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Novel Face Index for Benzenoid Hydrocarbons

Muhammad Kamran Jamil [1,2,*], Muhammad Imran [2,3] and Kanza Abdul Sattar [1]

[1] Department of Mathematics, Riphah Institute of Computing and Applied Sciences, Riphah International University, 14 Ali Road, 54000 Lahore, Pakistan; kanzasatter@gmail.com
[2] Department of Mathematical Sciences, College of Sciences, United Arab Emirates University, 15258 Al Ain, UAE; imrandhab@gmail.com
[3] Department of Mathematics, School of Natural Sciences, NUST, 44000 Islamabad, Pakistan
* Correspondence: m.kamran.sms@gmail.com; Tel.: +92-346-4105447

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Abstract: A novel topological index, the face index (FI), is proposed in this paper. For a molecular graph G, face index is defined as $FI(G) = \sum_{f \in F(G)} d(f) = \sum_{v \sim f, f \in F(G)} d(v)$, where $d(v)$ is the degree of the vertex v. The index is very easy to calculate and improved the previously discussed correlation models for $\pi - electron$ energy and boiling point of benzenoid hydrocarbons. The study shows that the multiple linear regression involving the novel topological index can predict the π-electron energy and boiling points of the benzenoid hydrocarbons with correlation coefficient $r > 0.99$. Moreover, the face indices of some planar molecular structures such as 2-dimensional graphene, triangular benzenoid, circumcoronene series of benzenoid are also investigated. The results suggest that the proposed index with good correlation ability and structural selectivity promised to be a useful parameter in QSPR/QSAR.

Keywords: vertex degree; face degree; faces of a graph; face index; polycyclic aromatic hydrocarbons; π-electron energy; boiling point.

1. Introduction

In application of mathematical and statistical methods one of the most important purposes is to find a relationship between molecular structure and values of physical, chemical and biological properties. As a result, quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) have been studied.

In QSPR/QSAR studies topological indices(molecular descriptors) are key tools [1–4]. A topological index is a graph invariant number calculated from a graph associated to a molecule.

Properties estimation can help to minimize the time and cost in producing new chemical materials with desired properties. For estimation some of the statistical tests are discussed in [5]. The physiochemical properties of molecular compounds are important in many fields. A lot of work has done on prediction of physiochemical properties of different compounds [6–11].

Molecules can be represented by molecular graphs, where vertices represent the atoms and edges represent the bonds between them. For a molecular graph $G = (V, E)$, V and E represent the set of vertices and the set of edges, respectively. The graph theory-based structure descriptors can be determined by considering graph edges, vertices, or both. Rather simple arithmetic operations are carried out to get numerical indices. These indices are suppose to comprise information on properties/activities of the molecules.

The vertex-connectivity index $\chi(G)$ of a (molecular) graph G was introduced by Randić in 1975 [12]:

$$\chi(G) = \sum_{uv \in E(G)} \left[d(u)d(v)\right]^{-1/2}$$

where $d(u)$ is the degree of the vertex u in G.

The edge-connectivity index $\epsilon(G)$ of a (molecular) graph G was introduced by Estrada [11]:

$$\epsilon(G) = \sum_{e \sim f} \left[d(e)d(f)\right]^{-1/2}$$

where $e \sim f$ shows that the edges e and f are adjacent and $d(e) = d(u) + d(v) - 2$ for $e = uv$.

In [13] Nikolić and Trinajstić made a comparison between the vertex and edge connectivity indices for benzenoid hydrocarbons. They showed that the π-electron energies (E) of benzenoids can be computed by means of either the vertex connectivity index or the edge connectivity index. Their best quadratic model based on the edge-connectivity index can predict the π-electron energies of benzenoids within the error range of 0.8%–2%. While their best structure-boiling point (bp) model was a quadratic model that can predict the boiling points of benzenoid hydrocarbons within the error range of 1.3%–4%. Their best models are as follows

$$E = 2.257(\pm 0.020)\epsilon + 1.486(\pm 0.229) \tag{1}$$

$n = 23; \quad r = 0.9993; \quad r^2(adjusted) = 0.9984; \quad s = 0.278; \quad F = 3276$

$$bp = -0.868(\pm 0.152)\epsilon^2 + 58.768(\pm 2.986) - 81.692(\pm 13.998) \tag{2}$$

$n = 23; \quad r = 0.9982; \quad r^2(adjusted) = 0.9962; \quad s = 8.0; \quad F = 2859$ where n is the number of benzenoids, r is the correlation coefficient, r^2(adjusted) is the adjusted correlation coefficient, s is the standard error of estimate and F is the Fisher ratio.

