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Computation of Neighborhood *M*-Polynomial of Cycloparaphenylene and Its Variants

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ABSTRACT: In the domains of materials and chemical and physical sciences, a significant aspiration is to design and synthesize extensively conjugated macrocycles possessing precisely defined structures. This objective bears substantial promise across a wide range of scientific and technological fields. These molecules offer a unique blend of structural complexity and electronic properties that make them particularly intriguing for both theoretical and practical reasons. Cycloparaphenylene (CPP) radial π-conjugated macrocycles is a specific example of a conjugated macrocycle that has garnered significant attention in the field of chemistry and materials science. It consists of a series of benzene rings linked together in a cyclic arrangement, forming a one-dimensional structure. CPP systems have been on the rise due to their novel and captivating characteristics, encompassing properties, such as electronic properties, heightened electrical conductivity, optoelectronic traits, and mechanical properties. Given the potential applications of CPP, it becomes essential to analyze this structure from a theoretical standpoint. Molecular descriptors play a crucial role in the theoretical analysis of such structures. Research on molecular descriptors has unequivocally demonstrated their significant correlation with the diverse properties of chemical compounds. This article illustrates the neighborhood sum *M*-polynomial-based descriptors' calculation using edge-partition techniques for CPP and its sidewalls consisting of pyrene and hexabenzocoronene units. The examination of these neighborhood sum *M*-polynomial-based descriptors for these structures has the potential to establish a foundational framework for delving deeper into CPP and its associated properties.
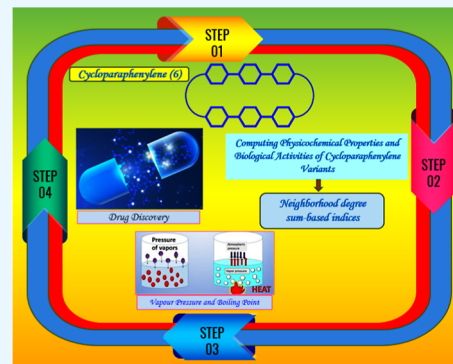
1. INTRODUCTION

Conjugated macrocycles are large cyclic molecules with a series of alternating single and multiple bonds, creating a conjugated π-electron system. These molecules exhibit unique electronic properties due to the delocalization of π-electrons across the cyclic structure.[1−6] Cycloparaphenylene is a term used in organic chemistry to refer to a family of hydrocarbon molecules composed of carbon atoms arranged in a ring structure that resembles a phenyl (C_6H_5) unit. The term "cycloparaphenylene" is often used to describe a series of macrocyclic compounds consisting of multiple phenyl rings connected together in a circular arrangement (see Figure 1).
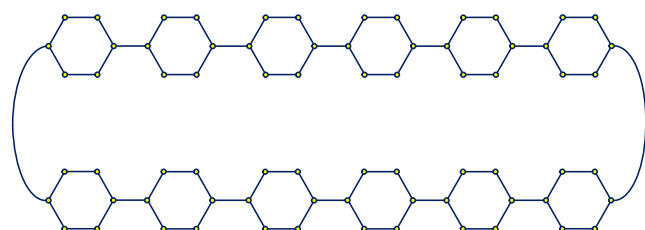

**Figure 1.** Cycloparaphenylene.[12]

These compounds are of interest in the fields of organic chemistry and materials science due to their unique geometric and electronic properties. Their cyclic structure gives them distinct properties that can be utilized in various applications, such as molecular electronics, nanotechnology, optoelectronics, molecular recognition and sensing, drug delivery, supramolecular chemistry, and materials science.[7−15] Cyclo-paraphenylenes (CPPs) have the potential to be used as molecular wires or components in molecular electronic devices due to their well-defined and tenable electronic properties. Their cyclic and planar structures could be employed in the creation of nanocircuits, nanosensors, and other nanoscale devices. Due to their distinctive optical characteristics, CPPs have the potential to be utilized in optoelectronic gadgets like organic photovoltaics (solar cells) and organic light-emitting diodes (OLEDs).[16−29] CPPs can be designed to exhibit
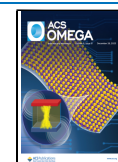
specific binding properties, making them useful in molecular recognition and sensing applications. CPPs could be incorporated into new materials with tailored properties, such as enhanced mechanical strength, thermal stability, or electronic conductivity.[30−35]

The term "CPP nanoring with graphene hexabenzocoronene sidewalls" describes a specific hybrid nanostructure that combines elements from two distinct types of carbon-based molecules: CPPs and hexabenzocoronenes (HBCs), which are commonly referred to as "coronenes". CPP nanoring refers to a cyclic carbon-based structure composed of multiple phenyl rings connected in a closed circular arrangement. Each phenyl ring consists of six carbon atoms arranged in a hexagonal pattern. These rings are linked together to form a ring structure. The term "CPP" refers to this type of structure. HBC is a type of polycyclic aromatic hydrocarbon (PAH) composed of six benzene rings fused together with a circular pattern. It resembles a molecular version of a hexagonal graphene lattice. HBCs are often used in organic electronics and materials due to their unique electronic properties and self-assembly capabilities. The phrase "CPP nanoring with graphene HBC sidewalls" suggests a nanostructure where a cyclic ring made of CPPs serves as the central core or "nanoring". The sides of this nanoring are modified or coated with HBC structures (see Figure 2). This hybrid structure combines the properties of
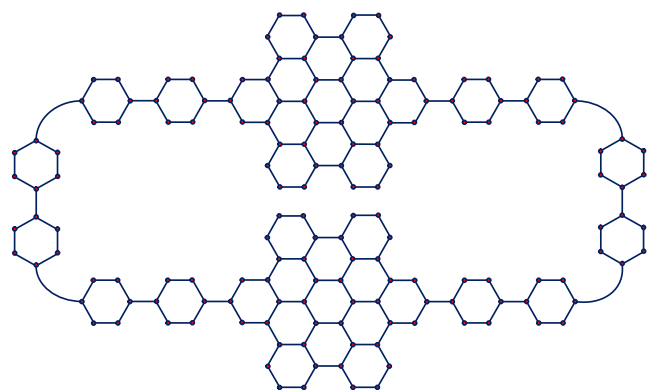
Figure 2. CPP nanoring with graphenic HBC sidewalls.[6]

