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Computation of Degree-Based Numerical Descriptors of Porous Graphene

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Abstract: Graph theory is attracting much attention due to the use of devices like topological indices. A topological graph index is defined according to a certain rule. After defining a new topological index, it must be checked for a possible correlation with the properties of a particular chemical substance along with a few mathematical properties. As most of the indices involve some data related to the degrees of the vertices, types of edges, and various details of the chemical compound under the study, it is very useful in chemistry applications. The applications include drug design, modeling of a compound, the study of structure relationships, etc. In this work, the redefined Zagreb indices, *ABC* index, *GA* index, Augmented Zagreb index, neighborhood version of redefined Zagreb indices, ABC_4 index, GA_5 index, and Sanskruti index is computed for the chemical compound called porous graphene. The work is concluded with a detailed conclusion of the study considered.

Keywords: topological index; porous graphene; cheminformatics.

1. Introduction

Graph theory is a very useful tool for chemistry, used to solve many problems in the theoretical part. By depicting a compound in terms of a graph, notions like the vertex degrees and types of edges offer information related to the properties of the compound. A topological index (TI) is a useful tool for obtaining information about a chemical compound. It provides numerous data on the compound used in QSAR and QSPR studies [1,2].

In mathematical chemistry, many tools such as TI's, matrices, and polynomials are used to categorize the properties of chemical compounds. In general, polynomials are used to relate two or more parameters that exist in the equation. Hosoya introduced the Hosoya polynomials from which the distance-based TI called Wiener index can be determined. The Hosoya polynomial has varied applications in chemistry because distance-based TI's can be computed from this polynomial [3,4].

The most privileged documented branch of science is chemistry, which provides most of the chemical information associated with the structure of the compound and its structural formula. Chemistry happens to be a potential branch of science worldwide. Chemists can communicate using chemical formulae irrespective of their mother tongues, i.e., as chemistry already has chemical formulae and chemical structures available, it is easy to retrieve the data

for any compounds. The graph theory is applied to chemistry because of the existence of isomers; useful information could be obtained using the topological indices.

Now we recall a few topological indices:

Estrada *et al*. [5] proposed the ABC index given by

$$ABC(G) = \sum_{v\omega \in E(G)} \sqrt{\frac{d_v + d_\omega - 2}{d_v d_\omega}}$$

M. Ghorbani *et al*. [6] proposed the fourth ABC index as

$$ABC_4(G) = \sum_{v\omega \in E(G)} \sqrt{\frac{S_v + S_\omega - 2}{S_v S_\omega}}$$

Vukicevic *et al*. [7] proposed the *GA* index as

$$GA(G) = \sum_{v\omega \in E(G)} \frac{2\sqrt{d_v d_\omega}}{d_v + d_\omega}$$

A. Graovac *et al*. [8] proposed the GA_5 index as

$$GA_5(G) = \sum_{v\omega \in E(G)} \frac{2\sqrt{S_v S_\omega}}{S_v + S_\omega}$$

Furtula *et al*. proposed the augmented Zagreb index [9] given by

$$AZI(G) = \sum_{v\omega \in E(G)} \left\{\frac{d_v d_\omega}{d_v + d_\omega - 2}\right\}^3$$

The Sanskruti index $S(G)$ is defined by Hosamani [10] as

$$S(G) = \sum_{v\omega \in E(G)} \left\{\frac{S_v S_\omega}{S_v + S_\omega - 2}\right\}^3$$

Redefined first, second, and third Zagreb indices were proposed by Ranjini *et al*., in 2016 [11,12] as

$$ReZG_1(G) = \sum_{v\omega \in E(G)} \frac{d_v + d_\omega}{d_v d_\omega}$$

$$ReZG_2(G) = \sum_{v\omega \in E(G)} \frac{d_v d_\omega}{d_v + d_\omega}$$

$$ReZG_3(G) = \sum_{v\omega \in E(G)} (d_v d_\omega)(d_v + d_\omega)$$

Shanmukha *et al*. [13] proposed the neighborhood versions of the redefined first and second Zagreb indices as follows:

