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FULL PAPER

Calculating the topological indices of Starphene graph *via* M-polynomial approach

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Chemical graph theory is related to the structure of different chemical compounds. A chemical graph represents the molecule of the substance. Chemical graph theory provides the connection between the real number and the different physical, chemical, and biological properties of the chemical species. By implementing the mathematical tools, a chemical graph is converted into a real number. This number can have the predicating ability about the properties of the molecule. In this article, we find some topological indices via M-polynomial for the Starphene graph.

KEYWORDS

Molecular graph; M-polynomial; Starphene; topological indices.

Introduction

In theoretical chemistry, topological indices have received substantial attention. The topological directories enable us to understand easily the different structural properties of the chemical substance. So, topological index has a key role, to demonstrate the chemical structure. These indices are obtained by using mathematical tools and are used to explain a molecule under testing.

Topological indices are worked out from their definition; however, these can also be deliberate by resources of their M-polynomial. Table 2 shows some important degree-based topological indices. M-polynomial is also a graph representative mathematical object. With the support of M-polynomial, we compute relatively a lot of degree dependent topological invariant that are represented in Table 3.

For a graph G, the well-known M-polynomial is defined as [6]:

$$M(G,a,b) = \sum_{\delta \le i \le j \le \Delta} m_{ij}(G) a^i b^j$$

Where $\delta = min\{d_v | v \in V(G)\}$, $\Delta = max\{d_v | v \in V(G)\}$ and $m_{ij}(G)$ is the number of edges $vu \in E(G)$ such that $\{d_v ; du\} = \{i; j\}$. Table 3 shows some well-known degree-based topological directories computed by the use of M-Polynomial. M-polynomial of various graphs has been previously introduced [1, 3-5,10,12, 14-30]. In this paper, we have computed M-polynomial and topological directories of *St(l,p,r)*.

Figures 1 and 2 show a Starphene *St(l,p,r)* which can be considered as a configuration acquired by merging three linear polyenes of length *l*, *p* and *r*, respectively.

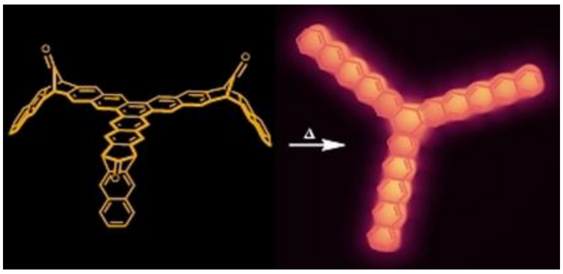


FIGURE 1 Starphene

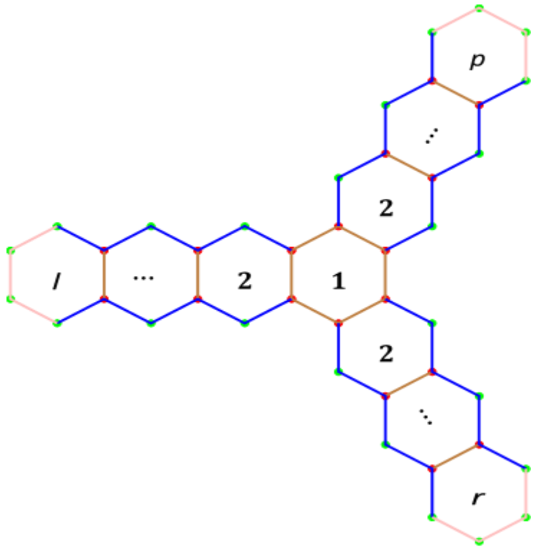


FIGURE 2 Starphene graph *St (l, p,r)*

TABLE 1 Edge partition of Starphene St (l, p, r)

(d_u; d_v)	*Number of edges*
(2,2)	*9*
(2,3)	*4(l+p+r)-18*
(3,3)	*(l+p+r)*
Total edges	*5(l+p+r)-9*

TABLE 2 Degree-based topological indices

First Zagreb index[14]	$M_1\left[St\left(\left(l,p,r\right)\right)\right]=\sum_{uv\in E\left[St(l,p,r)\right]}(d_u+d_v)$
Second Zagreb index[14]	$M_2\left[St\left(l,p,r\right)\right]=\sum_{uv\in E\left[St(l,p,r)\right]}(d_u.d_v)$
Randić Index[18]	$R_{-\frac{1}{2}}\left[St\left(l,p,r\right)\right]=\sum_{uv\in E\left[St(l,p,r)\right]}\frac{1}{\sqrt{d_u.d_v}}$

