Computing Neighborhood Degree based TI's of Supercoronene and Triangle-shaped Discotic Graphene through NM-polynomial

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Abstract

For a long time, the structure and characteristics of benzene and other arenes have piqued researchers curiosity in quantum chemistry. The structural features of polycyclic aromatic compounds, like the fundamental molecular topology, have a strong influence on their chemical and biological properties. Quantitative structure-activity and property relationship (QSAR/QSPR) techniques for predicting characteristics of polycyclic aromatic compounds (PAC) and related graphs from chemical structures have been developed in this approach. To obtain degree-based topological indices, we have many polynomials. The neighbourhood M-polynomial is one of these polynomials, which is used to produce a number of topological indices based on neighborhood degree sum. In this study, we offer the exact analytical expressions of neighborhood M-polynomial and their corresponding topological indices for supercoronene (SC), cove-hexabenzocoronene (cHBC), and triangular-shaped discotic graphene (TDG) with hexabenzocorenene (HBC) as the base molecule. The findings could help with the development of physicochemical characteristic prediction.

Key Words: Topological index; Neighborhood M-polynomial; supercoronene; cove-hexabenzocoronene; triangular-shaped discotic graphene.

1 Introduction

Chemical graph theory is a branch of graph theory aimed at the study of organic compounds and the understanding or prediction of certain properties of these compounds. The boiling points of molecules

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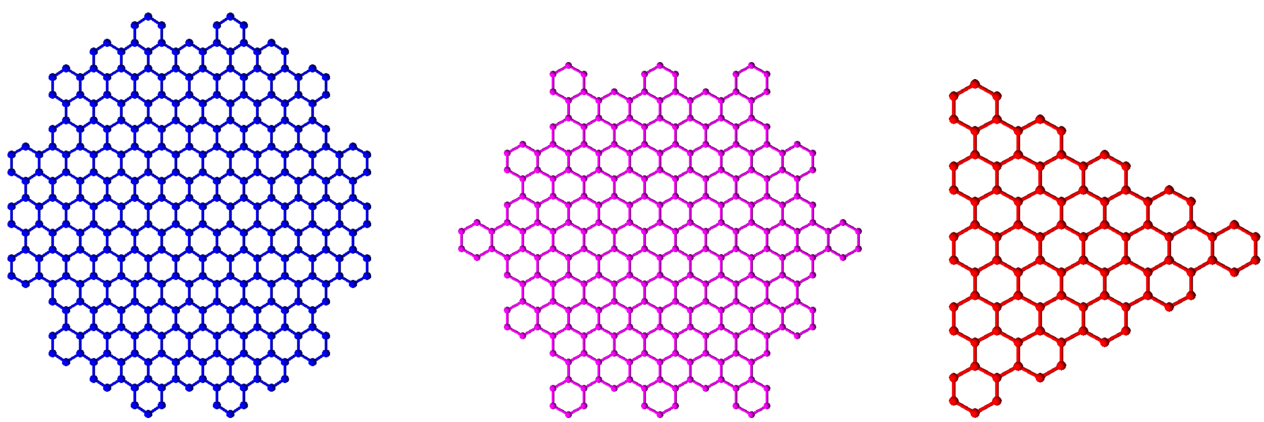
are predicted using molecular graph theory based on the number of components in a molecule and their inter-linkage. It is important in the chemical sciences because it connects the applications of graph theory to molecular problems. Chemists employ a variety of physical properties to figure out how molecules work. The concept of topological index was first introduced by H.Wiener in 1947 when he was investigating the boiling points of alkanes [1]. Following that, plenty of topological indices emerged. Most of the researchers are actively working on topological indices based on neighborhood degree sums of vertices because they have more isomer discrimination ability than degree-based indices.

Polycyclic aromatic hydrocarbons (PAHs), commonly referred to as polyarenes or polynuclear aromatic hydrocarbons, are common environmental pollutants. PAHs are chemical compounds with two or more fused benzene rings that make up a big group [2]. PAHs might theoretically have an endless number of benzene rings, and the arrangement of those benzene rings could result in a large range of isomers. Furthermore, the majority of PAHs investigated have eight or fewer rings, with seven or fewer being the most environmentally relevant [2, 3]. The common properties of PAHs are high melting points, lower vapour pressure, and very low aqueous solubility. PAHs, on the other hand, are very soluble in organic solvents due to their high lipophilicity. The functions of PAHs are physiological action, corrosion resistance, light sensitivity, and heat resistance. In addition, PAHs are used as intermediaries in pharmaceuticals, agricultural products, photographic products, thermosetting polymers, lubricating materials, and other chemical sectors [7]. Using hexa-peri-hexabenzocoronene (HBC) molecules as building blocks, the Müllens research group and others prepared so-called super-PAHs in the year 2000 [8]. Supernaphthalene, supertetracene, superphenalene, supertriphenylene, supertriangulene, and supercoronene are examples of super-PAHs that have two, three, or four superbenzenes bonded together. One important application of PAHs is their use as active materials in optoelectronic devices due to their attractive optical and electronic properties arising from delocalized π-conjugation structures. The delocalized electrons bring about decreased energy gaps and a strong tendency to self-assemble into supramolecular structures through π-π interactions. These properties could be further tuned by their molecular shapes, sizes, and edge structures.

Graphene structures using zig-zag edges have piqued a great deal of attention because they can alter molecular properties such as solubility, three-dimensional form, electrical properties, reactivity, stability, and in addition to causing nonbonding π-electron states in the zig-zag boundary regions. Disc shaped contorted PAHs clench great promise for potential electronic applications, whose functionality differs based on their high degree of extended conjugation, concave π-surfaces and tunable edge boundaries [9].

Fig.1a shows the structure of supercorenene $SC(2)$, which is a large PAHs with HBC as the basic molecule. Large polycyclics are made entirely of condensed hexagonal rings, either by circumscribing the benzene rings or by compressing the base molecule into dimers, trimers, and oligomers. The supercorenene system is made by circumscribing the HBC molecule on its own, and the structures periphery has both armchair and cove-typed edges. The second structure is cove-hexabenzocorenene (cHBC) depicted in Fig.1b, which has n coves on each side of HBC and contains cove type edges on the periphery. Next, we look into triangle-shaped discotic graphene (TDG), see Fig. 1c which is derived from triangulene and has the same amount of carbons as fullerene C_{60} and a big D_{3h} symmetric disc-shaped core [10].

