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Face-centered cubic lattice F C C (n) has received extensive consideration as of late, inferable from its recognized properties and non-poisonous nature, minimal effort, plenitude, and basic creation process. The graph of a face-centered cubic cross-section contains cube points and face centres. A topological index of a molecular graph G is a numeric amount identified with G, which depicts its topological properties. In this paper, using graph theory tools, we computed the molecular descriptors (topological indices)—to be specific, Zagreb-type indices, a forgotten index, a Balaban index, the fourth version of an atom?bond connectivity index, and the fifth version of a geometric arithmetic index for face-centered cubic lattice F C C (n) .

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On Molecular Descriptors of Face-Centered Cubic Lattice

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Abstract: Face-centered cubic lattice $FCC(n)$ has received extensive consideration as of late, inferable from its recognized properties and non-poisonous nature, minimal effort, plenitude, and basic creation process. The graph of a face-centered cubic cross-section contains cube points and face centres. A topological index of a molecular graph G is a numeric amount identified with G, which depicts its topological properties. In this paper, using graph theory tools, we computed the molecular descriptors (topological indices)—to be specific, Zagreb-type indices, a forgotten index, a Balaban index, the fourth version of an atom–bond connectivity index, and the fifth version of a geometric arithmetic index for face-centered cubic lattice $FCC(n)$.

Keywords: Zagreb-type indices; forgotten index; Balaban index; atom–bond connectivity index; geometric arithmetic index; face-centered cubic lattice $FCC(n)$

MSC: 05C12; 05C90

1. Introduction

Chemical graph theory is a branch of numerical science in which we apply apparatuses of a diagram hypothesis to demonstrate the compound marvel scientifically. This hypothesis contributes noticeably in the fields of chemical sciences. Through its assistance, some physical properties, e.g., the breaking point, can be anticipated in view of the structure of the atoms. Numerical and computational strategies are effectively used to display and foresee the structure of the issue at nuclear level [1]. The structures of atoms, from a numerical perspective, are graphs. Graph theory is utilized as part of relatively every field of science, and it is likewise vigorously utilized as a part of training, both for recreations and designing arrangements [2–4].

Each structural formula that incorporates covalent bonded compounds or atoms is a diagram. Thus, these are called molecular graphs or basic diagrams or, perhaps more accurately, constitutional graphs. In chemistry, graph theory provides the basis for the definition, numeration, systematization of the issue closeby, it paves the way toward organizing laws or standards as per a framework or arranging terminology, and it provides the association between compounds or atoms, and PC programming. The significance of graph theory for science can be found in the presence of isomerism, which is supported by chemical graph theory [5,6].

As a result, it was recently noted that topological indices are utilized for bringing together QSAR models with numerous objectives, such as for DNA examination, to consider protein successions, for 2D

RNA structures, to examine sedate–protein or medication–RNA quantitative structure-restricting relationships (QSBR), to encode protein surface data, and for protein association systems (PINs) [7–9].

A graph $G(V, E)$ is a collection of two sets, namely vertex set V and edge set E. For a graph G, the level of a vertex v is the quantity of edge episodes to v and signified by $\xi(v)$. A subatomic chart is a hydrogen-exhausted synthetic structure in which vertices signify iotas and edges indicate the bonds.

The possibility of a topological index came to light through the work of Wiener [10], while he was managing the limit of paraffin. He named this rundown the Wiener index. The Wiener index is the first and most thought-out topological file, both from a theoretical point of view and applications, and described as the entire of partitions between all arrangements of vertices in G; for further information, see [11].

Ghorbani and Azimi [12] defined the first and second multiple Zagreb index of a graph G as:

$$PM_1(G) = \prod_{wy \in E(G)} [\xi(w) + \xi(y)], \tag{1}$$

$$PM_2(G) = \prod_{wy \in E(G)} [\xi(w) \times \xi(y)]. \tag{2}$$

The first Zagreb index was presented by Gutman and Trinajstic in [13,14]. Taken after by the first and second Zagreb indices, Furtula and Gutman [15] presented the forgotten topological index as:

$$F(G) = \sum_{wy \in E(G)} (\xi(w)^2 + \xi(y)^2). \tag{3}$$

Gutman et al. argue that the prescient capacity, acentric factor, and entropy of the forgotten topological index are practically like those of thr first Zagreb index, and the correlation coefficients between these two are bigger than 0.95. Thus, the forgotten topological index is helpful to test the compound and pharmacological properties of medication subatomic structures. Sun et al. (2014) found some essential type of the forgotten topological index and announced that such an index can fortify the physicochemical flexibility of Zagreb indices. Recently, Gao et al. [16] showed the forgotten topological index of some noteworthy medication atomic structures.

Urtula [17] et al. introduced an augmented Zagreb index as:

$$AZI(G) = \sum_{wy \in E(G)} \left(\frac{\xi(w)\xi(y)}{\xi(w) + \xi(y) - 2} \right)^3. \tag{4}$$

Another topological index based on the vertex degree is the Balaban index [18,19]. This index for a graph G of order n, size m is defined as:

$$J(G) = \frac{m}{m - n + 2} \sum_{wy \in E(G)} \frac{1}{\sqrt{\xi(w)\xi(y)}}. \tag{5}$$