General Randić Index[18]	$R_\alpha\left[St(l,p,r)\right]=\sum_{uv\in E\left[St(l,p,r)\right]}(d_u.d_v)^\alpha$
Inverse Randić Index[18]	$RR_\alpha\left[St(l,p,r)\right]=\sum_{uv\in E\left[St(l,p,r)\right]}(\frac{1}{d_u.d_v})^\alpha$
Harmonic index[12]	$H\left[St(l,p,r)\right]=\sum_{uv\in E\left[St(l,p,r)\right]}(\frac{2}{d_u+d_v})$
Symmetric division index	$SSD\left[St(l,p,r)\right]=\sum_{uv\in E\left[St(l,p,r)\right]}(\frac{d_u}{d_v}+\frac{d_v}{d_u})$
Inverse sum index[4]	$I\left[St(l,p,r)\right]=\sum_{uv\in E\left[St(l,p,r)\right]}(\frac{d_u.d_v}{d_u+d_v})$
Augmented Zagreb index[13]	$A\left[St(l,p,r)\right]=\sum_{uv\in E\left[St(l,p,r)\right]}(\frac{d_u.d_v}{d_u+d_v-2})^3$

TABLE 3 Degree dependent topological directories

Topological index	Derivation from *M(G; a, b)*		
First Zagreb index	$M_1[St(l,p,r)]$	=	$(D_a+D_b)[f(a;b)]_{a=b=1}$
Second Zagreb index	$M_2[St(l,p,r)]$	=	$(D_aD_b)[f(a;b)]_{a=b=1}$
Modified second Zagreb index	$^mM_2[St(l,p,r)]$	=	$(S_aS_b)[f(a;b)]_{a=b=1}$
General Randić Index	$R_\alpha[St(l,p,r)]$	=	$(D_a^\alpha D_b^\alpha)[f(a;b)]_{a=b=1}$
Inverse Randić Index	$RR_\alpha[St(l,p,r)]$	=	$(S_a^\alpha S_b^\alpha)[f(a;b)]_{a=b=1}$
Symmetric division index	$SSD[St(l,p,r)]$	=	$(D_aS_b+S_aD_b)[f(a;b)]_{a=b=1}$
Harmonic index	$H[St(l,p,r)]$	=	$2S_aJ[f(a;b)]_{a=1}$
Inverse sum index	$I[St(l,p,r)]$	=	$S_aJD_aD_b[f(a;b)]_{a=1}$
Augmented Zagreb index	$A[St(l,p,r)]$	=	$S_a^3Q_{-2}JD_a^3D_b^3[f(a;b)]_{a=1}$

Where operator used are defined as

$$D_a f(a,b)=a\frac{\partial(f(a,b))}{\partial a},$$

$$D_b f(a,b)=b\frac{\partial(f(a,b))}{\partial y},$$

$$L_a f(a,b)=f(a^2,b),$$

$$L_b f(a,b)=f(a,b^2),$$

$$S_a f(a,b)=\int_0^a\frac{f(t,b)}{t}dt,$$

$$S_b f(a,b)=\int_0^b\frac{f(a,t)}{t}dt,$$

$$Jf(a,b) = f(a,a),$$

$$Q_\alpha f(a,b) = a^\alpha f(a,b),$$

$$D_a^{\frac{1}{2}} f(a,b) = \sqrt{a\frac{\partial(f(a,b))}{\partial a}}.\sqrt{f(a,b)},$$

$$D_b^{\frac{1}{2}} f(a,b) = \sqrt{b\frac{\partial(f(a,b))}{\partial b}}.\sqrt{f(a,b)},$$

$$S_a^{\frac{1}{2}} f(a,b) = \sqrt{\int_0^a \frac{f(t,b)}{t}dt}\cdot\sqrt{f(a,b)},$$

$$S_b^{\frac{1}{2}} f(a,b) = \sqrt{\int_0^b \frac{f(a,t)}{t}dt}\cdot\sqrt{f(a,b)}.$$

M-Polynomial of Starphene graph

Theorem 3.1. If Starphene is denoted by *St(l,p,r)* then for *l,p,r* ≥ 3, M-polynomial of *St(l,p,r)* is $M[St(l,p,r),a, b] = 9a^2b^2 + (4(l+p+r)-18)a^2b^3 + (l+p+r)a^3b^3$.