We introduced the novel topological index to improve the efficiency of the above equations.

1.1. **Definition of the Face Index**

When a connected graph can be drawn on the plane without crossing any edges, it is called a planar graph. When a planar graph is drawn in this way, it divides the plane into regions called faces. The unbounded region is called the infinite face.

Let $G = (V(G), E(G), F(G))$ be a finite simple connected planar graph, where $V(G)$, $E(G)$ and $F(G)$ represent the vertex, edge and face sets, respectively. A face $f \in F(G)$ is incident to an edge $e \in E(G)$ if e is one of those edges which surrounds the face. Similarly, a face $f \in F(G)$ is incident to a vertex v in G if v is at the end of one of those incident edges.

The molecular graph of benzene ring is a cycle consist of six vertices and edges each and two faces. The molecular graph of benzenoid hydrocarbons contain considerable number of faces.

In the present study, we introduced a new topological index, the *face index* (FI), using the degree of the vertices incident with the faces of a graph. For a planar graph G, FI can be defined as

$$FI(G) = \sum_{f \in F(G)} d(f) = \sum_{v \sim f, f \in F(G)} d(v)$$

$v \sim f$ represents the incidency of the vertex v with the face f.

In benzenoid graphs (BG), vertices have either degree two or three; the vertices with degree two are incident with two faces and vertices with degree three are incident with three faces. Let v_2 and v_3 denote the number of vertices with degree two and three in BG, then the definition of FI for BG becomes

$$FI(BG) = 2 \times 2 \times v_2 + 3 \times 3 \times v_3 = 4v_2 + 9v_3$$

Hence, FI of any BG can be investigated by just knowing the number of vertices of degree two and three. In case of perylene (P) as shown in Figure 1 $v_2 = 12$ and $v_3 = 8$, so $FI(P) = 120$. Authors in [14], discussed theoretical study of singlet fission in oligorylenes.

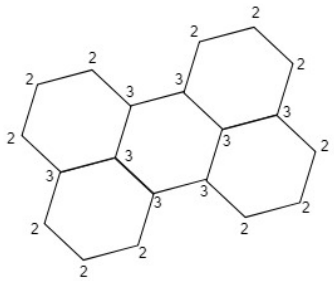

Figure 1. Vertices degree of the perylene benzenoid graph (P).

2. Discussion

The novel topological index is used to construct the structure-energy and structure-boiling point models and the obtained results are comparable with the results obtained in [10,13,15]. We computed FI for 21 common benzenoid hydrocarbons. The values of FI for these hydrocarbons are given in Table 1 along with the π-electron energies (β) and boiling points (°C). The π-electron energies have been taken from the tabulation of Coulson and Streiwieser [16] . The experimental values of boiling points were taken from Basak et al. [17].

Table 1. The face index (FI), Randić index (χ), edge-connectivity index (ε), π-electron energies (E) in β and boiling points (bp) in ^oC of studied benzenoid hydrocarbons.

Benzenoid Hydrocarbons	FI	χ	ϵ	E	bp
benzene	24	3	3	8	80.1
naphthalene	50	4.966	5.455	13.683	218.0
phenanthrene	76	6.95	7.926	19.448	338.0
anthracene	76	6.933	7.942	19.314	340.0
chrysene	102	8.933	10.247	25.192	431.0
benzanthracene	102	8.916	10.414	25.101	425.0
triphenylene	102	8.95	10.414	25.275	429.0
tetracene	102	8.899	10.43	25.188	440.0
benzo(a)pyrene	120	9.916	11.897	28.22	496.0
benzo(e)pyrene	120	9.933	11.897	28.336	493.0
perylene	120	9.933	11.897	28.245	497.0
anthanthrene	138	10.899	13.397	31.253	547.0
benzoperylene	146	10.916	13.379	31.425	542.0
dibenzo(a,c)anthracene	128	10.916	12.902	30.942	535.0
dibenzo(a,h)anthracene	128	10.899	12.885	30.881	535.0
dibenzo(a,i)anthracene	128	10.899	13.218	30.88	531.0
picene	128	10.915	12.686	30.943	519.0
coronene	156	11.899	14.863	34.572	590.0
dibenzo(a,h)pyrene	146	11.566	14.385	33.928	596.0
dibenzo(a,g)pyrene	146	11.491	14.385	33.954	594.0
pyrene	94	7.933	9.408	22.506	393.0

2.1. *Relationships between the Face Index and Vertex and Edge Connectivity Indices for Benzenoid Hydrocarbons*