$$NReZG_1(G) = \sum_{v\omega \in E(G)} \frac{S_v + S_\omega}{S_v S_\omega}$$

$$NReZG_2(G) = \sum_{v\omega \in E(G)} \frac{S_v S_\omega}{S_v + S_\omega}$$

Sourav Mondal *et al*. [14], introduced the neighborhood third NDe index defined by

$$NDe_3(G) = \sum_{v\omega \in E(G)} (S_v S_\omega)(S_v + S_\omega)$$

Here d_v denotes the degree of the vertex v and S_v denotes the sum of degrees of neighboring vertices of v .

Graph theory is not only applied in chemistry but also its applications are spread through various fields like computer networks to transfer the data and other information quickly with high accuracy. In this modern era, networks play a significant role in social networks; small worlds have come into existence. Graph theory plays a very important role in spatial networks or food web and other networks. More research work is happening in cheminformatics has potential applications in real life. It gives a deep insight into the QSAR and QSPR studies [15-22].

The most popular and oldest indices are the Randic index, Zagreb indices, ABC index, etc., see [23-28]. The properties of chemical compounds, like boiling point, enthalpy of vaporization, stability, etc., can be predicted using these indices. Several TI's defined in graph theory can model the geometric structure of chemical compounds [29-33].

ABC and ABC_4 indices have remarkable applications in the stability of alkanes and the strain energy of cycloalkanes. In [34], Wei Gao *et al*. have computed GA and ABC indexes for the octagonal, hexagonal, and square grids. A comparison is made for these indices with GA_5 and ABC_4 indices. In [35], K.C. Das *et al*. have found the extremal values for ABC index.

Numerous papers are available in the field of research on the pair of molecular descriptors known as the Zagreb indices. I. Gutman and N. Trinajstic derived the topological formula for total π-energy of conjugated molecules in 1972 [36]. Molecular complexity, ZE-isomerism, chirality, etc., have been used in the study of Zagreb indices. The multi-linear regression models are derived from these indices applications [37-52].

Several topological indices have vast applications in chemistry. In recent times, there have been numerous TI's, and few are applied in chemistry. The spectrum of the graph is defined using the Estrada index. Perhaps the oldest and the most famous index is the Wiener index, based on the topological distance of vertices in the respective graph. It was defined and used by Harold Wiener in 1947, which helped him to compare the boiling points of some alkane isomers.

2. Materials and Methods

The chemical compound porous graphene is modeled in this study by a simple graph. To compute the porous graphene structure's TI's, the methods employed are vertex partitioning, edge partitioning, neighborhood vertex partitioning, and computational techniques. The work is equipped with the MATLAB R2017A version to depict the results in graphs and verify computed results.

3. Results and Discussion

Graphene is an essential and intriguing chemical that draws theoretical and practical research. Graphene is useful in material science because of its unique properties and applications. Porous graphene is a plane-based composite of graphene-related materials with nanopores. Because of the presence of nanopores in the graphene plane, porous graphene has unique features. As a result, porous graphene has applications in gas separation, hydrogen storage, DNA sequencing, biosensors, diagnostics, DNA sensors that are useful in sensor applications and supercapacitors.

Graphene is an important and exciting material attracting theoretical and practical studies in chemistry. Graphene is useful in material science because of its extraordinary characteristics and uses. Porous graphene is a combination of graphene-related materials and

nanopores in the plane. The porous graphene has distinct properties because of the presence of nanopores in the graphene plane. Hence porous graphene has its applications in the separation of gas, storage of hydrogen, DNA sequencing, biosensors, diagnostics, and DNA sensors beneficial in the usage of sensors and supercapacitors [53-55].

The structure of porous graphene is illustrated in Figure 1. The structure includes six hexagons connected by an edge between two carbon atoms, and also, six hexagon structure is connected linearly row-wise and column-wise using carbon-carbon atoms [56,57].