Proof. Let *St(l,p,r)* be a Starphene then via Table 1 besides Figure 2, the edge partition of *St(l,p,r)* is

$E_{2;2}(St(l,p,r))=\{e=uv\in St(l,p,r)d_u=2;d_v=2\}$
$\rightarrow|E_{2;2}St(l,p,r)|=9$

$E_{2;3}(St(l,p,r))=\{e=uv\in St(l,p,r):d_u=2;d_v=3\}$
$\rightarrow|E_{2;3}St(l,p,r)|=(4(l+p+r)-18)$

$E_{3;3}(St(l,p,r))=\{e=uv\in St(l,p,r):d_u=3;d_v=3\}$
$\rightarrow|E_{3;3}St(l,p,r)|=(l+p+r)$

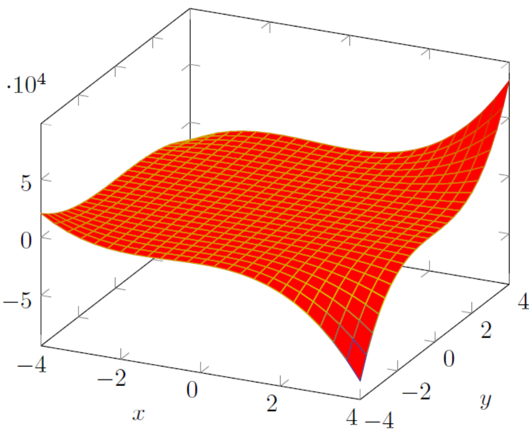


FIGURE 3 3D design of M-polynomial of Starphene (St (l, p, r)) for l=p=r=4.

The following outcome comes by applying the interpretation of M-polynomial

$$M(St(l,p,r);a,b) = \sum_{\delta\le i\le j\le\Delta} m_{ij}(St(l,p,r))a^ib^j,$$

$$M(St(l,p,r);a,b) = \sum_{2\le i\le j\le 3} m_{ij}(St(l,p,r))a^ib^j,$$

$$M(St(l,p,r);a,b) = \sum_{2\le 2} m_{22}(St(l,p,r))a^2b^2$$

$$+\sum_{2\le 3} m_{23}(St(l,p,r))a^2b^3 + \sum_{3\le 3} m_{33}(St(l,p,r))a^3b^3,$$

$$M(St(l,p,r);a,b) =|E_{2,2}|a^2b^2$$

$$+|E_{2,3}|a^2b^3+|E_{3,3}|a^3b^3$$

$$M(St(l,p,r);a,b) = 9a^2b^2 + (4(l+p+r)$$

$$-18)a^2b^3 + (l+p+r)a^3b^3.$$

Topological directories of Starphene

Theorem 4.1. Let St (l; p; z) be a Starphene:

$M[St(l,p,r);a;b]=9a^2b^2+(4(l+p+r)-18)a^2b^3$
$+(l+p+r)a^3b^3$

$$(1) M_1[St(l,p,r)] = 26(l+p+r)-54,$$

$$(2) M_2[St(l,p,r)] = 33(l+p+r)-72 = \frac{7}{9}(l+p+r)-\frac{3}{4},$$

$$(3)^m M_2[St(l,p,r)] = \frac{7}{9}(l+p+r)-\frac{3}{4}$$

$$(4) R_\alpha[St(l,p,r)] = (4\cdot 6^\alpha + 9^\alpha)(l+p+r)-(18\cdot 6^\alpha - 9\cdot 4^\alpha),$$

$$(5) RR_\alpha[St(l,p,r)] = (\frac{4}{6^\alpha}+\frac{1}{9^\alpha})(l+p+r)-(\frac{18}{6^\alpha}-\frac{9}{4^\alpha}),$$