We first considered the relationships between the face index and the vertex-connectivity index and between the face index and the edge connectivity index for benzenoid hydrocarbons. Plots of FI versus χ and FI versus ϵ for benzenoids is given in Figures 2 and 3 and the obtained mathematical models are:

$$FI = 0.68(\pm 0.002)\chi + 1.741(\pm 0.262) \quad (3)$$

$n = 21; \quad r = 0.9896; \quad r^2(adjusted) = 0.9783; \quad s = 4.8962; \quad F = 906.241$

$$FI = 0.091(\pm 0.002)\epsilon + 1.023(\pm 0.222) \tag{4}$$

$n = 21; \quad r = 0.996; \quad r^2(adjusted) = 0.991; \quad s = 3.1325; \quad F = 2241.371$

From above equations we can see that the face index is more closely related with edge connectivity index rather the vertex connectivity index.

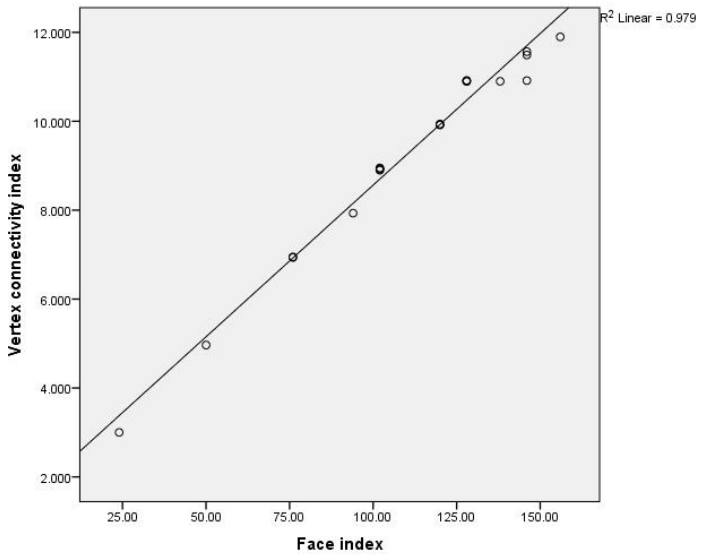

Figure 2. Plot of the face index versus vertex connectivity index for 21 benzenoid hydrocarbons.

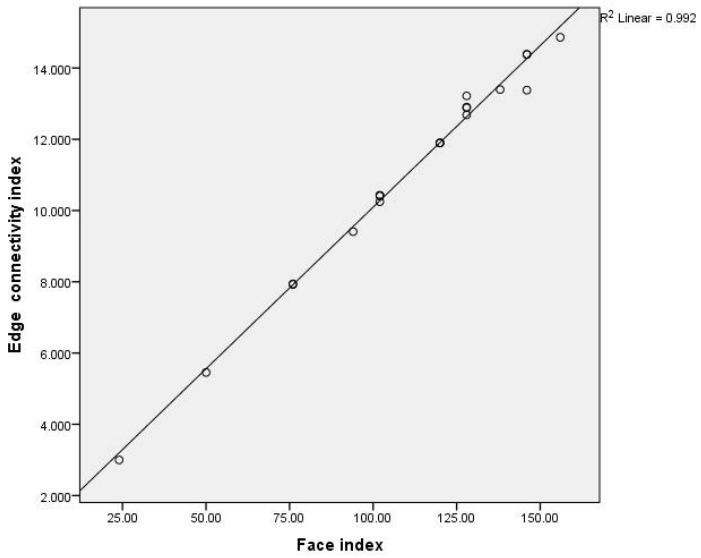

Figure 3. Plot of the face index versus edge connectivity index for 21 benzenoid hydrocarbons.

2.2. **Linear mathematical models of the face index (FI) for the π-electron energy (E).**

In this section, we constructed the linear and multiple linear relationships between the π-electron energies of considered benzenoid hydrocarbons and the face index. The linear and multiple linear correlation plots are shown in Figures 4 and 5.

The regression analysis gives the following relationships for π-electron energy (E):

Linear Correlation:

$$E = 0.074(\pm 0.003)FI + 5.491(\pm 0.766) \quad (5)$$

$n = 21; \quad r = 0.9933; \quad r^2(adjusted) = 0.9859; \quad s = 0.8129; \quad F = 1368.287$

Multivariate Correlation:

$$E = 0.002(\pm 0.016)FI + 1.123(\pm 0.308)\epsilon + 1.480(\pm 0.261)\chi + 0.095(\pm 0.294) \quad (6)$$

$n = 21; \quad r = 0.9996; \quad r^2(adjusted) = 0.9991; \quad s = 0.2015; \quad F = 7709.838$

The Equation (6) gives the best correlation with energy.

