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On Some Topological Indices of the Starphene Graph

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Abstract

The quantitative specifications which are used to narrate the atomic topology of graphs are usually entitled as topological indices in theoretical Chemistry. The features of physical and chemical properties like melting point, entropy, boiling point, energy generation and enthalpy of vaporisation of chemical compounds can be estimated by means of these topological indices. The field of Graph theory has a remarkable application of linking certain graphs with many types of topological indices. In this paper, we calculate a new set of topological indices based on M-polynomial of starphene graph. Further, the graphical representation of the M-polynomial and its corresponding topological indices are obtained.

Keywords: Starphene graph, reduced reciprocal randic, SK index, General sum-connectivity index, SK_1 index, First Zagrab index, Forgotten index, SK_2 index, Arithmetic geometric index, SCI_γ index.

1. INTRODUCTION

Chemical graph theory is a field which belongs to both mathematics and chemistry where it utilizes graph theory to model of chemical compound. The topological index is an invariable which illustrates the topology of molecular structure and converts it to a real number which estimates certain obvious properties like viscosity, freezing point, infrared spectrum, boiling point, melting point, density and electronic parameters which are termed as physico-chemical characteristics [1-3].

Starphene is a graph which are surrounded by three similar acene arms centered in a single benzene ring [4]. To use in high-quality octane gasoline and manufacture polymers the derivatives of benzene are produced in large scale, also to go through the trimerization of Nicatalyzed ortho-bromotetracene and orthodibromopentacene are used for the formation of starphene. The red starphene is a structure with one centre ring distributed with orange star which is made of total three hexacenes. In 1968, Mullen and Clar composed the largest unsubstituted derivatives of starphene called Decastarphene-(3,3,3) [5]. It is difficult to show that this is a complete aromatic coincidence which does not exist in substituent of starphene. It is a very interesting compound because of its physicochemical properties. They take over most of the properties from arenes, which are widely used in the study of optics and electronic devices for their interesting characteristics. In [6], Holec.et al mention its instability to manufacture larger starphene.

Graph theory as various branches, in which Chemical graph theory plays a very important role where a chemical compound is represented by simple graph called molecular graph in which atoms are vertices and atomic bounds are edges of a molecule. In recent times we see another emerging field that is Cheminformatics, in which the relationship between structural property and quantitative structural activities are studied to predict biological activities of the structure.

In 1947 Weiner first introduced topological indices, it is a process in which the data related to chemical compounds is converted to some numerical values. These topological indices have many applications in the field of chemistry and graph theory, precisely in QSAR and QSPR studies. Topological indices are divided majorly in to eccentricity-based, degree-based, distance-based, spectrum-based, and so on. The degree-based topological indices are obtained by degrees of the vertices of the molecular graph of the corresponding chemical structures.

Graph polynomials encode the information of a graph and build up various algebraic methods to find out the hidden information of a graph. Several important graph algebraic polynomials have been introduced. Some of them are Hosoye polynomial [7], Matching polynomial [8], M-polynomial [9], and so on.

To compute the numerical values of the topological indices, there are multiple methods such as by using integrals or derivatives or by graph polynomials. We see similar type of works done in [10-12]. In [13], Gutman and Furtula established a reduced reciprocal index in 2015.The reduced reciprocal randic index is defined as

$$RRR(G) = \sqrt{(d_s - 1)(d_l - 1)}\,.$$

In [12], Deutsch and Klawzar used the arithmetic geometric index which is defined as

$$AG_1(G) = \sum_{sl \in E(G)} \frac{d_s + d_l}{2\sqrt{d_s d_l}}$$

In 2016, Shegehalli and Kanabur used SK, SK_1, SK_2 indices which are defined as follows [14].

$$SK(G) = \sum_{sl \in E(G)} \frac{d_s + d_l}{2}$$

$$SK_1(G) = \sum_{sl \in E(G)} \frac{d_s d_l}{2}$$

$$SK_2(G) = \sum\nolimits_{sl \in E(G)} \left(\frac{d_s d_l}{2}\right)^2$$

First Zagreb index which was defined as follows and was introduced in 2014 [15].