$$(6) SSD[St(l,p,r)] = \frac{32}{3}(l+p+r)-21,$$

$$(7) H[St(l,p,r)] = \frac{29}{15}(l+p+r)-\frac{27}{10},$$

$$(8) I[St(l,p,r)] = \frac{63}{10}(l+p+r)-\frac{63}{5},$$

$$(9) A[St(l,p,r)] = \frac{2777}{64}(l+p+r)-72.$$

Proof. Let $M[St(l,p,r);a;b]=9a^2b^2+(4(l+p+r)-18)a^2b^3+(l+p+r)a^3b^3$

The first Zagreb index

$$f(a,b) = 9a^2b^2 + (4(l+p+r)-18)a^2b^3 + (l+p+r)a^3b^3,$$
$$D_a f(a,b) = 18a^2b^2 + 2(4(l+p+r)-18)a^2b^3 + 3(l+p+r)a^3b^3,$$
$$D_b f(a,b) = 18a^2b^2 + 3(4(l+p+r)-18)a^2b^3 + 3(l+p+r)a^3b^3,$$
$$(D_a + D_b) f(a,b) = 36a^2b^2 + 5(4(l+p+r)-18)a^2b^3 + 6(l+p+r)a^3b^3,$$
$$M_1[St(l,p,r)] = (D_a + D_b) f(a,b)_{a=b=1}, = 26(l+p+r)-54,$$

The second Zagreb index

$$f(a,b) = 9a^2b^2 + (4(l+p+r)-18)a^2b^3 + (l+p+r)a^3b^3,$$
$$D_b f(a,b) = 18a^2b^2 + 3(4(l+p+r)-18)a^2b^3 + 3(l+p+r)a^3b^3,$$
$$D_a D_b f(a,b) = 36a^2b^2 + 6(4(l+p+r)-18)a^2b^3 + 9(l+p+r)a^3b^3,$$
$$M_2[St(l,p,r)] = (D_a D_b) f(a,b)_{a=b=1}, = 33(l+p+r)-72,$$

The modified second Zagreb index

$$f(a,b) = 9a^2b^2 + (4(l+p+r)-18)a^2b^3 + (l+p+r)a^3b^3,$$
$$S_b f(a,b) = \frac{9}{2}a^2b^2 + \frac{1}{3}(4(l+p+r)-18)a^2b^3 + \frac{1}{3}(l+p+r)a^3b^3,$$
$$S_a S_b f(a,b) = \frac{9}{4}a^2b^2 + \frac{1}{6}(4(l+p+r)-18)a^2b^3 + \frac{1}{9}(l+p+r)a^3b^3,$$
$${}^{m}M_2[St(l,p,r)] = (S_a S_b) f(a,b)_{a=b=1} = \frac{7}{9}(l+p+r) - \frac{3}{4},$$

The general Randić index

$$f(a,b) = 9a^2b^2 + (4(l+p+r)-18)a^2b^3 + (l+p+r)a^3b^3,$$
$$D_b^{\alpha} f(a,b) = 2^{\alpha} \cdot 9a^2b^2 + 3^{\alpha} \cdot (4(l+p+r)-18)a^2b^3 + 3^{\alpha} \cdot (l+p+r)a^3b^3,$$
$$D_a^{\alpha} D_b^{\alpha} f(a,b) = 4^{\alpha} \cdot 9a^2b^2 + 6^{\alpha} \cdot (4(l+p+r)-18)a^2b^3 + 9^{\alpha} \cdot (l+p+r)a^3b^3,$$
$$R_{\alpha}[St(l,p,r)] = (D_a^{\alpha} D_b^{\alpha}) f(a,b)_{a=b=1}, = (4 \cdot 6^{\alpha} + 9^{\alpha})(l+p+r) - (18 \cdot 6^{\alpha} - 9 \cdot 4^{\alpha}),$$

The inverse Randić index

$$f(a,b) = 9a^2b^2 + (4(l+p+r)-18)a^2b^3 + (l+p+r)a^3b^3,$$
$$S_b^{\alpha} f(a,b) = \frac{9}{2^{\alpha}}a^2b^2 + \frac{1}{3^{\alpha}}(4(l+p+r)-18)a^2b^3 + \frac{1}{3^{\alpha}}(l+p+r)a^3b^3,$$
$$S_a^{\alpha} S_b^{\alpha} f(a,b) = \frac{9}{4^{\alpha}}a^2b^2 + \frac{1}{6^{\alpha}}(4(l+p+r)-18)a^2b^3 + \frac{1}{9^{\alpha}}(l+p+r)a^3b^3,$$
$$RR_{\alpha}[St(l,p,r)] = (S_a^{\alpha} S_b^{\alpha})[f(a,b)]_{a=b=1}, = (\frac{4}{6^{\alpha}} + \frac{1}{9^{\alpha}})(l+p+r) - (\frac{18}{6^{\alpha}} - \frac{9}{4^{\alpha}}),$$

