

COMPUTATION OF k^{th} ROOT TOPOLOGICAL INDEX OF GRAPHENE

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Abstract: The k^{th} Root Index is a newly defined degree based topological index. It is a generalized index which attempts to study a family of indices. In this paper the computation of k^{th} Root index of Graphene, an allotrope of carbon, is carried out without the aid of computer.

Keywords and Phrases: Molecular graph, k^{th} Root Index, Benzene ring and Graphene.

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1. Introduction

Graphene is an atomic scale honeycomb lattice made of carbon atoms. Among the known materials, Graphene is found to be the strongest material that could even withstand a speeding bullet. In fact Graphene is hundred times stronger than the strongest steel of same thickness. It is one million times thinner than a human hair and hence a single Graphene sheet is almost transparent. Graphene conducts heat and electricity efficiently. It absorbs light of all visible wave lengths. In 1962 Graphene was first observed in electron microscope but was studied only while supported on metal surfaces. It was in the year 2004, Andre Geim and Konstantin Novoselov isolated and characterized Graphene [1].

In the recent years, several topological indices of Graphene have been computed and studied. Here is a brief survey of the topological indices of Graphene with ‘t’

rows of benzene rings and 's' benzene rings in each row.

The First Zagreb index [3] of Graphene is given by

$$M_1(G) = \begin{cases} 26s - 2 & \text{if } t = 1 \\ 18ts + 8t + 8s - 10 & \text{if } t \neq 1 \end{cases} \quad (1)$$

The Second Zagreb index [3] of Graphene is given by

$$M_2(G) = \begin{cases} 33s - 9 & \text{if } t = 1 \\ 27ts + 7t + 6s - 17 & \text{if } t \neq 1 \end{cases} \quad (2)$$

The First Neighbourhood Zagreb index [6] of Graphene is given by

$$MN_1(G) = \begin{cases} 162st + 8s + 16t - 106 & \text{if } t > 1, s > 1 \\ 170s - 78 & \text{if } t = 1, s > 1 \\ 178t - 94 & \text{if } t > 1, s = 1 \\ 96 & \text{if } t = 1, s = 1 \end{cases} \quad (3)$$

The Second Neighbourhood Zagreb index [6] of Graphene is given by

$$MN_2(G) = \begin{cases} 243st - 30s - 11t - 147 & \text{if } t > 1, s > 1 \\ 217s - 133 & \text{if } t = 1, s > 1 \\ 233t - 166 & \text{if } t > 1, s = 1 \\ 96 & \text{if } t = 1, s = 1 \end{cases} \quad (4)$$

The First Multiple Zagreb index [3] of Graphene is given by

$$PM_1(G) = \begin{cases} (1.092267) \times 5^{4s} \times 6^s & \text{if } t = 1 \\ 2^{2t+8} \times 5^{4s+2t-4} \times 6^{3ts-2s-t-1} & \text{if } t \neq 1 \end{cases} \quad (5)$$

The Second Multiple Zagreb index [3] of Graphene is given by

$$PM_2(G) = \begin{cases} (0.351166) \times 6^{4s} \times 9^s & \text{if } t = 1 \\ 2^{2t+8} \times 6^{4s+2t-4} \times 3^{6ts-2t-4s-2} & \text{if } t \neq 1 \end{cases} \quad (6)$$

The Augmented Zagreb index [3] of Graphene is given by

$$AZI(G) = \begin{cases} (43.390625)s + 4.609375 & \text{if } t = 1 \\ (12.609375)t + (9.21875)s + (34.171875)ts - (11.390625) & \text{if } t \neq 1 \end{cases} \quad (7)$$

The Harmonic index [3] of Graphene is given by

$$H(G) = \begin{cases} (1.93333)s + 1.0667 & \text{if } t = 1 \\ (0.9667)t + (0.9334)s + ts + (0.0667) & \text{if } t \neq 1 \end{cases} \quad (8)$$

