On Degree Based Topological Indices of Self-Assembled Tetraphenylethylene and Terpyridine Rosettes

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Abstract

A technique is described to compute topological indices for supramolucular rosettes of tetraphenylethylene (TPE) and terpyridine (TPY) ligands with its applications on physicochemical and biological properties. This technique, we have applied to a self assembled TPE and TPY supramolucular graphs which is obtained in the form of rosette cycles. Also these type of rosettes graph finds significant applications in electrical sensors, light emitting diodes, bioimaging and photoelectric devices etc. As regarded to the next generation sensing applications with a typical induced aggregative emission behaviour, tetraphenylethylene can be utilised in constructing fluorescent probes. For this supramolucular systems we have done a work by computing some topological indices such as the variants of Zagreb index, Randić index, Sum Connectivity index, ABC index and Harmonic index.

Key Words: degree based topological indices, supramolucular rosettes, tetraphenylethylene, terpyridine.

1 Introduction

A particular discussion on co-ordination driven self-assemblies of molecular structures has revealed a powerful basement approach within the different fields of supramolecular chemistry in constructing several supramolecular architectures and structures varying from basic two dimensional 2D macrocycles to large three dimensional 3D cages with their increment of complexities [2] - [11], and one of a known example is the tetraphenylethylene and terpyridine (TPE-TPY) supramolucular rosettes [1].

Various application benefited by the perfect controlling of shape, size, and the metallo supramolecules makeup system has witnessed the depth and widened breadth of its scope [12] - [16]. Extensively three significant strategies have been approached by aiming to advance the comparative sophistication as biological self-assemblies with metallo supramolecules, those are designing newly built architectures with additionally increased complexity and host guest encapsulation, introduce functional moieties in addition with widened diversity into well explained supramolecular platforms [17] - [20]. Inside this boundry of research, the combination of metallo supramolecules with chromophores resulted as materials with light emitting property has gathered accountable observation due to their broad applications in photoelectric devices, sensors, diodes with light emmitting property, bioimaging extra [21]- [24]. Presently, the following frame works and abbreviated terms such as covalent organic frameworks (COFs) [28] - [30], metal organic frameworks (MOFs) [25]- [27], metallomacrocycles [31]- [34], an effect caused by the restriction of intramolecular rotation (RIR) [41] - [42], to construct luminescent materials based on aggregation induced emission (AIE) [40] using metallo cages [35] - [39], has incorporated tetraphenylethylene (TPE) as an archetypal fluorophore.

Restriction of intramolecular rotation was stored by anchoring TPE fluorophores to metal ions within stiff scaffolds in order to limit the non-radiative channel and activate the radiative decay, which was one of the most extreme situations of coordination system. For the coordination, typically TPE containing ligands consist of tiny replacements, such as pyridine or carboxylate. [22]. As a result, RIR was mostly attributed to metal coordination, which limits intramolecular movements to some extent. More specifically, we compute various degree-based topological indices for two-generation growths of AIE active ligands with full TPE-TPY conjugation [43] - [44], which is a faintly luminous material that is gaining popularity in metallo supramolecular chemistry for the self-assembly of co-ordination polymers and different supramolecular designs [45] - [48]. The TPY substituents' greater conjugation and bulky size cause intramolecular rotations to be somewhat inhibited even in solution, resulting in emission in both solution and aggregation states. TPE and TPY ligands are also combined with Cd(II) via coordination to introduce more RIR and immobilise fluorophores in metallo macrocycles, or rosettes, which act as scaffolds. A combination of macrocycles is generated using a ditopic ligand, but distinct double-layered hexameric and triple layered heptameric rosettes with increasing structural complexity are constructed using tetratopic and hexatopic ligands, respectively, via multivalent interactions.

From the subject of graph theory, the word topological index is a useful tool for generating a relationship between Mathematics and Chemistry. For some isomorphic graphs, the topological index is treated as a real number, with some specific constraints that remain constant linking it to a given graph. Topological indices also defines the molecular structure's topology. Topological indices play an

