Section A-Research paper
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Determination of Degree-Based Molecular Descriptors of Superphenalene and Supertriphenylene through M-Polynomial

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Abstract:

The objective of this article is to obtain degree-based molecular descriptors for super-polycyclic aromatic compounds like superphenalene and supertriphenylene, which are built upon the foundational molecule hexabenzocoronene. These descriptors will offer quantitative insights into the connectivity and structural properties of these compounds by analysing their degree of connectivity. These super-polycyclic aromatic compounds have been the focus of several studies due to their unprecedented mechanical lead to their remarkable thermoelectric conductivities, making graphene an obvious choice to replace other common materials in a variety of applications. With the help of M-polynomial, we were able to generate numerous degree-based descriptors in this study.

Key Words: M-polynomial; Superphenalene; Supertriphenylene; Molecular descriptors; Super-polycyclic aromatic compounds.

1: Introduction

Polycyclic aromatic hydrocarbons (PAHs) are broad family of chemical compounds that are persistent environmental pollutants with unique structures and varying toxicity. They comprise two or more fused aromatic rings and have a wide range of toxicity. Hundreds of individual PAHs are released into the environment because of both anthropogenic and natural processes [1]. Hexabenzocoronene (HBC) should be referred to as a superbenzene because of its hexagonal symmetry and peripheral benzene rings that each equate to one sp^2-carbon of benzene. Mullen's research group prepared super-PAHs in 2001 [2], incorporating well-known terminology for benzene substitution patterns, such as ortho, meta, and para. Superphenalene is essentially a PAH with the chemical formula $C_{96}H_{30}$, and it is widely believed to be composed of three trapped Hexa-peri-hexabenzocoronene (HBC) molecules. It is generally regarded as a structure consisting of three HBC molecules symmetrically associated around a central core [3].

These HBCs have been recognized as building blocks for molecular electronics since 2004, as they form self-assembled structures and nanotubes. The synthesis of HBCs has led to the formation of superacenes, such as supertriphenylene, through the cyclodehydrogenation of their corresponding twisted precursors [4].

In chemical graph theory, chemical structures are depicted as molecular graphs, which are simple graphs that illustrate the carbon atom skeleton of an organic molecule. The vertices of the molecular graph represent the carbon atoms, while the edges represent the carbon-carbon bonds [5]. A topological index, often referred to as a molecular structure descriptor, is a numerical value correlated with the chemical make-up of a molecule. These indices are employed to link chemical structure to a variety of physical attributes, chemical reactivity, or biological activity [5]. However, achieving consistent predictions often requires the use of multiple topological indices, as a single molecular graph may necessitate the identification of several indices.

The research conducted by Milan Randić et al. [6] focused on calculating the molecular resonance energy for superphenalene. They observed that as we move closer to the center of the molecule, the degree of difference between nearby rings decreases. Vandana Bhalla et al. [7] subsequently worked on the synthesis of supertriphenylene from triphenylene. In 2020, Prabhu et al. [8] conducted a study on the molecular structural characterization of both superphenalene and supertriphenylene. However, there has been no progress in computing degree-based topological indices using M-polynomials for super polycyclic aromatic hydrocarbons (PAHs) such as superphenalene and supertriphenylene. The following section will explain the computation of degree-based topological indices using M-polynomials and computing the corresponding mathematical expressions. Figure 1 illustrates the two-dimensional structure of Superphenalene and Supertriphenylene.

