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THE GENERALIZED ZAGREB INDEX OF SOME CARBON STRUCTURES

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Abstract: In chemical graph theory, chemical structures are model edthrough a graph where atoms are considered as vertices and edges are bonds between them. In chemical sciences, topological indices are used for understanding the physicochemical properties of molecules. In this work, we study the generalized Zagreb index for three types of carbon allotrope's theoretically.

Keywords: Vertex degree-based topological indices, Generalized Zagreb index, Carbon allotrope's

Introduction

A graph G is a ordered pair of two sets, namely vertex set $V(G)$ and edge set $E(G)$, that is $G = (V(G), E(G))$. The degree of a vertex $v \in V(G)$ is denoted by $d_G(v)$ and is defined as the number of adjacent vertices of v in G. In this study, we consider only finite, simple and connected graphs. A

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topological index is a real number obtained from the graph numerically or more generally it is a molecular descriptor that helps us to understand some, physicochemical properties of molecules such as stability, entropy, enthalpy, boiling point and so many other properties. In recent time more than hundreds of topological indices are introduced by various researchers, among which in this work, we study some well known degree based topological indices in a generalized approach. Here, we mainly derive the generalized Zagreb index or (a, b)-Zagreb index of some carbon structures such as allotrope's and hence as a special case we derive some explicit expressions of the same for other degree based topological indices such as Zagreb indices, forgotten topological index, redefined Zagreb index, general first Zagreb index, general Randic′index, symmetric division deg index. The Zagreb indices were introduced by Gutman and Trinajestic′in 1972,[1] to study the total π–electron energy (ϵ) of carbon atoms and are defined as

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2 = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

The "forgotten topological index" or F-index was introduced in the same paper,[1] where Zagreb indices were introduced and is defined as

$$F(G) = \sum_{v \in V(G)} d_G(v)^3 = \sum_{uv \in E(G)} [d_G(u)^2 + d_G(v)^2].$$

Ranjiniet al.[2] first redefined the Zagreb index in 2013 and is defined as

$$ReZM(G) = \sum_{uv \in E(G)} d_G(u) d_G(v)[d_G(u) + d_G(v)].$$

The concept of the general Zagreb index was first introduced by Li and Zheng in,[3] and is defined as

$$M^{\alpha}(G) = \sum_{u \in V(G)} d_G(u)^{\alpha}$$

where, $\alpha \neq 0, 1\ and \alpha \in R$. Clearly, when $\alpha = 2$ we get first Zagreb index and when $\alpha = 3$ it gives the F-index. Gutman and Lepovic′,[4] first generalized the Randic′ index in 2001 and is defined as

$$R_a = \sum_{uv \in E(G)} \{d_G(u) d_G(v)\}^{a}$$

where, $a \neq 0,\ a \in R$.

The Symmetric division deg index of a graph is defined as

$$SDD(G) = \sum_{uv \in E(G)} [\frac{d_G(u)}{d_G(v)} + \frac{d_G(v)}{d_G(u)}].$$

For further study about this index, we refer our reader to.[5-7] Azari et al.[8] introduced a generalized version of vertex degree based topological index, named as generalized Zagreb index or the (a, b) −Zagreb index in 2011 and is defined as

$$Z_{a,b}(G) = \sum_{uv \in E(G)} [d_G(u)^a d_G(v)^b + d_G(u)^b d_G(v)^a].$$

We refer our reader to[9-11] for further study about this index. It is clear that all the topological indices discussed previously, are derived from this (a, b)-Zagreb index for some particular values of a and b. The table 1 shows the relationship between this (a, b) −Zagreb index and some other topological indices. In this paper, we study the mathematical properties of (a, b) −Zagreb index for three types of carbon allotrope's such as graphene, carbon graphite and crystal cubic structure of carbon. A graphene is a hexagonal lattice of carbon atoms in a honeycomb-like structure and is the world's first 2D material. Graphene is flexible, thinnest and 200 times stronger than steel. As it is a superb conductor and can act as a perfect barrier not even helium can pass through it hence, it has many applications in electronics, sensors, biomedical, composites, and coatings. Graphene membranes could see huge progress in water purification technology. So, for this it has captured the attention of scientist, researchers and industry worldwide. G. Sridhara et al. studied some topological indices of graphene in,[12] V.S. Shigehalli et al. studied some new degree based topological indices for graphene in.[13]

Recently, S. Aktar et al. studied some topological indices of honycomb networks and grapheme networks in[14] and R.P. Kumar et al. studied some vertex degree based topological indices of graphene in.[15]

Table 1. Relations between (a,b)-Zagreb index with some other topological indices.