The Hyper Zagreb index [3] of Graphene is given by

$$HM(G) = \begin{cases} 136s - 40 & \text{if } t = 1 \\ 108ts + 30t + 28s - 72 & \text{if } t \neq 1 \end{cases} \quad (9)$$

The Atom-Bond Connectivity index [10] of Graphene is given by

$$ABC(G) = \begin{cases} \frac{(12+2\sqrt{2})s+(6-2\sqrt{2})}{(3\sqrt{2})} & \text{if } t = 1 \\ \frac{(12-4\sqrt{2})s+(9-2\sqrt{2})t+6\sqrt{2}ts-2\sqrt{2}}{(3\sqrt{2})} & \text{if } t \neq 1 \end{cases} \quad (10)$$

The Fourth Atom-Bond Connectivity index [10] of Graphene is given by

$$ABC_4(G) = \begin{cases} \frac{3\sqrt{6}}{2} & \text{if } t = 1, s = 1 \\ 2.541937s + 1.140265 & \text{if } t = 1, s > 1 \\ (1.217295)t + (1.212097)s + (1.333333)ts - 0.088070 & \text{if } t \neq 1 \end{cases} \quad (11)$$

The Randic Connectivity index [10] of Graphene is given by

$$R(G) = \begin{cases} \frac{(1+2\sqrt{6})s+(8-2\sqrt{6})}{3} & \text{if } t = 1 \\ \frac{(1+2\sqrt{6})t-4(1-\sqrt{6})s+6ts+10-4\sqrt{6}}{6} & \text{if } t \neq 1 \end{cases} \quad (12)$$

The Sum Connectivity index [10] of Graphene is given by

$$SCI(G) = \begin{cases} \frac{(\sqrt{5}+4\sqrt{6})s+(3\sqrt{30}-\sqrt{5}-4\sqrt{6})}{\sqrt{30}} & \text{if } t = 1 \\ \frac{(\sqrt{30}+4\sqrt{6}-2\sqrt{5})t+(8\sqrt{6}-4\sqrt{5})s+6\sqrt{5}ts+4\sqrt{30}-8\sqrt{6}-2\sqrt{5}}{2\sqrt{30}} & \text{if } t \neq 1 \end{cases} \quad (13)$$

The Geometric-Arithmetic index [10] of Graphene is given by

$$GA(G) = \begin{cases} \frac{(5+8\sqrt{6})s+(25-8\sqrt{6})}{5} & \text{if } t = 1 \\ \frac{(8\sqrt{6}-10)s+4\sqrt{6}t+15ts+15-8\sqrt{6}}{5} & \text{if } t \neq 1 \end{cases} \quad (14)$$

The Fifth geometric-arithmetic index [10] of Graphene is given by

$$GA_5(G) = \begin{cases} 6, & \text{if } t = 1, s = 1 \\ (4.988148)s + 0.942989, & \text{if } t = 1, s > 1 \\ (1.942554)t + (1.972462)s + 3ts - 0.998066 & \text{if } t \neq 1 \end{cases} \quad (15)$$

The First Arithmetic-Geometric index [9] of Graphene is given by

$$GA_1(G) = \begin{cases} \frac{(2\sqrt{6}+20)s+6\sqrt{6}-10}{2\sqrt{6}} & \text{if } t = 1 \\ \frac{(6\sqrt{6})st+(20-4\sqrt{6})s+10t-(20-6\sqrt{6})}{2\sqrt{6}} & \text{if } t \neq 1 \end{cases} \quad (16)$$

The SK index [9] of Graphene is given by

$$SK(G) = \begin{cases} \frac{26s-2}{2} & \text{if } t = 1 \\ \frac{18st+8s+8t-10}{2} & \text{if } t \neq 1 \end{cases} \quad (17)$$

The SK_1 index [9] of Graphene is given by

$$SK_1(G) = \begin{cases} \frac{33s-10}{2} & \text{if } t = 1 \\ \frac{27st+6s+7t-17}{2} & \text{if } t \neq 1 \end{cases} \quad (18)$$

