Research Article

Hong Yang, Muhammad Kamran Siddiqui, Muhammad Naeem*, Najma Abdul Rehman

Molecular Properties of Carbon Crystal Cubic Structures

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Abstract: Graph theory assumes an imperative part in displaying and planning any synthetic structure or substance organizer. Chemical graph theory facilitates in conception of the chemical graphs for their atomic properties. The graphical structure of a chemical involves atoms termed as vertices and the line segment between two different vertices are called edges. In this manuscript, our concentration is on the chemical graph of carbon graphite and cubic carbon. Additionally, we also define a procedure and calculate the degree based topological indices namely Zagreb type indices, Balaban, Forgotten and Augmented indices.

Keywords: Balaban; Forgotten and Augmented index; Re-defined Zagreb index; Carbon Graphite; Crystal Cubic.

1 Introduction

Graph theory is capable of forming and creating various chemical structures and networks. Chemical graph theory uses the theory of graphs in modelling chemical phenomena; this theory is very useful for the analysis of chemical structures. The examinations of structures of molecules and data are made possible by using chemical descriptors. A large number of topological descriptors are examined and utilized in theoretical chemistry [1, 2, 3].

A topological descriptor is a numerical value which demonstrates some valuable data related to chemical

structures. It is a numerical invariant of chemical graphs and is valuable to connect with the bioactivities and physicochemical properties of the structure. Scientists observed that these indices were an effective and valuable instrument in the portrayal of chemical graph. A few applications identified with topological descriptors of chemical graphs can be found in [4, 5, 6].

The analysts have used chemical graphs to describe the topological uses of carbons in a nano cones, in chains of extremal pentagons, tree like poly phenylene, spiro hexagonal frame-works, poly-phenylene dendrimers nano stars, and palomino's chain [7, 8, 9].

A large number of allotropes of carbon have been discovered such as nanotubes, buckminsterfullerenes and nanosheets. The uses of several allotropes of carbons are studied in [10, 11, 12].

The notion of topological index originated with the work of Wiener [13], whilst he discussed boiling points of paraffins. Soon after, this numeric quantity was retitled as Wiener index. The Wiener index was the earliest and highly studied topological index, both from putative perspectives and application, and is characterized as the cumulative of disjunctions among all the sets of vertices of *G*; for more subtle elements see [14, 15, 16].

A graph G=(V, E) where V is the set of vertices and E denotes the set of edges of G, the degree of a vertex \mathbf{u} is the total number of edges associated with \mathbf{u} and is denoted by $\lambda(\mathbf{u})$.

Furtula, along with Gutman [17] presented forgotten topological descriptor as u and v are two vertices of an edge E:

$$F(G) = \sum_{uv \in E(G)} (\lambda (u)^2 + \lambda (v)^2),$$
 (1)

where u, v are vertices. Inspired from the successful discovery of ABC index, Furtula et al. [18], presented the augmented Zagreb index as:

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{\lambda(u) \times \lambda(v)}{\lambda(u) + \lambda(v) - 2} \right)^{3}$$
 (2)

^{*}Corresponding author: Muhammad Naeem, Department of Mathematics and Statistics, Institute of Southern Punjab, Multan, 66000, Pakistan, E-mail: naeempkn@gmail.com

Hong Yang, School of Information Science and Engineering,
Chengdu University, Chengdu 610106, China

Muhammad Kamran Siddiqui, Department of Mathematics,
COMSATS University Islamabad, Lahore Campus, 54000, Pakistan

Najma Abdul Rehman, Department of Mathematics, COMSATS

University Islamabad, Sahiwal Campus, 57000, Pakistan

Balaban defined a new index for a graph G with order n and size m, called Balaban index as [19]:

$$J(G) = \frac{m}{m - n + 2} \sum_{uv \in E(G)} \frac{1}{\sqrt{\lambda(u) \times \lambda(v)}},$$
 (3)

where m, n are total number of vertices and total number of edges respectively. The re-defined Zagreb indices are introduced by Ranjini et al. [20] in the following way:

$$ReZG_1 \ (G) = \sum_{uv \in E(G)} \frac{\lambda(u) + \lambda(v)}{\lambda(u)\lambda(v)}$$
 (4)

$$ReZG_2(G) = \sum_{uv \in E(G)} \frac{\lambda(u)\lambda(v)}{\lambda(u) + \lambda(v)}$$
 (5)

$$ReZG_3$$
 $(G) = \sum_{uv \in E(G)} [\lambda(u) \times \lambda(v)] \times [(\lambda(u) + \lambda(v))]$

(6

2 Applications of Topological Descriptors

Furtula and Gutman [21] raise the insightful limit of forgotten topological index is moderately analogous to first Zagreb index. They designed it for the acentric factors, entropy and to gain relationships coefficient greater than 0.95. These facts highlight the significance of the forgotten index examining the manufactured and pharmacological characteristics of the atomic structure of medication.

Gao et al. [22] demonstrated the forgotten topological index of approximately gigantic drug nuclear compositions. The redefined Zagreb indices give a reasonable association with the steadfastness of unconventional alkane; the all-inclusive alkane and for enlisting the strain imperativeness of different cycloalkanes [3]. To relate with specific physico-chemical properties, Balaban topological descriptor has lot of favoured judicious command over the perceptive vitality of Randic index [23].

Sun et.al. discovered approximately fundamental properties of forgotten descriptor and uncovered that rundown can invigorate the physico-engineered versatility of Zagreb type indices.

The re-defined Zagreb type indices are used for figuring of the total π -electron energy of the molecules inside specific deduced verbalizations [24]. For further results, see [25].