Topological index	Corresponding (a,b)-Zagreb index
First Zagreb index $M_1(G)$	$Z_{1,0}(G)$
Second Zagreb index $M_2(G)$	$\frac{1}{2}Z_{1,1}(G)$
Forgotten topological index F(G)	$Z_{2,0}(G)$
Redefined Zagreb index ReZM(G)	$Z_{2,1}(G)$
General first Zagreb index $M^a(G)$	$Z_{a-1,0}(G)$
General Randic$'$ index $R_a(G)$	$\frac{1}{2}Z_{a,a}(G)$
Symmetric division deg index SDD(G)	$Z_{1,-1}(G)$

A graphene with m rows and n benzene rings in each row is shown in figure 1. Graphite is multiple layers of graphene. For some unique properties of graphite, it has many applications of different fields. As it has no melting point at atmospheric pressure, is a good conductor of heat and is resistant to many chemicals, which makes it an ideal material for crucibles. Crucibles are containers used in the production of metal, glass, and pigment. Recently, A.Q.

Baig et al. studied the connectivity index, geometric-arithmetic index for graphite in[16] and W. Gao et al. in,[17] studied the topological characterization of carbon graphite and crystal cubic carbon structures. The chemical graph of carbon graphite GG [r,s] for t levels of graphene layers is shown in figure 2, where, r and s is the number of rows and column respectively. Crystal cubic structure of carbon CCC[n] is a one of hypothetical allotrope's of carbon. The structure of crystal cubic of carbon for the first and second layer is shown in figure 3 and figure 4.

Main Results

In this section, we derived (a,b)-Zagreb index of some carbon allotrope's. First, we consider graphene G. The edge sets of graphene with $m$rows and n benzene ring in each row are divided into three parts and are shown as follows:

$$E_1(G) = \{e = uv \in E(G): d_G(u) = 2 \ and d_G(v) = 2\}$$

$$E_2(G) = \{e = uv \in E(G): d_G(u) = 2 \ and d_G(v) = 3\}$$

$$E_3(G) = \{e = uv \in E(G): d_G(u) = 3 \ and d_G(v) = 3\}$$

note that, $|E_1(G)| = (m + 4), |E_2(G)| = (4n + 2m - 4)$, $|E_3(G)| = (3mn - 2n - m - 1)$, so that $|E(G)| = (3mn + 2m + 2n - 1)$.The two dimensional structure of a graphene with n benzene ring and m rows is shown in figure 1.

Theorem 1.The(a, b)-Zagreb index of a graphene with n benzene ring and m rows is given by

$$Z_{a,b}(G) = (m + 4). 2^{a+b+1} + (4n + 2m - 4)\left(2^a. 3^b + 2^b. 3^a\right)$$

$$+(3mn - 2n - m - 1). 2.3^{a+b}.$$

Proof: Applying the definition of (a,b)-Zagreb index, we get

$$Z_{a,b}(G) = \sum_{uv\in E(G)} [d_G(u)^a d_G(b)^b + d_G(u)^b d_G(v)^a]$$

$$= \sum_{uv\in E_1(G)} (2^a.2^b + 2^b.2^a)$$

$$+ \sum_{uv\in E_2(G)} (2^a.3^b + 2^b.3^a) + \sum_{uv\in E_3(G)} (3^a.3^b + 3^b.3^a)$$

$$= |E_1(G)|(2^a.2^b + 2^b.2^a) + |E_2(G)|(2^a.3^b + 2^b.3^a) + |E_3(G)|(3^a.3^b + 3^b.3^a)$$

$$= (m+4).2^{a+b+1} + (4n+2m-4)(2^a.3^b + 2^b.3^a)$$

$$+ (3mn-2n-m-1).2.3^{a+b}.$$

Hence, the theorem.