The symmetric division index

$$f(a,b)=9a^2b^2+(4(l+p+r)-18)a^2b^3+(l+p+r)a^3b^3,$$
$$S_b f(a,b)=\frac{9}{2}a^2b^2+\frac{1}{3}(4(l+p+r)-18)a^2b^3+\frac{1}{3}(l+p+r)a^3b^3,$$
$$D_aS_b f(a,b)=9a^2y^2+\frac{2}{3}(4(l+p+r)-18)a^2b^3+(l+p+r)a^3b^3,$$
$$D_b f(a,b)=18a^2b^2+3(4(l+p+r)-18)a^2b^3+3(l+p+r)a^3b^3,$$
$$S_aD_b f(a,b)=9a^2b^2+\frac{3}{2}(4(l+p+r)-18)a^2b^3+(l+p+r)a^3b^3$$
$$(D_aS_b+S_aD_b)f(a,b)=18a^2b^2+\frac{13}{6}(4(l+p+r)-18)a^2b^3+2(l+p+r)a^3b^3$$
$$\mathrm{SDD[St(l;\ p;\ r)]}=(D_aS_b+S_aD_b)f(a,b)_{a=b=1}=\frac{32}{3}(l+p+r)-21$$

The harmonic index

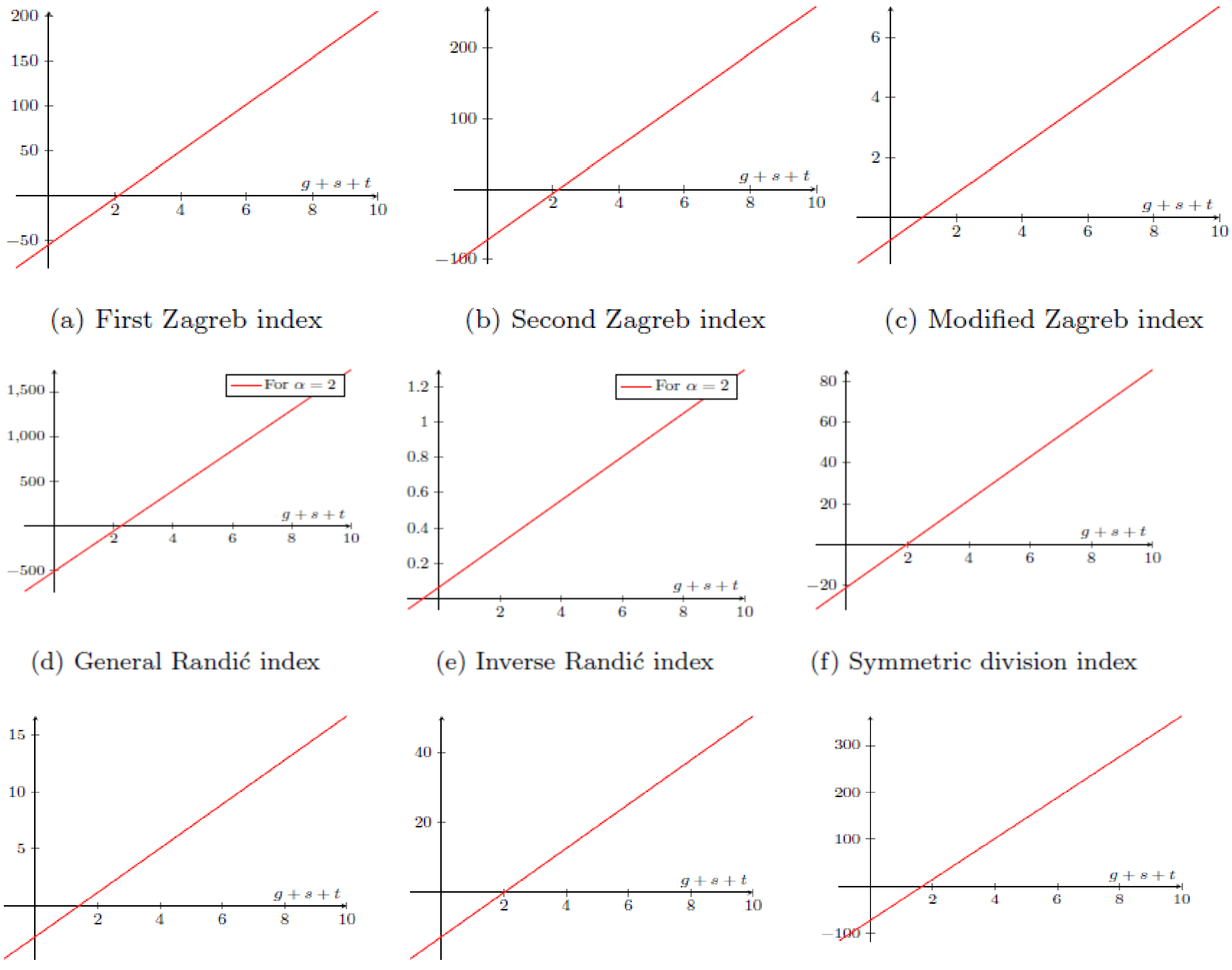
$$f(a,b)=9a^2b^2+(4(l+p+r)-18)a^2b^3+(l+p+r)a^3b^3,$$
$$Jf(a,b)=9a^4+(4(l+p+r)-18)a^5+(l+p+r)a^6,$$
$$S_aJf(a,b)=\frac{9}{4}a^4+\frac{1}{5}(4(l+p+r)-18)a^5+\frac{1}{6}(l+p+r)a^6,$$
$$2S_aJf(a,b)=\frac{9}{2}a^4+\frac{2}{5}(4(l+p+r)-18)a^5+\frac{1}{3}(l+p+r)a^6,$$
$$H[St(l,p,r)]=2S_aJf(a,b)_{a=1},=\frac{29}{15}(l+p+r)-\frac{27}{10},$$