There has been increasing interest in the research of graphitic materials such as graphene because of their electrical properties. Graphene is a 2D sheet of sp2 hybridized carbon atoms that has attracted many researchers because of its exceptional properties in various applications. Porous graphene may be prepared via various physical and chemical methods, resulting in various uses and structures. Chemists are solely responsible for the synthesis of this chemical molecule.

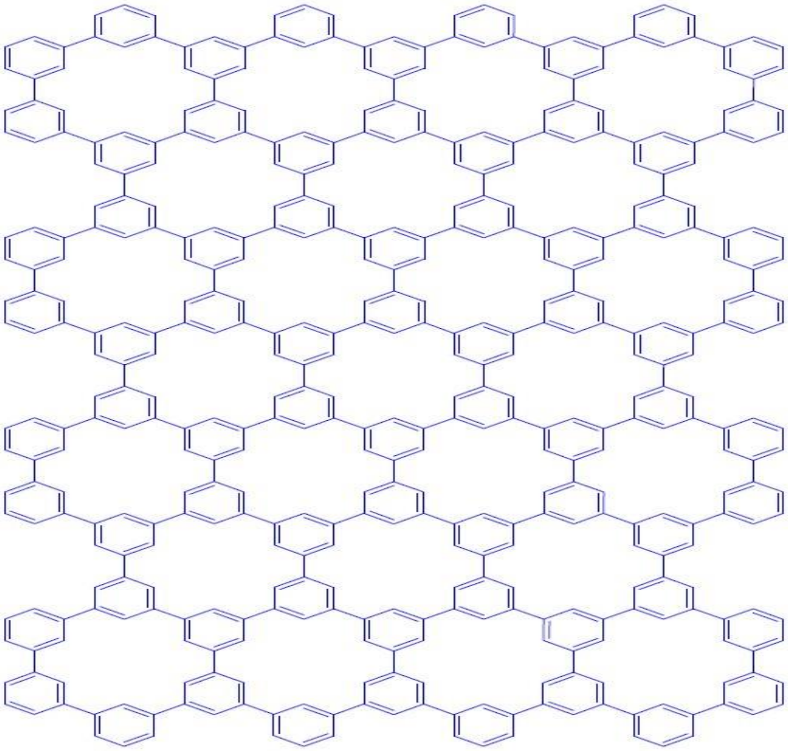


Figure 1. Porous Graphene Structure P[4, 4].

Figure 1 shows the molecular graph of porous graphene G = P[4, 4], a spatial six-carbon grate with four rows and four columns in the plane. In general, if the number of rows and columns are m and n, respectively. It can be seen that, then $|V(P[m,n])| = 12mn + 12m + 12n$ and $|E(P[m,n])| = 15mn + 14m + 14n - 1$.

3.1. Results for porous graphene graph using degrees of the end vertices.

The degree of incident vertices for a porous graphene graph can be computed using Figure 1. The collection of vertices has a cardinality of |V(P[m, n])=12mn+12m+12n. In Table 1, there are two vertices with degrees 2 and 3, respectively. Table 2 lists many types of edges.

Table 1. The vertex partition of porous graphene structure graph.

$d_v \backslash v \in V(G)$	No. of Vertices
2	6mn + 8m + 8n + 2
3	6mn + 4m + 4n − 2.

Table 2. The edge partition of a porous graphene graph based on the degrees of the end vertices of each edge.

(d_v, d_ω) where $v\omega \in E(G)$	No. of edges
$E_1 = (2,2)$	4m + 4n + 4
$E_2 = (2,3)$	12mn + 8m + 8n − 4
$E_3 = (3,3)$	3mn + 2m + 2n − 1

Theorem 3.1.1. The ABC(G) index of porous graphene graph is

$$ABC(G) = \frac{1049}{100}mn + \frac{491}{50}m + \frac{491}{50}n - \frac{2}{3}.$$