important role in determining various biological activities and physiochemical properties in the study of quantitative structure property relationship (QSPR) or quantitative structure activity relationship (QSAR), which aids in the discovery of computer-aided drug discovery. On going back to the analysis of past decade, QSAR/QSPR has seen a notable amount of results in model learning. To foretell and to do a analysing studty on quantum-theoretic and physicochemical properties of new compounds with predicted activities/properties the fact of QSAR/QSPR [59] aids in a possible way. The most significant three steps to learn QSAR/QSPR model are: (i) From a chemical graph, encoding it's statistical/mathematical/ datas, (ii) Estimating and calculating the properties of the structure encoded with the help of constructing a linear regression example and (iii) For certain existing compounds a training set is generated with evaluated properties. In the model learning of QSAR/ QSPR,on the first step molecular indices is involved as a significant part. All the compound's characteristics such as critical pressure, critical volume, enthalpy of formation, boiling point, enthalpy of vaporization, Kovat's retention index, and so on are included in the physicochemical properties. At the level of atomic and subatomic state quantum theoretical characterstics includes the properties of compounds. For certain physicochemical properties namely enthalpy of formation, standard boiling point of the compounds are well correlated wić with these degree based indices says Gutman and Tošović [60]. In a recent study, Hayat et al. [61] has shown that prediction potential efficiency for correlating with physicochemical properties of any degree based indices is relatively more important than the distance based indices. Also for the polycyclic aromatic hydrocarbons with p electronic energy (PAHs) Hayat et al. [62] has detected the prediction potential of distance based indices. The correlation potential of different kinds has been studied by Hayat and co-authors [63] - [65] for spectrum based indices for some p electronic energy of polycyclic aromatic hydrocarbons. S. Hayat and S. Khan [66] - [67] has investigated the measuring of physicochemical properties of polycyclic aromatic hydrocarbons using the prediction potential of the similar kinds of spectral indices. Moreover, Nikolic et al., [68] Chen [69] and Hayat et al. [70] have shown for benzenoid hydrocarbons with the p electronic energy are well correlated with degree based indices. On approaching the progress, it shows that the most successful kind of graph theoretic molecular indices are degree-based indices and it is an open concept on determining their correlation potential efficency to measure the PAHs physicochemical properties. Its application in many different branches namely biotechnology, nanoscience has a remarkable scope. This topic gathers the attraction of worldwide researcher's involvement. The Wiener index [55] was introduced by a chemist Harold Wiener in 1947, the year when topological index started it's journey. In the past decades various topological indices have been introduced related to the vertex degree of a molucular graph G. Inspired by those works, we have computed some degree based topological indices namely First Zagreb index, Second Zagreb, General Randić Index, Randic Index, Hyper Zagreb index, Sum

Table 1: **Degree based topological indices**

First Zagreb Index	$M_1(G)= \sum_{uv\in E(G)} [d_u + d_v]$
Second Zagreb Index	$M_2(G) = \sum_{uv\in E(G)} [d_u \times d_v]$
General Randić Index	$R_\alpha(G) = \sum_{uv\in E(G)} [d_u d_v]^\alpha$
Randić Index	$R(G) = \sum_{uv\in E(G)} [d_u d_v]^{\frac{-1}{2}}$
Hyper Zagreb Index	$HM(G) = \sum_{uv\in E(G)} [d_u + d_v]^2$
Sum Connectivity Index	$SCI_1(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}$
General Sum Connectivity Index	$\chi_\alpha(G) = \sum_{uv\in E(G)} [d_u + d_v]^\alpha$
Geometric Arithmetic Index	$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$
Atom Bond Connectivity Index	$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$
Harmonic Index	$H(G) = \sum_{uv\in E(G)} \frac{2}{d_u + d_v}$

connectivity Index, Generalized sum connectivity Index, Geometric arithemetic Index. The graphs considered in this work are only molecular graph [55] to [58]. A pictorial representation of chemical compound are called molecular graphs. For the graph G, $V(G)$ and $E(G)$ are used as vertex and edge sets, respectively, throughout this paper. The total number of edges intersecting with any vertex $u \in V$ in the graph, given by $d(u)$, is the vertex u's degree. Refer Table.1 for the indices which are used in this paper.

1.1 Tetraphenylethylene (TPE) Terpyridine (TPY) Supramolucular Rosettes Graph Structure

The supramolucular rosettes of tetraphenylethylene (TPE) and terpyridine (TPY) ligands is obtained due to bulky size of tetraphenylethylene substituent compounds, even in dilute solution the intramolecular rotations of ligands are restricted partially, therefore it leads to emissive activity in both aggregation states and solution. In addition, tetraphenylethylene and terpyridine get their ligands to assemble with Cd(cadimum) to generate more intramolecular rotation restrictions and immobilise fluorophores into rosette form of metallo supramolecules ranging from generation growths (G_1) and