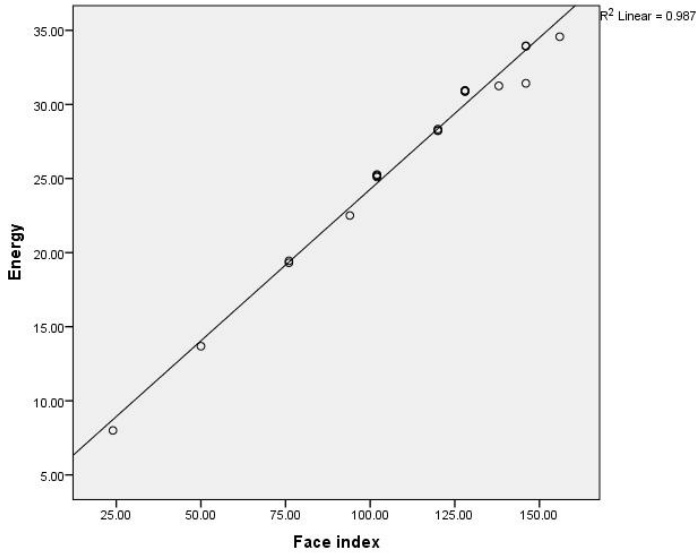

Figure 4. The linear correlation between the first face index and the energy for benzenoid hydrocarbons.

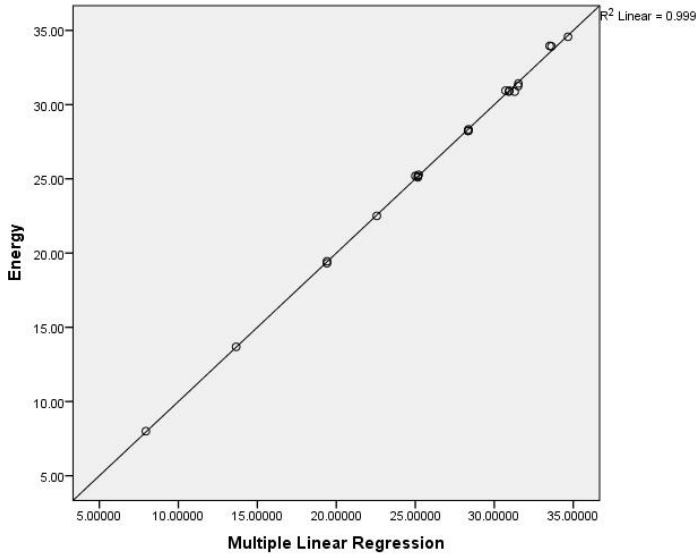

Figure 5. The multiple linear correlation for the energy of benzenoid hydrocarbons.

2.3. *Linear Mathematical Models of the Face Index (FI) for the Boiling Points (bp).*

We considered the linear and multiple linear relationships between the boiling points (bp) of benzenoid hydrocarbons and the face index. The corresponding plots of linear and multiple linear correlation is shown in Figures 6 and 7.

The regression analysis gives the following relationships for the boiling points (°C) of benzenoid hydrocarbons:

Linear Correlation:

$$bp = 3.822(\pm 0.136)FI + 30.881(\pm 15.878) \tag{7}$$

$n = 21$; $r = 0.9886$; $r^2(adjusted) = 0.9782$; $s = 19.8306$; $F = 784.290$

Multivariate Correlation:

$$bp = -0.008(\pm 0.001)FI^2 + 1.867(\pm 0.752)FI + 38.195(\pm 6.687)\epsilon - 68.627(\pm 11.542) \tag{8}$$

$n = 21$; $r = 0.9985$; $r^2(adjusted) = 0.9965$; $s = 7.5990$; $F = 1904.216$

Clearly, Equation (8) gives the best result.

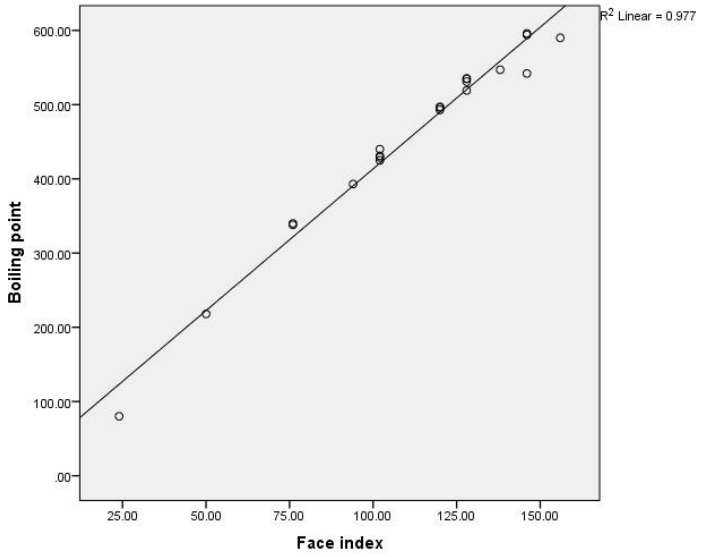

Figure 6. The linear correlation between the first face index and the boiling points for benzenoid hydrocarbons.