The redefined versions of the Zagreb indices were defined by Ranjini et al. [20], namely, the redefined first, second, and third Zagreb index for a graph G as:

$$ReZG_1(G) = \sum_{wy \in E(G)} \frac{\xi(w) + \xi(y)}{\xi(w)\xi(y)}, \tag{6}$$

$$ReZG_2(G) = \sum_{wy \in E(G)} \frac{\xi(w)\xi(y)}{\xi(w) + \xi(y)}, \tag{7}$$

$$ReZG_3(G) = \sum_{wy \in E(G)} (\xi(w)\xi(y))(\xi(w) + \xi(y)). \tag{8}$$

Fath-Tabar [21] defined the first Zagreb polynomial and second Zagreb polynomial of a graph G as:

$$M_1(G,x) = \sum_{wy \in E(G)} x^{[\xi(w)+\xi(y)]}, \tag{9}$$

$$M_2(G,x) = \sum_{wy \in E(G)} x^{[\xi(w)\times\xi(y)]}. \tag{10}$$

In 2017, Chaluvaraju et al. [22] defined the first and second hyper-Zagreb polynomials of a graph G as:

$$HM_1(G,x) = \sum_{wy \in E(G)} x^{[\xi(w)+\xi(y)]^2}, \tag{11}$$

$$HM_2(G,x) = \sum_{wy \in E(G)} x^{[\xi(w)\times\xi(y)]^2}. \tag{12}$$

The fourth version of the atom–bond connectivity index ABC_4 of a graph G was introduced by Ghorbhani et al. [23]. It was defined as:

$$ABC_4(G) = \sum_{wy \in E(G)} \sqrt{\frac{S_w + S_y - 2}{S_w S_y}}. \tag{13}$$

Another molecular descriptor is the fifth version of the geometric arithmetic index GA_5 of a graph G, introduced by Graovoc et al. [24]. It was defined as:

$$GA_5(G) = \sum_{wy \in E(G)} \frac{2\sqrt{S_w S_y}}{S_w + S_y}, \tag{14}$$

where $S_w = \sum\limits_{wy \in E(G)} \xi(y)$ and $S_y = \sum\limits_{wy \in E(G)} \xi(w)$.

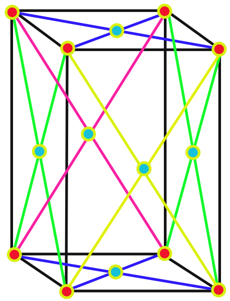
For more details about topological indices, see [25–29].

2. Face-Centered Cubic Lattice

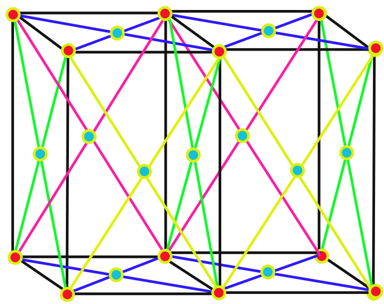
Face-centered cubic lattice $FCC(n)$ comprises unit cells that are 3D squares with an atom at each edge of the solid shape and a particle in the focal point of each face of the 3D shape, see Figure 1. In our diagrams, vertices (focuses) speak to the atoms; the terms 3D square vertices (block focuses) and confront focuses (or face centre points) will be utilized, individually. An unordered pair of nodes (atoms) that specify a line joining these two nodes (atoms) is said to form an edge. In fact, the $FCC(n)$ structure has the biggest pressing thickness in 3D space: This is a standout amongst the highest productive models to cover similar size circles in a volume [30,31], as can be found in Figure 1. Along these lines, this structure is otherwise called a cubic nearest pressed precious stone structure. Metals with an $FCC(n)$ structure include copper, aluminum, nickel silver, and gold. In this paper, we utilized graphs that speak to lines of unit cells of the $FCC(n)$ cross section (i.e., the measurement of our space is $(n \times 1 \times 1)$ unit cells), see Figure 2.

Methodology of Face-Centered Cubic Lattice $FCC(n)$ Formulas

The molecular graph of face-centered cubic lattice $FCC(n)$ adds up to $9n + 5$ vertices, among which the quantity of vertices of degree 4 is $5n + 1$, the quantity of vertices of degree 6 is 8, and the quantity of vertices of degree 9 is $4n - 4$. Likewise, then, adding up the number of edges again gives us $28n + 8$. To find the abstracted indices, we partition the edges of $FCC(n)$ The first edge segment contains 24 edges wy, where $\xi(w) = 4$ and $\xi(y) = 6$. The second edge segment contains $20n - 20$ edges wy, where $\xi(w) = 4$ and $\xi(y) = 9$. The third edge segment contains 8 edges wy, where $\xi(w) = 6$ and $\xi(y) = 6$. The fourth edge segment contains 8 edges wy, where $\xi(w) = 6$ and $\xi(y) = 9$. The fifth edge segment contains $8n-12$ edges wy, where $\xi(w)=\xi(y)=9$. Table 1 shows the edge partition of $FCC(n)$ with $n \geq 2$.



(a)



(b)

Figure 1. (**a**) Unit cell of $FCC(n)$; (**b**) Face-centered cubic lattice $FCC(2)$.

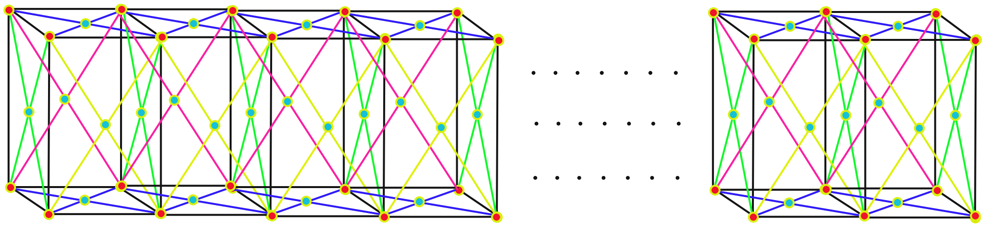


Figure 2. Face-centered cubic lattice $FCC(n)$.

Table 1. Degree-based partition of edges of face-centered cubic lattice $FCC(n)$.

$(\xi(w),\ \xi(y))$	Frequency	Edge Sets
(4, 6)	24	E_1
(4, 9)	$20n-20$	E_2
(6, 6)	8	E_3
(6, 9)	8	E_4
(9, 9)	$8n-12$	E_5

3. Main Results

In the next theorems, we computed the topological indices—to be specific, the Zagreb-type indices, the forgotten index, Balaban index, augmented Zagreb index, the fourth version of atom–bond connectivity index, and the fifth version of the geometric arithmetic index for face-centered cubic lattice $FCC(n)$. Moreover, to compute our results, we used the method of combinatorial computing, analytical techniques, the vertex partition method, edge partition method, graph theoretical tools, the degree counting method, and the sum of degrees of neighbours method. Moreover, we used MATLAB for mathematical calculations and verifications. We also used the maple to plot these mathematical results.