CPPs, graphene, and HBC potentially resulting in a material with tunable electronic properties, self-assembly behavior, and other unique characteristics.[37−41] It is important to note that the specific properties and potential applications of this hybrid nanostructure would depend on the arrangement, size, and interactions between the different components. This kind of advanced molecular architecture is of interest in fields such as nanotechnology, materials science, and electronics, where researchers are exploring ways to create new materials with tailored properties for various applications.

A pyrene-containing π-extended carbon nanoring refers to a specific type of carbon-based molecular structure that includes the aromatic hydrocarbon pyrene as part of a larger, cyclic π-extended carbon ring. Let us break down the components. Pyrene is a PAH composed of four fused benzene rings with linear arrangement, resulting in a total of 16 carbon atoms (see Figure 3). It is a common component in various organic compounds and materials due to its distinctive electronic and optical properties. A π-extended carbon nanoring is a cyclic arrangement of carbon atoms, where the π electrons (the delocalized electrons in the double bonds of aromatic systems)
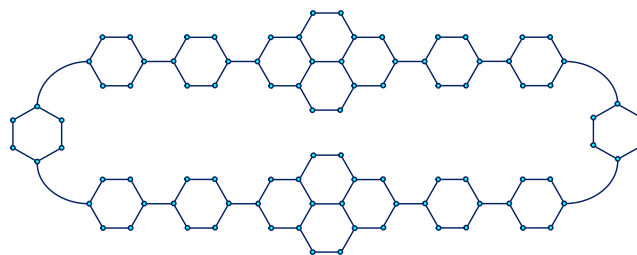
Figure 3. Pyrene-containing π-extended carbon nanoring.[5]

extend over the entire ring structure, contributing to its electronic properties. In this context, "π-extended" refers to the presence of conjugated double bonds that enable the delocalization of π electrons around the ring. This kind of structure could have potential applications in optoelectronics, molecular electronics, and materials science, where the arrangement of π-conjugated systems can influence the behavior and properties of the resulting materials. As with other complex molecular architectures, the specific properties and potential applications of a pyrene-containing π-extended carbon nanoring would depend on the arrangement, size, and interactions between the pyrene units and carbon ring.[42−44]

p-Phenylene refers to a specific arrangement of carbon atoms in an aromatic hydrocarbon molecule. In organic chemistry, the term "p-phenylene" is often used to describe a benzene ring where two adjacent carbon atoms are connected in a para-position (see Figures 4 and 5). The "p" indicates the para-
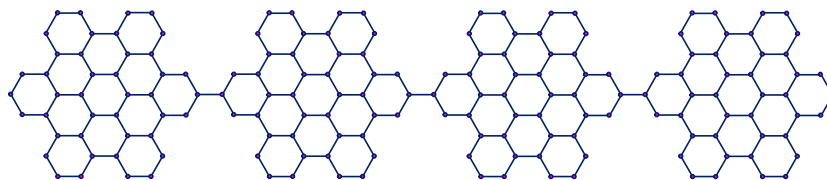
Figure 4. p-Phenylene.[5]

relationship between the carbon atoms. A benzene ring refers to a carbon ring consisting of six members, where single and double bonds alternate between the carbon atoms. In the case of p-phenylene, two carbon atoms within the ring are connected in the para-position, which means that they are located opposite each other in the ring.

The presence of p-phenylene units in molecules can influence their electronic and optical properties, making them important in the development of materials for applications in electronics, optoelectronics, and more.[31,45−47] It is important to note that the field of CPP and its substructure research is still evolving, and these potential applications are based on theoretical predictions and early experimental work.[18,29,31,36,48,51−54] The molecular descriptors are used to analyze these structures theoretically. In this research, the theoretical analysis of CPP and its substructure has been derived using the neighborhood sum M-polynomial-based descriptors. The computed results are compared to understand the behavioral patterns of various substances with respect to the underlying molecular structures. This study is a significant contributor to the existing literature on CPPs as this is the first time that the structures are analyzed using M-polynomial. This study will open up several avenues for exploring these structures from theoretical perspectives.

Figure 5. Poly-p-superphenylenes.[4]

2. GRAPH-THEORETICAL TERMINOLOGIES

A graph $\mathcal{G}$ is a set of vertices, called nodes which are connected by edges, called links. Thus, $\mathcal{G}=(V, E)$. In an undirected graph, a vertex degree is determined by the number of edges that are incident to it with the exception that a loop at a vertex doubles its degree. For an edge $e = uv \in E(\mathcal{G})$,

$$N_u(e|\mathcal{G}) = a \in V(\mathcal{G}): d_{\mathcal{G}(u,a)} \leq d_{\mathcal{G}(v,a)}$$

and

$$M_u(e|\mathcal{G}) = k \in E(\mathcal{G}): d_{\mathcal{G}(u,k)} \leq d_{\mathcal{G}(v,k)}$$

$N_u(e|\mathcal{G})$ and $M_u(e|\mathcal{G})$ are the number of vertices lying closer to the vertex u than v and the number of edges lying closer to the vertex u than v, respectively. It is denoted by $|N_u(e|\mathcal{G})| = n_u(e|\mathcal{G})$ and $|M_u(e|\mathcal{G})| = m_u(e|\mathcal{G})$ are their respective cardinalities.

