Turkish Journal of Computer and Mathematics Education *Vol.12 No.3(2021), 3642-3649*

Research Article

Degree based and neighbourhood degree-sum based topological indices of PAH(Dimer 1) in graphene context

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Article History: Received: 10 November 2020; Revised 12 January 2021 Accepted: 27 January 2021; Published online: 5 April 2021

Abstract: In this paper, twenty degree-based topological indices and seven neighbourhood degree-sum-based topological indices of Dimer 1 (two units of chrysene) [4] 0D & 1D in the graphene context are enumerated. The Oligomer Approach[3] is practiced here to explore the interconnection between PAH (cove type periphery based on 11, 11'-dibromo-5,5'-bis chrysene as a key monomer-Dimer 1) and graphene numerically through the indices.

Keywords: Neighbourhood degree, Degree of vertex, TIs (Topological Indices), NTIs (Neighbourhood Topological Indices), Oligomer Approach, cove-edged, (11, 11'-dibromo-5,5'-bischrysene), Dimer 1, Linear Chain(LCn), Radial Expansion, PAHs (Polycyclic Aromatic Hydrocarbons), GQDs (Graphene Quantum Dots), GNRs (Graphene Nano Ribbons), GNS (Graphene Nano Sheets)

1. Introduction

The separation of the Graphene (21st-century wonder material) layer from graphite is the recent revolution in the material science domain. Polycyclic aromatic hydrocarbons (*PAH*s or polyaromatic hydrocarbons or polynuclear aromatic hydrocarbons) are organic compounds having only carbon and hydrogen with the collection of multiple aromatic rings. In this paper, Dimer 1(*PAH*) is considered to evaluate in the graphene context. Graphene monomer (*GQD*,0*D*) is quasi-zero-dimensional nanographene cut-out. Graphene nanoribbon (*GNR*,1*D*) is quasi-one-dimensional (variation in one direction only) graphene cut out and Graphene nanosheet (*GNS*,2*D*) is quasi-two-dimensional graphene cut-out. "Oligomer approach" consists of few repeating finite units of monomers. In this paper, the focus on *PAH*s in "graphene context" resulting in 0*D* (*GQD*),1*D* (*GNR*) molecular structure-property related Topological index development.

Chemical graph theory(*CGT*) is the division of mathematical Chemistry and graph theory is used as the mathematical model of molecular structures to predict the physical properties of the molecules. Abundant studies specify that the relation between the chemical properties of the compounds and their molecular structures are significantly related. Topological indices demarcated on these molecular structures to predict the physicochemical properties and biological activity. Topological indices are engendered as new limits in quantitative structure-property relationship (*QSPR/QSAR*) models to encrypt the structural environment of each atom in a molecule. The two main branches of topological indices are distance-based and degree-based. The degree-based Topological indices (*TIs*) are stretched to neighbourhood degree sum topological indices (*NTIs*). The neighbourhood degree sum of a vertex v is the sum of the degrees of neighbourhood vertices of the vertex *v* and is denoted as S_v, whereas the degree of *v* is the number of edges meeting at v and is denoted as d_v Chemical graph theory (*CGT*) is a division of mathematical chemistry, pacts with the nontrivial applications of graph theory to crack molecular problems. At large, a molecular graph is used to characterize molecules by seeing the atoms as the vertices of the graph and the molecular bonds as the edges. *CGT* is to custom algebraic invariants to condense the topological structure of a molecule to a single number, which symbolizeseither the energy of the molecule as a whole or its orbitals.