Recently Prabhu et al. studied the molecular structural characterization of Supercorenene, and triangle-shaped discotic graphene. However, no progress has been made on computing neighborhood degree-based topological indices using M-polynomial for super polycyclic aromatic hydrocarbons like supercoronene and cove-hexaenzocoronene using M-polynomials. Compared to degree-based indices, neighborhood degree-based indices have a significant benefit because they have more isomer discrimination ability. As a result, there is a compelling need to compute neighborhood degree-based indices, which will make it easier to synthesis novel PAHs based on their features. In this article, we derive the analytical expression of NM-polynomial for the structures supercoronene $SC(n)$, cove-hexabenzocoronene $cHBC(n)$, and triangular-shaped discotic graphene $TDG(n)$. The numerical values are computed using the analytical expression of the descriptors, and their behavior is observed using 3D graphical plots.



(a) (b) (c)

Figure 1: (a) $SC(3)$; (c) $coveHBC(3)$; (c) $TDG(5)$

2 Preliminaries

We begin this section by defining some basic notions and notations that will be used throughout this study. Consider the carbon atoms and bonds of $SC(n)$, $cHBC(n)$, and $TDG(n)$ as the vertex set $V(G)$, and edge set $E(G)$ of a simple connected graph, respectively. The degree of a vertex b is defined as the total number of edges incident to b and is denoted by d_b. The degree sum of neighbors of a vertex a in G

is denoted by δ_a. We refer to the vertices that are adjacent to that vertex as its neighbors.

The M-polynomial of a graph G, is defined as [11],

$$M(G;x,y) = \sum_{i\leq j} m_{i,j} x^i y^j,$$

where $m_{i,j}$ is the total amount of edges $ab \in E(G)$ such that $\{d_a, d_b\} = \{i,j\}$.

The neighborhood M-polynomial of a graph G is defined as,

$$NM(G;x,y) = \sum_{i\leq j} \chi_{i,j} x^i y^j,$$

where $\chi_{i,j}$ is the total number of edges, where $ab \in E(G)$ such that $\{\delta_a, \delta_b\} = \{i,j\}$. In this article , we will refer to $NM(G;x,y)$ as $NM(G)$

Table 1: Formulation of topological indices for a graph G using neighborhood M-polynomial.

Topological Index	$h(\gamma(a),\gamma(b))$	Derivation from $NM(G:x,y)$
Neighborhood general Randić index (NR_α) [15–19]	$\sum_{ab\in E} = \gamma(a)^\alpha \gamma(b)^\alpha$	$(D_x^\alpha D_y^\alpha)(h(x,y))_{y=1=x}$
Neighborhood general Reciprocal Randić index (NRR_α) [15–19]	$\sum_{ab\in E} = \frac{1}{(\gamma(a)\gamma(b))^\alpha}$	$(S_x^\alpha S_y^\alpha)(h(x,y))_{y=1=x}$
Neighborhood first Zagreb index (NM_1) [20–22]	$\sum_{ab\in E} = \gamma(a) + \gamma(b)$	$(D_x + D_y)(h(x,y))_{y=1=x}$
Neighborhood second Zagreb index (NM_2) [20–22]	$\sum_{ab\in E} = \gamma(a)\cdot\gamma(b)$	$(D_x D_y)(h(x,y))_{y=1=x}$
Neighborhood second modified Zagreb index (NM_2^m) [20–22]	$\sum_{ab\in E} = \frac{1}{(\gamma(a)\gamma(b))}$	$(S_x S_y)(h(x,y))_{y=1=x}$
Third ND_e index ND_3 [23]	$\sum_{ab\in E} = \gamma(a)\gamma(b)(\gamma(a)+\gamma(b))$	$D_x D_y (D_x + D_y)(h(x,y))_{y=1=x}$
Fifth ND_e index (ND_5) [23]	$\sum_{ab\in E} = \frac{\gamma^2(a)+\gamma^2(b)}{\gamma(a)\gamma(b)}$	$(D_x S_y + S_x D_y)(h(x,y))_{y=1=x}$
Neighborhood forgotten topological index (NF) [20, 24]	$\sum_{ab\in E} = \gamma^2(a) + \gamma^2(b)$	$(D_x^2 + D_y^2)(h(x,y))_{y=1=x}$
Neighborhood Harmonic index (NH) [25]	$\sum_{ab\in E} = \frac{2}{\gamma(a)+\gamma(b)}$	$2S_x J(h(x,y))_{x=1}$
Neighborhood inverse sum index (NI) [25]	$\sum_{ab\in E} = \frac{\gamma(a)\gamma(b)}{\gamma(a)+\gamma(b)}$	$S_x J D_x D_y (h(x,y))_{x=1}$
Sanskruti index (S) [26]	$\sum_{ab\in E} = \left[\frac{\gamma(a)\gamma(b)}{\gamma(a)+\gamma(b)-2}\right]^3$	$S_x^3 Q_{-2} J D_x^3 D_y^3 (h(x,y))_{x=1}$

$$D_x = x\frac{\partial(h(x,y))}{\partial x}, D_y = y\frac{\partial(h(x,y))}{\partial y},$$

$$S_x = \int_0^x \frac{(h(x,y))|_{x=z}}{z} dz,$$

$$S_y = \int_0^y \frac{(NM(G))|_{y=z}}{z} dz,$$

$$J(h(x,y)) = h(x,x), Q_\alpha = x^\alpha h(x,y)$$

To know more about neighborhood degree based topological indices and its applications reader can refer [27–41].

3 Methodology

The chemical structure of supercoronene and its derivatives is treated as a simple graph in this work, and topological indices are computed using the NM-polynomial. Edge partition, neighborhood vertex partition, and other combinatorial techniques are employed in the computation of the findings. The numerical values of NM-polynomial graphs are represented using ORIGIN software.

4 Supercoronene

In this section, we discuss the neighborhood M-polynomial and degree sum based topological indices of supercorenene. Let G_1 be a graph of supercoronene represented as $SC(n)$, $n \geq 1$. Then the total number of vertices and edges of the $SC(n)$ are $18n^2 + 54n + 6$, and $27n^2 + 57n - 24$ respectively.

Table 2: The edge partition of $SC(n)$ based on the neighborhood degree-sum of adjacent vertices.