The SK_2 index [9] of Graphene is given by

$$SK_2(G) = \begin{cases} \frac{136s-42}{4} & \text{if } t = 1 \\ \frac{108st+28s+30t-72}{4} & \text{if } t \neq 1 \end{cases} \quad (19)$$

For more results on Graphene one may refer [1, 2, 7, 11, 13]

1.1. Definition

The k^{th} Root index is an attempt to generalize a class of topological indices. It is a degree based topological index with a variable $k=1, 2, 3, \dots$. If $G = (V, E)$ is a molecular graph and $d(u)$ is the degree of the vertex u , then k^{th} Root index of G denoted by $R_k(G)$ is defined as

$$R_k(G) = \sum_{uv \in E} (d(u)^k + d(v)^k)^{\frac{1}{k}}$$

When $k=1$ the k^{th} Root index is the First Zagreb index.

$$R_1(G) = \sum_{uv \in E} (d(u) + d(v))$$

When $k=2$,

$$R_2(G) = \sum_{uv \in E} (d(u)^2 + d(v)^2)^{\frac{1}{2}}$$

When $k=3$,

$$R_3(G) = \sum_{uv \in E} (d(u)^3 + d(v)^3)^{\frac{1}{3}}$$

1.2. Significance of k^{th} Root Index in QSPR Studies

Topological indices are a convenient means of translating chemical constitution into numerical values which can be used to predict the physiochemical properties in quantitative structure property/activity relationship (QSPR/QSAR) studies. In the last few years, the number of proposed molecular descriptors is rapidly growing due to the chemical significance of these indices.

A brief study on QSPR analysis of k^{th} Root index on the physiochemical properties of octane isomers reveals that there exists good correlation between the k^{th} Root index and the physiochemical properties of octane isomers. The k^{th} Root index highly correlates with acentric factor of octane isomers, the highest correlation coefficient being $r = -0.973$ for the 1st Root index. The 1st Root index is also an useful tool to predict the entropy with correlation coefficient value $r = -0.954$. The 6th and the higher Root indices show good correlation with heat of formation with correlation coefficient value $r = 0.81$. From practical point of view, topological indices for which the absolute value of correlation coefficient is less than 0.8 can be considered as inefficient. The QSPR study of the k^{th} Root index with physiochemical properties of octane isomers helps us to determine the value of k for which the k^{th} Root index is most efficient.

2. Main Results

Consider a Graphene structure with “ $t > 1$ ” rows and “ s ” benzene rings in each row as shown in (fig.1). Let E_{ij} denote the number of edges connecting the vertices of degree i and j . The two dimensional structure of Graphene with $t > 1$ contains $E_{22} + E_{23} + E_{33}$ number of edges. The values of E_{22} , E_{23} and E_{33} in each row are mentioned in Table.1.

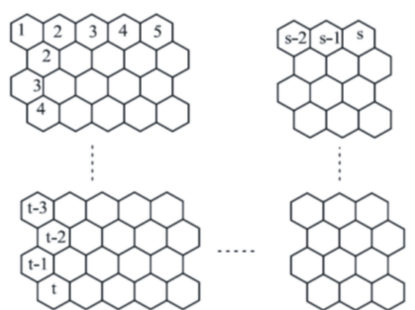
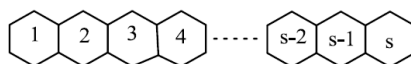


Figure 1: 2D Structure of Graphene for $t > 1$

Figure 2: 2D Structure of Graphene for $t = 1$

Row	E_{22}	E_{23}	E_{33}
1	3	$2s$	$3s-2$
2	1	2	$3s-1$
3	1	2	$3s-1$
4	1	2	$3s-1$
-	-	-	-
-	-	-	-
-	-	-	-
-	-	-	-
t	3	$3s$	$s-1$
Total	$t+4$	$4s+2t-4$	$3ts-2s-t-1$

Table 1: Values of E_{ij} in 2D Structure of Graphene for $t > 1$

Row	E_{22}	E_{23}	E_{33}
1	6	$4s-4$	$s-1$

Table 2: Values of E_{ij} in 2D Structure of Graphene for $t=1$

The two dimensional structure of Graphene having “ $t = 1$ ” row with “ s ” benzene rings, as shown in (fig.2), contains $E_{22} + E_{23} + E_{33}$ number of edges. The values of E_{22} , E_{23} and E_{33} in the row are mentioned in Table.2.