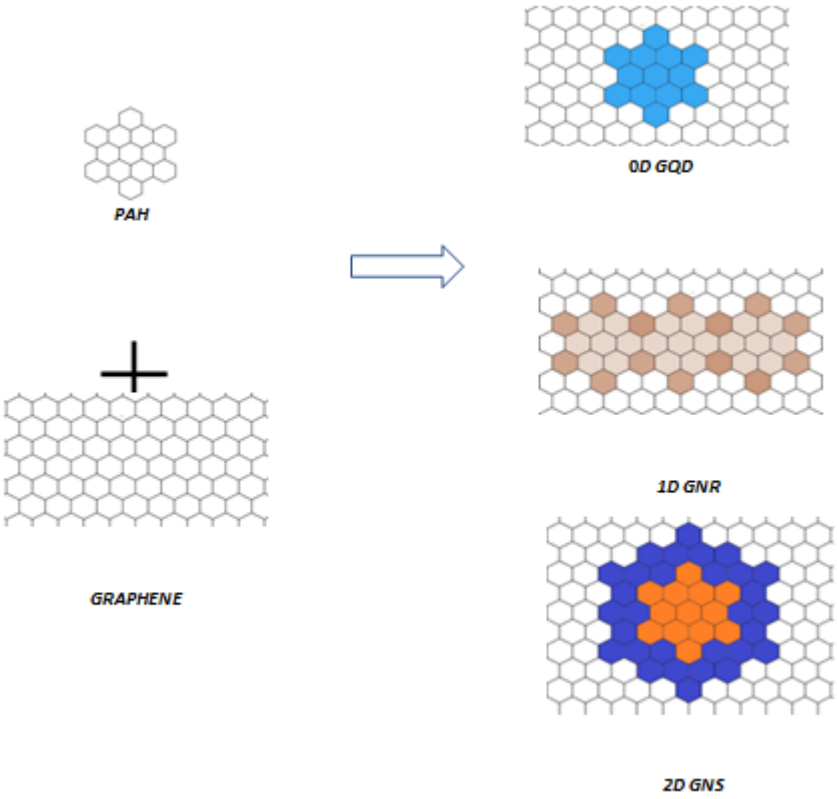


Figure 1. Example of diagrammatical representation of *PAH*s in "graphene context" describing 0*D* (*GQD*),1*D* (*GNR*), 2*D* (*GNS*) molecular structures respectively.

2. Preliminaries

Let *D*(*Dimer*1) denotes a molecular graph of a distinct unit of cove type periphery based on 11, 11'-dibromo-5,5'-bis chrysene as a key monomer-dimer 1 (0 *D* oligomers). Let LC_n (*Dimer* 1) denotes a molecular graph of a linear chain of n number of monomers of *Dimer* 1 where the chemical structure is treated as a single unit and n number of units (1 *D* oligomers) are linearly arranged like a ribbon. We determined here, GNR containing n number of subunits of *Dimer* 1as Linear Chain of *Dimer* 1 (*LCn*)

Let $\aleph(V, E)$ is a simple, connected graph where $V(\aleph)$ is its vertex set and $E(\aleph)$ is its edge set for any vertex $\kappa \in V(\aleph)$ and for any edge $\kappa,\vartheta \in E(\aleph)$. The degree of vertex $\kappa \in V$ denotes as (κ) and the neighbourhood degree sum of $\kappa \in V$ denotes as $S(\kappa)$

Here, we have tabulated the twenty degree-based topological indices and seven neighbourhood degree-based topological indices along with their notations and descriptions. Based on the listed *TI*s and *NTI*s, *D*(*Dimer* 1), LC_n (*Dimer* 1) are enumerated.

Table 1 & 2. The notations and Descriptions of twenty TIs and seven *NTI*s are listed here.

Table1.

Topological Indices - *TI*s	Notations & Descriptions
[8] Randi**ć** Index	$R(\aleph) = \sum_{\kappa,\vartheta \in E} \frac{1}{\sqrt{\eta(\kappa)\eta(\vartheta)}}$
[8] Generalise$_d$ Randi**ć** Index	$R_\alpha(\aleph) = \sum_{\kappa,\vartheta \in E} (\eta(\kappa)\eta(\vartheta))^\alpha$
[11] Reciprocal Randi**ć**Index	$RR(\aleph) = \sum_{\kappa,\vartheta \in E} \sqrt{(\eta(\kappa)\eta(\vartheta))}$
[11] Reduced Reciprocal Randi**ć** Index	$RRR(\aleph) = \sum_{\kappa,\vartheta \in E} \sqrt{(\eta(\kappa)-1)(\eta(\vartheta)-1)}$