(δ_a, δ_b) Where $ab \in E(G_1)$	Total number of edges
$(4, 5)$	24
$(5, 5)$	$6n - 12$
$(5, 8)$	$12n$
$(6, 8)$	12
$(8, 8)$	$6n + 6$
$(8, 9)$	$12n + 12$
$(9, 9)$	$27n^2 + 39n - 42$

4.1 NM-polynomial of Supercoronene $SC(n)$

Consider a chemical graph G_1 for supercoronene. By using NM-polynomial definition and Table 2, we arrive at

$$\begin{aligned}
NM(G_1, x, y) &= \sum_{i \leq j} E_{i,j}(G_1) x^i y^j \\
&= \sum_{4 \leq 5} |E_{4,5}|(G_1) x^4 y^5 + \sum_{5 \leq 5} |E_{5,5}|(G_1) x^5 y^5 + \sum_{5 \leq 8} |E_{5,8}|(G_1) x^5 y^8 + \sum_{6 \leq 8} |E_{6,8}|(G_1) x^6 y^8 \\
&\quad + \sum_{8 \leq 8} |E_{8,8}|(G_1) x^8 y^8 + \sum_{8 \leq 9} |E_{8,9}|(G_1) x^8 y^9 + \sum_{9 \leq 9} |E_{9,9}|(G_1) x^9 y^9 \\
&= 24x^4y^5 + (6n - 12)x^5y^5 + (12n)x^5y^8 + 12x^6y^8 + (6n + 6)x^8y^8 \\
&\quad + (12n + 12)x^8y^9 + (27n^2 + 39n - 42)x^9y^9
\end{aligned}$$

4.2 Neighborhood degree-based topological indices of supercoronene graph

The NM-polynomial of supercoronene graph G_1 is as follows:

$$\begin{aligned} NM(G_1,x,y) &= 24x^4y^5+(6n-12)x^5y^5+(12n)x^5y^8+12x^6y^8+(6n+6)x^8y^8 \\ &\quad +(12n+12)x^8y^9+(27n^2+39n-42)x^9y^9 \end{aligned}$$

Then,

$$\begin{aligned}
D_xh(x,y) &= 96x^4y^5+5(6n-12)x^5y^5+60nx^5y^8+72x^6y^8+8(6n+6)x^8y^8 \\
&\quad +8(12n+12)x^8y^9+9(27n^2+39n-42)x^9y^9 \\
D_yh(x,y) &= 120x^4y^5+5(6n-12)x^5y^5+96nx^5y^8+96x^6y^8+8(6n+6)x^8y^8 \\
&\quad +9(12n+12)x^8y^9+9(27n^2+39n-42)x^9y^9 \\
(D_x+D_y)h(x,y) &= 216x^4y^5+10(6n-12)x^5y^5+156nx^5y^8+168x^6y^8+16(6n+6)x^8y^8 \\
&\quad +17(12n+12)x^8y^9+18(27n^2+39n-42)x^9y^9 \\
D_xD_yh(x,y) &= 480x^4y^5+25(6n-12)x^5y^5+480nx^5y^8+576x^6y^8+64(6n+6)x^8y^8 \\
&\quad +72(12n+12)x^8y^9+81(27n^2+39n-42)x^9y^9 \\
(D_x^2+D_y^2)h(x,y) &= 984x^4y^5+50(6n-12)x^5y^5+1068nx^5y^8+1200x^6y^8+128(6n+6)x^8y^8 \\
&\quad +145(12n+12)x^8y^9+162(27n^2+39n-42)x^9y^9 \\
(D_x^\alpha D_y^\alpha)h(x,y) &= (24)(20^\alpha)x^4y^5+25^\alpha(6n-12)x^5y^5+(12n)(40^\alpha)x^5y^8+(12)6^\alpha 8^\alpha x^6y^8 \\
&\quad +(6n+6)(64^\alpha)x^8y^8+(12n+12)8^\alpha 9^\alpha x^8y^9 \\
&\quad +(27n^2+39n-42)(81^\alpha)x^9y^9 \\
(D_x+D_y)(D_x+D_y)h(x,y) &= 4320x^4y^5+250(6n-12)x^5y^5+6240nx^5y^8+8064x^6y^8+1024(6n+6)x^8y^8 \\
&\quad +1224(12n+12)x^8y^9+1458(27n^2+39n-42)x^9y^9 \\
S_xS_yh(x,y) &= 24\frac{x^4}{4}\frac{y^5}{5}+(6n-12)\frac{x^5}{5}\frac{y^5}{5}+12n\frac{x^5}{5}\frac{y^8}{8}+12\frac{x^6}{6}\frac{y^8}{8}+(6n+6)\frac{x^8}{8}\frac{y^8}{8} \\
&\quad +(12n+12)\frac{x^8}{8}\frac{y^9}{9}+(27n^2+39n-42)\frac{x^9}{9}\frac{y^9}{9} \\
S_x^\alpha S_y^\alpha h(x,y) &= (24)\frac{x^4}{4^\alpha}\frac{y^5}{5^\alpha}+(6n-12)\frac{x^5}{5^\alpha}\frac{y^5}{5^\alpha}+12n\frac{x^5}{5^\alpha}\frac{y^8}{8^\alpha}+(12)\frac{x^6}{6^\alpha}\frac{x^8}{8^\alpha} \\
&\quad +(6n+6)\frac{x^8}{8^\alpha}\frac{y^8}{8^\alpha}+(12n+12)\frac{x^8}{8^\alpha}\frac{y^9}{9^\alpha}+(27n^2+39n-42)\frac{x^9}{9^\alpha}\frac{y^9}{9^\alpha} \\
(S_yD_x+S_xD_y)h(x,y) &= \left(\frac{246}{5}\right)x^4y^5+(12n-24)x^5y^5+\left(\frac{1068}{40}\right)nx^5y^8+25x^6y^8 \\
&\quad +\left(\frac{1740}{72}n+\frac{1740}{72}\right)x^8y^9+\left(54n^2+78n-84\right)x^9y^9 \\
2S_xJh(x,y) &= 2\Bigg[\left(\frac{24}{9}\right)x^9+\left(\frac{1}{10}\right)(6n-12)x^{10}+\left(\frac{12}{13}\right)nx^{13}+\left(\frac{12}{14}\right)x^{14}
\end{aligned}$$