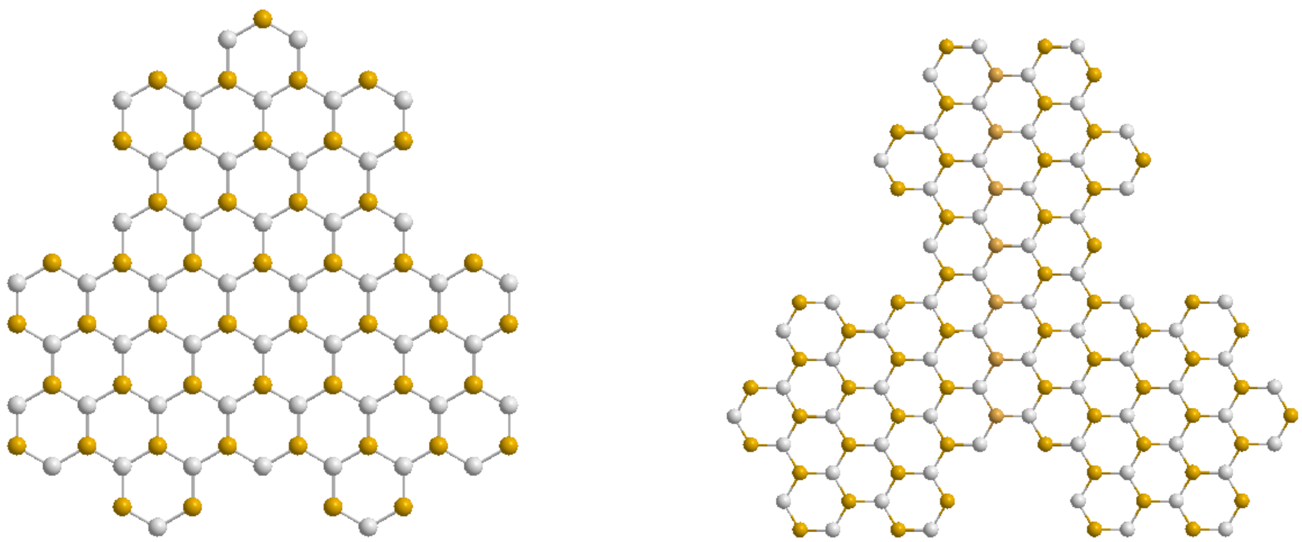

Figure 1: (a) Superphenalene $SP(2)$; (b) Supertriphenylene $STP(2)$

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2: Mathematical Terminologies

We calculate the degree-based topological indices using the degree of the vertices of molecular graph. The M-polynomial was proposed as a substitute for the Hosoya polynomial by Deutsch et al. in [9]. The M-polynomial offers a distinct advantage as it carries significant information on degree-based graph invariants. In this context, Γ represents a simple connected graph, while V and Ω represent the vertex set and edge set, respectively. The degree of a vertex v in a graph Γ is denoted as $deg\Gamma(v)$ and represents the number of edges adjacent to that vertex. Table 1 demonstrates the derivation of specific degree-based topological descriptors from M-polynomials.

The M-polynomial of a graph Γ is defined as,

$$M(\Gamma;u,v) = \sum_{\delta \le i \le j \le \Delta} m_{ij}(\Gamma) u^i v^j ------- (1)$$

where $m_{ij}(\Gamma)$ is the number of edges $rs \in \Omega(\Gamma)$ such that $\{d_r, d_s\} = \{i,j\}, \delta = min\{d_s | s \in V(\Gamma)\}$,and $\Delta = max\{d_s | s \in V(\Gamma)\}$. Let $M(\Gamma;u,v) = f(u,v)$ and Table 1 shows expression of M-polynomial for different TI's, where.

$$D_u\big(f(u,v)\big) = u\frac{\partial f(u,v)}{\partial u}$$

$$D_v\big(f(u,v)\big) = v\frac{\partial f(u,v)}{\partial v}$$

$$S_u\big(f(u,v)\big) = \int_0^u \frac{f(t,v)}{t} dt$$

$$S_v\big(f(u,v)\big) = \int_0^v \frac{f(u,t)}{t} dt$$

$$J\big(f(u,v)\big) = f(u,v)$$

$$Q_\alpha\big(f(u,v)\big) = x^\alpha f(u,v), \alpha \neq 0$$

For more properties and applications on the above indices refer [10–20].

Table 1: The extraction of some degree-based topological descriptors from M-polynomials.