[12] Sum Connectivity Index	$S(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} \frac{1}{\sqrt{\eta(\kappa)+\eta(\vartheta)}}$
[6] First Zagreb Index	$M_1(\mathcal{N}) = \sum_{\kappa \in V} \eta(\kappa)^2$ or $M_1(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} \eta(\kappa) + \eta(\vartheta)$
[6] Second Zagreb Index	$M_2(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} \eta(\kappa)\eta(\vartheta)$
[7] Third Zagreb Index	$M_3(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} \lvert \eta(\kappa) - \eta(\vartheta) \rvert$
[5] Reclassified Zagreb Index 1	$ReZ_1(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} \frac{\eta(\kappa)\eta(\vartheta)}{\eta(\kappa)+\eta(\vartheta)}$
[5] Reclassified Zagreb Index 2	$ReZ_2(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} \frac{\eta(\kappa)+\eta(\vartheta)}{\eta(\kappa)\eta(\vartheta)}$
[5] Reclassified Zagreb Index 3	$ReZ_3(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} (\eta(\kappa) + \eta(\vartheta))(\eta(\kappa)\eta(\vartheta))$
[11] Reduced Second Zagreb Index	$RM_2(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} (\eta(\kappa) - 1)(\eta(\vartheta) - 1)$
[14] Hyper Zagreb Index 1	$HM_1(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} (\eta(\kappa) + \eta(\vartheta))^2$
[14] Hyper Zagreb Index 2	$HM_2(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} (\eta(\kappa)\eta(\vartheta))^2$
[16] Augmented Zagreb Index	$AZ(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} \left(\frac{\eta(\kappa)\eta(\vartheta)}{\eta(\kappa)+\eta(\vartheta)-2}\right)^3$
[15] Harmonic Index	$H(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} \frac{2}{(\eta(\kappa)+\eta(\vartheta))}$
[2] Atom Bond Connectivity Index	$ABC(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} \left(\sqrt{\frac{(\eta(\kappa)+\eta(\vartheta))-2}{(\eta(\kappa)\eta(\vartheta))}}\right)$
[3] Geometric Arithmetic Index	$GA(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} \left(\frac{2\sqrt{(\eta(\kappa)\eta(\vartheta))}}{(\eta(\kappa)+\eta(\vartheta))}\right)$
[28] Forgotten Index	$F(\mathcal{N}) = \sum_{\kappa \in V} (\eta(\kappa))^3$ or $\sum_{\kappa,\vartheta \in E} \eta(\kappa)^2 + \eta(\vartheta)^2$
[14] Symmetric Division Index	$SDD(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} \left(\left(\frac{max((\eta(\kappa),\eta(\vartheta))}{min((\eta(\kappa),\eta(\vartheta))} + \frac{min((\eta(\kappa),\eta(\vartheta))}{max((\eta(\kappa),\eta(\vartheta))}\right)\right)$

Table 2.

Neighbourhood Topological Indices	Notations & Descriptions
[40] Fourth Atom Bond Connectivity Index	$ABC_4(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} \sqrt{\frac{S(\kappa)+S(\vartheta)-2}{S(\kappa)\ S(\vartheta)}}$
[40] Fifth Geometric Arithmetic Index	$GA_5(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} \frac{2\sqrt{S(\kappa)\ S(\vartheta)}}{S(\kappa)+S(\vartheta)}$
[32,33] Sanskruti Index	$SK(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} \left(\frac{S(\kappa)\ S(\vartheta)}{S(\kappa)+S(\vartheta)-2}\right)^3$
[14] Neighbourhood Version Of Forgotten Index	$F_N(\mathcal{N}) = \sum_{\kappa \in V} S(\kappa)^3$
[14] Modified Neighbourhood Version Of Forgotten Index	$F_N^*(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} (S(\kappa)^2 + S(\kappa)^2)$
[14] Neighbourhood Version Of Second Zagreb Index	$M_2^*(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} S(\kappa)\ S(\vartheta)$
[14] Neighbourhood Version Of Hyper Zagreb Index	$HM_N(\mathcal{N}) = \sum_{\kappa,\vartheta \in E} (S(\kappa) + S(\vartheta))^2$