$$+\left(\frac{1}{16}\right)(6n+6)x^{16}+\left(\frac{1}{17}\right)(12n+12)x^{17}$$
$$+\left(\frac{1}{18}\right)(27n^2+39n-42)x^{18}\Bigg]$$
$$S_xJD_xD_yh(x,y)=\left[\left(\frac{480}{9}\right)x^9+\left(\frac{25}{10}\right)(6n-12)x^{10}+\left(\frac{480}{13}\right)nx^{13}+\left(\frac{576}{14}\right)x^{14}\right.$$
$$+\left(\frac{64}{16}\right)(6n+6)x^{16}+\left(\frac{72}{17}\right)(12n+12)x^{17}$$
$$\left.+\left(\frac{81}{18}\right)(27n^2+39n-42)x^{18}\right]$$
$$S_x^3Q_{-2}JD_x^3D_y^3h(x,y)=\left[\left(\frac{192000}{343}\right)x^7+\left(\frac{15625}{512}\right)(6n-12)x^8+\left(\frac{768000n}{1331}\right)x^{11}+\left(\frac{110592}{1728}\right)x^{12}\right.$$
$$+\left(\frac{262144}{2744}\right)(6n+6)x^{14}+\left(\frac{373248}{3375}\right)(12n+12)x^{15}$$
$$\left.+\left(\frac{531441}{4096}\right)(27n^2+39n-42)x^{16}\right]$$

Using the above results in Table 1, we obtain

(i) $NM_1(G_1)=486n^2+1218n-192.$

(ii) $NM_2(G_1=2187n^2+5037n-1398.$

(iii) ${}^mNM_2(G_1)=\frac{1}{3}n^2+\frac{27689}{21600}n+\frac{15377}{21600}.$

(iv) $ND_3(G_1)=39366n^2+85434n-31020.$

(v) $NF(G_1)=4374n^2+10194n-2712.$

(vi) $NR_\alpha(G_1)=24(20)^\alpha+(6n-12)(25)^\alpha+12n(40)^\alpha+12(48)^\alpha+(6n+6)(64)^\alpha+(12n+12)(72)^\alpha$
$+(27n^2+39n-42)(81)^\alpha.$

(vii) $NRR_\alpha(G_1)=24\big(\frac{1}{20^\alpha}\big)+(6n-12)(\frac{1}{25^\alpha})+12n(\frac{1}{40^\alpha})+12(\frac{1}{48^\alpha})+(6n+6)(\frac{1}{64^\alpha})+(12n+12)(\frac{1}{72^\alpha})$
$+(27n^2+39n-42)(\frac{1}{81^\alpha}).$

(viii) $ND_5(G_1)=54n^2+\frac{26247}{10}n+\frac{12371}{5}.$

(ix) $NH(G_1)=3n^2+\frac{477}{50}n+\frac{107}{50}.$

(x) $NI(G_1)=\frac{243}{2}n^2+\frac{3542}{5}n-\frac{497}{10}.$

(xi) $S(G_1)=\frac{17516}{5}n^2+\frac{15441}{2}n+107240.$

5 Cove-hexabenzocoronene

In this section, we discuss the neighborhood M-polynomial and degree sum based topological indices of cove-hexabenzocoronene. Let G_2 be a graph of cove-hexabenzocoronene is represented as $cHBC(n)$, $n \geq 1$. Then the total number of vertices and edges of the $covHBC(n)$ are $54n^2 - 90n + 42$, and $81n^2 - 147n + 72$ respectively.

Table 3: The edge partition of $cHBC(n)$ based on the neighborhood degree-sum of adjacent vertices.

(δ_a, δ_b) Where $ab \in E(G_2)$	Total number of edges
$(4,4)$	6
$(4,5)$	$12n - 12$
$(5,8)$	$12n - 12$
$(6,8)$	$12n - 12$
$(8,8)$	$6n + 6$
$(8,9)$	$24n - 36$
$(9,9)$	$81n^2 - 213n + 132$

5.1 NM-polynomial of cove-hexabenzocoronene($cHBC(n)$)

Consider a chemical graph G_2 for cove-hexabenzocoronene. By using NM-polynomial definition and Table 3, we arrive at

$$\begin{aligned}
NM(G_2, x, y) &= \sum_{i \leq j} E_{i,j}(G_2) x^i y^j \\
&= \sum_{4 \leq 4} |E_{4,4}|(G_2) x^4 y^4 + \sum_{4 \leq 5} |E_{4,5}|(G_2) x^4 y^5 + \sum_{5 \leq 8} |E_{5,8}|(G_2) x^5 y^8 \\
&\quad + \sum_{6 \leq 8} |E_{6,8}|(G_2) x^6 y^8 + \sum_{8 \leq 8} |E_{8,8}|(G_2) x^8 y^8 + \sum_{8 \leq 9} |E_{8,9}|(G_2) x^8 y^9 + \sum_{9 \leq 9} |E_{9,9}|(G_2) x^9 y^9 \\
&= 6x^4y^4 + (12n - 12)x^4y^5 + (12n - 12)x^5y^8 + (12n - 12)x^6y^8 + (6n + 6)x^8y^8 \\
&\quad + (24n - 36)x^8y^9 + (81n^2 - 213n + 132)x^9y^9
\end{aligned}$$

5.2 Neighborhood degree-based topological indices of cove-hexabenzocoronene using NM-polynomial

The NM-polynomial of cove-hexabenzocoronene graph G_2 is as follows:

$$NM(G_2, x, y) = 6x^4y^4 + (12n - 12)x^4y^5 + (12n - 12)x^5y^8 + (12n - 12)x^6y^8 + (6n + 6)x^8y^8$$