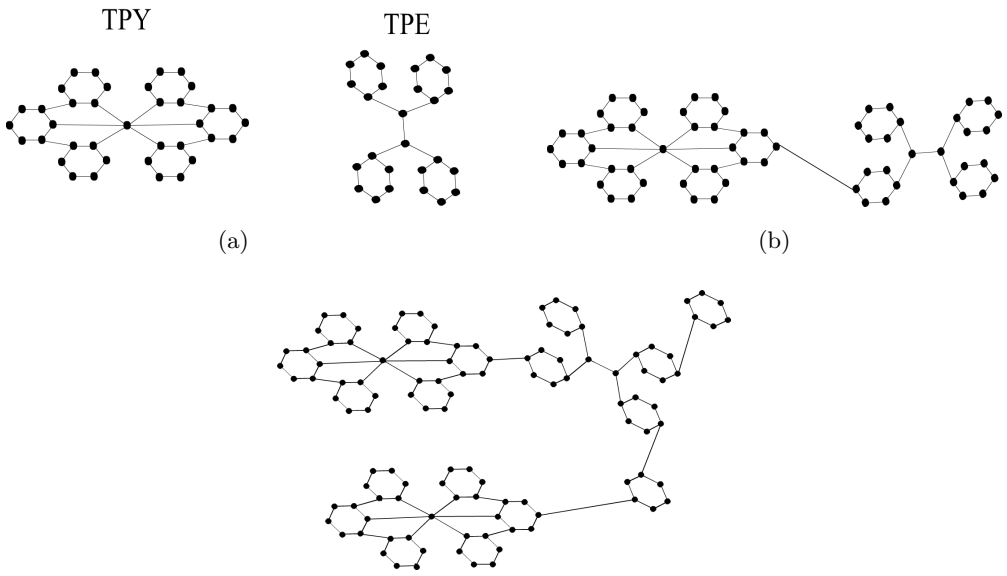


Figure 1: (a) Compounds TPE and TPY (b) Connected section of TPE and TPY for G_1 (c) Connected section of TPE and TPY for G_2

(G_2) [2] - [4]. From the graphical point of view, the supramolucular rosettes structure of TPE and TPY ligands is obtained by connecting the (TPE -TPY) scections (See Figure 1) of regular hexagons in a n dimensional cyclic rosette sequence form as shown in (See Figures 2 and 3). As an exapmple the base form of (TPE -TPY) rosette cycle with dimension $n = 1$ is obtained by connecting three sections of (TPE -TPY) in the form of a cycle C_3. In this paper we compute some degree based topological indices by dividing and splitting the molecular graph in to four classes of edge partitions and calculating their molecular parameter for two growth of TPE and TPY supramolucular rosettes structures namely G_1 and G_2 (See Figures 2 and 3).

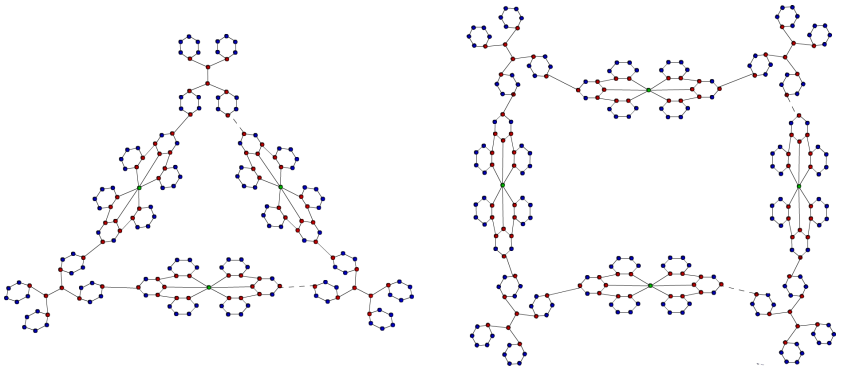
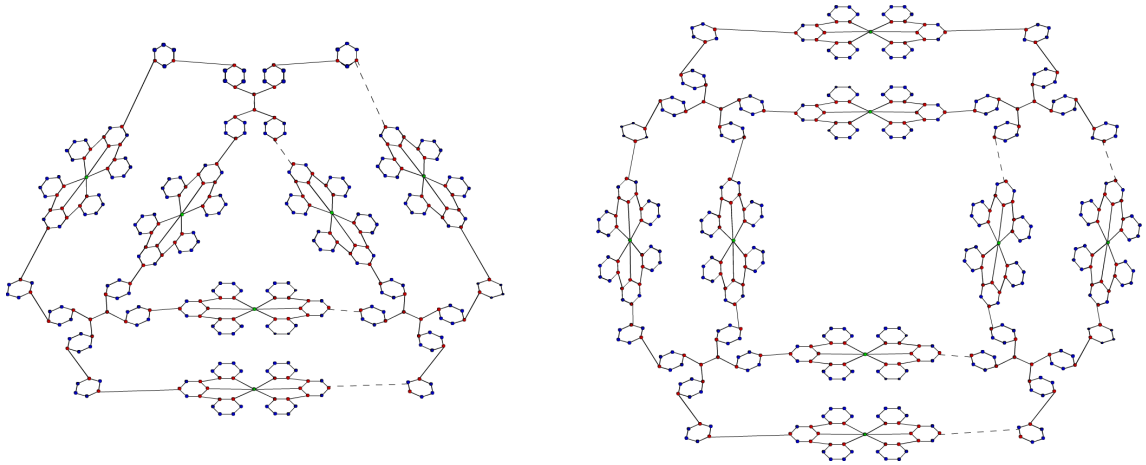