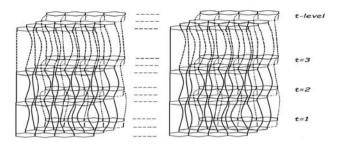


Figure 1: Carbon graphite *CG*(*m*,*n*) *t*-levels.

3 Methods

To compute our results, we utilize the strategy for combinatorial techniques, vertex and edge based partitions. Matlab was used for scientific computations and verifications. We used maple for plotting these mathematical results.

4 Structure of Carbon Graphite *CG*(*m*,*n*)

Graphite is an amalgamation of carbon. The chemical graph of carbon graphite CG(m,n) is comprised of a hexagon silhouettes. Carbon graphite is comprised of hexagons as layers in a steady progression and amid these strata there is a frail [3]. The chemical graph of carbon graphite CG(m,n) for it-levels is delineated in Figure 1.

4.1 Methodology of Carbon: Graphite CG(m,n) Formulas

There are 2t(mn + m + n) vertices and 2n(2mt+t)+m(3t-n)-t-m edges in CG(m,n). A solitary stratum in carbon graphite delineates the graphene layer. Carbon graphite is comprised of various stratum of graphene. The t is the stratum that delineates graphene stratums in carbon graphite, m is the quantity of lines and n is the quantity of: sections in each layer with m is taken as n duplicates of hexagon consecutively and n is taken as m duplicates of hexagons in segment see Figure 1 (see [25]).

In CG(m,n), there are 2(1 + nt + m) vertices of degree 2, 2t - 4 + 2mt - 2m + 2mn vertices of degree 3 and 2mnt-2t+2-2mn vertices of degree 4. The edge set of CG(m,n) is isolated hooked on six allotments in light of the level of termination vertices. Table 1 represents edge parcel of CG(m,n).

4.2 Main Results for carbon graphite CG(m,n)

Theorem 1. If G is a graph of carbon graphite CG(m,n). Then its forgotten topological index is F(G) = 36 - 74t + 16nt-38m - 74mn + 54mt + 128mnt

Proof: Now using equation (1), and Table 1, we have:

$$\begin{split} F(G) &= \sum_{u,v \in E(G)} \left(\lambda(u)^2 + \lambda(v)^2\right) \\ F(CG(m,n)) &= \sum_{uv \in E_1} \left[\lambda(u)^2 + \lambda(v)^2\right] + \sum_{uv \in E_2} \left[\lambda(u)^2 + \lambda(v)^2\right] \\ &+ \sum_{uv \in E_3} \left[\lambda(u)^2 + \lambda(v)^2\right] + \sum_{uv \in E_4} \left[\lambda(u)^2 + \lambda(v)^2\right] \\ &+ \sum_{uv \in E_5} \left[\lambda(u)^2 + \lambda(v)^2\right] + \sum_{uv \in E_6} \left[\lambda(u)^2 + \lambda(v)^2\right] \\ &= 8|E_1(CG(m,n))| + 13|E_2(CG(m,n))| + \\ &+ 20|E_3(CG(m,n))| + 18|E_4(CG(m,n))| + \\ &+ 25|E_5(CG(m,n))| + 32|E_6(CG(m,n))| \\ &= 8(4) + 13(4n + 4t - 4) + 20(4nt + 4m - 4n - 4t) \\ &+ 18(4t - 10 + 4m) + +25(4t - 10 + 4m) \\ &+ 32(4mtn - 3tm - 2tn + t - 2 - 7mn + 5m + 4n) \\ &= 36 - 74t + 16nt - 38m - 74mn + 54mt + 128mnt. \end{split}$$

Theorem 2. If G is a graph of carbon graphite CG(m,n). Then its Augmented Zagreb index is:

$$\begin{split} AZI(G) = \frac{1518029}{108000} + \frac{69376}{3375}n - \frac{994601}{54000}t - \frac{160}{27}nt - \frac{1142569}{54000}m - \frac{168064}{3375}mn + \\ + \frac{29312}{1125}mt + \frac{2048}{27}mnt. \end{split}$$

Proof: Now using equation (2), and Table 1, we have:

$$\begin{split} AZI(G) &= \sum_{u,v \in E(G)} \left(\frac{\lambda(u) \times \lambda(v)}{\lambda(u) + \lambda(v) - 2} \right)^3 \\ AZI(CG(m,n)) &= \sum_{uv \in E_1} \left(\frac{\lambda(u) \times \lambda(v)}{\lambda(u) + \lambda(v) - 2} \right)^3 + \sum_{uv \in E_2} \left(\frac{\lambda(u) \times \lambda(v)}{\lambda(u) + \lambda(v) - 2} \right)^3 + \sum_{uv \in E_3} \left(\frac{\lambda(u) \times \lambda(v)}{\lambda(u) + \lambda(v) - 2} \right)^3 + \sum_{uv \in E_4} \left(\frac{\lambda(u) \times \lambda(v)}{\lambda(u) + \lambda(v) - 2} \right)^3 + \sum_{uv \in E_5} \left(\frac{\lambda(u) \times \lambda(v)}{\lambda(u) + \lambda(v) - 2} \right)^3 + \sum_{uv \in E_6} \left(\frac{\lambda(u) \times \lambda(v)}{\lambda(u) + \lambda(v) - 2} \right)^3 \\ &= 8|E_1(CG(m, n))| + 8|E_2(CG(m, n))| + \\ + 8|E_3(CG(m, n))| + \frac{729}{64}|E_4(CG(m, n))| + \\ + \frac{1728}{125}|E_5(CG(m, n))| + \frac{512}{27}|E_6(CG(m, n))| \\ &= 8(4) + 8(4n + 4t - 4)) + 8(4nt + 4m - 4n - 4t) \\ &+ \frac{729}{64}(4t - 10 + 4m) \\ &+ \frac{1728}{125}(12 - 6t + 6mn - 14m - 4n + 6mt) \\ + \frac{512}{27}(4mtn - 3tm - 2tn + t - 2 - 7mn + 5m + 4n) \\ &= \frac{1518029}{108000} + \frac{69376}{3375}n - \frac{994601}{54000}t - \frac{160}{27}nt - \frac{1142569}{54000}m \\ &- \frac{168064}{3375}mn + \frac{29312}{1125}mt + \frac{2048}{27}mnt. \end{split}$$