$$+ (24n-36)x^8y^9 + (81n^2-213n+132)x^9y^9$$

Then,

$$\begin{aligned}
D_xh(x,y) &= 24x^4y^4 + 4(12n-12)x^4y^5 + 5(12n-12)x^5y^8 + 6(12n-12)x^6y^8 \\
&\quad + 8(6n+6)x^8y^8 + 8(24n-36)x^8y^9 + 9(81n^2-213n+132)x^9y^9 \\
D_yh(x,y) &= 24x^4y^4 + 5(12n-12)x^4y^5 + 8(12n-12)x^5y^8 + 8(12n-12)x^6y^8 \\
&\quad + 8(6n+6)x^8y^8 + 9(24n-36)x^8y^9 + 9(81n^2-213n+132)x^9y^9 \\
(D_x+D_y)h(x,y) &= 48x^4y^4 + 9(12n-12)x^4y^5 + 13(12n-12)x^5y^8 + 14(12n-12)x^6y^8 \\
&\quad + 16(6n+6)x^8y^8 + 17(24n-36)x^8y^9 + 18(81n^2-213n+132)x^9y^9 \\
D_xD_yh(x,y) &= 96x^4y^4 + 20(12n-12)x^4y^5 + 40(12n-12)x^5y^8 + 48(12n-12)x^6y^8 \\
&\quad + 64(6n+6)x^8y^8 + 72(24n-36)x^8y^9 + 81(81n^2-213n+132)x^9y^9 \\
(D_x^2+D_y^2)h(x,y) &= 192x^4y^4 + 41(12n-12)x^4y^5 + 89(12n-12)x^5y^8 + 100(12n-12)x^6y^8 \\
&\quad + 128(6n+6)x^8y^8 + 145(24n-36)x^8y^9 + 162(81n^2-213n+132)x^9y^9 \\
(D_x^\alpha D_y^\alpha)h(x,y) &= (6)(16^\alpha)x^4y^4 + 20^\alpha(12n-12)x^4y^5 + 40^\alpha(12n-12)x^5y^8 + 48^\alpha(12n-12)x^6y^8 \\
&\quad + 64^\alpha(6n+6)x^8y^8 + 72^\alpha(24n-36)x^8y^9 + 81^\alpha(81n^2-213n+132)x^9y^9 \\
(D_xD_y)(D_x+D_y)h(x,y) &= 768x^4y^4 + 180(12n-12)x^4y^5 + 520(12n-12)x^5y^8 + 672(12n-12)x^6y^8 \\
&\quad + 1024(6n+6)x^8y^8 + 1224(24n-36)x^8y^9 + 1458(81n^2-213n+132)x^9y^9 \\
S_xS_yh(x,y) &= 6\frac{x^4}{4}\frac{y^4}{4} + (12n-12)\frac{x^4}{4}\frac{y^5}{5} + (12n-12)\frac{x^5}{5}\frac{y^8}{8} + (12n-12)\frac{x^6}{6}\frac{y^8}{8} \\
&\quad + (6n+6)\frac{x^8}{8}\frac{y^8}{8} + (24n-36)\frac{x^8}{8}\frac{y^9}{9} + (81n^2-213n+132)\frac{x^9}{9}\frac{y^9}{9} \\
S_x^\alpha S_y^\alpha h(x,y) &= 6\frac{x^4}{4^\alpha}\frac{y^4}{4^\alpha} + (12n-12)\frac{x^4}{4^\alpha}\frac{y^5}{5^\alpha} + (12n-12)\frac{x^5}{5^\alpha}\frac{y^8}{8^\alpha} + (12n-12)\frac{x^6}{6^\alpha}\frac{y^8}{8^\alpha} \\
&\quad + (6n+6)\frac{x^8}{8^\alpha}\frac{y^8}{8^\alpha} + (24n-36)\frac{x^8}{8^\alpha}\frac{y^9}{9^\alpha} + (81n^2-213n+132)\frac{x^9}{9^\alpha}\frac{y^9}{9^\alpha} \\
(S_yD_x+S_xD_y)h(x,y) &= 12x^4y^4 + (\frac{41}{20})(12n+12)x^4y^5 + (\frac{89}{40})(12n+12)x^5y^8 + (\frac{100}{48})(12n+12)x^6y^8 \\
&\quad + (12n+12)x^8y^8 + (\frac{145}{72})(24n-36)x^8y^9 + 2(81n^2-213n+132)x^9y^9 \\
2S_xJh(x,y) &= 2\Bigg[\left(\frac{6}{8}\right)x^8 + \left(\frac{1}{9}\right)(12n-12)x^9 + \left(\frac{1}{13}\right)(12n-12)x^{13} + \left(\frac{1}{14}\right)(12n-12)x^{14} \\
&\quad + \left(\frac{1}{16}\right)(6n+6)x^{16} + \left(\frac{1}{17}\right)(24n-36)x^{17} \\
&\quad + \left(\frac{1}{18}\right)(81n^2-213n+132)x^{18}\Bigg] \\
S_xJD_xD_yh(x,y) &= \Bigg[\left(\frac{96}{8}\right)x^8 + \left(\frac{20}{9}\right)(12n-12)x^9 + \left(\frac{40}{13}\right)(12n-12)x^{13} + \left(\frac{48}{14}\right)(12n-12)x^{14}
\end{aligned}$$

$$+\left(\frac{64}{16}\right)(6n+6)x^{16}+\left(\frac{72}{17}\right)(24n-36)x^{17}$$
$$+\left(\frac{81}{18}\right)(81n^2-213n+132)x^{18}\Bigg]$$

$$S_x^3Q_{-2}JD_x^3D_y^3h(x,y)=\Bigg[\left(\frac{24576}{216}\right)x^8+\left(\frac{800}{343}\right)(12n-12)x^9+\left(\frac{64000}{1331}\right)(12n-12)x^{13}$$
$$+\left(\frac{110592}{1728}\right)(12n-12)x^{14}+\left(\frac{262144}{2744}\right)(6n+6)x^{16}+\left(\frac{373248}{3375}\right)(24n-36)x^{17}$$
$$+\left(\frac{531441}{4096}\right)(81n^2-2123n+1322)x^{18}\Bigg]$$

Using the above results in Table 1, we get

(i) $NM_1(G_2)=1458n^2-2898n+1476$.

(ii) $NM_2(G_2=6561n^2-1384n+7284$.

(iii) ${}^mNM_2(G_2)=n^2-\frac{21}{20}n+\frac{11}{25}$.

(iv) $ND_3(G_2)=118098n^2-258570n+138840$.

(v) $NF(G_2)=13122n^2-27498n+14364$.

(vi) $NR_\alpha(G_2)=6(16)^\alpha+(12n-12)(20)^\alpha+(12n-12)(40)^\alpha+(12n-12)(48)^\alpha+(6n+6)(64)^\alpha$
$+(24n-36)(72)^\alpha+(81n^2-213n+132)(81)^\alpha$

(vii) $NRR_\alpha(G_2)=6\big(\frac{1}{16^\alpha}\big)+(12n-12)(\frac{1}{20^\alpha})+(12n-12)(\frac{1}{40^\alpha})+(12n-12)(\frac{1}{48^\alpha})+(6n+6)(\frac{1}{64^\alpha})$
$+(24n-36)(\frac{1}{72^\alpha})+(81n^2-213n+132)(\frac{1}{81^\alpha})$.