Theorem 2.1. *The k^{th} Root index R_k of Graphene with “ t ” rows of benzene rings and “ s ” benzene rings in each row is given by*

$$R_k(G) = \begin{cases} (12)2^{\frac{1}{k}} + (4s-4)(2^k + 3^k)^{\frac{1}{k}} + 3(s-1)2^{\frac{1}{k}} & \text{if } t = 1 \\ 2(t+4)2^{\frac{1}{k}} + (4s+2t-4)(2^k + 3^k)^{\frac{1}{k}} + 3(3ts-2s-t-1)2^{\frac{1}{k}} & \text{if } t \neq 1 \end{cases} \quad (20)$$

Proof. Consider a Graphene with “ t ” rows and “ s ” benzene rings in each row.

Case 1: When $t \neq 1$

The two dimensional structure of Graphene (Fig.1) contains $E_{22} + E_{23} + E_{33}$

edges where $E_{22} = (t+4)$, $E_{23} = (4s+2t-4)$ and $E_{33} = (3ts-2s-t-1)$ as mentioned in Table.1. Therefore the k^{th} Root index R_k of Graphene is given by

$$\begin{aligned}
 R_k(G) &= \sum_{uv \in E} (d(u)^k + d(v)^k)^{\frac{1}{k}} \\
 &= E_{22}(2^k + 2^k)^{\frac{1}{k}} + E_{23}(2^k + 3^k)^{\frac{1}{k}} + E_{33}(3^k + 3^k)^{\frac{1}{k}} \\
 &= (t+4)(2^k + 2^k)^{\frac{1}{k}} + (4s+2t-4)(2^k + 3^k)^{\frac{1}{k}} + (3ts-2s-t-1)(3^k + 3^k)^{\frac{1}{k}} \\
 &= 2(t+4)2^{\frac{1}{k}} + (4s+2t-4)(2^k + 3^k)^{\frac{1}{k}} + 3(3ts-2s-t-1)2^{\frac{1}{k}}
 \end{aligned}$$

Case 2: When $t = 1$

The two dimensional structure of Graphene (Fig.2) contains $E_{22} + E_{23} + E_{33}$ edges where $E_{22} = 6$, $E_{23} = (4s-4)$ and $E_{33} = (s-1)$ as mentioned in Table.2. Therefore the k^{th} Root index R_k of Graphene is given by

$$\begin{aligned}
 R_k(G) &= \sum_{uv \in E} (d(u)^k + d(v)^k)^{\frac{1}{k}} \\
 &= E_{22}(2^k + 2^k)^{\frac{1}{k}} + E_{23}(2^k + 3^k)^{\frac{1}{k}} + E_{33}(3^k + 3^k)^{\frac{1}{k}} \\
 &= 6(2^k + 2^k)^{\frac{1}{k}} + (4s-4)(2^k + 3^k)^{\frac{1}{k}} + (s-1)(3^k + 3^k)^{\frac{1}{k}} \\
 &= (12)2^{\frac{1}{k}} + (4s-4)(2^k + 3^k)^{\frac{1}{k}} + 3(s-1)2^{\frac{1}{k}}
 \end{aligned}$$

Corollary 2.2. *The First Root index R_1 of Graphene with “t” rows of benzene rings and “s” benzene rings in each row is given by*

$$R_1(G) = \begin{cases} 26s - 2 & \text{if } t = 1 \\ 18ts + 8t + 8s - 10 & \text{if } t \neq 1 \end{cases} \quad (21)$$

Proof. Consider a Graphene with “t” rows and “s” benzene rings in each row.