$$EM_1(G) = \sum_{sl \in E(G)} (d_{sl})^2$$

In [16], Du.et.al introduced sum connectivity index which is defined as

$$SCI(G) = \sum_{sl \in E(G)} \frac{1}{\sqrt{d_s + d_l}}$$

Du.et.al also introduced SCI_γ index which is defined as [16]

$$SCI_\gamma(G) = \sum_{sl \in E(G)} (d_s + d_l)^\gamma$$

In 2015, Gutman and Furtula introduced forgotten index which is defined as

$$F(G) = \sum_{sl \in E(G)} (d_s^2 + d_l^2)$$

The M-polynomial is introduced in 2015 [12] defined as

$$M_f(G, x, y) = \sum_{\mu \le s \le l \le \xi} f_{sl}\,(G) x^s y^l$$

Where $\mu = \max\{\, d_i : i \in V(G)\}$, $\xi = \min\{d_i : i \in V(G)\}$ and $f_{sl}(G)$ is the set of all edges such that $\{d_g, d_h\} = \{s, l\}$.

Lately, many researchers have examined the M-polynomials of several graph structures. In [17], the M-polynomial of the two-dimensional three-layered single-walled titania nanotube lattice was studied by Raheem *et al*., The topological indices through M-polynomial of book graphs were found by Khalaf *et al*., [18]. Some other works related to M-polynomials was also found in [19, 20]. In this paper, we compute the topological indices of starphene graph with the help of M-polynomial.

In Table 1, degree-dependent topological indices via M-polynomial are provided

Table 1:

Topological Index	**Resulting from $\mathbf{M_f(G, x, y)}$**
1. Reduced reciprocal randic	$RRR(G) = D_x{}^{(1/2)} D_y{}^{(1/2)} Q_{y(-1)}\, Q_{x(-1)} [g(x, y)]_{x=y=1}$
2. Arithmetic geometric index	$AG_1(G) = (1/2) D_x J S_x{}^{(1/2)} S_y{}^{(1/2)} [g(x, y)]_{x=1}$
3. SK index	$SK(G) = (1/2)(D_x + D_y)\ [g(x, y)]_{x=y=1}$
4. SK_1 index	$SK_1(G) = (1/2)(D_x D_y)[g(x, y)]_{x=y=1}$
5. SK_2 index	$SK_2(G) = (1/4)(D_x{}^2) J [g(x, y)]_{x=y=1}$
6. First Zagrab index	$EM_1(G) = D_x^2 Q_{x(-2)} J [g(x, y)]_{x=1}$
7. General sum connectivity index	$SCI(G) = S_x^{(1/2)}\ J [g(x, y)]_{x=1}$
8. Forgotten index	$F(G) = (D_x^2 + D_y^2)\ [g(x, y)]_{x=y=1}$

Where,

$$D_x g(x,y) = x\frac{\partial\big(g(x,y)\big)}{\partial x};\ D_y g(x,y)$$
$$= y\frac{\partial\big(g(x,y)\big)}{\partial y};\ Jg(x,y)$$
$$= \quad g(x,x); \quad Q_{x(\alpha)} g(x,y) = x^{\alpha} g(x,y); \quad D_x^{(1/2)}\big(g(x,y)\big)$$
$$= \sqrt{x\frac{\partial\big(g(x,y)\big)}{\partial x}}\sqrt{g(x,y)};\ D_y^{(1/2)}\big(g(x,y)\big)$$
$$= \sqrt{y\frac{\partial\big(g(x,y)\big)}{\partial y}}\sqrt{g(x,y)}; \quad S_x^{(1/2)}\big(g(x,y)\big)$$
$$= \sqrt{\int_0^x \frac{g(t,y)}{t}dt}\sqrt{g(x,y)}\ ; \quad S_y^{(1/2)}\big(g(x,y)\big)$$
$$= \sqrt{\int_0^y \frac{g(x,t)}{t}dt}\sqrt{g(x,y)}$$

2. STRUCTURE OF STARPHENE GRAPH

Starphene graph $St(n,m,l)$, where n,m,l represents the total number of hexagons in every linear chain joined by a single together by central hexagon. It is a class of benzenoid system, it is colourless with melting point of $198^0\,C$. If the benzenoid structure are connected together by three hexagons with a common vertex, then it is called peri-condensed, otherwise, it is called catacondensed. The molecular structure of starphene is depicted in Fig. 1.