Figure 2: (a) (TPE -TPY) rosette of G_1 with dimension $n = 1$ and $n = 2$,



(a)

Figure 3: (a) (TPE -TPY) rosette of G_2 with dimension $n = 1$ and $n = 2$

2 Computational Strategies

2.1 Computational Methods for (TPE- TPY) Supramolucular Rosette Growths G_1 and G_2

This section deals on some computation methods of degree based topological indices for (TPE- TPY) Supramolucular rosette growths G_1 and G_2 with their corresponding edge partitions $E_i(G_1)$ and $E_i(G_2)$

$$|E_i(G_1)| = 154 + 77n$$
$$|E_i(G_2)| = 278 + 139n$$

Table 2: **Edge Partitions of TPE** G_1

Edge Type	(2,2)	(2,3)	(3,3)	(3,6)
$\lvert E_i(G_1)\rvert$	$\lvert E_1\rvert = 48 + 24n$	$\lvert E_2\rvert = 56 + 28n$	$\lvert E_3\rvert = 38 + 19n$	$\lvert E_4\rvert = 12 + 6n$

Table 3: **Edge Partitions of TPE** G_2

Edge Type	(2,2)	(2,3)	(3,3)	(3,6)
$\lvert E_i(G_2)\rvert$	$\lvert E_1\rvert = 84 + 36n$	$\lvert E_2\rvert = 100 + 56n$	$\lvert E_3\rvert = 70 + 35n$	$\lvert E_4\rvert = 24 + 12n$

3 Main Results

Theorem 1. *Let G_1 be the growth of n dimensional tetraphenylethylene supramolucular rosettes graph TPE_n then*

1. $M_1(TPE_n) = 404n + 808$
2. $M_2(TPE_n) = 543n + 1086$
3. $R(TPE_n) \quad = \frac{55n}{3} + \frac{\sqrt{2}(6n+12)}{6} + \frac{\sqrt{6}(28n+56)}{6} + \frac{110}{3}$
4. $R_\alpha(TPE_n) \quad = \frac{55n}{3} + \frac{\sqrt{2}(6n+12)}{6} + \frac{\sqrt{6}(28n+56)}{6} + \frac{110}{3}$
5. $HM(TPE_n) \;\; = (2254 + 4508n)$
6. $SCI_1(TPE_n) = 14n + \frac{\sqrt{6}(19n+38)}{6} + \frac{\sqrt{5}(28n+56)}{5} + 28$
7. $\chi_\alpha(TPE_n) = 14n + \frac{\sqrt{6}(19n+38)}{6} + \frac{\sqrt{5}(28n+56)}{5} + 28$
8. $GA(TPE_n) = (48 + 24n) + \frac{2\sqrt{6}}{5}(56 + 28n) + (38 + 19n) + \frac{2\sqrt{18}}{9}(12 + 6n)$
9. $ABC(TPE_n) = \frac{38n}{3} + \frac{\sqrt{14}(6n+12)}{6} + \frac{\sqrt{2}(24n+48)}{2} + \frac{\sqrt{2}(28n+56)}{2} + \frac{76}{3}$
10. $H(TPE_n) = \frac{463n}{15} + \frac{926}{15}$

Proof. Let the cardinality of vertex set and edge set of the n dimensional (TPE) and (TPY) supramolucular rosettes graph G_1 be $|V(TPE_n)| = 126+63n$ and $|E(TPE_n)| = 154+77n$ respectively. Consider the edge partitions of the graph related to the degrees of the terminal vertices of each and every edge. By applying the formulae of the indices above, we compute all the indices.
Further from Table 2

$$\begin{aligned}
1.M_1(TPE_n) &= (2+2)(|E_1|) + (2+3)(|E_2|) + (3+3)(|E_3|) \\
&\quad + (3+6)(|E_4|) \\
&= 404n + 808 \\
2.M_2(TPE_n) &= (2\times 2)(|E_1|) + (3\times 2)(|E_2|) + (3\times 3)(|E_3|) \\
&\quad + (3\times 6)(|E_4|) \\
&= 543n + 1086 \\
3.R(TPE_n) &= \frac{1}{\sqrt{2\times 2}}(|E_1|) + \frac{1}{\sqrt{2\times 3}}(|E_2|) + \frac{1}{\sqrt{3\times 3}}(|E_3|) \\
&\quad + \frac{1}{\sqrt{3\times 6}}(|E_4|)
\end{aligned}$$

$$= \frac{55n}{3} + \frac{\sqrt{2}(6n+12)}{6} + \frac{\sqrt{6}(28n+56)}{6} + \frac{110}{3}$$