Theorem 3. If G is a graph of carbon graphite CG(m,n). Then its Balaban index is

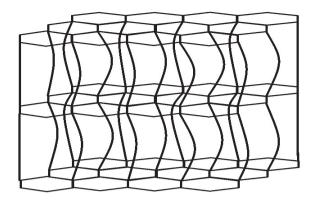


Figure 2: Carbon graphite graph for m=4 and t=3 [25].

Table 1: Edge divider of Carbon graphite graph CG(m,n).

$(\lambda(u), \lambda(v))$	Frequency
(2,i2)	4
(2,3)	4n + 4t - 4
(2,4)	4nt + 4m - 4n - 4t
(3,3)	4t - 10 + 4m
(3,4)	12-6t + 6mn - 14m - 4n + 6mt
(4,4)	4mtn - 3tm - 2tn + t - 2 - 7mn + 5m + 4n

$$\begin{split} J(G) &= \frac{3mt + 2nt + 4mnt + -mn - m - t}{2mnt + mt - mn - m - t + 2} \left[\frac{-11}{6} + \frac{2\sqrt{6}}{3}(n + t - 1) \right] + \\ &+ \frac{3mt + 2nt + 4mnt + -mn - m - t + 2}{2mnt + mt - mn - m - t + 2} \left[\sqrt{2}(nt + m - n - t) + \frac{31}{12}m + \frac{19}{12}t \right] + \\ &+ \frac{3mt + 2nt + 4mnt + -mn - m - t}{2mnt + mt - mn - m - t} \left[\frac{1}{6}\sqrt{3}(12 - 6t + 6mn - 14m - 4n + 6mt) \right] \\ &+ \frac{3mt + 2nt + 4mnt + -mn - m - t}{2mnt + mt - mn - m - t + 2} \left[mnt - \frac{3}{4}mt - \frac{1}{2}nt - \frac{7}{4}mn + n \right]. \end{split}$$

Proof: Now using equation (3), and Table 1, we have:

$$J(G) = \frac{m}{m-n+2} \sum_{u,v \in E(G)} \frac{1}{\sqrt{\lambda(u) \times \lambda(v)}}$$

$$J(CG(m, n)) = \frac{m}{m-n+2} \left[\sum_{uv \in E_1} \frac{1}{\sqrt{\lambda(u) \times \lambda(v)}} + \sum_{uv \in E_2} \frac{1}{\sqrt{\lambda(u) \times \lambda(v)}} \right] + \frac{m}{m-n+2} \left[\sum_{uv \in E_3} \frac{1}{\sqrt{\lambda(u) \times \lambda(v)}} + \sum_{uv \in E_4} \frac{1}{\sqrt{\lambda(u) \times \lambda(v)}} \right] + \frac{m}{m-n+2} \left[\sum_{uv \in E_3} \frac{1}{\sqrt{\lambda(u) \times \lambda(v)}} + \sum_{uv \in E_6} \frac{1}{\sqrt{\lambda(u) \times \lambda(v)}} \right]$$

$$= \frac{3mt + 2nt + 4mnt + -mn - m - t}{2mnt + mt - mn - m - t + 2} \left[\frac{1}{2} |E_1(CG(m, n))| + \frac{1}{\sqrt{6}} |E_2(CG(m, n))| \right] + \frac{3mt + 2nt + 4mnt + -mn - m - t}{2mnt + mt - mn - m - t + 2} \left[\frac{1}{\sqrt{12}} |E_5(CG(m, n))| + \frac{1}{4} |E_6(CG(m, n))| \right]$$

$$= \frac{3mt + 2nt + 4mnt + -mn - m - t}{2mnt + mt - mn - m - t + 2} \left[\frac{1}{\sqrt{12}} |E_5(CG(m, n)) + \frac{1}{4} |E_6(CG(m, n))| \right]$$

$$= \frac{3mt + 2nt + 4mnt + -mn - m - t}{2mnt + mt - mn - m - t + 2} \left[\frac{1}{\sqrt{8}} (4nt + 4m - 4n - 4t) + \frac{1}{3} (4t - 10 + 4m) \right]$$

$$+ \frac{3mt + 2nt + 4mnt + -mn - m - t}{2mnt + mt - mn - m - t + 2} \left[\frac{1}{\sqrt{8}} (4nt + 4m - 4n - 4t) + \frac{1}{3} (4t - 10 + 4m) \right]$$

$$+ \frac{3mt + 2nt + 4mnt + -mn - m - t}{2mnt + mt - mn - m - t + 2} \left[\frac{1}{\sqrt{12}} (12 - 6t + 6mn - 14m - 4n + 6mt) \right]$$

$$+ \frac{3mt + 2nt + 4mnt + -mn - m - t + 2}{2mnt + mt - mn - m - t + 2} \left[\frac{1}{\sqrt{12}} (12 - 6t + 6mn - 14m - 4n + 6mt) \right]$$

$$+ \frac{3mt + 2nt + 4mnt + -mn - m - t + 2}{2mnt + mt - mn - m - t + 2} \left[\frac{1}{\sqrt{12}} (12 - 6t + 6mn - 14m - 4n + 6mt) \right]$$