(viii) $ND_5(G_2)=162n^2-\frac{7234}{25}n+\frac{696}{5}$.

(ix) $NH(G_2)=9n^2-\frac{693}{50}n+\frac{129}{20}$.

(x) $NI(G_2)=\frac{729}{2}n^2-\frac{18203}{25}n+\frac{37279}{100}$.

(xi) $S(G_2)=10509n^2-22784n+12207$.

6 Triangel-shaped discotic graphene

In this section, we discuss the neighborhood M-polynomial and degree sum based topological indices of triangle-shaped discotic graphene. Let G_3 be a graph of triangle-shaped discotic graphene is represented as $TDG(n)$, n is odd. Then the total number of vertices and edges of the $TDG(n)$ are $3n^2+3n$, and $(9n^2+3n)/2$ respectively.

6.1 NM-polynomial of triangle-shaped discotic graphene $TDG(n)$

Table 4: The edge partition of $TDG(n)$ based on the neighborhood degree-sum of adjacent vertices.

(δ_a, δ_b) Where $ab \in E(G_3)$	Total number of edges
$(4,4)$	3
$(4,5)$	6
$(5,5)$	$3n-6$
$(5,8)$	$6n-6$
$(8,8)$	$3n$
$(8,9)$	$6n-12$
$(9,9)$	$\frac{9}{2}n^2 - \frac{33}{2}n + 15$

Consider a chemical graph G_3 for $TDG(n)$, by using NM-polynomial definition and Table 4, we arrive at

$$
\begin{aligned}
NM(G_3,x,y) &= \sum_{i\leq j} E_{i,j}(G_3)x^iy^j \\
&= \sum_{4\leq 4} |E_{4,4}|(G_3)x^4y^4 + \sum_{4\leq 5} |E_{4,5}|(G_3)x^4y^5 + \sum_{5\leq 5} |E_{5,5}|(G_3)x^5y^5 + \sum_{5\leq 8} |E_{5,8}|(G_3)x^5y^8 \\
&\quad + \sum_{8\leq 8} |E_{8,8}|(G_3)x^8y^8 + \sum_{8\leq 9} |E_{8,9}|(G_3)x^8y^9 + \sum_{9\leq 9} |E_{9,9}|(G_3)x^9y^9 \\
&= 3x^4y^4 + 6x^4y^5 + (3n-6)x^5y^8 + (6n-6)x^6y^8 + (3n)x^8y^8 \\
&\quad + (6n-12)x^8y^9 + \frac{1}{2}(9n^2-33n+30)x^9y^9
\end{aligned}
$$

6.2 Neighborhood degree-based topological indices of triangle-shaped discotic graphene graph

The NM-polynomial of triangle-shaped discotic graphene graph G_3 is as follows:

$$
\begin{aligned}
NM(G_3,x,y) = 3x^4y^4 + 6x^4y^5 + (3n-6)x^5y^8 + (6n-6)x^6y^8 + (3n)x^8y^8 \\
+ (6n-12)x^8y^9 + \frac{1}{2}(9n^2-33n+30)x^9y^9
\end{aligned}
$$

Then,

$$
\begin{aligned}
D_xh(x,y) &= 12x^4y^4 + 24x^4y^5 + 5(3n-6)x^5y^5 + 5(6n-6)x^5y^8 + (24n)x^8y^8 \\
&\quad + 8(6n-12)x^8y^9 + \frac{9}{2}(9n^2-33n+30)x^9y^9 \\
D_yh(x,y) &= 12x^4y^4 + 30x^4y^5 + 5(3n-6)x^5y^5 + 8(6n-6)x^5y^8 + (24n)x^8y^8
\end{aligned}
$$

$$
\begin{aligned}
&+ 9(6n-12)x^8y^9 + \frac{9}{2}(9n^2-33n+30)x^9y^9 \\
(D_x+D_y)h(x,y) &= 24x^4y^4 + 54x^4y^5 + 10(3n-6)x^5y^5 + 13(6n-6)x^5y^8 + (48n)x^8y^8 \\
&+ 17(6n-12)x^8y^9 + 9(9n^2-33n+30)x^9y^9 \\
D_xD_yh(x,y) &= 48x^4y^4 + 120x^4y^5 + 25(3n-6)x^5y^5 + 40(6n-6)x^5y^8 + (192n)x^8y^8 \\
&+ 72(6n-12)x^8y^9 + \frac{81}{2}(9n^2-33n+30)x^9y^9 \\
(D_x^2+D_y^2)h(x,y) &= 96x^4y^4 + 216x^4y^5 + 50(3n-6)x^5y^5 + 65(6n-6)x^5y^8 + (384n)x^8y^8 \\
&+ 136(6n-12)x^8y^9 + 81(9n^2-33n+30)x^9y^9 \\
(D_x^\alpha D_y^\alpha)h(x,y) &= (3)(16^\alpha)x^4y^4 + (6)20^\alpha x^4y^5 + (3n-6)(25^\alpha)x^5y^5 + (6n-6)(40^\alpha)x^5y^8 \\
&+ (3n)(64^\alpha)x^8y^8 + (6n-12)(72^\alpha)x^8y^9 \\
&+ \frac{1}{2}(9n^2-33n+30)(81^\alpha)x^9y^9 \\
(D_x+D_y)(D_x+D_y)h(x,y) &= 384x^4y^4 + 1080x^4y^5 + 250(3n-6)x^5y^5 + 520(6n-6)x^5y^8 + (3072n)x^8y^8 \\
&+ 1224(6n-12)x^8y^9 + 729(9n^2-33n+30)x^9y^9 \\
S_xS_yh(x,y) &= 3\frac{x^4}{4}\frac{y^4}{4} + 6\frac{x^4}{4}\frac{y^5}{5} + (3n-6)\frac{x^5}{5}\frac{y^5}{5} + (6n-6)\frac{x^5}{5}\frac{y^8}{8} + (3n)\frac{x^8}{8}\frac{y^8}{8} \\
&+ (6n-12)\frac{x^8}{8}\frac{y^9}{9} + \frac{1}{2}(9n^2-33n+40)\frac{x^9}{9}\frac{y^9}{9} \\
S_x^\alpha S_y^\alpha h(x,y) &= 3\frac{x^4}{4^\alpha}\frac{y^4}{4^\alpha} + 6\frac{x^4}{4^\alpha}\frac{y^5}{5^\alpha} + (3n-6)\frac{x^5}{5^\alpha}\frac{y^5}{5^\alpha} + (6n-6)\frac{x^5}{5^\alpha}\frac{y^8}{8^\alpha} + (3n)\frac{x^8}{8\alpha}\frac{y^8}{8^\alpha} \\
&+ (6n-12)\frac{x^8}{8^\alpha}\frac{y^9}{9^\alpha} + \frac{1}{2}(9n^2-33n+40)\frac{x^9}{9^\alpha}\frac{y^9}{9^\alpha} \\
(S_yD_x+S_xD_y)h(x,y) &= 6x^4y^4 + (\frac{246}{20})x^4y^5 + (6n-12)x^5y^5 + \frac{89}{40}(6n-6)x^5y^8 + (6n)x^8y^8 \\
&+ \frac{145}{72}(6n-12)x^8y^9 + (9n^2-33n+30)x^{9y^9} \\
2S_xJh(x,y) &= 2\Bigg[\left(\frac{3}{8}\right)x^8 + \left(\frac{1}{10}\right)(3n-16)x^{10} + \left(\frac{1}{13}\right)(6n-6)x^{13} + \left(\frac{1}{16}(3n)\right)x^{16} \\
&+ \left(\frac{1}{17}\right)(6n-12)x^{17} + \left(\frac{1}{36}\right)(9n^2-33n+30)x^{18} \\
&+ \left(\frac{1}{18}\right)(27n^2+39n-42)x^{18}\Bigg] \\
S_xJD_xD_yh(x,y) &= \Bigg[\left(\frac{48}{8}\right)x^8 + \left(\frac{120}{9}\right)x^9 + \left(\frac{25}{10}\right)(3n-6)x^{10} + \left(\frac{40}{13}(6n-6)\right)x^{13} \\
&+ \left(\frac{192}{16}\right)(n)x^{16} + \left(\frac{72}{17}\right)(6n-12)x^{17} \\
&+ \left(\frac{81}{36}\right)(9n^2-33n+30)x^{18}\Bigg] \\
S_x^3Q_{-2}JD_x^3D_y^3h(x,y) &= \Bigg[\left(\frac{12288}{216}\right)x^6 + \left(\frac{48000}{347}\right)x^7 + \left(\frac{15625(3n-6)}{512}\right)x^8 + \left(\frac{40000(6n-6)}{1331}\right)x^{11}
\end{aligned}
$$