Topological Index	Extraction From $M(\Gamma;x,y)$
First Zagreb Index	$D_u + D_v\big(M(\Gamma;\mathrm{u},\mathrm{v})\big)\vert_{\mathrm{u=v=1}}$
Second Zagreb Index	$D_u D_v\big(M(\Gamma;\mathrm{u},\mathrm{v})\big)\vert_{\mathrm{u=v=1}}$

Modified Second Zagreb Index	$S_u S_v\big(M(\Gamma;\mathrm{u},\mathrm{v})\big)\vert_{\mathrm{u}=\mathrm{v}=1}$
General Randić Index	$D_u^{\alpha} D_v^{\alpha}\big(M(\Gamma;\mathrm{u},\mathrm{v})\big)\vert_{\mathrm{u}=\mathrm{v}=1}$
Inverse Randić Index	$S_u^{\alpha} S_v^{\alpha}\big(M(\Gamma;\mathrm{u},\mathrm{v})\big)\vert_{\mathrm{u}=\mathrm{v}=1}$
Symmetric Division Index	$(D_u S_v + D_v S_u)\big(M(\Gamma;\mathrm{u},\mathrm{v})\big)\vert_{\mathrm{u}=\mathrm{v}=1}$
Harmonic Index	$2S_u J\big(M(\Gamma;\mathrm{u},\mathrm{v})\big)\vert_{\mathrm{u}=1}$
Inverse Sum Index	$S_u J D_u D_v\big(M(\Gamma;\mathrm{u},\mathrm{v})\big)\vert_{\mathrm{u}=1}$
Augmented Zagreb Index	$S_u^3 Q_{-2} J D_u^3 D_v^3\big(M(\Gamma;\mathrm{u},\mathrm{v})\big)\vert_{\mathrm{u}=1}$
Forgotten Index	$(D_u^2 + D_v^2)\big(M(\Gamma;\mathrm{u},\mathrm{v})\big)\vert_{\mathrm{u}=\mathrm{v}=1}$
Reduced Second Zagreb Index	$(D_u - 1)(D_v - 1)\big(M(\Gamma;\mathrm{u},\mathrm{v})\big)\vert_{\mathrm{u}=\mathrm{v}=1}$
Sigma Index	$(D_u - D_v)^2\big(M(\Gamma;\mathrm{u},\mathrm{v})\big)\vert_{\mathrm{u}=\mathrm{v}=1}$
Hyper-Zagreb Index	$(D_u + D_v)^2\big(M(\Gamma;\mathrm{u},\mathrm{v})\big)\vert_{\mathrm{u}=\mathrm{v}=1}$
Albertson Index	$(D_v - D_u)\big(M(\Gamma;\mathrm{u},\mathrm{v})\big)\vert_{\mathrm{u}=\mathrm{v}=1}$

3: The Topological Descriptors for Superphenalene $SP(t)$

Let Γ_1 be a graph of superphenalene is represented as $SP(t)$, $t \geq 2$, Then the total number of vertices and edges of the superphenalene $SP(t)$ are $54t^2 - 72t + 24$ and $81t^2 - 120t + 45$ respectively. Table 2 gives the edge partition of $SP(t)$**.**

Table 2: The edge partition of SP(t)

$(\boldsymbol{d_r}, \boldsymbol{d_s})$ ***Where*** $\boldsymbol{rs} \in \boldsymbol{\Omega}(\boldsymbol{\Gamma_1})$	***Total Number of Edges***
$(\mathbf{2},\mathbf{2})$	$12t - 6$
$(\mathbf{2},\mathbf{3})$	$24t - 24$
$(\mathbf{3},\mathbf{3})$	$81t^2 - 156t + 75$

Theorem 1. *Let* $SP(t)$, $t \geq 2$, *be a superphenalene, Then* $M(SP(t);u,v) = (12t - 6)u^2v^2 + (24t - 24)u^2v^3 + (81t^2 - 156t + 75)u^3v^3$.

Proof: The intended outcome is achieved by using the definition of the M-Polynomial for SP(t) as

$$\begin{aligned} M(SP(t)) &= \sum_{i\le j} m_{ij}\,(SP(t))u^i v^j \\ &= \sum_{2\le 2} m_{2,2}\,(SP(t))u^2v^2 + \sum_{2\le 3} m_{2,3}\,(SP(t))u^2v^3 + \sum_{3\le 3} m_{3,3}\,(SP(t))u^3v^3 \\ &= (12t-6)u^2v^2 + (24t-24)u^2v^3 + (81t^2-156t+75)u^3v^3. \end{aligned}$$

Figure 2 gives the 3D plot of M-polynomial for $\boldsymbol{SP(t)}$.