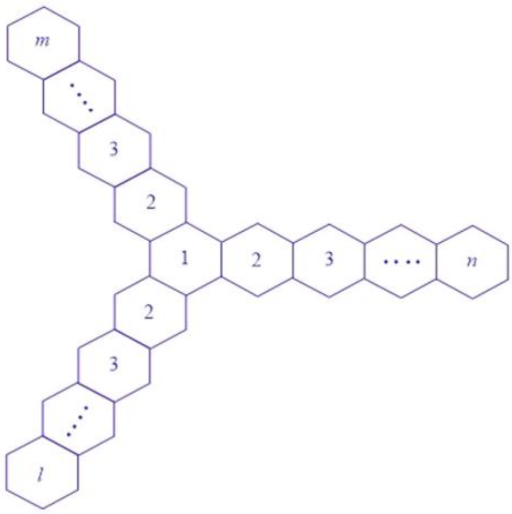


Figure1: The structure of $\boldsymbol{St(n,m,l)}$.

The structure of starphene $St(n,m,l)$ has $2(2m+2n+2l-3)$ vertices and $(5m+5n+5l-9)$ edges. Let the vertex of $St(n,l,m)$ be V_i having vertices of degree i. The vertex set of $V(G)$ is divided in to V_2 and V_3 having cardinality of $(2m+2n+2l)$ and $(2m+2n+2l-6)$ vertices. Let ω_{ij} be the edge set having degree i and j as the end vertices. The edge set of graphs can be partitioned in to $\omega_{(2,2)}$ with 9 edges, $\omega_{(2,3)}$ having $2(2m+2n+2l-9)$ edges and $\omega_{(3,3)}$ with $(m+n+l)$ edges. In this paper, the M-polynomial of starphene graph is found and this polynomial is used to derive few degree-based topological indices

3. TOPOLOGICAL INDICES OF STARPHENE GRAPH

Theorem 1. Let $St(g,s,t)$ be the Starphene graph. The $M-$polynomial is

$$M_f(St(g,s,t),x,y) = 9x^2y^2 + [4(g+s+t)-18]x^2y^3 + (g+s+t)x^3y^3.$$

Then,

1. $RRR(G) = \left(4\sqrt{2}+2\right)(g+s+t) + \left(9-18\sqrt{2}\ \right).$
2. $AG_1(G) = \left(\frac{10}{\sqrt{6}}+1\right)(g+s+t) + \left(9-\frac{45}{\sqrt{6}}\right).$
3. $SK(G) = 13(g+s+t) - 27.$
4. $SK_1(G) = \frac{33}{2}(g+s+t) - 36.$
5. $SK_2(G) = 34(g+s+t) - \frac{153}{2}.$
6. $EM_1(G) = 52(g+s+t) - 126.$
7. $SCI(G) = \left(\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{6}}\right)(g+s+t) + \left(\frac{9}{2}-\frac{18}{\sqrt{5}}\right).$
8. $F(G) = 70(g+s+t) - 162.$

Proof: Let $M_f(St(g,s,t),x,y) = f(x,y)$

1. Reduced reciprocal randic index is

$$D_y^{(1/2)} Q_{y(-1)} Q_{x(-1)}\big(f(x,y)\big) = 9xy + \sqrt{2}(\,4(g+s+t)-18)xy^2 + \quad \sqrt{2}\,(g+s+t)x^2y^2.$$

$$D_x^{(1/2)} D_y^{(1/2)} Q_{y(-1)} Q_{x(-1)}\big(f(x,y)\big) = 9xy + \sqrt{2}(\,4(g+s+t)-18)xy^2 + \quad 2(g+s+t)x^2y^2.$$

$$RRR(G) = D_x{}^{(1/2)} D_y{}^{(1/2)} Q_{y(-1)}\, Q_{x(-1)}[g(x,y)]_{x=y=1} = \left(4\sqrt{2}+2\right)(g+s+t) + \left(9-18\sqrt{2}\ \right)$$