$$+\left(\frac{786432n}{2744}\right)x^{14}+\left(\frac{373248(6n-12)}{3375}\right)x^{15}$$
$$\left.+\left(\frac{531441}{8192}(27n^2+39n-42)\right)x^{16}\right]$$

Using the above results in Table 1, we get

(i) $NM_1(G_3) = 81n^2 - 39n + 6$.

(ii) $NM_2(G_3 = \frac{729}{2}n^2 - \frac{795}{2}n + 129$.

(iii) ${}^{m}NM_2(G_3) = \frac{139}{2500}n^2 + \frac{393}{2000}n - \frac{29}{250}$.

(iv) $ND_3(G_3) = 6561n^2 - 9771n + 4026$.

(v) $NF(G_3) = 729n^2 - 735n + 108$.

(vi) $NR_\alpha(G_3) = (3)(16^\alpha) + (6)20^\alpha + (3n-6)(25^\alpha) + (6n-6)(40^\alpha) + (3n)(64^\alpha)$
$+ (6n-12)(72^\alpha) + \frac{1}{2}(9n^2 - 33n + 30)(81^\alpha)$.

(vii) $NRR_\alpha(G_3) = 3\left(\frac{1}{16^\alpha}\right) + 6(\frac{1}{20^\alpha}) + (3n-6)(\frac{1}{25^\alpha}) + (6n-6)(\frac{1}{40^\alpha}) + (3n)(\frac{1}{64^\alpha}) + (6n-12)(\frac{1}{72^\alpha})$
$+ \frac{1}{2}(9n^2 - 33n + 30)(\frac{1}{81^\alpha})$.

(viii) $ND_5(G_3) = 9n^2 + \frac{44333}{10000}n - \frac{12167}{10000}$.

(ix) $NH(G_3) = \frac{1}{2}n^2 + \frac{1169}{1517}n + \frac{269}{1250}$.

(x) $NI(G_3) = \frac{81}{4}n^2 - \frac{108767}{10000}n + \frac{20761}{8147}$.

(xi) $S(G_3) = \frac{116771}{100}n^2 - \frac{305961}{100}n + \frac{56469}{25}$.

Table 5: Numerical comparison of neighborhood degree-based indices of the molecular graph $SC(n)$.

n	M_1	M_2	M_2^{nm}	S	NI	$NR_{-\frac{1}{2}}$	$NRR_{-\frac{1}{2}}$	ND_5	NH	NF	ND_3
2	4188	17424	4.59	136690	1853.1	35.63	2087.7	7939.6	33.22	35172	297312
3	7836	33396	7.52	161930	3169	60.98	3909.4	10834	57.76	67236	579576
4	12456	53742	11.11	194170	4727.9	92.32	6217.2	13837	88.30	108048	940572
5	18048	78462	15.36	233420	6529.8	129.67	9010.9	16948	124.84	157608	1380300
6	24612	107556	20.27	279680	8574.7	173.01	12291	20166	167.38	215916	1898760

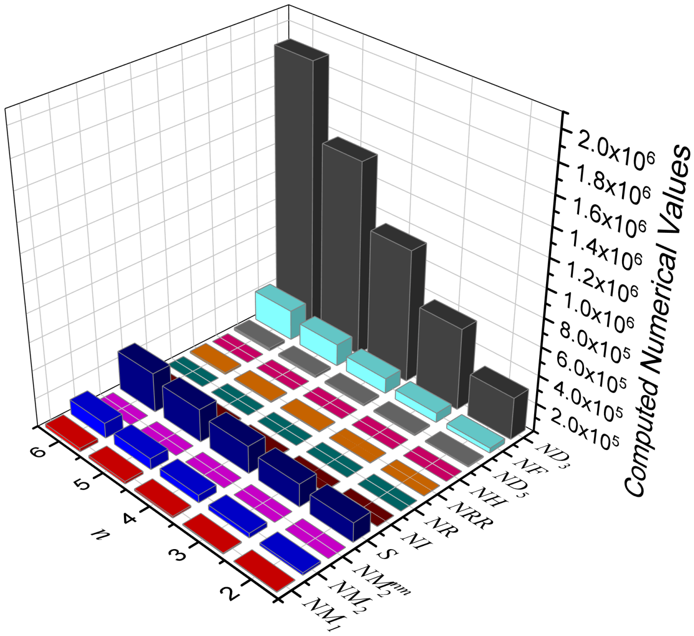


Figure 2: Visualization of numerical values for $SC(n)$ formulated on degree-sum based descriptors.