Theorem 1. *Consider face-centered cubic lattice $FCC(n)$, then its multiple Zagreb indices are:*

$$PM_1(FCC(n)) = 10^{24} \times 13^{(20n-20))} \times 16^8 \times 15^8 \times 18^{(8n-12)},$$
$$PM_2(FCC(n)) = 24^{24} \times 36^{(20n-20))} \times 36^8 \times 54^8 \times 81^{(8n-12)}.$$

Proof. Let G be the graph of face-centered cubic lattice $FCC(n)$. Now, using Table 1 and Equation (1), add Equation (2) to the following computation:

$$
\begin{aligned}
PM_1(G) &= \prod_{wy \in E(G)} [\xi(w)+\xi(y)] \\
PM_1(FCC(n)) &= \prod_{wy \in E_1(G)} [\xi(w)+\xi(y)] \times \prod_{wy \in E_2(G)} [\xi(w)+\xi(y)] \times \prod_{wy \in E_3(G)} [\xi(w)+\xi(y)] \\
&\times \prod_{wy \in E_4(G))} [\xi(w)+\xi(y)] \times \prod_{wy \in E_5(G))} [\xi(w)+\xi(y)] \\
&= 10^{24} \times 13^{(20n-20))} \times 16^8 \times 15^8 \times 18^{(8n-12)} \\
PM_2(G) &= \prod_{wy \in E(G)} [\xi(w) \times \xi(y)] \\
PM_2(FCC(n)) &= \prod_{wy \in E_1(G)} [\xi(w) \times \xi(y)] \times \prod_{wy \in E_2(G)} [\xi(w) \times \xi(y)] \times \prod_{wy \in E_3(G)} [\xi(w) \times \xi(y)] \\
&\times \prod_{wy \in E_4(G))} [\xi(w) \times \xi(y)] \times \prod_{wy \in E_5(G))} [\xi(w) \times \xi(y)] \\
&= 24^{24} \times 36^{(20n-20))} \times 36^8 \times 54^8 \times 81^{(8n-12)}
\end{aligned}
$$

□

Theorem 2. *Consider face-centered cubic lattice $FCC(n)$, then its forgotten topological index is equal to:*

$$F(G) = 3236n - 1124.$$

Proof. Let G be a the graph of face-centered cubic lattice $FCC(n)$. Now, using Table 1 and Equation (3), the $F(G)$ index can be calculated as:

$$
\begin{aligned}
F(G) &= \sum_{wy \in E(G)} \left(\xi(w)^2+\xi(y)^2\right) \\
F(G) &= \sum_{wy \in E_1(G)} \left(\xi(w)^2+\xi(y)^2\right) + \sum_{wy \in E_2(G)} \left(\xi(w)^2+\xi(y)^2\right) + \sum_{wy \in E_3(G)} \left(\xi(w)^2+\xi(y)^2\right) \\
&+ \sum_{wy \in E_4(G)} \left(\xi(w)^2+\xi(y)^2\right) + \sum_{wy \in E_5(G)} \left(\xi(w)^2+\xi(y)^2\right) \\
&= (24)\left(4^2+6^2\right) + (20n-20)\left(4^2+9^2\right) + (8)\left(6^2+6^2\right) + (8)\left(6^2+9^2\right) + (8n-12)\left(9^2+9^2\right) \\
&= (52)(24) + (97)(20n-20) + (72)(8) + (117)(8) + (162)(8n-12) = 3236n - 1124.
\end{aligned}
$$

□

Theorem 3. *Consider face-centered cubic lattice $FCC(n)$, then its augmented Zagreb index is:*

$$AZI(G) = \; = \frac{1185105411n}{681472} - \frac{248308379068617}{374298496000}.$$

Proof. Let G be a the graph of face-centered cubic lattice $FCC(n)$. Now, using Table 1 and Equation (4), $AZI(G)$ can be calculated as:

$$
\begin{aligned}
AZI(G) &= \sum_{wy \in E(G)} \left(\frac{\xi(w)\xi(y)}{\xi(w)+\xi(y)-2}\right)^3 \\
AZI(G) &= \sum_{wy \in E_1(G)} \left(\frac{\xi(w)\xi(y)}{\xi(w)+\xi(y)-2}\right)^3 + \sum_{wy \in E_2(G)} \left(\frac{\xi(w)\xi(y)}{\xi(w)+\xi(y)-2}\right)^3 + \sum_{wy \in E_3(G)} \left(\frac{\xi(w)\xi(y)}{\xi(w)+\xi(y)-2}\right)^3 \\
&+ \sum_{wy \in E_4(G)} \left(\frac{\xi(w)\xi(y)}{\xi(w)+\xi(y)-2}\right)^3 + \sum_{wy \in E_5(G)} \left(\frac{\xi(w)\xi(y)}{\xi(w)+\xi(y)-2}\right)^3
\end{aligned}
$$

$$
\begin{aligned}
AZI(G) &= (24)\left(\tfrac{4\times 6}{4+6-2}\right)^3 + (20n-20)\left(\tfrac{4\times 9}{4+9-2}\right)^3 + (8)\left(\tfrac{6\times 6}{6+6-2}\right)^3 \\
&+ (8)\left(\tfrac{6\times 9}{6+9-2}\right)^3 + (8n-12)\left(\tfrac{9\times 9}{9+9-2}\right)^3 \\
&= \tfrac{1185105411n}{681472} - \tfrac{248308379068617}{374298496000}.
\end{aligned}
$$