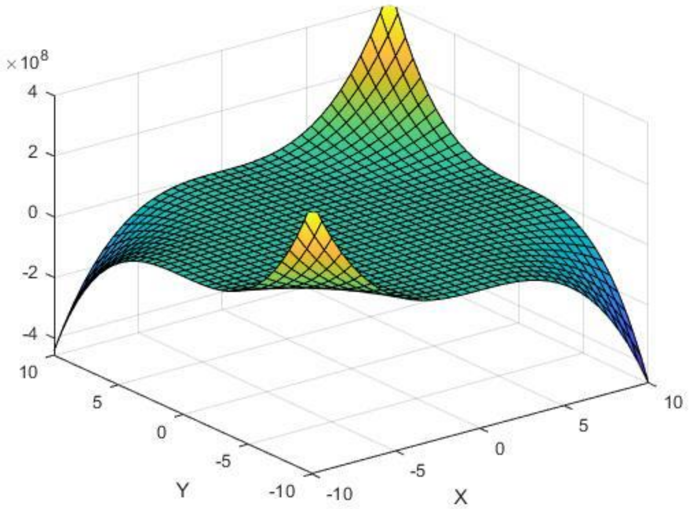


Figure 2: 3-dimensional plot of M-polynomial for $\boldsymbol{SP(t)}$

Theorem 2. Let $SP(t), t \geq 2$ be superphenalene. Then

i. $M_1(SP(t)) = 486t^2 - 768t + 306.$

ii. $M_2(SP(t)) = 729t^2 - 1212t + 507.$

iii. $M_2^m(SP(t)) = 81t^2 - 140t + 65.$

iv. $R_\alpha(SP(t)) = 4^\alpha(12t-6) + 6^\alpha(24t-24) + 9^\alpha(81t^2-156t+75).$

v. $RR_\alpha(SP(t)) = \frac{1}{4^\alpha}(12t-6) + \frac{1}{6^\alpha}(24t-24) + \frac{1}{9^\alpha}(81t^2-156t+75).$

vi. $SDD(SP(t)) = 162t^2 - 236t + 86.$

vii. $H(SP(t)) = 243t^2 - 384t + 153.$

viii. $I(SP(t)) = 54t^2 - 72t + 24.$

ix. $AZI(SP(t)) = \frac{64t^2}{9} + \frac{14168t}{243} - \frac{12980}{243}$.

x. $F(SP(t)) = 1458t^2 - 2400t + 990$.

xi. $RM_2(t) = 324t^2 - 876t + 510$.

xii. $\sigma(SP(t)) = 24t - 24$.

xiii. $HM(SP(t)) = 2916t^2 - 4824t + 2004$.

xiv. $A(SP(t)) = 24t - 24$.

Proof: Let $f(u,v) = M(SP(t);u,v) = (12t-6)u^2v^2 + (24t-24)u^2v^3 + (81t^2 - 156t + 75))u^3v^3$

By making use of Table 1 and Table 2, we get the required result.