Case 1: When $t \neq 1$

The two dimensional structure of Graphene (Fig.1) contains $E_{22} + E_{23} + E_{33}$ edges where $E_{22} = (t+4)$, $E_{23} = (4s+2t-4)$ and $E_{33} = (3ts-2s-t-1)$ as mentioned in Table.1. Therefore the First Root index R_1 of Graphene is given by

$$\begin{aligned}
 R_1(G) &= \sum_{uv \in E} (d(u) + d(v)) \\
 &= E_{22}(2 + 2) + E_{23}(2 + 3) + E_{33}(3 + 3) \\
 &= (t+4)(2 + 2) + (4s+2t-4)(2 + 3) + (3ts-2s-t-1)(3 + 3) \\
 &= (t+4)4 + (4s+2t-4)5 + (3ts-2s-t-1)6 \\
 &= (4t + 16) + (20s + 10t - 20) + (18ts - 12s - 6t - 6) \\
 &= 18ts + 8t + 8s - 10
 \end{aligned}$$

Case 2: When $t = 1$

The two dimensional structure of Graphene (Fig.2) contains $E_{22} + E_{23} + E_{33}$ edges where $E_{22} = 6$, $E_{23} = (4s-4)$ and $E_{33} = (s-1)$ as mentioned in Table.2. Therefore the First Root index R_1 of Graphene is given by

$$\begin{aligned}
 R_1(G) &= \sum_{uv \in E} (d(u) + d(v)) \\
 &= E_{22}(2 + 2) + E_{23}(2 + 3) + E_{33}(3 + 3) \\
 &= 6(2 + 2) + (4s - 4)(2 + 3) + (s - 1)(3 + 3) \\
 &= 24 + 5(4s - 4) + 6(s - 1) \\
 &= 24 + 20s - 20 + 6s - 6 \\
 &= 26s - 2
 \end{aligned}$$

Corollary 2.3. *The Second Root index R_2 of Graphene with “t” rows of benzene rings and “s” benzene rings in each row is given by*

$$R_2(G) = \begin{cases} (4\sqrt{13} + 3\sqrt{2})s - 4\sqrt{13} + 9\sqrt{2} & \text{if } t = 1 \\ 9\sqrt{2}ts + (2\sqrt{13} - \sqrt{2})t + (4\sqrt{13} - 6\sqrt{2})s + 5\sqrt{2} - 4\sqrt{13} & \text{if } t \neq 1 \end{cases} \quad (22)$$

Proof. Consider a Graphene with “t” rows and “s” benzene rings in each row.

Case 1: When $t \neq 1$

The two dimensional structure of Graphene (Fig.1) contains $E_{22} + E_{23} + E_{33}$ edges where $E_{22} = (t+4)$, $E_{23} = (4s+2t-4)$ and $E_{33} = (3ts-2s-t-1)$ as mentioned in Table.1. Therefore the Second Root index R_2 of Graphene is given by

$$\begin{aligned}
 R_2(G) &= \sum_{uv \in E} (d(u)^2 + d(v)^2)^{\frac{1}{2}} \\
 &= E_{22}(2^2 + 2^2)^{\frac{1}{2}} + E_{23}(2^2 + 3^2)^{\frac{1}{2}} + E_{33}(3^2 + 3^2)^{\frac{1}{2}} \\
 &= (t + 4)(2^2 + 2^2)^{\frac{1}{2}} + (4s + 2t - 4)(2^2 + 3^2)^{\frac{1}{2}} + (3ts - 2s - t - 1)(3^2 + 3^2)^{\frac{1}{2}} \\
 &= 2\sqrt{2}(t + 4) + \sqrt{13}(4s + 2t - 4) + 3\sqrt{2}(3ts - 2s - t - 1) \\
 &= 2\sqrt{2}t + 8\sqrt{2} + 4\sqrt{13}s + 2\sqrt{13}t - 4\sqrt{13} + 9\sqrt{2}ts - 6\sqrt{2}s - 3\sqrt{2}t - 3\sqrt{2} \\
 &= 9\sqrt{2}ts + (2\sqrt{13} - \sqrt{2})t + (4\sqrt{13} - 6\sqrt{2})s + 5\sqrt{2} - 4\sqrt{13}
 \end{aligned}$$