□

Theorem 4. *Consider face-centered cubic lattice $FCC(n)$, then its Balaban index $J(G)$ index is:*

$$J(G) = \frac{1064n^2 + (616n+176)\sqrt{6} - 536n - 240}{171n+27}.$$

Proof. Let G be the graph of face-centered cubic lattice $FCC(n)$. The above result can be proven using Table 1 and Equation (5) in the following computation:

$$
\begin{aligned}
J(G) &= \tfrac{m}{m-n+2}\sum_{wy\in E(G)} \tfrac{1}{\sqrt{\xi(w)\xi(y)}} \\
J(G &= \tfrac{m}{m-n+2}\left[\sum_{wy\in E_1(G)} \tfrac{1}{\sqrt{\xi(w)\xi(y)}} + \sum_{wy\in E_2(G)} \tfrac{1}{\sqrt{\xi(w)\xi(y)}} + \sum_{wy\in E_3(G)} \tfrac{1}{\sqrt{\xi(w)\xi(y)}}\right] \\
&+ \tfrac{m}{m-n+2}\left[\sum_{wy\in E_4(G)} \tfrac{1}{\sqrt{\xi(w)\xi(y)}} + \sum_{wy\in E_5(G)} \tfrac{1}{\sqrt{\xi(w)\xi(y)}}\right] \\
&= \tfrac{28n+8}{19n+3}\left[\tfrac{24}{\sqrt{4\times 6}} + \tfrac{20n-20}{\sqrt{4\times 9}} + \tfrac{8}{\sqrt{6\times 6}} + \tfrac{8}{\sqrt{6\times 9}} + \tfrac{8n-12}{\sqrt{9\times 9}}\right] \\
&= \tfrac{1064n^2+(616n+176)\sqrt{6}-536n-240}{171n+27}.
\end{aligned}
$$

□

Theorem 5. *Consider the graph of face-centered cubic lattice $FCC(n)$, then its redefined Zegreb indices are:*

$$
\begin{aligned}
ReZG_1(G) &= 9n+5, \\
ReZG_2(G) &= \frac{5940n+33}{13}, \\
ReZG_3(G) &= 21024n - 11160.
\end{aligned}
$$

Proof. Let G be the graph of $FCC(n)$. Then, using Equation (6) and Table 1, the first, second, and third redefine Zagreb indices are computed as below:

$$
\begin{aligned}
ReZG_1(G) &= \sum_{wy\in E(G)} \frac{\xi(w)+\xi(y)}{\xi(w)\xi(y)} \\
&= \sum_{wy\in E_1(G)} \frac{\xi(w)+\xi(y)}{\xi(w)\xi(y)} + \sum_{wy\in E_2(G)} \frac{\xi(w)+\xi(y)}{\xi(w)\xi(y)} + \sum_{wy\in E_3(G)} \frac{\xi(w)+\xi(y)}{\xi(w)\xi(y)} \\
&+ \sum_{wy\in E_4(G)} \frac{\xi(w)+\xi(y)}{\xi(w)\xi(y)} + \sum_{wy\in E_5(G)} \frac{\xi(w)+\xi(y)}{\xi(w)\xi(y)} \\
&= (24)\left(\frac{4+6}{4\times 6}\right) + (20n-20)\left(\frac{4+9}{4\times 9}\right) + (8)\left(\frac{6+6}{6\times 6}\right) \\
&+ (8)\left(\frac{6+9}{6\times 9}\right) + (8n-12)\left(\frac{9+9}{9\times 9}\right) \\
&= 9n+5.
\end{aligned}
$$

□

Using Equation (7) and Table 1, the second redefined Zagreb index is computed as below:

$$\begin{aligned}
ReZG_2(G) &= \sum_{wy \in E(G)} \frac{\xi(w)\xi(y)}{\xi(w)+\xi(y)} \\
&= \sum_{wy \in E_1(G)} \frac{\xi(w)\xi(y)}{\xi(w)+\xi(y)} + \sum_{wy \in E_2(G)} \frac{\xi(w)\xi(y)}{\xi(w)+\xi(y)} + \sum_{wy \in E_3(G)} \frac{\xi(w)\xi(y)}{\xi(w)+\xi(y)} \\
&+ \sum_{wy \in E_4(G)} \frac{\xi(w)\xi(y)}{\xi(w)+\xi(y)} + \sum_{wy \in E_5(G)} \frac{\xi(w)\xi(y)}{\xi(w)+\xi(y)}
\end{aligned}$$

$$\begin{aligned}
ReZG_2(G) &= (24)\left(\frac{4\times 6}{4+6}\right) + (20n-20)\left(\frac{4\times 9}{4+9}\right) + (8)\left(\frac{6\times 6}{6+6}\right) \\
&+ (8)\left(\frac{6\times 9}{6+9}\right) + (8n-12)\left(\frac{9\times 9}{9+9}\right) \\
&= \frac{5940n+33}{13}.
\end{aligned}$$

Now, using Equation (8) and Table 1, the third redefined Zagreb index is computed as below:

$$\begin{aligned}
ReZG_3(G) &= \sum_{wy \in E(G)} (\xi(w)\xi(y))(\xi(w)+\xi(y)) \\
&= \sum_{wy \in E_1(G)} (\xi(w)\xi(y))(\xi(w)+\xi(y)) + \sum_{wy \in E_2(G)} (\xi(w)\xi(y))(\xi(w)+\xi(y)) \\
&+ \sum_{wy \in E_3(G)} (\xi(w)\xi(y))(\xi(w)+\xi(y)) + \sum_{wy \in E_4(G)} (\xi(w)\xi(y))(\xi(w)+\xi(y)) \\
&+ \sum_{wy \in E_5(G)} (\xi(w)\xi(y))(\xi(w)+\xi(y)) \\
&= (24)\Big((4\times 6)(4+6)\Big) + (20n-20)\Big((4\times 9)(4+9)\Big) + (8)\Big((6\times 6)(6+6)\Big) \\
&+ (8)\Big((6\times 9)(6+9)\Big) + (8n-12)\Big((9\times 9)(9+9)\Big) \\
&= 21024n - 11160.
\end{aligned}$$