The inverse sum index

$$f(a,b)=9a^2b^2+(4(l+p+r)-18)a^2b^3+(l+p+r)a^3b^3,$$
$$D_b f(a,b)=18a^2b^2+3(4(l+p+r)-18)a^2b^3+3(l+p+r)a^3b^3,$$
$$D_aD_b f(a,b)=36a^2b^2+6(4(l+p+r)-18)a^2b^3+9(l+p+r)a^3b^3,$$
$$JD_aD_b f(a,b)=36a^4+6(4(l+p+r)-18)a^5+9(l+p+r)a^6,$$
$$S_aJD_aD_b f(a,b)=9a^4+\frac{6}{5}(4(l+p+r)-18)a^5+\frac{3}{2}(l+p+r)a^6,$$
$$I[St(l,p,r)]=(S_aJD_aD_b)f(a,b)_{a=1},=\frac{63}{10}(l+p+r)-\frac{63}{5},$$

The augmented Zagreb index

$$f(a,b) = 9a^2b^2 + (4(l+p+r)-18)a^2b^3 + (l+p+r)a^3b^3,$$
$$D_b^3 f(a,b) = 72a^2b^2 + 27(4(l+p+r)-18)a^2b^3 + 27(l+p+r)a^3b^3,$$
$$D_a^3 D_b^3 f(a,b) = 576a^2b^2 + 216(4(l+p+r)-18)a^2b^3 + 729(l+p+r)a^3b^3,$$
$$JD_a^3 D_b^3 f(a,b) = 576a^4 + 216(4(l+p+r)-18)a^5 + 729(l+p+r)a^6,$$
$$Q_{-2}JD_a^3 D_b^3 f(a,b) = 576a^2 + 216(4(l+p+r)-18)a^3 + 729(l+p+r)a^4,$$
$$S_a^3 Q_{-2}JD_a^3 D_b^3 f(a,b) = 72a^2 + 8(4(l+p+r)-18)a^3 + \frac{729}{64}(l+p+r)a^4,$$
$$A[St(l,p,r)] = S_a^3 Q_{-2}JD_a^3 D_b^3 f(a,b)_{a=1} = \frac{2777}{64}(l+p+r) - 72.$$



(a) First Zagreb index (b) Second Zagreb index (c) Modified Zagreb index

(d) General Randić index (e) Inverse Randić index (f) Symmetric division index

(g) Harmonic index (h) Inverse sum index (i) Augmented Zagreb index

FIGURE 4 The chart of topological indices of St(l,p,r)

A graphical sketch of topological indices of St(l,p,r) is shown in Figure 4. By means of graphs, we hold up the performance of the topological indices along different parameters. Although the graphs look to be identical, they in fact have distinct gradients.

Conclusion

In the current article, we worked out a closed-form of M-polynomial for the graph Starphene and then we derived numerous degree-based topological directories as well. Topological indices help to reduce the number of experiments. These topological indices can help to understand more about the biological, chemical, and physical characteristics of a molecule. The topological index has a significant role that represents the chemical structure of a molecule to a real number. It is used to express the molecule which is under deliberation. These results are very helpful in estimating the physico-chemical properties for these chemical structures.

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