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$$\begin{split} &=\frac{3mt+2nt+4mnt+-mn-m-t}{2mnt+mt-mn-m-t+2}\left[\frac{-11}{6}+\frac{2\sqrt{6}}{3}\left(n+t-1\right)\right]\\ &+\frac{3mt+2nt+4mnt+-mn-m-t}{2mnt+mt-mn-m-t+2}\left[\sqrt{2}\left(nt+m-n-t\right)+\frac{31}{12}m+\frac{19}{12}t\right]\\ &+\frac{3mt+2nt+4mnt+-mn-m-t}{2mnt+mt-mn-m-t}\left[\frac{1}{6}\sqrt{3}\left(12-6t+6mn-14m-4n+6mt\right)\right]\\ &+\frac{3mt+2nt+4mnt+-mn-m-t}{2mnt+mt-mn-m-t+2}\left[mnt-\frac{3}{4}mt-\frac{1}{2}nt-\frac{7}{4}mn+n\right]. \end{split}$$

Theorem 4. The redefined Zagreb indices of carbon graphite CG(m,n) are:

$$\begin{aligned} ReG_1(G) &= 2nt + 2mt + 2mnt, \\ ReG_2(G) &= \frac{27}{35} - \frac{64}{105}n - \frac{296}{105}t + \frac{4}{3}nt - \frac{8}{3}m - \frac{26}{7}mn + \frac{30}{7}mt + 8mnt, \\ ReG_3(G) &= 156 + 104n - 232t - 64nt - 128m - 392mn + 120mt + 512mnt. \end{aligned}$$

Proof: Now using equations [(4), (5), (6)], and Table 1, we have:

Redefine first Zagreb index

$$\begin{split} ReG_1(CG(m,n)) &= \sum_{uv \in E_1} \frac{\lambda(u) + \lambda(v)}{\lambda(u)\lambda(v)} \\ &= \sum_{uv \in E_1} \frac{\lambda(u) + \lambda(v)}{\lambda(u)\lambda(v)} + \sum_{uv \in E_2} \frac{\lambda(u) + \lambda(v)}{\lambda(u)\lambda(v)} + \sum_{uv \in E_3} \frac{\lambda(u) + \lambda(v)}{\lambda(u)\lambda(v)} \\ &+ \sum_{uv \in E_4} \frac{\lambda(u) + \lambda(v)}{\lambda(u)\lambda(v)} + \sum_{uv \in E_5} \frac{\lambda(u) + \lambda(v)}{\lambda(u)\lambda(v)} + \sum_{uv \in E_6} \frac{\lambda(u) + \lambda(v)}{\lambda(u)\lambda(v)} \\ &= 1|E_1(CG(m,n))| + \frac{5}{6}|E_2(CG(m,n))| + \frac{3}{4}|E_3(CG(m,n))| + \\ &+ \frac{2}{3}|E_4(CG(m,n))| + \frac{7}{12}|E_5(CG(m,n))| + \frac{1}{2}|E_6(CG(m,n))| \\ &= 1(4) + \frac{5}{6}(4n + 4t - 4) + \frac{3}{4}(4nt + 4m - 4n - 4t) + \frac{2}{3}(4t - 10 + 4m) + \\ &+ \frac{7}{12}(12 - 6t + 6mn - 14m - 4n + 6mt) \\ &+ \frac{1}{2}(4mtn - 3tm - 2tn + t - 2 - 7mn + 5m + 4n) \end{split}$$

• Redefine second Zagreb Index

$$\begin{split} ReG_2(CG(m,n)) &= \sum_{uv \in E(G)} \frac{\lambda(u)\lambda(v)}{\lambda(u) + \lambda(v)} \\ &= \sum_{uv \in E_1} \frac{\lambda(u)\lambda(v)}{\lambda(u) + \lambda(v)} + \sum_{uv \in E_2} \frac{\lambda(u)\lambda(v)}{\lambda(u) + \lambda(v)} + \sum_{uv \in E_3} \frac{\lambda(u)\lambda(v)}{\lambda(u) + \lambda(v)} \\ &+ \sum_{uv \in E_4} \frac{\lambda(u)\lambda(v)}{\lambda(u) + \lambda(v)} + \sum_{uv \in E_5} \frac{\lambda(u)\lambda(v)}{\lambda(u) + \lambda(v)} + \sum_{uv \in E_6} \frac{\lambda(u)\lambda(v)}{\lambda(u) + \lambda(v)} \\ &= 1|E_1(CG(m,n))| + \frac{6}{5}|E_2(CG(m,n))| + \frac{4}{3}|E_3(CG(m,n))| + \\ &+ \frac{3}{2}|E_4(CG(m,n))| + \frac{12}{7}|E_5(CG(m,n))| + 2|E_6(CG(m,n))| \\ &= 1(4) + \frac{6}{5}(4n + 4t - 4) + \frac{4}{3}(4nt + 4m - 4n - 4t) + \\ &+ \frac{3}{2}(4t - 10 + 4m) + \frac{12}{7}(12 - 6t + 6mn - 14m - 4n + 6mt) + \\ &+ 2(4mtn - 3tm - 2tn + t - 2 - 7mn + 5m + 4n) \\ &= \frac{27}{35} - \frac{64}{105}n - \frac{296}{105}t + \frac{4}{3}nt - \frac{8}{3}m - \frac{26}{7}mn + \frac{30}{7}mt + 8mnt. \end{split}$$