Theorem 6. *Consider face-centered cubic lattice $FCC(n)$, then its first and second Zagreb polynomials are equal to:*

$$\begin{aligned}
M_1(G,x) &= 24x^{10} + (20n-20)x^{13} + 8x^{12} + 8x^{15} + (12n-8)x^{18}, \\
M_2(G,x) &= 24x^{24} + (20n-20)x^{36} + 8x^{36} + 8x^{54} + (12n-8)x^{81}.
\end{aligned}$$

Proof. Let G be the graph of $FCC(n)$. Now, using Table 1 and Equations (9) and (10), the Zagreb polynomials are computed as below:

$$\begin{aligned}
M_1(G,x) &= \sum_{wy \in E(G)} x^{(\xi(w)+\xi(y))} \\
M_1(G,x) &= \sum_{wy \in E_1(G)} x^{(\xi(w)+\xi(y))} + \sum_{wy \in E_2(G)} x^{(\xi(w)+\xi(y))} + \sum_{wy \in E_3(G)} x^{(\xi(w)+\xi(y))} \\
&+ \sum_{wy \in E_4(G)} x^{(\xi(w)+\xi(y))} + \sum_{wy \in E_5(G)} x^{(\xi(w)+\xi(y))} \\
&= (24)x^{(4+6)} + (20n-20)x^{(4+9)} + (8)x^{(6+6)} + (8)x^{(6+9)} + (12n-8)x^{(9+9)} \\
&= 24x^{10} + (20n-20)x^{13} + 8x^{12} + 8x^{15} + (12n-8)x^{18}
\end{aligned}$$

$$
\begin{aligned}
M_2(G,x) &= \sum_{wy\in E(G)} x^{(\xi(w)\times\xi(y))} \\
M_2(G,x) &= \sum_{wy\in E_1(G)} x^{(\xi(w)\times\xi(y))} + \sum_{wy\in E_2(G)} x^{(\xi(w)\times\xi(y))} + \sum_{wy\in E_3(G)} x^{(\xi(w)\times\xi(y))} \\
&+ \sum_{wy\in E_4(G)} x^{(\xi(w)\times\xi(y))} + \sum_{wy\in E_5(G)} x^{(\xi(w)\times\xi(y))} \\
&= (24)x^{(4\times 6)} + (20n-20)x^{(4\times 9)} + (8)x^{(6\times 6)} + (8)x^{(6\times 9)} + (12n-8)x^{(9\times 9)} \\
&= 24x^{24} + (20n-20)x^{36} + 8x^{36} + 8x^{54} + (12n-8)x^{81}.
\end{aligned}
$$

□

Theorem 7. *Consider face-centered cubic lattice $FCC(n)$, then its first and second hyper-Zagreb polynomials are equal to:*

$$
\begin{aligned}
HM_1(G,x) &= 24x^{100} + (20n-20)x^{169} + 8x^{1296} + 8x^{225} + (12n-8)x^{324}, \\
HM_2(G,x) &= 24x^{576} + (20n-20)x^{1296} + 8x^{1296} + 8x^{2916} + (12n-8)x^{6561}.
\end{aligned}
$$

Proof. Let G be the graph of $FCC(n)$. Now, using Table 1 and Equations (11) and (12), the hyper-Zagreb polynomials are computed as:

$$
\begin{aligned}
HM_1(G,x) &= \sum_{wy\in E(G)} x^{(\xi(w)+\xi(y))^2} \\
HM_1(G,x) &= \sum_{wy\in E_1(G)} x^{(\xi(w)+\xi(y))^2} + \sum_{wy\in E_2(G)} x^{(\xi(w)+\xi(y))^2} + \sum_{wy\in E_3(G)} x^{(\xi(w)+\xi(y))^2} \\
&+ \sum_{wy\in E_4(G)} x^{(\xi(w)+\xi(y))^2} + \sum_{wy\in E_5(G)} x^{(\xi(w)+\xi(y))^2} \\
&= (24)x^{(4+6)^2} + (20n-20)x^{(4+9)^2} + (8)x^{(6+6)^2} + (8)x^{(6+9)^2} + (12n-8)x^{(9+9)^2} \\
&= 24x^{100} + (20n-20)x^{169} + 8x^{144} + 8x^{225} + (12n-8)x^{324}
\end{aligned}
$$

$$
\begin{aligned}
HM_2(G,x) &= \sum_{wy\in E(G)} x^{(\xi(w)\times\xi(y))^2} \\
HM_2(G,x) &= \sum_{wy\in E_1(G)} x^{(\xi(w)\times\xi(y))^2} + \sum_{wy\in E_2(G)} x^{(\xi(w)\times\xi(y))^2} + \sum_{wy\in E_3(G)} x^{(\xi(w)\times\xi(y))^2} \\
&+ \sum_{wy\in E_4(G)} x^{(\xi(w)\times\xi(y))^2} + \sum_{wy\in E_5(G)} x^{(\xi(w)\times\xi(y))^2} \\
&= (24)x^{(4\times 6)^2} + (20n-20)x^{(4\times 9)^2} + (8)x^{(6\times 6)^2} + (8)x^{(6\times 9)^2} + (12n-8)x^{(9\times 9)^2} \\
&= 24x^{576} + (20n-20)x^{1296} + 8x^{1296} + 8x^{2916} + (12n-8)x^{6561}.
\end{aligned}
$$

□

Table 2 shows the partition of the edges of the graph face-centered cubic lattice $FCC(n)$ depending on the sum of degrees of the neighboring vertices of the end vertices of each edge. The next theorem shows the exact value of the fourth version of atom–bond connectivity index ABC_4 of $FCC(n)$.