3. Computational Techniques for the Face Index

In this section, we computed the face index of some planar molecular graphs. Method of partitioning of face set based on the degrees of the faces in the graph is used to find the face index. f^{∞} will denote the unbounded face of the graph. The face index of graphene, triangular benzenoid and circumcoronene series of benzenoid is computed in the following subsections. There are several papers in which authors used different techniques to calculate the certain topological indices of some special molecular graphs [18–25].

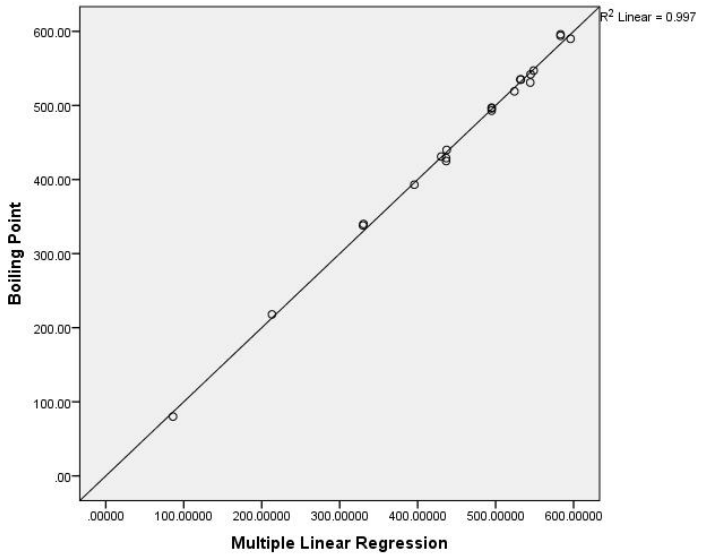

Figure 7. The multiple linear correlation for the boiling points for benzenoid hydrocarbons.

3.1. *Face Index of Graphene* $G(n, s)$

Graphene is a 2-dimensional planar sheet of carbon atoms which is densely packed in a honeycomb crystal lattice, and it is the major element of certain carbon allotropes including charcoal, fullerenes and graphite, see Figure 8. It is represented by $G(s, n)$ where n is number of rows and s is number of benzene rings in each row. In the review [26], authors gave a brief introduction on the recent advances in the study of graphene edges, including edge formation energy, edge reconstruction, method of graphene edge synthesis and the recent progress on metal-passivated graphene edges.

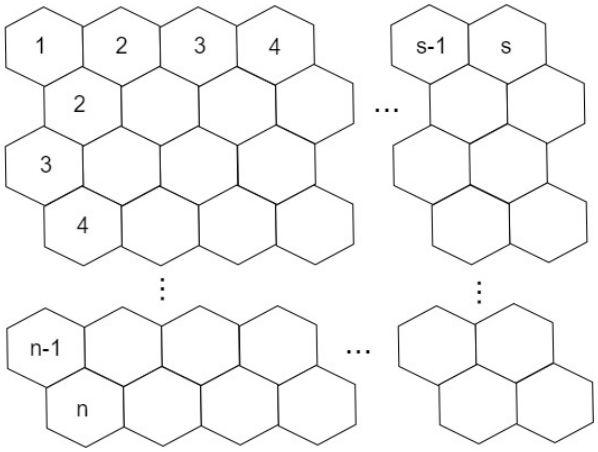

Figure 8. 2D graphene structure with 'n' rows and 's' benzene rings in each row.