Proof. Let the edges of the porous graphene graph be denoted by $e_{i,j}$ with $i = d_v$ and $j = d_\omega$. It is observed from Figure 1, that the number of vertices and edges of the porous graphene graph structure G = P[m, n] are |V (P[m, n])| = 12mn+12m+12n and |E(P[m, n])| = 15mn + 14m + 14n − 1 respectively. The edges of the porous graphene graph are classified into 3 edge types, $e_{2,2}, e_{2,3}, e_{3,3}$ as shown in Table 2. Hence the ABC index is

$$ABC(G) = \sum_{v\omega \in E(G)} \sqrt{\frac{d_v + d_\omega - 2}{d_v d_\omega}}$$

$$= e_{2,2}\sqrt{\frac{2+2-2}{2\times 2}} + e_{2,3}\sqrt{\frac{2+3-2}{2\times 3}} + e_{3,3}\sqrt{\frac{3+3-2}{3\times 3}}$$

$$= (4m + 4n + 4)\left(\sqrt{\frac{1}{2}}\right) + (12mn + 8m + 8n - 4)\left(\sqrt{\frac{1}{2}}\right)$$

$$+ (3mn + 2m + 2n - 1)\left(\sqrt{\frac{4}{9}}\right)$$

$$= \frac{1049}{100}mn + \frac{491}{50}m + \frac{491}{50}n - \frac{2}{3}.$$

Theorem 3.1.2. The GA(G) index of the porous graphene graph is

$$\mathrm{GA(G)} = \frac{369}{25}\mathrm{mn} + \frac{346}{25}\mathrm{m} + \frac{346}{25}\mathrm{n} - \frac{1149}{1250}.$$

Proof. Using the definition of GA index, the result follows by Table 2 as

$$GA(G) = \frac{369}{25}mn + \frac{346}{25}m + \frac{346}{25}n - \frac{1149}{1250}.$$

Theorem 3.1.3. The augmented Zagreb index of the porous graphene graph is

$$AZI(G) = \frac{13017}{100}mn + \frac{5939}{50}m + \frac{5939}{50}n - \frac{1139}{100}.$$

Proof. The result similarly follows.

Theorem 3.1.4**.** The redefined Zagreb indices of the porous graphene graph are

$$\mathrm{ReZG_1(G)} = 12\mathrm{mn} + 12\mathrm{m} + 12\mathrm{n}.$$

$$\mathrm{ReZG_2(G)} = \frac{189}{10}\mathrm{mn} + \frac{83}{5}\mathrm{m} + \frac{83}{5}\mathrm{n} - \frac{23}{10}.$$

$$\mathrm{ReZG_3(G)} = 522\mathrm{mn} + 412\mathrm{m} + 412\mathrm{n} - 110.$$

Proof. Using the definitions of redefined Zagreb indices and Table 2, the results follow.

3.2. Results for porous graphene graph using neighborhood degrees of the end vertices.

From Figure 1, the degrees of neighboring vertices are calculated for the porous graphene graph. The cardinality of the vertex set is |V (P[m, n])| = 12mn + 12m + 12n. There are four types of vertices of degrees 4, 5, 6, and 7, as tabulated in Table 3. The types of edges in the neighbor degree of vertices are tabulated in Table 4.

Table 3. The Vertex partition of Porous Graphene Structure Graph.

$S_v \backslash v \in E(G)$	No. of Vertices
4	2m + 2n + 2
5	4m + 4n + 4
6	6mn + 2m + 2n − 4
7	6mn + 4m + 4n − 2

Table 4. The edge partition of a porous graphene graph based on the sum of neighbor degrees of the end vertices of each edge.

(S_v, S_ω) where $v\omega \in E(G)$	No. of Edges
$E_1 = (4,5)$	4m + 4n + 4
$E_2 = (5,7)$	4m + 4n + 4
$E_3 = (6,7)$	12mn + 4m + 4n − 8
$E_4 = (7,7)$	3mn + 2m + 2n − 1.

Theorem 3.2.1. For the porous graphene graph, the $ABC_4(G)$ index is

$$ABC_4(G) = \frac{3813}{500}mn + \frac{377}{50}m + \frac{377}{50}n - \frac{169}{2000}.$$

Proof. Let the edges of the porous graphene graph be denoted by $e_{i,j}$ with $i = S_v$ and $j = S_\omega$. It is observed from Figure 1, that the number of vertices and edges of the porous graphene graph are |V (P[m, n])| = 12mn + 12m + 12n and |E(P[m, n])| = 15mn + 14m + 14n − 1 respectively and the sum of the degrees of neighboring vertices of each edge of the porous graphene graph have 4 edge types $e_{4,5}, e_{5,7}, e_{6,7}$ and $e_{7,7}$ as shown in Table 4.