Table 2. Degree-based partition of edges of $FCC(n)$, for $n \geq 2$.

(S_u, S_v)	Number of Edges	Edge Sets
(33, 33)	8	$E_1(G)$
(24, 33)	8	$E_2(G)$
(30, 33)	16	$E_3(G)$
(36, 53)	24	$E_4(G)$
(30, 53)	16	$E_5(G)$
(33, 53)	8	$E_6(G)$
(53, 53)	8	$E_7(G)$
(53, 56)	8	$E_8(G)$
(56, 56)	8n-28	$E_9(G)$
(36, 56)	20n-60	$E_{10}(G)$

Theorem 8. *Consider the graph $G \cong FCC(n)$, then the fourth version of index ABC_4 for $FCC(n)$ is:*

$$ABC_4(G) = 5.72406962n + 3.6455090.$$

Proof. Let G be the graph structure of $FCC(n)$. Then, using Table 2 and Equation (13), the fourth version of index ABC_4 is computed as follows:

$$\begin{aligned}
S(G) &= \sum_{wy \in E(G)} \sqrt{\frac{S_w + S_y - 2}{S_w \times S_y}} \\
ABC_4(G) &= \sum_{wy \in E_1(G)} \sqrt{\frac{S_w + S_y - 2}{S_w \times S_y}} + \sum_{wy \in E_2(G)} \sqrt{\frac{S_w + S_y - 2}{S_w \times S_y}} + \sum_{wy \in E_3(G)} \sqrt{\frac{S_w + S_y - 2}{S_w \times S_y}} \\
&+ \sum_{wy \in E_4(G)} \sqrt{\frac{S_w + S_y - 2}{S_w \times S_y}} + \sum_{wy \in E_5(G)} \sqrt{\frac{S_w + S_y - 2}{S_w \times S_y}} + \sum_{wy \in E_6(G)} \sqrt{\frac{S_w + S_y - 2}{S_w \times S_y}} \\
&+ \sum_{wy \in E_7(G)} \sqrt{\frac{S_w + S_y - 2}{S_w \times S_y}} + \sum_{wy \in E_8(G)} \sqrt{\frac{S_w + S_y - 2}{S_w \times S_y}} + \sum_{wy \in E_9(G)} \sqrt{\frac{S_w + S_y - 2}{S_w \times S_y}} \\
&+ \sum_{wy \in E_{10}(G)} \sqrt{\frac{S_w + S_y - 2}{S_w \times S_y}}
\end{aligned}$$

$$\begin{aligned}
ABC_4(G) &= (8)\sqrt{\frac{33+33-2}{33 \times 33}} + (8)\sqrt{\frac{24+33-2}{24 \times 33}} + (16)\sqrt{\frac{30+33-2}{30 \times 33}} \\
&+ (24)\sqrt{\frac{36+53-2}{36 \times 53}} + (16)\sqrt{\frac{30+53-2}{30 \times 53}} + (8)\sqrt{\frac{33+53-2}{33 \times 53}} \\
&+ (8)\sqrt{\frac{53+53-2}{53 \times 53}} + (8)\sqrt{\frac{53+56-2}{53 \times 56}} + (8n-28)\sqrt{\frac{56+56-2}{56 \times 56}} \\
&+ (20n-60)\sqrt{\frac{36+56-2}{36 \times 56}} \\
&= 5.72406962n + 3.6455090.
\end{aligned}$$

□

Theorem 9. *Consider the graph $G \cong FCC(n)$, then the fifth version of geometric arithmetic index GA_5 of $FCC(n)$ is:*

$$GA_5(G) = 9.53740238n + 7.3250487.$$

Proof. Let G be the graph structure of $FCC(n)$. Then, using Table 2 and Equation (14), the fifth version of geometric arithmetic index GA_5 is computed as follows:

$$\begin{aligned}
GA_5(G) &= \sum_{wy \in E(G)} \frac{2\sqrt{S_w S_y}}{S_w + S_y} \\
&= \sum_{wy \in E_1(G)} \frac{2\sqrt{S_w S_y}}{S_w + S_y} + \sum_{wy \in E_2(G)} \frac{2\sqrt{S_w S_y}}{S_w + S_y} + \sum_{wy \in E_3(G)} \frac{2\sqrt{S_w S_y}}{S_w + S_y} \\
&+ \sum_{wy \in E_4(G)} \frac{2\sqrt{S_w S_y}}{S_w + S_y} + \sum_{wy \in E_5(G)} \frac{2\sqrt{S_w S_y}}{S_w + S_y} + \sum_{wy \in E_6(G)} \frac{2\sqrt{S_w S_y}}{S_w + S_y} \\
&+ \sum_{wy \in E_7(G)} \frac{2\sqrt{S_w S_y}}{S_w + S_y} + \sum_{wy \in E_8(G)} \frac{2\sqrt{S_w S_y}}{S_w + S_y} + \sum_{wy \in E_9(G)} \frac{2\sqrt{S_w S_y}}{S_w + S_y} \\
&+ \sum_{wy \in E_{10}(G)} \frac{2\sqrt{S_w S_y}}{S_w + S_y}
\end{aligned}$$

$$\begin{aligned}
GA_5(G) &= (8)\frac{2\sqrt{33 \times 33}}{33 + 33} + (8)\frac{2\sqrt{24 \times 33}}{24 + 33} + (16)\frac{2\sqrt{30 \times 33}}{30 + 33} \\
&+ (24)\frac{2\sqrt{36 \times 53}}{36 + 53} + (16)\frac{2\sqrt{30 \times 53}}{30 + 53} + (8)\frac{2\sqrt{33 \times 53}}{33 + 53} \\
&+ (8)\frac{2\sqrt{53 \times 53}}{53 + 53} + (8)\frac{2\sqrt{53 \times 56}}{53 + 56} + (8n - 28)\frac{2\sqrt{56 \times 56}}{56 + 56} \\
&+ (20n - 60)\frac{2\sqrt{36 \times 56}}{36 + 56} \\
&= 9.53740238n + 7.3250487.
\end{aligned}$$

□

4. Comparisons and Discussion

In this section, we computed all the indices for different values of n for face-centered cubic lattice $FCC(n)$. In addition, we constructed Tables 3 and 4 for small values of n for these topological indices to the structure of face-centered cubic lattice $FCC(n)$. Now, from Tables 3 and 4, we can easily see that all indices are in increasing order as the value of n are increases.