$$\begin{aligned}
D_u(f(u,v)) &= 2(12t-6)u^2v^2 + 2(24t-24)u^2v^3 + 3(81t^2-156t+75)u^3v^3 \\
D_v(f(u,v)) &= 2(12t-6)u^2v^2 + 3(24t-24)u^2v^3 + 3(81t^2-156t+75)u^3v^3 \\
D_u^2(f(u,v)) &= 4(12t-6)u^2v^2 + 4(24t-24)u^2v^3 + 9(81t^2-156t+75)u^3v^3 \\
D_v^2(f(u,v)) &= 4(12t-6)u^2v^2 + 9(24t-24)u^2v^3 + 9(81t^2-156t+75)u^3v^3 \\
D_u + D_v(f(u,v)) &= 4(12t-6)u^2v^2 + 5(24t-24)u^2v^3 + 6(81t^2-156t+75)u^3v^3 \\
D_u \cdot D_v(f(u,v)) &= 4(12t-6)u^2v^2 + 6(24t-24)u^2v^3 + 9(81t^2-156t+75)u^3v^3 \\
S_u(f(u,v)) &= (6t-3)u^2v^2 + (12t-12)u^2v^3 + (27t^2-52t+25)u^3v^3 \\
S_v(f(u,v)) &= (6t-3)u^2v^2 + (8t-8)u^2v^3 + (27t^2-52t+25)u^3v^3 \\
S_v \cdot S_u(f(u,v)) &= \frac{(6t-3)}{2}u^2v^2 + (4t-4)u^2v^3 + \frac{(27t^2-52t+25)}{3}u^3v^3 \\
D_u^\alpha \cdot D_v^\alpha(f(u,v)) &= 4^\alpha(12t-6)u^2v^2 + 6^\alpha(24t-24)u^2v^3 + 9^\alpha(81t^2-156t+75)u^3v^3 \\
S_u^\alpha \cdot S_v^\alpha(f(u,v)) &= \frac{(12t-6)}{4^\alpha}u^2v^2 + \frac{(24t-24)}{6^\alpha}u^2v^3 + \frac{(81t^2-152t+75)}{9^\alpha}u^3v^3 \\
S_v \cdot D_u(f(u,v)) &= (12t-6)u^2v^2 + (16t-16)u^2v^3 + (81t^2-156t+75)u^3v^3 \\
S_u \cdot D_v(f(u,v)) &= (12t-6)u^2v^2 + (36t-36)u^2v^3 + (81t^2-156t+75)u^3v^3 \\
Jf(u,v) &= f(u,u) = (12t-6)u^4 + (24t-24)u^5 + (81t^2-156t+75)u^6 \\
S_u \cdot Jf(u,v) &= f(u,u) = \frac{(12t-6)}{4}u^4 + \frac{(24t-24)}{5}u^5 + \frac{(81t^2-156t+75)}{6}u^6 \\
S_uJD_vD_v(f(u,v)) &= (12t-6)u^4 + \frac{6}{5}(24t-24)u^5 + \frac{3}{2}(81t^2-156t+75)u^6 \\
S_u^3Q_{-2}JD_u^3D_v^3(f(u,v)) &= 8(12t-6) + 8(24t-24) + \frac{729(81t^2-156t+75)}{64}
\end{aligned}$$

4: The Topological Descriptors for $STP(t)$

Let Γ_2 be a graph of Supertriphenylene is represented as $STP(t)$, $t \geq 2$. Then the total number of vertices and edges of the supertriphenylene $STP(t)$ are $72t^2 - 90t + 24$ and $108t^2 - 153t + 51$ respectively. Table 3 represents the edge partition of $\boldsymbol{SPT(t)}$.

Table 3: The edge partition of $SPT(t)$.

(d_r, d_s) ***Where*** $rs \in \Omega(\Gamma_2)$	***Total Number of Edges***
$(2,2)$	$18t - 12$
$(2,3)$	$36t - 36$
$(3,3)$	$108t^2 - 207t + 99$

Theorem 3. *Let $STP(t)$, $t \geq 2$, be a supertriphenylene. Then,* $M(STP(t); u, v) = (18t - 12)u^2v^2 + (36t - 36)u^2v^3 + (108t^2 - 207t + 99)u^3v^3$

Proof: Using Equation (1) for $STP(t)$, the desired result is obtained as follows,

$$\begin{aligned} M(STP(t); u, v) &= \textstyle\sum_{i \leq j} m_{ij}\left(STP(t)\right)u^i v^j \\ &= \textstyle\sum_{2\leq 2} m_{2,2}\left(STP(t)\right)u^2v^2 + \sum_{2\leq 3} m_{2,3}\left(STP(t)\right)u^2v^3 + \sum_{3\leq 3} m_{3,3}\left(STP(t)\right)u^3v^3 \\ &= (18t - 12)u^2v^2 + (36t - 36)u^2v^3 + (108t^2 - 207t + 99)u^3v^3 \end{aligned}$$

Figure 3 gives the 3D plot of M-polynomial for $\boldsymbol{STP(t)}$.