Table 6: Numerical comparison of neighborhood degree-based indices of the molecular graph $cHBC(n)$.

n	M_1	M_2	M_2^{nm}	S	NI	$NR_{-\frac{1}{2}}$	$NRR_{-\frac{1}{2}}$	ND_5	NH	NF	ND_3
2	1512	30760	2.34	8675	374.55	31.65	2004.6	208.48	14.73	11856	94092
3	5904	62181	6.29	38436	1468.9	56.24	3826.3	729.12	45.87	49968	426012
4	13212	106724	12.24	89215	3292.3	86.84	6134	1573.8	95.01	114324	994128
5	23436	164389	20.19	161012	5844.7	123.43	8927.7	2742.4	162.15	204924	1798440
6	36576	235176	30.14	253827	9126.1	166.03	12207	4235	247.29	321768	2838948

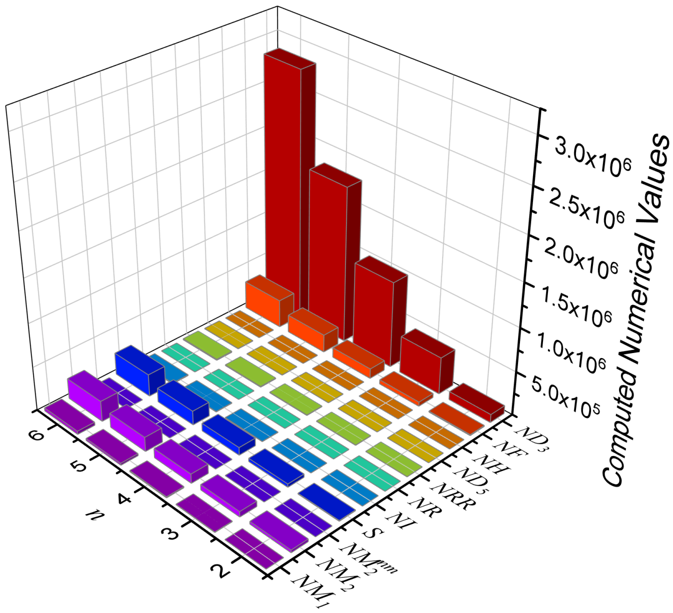


Figure 3: Visualization of numerical values for $cHBC(n)$ formulated on degree-sum based descriptors.

Table 7: Numerical comparison of neighborhood degree-based indices of the molecular graph $TDG(n)$.

n	M_1	M_2	M_2^{nm}	S	NI	$NR_{-\frac{1}{2}}$	$NRR_{-\frac{1}{2}}$	ND_5	NH	NF	ND_3
2	252	792	0.49	810.38	61.79	3.79	124.78	43.64	3.75	1554	10728
3	618	2217	0.97	3589.3	152.16	7.08	306.63	93.08	7.02	4464	33762
4	1146	4371	1.55	8703.7	283.04	11.38	569.49	160.51	11.29	8832	69918
5	1836	7254	2.25	16153	454.41	16.68	913.35	245.94	16.56	14658	119196
6	2688	10866	3.06	25939	666.28	22.98	1338	349.38	22.83	21942	181596

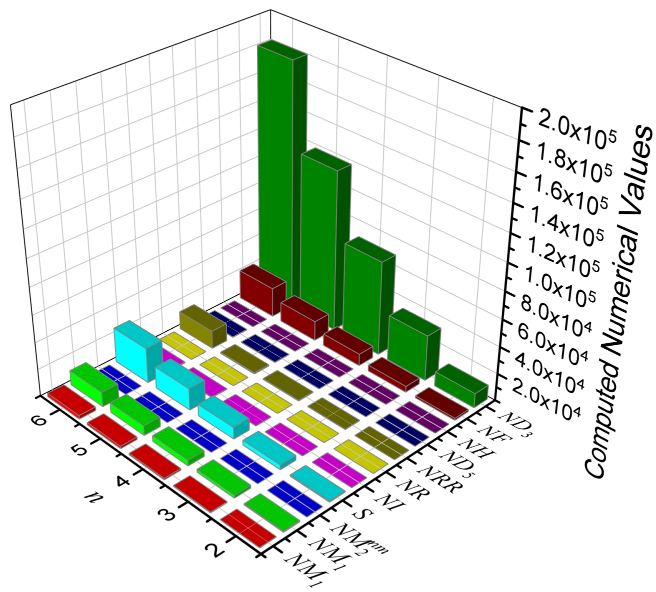


Figure 4: Visualization of numerical values for $TDG(n)$ formulated on degree-sum based descriptors.

7 Conclusion

NM-polynomial methods are used to compute various neighborhood degree based topological indices for the supercoronene, cove-hexabenzocoronene, and triangular-shaped discotic graphene in sections 4, 5 and 6. From Table 5,6, and 7 different values of n are investigated to check the behaviour of indices. The values of topological indices grow as n increases, as shown in Figure 2,3 and 4. Also, among the 11 neighborhood degree based indices evaluated in this study, it is clear that ND_3 has the largest numerical value and that NM_2^m has the lowest value for every *n=1* to *10*. Polycyclic aromatic hydrocarbon compounds (PAH) represent molecules comprising at least two consolidated aromatic rings. They are currently of extraordinary interest as potential semiconducting materials for organic field-effect transistors, light-emitting diodes, and solar panels. Finding topological indices are useful to get the physicochemical properties of PAHs. As the molecular descriptors describe the compounds structural properties, the results obtained here act as a vital tool for understanding the significance of these large-sized aromatic compounds in various fields including predictive toxicology, materials science, astrochemistry, and drug discovery. The values presented in this article would reduce the routine laboratory work in the study of the physicochemical properties of supercoronene, cove-hexabenzocoronene, and triangle-shaped discotic graphene.

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