2. Arithmetic Geometric index is

$$S_x^{(1/2)} S_y^{(1/2)}\big(f(x,y)\big) = \frac{9}{2}x^2y^2 + (4(g+s+t)-18)\frac{1}{\sqrt{6}}x^2\,y^3 + \quad \frac{1}{3}(g+s+t)x^3y^3.$$

$$JS_x^{(1/2)} S_y^{(1/2)}\big(f(x,y)\big) = \frac{9}{2}x^4 + (4(g+s+t)-18)\frac{1}{\sqrt{6}}x^5 + \frac{1}{3}(g+s+t)x^6.$$

$$(1/2)D_x JS_x{}^{(1/2)} S_y{}^{(1/2)}\big(g(x,y)\big) = 9x^4 + (2(g+s+t)-9)\frac{5}{\sqrt{6}}x^5 + \quad (g+s+t)x^6.$$

$$AG_1(G) = (1/2)D_x JS_x{}^{(1/2)} S_y{}^{(1/2)}[g(x,y)]_{x=1} = \left(\frac{10}{\sqrt{6}}+1\right)(g+s+t) + \left(9-\frac{45}{\sqrt{6}}\right).$$

3. SK index is

$$D_x(f(x,y)) = 18x^2y^2 + 2(4(g+s+t)-18)x^2y^3 + 3(g+s+t)x^3y^3.$$

$$D_y(f(x,y)) = 18x^2y^2 + 3(4(g+s+t)-18)x^2y^3 + 3(g+s+t)x^3y^3.$$

$$\frac{1}{2}(D_x+D_y)\left(f(x,y)\right) = 18x^2y^2 + \frac{5}{2}[4(g+s+t)-18]x^2y^3 + 3(g+s+t)x^3y^3.$$

$$SK(G) = (1/2)(D_x+D_y)\ [g(x,y)]_{x=y=1} = 13(g+s+t)-27.$$

4. SK_1 index is

$$\frac{1}{2}(D_xD_y)\left(f(x,y)\right) = 18x^2y^2 + 3[4(g+s+t)-18]x^2y^3 + \frac{9}{2}(g+s+t)x^3y^3.$$

$$SK_1(G) = (1/2)(D_xD_y)\ [g(x,y)]_{x=y=1} = \frac{33}{2}(g+s+t)-36.$$

5. SK_2 index is

$$J(f(x,y)) = 9x^4 + [4(g+s+t)-18]x^5 + (g+s+t)x^6.$$

$$(1/4)D_x^2J(f(x,y)) = 36x^4 + \frac{25}{2}[2(g+s+t)-9]x^5 + 9(g+s+t)x^6.$$

$$SK_2(G) = (1/4)({D_x}^2)J[g(x,y)]_{x=y=1} = 34(g+s+t) - \frac{153}{2}.$$

6. First zagrab index is

$$Q_{x(-2)}J(f(x,y)) = 9x^2 + [4(g+s+t)-18]x^3 + (g+s+t)x^4.$$

$$D_x^2Q_{x(-2)}J(f(x,y)) = 36x^2 + 9\,[4(g+s+t)-18]x^3 + 16(g+s+t)x^4.$$

$$EM_1(G) = D_x^2Q_{x(-2)}J[g(x,y)]_{x=1} = 52(g+s+t)-126.$$

7. General sum connectivity index is

$$S_x^{(1/2)}J(f(x,y)) = \frac{9}{2}x^4 + \frac{1}{\sqrt{5}}[4(g+s+t)-18]x^5 + \frac{1}{\sqrt{6}}(g+s+t)x^6.$$

$$SCI(G) = S_x^{(1/2)}\ J[g(x,y)]_{x=1} = \left(\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{6}}\right)(g+s+t) + \left(\frac{9}{2}-\frac{18}{\sqrt{5}}\right).$$