$$4.R_\alpha(TPE_n) = (2\times 2)^\alpha(|E_1|) + (3\times 2)^\alpha(|E_2|) +$$
$$(3\times 3)^\alpha(|E_3|) + (3\times 6)^\alpha(|E_4|)$$
$$= \frac{55n}{3} + \frac{\sqrt{2}(6n+12)}{6} + \frac{\sqrt{6}(28n+56)}{6} + \frac{110}{3}$$

$$5.HM(TPE_n) = (2+2)^2(|E_1|) + (2+3)^2(|E_2|) + (3+3)^2(|E_3|)$$
$$+ (3+6)^2(|E_4|)$$
$$= (2254 + 4508n)$$

$$6.SCI_1(TPE_n) = \frac{1}{\sqrt{2+2}}(|E_1|) + \frac{1}{\sqrt{2+3}}(|E_2|) + \frac{1}{\sqrt{3+3}}(|E_3|)$$
$$+ \frac{1}{\sqrt{3+6}}(|E_4|)$$
$$= 14n + \frac{\sqrt{6}(19n+38)}{6} + \frac{\sqrt{5}(28n+56)}{5} + 28$$

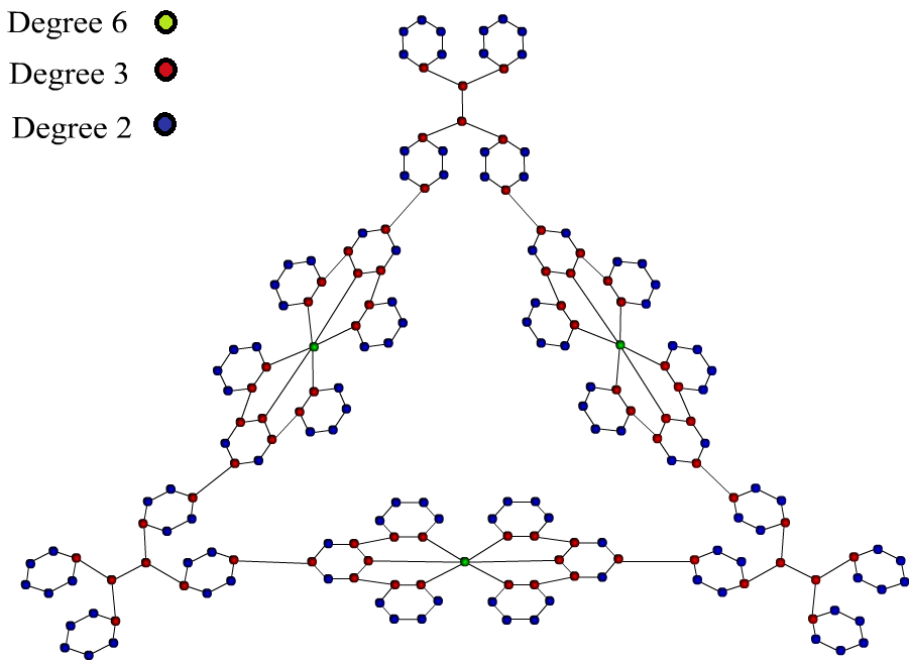
$$7.\chi_\alpha(TPE_n) = (2+2)^\alpha(|E_1|) + (3+2)^\alpha(|E_2|) + (3+3)^\alpha(|E_3|)$$
$$+ (3+6)^\alpha(|E_4|)$$
$$= 66n + \sqrt{6}(19n+38) + \sqrt{5}(28n+56) + 132$$

$$8.GA(TPE_n) = \frac{2\sqrt{2\times 2}}{2+2}(|E_1|) + \frac{2\sqrt{3\times 2}}{3+2}(|E_2|) + \frac{2\sqrt{3\times 3}}{3+3}(|E_3|)$$
$$+ \frac{2\sqrt{3\times 6}}{3+6}(|E_4|)$$
$$= (48+24n) + \frac{2\sqrt{6}}{5}(56+28n) + (38+19n) + \frac{2\sqrt{18}}{9}(12+6n)$$

$$9.ABC(TPE_n) = \sqrt{\frac{2+2-2}{2\times 2}}(|E_1|) + \sqrt{\frac{2+3-2}{2\times 3}}(|E_2|) + \sqrt{\frac{3+3-2}{3\times 3}}(|E_3|)$$
$$+ \sqrt{\frac{3+6-2}{3\times 6}}(|E_4|)$$

$$10.H(TPE_n) = \frac{2}{2+2}(|E_1|) + \frac{2}{2+3}(|E_2|) + \frac{2}{3+3}(|E_3|) + \frac{2}{3+6}(|E_4|)$$
$$= \frac{463n}{15} + \frac{926}{15}$$

Hence we have computed all the ten indices (See Table 1) for the n dimensional TPE growth G_1. The TPE growth G_1 with dimension $n = 1$ is shown in Figure 4. □



(a)