Corollary 1. Using theorem 1, the following results follows:

(i)$M_1(G) = Z_{1,0}(G) = 4(m+4) + 5(4n+2m-4)$

$$+6(3mn-2n-m-1),$$

(ii)$M_2(G) = \frac{1}{2}Z_{1,1}(G) = 4(m+4) + 6(4n+2m-4)$

$$+9(3mn-2n-m-1),$$

(iii) $F(G) = Z_{2,0}(G) = 8(m+4) + 13(4n+2m-4)$

$$+18(3mn-2n-m-1),$$

(iv)$ReZM(G) = Z_{2,1}(G) = 16(m+4) + 30(4n+2m-4)$

$$+54(3mn-2n-m-1),$$

(v) $M^a(G) = Z_{a-1,0}(G) = 2^a(m+4) + (2^{a-1} + 3^{a-1})(4n+2m-4)$

$$+2.3^{a-1}(3mn-2n-m-1)$$

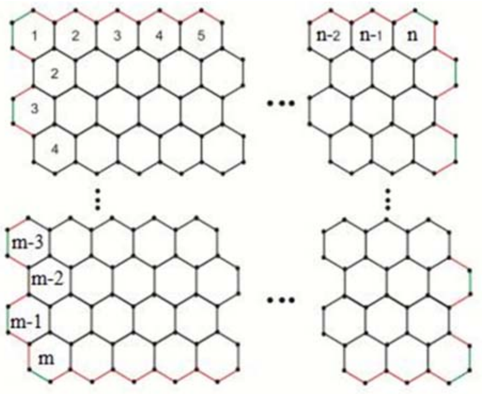

Figure 1.The two dimensional structure of graphene with$m$ rows and n benzene ring.

(iv)$ReZM(G) = Z_{2,1}(G) = 16(m+4) + 30(4n+2m-4) + 54(3mn-2n-m-1),$

(v) $M^a(G) = Z_{a-1,0}(G) = 2^a(m+4) + (2^{a-1}+3^{a-1})(4n+2m-4) + 2.3^{a-1}(3mn-2n-m-1),$

(vi)$R^a(G) = \frac{1}{2}Z_{a,a}(G) = 2^{2a}(m+4) + 2^a.3^a(4n+2m-4) + 3^{2a}(3mn-2n-m-1),$

(vii) $SDD(G) = Z_{1,-1}(G) = 2(m+4) + \frac{13}{6}(4n+2m-4) + 2(3mn-2n-m-1).$

Now, we consider the carbon graphite $CG[r,s]$ for t-levels and obtained the (a,b)-Zagreb index of this structure. Note that, $|V(CG[r,s])| = 2t(rs+r+s)$ and $|E(CG[r,s])| = (4rst+3rt+2st-rs-r-t-2)$.The structure of carbon graphite $CG[r,s]$for t -levels is shown in figure 2.The edge sets of carbon graphite $CG[r,s]$for t-levels can be partitioned as follows:

$$E_1(CG[r,s]) = \{e = uv \in E(CG[r,s]): d_{CG[r,s]}(u) = 2 \, and d_{CG[r,s]}(v) = 2\}$$

$$E_2(CG[r,s]) = \{e = uv \in E(CG[r,s]): d_{CG[r,s]}(u) = 2 \, and d_{CG[r,s]}(v) = 3\}$$

$$E_3(CG[r,s]) = \{e = uv \in E(CG[r,s]): d_{CG[r,s]}(u) = 2 \, and d_{CG[r,s]}(v) = 4\}$$

$$E_4(CG[r,s]) = \{e = uv \in E(CG[r,s]): d_{CG[r,s]}(u) = 3 \, and d_{CG[r,s]}(v) = 3\}$$

$$E_5(CG[r,s]) = \{e = uv \in E(CG[r,s]): d_{CG[r,s]}(u) = 3 \, and d_{CG[r,s]}(v) = 4\}$$

$$E_6(CG[r,s]) = \{e = uv \in E(CG[r,s]): d_{CG[r,s]}(u) = 4 \, and d_{CG[r,s]}(v) = 4\}$$