8. Forgotten index is

$$D_x^2(f(x,y)) = 36x^2y^2 + 4[\ 4(g+s+t)-18]x^2y^3 + 9(g+s+t)x^3y^3.$$

$$D_y^2(f(x,y)) = 36x^2y^2 + 9[\ 4(g+s+t)-18]x^2y^3 + 9(g+s+t)x^3y^3.$$

$$(D_x^2+D_y^2)(f(x,y)) = 72x^2y^2 + 13[4(g+s+t)-18]x^2y^3 + 18(g+s+t)x^3y^3.$$

$$F(G) = (D_x^2+D_y^2)\ [g(x,y)]_{x=y=1} = 70(g+s+t)-162.$$

The topological values obtained through M-polynomial have different functioning with respect to the parameters x and y used. The values of M-polynomial can be modulated by the parameters x and y.

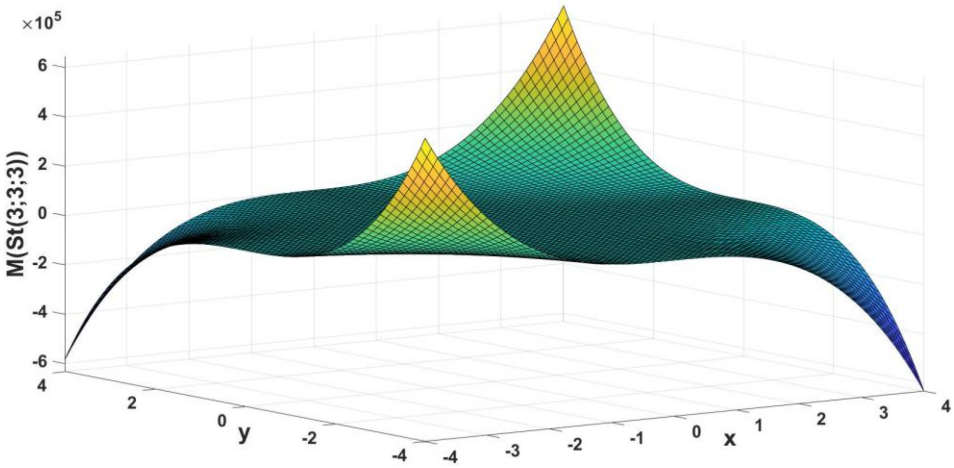
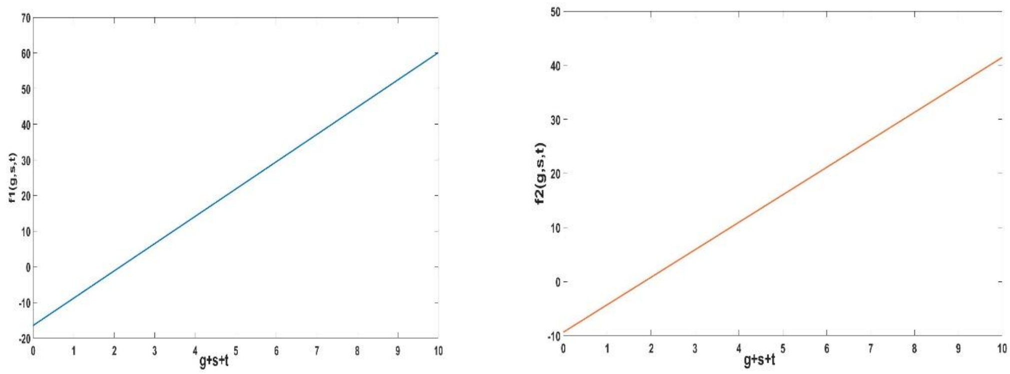
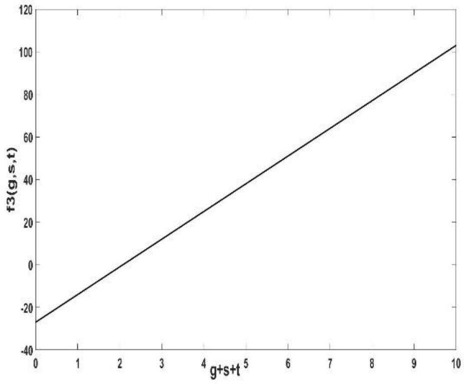