Figure 4: Growth G_1 Tetraphenykethylene TPE_1

Theorem 2. *Let G_2 be the growth of n dimensional supramolucular rosettes graph TPE_n then*

$$1.M_1(TPE_n) = 742n + 1472$$

$$2.M_2(TPE_n) = 1011n + 1998$$

$$3.R(TPE_n) = \frac{89n}{3} + \frac{\sqrt{2}(12n+24)}{6} + \frac{\sqrt{6}(56n+100)}{6} + \frac{196}{3}$$

$$4.R_\alpha(TPE_n) = \frac{89n}{3} + \frac{\sqrt{2}(12n+24)}{6} + \frac{\sqrt{6}(56n+100)}{6} + \frac{196}{3}$$

$$5.HM(TPE_n) = (4208 + 8308n)$$

$$6.SCI_1(TPE_n) = 22n + \frac{\sqrt{6}(35n+70)}{6} + \frac{\sqrt{5}(56n+100)}{5} + 50$$

$$7.\chi_\alpha(TPE_n) = 22n + \frac{\sqrt{6}(35n+70)}{6} + \frac{\sqrt{5}(56n+100)}{5} + 50$$

$$8.GA(TPE_n) = (84 + 36n) + \frac{2\sqrt{6}}{5}(100 + 56n) + (70 + 35n) + \frac{2\sqrt{18}}{9}(24 + 12n)$$

$$9.ABC(TPE_n) = \frac{70n}{3} + \frac{\sqrt{14}(12n+24)}{6} + \frac{\sqrt{2}(36n+84)}{2} + \frac{\sqrt{2}(56n+100)}{2} + \frac{140}{3}$$

$$10.H(TPE_n) = \frac{821n}{15} + \frac{332}{3}$$

Proof. Let the cardinality of vertex set and edge set of the n dimensional (TPE) and (TPY) supramolucular rosettes graph G_2 be $|V(TPE_n)| = 224 + 112n$ and $|E(TPE_n)| = 278 + 139n$ respectively. Consider the edge partitions of the graph related to the degrees of the terminal vertices of each and every

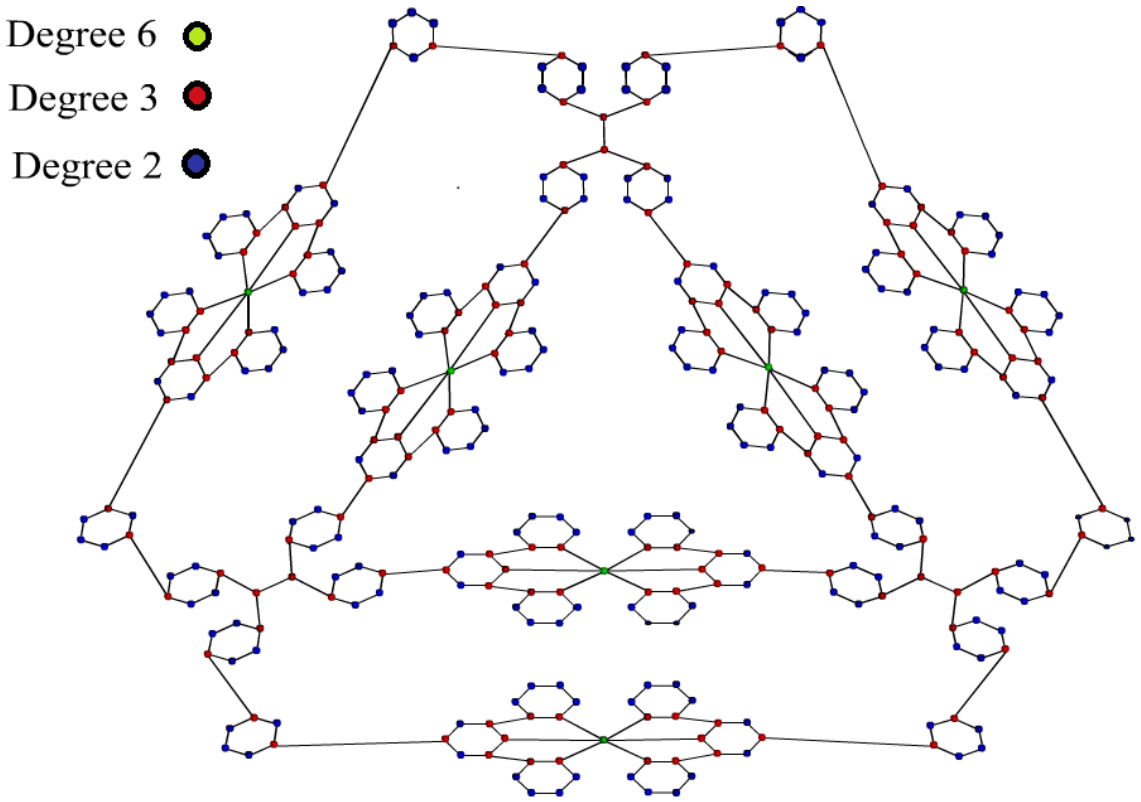
edge. By applying the formulae of the indices above, we compute all the indices.