The M-polynomial of a graph $\mathcal{G}$ is defined as

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

where $N_{i,j}$ is the total number of edges. $uv \in E(\mathcal{G})$ number such that $d\mathcal{G}(u), d\mathcal{G}(v) = i, j$. The NM-polynomial of a graph $\mathcal{G}$ is defined as

$$NM(\mathcal{G}) = \sum_{i \leq j} m_{ij}(\mathcal{G}) x^i y^j$$

where m_{ij} is the total number of edges and $uv \in E(\mathcal{G})$ number such that $\delta\mathcal{G}(u), \delta\mathcal{G}(v) = i, j$.

Now we will discuss an example.

In Figure 6, we have $d_{u1} = 1$, $d_{u2} = 4$, $d_{u3} = 2$, $d_{u4} = 3$, $d_{u5} = 1$, $d_{u6} = 1$, $d_{u7} = 1$, $d_{u8} = 1$, $\delta_{u1} = 4$, $\delta_{u2} = 5$, $\delta_{u3} = 7$, $\delta_{u4} = 4$, $\delta_{u5} = 3$,
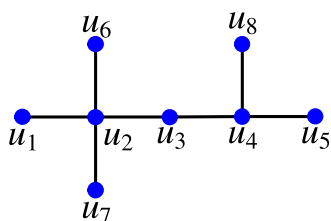

Figure 6. Carbon tree of isooctane.

$\delta_{u6} = 4$, $\delta_{u7} = 4$, and $\delta_{u8} = 3$. Thus, we have $N_{(1,4)} = 3$, $N_{(1,3)} = 2$, $N_{(2,4)} = 1$, $N_{(2,3)} = 1$, $m_{(4,5)} = 3$, $N_{(5,7)} = 1$, $N_{(4,7)} = 1$, and $N_{(3,4)} = 2$. Therefore, the M-polynomial for the carbon tree of isooctane is

$$M(G) = 3xy^4 + 2xy^3 + x^2y^3 + x^2y^4$$

and the NM-polynomial for the carbon tree of isooctane is

$$NM(G) = 3x^4y^5 + x^5y^7 + x^4y^7 + 2x^3y^4$$

Neighborhood degree sum-based topological indices[49,50] defined on edge collection of a graph $\mathcal{G}$ can be represented as

$$I(\mathcal{G}) = \sum_{xy \in E(\mathcal{G}) \varphi(d_x, d_y)}$$

The function of d_x, d_y which is utilized in Table 1 is to build neighborhood degree sum-based indices.

Table 1. Formulation of Topological Indices for a Graph $\mathcal{G}$ Using Neighborhood M-Polynomial

topological Indices	$\varphi(x, y)$	derivation from $NM(\mathcal{G})$
Neighborhood First Zagreb Index[56] $M_1(\mathcal{G})$	$x + y$	$D_x + D_y(NM(\mathcal{G}))|x = y = 1$
Neighborhood Second Zagreb Index[57] $M_2(\mathcal{G})$	xy	$D_x D_y(NM(\mathcal{G}))|x = y = 1$
Neighborhood Second Modified Zagreb Index[57] $M_2^{nm}(\mathcal{G})$	$\dfrac{1}{xy}$	$S_x S_y(NM(\mathcal{G})|x = y = 1$
Neighborhood Forgotten Topological Index[57] $F_N(\mathcal{G})$	$x^2 + y^2$	$D_x^2 + D_y^2(NM(\mathcal{G}))|x = y = 1$
Third Neighborhood Index[57] $ND_3(\mathcal{G})$	$xy(x + y)$	$D_x D_y(D_x + D_y)(NM(\mathcal{G}))|x = y = 1$
Symmetric Division Index[57] $ND_5(\mathcal{G})$	$\left(\dfrac{x^2 + y^2}{xy}\right)$	$(D_x S_y + S_x D_y)(NM(\mathcal{G}))|x = y = 1$
Neighborhood General Randic Index[57] $NR_\alpha(\mathcal{G})$	$x^\alpha y^\alpha$	$D_x^\alpha D_y^\alpha(NM(\mathcal{G}))|x = y = 1$
Neighborhood Harmonic Index[57] $NH(\mathcal{G})$	$\dfrac{2}{x + y}$	$2S_x J(NM(\mathcal{G}))|x = 1$
Neighborhood Inverse Sum Index[57] $NI(\mathcal{G})$	$xyx + y$	$S_x J D_x D_y(NM(\mathcal{G}))|x = 1 y = 1$
Sanskruti Index[55] $S(\mathcal{G})$	$\left(\dfrac{xy}{x + y - 2}\right)^2$	$S_x^3 J D_x^3 D_y^3(NM(\mathcal{G}))|x = 1 y = 1$

3. RESULTS AND DISCUSSION

In this section, we provide accurate expressions for several kinds of CPP-based neighborhood M-polynomial topological indices.