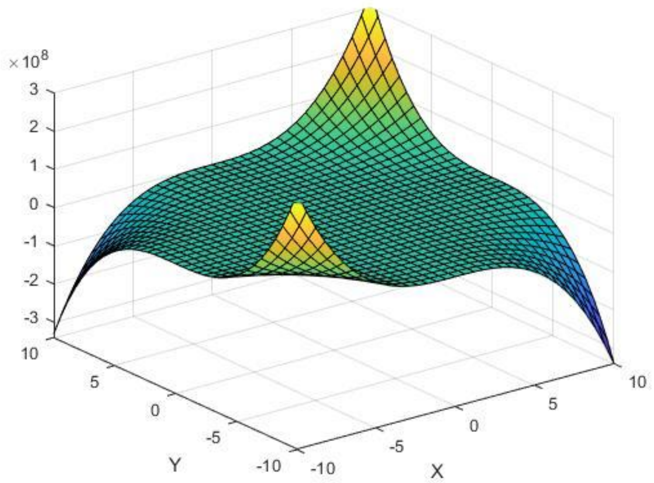


Figure 3: 3D plot of M-polynomial for $STP(t)$

Theorem 4. *Let $STP(t)$, $t \geq 2$ be a supertriphenylene. Then*

i. $M_1\big(STP(t)\big) = 648t^2 - 990t + 366$.

ii. $M_2\big(STP(t)\big) = 972t^2 - 1575t + 627$.

iii. $M_2^m\big(STP(t)\big) = 12t^2 + 55t - 43$.

iv. $R_\alpha\big(STP(t)\big) = 4^\alpha(18t - 12) + 6^\alpha(36t - 36) + 9^\alpha(108t^2 - 207t + 99)$.

v. $RR_\alpha\big(STP(t)\big) = \frac{1}{4^\alpha}(18t - 12) + \frac{1}{6^\alpha}(36t - 36) + \frac{1}{9^\alpha}(108t^2 - 207t + 99)$.

vi. $SDD\big(STP(t)\big) = 216t^2 - 300t + 96$.

vii. $H\big(STP(t)\big) = 1296t^2 - 1980t + 732$.

viii. $I\big(STP(t)\big) = 72t^2 - 90t + 24$.

ix. $AZI\big(STP(t)\big) = \frac{256t^2}{27} + \frac{7276t}{81} - \frac{7072}{81}$.

x. $F\big(STP(t)\big) = 1944t^2 - 3114t + 1218$.

xi. $RM_2\big(STP(t)\big) = 432t^2 - 738t + 312$.

xii. $\sigma\big(STP(t)\big) = 36t - 36$.

xiii. $HM\big(STP(t)\big) = 3888t^2 - 6264t + 2472$.

xiv. $A\big(STP(t)\big) = 36t - 36$.

Proof: Let $f(u,v) = M(STP(t);u,v) = (18t - 12)u^2v^2 + (36t - 36)u^2v^3 + (108t^2 - 207t + 99)u^3v^3$. Then by using Table 1 and Table 3 we obtain the necessary outcomes.