Theorem 1. *Let $G(n, s)$ be a graphene structure, where 'n' is the number of rows and 's' is the benzene rings in each row and $n \geq 1$ and $s \geq 1$. The face index of $G(n, s)$ is given as*

$$FI(G(n,s)) = \begin{cases} 18ns + 8(n+s) - 10, & \text{if } n \neq 1, \\ 26s - 2, & \text{if } n = 1. \end{cases}$$

Proof. Consider the graphene structure, $G(n, s)$, with 'n' rows and each row has 's' benzene rings. Let f_j denotes a face having degree j, i.e., $\sum_{v \sim f} d(v) = j$ and $|f_j|$ denotes the number of faces with degree j. 2-dimensional structure of graphene (shown in Figure 8) contains five types of internal faces f_{14}, f_{15}, f_{16}, f_{17}, f_{18} and an external face. For $n = 1$ sum of degrees of vertices of external face is $10s + 2$, For

$n = 2$ sum of degrees of vertices of external face is $10s + 12$, for $n = 3$ sum of degrees of vertices of external face is $10s + 22$ and similarly when graphene structure has n rows then sum of degrees of vertices of external face is $10(n + s) - 8$. Table 2 shows the details of the number of faces with a degree in each row.

Case 1. From the definition of face index and Table 2 for $n \neq 1$, we have

$$\begin{aligned} FI(G(n,s)) &= \sum_{v\sim f\in F(G)} d(v) \\ &= \sum_{v\sim f_{15}\in F(G)} d(v) + \sum_{v\sim f_{16}\in F(G)} d(v) + \sum_{v\sim f_{17}\in F(G)} d(v) + \sum_{v\sim f_{18}\in F(G)} d(v) \\ &+ \sum_{v\sim f^{\infty}\in F(G)} d(v) \\ &= |f_{15}|(15) + |f_{16}|(16) + |f_{17}|(17) + |f_{18}|(18) + 10n + 10s - 8 \\ &= 2(15) + n(16) + 2(s-2)(17) + (n-2)(s-1)(18) + 10n + 10s - 8 \\ &= 18ns + 8(n+s) - 10 \end{aligned}$$

Table 2. Numbers of f_{14}, f_{15}, f_{16}, f_{17}, f_{18} in each row.

Rows	$\|f_{14}\|$	$\|f_{15}\|$	$\|f_{16}\|$	$\|f_{17}\|$	$\|f_{18}\|$
1	2	-	s-2	-	-
2	-	2	2	2(s-2)	-
3	-	2	3	2(s-2)	(s-1)
4	-	2	4	2(s-2)	2(s-1)
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
n	-	2	n	2(s-2)	(n-2)(s-1)

Case 2. When 2-dimensional structure of graphene has just 1 row then it has two types of internal faces $|f_{14}|$, $|f_{16}|$ and one external face whose sum of degrees is $10s + 2$.

For $n = 1$, $|f_{14}| = 2$ and $|f_{16}| = s - 2$ as shown in Figure 9, and the face index is

$$\begin{aligned} FI(G(n,s)) &= \sum_{v\sim f\in F(G)} d(v) \\ &= \sum_{v\sim f_{14}\in F(G)} d(v) + \sum_{v\sim f_{16}\in F(G)} d(v) \\ &= |f_{14}|(14) + |f_{16}|(16) + 10s + 2 \\ &= 2(14) + (s-2)(16) + 10s + 2 \\ &= 26s - 2 \end{aligned}$$

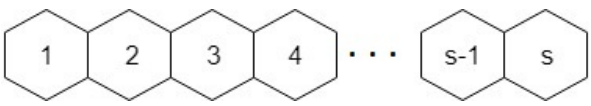

Figure 9. 2-dimensional structure of graphene with one row having s benzene rings.

This completes the proof.

□

3.2. *Face index of Triangular Benzenoid $T(n)$*

Now, we calculate the face index of a triangular benzenoid graph $T(n)$ where n represents the number of rows depicted in Figure 10. For synthesis and characterization of π-extended triangulene we refer [27].

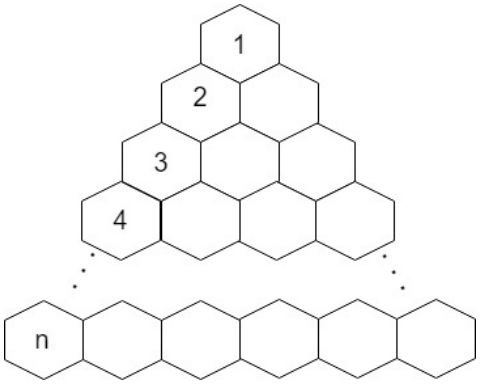

Figure 10. Molecular graph of triangular benzenoid.