3.1. Lemma 1. If $\mathcal{G}_1$ is the molecular graph of $[n]$CPP, then the NM-polynomial is presented as

$$NM(\mathcal{G}_1) = 2nx^5y^5 + 4nx^5y^7 + nx^7y^7$$

.

3.1.1. Proof. The molecular graph of $[n]$CPP has $6n$ vertices and $7n$ edges. The following categories are used to group its edge frequency. Now, NM-polynomial of $\mathcal{G}_1$ is acquired as follows.

$$NM(\mathcal{G}_1) = \sum_{i \leq j} m_{ij}(\mathcal{G}_1)x^i y^j$$

$$= m_{5,5}x^5 y^5 + m_{5,7}x^5 y^7 + m_{7,7}x^7 y^7$$

$$= 2nx^5 y^5 + 4nx^5 y^7 + nx^7 y^7$$

3.2. Theorem 1. Let $\mathcal{G}_1$ be a molecular graph of $[n]$CPP, then

(i)

$$M_1(\mathcal{G}_1) = 82n$$

(ii)

$$M_2(\mathcal{G}_1) = 239n$$

(iii)

$$M_2{}^{nm}(\mathcal{G}_1) = 0.2147n$$

(iv)

$$F_N(\mathcal{G}_1) = 494n$$

(v)

$$ND_3(\mathcal{G}_1) = 2866n$$

(vi)

$$ND_5(\mathcal{G}_1) = 14.4571n$$

(vii)

$$NR_\alpha(\mathcal{G}_1) = (2(25)^\alpha + 4(35)^\alpha + (49)^\alpha)_n$$

(viii)

$$NH(\mathcal{G}_1) = 0.6048n$$

(ix)

$$NI(\mathcal{G}_1) = 20.1667n$$

(x)

$$S(\mathcal{G}_1) = 300.6191n$$

3.2.1. Proof.

$$(D_x + D_y)(\varphi(x, y)) = 20nx^5 y^5 + 48nx^5 y^7 + 14nx^7 y^7$$

$$D_x D_y(\varphi(x, y)) = 50nx^5 y^5 + 140nx^5 y^7 + 49nx^7 y^7$$

$$S_x S_y(\varphi(x, y)) = \frac{2}{25}nx^5 y^5 + \frac{4}{35}nx^5 y^7 + \frac{1}{49}nx^7 y^7$$

$$(D_x^2 + D_y^2)(\varphi(x, y)) = 100nx^5 y^5 + 296nx^5 y^7 + 98nx^7 y^7$$

$$D_x D_y(D_x + D_y)(\varphi(x, y)) = 500nx^5 y^5 + 1680nx^5 y^7 + 686nx^7 y^7$$

$$(D_x S_y + S_x D_y)(\varphi(x, y)) = 4nx^5 y^5 + \frac{296}{35}nx^5 y^7 + 2nx^7 y^7$$

$$D_x^\alpha D_y^\alpha(\varphi(x, y)) = 2(25)^\alpha nx^5 y^5 + 4(35)^\alpha nx^5 y^7 + (49)^\alpha nx^7 y^7$$

$$S_x J(\varphi(x, y)) = \frac{2}{10}nx^{10} + \frac{4}{12}nx^{12} + \frac{1}{14}nx14$$

$$S_x J D_x D_y(\varphi(x, y)) = \frac{50}{10}nx^{10} + \frac{140}{12}nx^{12} + \frac{49}{14}nx14$$

$$S_x^3 Q_{-2} J D_x^3 D_y^3(\varphi(x, y)) = \frac{31,250}{512}nx^8 + \frac{171,500}{1000}nx^{10} + \frac{117,649}{1728}nx^{12}$$

3.3. Lemma 2. If $\mathcal{G}_2$ is the CPP nanoring with graphenic HBC sidewalls, then the NM-polynomial is presented as

$$NM(\mathcal{G}_2) = 16x^4 y^5 + 4nx^5 y^5 + 8nx^5 y^7 + 16x^5 y^8 + 8x^6 y^7 + 8x^6 y^8 + (2n+2)x^7 y^7 + 12x^8 y^8 + 24x^8 y^9 + 24x^9 y^9$$

3.3.1. Proof. The molecular graph of CPP(HBC) has $12n + 84$ vertices and $14n + 110$ edges. The following categories are used to group its edge frequency. Now, NM-polynomial of $\mathcal{G}_2$ is acquired as follows.

$$NM(\mathcal{G}_2) = \sum_{i \leq j} m_{ij}(\mathcal{G}_2)x^i y^j$$

$$= m_{4,5}x^4 y^5 + m_{5,5}x^5 y^5 + m_{5,7}x^5 y^7 + m_{5,8}x^5 y^8 + m_{6,7}x^6 y^7 + m_{6,8}x^6 y^8 + m_{7,7}x^7 y^7 + m_{8,8}x^8 y^8 + m_{8,9}x^8 y^9 + m_{9,9}x^9 y^9$$

$$= 16x^4 y^5 + 4nx^5 y^5 + 8nx^5 y^7 + 16x^5 y^8 + 8x^6 y^7 + 8x^6 y^8 + (2n+2)x^7 y^7 + 12x^8 y^8 + 24x^8 y^9 + 24x^9 y^9$$

