{CNBH}), \qquad n \geq 2.$$

Similarly, analogous inequalities hold for the second Zagreb connection index, forgotten index, redefined Zagreb connection index, and symmetric division degree index. These inequalities indicate the stronger connectivity characteristics of FCC lattices.
Further,

$$C_1^{(2)}(\text{CNBH}) = 184n + 44$$

and

$$C_1^{(2)}(\text{FCC}) = 1368n - 576.$$

Hence,

$$\lim_{n\to\infty} \frac{C_1^{(2)}(\text{FCC})}{C_1^{(2)}(\text{CNBH})} = \frac{1368}{184} \approx 7.43.$$

which implies that the first Zagreb connection index of the FCC lattice grows approximately 7.43 times faster than that of the CNBH structure for large values of n, indicating a denser and more highly interconnected topology.
Bounds:
Since all obtained connection indices are linear in n, they admit simple linear bounds. For example,

$$184n < C_1^{(2)}(\text{CNBH}) = 184n + 44,$$

and

$$1368n - 576 < C_1^{(2)}(\text{FCC}) < 1368n.$$

Hence, both graph families exhibit linear growth with respect to the structural parameter n. Therefore,

$$C_1^{(2)}(\text{CNBH}) = O(n)$$

and

$$C_1^{(2)}(\text{FCC}) = O(n).$$

Therefore, the growth order of both structures is $O(n)$ and the same asymptotic behavior is observed for the remaining investigated connection indices.

6.3 Computational Complexity

An important advantage of the obtained formulas is their computational efficiency. Since all considered indices are derived in closed form as explicit functions of the parameter n, their evaluation does not require repeated edge-partition computations. Therefore, once n is specified, the computational complexity is $O(1)$. This property makes the proposed formulas applicable even for very large graph instances.

7 Conclusions

This work focuses on the exploration of topological indices for two specific structures: the Concealed Non-Kekulean Benzenoid Hydrocarbon and the Face Centered Cubic Lattice. Various topological indices, with particular emphasis on the Zagreb connection index denoted as $C^2_{p,q}(\Upsilon)$ for the Metallic framework Υ with an aspect of n (where $n \geq 2$) in the scenario of the Face Centered Cubic Lattice has been investigated.

The analysis of these topological indices provides valuable insights into the structural characteristics and properties of the studied systems. The results demonstrate the effectiveness of the Zagreb connection index in capturing important features of the Concealed Non-Kekulean Benzenoid Hydrocarbon and the Face Centered Cubic Lattice. The aforementioned findings enhance our knowledge of the connection and functioning of these systems. In future, one can study distance based topological indices for these structures to further elevate their significance.

Beyond the calculation of individual topological indices, the obtained generalized formulations provide a unified analytical framework for investigating connection-based descriptors of chemical and metallic structures. The closed-form expressions allow efficient computation for arbitrary values of n and facilitate direct comparison of different graph families. Moreover, the asymptotic growth of the derived indices demonstrates that the FCC lattice exhibits substantially higher connectivity characteristics than the CNBH structure. These findings contribute to a deeper understanding of the structural organization of complex molecular networks and provide a basis for future theoretical investigations involving generalized connection indices.

Despite these contributions, the present study has certain limitations. The analysis is restricted to two specific graph families, namely CNBH(n) and FCC(n). Moreover, only connection-based topological descriptors corresponding to the case $j = 2$ have been considered. The work focuses on theoretical derivations and does not include experimental, physicochemical, QSAR, or QSPR validation of the obtained descriptors.

The obtained generalized Zagreb connection indices may provide useful molecular descriptors for future QSAR/QSPR investigations. However, the incorporation of experimental physicochemical properties and predictive regression models remains beyond the scope of the present study and constitutes an interesting direction for future research.

8 Future Research Directions

Future investigations may extend the proposed methodology to other classes of chemical, biological, and material networks. It would also be interesting to study generalized Zagreb connection indices for higher-distance neighborhoods ($j > 2$), establish bounds and extremal properties, and explore relationships with other graph invariants. Furthermore, the incorporation of experimental physicochemical data and the development of QSAR/QSPR models based on the derived descriptors constitute promising directions for future research.

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