3. Methods and Main Results

In this section, twenty degree-based topological indices and seven degree-sum-based topological indices mentioned in Table 1&2 are computed in 3 divisions based on 0*D*,1*D*& 2*D* oligomers. For getting the results, we have employed vertex partition, edge partition, vertex partition of neighbourhood degree sum & edge partition of neighbourhood degree sum and are displayed in the Tables 3,4,5& 6

The results of Distinct unit (0 *D* approach) & Linear Chain (1*D* approach) at *n* number of molecular graphs of the cove type periphery based on 11, 11'-dibromo-5,5'-bis chrysene as a key monomer-*Dimer* 1 are presented in an elaborated manner.

Table 3 & 4. Vertex partition and neighbourhood degree sum partition of each vertex ofLC_n(*Dimer* 1), based on the degree of end vertices of each edge.

Table 5 & 6. Edge partition based on degrees of end vertices and degree sum of neighbours of end vertices ofLC_n.

Table 3.

$\|V(LC_n)\|$	Cardinality
$\|V_2\|$	$12n + 6$
$\|V_3\|$	$24n - 6$
$\|V\|$	$30n$

Table 4.

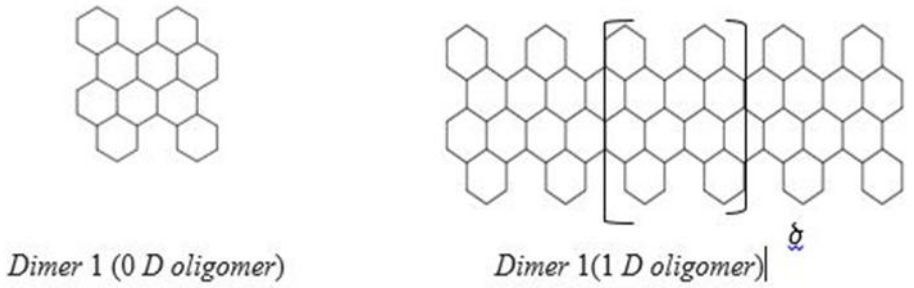
$\|S(LC_n)\|$	Cardinality
$\|S_4\|$	$4n + 2$
$\|S_5\|$	$8n + 4$
$\|S_7\|$	2
$\|S_8\|$	$8n$
$\|S_9\|$	$16n - 8$
$\|S_\kappa\|$	$36n$

Table 5.

$\|E_{(\kappa,\vartheta)}\|$	Cardinality
$\|E_{(2,2)}\|$	$8n + 4$
$\|E_{(2,3)}\|$	$8n + 4$
$\|E_{(3,3)}\|$	$32n - 11$
No. Of Edges	$48n - 3$

Table 6.

$\|S_{(\kappa,\vartheta)}\|$	Cardinality
$\|S_{(4,4)}\|$	**2**
$\|S_{(4,5)}\|$	$8n$
$\|S_{(5,5)}\|$	2
$\|S_{(5,7)}\|$	4
$\|S_{(5,8)}\|$	$8n$
$\|S_{(8,8)}\|$	4
$\|S_{(8,9)}\|$	$16n - 8$
$\|S_{(7,9)}\|$	2
$\|S_{(9,9)}\|$	$16n - 9$
No. of edges	$48n - 3$



Dimer 1 (0 *D oligomer*) *Dimer* 1(1 *D oligomer*)

Figure 2&3 show the monomer of cove type periphery based on 11, 11'-dibromo-5,5' - bis chrysene (0 *D*) and the Linear Chain at ð number of the monomers (1 *D*).