3.4. Theorem 2. Let $\mathcal{G}_2$ be a CPP nanoring with graphenic HBC sidewalls, then

(i)

$$M_1(\mathcal{G}_2) = 164n + 1628$$

(ii)

$$M_2(\mathcal{G}_2) = 478n + 6218$$

(iii)

$$M_2{}^{nm}(\mathcal{G}_2) = (75{,}744n+1{,}628{,}155)/176{,}400$$

(iv)

$$F_N(\mathcal{G}_2)=988n+12{,}660$$

(v)

$$ND_3(\mathcal{G}_2)=5732n+98{,}972$$

(vi)

$$ND_5(\mathcal{G}_2) = (3036n+23{,}687)/105$$

(vii)

$$NR_\alpha(\mathcal{G}_2) = (4(25)^\alpha+8(35)^\alpha+2(49)^\alpha+16(20)^\alpha)_n$$
$$+16(40)^\alpha+8(42)^\alpha+8(48)^\alpha+2(49)^\alpha$$
$$+12(64)^\alpha+24(72)^\alpha+24(81)^\alpha$$

(viii)

$$NH(\mathcal{G}_2) = (831{,}844n+1{,}686{,}225)/278{,}460$$

(ix)

$$NI(\mathcal{G}_2) = (150{,}943n+691{,}623)/1989$$

(x)

$$S(\mathcal{G}_2)=974.42n+8777.34$$

3.4.1. Proof.

3.5. Lemma 3. If $\mathcal{G}_3$ is the pyrene-containing π-extended carbon nanoring, then the NM-polynomial is presented as

$$NM(\mathcal{G}_3) = (4n+4)x^5y^5 + (8n+8)x^5y^7+16x^6y^7$$
$$+ (2n+2)x^7y^7+8x^7y^9+2x^9y^9$$

3.5.1. Proof. The molecular graph of $\mathcal{G}_3$ has $12n + 32$ vertices and $14n + 40$ edges. The following categories are used to group its edge frequency. Now, NM-polynomial of $\mathcal{G}_3$ is acquired as follows.

$$NM(\mathcal{G}_3) = \sum_{i\leq j} m_{ij}(\mathcal{G})x^iy^j$$
$$= m_{5,5}x^5y^5 + m_{5,7}x^5y^7 + m_{6,7}x^6y^7 + m_{7,7}x^7y^7$$
$$+ m_{7,9}x^7y^9 + m_{9,9}x^9y^9$$
$$= (4n+4)x^5y^5 + (8n+8)x^5y^7+16x^6y^7$$
$$+ (2n+2)x^7y^7+8x^7y^9+2x^9y^9$$

3.6. Theorem 3. Let $\mathcal{G}_3$ be a pyrene-containing π-extended carbon nanoring. Then

(i)

$$M_1(\mathcal{G}_3)=164n+536$$

(ii)

$$M_2(\mathcal{G}_3)=478n+1816$$

(iii)

$$M_2{}^{nm}(\mathcal{G}_3) = (42{,}606n+95{,}456)/99{,}225$$

(iv)

$$F_N(\mathcal{G}_3)=1420n+4144$$

(v)

$$ND_3(\mathcal{G}_3)=5732n+25{,}448$$

(vi)

$$ND_5(\mathcal{G}_3) = (9108n+25{,}118)/315$$

(vii)

$$NR_\alpha(\mathcal{G}_3)=4n(25)^\alpha+8n(35)^\alpha+2n(49)^\alpha+4(25)^\alpha+8$$
$$(35)^\alpha+16(42)^\alpha+2(49)^\alpha+8(63)^\alpha+2$$
$$(81)^\alpha$$

(viii)

$$NH(\mathcal{G}_3) = (9906n+24{,}991)/8190$$

(ix)

$$NI(\mathcal{G}_3) = (3146n+10{,}337)/78$$

(x)

$$S(\mathcal{G}_3)=601.2381n+2480.3454$$

3.6.1. Proof.

3.7. Lemma 4. If $\mathcal{G}_4$ is the p-phenylene, then the NM-polynomial is presented as

$$NM(\mathcal{G}_4)=4x^4y^4+4x^4y^5 + (2n-4)x^5y^5 + (4n-4)x^5y^7$$
$$+ (n-1)x^7y^7$$

3.7.1. Proof. The molecular graph of $\mathcal{G}_4$ has $6n$ vertices and $7n - 1$ edges. The following categories are used to group its edge frequency. Now, NM-polynomial of $\mathcal{G}_4$ is acquired as follows.

$$NM(\mathcal{G}_4) = \sum_{i\leq j} m_{ij}(\mathcal{G}_4)x^iy^j$$
$$= m_{4,4}x^4y^4 + m_{4,5}x^4y^5 + m_{5,5}x^5y^5 + m_{5,7}x^5y^7$$
$$+ m_{7,7}x^7y^7$$
$$= 4x^4y^4+4x^4y^5 + (2n-4)x^5y^5 + (4n-4)x^5y^7$$
$$+ (n-1)x^7y^7$$

3.8. Theorem 4. Let $\mathcal{G}_4$ be a p-phenylene. Then

(i)

$$M_1(\mathcal{G}_4)=82n-34$$

Table 2. Computed Numerical Values for $[n]$CPP

n	$M_1(\mathcal{G}_1)$	$M_2(\mathcal{G}_1)$	$M_2^{nm}(\mathcal{G}_2)$	$F_N(\mathcal{G}_1)$	$ND_3(\mathcal{G}_1)$	$ND_5(\mathcal{G}_1)$	$NR_1(\mathcal{G}_1)$	$NH(\mathcal{G}_1)$	$NI(\mathcal{G}_1)$	$S(\mathcal{G}_1)$
1	82	239	0	494	2866	14	239	1	20	301
2	164	478	0	988	5732	29	478	1	40	601
3	246	717	1	1482	8598	43	717	2	61	902
4	328	956	1	1976	11,464	58	956	2	81	1202
5	410	1195	1	2470	14,330	72	1195	3	101	1503
6	492	1434	1	2964	17,196	87	1434	4	121	1804
7	574	1673	2	3458	20,062	101	1673	4	141	2104
8	656	1912	2	3952	22,928	116	1912	5	161	2405
9	738	2151	2	4446	25,794	130	2151	5	182	2706
10	820	2390	2	4940	28,660	145	2390	6	202	3006