• Redefine third Zagreb Index

$$ReG_{3}(CG(m,n)) = \sum_{uv \in E(G)} [\lambda(u) \times \lambda(v)] \times [(\lambda(u) + \lambda(v))]$$

$$= \sum_{uv \in E_{1}} [\lambda(u) \times \lambda(v)] \times [(\lambda(u) + \lambda(v))]$$

$$+ \sum_{uv \in E_{2}} [\lambda(u) \times \lambda(v)] \times [(\lambda(u) + \lambda(v))] +$$

$$+ \sum_{uv \in E_{3}} [\lambda(u) \times \lambda(v)] \times [(\lambda(u) + \lambda(v))]$$

$$+ \sum_{uv \in E_{4}} [\lambda(u) \times \lambda(v)] \times [(\lambda(u) + \lambda(v))] +$$

$$+ \sum_{uv \in E_{4}} [\lambda(u) \times \lambda(v)] \times [(\lambda(u) + \lambda(v))] +$$

$$+ \sum_{uv \in E_{5}} [\lambda(u) \times \lambda(v)] \times [(\lambda(u) + \lambda(v))]$$

$$= 16|E_{1}(CG(m, n))| + 30|E_{2}(CG(m, n))| + 48|E_{3}(CG(m, n))|$$

$$+ 54|E_{4}(CG(m, n))| + 84|E_{5}(CG(m, n))| + 128|E_{6}(CG(m, n))|$$

$$+ 54(4t - 10 + 4m) + 84(12 - 6t + 6mn - 14m - 4n - 4t)|$$

$$+ 54(4t - 10 + 4m) + 84(12 - 6t + 6mn - 14m - 4n + 6mt)$$

$$+ 128(4mtn - 3tm - 2tn + t - 2 - 7mn + 5m + 4n)$$

$$= 156 + 104n - 232t - 64nt - 128m - 392mt + 120mt + 512mt.$$

5 Structure of Crystal Cubic Carbon

The organisation of crystal cubic carbon comprises of cubes. The chemical graph of precious stone cubic carbon CCC(n) for first glassy is portrayed in Figure 3 (see [25]). For second glassy, the shape is built at each end vertex of first glassy. The second glassy of CCC(n) is portrayed in Figure 4 (see [25]). So proceeding with this methodology to get the following level (see [25]).

5.1 Methodology of crystal cubic carbon *CCC(n)* Formulas

The total number of vertices and edges for CCC(n) are presented in following formulas:

$$|V(CCC(n))| = 2(24\sum_{r=3}^{n} (2^3 - 1)^{r-3} + 31(2^3 - 1)^{n-2} + 2\sum_{r=0}^{n-2} (2^3 - 1)^r + 3)$$

$$|E(CCC(n))| = 4(24\sum_{r=3}^{n} (2^3 - 1)^{r-3} + 24(2^3 - 1)^{n-2} + 2\sum_{r=0}^{n-2} (2^3 - 1)^r + 3)$$

In CCC(n), $8(2^3 - 1)^{n-1}$ vertices of degree 3 and there are

$$2(24\sum_{r=3}^{n} (2^3 - 1)^{r-3} + 3((2^3 - 1)^{n-2} + 1) + 2\sum_{r=0}^{n-2} (2^3 - 1)^r + 3)$$

vertices of degree 4. The edge set of CCC(n) is isolated into three parcels see Table 2.

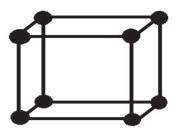


Figure 3: For n=1, Crystal Structure of Cubic Carbon.

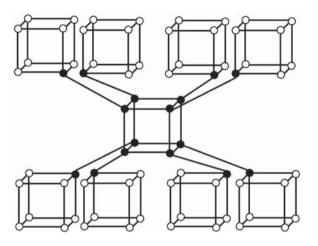


Figure 4: For n=3, Crystal Structure of Cubic Carbon.

Table 2: Edge partition of CCC(n) based on degrees of end vertices of each edge.

$(\lambda(u),\lambda(v))$	Frequency		
(3,3)	504n ⁻²		
(3,4)	108 <i>n</i> -²		
(4,4)	$12\left(1+\sum_{r=3}^{n}2^{3}(2^{3}-1)^{r-3}\right)+8\sum_{r=0}^{n-2}(2^{3}-1)^{r}$		

5.2 Main Results for Crystal Cubic Carbon CCC(n)

Theorem.5. If G be a graph of carbon graphite CCC(n). Then its Forgotten index is:

$$F(G) = 384 + 1896((2^{3} - 1)n^{-2}) + 384\left(\sum_{r=3}^{n} 2^{3}(2^{3} - 1)^{r-3}\right) + 256\left(\sum_{r=0}^{n-2} (2^{3} - 1)^{r}\right)$$

Proof: Now using equations (1), and Table 2, we have:

$$\begin{split} F(G) &= \sum_{u,v \in E(G)} (\lambda(u)^2 + \lambda(v)^2) \\ F(G) &= \sum_{uv \in E_1} [\lambda(u)^2 + \lambda(v)^2] \\ &+ \sum_{uv \in E_2} [\lambda(u)^2 + \lambda(v)^2] + \sum_{uv \in E_3} [\lambda(u)^2 + \lambda(v)^2] \\ &= 18|E_1(G)| + 25|E_2(G)| + 32|E_3(G)| \\ &= 18(504n^{-2}) + 25(108n^{-2}) + \\ &+ 32\left(12(1 + \sum_{r=3}^n 2^3(2^3 - 1)^{r-3}) + 8\sum_{r=0}^{n-2} (2^3 - 1)^r\right) \\ &= 384 + 1896\left((2^3 - 1)n^{-2}\right) + 384\left(\sum_{r=3}^n 2^3(2^3 - 1)^{r-3}\right) + \\ &+ 256\left(\sum_{r=0}^{n-2} (2^3 - 1)^r\right). \end{split}$$