The graphical representation of the $PM_1(G)$ and $PM_2(G)$ indices is depicted in Figure 3, that of the forgotten topological index in Figure 4, that of the augmented Zagreb index in Figure 5, that of the Balaban index in Figure 6, that of the first, second, and third Zagreb indices in Figure 7, that of Zagreb polynomials $M_1(G,x)$ and $M_2(G,x)$ in Figure 8, that of hyper-Zagreb polynomials in Figure 9, and that of the ABC_4 index and GA_5 index in Figure 10.

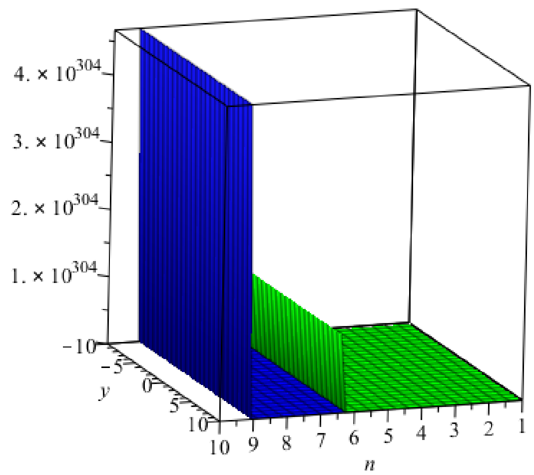


Figure 3. The graphical representation of the $PM_1(G)$ and $PM_2(G)$ indices.

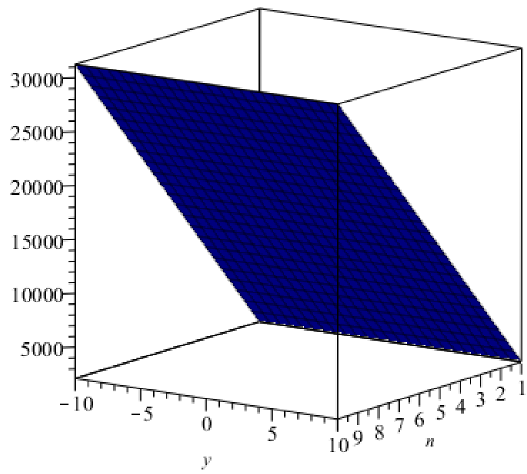


Figure 4. The graphical representation of the forgotten topological index.

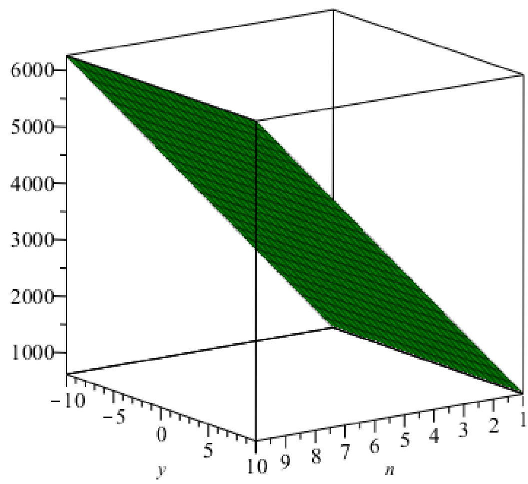


Figure 5. The graphical representation of the augmented Zagreb index.

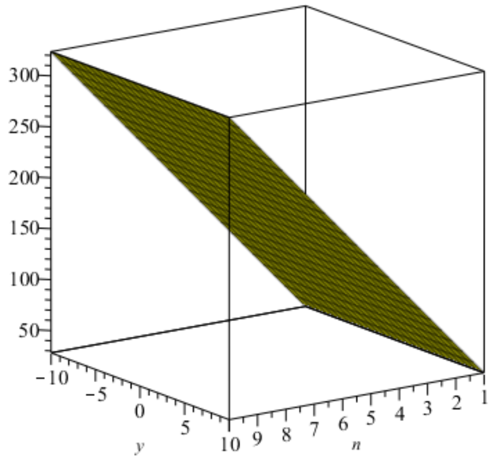


Figure 6. The graphical representation of Balaban index.

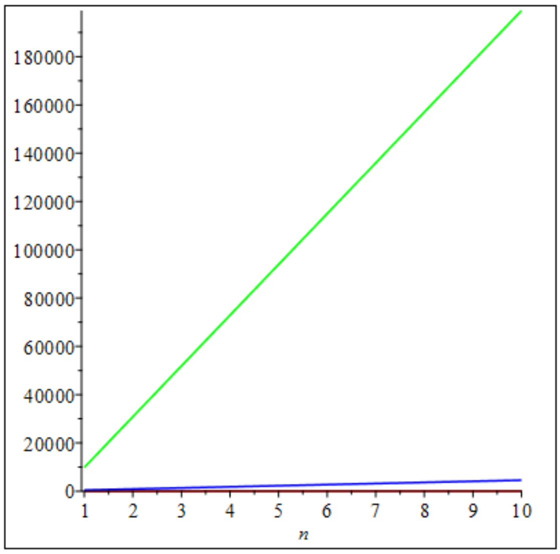


Figure 7. The graphical representation of the first, second, and third Zagreb indices of $FCC(n)$. The red, blue, and green colors represent $ReZG_1(G)$, $ReZG_2(G)$, and $ReZG_3(G)$, respectively.