(ii)
$$M_2(\mathcal{G}_4)=239n-145$$

(iii)
$$M_2^{nm}(\mathcal{G}_4) = (952n+961)/4900$$

(iv)
$$F_N(\mathcal{G}_4)=494n-302$$

(v)
$$ND_3(\mathcal{G}_4)=2866n-2134$$

(vi)
$$ND_5(\mathcal{G}_4) = (506n-79)/35$$

(vii)
$$NR_\alpha(\mathcal{G}_4) = (2(25)^\alpha+4(35)^\alpha + (49)^\alpha)$$
$$n+4(16)^\alpha+4(20)^\alpha-4(25)^\alpha-4(35)^\alpha$$
$$- (49)^\alpha$$

(viii)
$$NH(\mathcal{G}_4) = (381n+88)/630$$

(ix)
$$NI(\mathcal{G}_4) = (363n-149)/18$$

(x)
$$S(\mathcal{G}_4)=300.6191n+262.4788$$

3.8.1. Proof.

3.9. Lemma 5. If $\mathcal{G}_5$ is the super p-phenylene, then the *NM*-polynomial is presented as

$$NM(\mathcal{G}_5) = (8n+4)x^4y^5 + (8n+4)x^5y^8 + (4n-4)x^6y^7$$
$$+ (4n-4)x^6y^8 + (n-1)x^7y^7 + 6nx^8y^8 + 12nx^8y^9$$
$$+ 12nx^9y^9$$

3.9.1. Proof. The molecular graph of super p-phenylene has $42n$ vertices and $55n - 1$ edges. The following categories are used to group its edge frequency. Now, *NM*-polynomial of $\mathcal{G}_5$ is acquired as follows.

$$NM(\mathcal{G}_5) = \sum_{i \leq j} m_{ij}(\mathcal{G}_5)x^i y^j$$

$$= m_{4,5}x^4y^5 + m_{5,8}x^5y^8 + m_{6,7}x^6y^7 + m_{6,8}x^6y^8$$
$$+ m_{7,7}x^7y^7 + m_{8,8}x^8y^8 + m_{8,9}x^8y^9 + m_{9,9}x^9y^9$$

$$= (8n+4)x^4y^5 + (8n+4)x^5y^8 + (4n-4)x^6y^7$$
$$+ (4n-4)x^6y^8 + (n-1)x^7y^7 + 6nx^8y^8 + 12n$$
$$x^8y^9 + 12nx^9y^9$$

3.10. Theorem 5. Let $\mathcal{G}_5$ be a super p-phenylene, then

(i)
$$M_1(\mathcal{G}_5)=598n+182$$

(ii)
$$M_2(\mathcal{G}_5)=2137n+803$$

(iii)
$$M_2^{nm}(\mathcal{G}_5) = (255,613n+21,384)/211,680$$

(iv)
$$F_N(\mathcal{G}_5)=4386n+1626$$

(v)
$$ND_3(\mathcal{G}_5)=31,990n+14,738$$

(vi)
$$ND_5(\mathcal{G}_5) = (23,687n+3221)/210$$

(vii)
$$NR_\alpha(\mathcal{G}_5) = (8(20)^\alpha+8(40)^\alpha+4(42)^\alpha+4(48)^\alpha$$
$$+ (49)^\alpha+6(64)^\alpha+12(72)^\alpha+12(81)^\alpha)$$
$$n+4(20)^\alpha + 4(40)^\alpha-4(42)^\alpha-4(48)^\alpha$$
$$- (49)^\alpha$$

(viii)
$$NH(\mathcal{G}_5) = (436,253n+9724)/111,384$$

Table 3. Computed Numerical Values for Cycloparaphenylene Nanoring with Graphenic HBC Sidewalls

n	$M_1(G_2)$	$M_2(G_2)$	$M_2^{nm}(G_2)$	$F_N(G_2)$	$ND_3(G_2)$	$ND_5(G_2)$	$NR_1(G_2)$	$NH(G_2)$	$NI(G_2)$	$S(G_2)$
1	1792	6696	10	13,648	104,704	255	6320	9	424	9752
2	1956	7174	10	14,636	110,436	283	7118	12	500	10,726
3	2120	7652	11	15,624	116,168	312	7916	15	575	11,701
4	2284	8130	11	16,612	121,900	341	8714	18	651	12,675
5	2448	8608	11	17,600	127,632	370	9512	21	727	13,649
6	2612	9086	12	18,588	133,364	399	10,310	24	803	14,624
7	2776	9564	12	19,576	139,096	428	11,108	27	879	15,598
8	2940	10,042	13	20,564	144,828	457	11,906	30	955	16,573
9	3104	10,520	13	21,552	150,560	486	12,704	33	1031	17,547
10	3268	10,998	14	22,540	156,292	515	13,502	36	1107	18,522