Theorem 1.1: The Randić Indices of Linear Chain of (*Dimer* 1) is given by

(i) $R(LC_n) = 17.93266n - 0.03368$

(ii) $R_\alpha(LC_n) = (8n + 4)\,4^\alpha + (8n + 4)\,6^\alpha + (32n - 11)\,9^\alpha$

(iii) $RR(LC_n) = 131.59592n - 15.20204$

(iv) $RRR(LC_n) = 83.3137n - 12.34315$

Proof: Let $\kappa, \in E(LCn)$ and (κ) and $\eta(\vartheta)$are the degree of κ and degree of ϑ respectively,

(i) $R(LC_n) = \frac{(8n+4)}{2} + \frac{(8n+4)}{\sqrt{6}} + \frac{(32n-11)}{3} = 17.93266n - 0.03368$

(ii) $R_a(LC_n) = (8n + 4)\,4^\alpha + (8n + 4)\,6^\alpha + (32n - 11)\,9^\alpha$

(iii) $RR(LC_n) = 2(8n + 4) + \sqrt{6}(8n + 4) + 3(32n - 11) = 131.59592n – 15.20204$

(iv) $RRR(LC_n) = 8n + 4 + \sqrt{2}(8n + 4) + 2(32n – 1) = 83.3137n – 12.34315$

Theorem 1.2: The Sum Connectivity Index of Linear Chain of (*Dimer* 1) is given by

$S(LC_n) = 20.64166n – 0.70188$

Proof: $\frac{(8n+4)}{2} + \frac{(8n+4)}{\sqrt{5}} + \frac{(32n-11)}{\sqrt{6}} = 20.64166n – 0.70188$

Theorem 1.3: The Zagreb Indices and their redefined version indices of Linear Chain of (*Dimer* 1) is given by

(i) $M_1(LC_n) = 264n – 30$

(ii) $M_2(LC_n) = 368n – 59$

(iii) $M_3(LC_n) = 8n + 4$

(iv) $ReZ_1(LC_n) = 65.6n – 7.7$

(v) $ReZ_2(LC_n) = 36n$

(vi) $ReZ_3(LC_n) = 2000n – 458$

(vii) $RM_2(LC_n) = 152n – 32$

(viii) $HM_1(LC_n) = 1480n – 232$

(ix) $HM_2(LC_n) = 3008n – 683$

(x) $AZ(LC_n) = 492.39063n – 61.29688$

Proof: For getting the result of First Zagreb index, we can use the vertex partition and edge partition methods and other *TI*s were getting through edge partition method.

(i) (a) $M_1(LC_n) = 4(12n + 6) + 9(24n - 6) = 264n – 30$

(b) $M_1(LC_n) = 4(8n + 4) + 5(8n + 4) + 6(32n – 11) = 264n – 30$

(ii) $M_2(LC_n) = 4(8n + 4) + 6(8n + 4) + 9(32n – 11) = 368n – 59$

(iii) $M_3(LC_n) = 8n + 4$

(iv) $ReZ_1(LC_n) = (8n + 4) + \frac{6(8n+4)}{5} + \frac{3(32n-11)}{2} = 65.6n + 7.7$

(v) $ReZ_2(LC_n) = (8n + 4) + \frac{5(8n+4)}{6} + \frac{2(32n-11)}{3} = 36n$

(vi) $ReZ_3(LC_n) = 16(8n + 4) + 30(8n + 4) + 54(32 – 11) = 2000n – 458$

(vii) $RM_2(LC_n) = (8n + 4) + 2(8n + 4) + 4(32n – 11) = 152n – 32$

(viii) $HM_1(LC_n) = 16(8n + 4) + 25(8n + 4) + 36(32n – 11) = 1480n – 232$

(ix) $HM_2(LC_n) = 16(8n + 4) + 36(8n + 4) + 81(32n – 11) = 3008n – 683$

(x) $AZ(LC_n) = 8(8n+4)+8(8n+4)+11.390625(32n – 11) = 492.39063n – 61.29688$

Theorem 1.4: The Harmonic Index of Linear Chain is given by $H(LC_n) = 17.86667n – 0.06667$

Proof: This index is calculated through edge partition method where $\kappa, \in E\&\kappa, \vartheta$ are the vertices of Linear chain of (*Dimer* 1).

$H(LC_n) = \frac{8n+4}{2} + \frac{2(8n+4)}{5} + \frac{(32n-11)}{3} = 17.86667n – 0.06667$

Theorem 1.5: The Atom Bond Connectivity Index of *LCn*is given by,

$ABC(LC_n) = 32.64704n – 1.67648$

Proof: This index is calculated through edge partition method where κ and ϑ are adjacent vertices of Linear Chain of *Dimer* 1.