$$
\begin{aligned}
D_u(f(u,v)) &= 2(18t-12)u^2v^2 + 2(36t-36)u^2v^3 + 3(108t^2-207t+99)u^3v^3\\
D_v(f(u,v)) &= 2(18t-12)u^2v^2 + 3(36t-36)u^2v^3 + 3(108t^2-207t+99)u^3v^3\\
D_u^2(f(u,v)) &= 4(18t-12)u^2v^2 + 4(36t-36)u^2v^3 + 9(108t^2-207t+99)u^3v^3\\
D_v^2(f(u,v)) &= 4(18t-12)u^2v^2 + 9(36t-36)u^2v^3 + 9(108t^2-207t+99)u^3v^3\\
D_u + D_v(f(u,v)) &= 4(18t-12)u^2v^2 + 5(36t-36)u^2v^3 + 6(108t^2-207t+99)u^3v^3\\
D_u \cdot D_v(f(u,v)) &= 4(18t-12)u^2v^2 + 6(36t-36)u^2v^3 + 9(108t^2-207t+99)u^3v^3\\
S_u(f(u,v)) &= \frac{(18t-12)}{2}u^2v^2 + \frac{(36t-36)}{2}u^2v^3 + \frac{(108t^2-207t+99)}{3}u^3v^3\\
S_v(f(u,v)) &= \frac{(18t-12)}{2}u^2v^2 + \frac{(36t-36)}{3}u^2v^3 + \frac{(108t^2-207t+99)}{3}u^3v^3\\
S_v \cdot S_u(f(u,v)) &= \frac{(18t-12)}{4}u^2v^2 + \frac{(36t-36)}{6}u^2v^3 + \frac{(108t^2-207t+99)}{9}u^3v^3\\
D_u^\alpha . D_v^\alpha(f(u,v)) &= 4^\alpha(18t-12)u^2v^2 + 6^\alpha(36t-36)u^2v^3 + 9^\alpha(108t^2-207t+99)u^3v^3\\
S_u^\alpha \cdot S_v^\alpha(f(u,v)) &= \frac{(18t-12)}{4^\alpha}u^2v^2 + \frac{(36t-36)}{6^\alpha}u^2v^3 + \frac{(108t^2-207t+99)}{9^\alpha}u^3v^3\\
S_v \cdot D_u(f(u,v)) &= (18t-6)u^2v^2 + \frac{2(36t-36)}{3}u^2v^3 + (108t^2-207t+99)u^3v^3\\
S_u \cdot D_v(f(u,v)) &= (18t-12)u^2v^2 + \frac{3(36t-36)}{2}u^2v^3 + (108t^2-207t+99)u^3v^3\\
Jf(u,v) &= f(u,u) = (18t-12)u^4 + (36t-36)u^5 + (108t^2-207t+99)u^6\\
S_uJf(u,v) &= \frac{(18t-12)}{4}u^4 + \frac{(36t-36)}{5}u^5 + \frac{(108t^2-207t+99)}{6}u^6\\
S_uJD_uD_v(f(u,v)) &= (18t-12)u^4 + \frac{6(36t-36)}{5}u^5 + \frac{3(108t^2-207t+99)}{2}u^6\\
S_u^3Q_{-2}JD_u^3D_u^3(f(u,v)) &= 8(18t-12) + 8(36t-36) + \frac{729(108t^2-207t+99)}{64}
\end{aligned}
$$

5: Numerical Results and Discussions

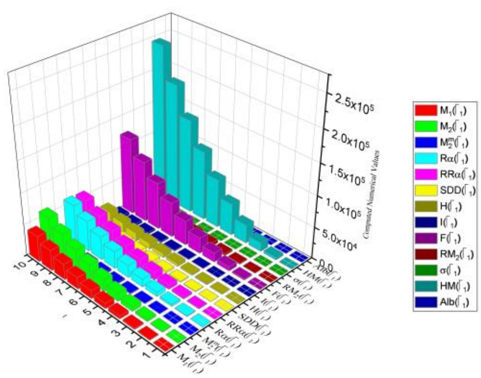
The statistical results for superphenalene and supertriphenylene are reported in this part, which are derived from the computation of degree-based topological descriptors with the help of M-polynomial. The degree-based topological indices for different values of *n* are given below for numerical comparison. These values are plotted using the ORIGIN 2020b software. Tables 4 andv5 give the numerical values and Figure 4 is its graphical representations.