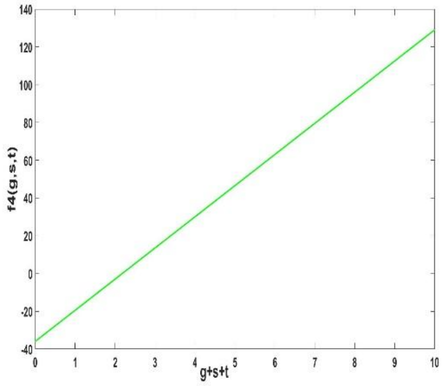
Figure 2: Plot of M-polynomial of Starphene graph $St(3,3,3)$.

Now we plot the graphs of degree based topological indices of $St(3,3,3)$.

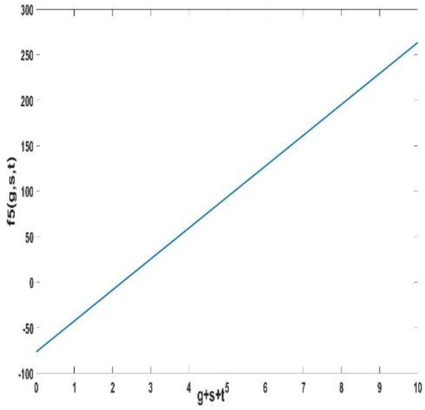


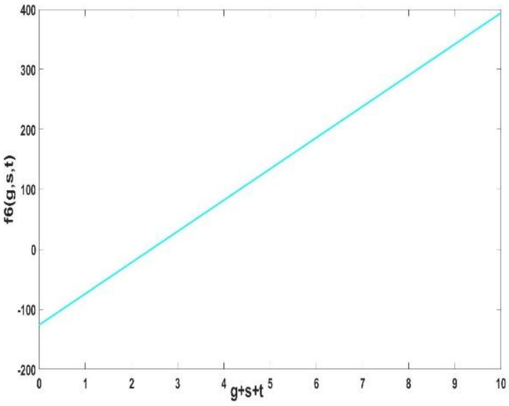
(a) **(b)**



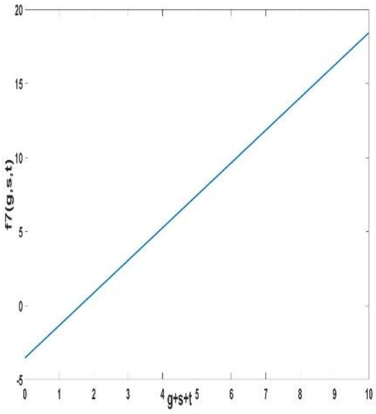


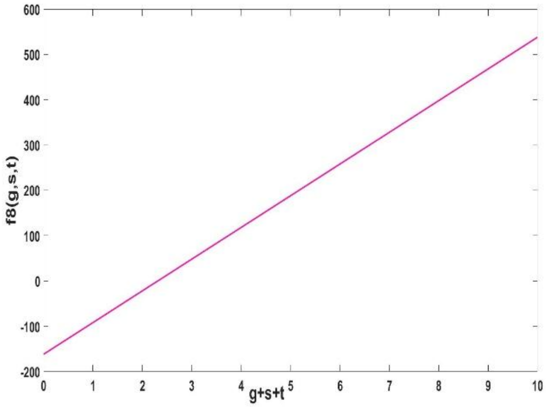
(c) **(d)**





(e) **(f)**





(g) **(h)**

Figure 3: Plots of Topological indices of Starphene graph. (a) $RRR(G)$).(b) $AG_1(G)$).(c) $SK(G)$).(d) $SK_1(G)$).(e) $SK_2(G)$).(f) $EM_1(G)$).(g) $SCI(G)$).(h) $F(G)$.

4. CONCLUSION

A topological index acts as a core instrument which maps every molecular structure to a mathematical number also it can be thought as a description of an entire molecular structure under testing. In this article, the degree based topological indices of Starphene graph are calculated through M-polynomials. The graphs of these topological indices are plotted, which concludes that these indices are associated with structural parameters s, t and g as considered.

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