Hence

$$ABC_4(G) = \sum_{v\omega \in E(G)} \sqrt{\frac{S_v + S_\omega - 2}{S_v S_\omega}}$$

$$= e_{4,5}\sqrt{\frac{4+5-2}{4\times5}} + e_{5,7}\sqrt{\frac{5+7-2}{5\times7}} + e_{6,7}\sqrt{\frac{6+7-2}{6\times7}} + e_{7,7}\sqrt{\frac{7+7-2}{7\times7}}$$

$$= (4m + 4n + 4)\left(\sqrt{\frac{7}{20}}\right) + (4m + 4n + 4)\left(\sqrt{\frac{10}{35}}\right) + (12mn + 4m + 4n - 8)\left(\sqrt{\frac{11}{42}}\right)$$

$$+ (3mn + 2m + 2n - 1)\left(\sqrt{\frac{12}{49}}\right)$$

$$= \frac{3813}{500}mn + \frac{377}{50}m + \frac{377}{50}n - \frac{169}{2000}.$$

Theorem 3.2.2. For the porous graphene graph, GA_5 index is

$$GA_5(G) = \frac{3741}{250}mn + \frac{1391}{100}m + \frac{1391}{100}n - \frac{1057}{1000}.$$

Proof. The result follows by Table 4, using the GA index definition.

Theorem 3.2.3. The Sanskruti index of the porous graphene graph is

$$S(G) = \frac{872213}{1000}mn + \frac{311808}{500}m + \frac{311808}{500}n - \frac{1243}{5}.$$

Proof. It follows similarly.

Theorem 3.2.4. The neighborhood version of the redefined first Zagreb index of the porous graphene graph is

$$\mathrm{NReZ}_1(\mathrm{G}) = \frac{457}{100}\mathrm{mn} + \frac{4981}{1000}\mathrm{m} + \frac{4981}{1000}\mathrm{n} + \frac{819}{2000}.$$

Proof. By Table 4, using the definition of the neighborhood version of the redefined first Zagreb index, the result follows.

Theorem 3.2.5. The neighborhood version of the redefined second Zagreb index of the porous graphene graph is

$$\mathrm{NReZ}_2(\mathrm{G}) = \frac{49269}{1000}\mathrm{mn} + \frac{40479}{1000}\mathrm{m} + \frac{40479}{1000}\mathrm{n} - \frac{8791}{1000}.$$

Proof. In Table 4, using the definition of the neighborhood version of the redefined second Zagreb index, the result follows.

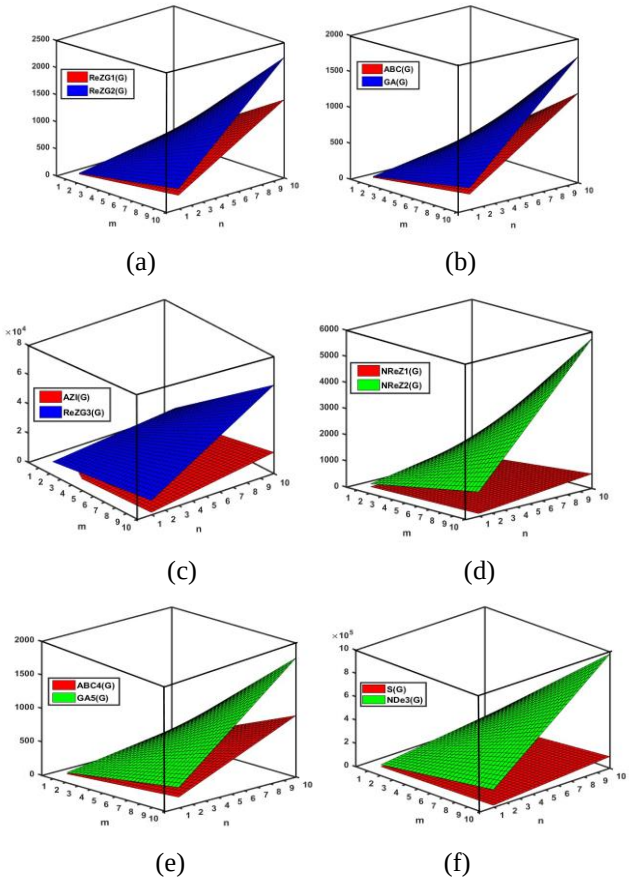
Theorem 3.2.6. The neighborhood version of the third NDe index of the porous graphene graph is