Table 4: Numerical computation for TI's of $SP(t)$.

t	$M_1(\Gamma_1)$	$M_2(\Gamma_1)$	$M_2^m(\Gamma_1)$	$R_\alpha(\Gamma_1)$	$RR_\alpha(\Gamma_1)$	$SDD(\Gamma_1)$	$H(\Gamma_1)$	$I(\Gamma_1)$	$AZI(\Gamma_1)$	$F(\Gamma_1)$	$RM_2(\Gamma_1)$	$\sigma(\Gamma_1)$	$HM(\Gamma_1)$	$Alb(\Gamma_1)$
1	24	24	6	24	24	12	12	6	12	48	6	0	96	0
2	714	999	109	999	859	262	357	96	92	2022	414	24	4020	24
3	2376	3432	374	3432	3152	836	1188	294	186	6912	1470	48	13776	48
4	5010	7323	801	7323	6903	1734	2505	600	294	14718	3174	72	29364	72
5	8616	12672	1390	12672	12112	2956	4308	1014	416	25440	5526	96	50784	96
6	13194	19479	2141	19479	18779	4502	6597	1536	522	39078	8526	120	78036	120
7	18744	27744	3054	27744	26904	6372	9372	2166	703	55632	12174	144	111120	144
8	25266	37467	4129	37467	36487	8566	12633	2904	868	75102	16470	168	150036	168
9	32760	48648	5366	48648	47528	11084	16380	3750	1047	97488	21414	192	194784	192
10	41226	61287	6765	61287	60027	13926	20613	4704	1240	122790	27006	216	245364	216

Table 5: Numerical computation for TI's of $STP(t)$.

t	$M_1(\Gamma_2)$	$M_2(\Gamma_2)$	$M_2^m(\Gamma_2)$	$R_\alpha(\Gamma_2)$	$RR_\alpha(\Gamma_2)$	$SDD(\Gamma_2)$	$H(\Gamma_2)$	$I(\Gamma_2)$	$A(\Gamma_2)$	$F(\Gamma_2)$	$RM_2(\Gamma_2)$	$\sigma(\Gamma_2)$	$HM(\Gamma_2)$	$Alb(\Gamma_2)$
1	24	24	24	24	24	12	48	6	12	48	6	0	96	0
2	978	1365	115	1365	1155	360	1956	132	130	2766	564	36	5496	36
3	3228	4650	230	4650	4230	1140	6456	402	267	9372	1986	72	18672	72
4	6774	9879	369	9879	4429	2352	13548	816	424	19866	4272	108	39624	108
5	11616	17052	532	17052	16212	3996	23232	1374	599	34248	7422	144	68352	144
6	17754	26169	719	26169	25119	6072	35508	2076	793	52518	11436	180	104856	180
7	25188	37230	930	37230	35970	8580	50376	2922	1006	74676	16314	216	149136	216
8	33918	50235	1165	50235	48765	11520	67836	3912	1238	100722	22056	252	201192	252
9	43944	65184	1424	65184	63504	14892	87888	5046	1489	130656	28662	288	261024	288
10	55266	82077	1707	82077	80187	18696	110532	6324	1759	164478	36132	324	328632	324



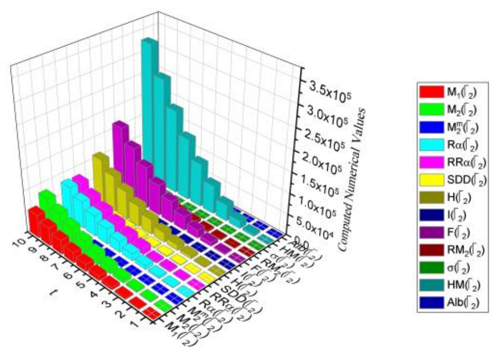


Figure 4: (a) Graphical Representation of different degree-based indices of $SP(t)$;

(b) Graphical Representation of different degree-based indices of $STP(t)$

6: Conclusion

In this paper, the M-polynomial has been employed to calculate fourteen degree-based topological indices. These descriptors provide further insights into the molecular structure and enable chemists to predict various properties of molecular compounds without the need for expensive and time-consuming experiments. The findings of this study have implications for the development of quantitative structure-activity relationship (QSAR) models in pharmaceutical and chemical science. By incorporating these degree-based topological indices into QSAR models, researchers can enhance their predictive capabilities and gain valuable insights into the properties and behaviours of molecular compounds. Furthermore, the paper highlights the potential for future research on computing graph entropies using topological indices specifically for superphenalene and supertriphenylene. Graph entropies provide measures of complexity and information content in molecular structures and can offer further understanding of their properties.

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