such that, $|E_1(CG[r,s])| = 4, |E_2(CG[r,s])| = 4(s+t-1),$

$|E_3(CG[r,s])| = 4(st+r-s-t),$

$|E_4(CG[r,s])| = (4r+4t-10),$

$|E_5(CG[r,s])| = 6rs+6rt-14r-4s-6t+12,$

$|E_6(CG[r,s])| = (4rs-3r-2s+1)t-7rs+5r+4s-2.$

Theorem 2. The (a,b) −Zagreb index of carbon graphite $CG[r,s]$ for t-levels is given by

$$Z_{a,b}(CG[r,s]) = 2^{a+b+3} + 4(s+t-1)(2^a.3^b + 2^b.3^a)$$
$$+ 4(st+r-s-t).2^{2ab+3}$$
$$+(6rs+6rt-14r-4s-6t+12)(3^a.4^b + 3^b.4^a)$$
$$+ (4r+4t-10).2.3^{a+b}$$
$$+\{(4rs-3r-2s+1)t-7rs+5r+4s-2\}.2^{2(a+b)+1}.$$

Proof: Using the definition of (a,b) −Zagreb index, we get

$$Z_{a,b}(CG[r,s]) = \sum_{uv\in E(CG[r,s])} [d_{CG[r,s]}(u)^a d_{CG[r,s]}(b)^b + d_{CG[r,s]}(u)^b d_{CG[r,s]}(v)^a]$$

$$= \sum_{uv\in E_1(CG[r,s])} (2^a.2^b + 2^b.2^a) + \sum_{uv\in E_2(CG[r,s])} (2^a.3^b + 2^b.3^a)$$

$$+ \sum_{uv\in E_3(CG[r,s])} (2^a.4^b + 2^b.4^a) + \sum_{uv\in E_4(CG[r,s])} (3^a.3^b + 3^b.3^a)$$

$$+ \sum_{uv\in E_5(CG[r,s])} (3^a.4^b + 3^b.4^a) + \sum_{uv\in E_6(CG[r,s])} (4^a.4^b + 4^b.4^a)$$

$$= |E_1(CG[r,s])|(2^a.2^b + 2^b.2^a) + |E_2(CG[r,s])|(2^a.3^b + 2^b.3^a)$$
$$+|E_3(CG[r,s])|(2^a.4^b + 2^b.4^a) + |E_4(CG[r,s])|(3^a.3^b + 3^b.3^a)$$
$$+|E_5(CG[r,s])|(3^a.4^b + 3^b.4^a) + |E_6(CG[r,s])|(4^a.4^b + 4^b.4^a)$$

$$= 4.2^{a+b+1} + 4(s+t-1)(2^a.3^b + 2^b.3^a) + 4(st+r-s-t)(2^a.4^b + 2^b.4^a)$$
$$+(4r+4t-10).2.3^{a+b} + (6rs+6rt-14r-4s-6t+12)(3^a.4^b + 3^b.4^a)$$
$$+\{(4rs-3r-2s+1)t-7rs+5r+4s-2\}2.4^{a+b}.$$

This is the required theorem.

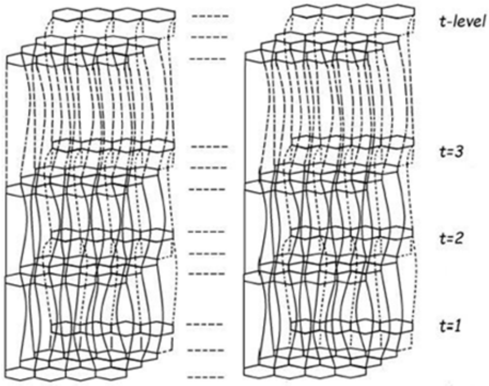

Figure 2. Carbon graphite *CG*[*r, s*] for *t*-levels.

Corollary 2. We derive the following results by using theorem 2, as follows:

(i)$M_1(CG[r,s]) = Z_{1,0}(CG[r,s]) = 16 + 20(s + t - 1) + 8(st + r - s - t) + 6(4r + 4t - 10) + 7(6rs + 6rt - 14r - 4s - 6t + 12) + 8\{(4rs - 3r - 2s + 1)t - 7rs + 5r + 4s - 2\}$,

(ii) $M_2(CG[r,s]) = \frac{1}{2}Z_{1,1}(CG[r,s]) = 16 + 24(s + t - 1) + 16(st + r - s - t) + 9(4r + 4t - 10) + 12(6rs + 6rt - 14r - 4s - 6t + 12) + 16\{(4rs - 3r - 2s + 1)t - 7rs + 5r + 4s - 2\}$,