Theorem.6. If G be a graph of carbon graphite CCC(n). Then its Augmented Zagreb index is:

$$\frac{AZI(G) =}{\frac{2048}{9} - \frac{1151901}{1000} (2^3 - 1)n^{-2} - \frac{2048}{9} \sum_{r=3}^{n} 2^3 (2^3 - 1)^{r-3} + \frac{4096}{27} \sum_{r=0}^{n-2} (2^3 - 1)^r. }$$

Proof: Now using equations (2), and Table 2, we have:

$$\begin{split} AZI(G) &= \sum_{u,v \in E(G)} \left(\frac{\lambda(u) \times \lambda(v)}{\lambda(u) + \lambda(v) - 2} \right)^3 \\ AZI(CCC(n)) &= \sum_{uv \in E_1} \left(\frac{\lambda(u) \times \lambda(v)}{\lambda(u) + \lambda(v) - 2} \right)^3 + \sum_{uv \in E_2} \left(\frac{\lambda(u) \times \lambda(v)}{\lambda(u) + \lambda(v) - 2} \right)^3 + \\ &\quad + \sum_{uv \in E_3} \left(\frac{\lambda(u) \times \lambda(v)}{\lambda(u) + \lambda(v) - 2} \right)^3 \\ &= \frac{729}{64} |E_1(CCC(n))| + \frac{1728}{125} |E_2(CCC(n))| + \frac{512}{27} |E_3(CCC(n))| \\ &\quad = \frac{729}{64} (504n^{-2}) + \frac{1728}{125} (108n^{-2}) \\ &\quad + \frac{512}{27} \left(12(1 + \sum_{r=3}^n 2^3(2^3 - 1)^{r-3}) + 8 \sum_{r=0}^{n-2} (2^3 - 1)^r \right) \\ &\quad = \frac{2048}{9} - \frac{1151901}{1000} (2^3 - 1)n^{-2} - \frac{2048}{9} \sum_{r=3}^n 2^3(2^3 - 1)^{r-3} \\ &\quad + \frac{4096}{27} \sum_{r=3}^{n-2} (2^3 - 1)^r. \end{split}$$

Theorem.7. If G be a graph of carbon graphite CCC(n). Then its Balaban index is:

$$\begin{split} J(G) &= \frac{4[24\sum_{r=3}^{n} (2^3-1)^{r-3} + 24(2^3-1)^{n-2} + 2\sum_{r=0}^{n-2} (2^3-1)^r + 3]}{48\sum_{r=3}^{n} (2^n-1)^{r-3} + 34(2^3-1)^{n-2} + 4\sum_{r=0}^{n-2} (2^3-1)^r + 8} \times \\ &\times \left(3 + 24(2^3-1)n^{-2} + \frac{12\sqrt{3}}{3}(2^3-1)n^{-2} + 3\sum_{r=3}^{n} 2^3(2^3-1)^{r-3} \right. \\ &\qquad \qquad + \\ &\qquad \qquad + 2\sum_{r=0}^{n-2} (2^3-1)^r \bigg). \end{split}$$

Proof: Now using equation (3), and Table 2, we have:

$$J(G) = \frac{m}{m-n+2} \sum_{u,v \in E(G)} \frac{1}{\sqrt{\lambda(u) \times \lambda(v)}}$$

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$$\begin{split} J(G) &= \frac{m}{m-n+2} \Biggl[\sum_{uv \in E_1} \frac{1}{\sqrt{\lambda(u) \times \lambda(v)}} + \sum_{uv \in E_2} \frac{1}{\sqrt{\lambda(u) \times \lambda(v)}} \Biggr] + \\ &+ \frac{m}{m-n+2} \Biggl[\sum_{uv \in E_3} \frac{1}{\sqrt{\lambda(u) \times \lambda(v)}} \Biggr] + \\ &= \frac{4[24 \sum_{r=3}^n (2^3-1)^{r-3} + 24(2^3-1)^{n-2} + 2 \sum_{r=0}^{n-2} (2^3-1)^r + 3]}{48 \sum_{r=3}^n (2^n-1)^{r-3} + 34(2^3-1)^{n-2} + 4 \sum_{r=0}^{n-2} (2^3-1)^r + 8} \times \\ &\times \left[\frac{1}{3} |E_1(G)| \right] + \frac{1}{\sqrt{12}} |E_2(G)| + \frac{1}{4} |E_3(G)| \Biggr] \\ &= \frac{4[24 \sum_{r=3}^n (2^3-1)^{r-3} + 24(2^3-1)^{n-2} + 2 \sum_{r=0}^{n-2} (2^3-1)^r + 3]}{48 \sum_{r=3}^n (2^n-1)^{r-3} + 34(2^3-1)^{n-2} + 4 \sum_{r=0}^{n-2} (2^3-1)^r + 8} \times \\ &\times \left[\frac{1}{3} (72(2^3-1)n^{-2}) + \frac{1}{\sqrt{12}} (24(2^3-1)n^{-2}) \right. \\ &+ \frac{1}{4} \Biggl(12(1 + \sum_{r=3}^n 2^3(2^3-1)^{r-3} + 24(2^3-1)^{n-2} + 2 \sum_{r=0}^{n-2} (2^3-1)^r + 8 \right] \times \\ &= \frac{4[24 \sum_{r=3}^n (2^3-1)^{r-3} + 24(2^3-1)^{n-2} + 2 \sum_{r=0}^{n-2} (2^3-1)^r + 3]}{48 \sum_{r=3}^n (2^n-1)^{r-3} + 34(2^3-1)^{n-2} + 4 \sum_{r=0}^{n-2} (2^3-1)^r + 8} \times \\ &\times \left(3 + 24(2^3-1)n^{-2} + \frac{12\sqrt{3}}{3} (2^3-1)n^{-2} + 3 \sum_{r=3}^n 2^3(2^3-1)^{r-3} + 2 \sum_{r=0}^{n-2} (2^3-1)^r + 8 \right] \times \\ &\times \left(3 + 24(2^3-1)n^{-2} + \frac{12\sqrt{3}}{3} (2^3-1)n^{-2} + 3 \sum_{r=3}^n 2^3(2^3-1)^{r-3} + 2 \sum_{r=0}^{n-2} (2^3-1)^r + 8 \right] \times \\ &\times \left(3 + 24(2^3-1)n^{-2} + \frac{12\sqrt{3}}{3} (2^3-1)n^{-2} + 3 \sum_{r=3}^n 2^3(2^3-1)^{r-3} + 2 \sum_{r=0}^n (2^3-1)^r + 8 \right) \times \\ &\times \left(3 + 24(2^3-1)n^{-2} + \frac{12\sqrt{3}}{3} (2^3-1)n^{-2} + 3 \sum_{r=3}^n 2^3(2^3-1)^{r-3} + 2 \sum_{r=0}^n (2^3-1)^r + 8 \right) \times \\ &\times \left(3 + 24(2^3-1)n^{-2} + \frac{12\sqrt{3}}{3} (2^3-1)n^{-2} + 3 \sum_{r=3}^n 2^3(2^3-1)^{r-3} + 2 \sum_{r=0}^n (2^3-1)^r + 8 \right) \times \\ &\times \left(3 + 24(2^3-1)n^{-2} + \frac{12\sqrt{3}}{3} (2^3-1)n^{-2} + 3 \sum_{r=3}^n 2^3(2^3-1)^{r-3} + 2 \sum_{r=0}^n (2^3-1)^r + 8 \right) \times \\ &\times \left(3 + 24(2^3-1)n^{-2} + \frac{12\sqrt{3}}{3} (2^3-1)n^{-2} + 3 \sum_{r=3}^n 2^3(2^3-1)^{r-3} + 2 \sum_{r=0}^n (2^3-1)^r + 3 \right) \right] \times \\ &\times \left(3 + 24(2^3-1)n^{-2} + \frac{12\sqrt{3}}{3} (2^3-1)n^{-2} + 3 \sum_{r=3}^n 2^3(2^3-1)^{r-3} + 2 \sum_{r=0}^n (2^3-1)^r + 3 \right) \times \\ &\times \left(3 + 24(2^3-1)n^{-2} + \frac{12\sqrt{3}}{3} (2^3-1)n^{-2} + 3 \sum_{r=3}^n 2^3(2^3-1)^r + 3 \right) \right) \right) + \frac{1}{2} \left(2^3 + 24(2^3-1)n^{-2} + 3 \sum_{r=3}^n 2^3(2^3-1$$

