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# ON AUGMENTED POLYNOMIALS OF GRAPHENE

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***Abstract:*** *Graphene is a honeycomb lattice of carbon atoms. Graphene's hexagonal lattice can be regarded as two interleaving triangular lattices. A topological index for molecular graph is a numerical quantity which is invariant under automophisms of the graph. The topological indices can be obtained from the corresponding topological polynomials. In this paper augmented polynomial, augmented Revan polynomial, augmented reverse polynomial and Second hyper-Revan polynomial are investigated for graphene.*
***Keywords:*** *Augmented Revan polynomial, degree, graphene, molecular graph.*

## Introduction

On the basis of Wiener index, H.Hosoya introduced the wiener polynomial (Hosoya polynomial) in 1988 [1].The Hosoya polynomial is defined as:

$$H(G,x) = ½ \sum_{u\,v\, \in E\,(G)} x^{d(v,u)}$$

A topological index is a numerical parameter mathematically derived from the graph structure. The topological indices of graphene are studied by G. Sridhara [2-3]. The fourth and sixth Zagreb polynomials for nanostar dendrimers are studied by W.Gao [4]. The Schultz polynomials of molecular graphs are studied by [5-6]. Augmented Revan Index and its polynomial of certain families of benzenoid systems, Hyper-Revan Indices and their polynomials of silicate networks and Arithmetic–geometric reverse indices of certain networks are studied by V. R. Kulli [7-9]. Revan and hyper-Revan indices of octahedral and icosahedral networks are studied by Abdul Qudair Baig et al [10]. Hosoya Polynomial and Topological Indices of the Jahangir Graph $J_{7,\,m}$ are studied by A.R. Nizami et al [11]. Many topological polynomials appear in the molecular topology [12-15]. Our notations are standard and mainly taken from standard books of topology [16].



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In this paper augmented polynomial, augmented Revan polynomial, augmented reverse polynomial and Second hyper-Revan polynomial are investigated for graphene.

## 2. Materials and method

A molecular graph is constructed by representing each atom of a molecule by a vertex and bonds between atoms by edges. A molecular graph is a simple graph related to the structure of a chemical compound. Let G be a graph with vertex set V(G) and edge set E(G). Let deg(u) denote the degree of the vertex u in G. Graphene is an atomic scale honeycomb lattice made of carbon atoms. The structure of graphene G(m,n) with n rows and m columns is shown in figure (1).

For $n \geq 2$ and $m \geq 1$, the partition of edge set of G(m,n) are:

$E_1 = \{uv \mid d_u = d_v = 2\}$, $E_2 = \{uv \mid d_u = 2, d_v = 3\}$ and $E_3 = \{uv \mid d_u = d_v = 3\}$.

From structural analysis it is observed that $|E_1| = n+4$, $|E_2| = 4m+2n-4$ and $|E_3| = 3mn-2m-n-1$.

Let $\Delta(G)$, $\delta(G)$ denote the maximum and minimum degree of among vertices of G. The Revan vertex degree of a vertex v in G is defined as: $r_G(v) = \Delta(G) + \delta(G) - d_G(v)$, where $d_G(v)$ is the degree of a vertex v in G and the reverse index degree of a vertex v in G is defined as $c_G(v) = \Delta(G) - d_G(v) + 1$. The reverse edge connecting the vertices u and v will be denoted by uv.

## 3. Results and discussion

The method explained to compute the polynomial of first Zagreb index by Sulemani can used to compute the augmented polynomials [17].

The augmented polynomial is defined as:

$$AP(G,x) = \sum_{uv\in E(G)} x^{\left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3}.$$

The augmented Revan polynomial is defined as:

$$ARI(G,x) = \sum_{uv\in E(G)} x^{\left(\frac{r_G(u)\, r_G(v)}{r_G(u) + r_G(v) - 2}\right)^{3}3}.$$

The arithmetic-geometric reverse index of a graph is defined as:

$$AGC(G) = \sum_{uv\in E(G)} \frac{c_u c_v}{2\sqrt{c_u c_v}}.$$

In the same way the augmented reverse polynomial can be defined as:

$$ARC(G,x) = \sum_{uv\in E(G)} x^{\left(\frac{c_u c_v}{c_u + c_v - 2}\right)^3}.$$

And the Second hyper-Revan polynomial of graph G is defined as:

$$HR_2(G,x) = \sum_{uv\in E(G)} x^{(r_G(u)\ r_G(v))^2}.$$

The structure of graphene G(m,n) with n rows and m columns is shown in figure (1). The partition edge set of G(m,n) are: $E_1 = \{uv \mid d_u = d_v = 2\}$, $E_2 = \{uv \mid d_u = 2, d_v =$

3}and $E_3$= {uv| $d_u$ = $d_v$= 3}.From the structural analysis of graphene it is observed that $|E_1|$ = n+4, $|E_2|$ = 4m+2n-4 and $|E_3|$ = 3mn-2m-n-1 [18].

**3.1 Augmented Revan polynomial**

The augmented Revan polynomial is computed as:

The Revan vertex-degree of a vertex v in G is defined as: $r_G(v)$= $\Delta$(G)+$\delta$(G)-$d_G(v)$,where $d_G(v)$ is the degree of a vertex v in G and the reverse index degree of a vertex v in G is defined as:

$c_G(v)$= $\Delta$(G)-$d_G(v)$+1.The reverse edge connecting the vertices u and v will be denoted by uv. From structural analysis of graphene, $\Delta$(G) = 3, $\delta$(G) = 2 and $E_1$= {uv| $d_u$ = $d_v$= 2},
$E_2$= {uv| $d_u$ = 2, $d_v$ = 3}and $E_3$= {uv| $d_u$ = $d_v$= 3}.