(iii) $F(CG[r,s]) = Z_{2,0}(CG[r,s]) = 32 + 52(s + t - 1) + 8(st + r - s - t) + 18(4r + 4t - 10) + 25(6rs + 6rt - 14r - 4s - 6t + 12) + 32\{(4rs - 3r - 2s + 1)t - 7rs + 5r + 4s - 2\}$,

(iv)$ReZM(CG[r,s]) = Z_{2,1}(CG[r,s]) = 64 + 120(s + t - 1) + 128(st + r - s - t) + 54(4r + 4t - 10) + 184(6rs + 6rt - 14r - 4s - 6t + 12) + 128\{(4rs - 3r - 2s + 1)t - 7rs + 5r + 4s - 2\}$,

(v) $M^a(CG[r,s]) = Z_{a-1,0}(CG[r,s]) = 2^{a+2} + 4(s + t - 1)(2^{a-1} + 3^{a-1}) + 8(st + r - s - t) + 2.3^{a-1}(4r + 4t - 10) + (3^{a-1} + 4^{a-1})(6rs + 6rt - 14r - 4s - 6t + 12) + 2^{2a-1}\{(4rs - 3r - 2s + 1)t - 7rs + 5r + 4s - 2\}$

(vi) $R^a(CG[r,s]) \quad = \frac{1}{2} Z_{a,a}(CG[r,s]) = 2^{2a+2} + 2^{a+2}.3^a(s+t-1)$

$$+2^{2(a^2+1)}(st+r-s-t) + 3^{2a}(4r+4t-10)$$
$$+3^a.4^a(6rs+6rt-14r-4s-6t+12)$$
$$+2^{4a}\{(4rs-3r-2s+1)t-7rs+5r+4s-2\}$$

(vii) $SDD(CG[r,s]) = Z_{1,-1}(CG[r,s]) = 8 + \frac{26}{3}(s+t-1) + 2(st+r-s-t)$

$$+2(4r+4t-10) + \frac{25}{12}(6rs+6rt-14r-4s-6t+12)$$
$$+2\{(4rs-3r-2s+1)t-7rs+5r+4s-2\}.$$

Finally, we obtained the (a,b) −Zagreb index for crystal cubic structure of carbon $CCC[n]$ with n-layers. Note that,

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

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

The structure of $CCC[n]$ is shown in figure 3 and figure 4. The edge sets of $CCC[n]$ are divided as follows:

$$E_1(CCC[n]) = \{e = uv \in E(CCC[n]) : d_{CCC[n]}(u) = 3\ and d_{CCC[n]}(v) = 3\}$$
$$E_2(CCC[n]) = \{e = uv \in E(CCC[n]) : d_{CCC[n]}(u) = 3\ and d_{CCC[n]}(v) = 4\}$$
$$E_3(CCC[n]) = \{e = uv \in E(CCC[n]) : d_{CCC[n]}(u) = 4\ and d_{CCC[n]}(v) = 4\}$$

where, $|E_1(CCC[n])| = 72(2^3-1)n^{-2}, |E_2(CCC[n])| = 24.(2^3-1)n^{-2}$,

$$|E_3(CCC[n])| = 12.\left(1 + \sum_{i=3}^{n} 2^3\,(2^3-1)^{i-3}\right) + 8\sum_{i=0}^{n-2}(2^3-1)^i.$$

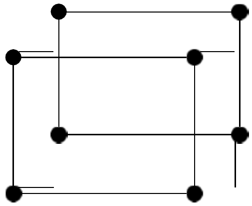

Figure 3. Crystal cubic structure of carbon CCC(1).