Further from Table 3

$$
\begin{aligned}
1.M_1(TPE_n) &= (2+2)(|E_1|) + (3+2)(|E_2|) + (3+3)(|E_3|) + (3+6)(|E_4|) \\
&= 742n + 1472 \\
2.M_2(TPE_n) &= (2\times 2)(|E_1|) + 2(|E_2|) + (3\times 3)(|E_3|) \\
&+ (3\times 6)(|E_4|) \\
&= 1011n + 1998 \\
3.R(TPE_n) &= \frac{1}{\sqrt{2\times 2}}(|E_1|) + \frac{1}{\sqrt{2\times 3}}(|E_2|) + \frac{1}{\sqrt{3\times 3}}(|E_3|) \\
&+ \frac{1}{\sqrt{3\times 6}}(|E_4|) \\
&= \frac{89n}{3} + \frac{\sqrt{2}(12n+24)}{6} + \frac{\sqrt{6}(56n+100)}{6} + \frac{196}{3} \\
4.R_\alpha(TPE_n) &= (2\times 2)^\alpha(|E_1|) + (2\times 2)^\alpha(|E_2|) \\
&+ (3\times 3)^\alpha(|E_3|) + (3\times 6)^\alpha(|E_4|) \\
&= \frac{89n}{3} + \frac{\sqrt{2}(12n+24)}{6} + \frac{\sqrt{6}(56n+100)}{6} + \frac{196}{3} \\
5.HM(TPE_n) &= (2+2)^2(|E_1|) + (2+3)^2(|E_2|) + (3+3)^2(|E_3|) \\
&+ (3+6)^2(|E_4|) \\
&= 16(84+36n) + 25(100+56n) + 36(70+35n) + 81(24+12n) \\
&= (4208 + 8308n) \\
6.SCI_1(TPE_n) &= \frac{1}{\sqrt{2+2}}(|E_1|) + \frac{1}{\sqrt{2+3}}(|E_2|) + \frac{1}{\sqrt{3+3}}(|E_3|) \\
&+ \frac{1}{\sqrt{3+6}}(|E_4|) \\
&= 22n + \frac{\sqrt{6}(35n+70)}{6} + \frac{\sqrt{5}(56n+100)}{5} + 50 \\
7.\chi_\alpha(TPE_n) &= (2+2)^\alpha(|E_1|) + (3+2)^\alpha(|E_2|) + (3+3)^\alpha(|E_3|) \\
&+ (3+6)^\alpha(|E_4|) \\
&= 108n + \sqrt{6}(12n+24) + \sqrt{5}(56n+100) + 240 \\
8.GA(TPE_n) &= \frac{2\sqrt{2\times 2}}{2+2}(|E_1|) + \frac{2\sqrt{3\times 2}}{3+2}(|E_2|) + \frac{2\sqrt{3\times 3}}{3+3}(|E_3|) \\
&+ \frac{2\sqrt{3\times 6}}{3+6}(|E_4|) \\
&= (84+36n) + \frac{2\sqrt{6}}{5}(100+56n) + (70+35n) + \frac{2\sqrt{18}}{9}(24+12n)
\end{aligned}
$$

$$
\begin{aligned}
9.ABC(TPE_n) &= \sqrt{\frac{2+2-2}{2\times 2}}(|E_1|) + \sqrt{\frac{2+3-2}{2\times 3}}(|E_2|) + \sqrt{\frac{3+3-2}{3\times 3}}(|E_3|) \\
&+ \sqrt{\frac{3+6-2}{3\times 6}}(|E_4|) \\
&= \frac{70n}{3} + \frac{\sqrt{14}(12n+24)}{6} + \frac{\sqrt{2}(36n+84)}{2} + \frac{\sqrt{2}(56n+100)}{2} + \frac{140}{3} \\
10.H(TPE_n) &= \frac{2}{2+2}(|E_1|) + \frac{2}{2+3}(|E_2|) + \frac{2}{3+3}(|E_3|) + \frac{2}{3+6}(|E_4|) \\
&= \frac{821n}{15} + \frac{332}{15}
\end{aligned}
$$

Hence we have computed all the ten indices (See Table 1) for the n dimensional TPE growth G_2. The TPE growth G_2 with dimension $n = 1$ is shown in Figure 5. □



(a)