1)$E_1$= {uv| $d_u$ = $d_v$= 2}, $r_G(v)$= $\Delta$(G)+$\delta$(G)-$d_G(v)$ , $r_G(u)$=3+2-2 = 3, $r_G(v)$= 3+2-2=3,

2)$E_2$= {uv| $d_u$ = 2, $d_v$ = 3}, $r_G(v)$= $\Delta$(G)+$\delta$(G)-$d_G(v)$, , $r_G(u)$=3+2-2 = 3, $r_G(v)$= 3+2-3=2,

3)$E_2$= {uv| $d_u$ = 3, $d_v$ = 3}, $r_G(v)$= $\Delta$(G)+$\delta$(G)-$d_G(v)$, $r_G(u)$=3+2-3 = 2, $r_G(v)$= 3+2-3=2,

$$ARI(G,x) = \sum_{uv\in E(G)} x^{\left(\frac{r_G(u) r_G(v)}{r_G(u)+r_G(v)-2}\right)^{3_3}}$$

$$= \sum_{uv\in E_1(G)} x^{\left(\frac{r_G(u) r_G(v)}{r_G(u)+ r_G(v)-2}\right)^{3_3}} + \sum_{uv\in E_2(G)} x^{\left(\frac{r_G(u) r_G(v)}{r_G(u)+r_G(v)-2}\right)^{3}} + \sum_{uv\in E_3(G)} x^{\left(\frac{r_G(u) r_G(v)}{r_G(u)+r_G(v)-2}\right)^{3}}.$$

$$= (n+4)\, x^{\left(\frac{3*3}{3+3-2}\right)^3} + (4m+2n-4)x^{\left(\frac{3*2}{3+2-2}\right)^3} + (3mn-2m-n-1)\, x^{\left(\frac{2*2}{2+2-2}\right)^{3_3}}.$$

$$= (n+4)x^{\left(\frac{9}{4}\right)^3} + (4m+2n-4)x^{\left(\frac{6}{3}\right)^3} + (3mn-2m-n-1)\, x^{\left(\frac{4}{2}\right)^{3_3}}.$$

**3.2 Augmented reverse polynomial**

Augmented reverse polynomial can be computed as:

$$ARC(G,x) = \sum_{uv\in E(G)} x^{\left(\frac{c_u c_v}{c_u+c_v-2}\right)^3}$$

1)$E_1$= {uv| $d_u$ = $d_v$= 2}, $c_G(v)$= $\Delta$(G)-$d_G(v)$+1, $c_G(v)$= 3-2+1=2, $c_G(u)$= 3-2+1=2.

2)$E_2$= {uv| $d_u$ = 2, $d_v$ = 3}, $c_G(v)$= $\Delta$(G)-$d_G(v)$+1, $c_G(v)$= 3-3+1=1, $c_G(u)$= 3-2+1=2.

3)$E_2$= {uv| $d_u$ = 3, $d_v$ = 3}, $c_G(v)$= $\Delta$(G)-$d_G(v)$+1, $c_G(v)$= 3-3+1=1, $c_G(u)$= 3-3+1=1.

ARC(G,x) = $\sum_{uv\in E(G)} x^{\left(\frac{c_u c_v}{c_u+c_v-2}\right)^3}$

$= \sum_{22\in E_1(G)} x^{\left(\frac{c_u c_v}{c_u+c_v-2}\right)^3} + \sum_{23 E_2(G)} x^{\left(\frac{c_u c_v}{c_u+c_v-2}\right)^3} + \sum_{33\in E_3(G)} x^{\left(\frac{c_u c_v}{c_u+c_v-2}\right)^3}$.

$= (n+4)x^{\left(\frac{2*2}{2+2-2}\right)^3} + (4m+2n-4)x^{\left(\frac{2*1}{2+1-2}\right)^3} + (3mn-2m-n-1)x^{\left(\frac{1*1}{1+1-2}\right)^3}$

.

$= (n+4)x^2 + (4m+2n-4)x^2 + (3mn-2m-n-1)$.

The augmented polynomial and second hyper-Revan polynomial are computed from degree- vertices and Revan vertices and represented in table (1).

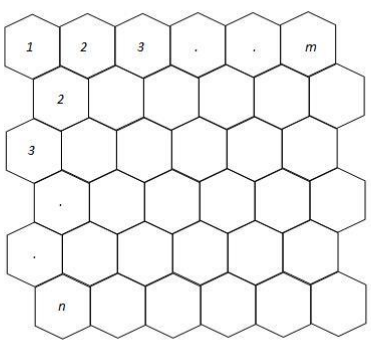


Fig.1. Dimensional graph of graphene sheet G(m,n).

Table 1.The vertices degree, Revan vertices and reverse-vertices based polynomials of graphene.

| Polynomials | Topological polynomials |
|---|---|
| Augmented polynomial | $(n+4)\ x^2 + (4m+2n-4)x^2+(3mn-2m-n-1)\ x^{(9/4)}$ |
| Augmented Revan polynomial | $(n+4)x^{\left(\frac{9}{4}\right)^3} + (4m+2n-4)x^8 + (3mn-2m-n-1)\ x^8$ |
| Augmented reverse polynomial | $(3mn-2m-n-1) + (n+4)x^2 + (4m+2n-4)x^2$ |
| Second hyper-Revan polynomial | $(3mn\text{-}2m\text{-}n\text{-}1)\ x^{16} + (4m+2n\text{-}4)\ x^{36} + (n+4)\ x^{81}$ |

**4. Conclusion**

The vertices degree-based topological polynomials and topological indices play vital role in QSPR/QSAR. The topological polynomials: augmented polynomial augmented Revan polynomial, augmented reverse polynomial and Second hyper-Revan polynomial are investigated for graphene.

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