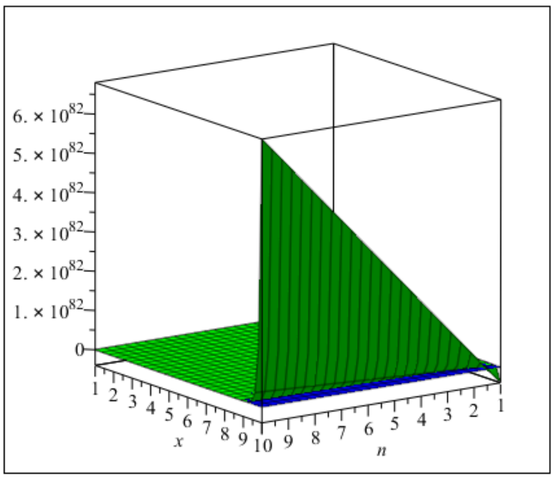


Figure 8. The graphical representation of $M_1(G,x)$ and $M_2(G,x)$ polynomials of face-centered cubic lattice $FCC(n)$. The colors blue and green represent $M_1(G,x)$ and $M_2(G,x)$, respectively.

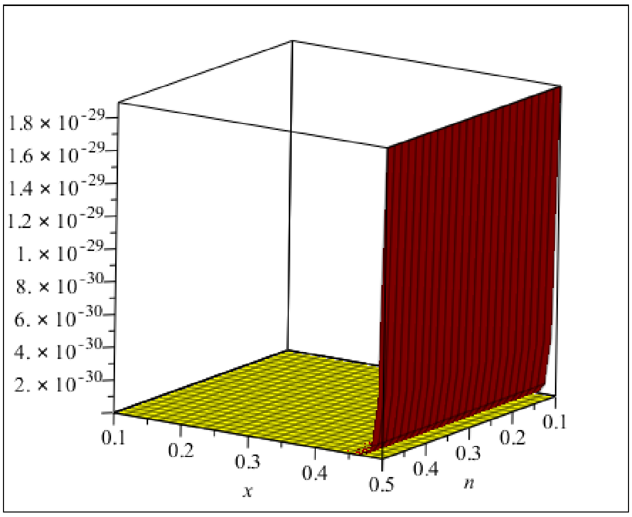


Figure 9. The graphical representation of the first and second hyper-Zagreb polynomial in a 2*D* structure of face-centered cubic lattice $FCC(n)$. The colors blue and green represent $HM_1(G,x)$ and $HM_2(G,x)$, respectively.

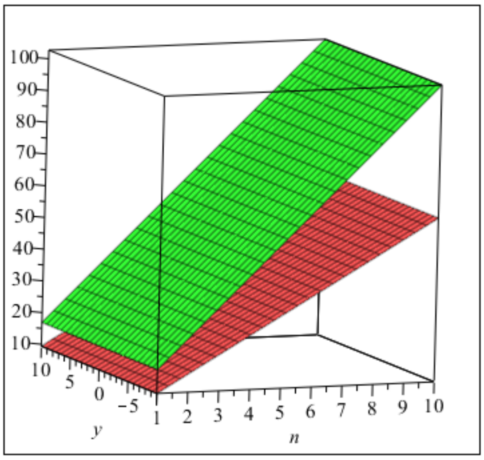


Figure 10. The graphical representation of ABC_4 index and GA_5 index of face-centered cubic lattice $FCC(n)$. The colors brown and green represent ABC_4 and GA_5, respectively.

Table 3. Comparison of all indices for face-centered cubic lattice $FCC(n)$.

n	$PM_1(FCC(n))$	$PM_2(FCC(n))$	$F(FCC(n))$	$AZI(FCC(n))$	$J(FCC(n))$
1	1.4×10^{38}	2.5×10^{18}	2112	49.31	8.9
2	3.7×10^{66}	3.4×10^{38}	5348	60.34	29.8
3	6.5×10^{89}	5.6×10^{57}	8548	80.41	61.4
4	7.6×10^{95}	7.4×10^{76}	11820	97.18	97.6
5	9.4×10^{110}	6.2×10^{95}	15056	115.08	105.7
6	5.8×10^{125}	8.5×10^{119}	18292	135.21	125.5

Table 4. Comparison of all indices for face-centered cubic lattice $FCC(n)$.

n	$ReZ_1(FCC(n))$	$ReZ_2(FCC(n))$	$ReZ_3(FCC(n))$	$ABC_4(FCC(n))$	$GA_5(FCC(n))$
1	14	459.6	9864	59.31	47.42
2	23	916.38	30888	62.34	65.18
3	32	1373.5	51912	81.41	81.23
4	41	1830.5	72936	95.11	97.04
5	50	2287.6	93960	107.12	117.31
6	59	2744.5	114984	1157.31	137.24

5. Conclusions

In this paper, we studied a reputable lattice, namely face-centered cubic lattice $FCC(n)$, and we determined the topological indices, namely the Zagreb-type indices, the forgotten index, Balaban index, the fourth version of AB_4, and the fifth version of the geometric arithmetic index for face-centered cubic lattice $FCC(n)$.

Since the first and second multiple Zagreb indices, redefined Zagreb indices were found to occur for computation of the total π-electron energy of the molecules; in the case of face-centered cubic lattice $FCC(n)$, their values provide total π-electron energy in increasing order for higher values of n. Moreover, the forgotten topological index, Balaban index, and augmented Zagreb index announced that the physicochemical flexibility of face-centered cubic lattice $FCC(n)$ is fruitful for chemical reactions. Further, the fourth atom–bond connectivity ABC_4 and the fifth version of the geometric arithmetic index GA_5 index provide a very good correlation for computing the strain energy of molecules; one can easily see that the strain energy of face-centered cubic lattice $FCC(n)$ is higher as the values of n increases. Additionally, these result are helpful from a chemical point of view as well as in pharmaceutical science. However, computing the distance-based and counting-related topological indices for these symmetrical chemical structures still remains open for investigation and a challenge for researchers.

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