Theorem 2. *Let $T(n)$ be a triangular benzenoid gragh where n represents the number of rows and $n \geq 1$. The face index of $T(n)$ is equal to*

$$FI(T(n)) = 9n^2 + 21n - 6.$$

Proof. Let f_j denotes the face having degree j, i.e., $\sum_{v \sim f_j} d(v) = j$. Triangular benzenoid graph contains four types of internal faces f_{14}, f_{15}, f_{17} and f_{18} and an external face. When triangular benzenoid has just 1 row then sum of degrees of vertices of external face is 12, when triangular benzenoid has 2 rows then sum of degrees of vertices of external face is 27, when triangular benzenoid has 3 rows then sum of degrees of vertices of external face is 42, and similarly when triangular benzenoid has n rows then sum of degrees of vertices of external face is $15n - 3$. The number of internal faces with the degree in each row is mentioned in Table 3.

From Table 3 and according to the definition of face index, we have

$$\begin{aligned} FI(T(n)) &= \sum_{v \sim f \in F(G)} d(v) \\ &= \sum_{v \sim f_{15} \in F(G)} d(v) + \sum_{v \sim f_{17} \in F(G)} d(v) + \sum_{v \sim f_{18} \in F(G)} d(v) + \sum_{v \sim f^{\infty} \in F(G)} d(v) \\ &= |f_{15}|(15) + |f_{17}|(17) + |f_{18}|(18) + 15n - 3 \\ &= 3(15) + 3(n-2)(17) + \frac{n^2 - 5n + 6}{2}(18) + 15n - 3 \\ &= 9n^2 + 21n - 6 \end{aligned}$$

Hence, this is our required result. □

Table 3. Number of f_{14}, f_{15}, f_{17}, f_{18} in each row.

Rows	$\|f_{12}\|$	$\|f_{15}\|$	$\|f_{17}\|$	$\|f_{18}\|$
1	1	-	-	-
2	-	3	-	-
3	-	3	3	-
4	-	3	6	1
5	-	3	9	3
6	-	3	12	6
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.
n	-	3	3(n-2)	$\frac{1}{2}(n-3)(n-2)$

3.3. *Face Index of Circumcoronene Series of Benzeniod H_k*

A circumcoronene homologous series of benzenoid H_k (k is the number of generations) consist of many copies of benzene C_6 on circumference. First three molecule of this series is shown in Figure 11 and the generalized circumcoronene series is shown in Figure 12.

Theorem 3. *Let H_k be a molecular graph of circumcoronene series of benzenoid, where $k \geq 1$. The face index of this graph is given by*

$$FI(H_k) = 54k^2 - 30k.$$

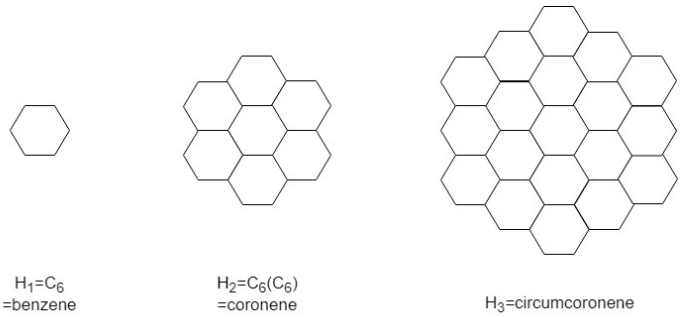

Figure 11. The first, second and third molecular graphs H_1, H_2 and H_3 from the circumcoronene series of benzenoid.

Proof. First we consider a circumcoronene series of benzeniod H_k for $k = 1, 2, 3$ presented in Figure 11 where k denotes the number of generations. Let f_j denotes a face having $\sum_{v \sim f_j} d(v) = j$ and $|f_j|$ denotes the number of faces having degree j. In H_1 both internal and external faces have degree 12. In H_2 there is two types of internal faces f_{18}, f_{16} and 1 external face f_{42}. In H_3 there are 3 types of internal faces f_{18}, f_{17} , f_{16} and 1 external face f_{72}. Figure 12 shown the circumcoronene series of benzenoid H_k for $k \geq 1$.

$$\begin{aligned}
FI(H_1) &= \sum_{w \sim f_{12} \in F(G)} d_w + \sum_{w \sim f^{\infty} \in F(G)} d_w \\
&= |f_{12}|(12) + 12 = 24 \\
FI(H_2) &= \sum_{w \sim f_{18} \in F(G)} d_w + \sum_{w \sim f_{16} \in F(G)} d_w + \sum_{w \sim f^{\infty} \in F(G)} d_w \\
&= |f_{18}|(18) + |f_{16}|(16) + |f_{42}|(42) \\
&= 1(18) + 6(16) + 42 \\
&= 156
\end{aligned}$$