Table 4. Computed Numerical Values for Pyrene-Containing π-Extended Carbon Nanoring

n	$M_1(G_3)$	$M_2(G_3)$	$M_2^{nm}(G_3)$	$F_N(G_3)$	$ND_3(G_3)$	$ND_5(G_3)$	$NR_1(G_3)$	$NH(G_3)$	$NI(G_3)$	$S(G_3)$
1	700	2294	1	5564	31,180	109	2294	4	173	3082
2	864	2772	2	6984	36,912	138	2772	5	213	3683
3	1028	3250	2	8404	42,644	166	3250	7	254	4284
4	1192	3728	3	9824	48,376	195	3728	8	294	4885
5	1356	4206	3	11,244	54,108	224	4206	9	334	5487
6	1520	4684	4	12,664	59,840	253	4684	10	375	6088
7	1684	5162	4	14,084	65,572	282	5162	12	415	6689
8	1848	5640	4	15,504	71,304	311	5640	13	455	7290
9	2012	6118	5	16,924	77,036	340	6118	14	496	7891
10	2176	6596	5	18,344	82,768	369	6596	15	536	8493

Table 5. Computed Numerical Values for p-Phenylene

n	$M_1(G_4)$	$M_2(G_4)$	$M_2^{nm}(G_4)$	$F_N(G_4)$	$ND_3(G_4)$	$ND_5(G_4)$	$NR_1(G_4)$	$NH(G_4)$	$NI(G_4)$	$S(G_4)$
1	48	94	0	192	732	12	94	1	12	563
2	130	333	1	686	3598	27	333	1	32	864
3	212	572	1	1180	6464	41	572	2	52	1164
4	294	811	1	1674	9330	56	811	3	72	1465
5	376	1050	1	2168	12,196	70	1050	3	93	1766
6	458	1289	1	2662	15,062	84	1289	4	113	2066
7	540	1528	2	3156	17,928	99	1528	4	133	2367
8	622	1767	2	3650	20,794	113	1767	5	153	2667
9	704	2006	2	4144	23,660	128	2006	6	173	2968
10	786	2245	2	4638	26,526	142	2245	6	193	3269

Table 6. Computed Numerical Values for Super p-Phenylene

n	$M_1(G_5)$	$M_2(G_5)$	$M_2^{nm}(G_5)$	$F_N(G_5)$	$ND_3(G_5)$	$ND_5(G_5)$	$NR_1(G_5)$	$NH(G_5)$	$NI(G_5)$	$S(G_5)$
1	780	2940	1	6012	46,728	128	2940	4	192	4314
2	1378	5077	3	10,398	78,718	241	6049	8	394	8889
3	1976	7214	4	14,784	110,708	354	9158	12	595	13,465
4	2574	9351	5	19,170	142,698	467	12,267	16	796	18,040
5	3172	11,488	6	23,556	174,688	579	15,376	20	998	22,615
6	3770	13,625	7	27,942	206,678	692	18,485	24	1199	27,190
7	4368	15,762	9	32,328	238,668	805	21,594	28	1401	31,766
8	4966	17,899	10	36,714	270,658	918	24,703	31	1602	36,341
9	5564	20,036	11	41,100	302,648	1030	27,812	35	1803	40,916
10	6162	22,173	12	45,486	334,638	1143	30,921	39	2005	45,492

(ix)

$$NI(G_5) = (5{,}606{,}905n - 248{,}965)/27{,}846$$

(x)

$$S(G_5) = 4575.2609n - 261.1065$$

3.10.1. Proof.

The graphical representations of various topological indices for a graph G using neighborhood M-polynomial and their comparative analysis are represented in Tables 2−6 and Figures 7−11.
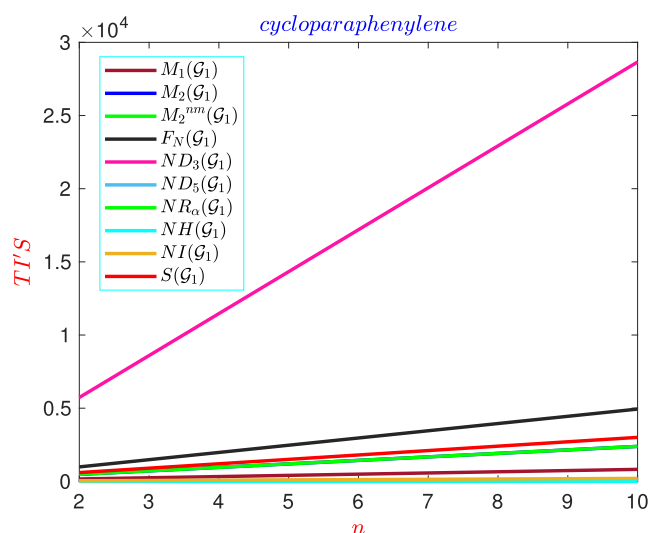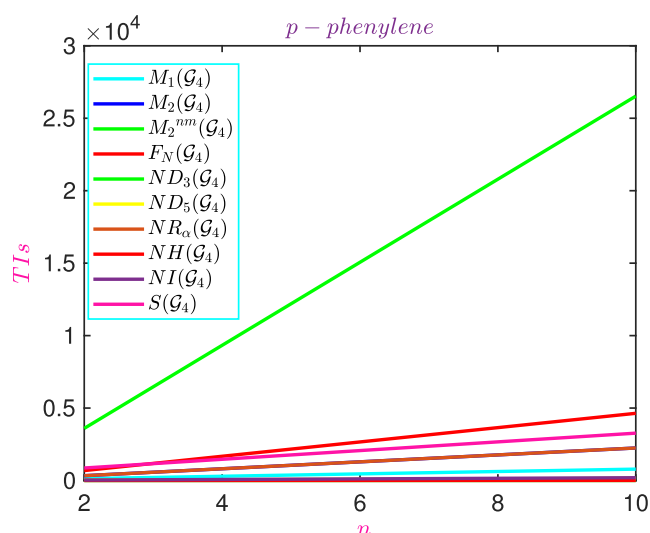
Figure 7. Graphical representation of Table 2.
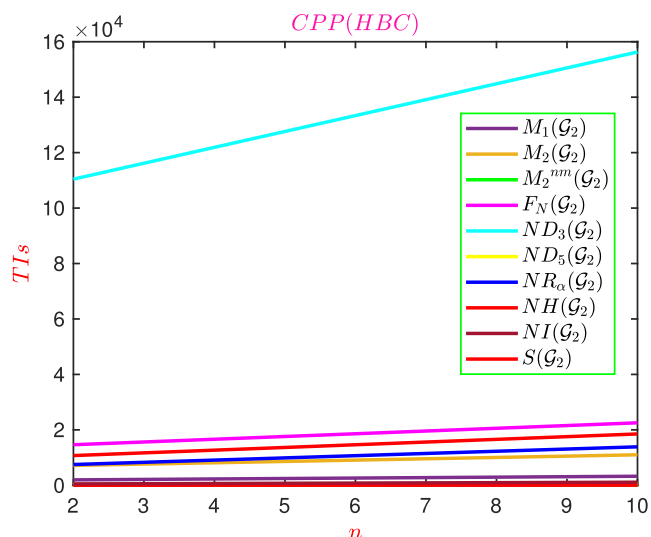