Theorem 3. The (a,b)-Zagreb index of CCC[n] is given by

$$Z_{a,b}\,(CCC[n]) = 72(2^3-1)n^{-2}.2.3^{a+b} + 24(2^3-1)n^{-2}\left(3^a.4^b+3^b.4^a\right)$$
$$+\{12\left(1+\sum_{i=3}^{n}2^3\,(2^3-1)^{i-3}\right)+8\sum_{i=0}^{n-2}(2^3-1)^i\}\,2^{2(a+b)+1}.$$

Proof: From definition of (a,b)-Zagreb index, we get

$$Z_{a,b}\,(CCC[n]) = \sum_{uv\in E(CCC[n])}[d_{CCC[n]}(u)^a d_{CCC[n]}(b)^b + d_{CCC[n]}(u)^b d_{CCC[n]}(v)^a]$$
$$= \sum_{uv\in E_1(CCC[n])}\left(3^a.3^b+3^b.3^a\right) + \sum_{uv\in E_2(CCC[n]}\left(3^a.4^b+3^b.4^a\right)$$
$$+\sum_{uv\in E_3(CCC[n])}\left(4^a.4^b+4^b.4^a\right)$$
$$= |E_1(CCC[n])|\left(3^a.3^b+3^b.3^a\right)+|E_2(G)|\left(3^a.4^b+3^b.4^a\right)$$
$$+|E_3(G)|\left(4^a.4^b+4^b.4^a\right)$$
$$= 72(2^3-1)n^{-2}.2.3^{a+b} + 24(2^3-1)n^{-2}\left(3^a.4^b+3^b.4^a\right)$$
$$+\{12\left(1+\sum_{i=3}^{n}2^3\,(2^3-1)^{i-3}\right)+8\sum_{i=0}^{n-2}(2^3-1)^i\}.2.4^{a+b}.$$

Hence, the theorem.

Corollary 3. Using theorem 3, we obtain following results as follows:

(i)$M_1(CCC[n]) \quad = Z_{1,0}(CCC[n]) = 152(2^3-1)n^{-2} + 168(2^3-1)n^{-2}$

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

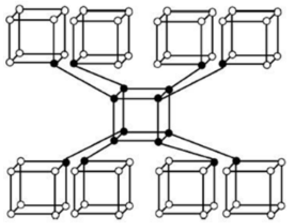

Figure4. CrystalcubicstructureofcarbonCCC(2).

(ii) $M_2(CCC[n]) \quad = \frac{1}{2}Z_{1,1}(CCC[n]) = 648(2^3-1)n^{-2} + 288(2^3-1)n^{-2}$

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

(iii) $F(CCC[n]) \quad = Z_{2,0}(CCC[n]) = 1296(2^3-1)n^{-2} + 600(2^3-1)n^{-2}$

$$+32\{12\left(1+\sum_{i=3}^{n} 2^3\,(2^3-1)^{i-3}\right)+8\sum_{i=0}^{n-2}(2^3-1)^i\},$$

(iv)$ReZM(CCC[n]) = Z_{2,1}(CCC[n]) = 3888(2^3-1)n^{-2} + 2016(2^3-1)n^{-2}$

$$+128\{12\left(1+\sum_{i=3}^{n} 2^3\,(2^3-1)^{i-3}\right)+8\sum_{i=0}^{n-2}(2^3-1)^i\},$$

(v) $M^a(CCC[n]) \quad = Z_{a-1,0}(CCC[n]) = 144.3^{a-1}(2^3-1)n^{-2}$

$$+24(3^{a-1}+4^{a-1})(2^3-1)n^{-2}$$

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

(vi) $R^a(CCC[n]) = \frac{1}{2}Z_{a,a}\,(CCC[n]) = 144.3^{2a}.\,(2^3-1)n^{-2}\ +$

$$+48.3^a.\,4^a.\,(2^3-1)n^{-2} + 2^{4a+1}\{12\left(1+\sum_{i=3}^{n} 2^3\,(2^3-1)^{i-3}\right)+8\sum_{i=0}^{n-2}(2^3-1)^i\},$$

(vii) $SDD(CCC[n]) \ = Z_{1,-1}(CCC[n]) = 144(2^3-1)n^{-2} + 50(2^3-1)n^{-2}$

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

Conclusions

In this study, we derive some explicit expressions of the (a,b)-Zagreb index of some carbon allotrope's such as graphene, graphite and crystal cubic structure of carbon and hence for some particular values of a and b some other important degree based topological indices are also obtained from the derived results. As different allotrope's of carbon plays an important role in chemical sciences, so this study will help to researchers understand their physicochemical properties, chemical reactivity and biological activity theoretically. For further study the (a,b)-Zagreb index of some other chemical structures can be obtained.

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