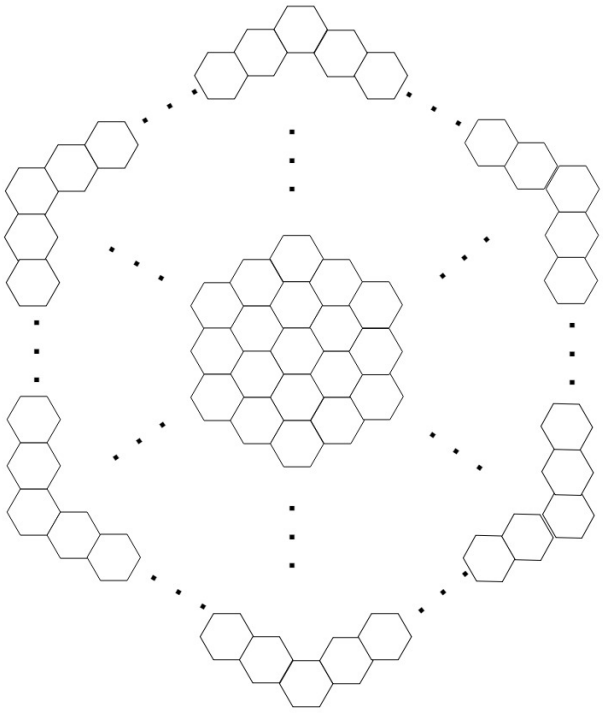

Figure 12. The circumcoronene series of benzenoid H_k for $k \geq 1$.

Now we calculate the face index FI for H_1, H_2 ... H_5.

$$\begin{aligned}
FI(H_3) &= \sum_{w\sim f_{18}\in F(G)} d_w + \sum_{w\sim f_{16}\in F(G)} d_w + \sum_{w\sim f_{17}\in F(G)} d_w + \sum_{w\sim f^{\infty}\in F(G)} d_w \\
&= |f_{18}|(18) + |f_{16}|(16) + |f_{17}|(17) + |f_{72}|(72) \\
&= 7(18) + 6(16) + 6(17) + 72 \\
&= 396 \\
FI(H_4) &= \sum_{w\sim f_{18}\in F(G)} d_w + \sum_{w\sim f_{16}\in F(G)} d_w + \sum_{w\sim f_{17}\in F(G)} d_w + \sum_{v\sim f^{\infty}\in F(G)} d_w \\
&= |f_{18}|(18) + |f_{16}|(16) + |f_{17}|(17) + |f_{102}|(102) \\
&= 19(18) + 6(16) + 12(17) + 102 \\
&= 744 \\
FI(H_5) &= \sum_{w\sim f_{18}\in F(G)} d_w + \sum_{w\sim f_{16}\in F(G)} d_w + \sum_{w\sim f_{17}\in F(G)} d_w + \sum_{w\sim f^{\infty}\in F(G)} d_w \\
&= |f_{18}|(18) + |f_{16}|(16) + |f_{17}|(17) + |f_{132}|(132) \\
&= 37(18) + 6(16) + 18(17) + 132 \\
&= 1200
\end{aligned}$$

From above information we get a recurrence relation;

$$FI(H_k) = FI(H_{k-1}) + 108k - 84$$

By solving this recurrence relation we get the following;

$$FI(H_k) = 54k^2 - 30k$$

This is our required result. □

From above result we can obtain the face index of circumcoronene with a window which is $FI(CW_k) = 54k^2 - 30k - 232$. Where CW_k is the molecular structure of circumcoronene with a window as shown in Figure 13.

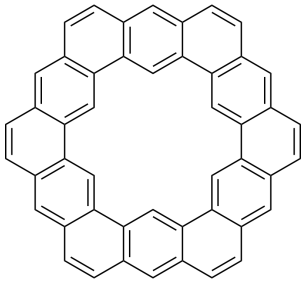

Figure 13. Molecular structure of circumcoronene with a window.

4. Conclusions

In this paper a new topological index, the face index (FI), is proposed which is based on the degrees of the vertices incident to the face of a graph. We showed that novel face index can be computed by the vertex and edge connectivity indices within the error of 6%–9% and 2%–6%, respectively. Which shows that the novel index is more closely correlate with edge connectivity index. The model Equation (6) involve the face index that improved the Nikolić Equation (1) and can predict the energy of the benzenoid within the error range of 0.6%–1.5%. Equation (8) improved the Nikolić Equation (2) and can compute the boiling point within the range of 1.2%–3.5%. The results warrant further studies on the properties and uses of the face index. In the later section, we considered 2-dimensional graphene, triangular benzenoid and circumcoronene series of benzenoid to study the topological property using their faces. The analytical closed formulas of FI for these molecular graphs are determined.

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