Theorem.8. If G be a graph of carbon graphite CCC(n). Then its redefined Zagreb indices are:

$$\begin{split} ReG_1(G) &= 6 + 62(2^3 - 1)n^{-2} + 6\sum_{r=3}^n 2^3(2^3 - 1)^{r-3} + 4\sum_{r=3}^{n-2} (2^3 - 1)^r, \\ ReG_2(G) &= 24 + \frac{1044}{7}(2^3 - 1)n^{-2} + 24\sum_{r=3}^n 2^3(2^3 - 1)^{r-3} + 16\sum_{r=0}^{n-2} (2^3 - 1)^r, \\ ReG_3(G) &= 1536 + 5904(2^3 - 1)n^{-2} + 1536\sum_{r=3}^n 2^3(2^3 - 1)^{r-3} + 1024\sum_{r=0}^{n-2} (2^3 - 1)^r. \end{split}$$

Proof: Now using equations [(4), (5), (6)], and Table 2, we have:

• Redefine first Zagreb index

$$\begin{aligned} ReG_1(CCC(n)) &= \sum_{e=uv \in E(G)}^{\infty} \frac{\lambda(u) + \lambda(v)}{\lambda(u)\lambda(v)} \\ &= \sum_{uv \in E_1} \frac{\lambda(u) + \lambda(v)}{\lambda(u)\lambda(v)} + \sum_{uv \in E_2} \frac{\lambda(u) + \lambda(v)}{\lambda(u)\lambda(v)} + \sum_{uv \in E_3} \frac{\lambda(u) + \lambda(v)}{\lambda(u)\lambda(v)} + \\ &= \frac{2}{3} |E_1(G)| + \frac{7}{12} |E_2(G)| + \frac{1}{2} |E_3(G)| \\ &= \frac{2}{3} (72(2^3 - 1)n^{-2}) + \frac{7}{12} (24(2^3 - 1)n^{-2}) \\ &+ \frac{1}{2} (12(1 + \sum_{r=3}^{n} 2^3(2^3 - 1)^{r-3}) + 8 \sum_{r=0}^{n-2} (2^3 - 1)^r) \\ &= 6 + 62(2^3 - 1)n^{-2} + 6 \sum_{r=3}^{n} 2^3(2^3 - 1)^{r-3} + 4 \sum_{r=0}^{n-2} (2^3 - 1)^r \end{aligned}$$

Redefine second Zagreb index

$$\begin{split} ReG_2(G) &= \sum_{e=uv\in E(G)} \frac{\lambda(u)\lambda(v)}{\lambda(u) + \lambda(v)} \\ &= \sum_{uv\in E_1} \frac{\lambda(u)\lambda(v)}{\lambda(u) + \lambda(v)} + \sum_{uv\in E_2} \frac{\lambda(u)\lambda(v)}{\lambda(u) + \lambda(v)} + \sum_{uv\in E_3} \frac{\lambda(u)\lambda(v)}{\lambda(u) + \lambda(v)} \\ &= \frac{3}{2} |E_1(CCC(n))| + \frac{12}{7} |E_2(CCC(n))| + 2|E_3(CCC(n))| \\ &= \frac{3}{2} (508n^{-2}) + \frac{12}{7} (104n^{-2}) \\ &+ 2 \left(12(1 + \sum_{r=3}^n 2^3(2^3 - 1)^{r-3}) + 8 \sum_{r=0}^{n-2} (2^3 - 1)^r \right) \\ &= 24 + \frac{1044}{7} (2^3 - 1)n^{-2} + 24 \sum_{r=3}^n 2^3(2^3 - 1)^{r-3} + 16 \sum_{r=0}^{n-2} (2^3 - 1)^r. \end{split}$$