$$\mathrm{NDe}_3(\mathrm{G}) = 8610\mathrm{mn} + 5956\mathrm{m} + 5956\mathrm{n} - 2654.$$

Proof. It follows similarly to the above indices.

3.3. Comparison of indices.

In Section 3, 12 topological indices for the molecular graph of porous graphene structure are computed. Different values of m = n are investigated to see how the indices behave. The values of topological indices grow as the m = n value increases, as shown in Table 5. As illustrated in Figure 2, the derived topological indices are graphically depicted in 3D for various values of m = n.



(a) (b) (c) (d) (e) (f)

Figure 2. Graphical comparison of twelve topological indices.

Table 5. Numerical comparison for m = n = 1 to 10.

[m, n]	ABC	GA	AZI	$ReZG_1$	$ReZG_2$	$ReZG_3$	ABC_4	S	$NReZ_1$	$NReZ_2$	$NReZ_3$	GA_5
[1,1]	29.463	41.521	356.34	36	49.8	1236	22.622	1870.8	14.942	121.44	17865	41.727
[2,2	80.573	113.481	984.41	96	139.7	3626	60.58	5734.7	38.614	350.201	55607	114.439
[3,3]	152.663	214.961	1872.8	180	267.4	7060	113.79	11343	71.426	677.504	110569	217.079
[4,4]	245.733	345.961	3021.6	288	432.9	11538	182.252	18696	113.378	1103.3	182751	349.647
[5,5]	359.783	506.481	4430.7	420	636.2	17060	265.966	27793	164.47	1627.7	272153	512.143
[6,6]	494.813	696.521	6100.1	576	877.3	23626	364.932	38634	224.702	2250.6	378775	704.567
[7,7]	650.823	916.081	8029.9	756	1156.2	31236	479.15	51220	294.074	2972.1	502617	926.919
[8,8]	827.813	1165.2	10220	960	1472.9	39890	608.62	65551	372.586	3792.1	643679	1179.2
[9,9]	1025.8	1443.8	12670	1188	1827.4	49588	753.342	81626	460.238	4710.6	801961	1461.4
[10,10]	1244.7	1751.9	15381	1440	2219.7	60330	913.316	99445	557.03	5727.7	977463	1773.5

It is evident from Table 5 and 6 graphs depicted in Figure 2 give the graphical comparison of twelve TI'S. In the above six graphs, three graphs give a comparison between degree-based indices $ReZG_1$ against $ReZG_2$, ABC against GA, and AZI against $ReZG_3$. Similarly, neighborhood versions of the indices such as $NReZ_1$ against $NReZ_2$, ABC_4 against GA_5, and S against NDe_3 are plotted. It is observed from the graph that the indices are linear increases as m = n increases.

4. Conclusions

This paper presents the values of twelve degree-based TI's, such as redefined Zagreb indices, augmented Zagreb index, neighborhood redefined first and second Zagreb indices, neighborhood third NDe index, Sanskruti index, and reciprocal Sanskruti index, are computed for porous graphene structure. The porous graphene structure has a wide range of applications in biosensors, diagnostics, and DNA sensors, all of which are useful for sensor utilization. These findings will help researchers to learn more about this chemical structure and its potential applications.

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Conflicts of Interest

The authors declare no conflict of interest.

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