Figure 8. Graphical representation of Table 3.

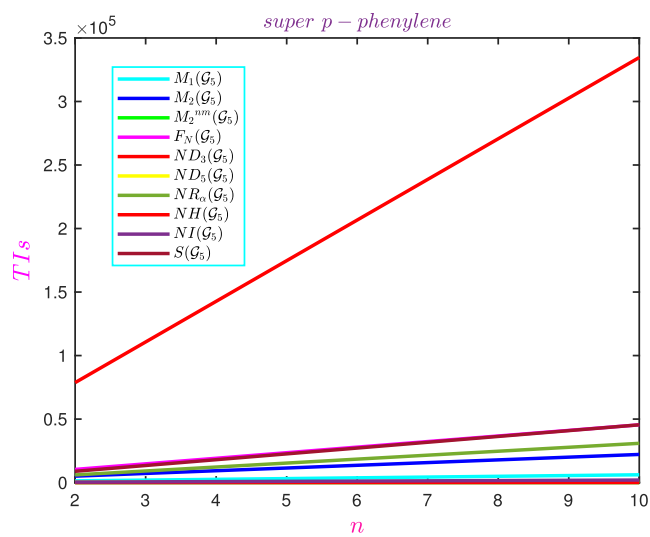**Figure 9.** Graphical representation of Table 4.

Figure 10. Graphical representation of Table 5.

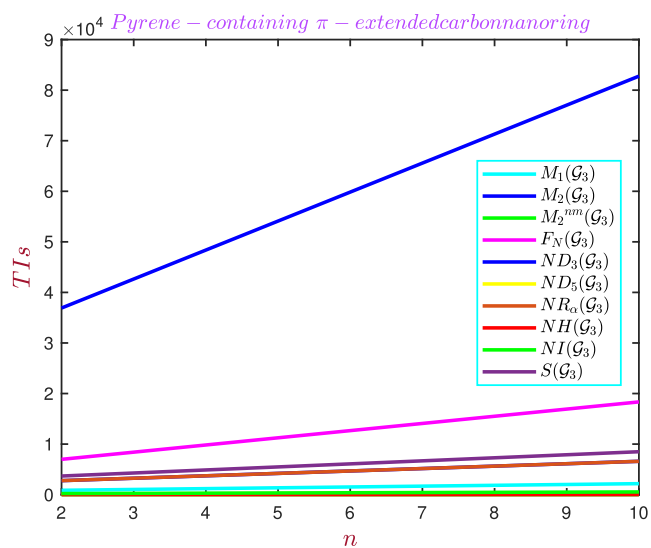**Figure 11.** Graphical representation of Table 6.

4. CONCLUSIONS

In this research, the exact expressions of the neighborhood sum-based molecular descriptors have been theoretically derived for the families of CPP chemical structures. CPP systems and their derivatives have garnered significant interest in various scientific domains, including porous molecular solids and organic electronics boasting of remarkable optoelectronic characteristics. This enduring fascination with CPP systems and their derivatives has persisted for several years, captivating the interest among researchers to explore new kinds of chemical compounds with similar properties. The theoretical investigations on these structures will enable chemists to explore new types of CPP systems using computed indices. As a result, it is possible that the computed results will be extremely useful in predicting the features and characteristics of the CPP systems. Additionally, this review also presents the calculated outcomes in graphical representations and compares them numerically, which is helpful for both theoretical chemists and experts in the field of chemistry. Computing eccentricity-based topological indices and other degree-based indices such as Revan and inverse of Revan indices, Sombor

indices, Banhatti indices, and irregularity-based indices for these CPP systems can also be explored. This problem remains open to future researchers.

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Notes

The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

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