Redefine third Zagreb index

$$ReG_{3}(G) = \sum_{uv \in E(G)} [\lambda(u) \times \lambda(v)] \times [(\lambda(u) + \lambda(v))]$$

$$= \sum_{uv \in E_{1}} [\lambda(u) \times \lambda(v)] \times [(\lambda(u) + \lambda(v))]$$

$$+ \sum_{uv \in E_{2}} [\lambda(u) \times \lambda(v)] \times [(\lambda(u) + \lambda(v))]$$

$$+ \sum_{uv \in E_{3}} [\lambda(u) \times \lambda(v)] \times [(\lambda(u) + \lambda(v))]$$

$$= 9(6)|E_{1}(CCC(n))| + 12(7)|E_{2}(CCC(n))| + 16(8)|E_{3}(CCC(n))|$$

$$= 9(6)(72(2^{3} - 1)n^{-2}) + 12(7)(24(2^{3} - 1)n^{-2})$$

$$+16(8)\left(12(1 + \sum_{r=3}^{n} 2^{3}(2^{3} - 1)^{r-3}) + 8\sum_{r=0}^{n-2} (2^{3} - 1)^{r}\right)$$

$$= 1536 + 5904(2^{3} - 1)n^{-2} + 1536\sum_{r=3}^{n} 2^{3}(2^{3} - 1)^{r-3}$$

$$+1024\sum_{r=0}^{n-2} (2^{3} - 1)^{r}.$$

6 Comparisons and Discussion

In this fragment, we have calculated all indices for altered tenets of m, n, t for mutual organisations CG(m, n). In accumulation, we build Table 3. The graphical demonstrations of topological indices are portrayed in Figures 5 and Figures 6, for certain values of m, t, n.

The numerical and graphical representations of topological indices of CCC(n) are depicted in Table 4, Figure 7 and Figure 8 respectively, for certain values of n.

Table 3: Comparison of all indices for CG(m, n).

[<i>m</i> , <i>n</i> , <i>t</i>]	F(G)	AZI(G)	J(G)	ReG ₁ (G)	ReG ₂ (G)	ReG ₃ (G)
[1,1,1]	48	7.7	11.41	6	17.42	76
[2,2,2]		35.5	86.32	32	45.18	2396
[3,3,3]	386	35.5	86.32	32	45.18	2396
[4,4,4]		176.6	529.12	192	107.04	17850
	759	92.3	218.11	116	81.23	10420
	1186	176.6	529.12	192	107.04	17850

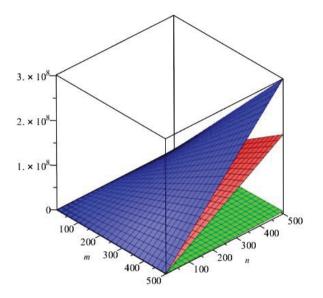


Figure 5: Blue, red and green colors represents F(G), AZI(G) and J(G) individually. Comparatively, in the specified territory F(G) is dictating.

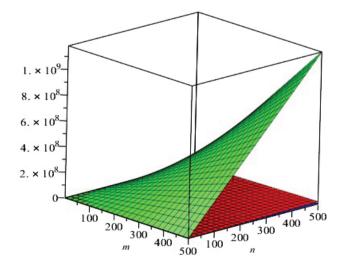


Figure 6: Red green and blue colours epitomise $ReG_1(G)$, $ReG_2(G)$ and $ReG_3(G)$, respectively. Its easy to see that $ReG_3(G)$ is more dominating in the given domain.

Table 4: Comparison of all indices for *CCC*(*n*).

[<i>m</i> , <i>n</i> , <i>t</i>]	F(G)	AZI(G)	J(G)	ReG ₁ (G)	ReG ₂ (G)	ReG ₃ (G)
[1,1,1]	138	17.27	14.26	42	22.36	86
[2,2,2]	986	65.15	98.44	112	48.23	2498
[3,3,3]	1850	186.4	416.12	456	96.24	12426
[4,4,4]	2488	356.8	728.44	886	204.18	19868

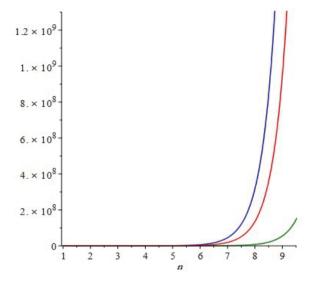


Figure 7: Comparison of F(G), AZI(G) and J(G) of CCC(n). As F(G) is dominating.

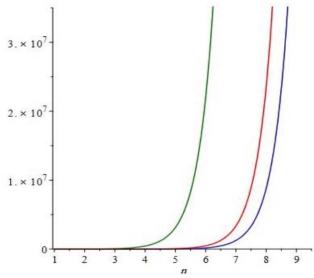


Figure 8: Green, red and blue represent $ReG_1(G)$, $ReG_2(G)$ and $ReG_3(G)$, respectively. Now $ReG_3(G)$ more dominating.

7 Conclusions

In this paper, we have studied and calculated degree based topological indices, mainly Forgotten index, Augmented Zagreb index, Balban index and redefined Zagreb indices for CG(m, n) and CCC(n).

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