Figure 5: Growth G_2 Tetraphenykethylene TPE_1

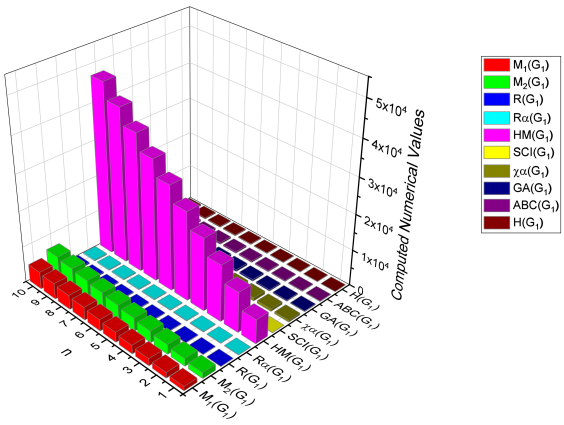
3.1 Computer Based Techniques for tetraphenylethylene (TPE)Supramolecular Rosettes Growth G_1 and G_2

Here we have done the computer based numerical computation work of the growths G_1 and G_2 for all the ten indices which are illustrated in Tables 4 and 5 and the graphical representation of those

numerical values are illustrated in Figures 6 and 7.

Table 4: **Degree based numerical computation for TPE** G_1

n	M_1	M_2	R	R_α	HM	SCI_1	χ_α	GA	ABC	H
1	1212	1629	93.5355	93.5355	6762	102.83	102.83	228.2734	159.5336	92.6000
2	1616	2172	124.714	124.714	11270	137.11	137.11	304.3646	212.7115	123.4667
3	2020	2715	155.8925	155.8925	15778	171.39	171.39	380.4557	265.8894	154.3333
4	2424	3258	187.071	187.071	20286	205.67	205.67	456.5468	319.0673	185.2000
5	2828	3801	218.2495	218.2495	24794	239.95	239.95	532.638	372.2451	216.0667
6	3232	4344	249.428	249.428	29302	274.22	274.22	608.7291	425.4230	246.9333
7	3636	4887	280.6065	280.6065	33810	308.50	308.50	684.8203	478.6009	277.8000
8	4040	5430	311.785	311.785	38318	342.78	342.78	760.9114	531.7788	308.6667
9	4444	5973	342.9635	342.9635	42826	377.06	377.06	837.0025	584.9566	339.5333
10	4848	6516	374.142	374.142	47334	411.34	411.34	913.0937	638.1345	370.4000

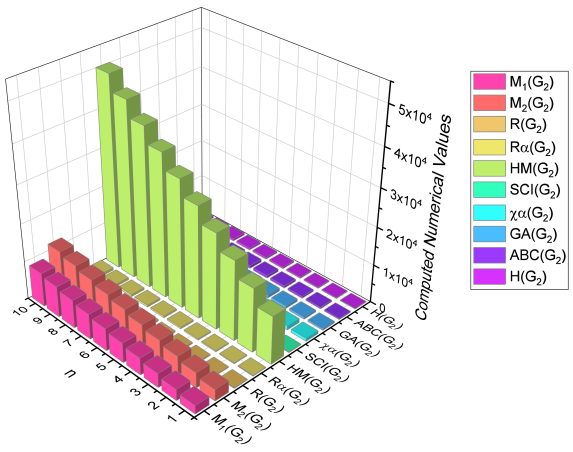


(a)

Figure 6: Graphical representation of numerical computation

Table 5: **Degree based numerical computation for TPE G_2**

n	M_1	M_2	R	R_α	HM	SCI_1	χ_α	GA	ABC	H
1	2214	3009	167.172	167.172	12516	184.63	184.63	411.8	287.6	165.4000
2	2956	4020	222.529	222.529	16724	245.96	245.96	549	383.5	220.1333
3	3698	5031	277.886	277.886	20932	307.29	307.29	686.2	479.4	274.8667
4	4440	6042	333.243	333.243	25140	368.62	368.62	823.3	575.2	329.6000
5	5182	7053	388.6	388.6	29348	429.96	429.96	960.5	671.1	384.3333
6	5924	8064	443.957	443.957	33556	491.29	492.29	1097.7	767.0	439.0667
7	6666	9075	499.314	499.314	37764	552.62	552.62	1234.9	862.8	493.8000
8	7408	10086	554.671	554.671	41972	613.96	613.96	1372.1	958.7	548.5333
9	8150	11097	610.028	610.028	46180	675.29	675.29	1509.2	1054.6	603.2667
10	8892	12108	665.385	665.385	50388	736.62	736.62	1646.4	1150.4	658.0000



(a)

Figure 7: Graphical representation of numerical computation

4 Conclusion

On approaching the conclusion, the degree based topological indices for self built TPE and TPY supramolucular rosettes structures with rosette cycles G_1 and G_2 were found using the edge partitioning technique. Apart from the computation of ten indices the Hyper Zagreb index [71] shows a high level of increasing numerical value from the graphical representation, such that it might give a significant change in the physicochemical properties of TPE and TPY compounds. By any of those high level changes in these compounds, the luminascent efficiency could be developed for future applications.

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