Case 2: When $t = 1$

The two dimensional structure of Graphene (Fig.2) contains $E_{22} + E_{23} + E_{33}$ edges where $E_{22} = 6$, $E_{23} = (4s-4)$ and $E_{33} = (s-1)$ as mentioned in Table.2. Therefore

the First Root index R_1 of Graphene is given by

$$\begin{aligned}
 R_2(G) &= \sum_{uv \in E} (d(u)^2 + d(v)^2)^{\frac{1}{2}} \\
 &= E_{22}(2^2 + 2^2)^{\frac{1}{2}} + E_{23}(2^2 + 3^2)^{\frac{1}{2}} + E_{33}(3^2 + 3^2)^{\frac{1}{2}} \\
 &= 6(2^2 + 2^2)^{\frac{1}{2}} + (4s - 4)(2^2 + 3^2)^{\frac{1}{2}} + (s - 1)(3^2 + 3^2)^{\frac{1}{2}} \\
 &= 12\sqrt{2} + \sqrt{13}(4s - 4) + 3\sqrt{2}(s - 1) \\
 &= 12\sqrt{2} + 4\sqrt{13}s - 4\sqrt{13} + 3\sqrt{2}s - 3\sqrt{2} \\
 &= (4\sqrt{13} + 3\sqrt{2})s - 4\sqrt{13} + 9\sqrt{2}
 \end{aligned}$$

Illustration 1. Consider a Graphene structure with 5 rows and 6 Benzene rings in each row. Then the First Root index of Graphene is given by

$$\begin{aligned}
 R_k(G) &= 2(t + 4)2^{\frac{1}{k}} + (4s + 2t - 4)(2^k + 3^k)^{\frac{1}{k}} + 3(3ts - 2s - t - 1)2^{\frac{1}{k}} \\
 R_1(G) &= 2(t + 4)2 + (4s + 2t - 4)(5) + 3(3ts - 2s - t - 1)2 \\
 &= 2(5 + 4)2 + (4(6) + 2(5) - 4)(5) + 3(3(5)(6) - 2(6) - 5 - 1)2 \\
 &= 4(9) + 5(30) + 6(72) \\
 &= 36 + 150 + 432 \\
 &= 618
 \end{aligned}$$

Illustration 2. Consider a Graphene structure with 5 rows and 5 Benzene rings in each row. Then the Second Root index of Graphene is given by

$$\begin{aligned}
 R_k(G) &= 2(t + 4)2^{\frac{1}{k}} + (4s + 2t - 4)(2^k + 3^k)^{\frac{1}{k}} + 3(3ts - 2s - t - 1)2^{\frac{1}{k}} \\
 R_2(G) &= 2(t + 4)2^{\frac{1}{2}} + (4s + 2t - 4)(2^2 + 3^2)^{\frac{1}{2}} + 3(3ts - 2s - t - 1)2^{\frac{1}{2}} \\
 &= 2(5 + 4)2^{\frac{1}{2}} + (4(5) + 2(5) - 4)(2^2 + 3^2)^{\frac{1}{2}} + 3(3(5)(5) - 2(5) - (5) - 1)2^{\frac{1}{2}} \\
 &= 18\sqrt{2} + 26\sqrt{13} + 177\sqrt{2} \\
 &= 195\sqrt{2} + 26\sqrt{13}
 \end{aligned}$$

3. Conclusion

A generalized formula for the k^{th} Root index of Graphene is derived for k with $k=1$ and $k=2$. In the generalized formula, k can also be replaced by any other desired values.

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