$ABC(LC_n) = \frac{(8n+4)}{\sqrt{2}} + \frac{(8n+4)}{\sqrt{2}} + \frac{2(32n-11)}{3} = 32.64704n - 1.67648$

Theorem 1.6: The Geometric Arithmetic Index of the Linear Chain of *Dimer* 1 is given by

$GA(LC_n) = 37.1717n + 0.58585$

Proof: Here, we have used edge partition method for finding $GA(LC_n)$

$$= (8n+4) + \frac{2\sqrt{6}}{5}(8n+4) + (32n - 11) = 37.1717n + 0.58585$$

Theorem 1.7: The Forgotten Index of the linear chain is given by

$F(LC_n) = 744n - 114$

Proof: Here, for getting the result of $F(LC_n)$, we can use vertex partition and edge partition methods.

(a) By vertex partition method, u $\in V(LC_n)$

$F(LC_n) = 8(12n+6) + 27(24n - 6) = 744n - 114$

(b) By edge partition method, $\kappa, \vartheta \in E(LC_n)$

$F(LC_n) = 8(8n+4) + 13(8n+4) + 18(32n - 11) = 744n - 114.$

Theorem 1.8: The Symmetric Division Index of the Linear Chain is given by,

$SDD(LC_n) = 97.33333n - 5.33333$

Proof: The result of $SDD(LC_n)$is done by edge partition method where $\kappa, \vartheta \in E(LC_n)$.

$SDD(LC_n) = 2(8n+4) + \left(\frac{13}{6}\right)(8n+4) + 2(32n - 11) = 97.33333n - 5.33333$

Theorem 2.1: The fourth Atom Bond Connectivity Index of the Linear Chain of *Dimer* 1 is given by,

$ABC_4(LC_n) = 23.34218n - 0.34365$

Proof: Here, we have calculated ABC_4 Index by using degree sum of neighbourhood method.

$ABC_4(LC_n) = 2\sqrt{\frac{6}{16}} + (8n)\sqrt{\frac{7}{20}} + 0.4\sqrt{8} + 4\sqrt{\frac{10}{25}} + (8n)\sqrt{\frac{11}{40}} + 0.5\sqrt{14} + (16n - 8)\sqrt{\frac{15}{72}} + 2\sqrt{\frac{14}{63}} + (16n - 9)\frac{4}{9} = 23.34218n - 0.34365$

Theorem 2.2: The fifth version of Geometric Arithmetic Index of $LC_n$of is given by,

$GA_5(LC_n) = 47.70682n - 3.05779$

Proof: Let $\kappa, \in E$ and the neighbourhood degree of κ and ϑ are denoted as $S(\kappa)$ and $S(\vartheta)$ respectively. The procedure of getting the result is as follows:

$GA_5(LC_n) = 2 + (16n)\ \frac{\sqrt{20}}{9} + 2 + \frac{8\sqrt{35}}{12} + (16n)\ \frac{\sqrt{40}}{13} + 4 + (32n - 16)\ \frac{\sqrt{72}}{17} + \frac{\sqrt{63}}{4} + (16n - 9)$

$= 47.70682n - 3.05779.$

Theorem 2.3: The Sanskruti Index of linear chain is given by,

$SK(LC_n) = 4416.67551n - 1217.60784$

Proof: The Sanskruti Index is calculated based on degree sum of neighbourhood method where $\kappa, \vartheta \in E(LC_n)$.

$SK(LC_n) = \sum_{u,v \in} \left(\frac{S_u . S_v}{S_u + S_v - 2}\right)^3 = 2\left(\frac{16}{6}\right)^3 + (8n)\ \left(\frac{20}{7}\right)^3 + 2\ (30.51757) + 4(42.875) + \left(\frac{40}{11}\right)^3 (8n) + 4(95.53352) + \left(\frac{72}{15}\right)^3 (16n - 8) + 2\left(\frac{63}{14}\right)^3 + \left(\frac{81}{16}\right)^3 (16n - 9) = 4416.67551n - 1217.60784.$

Theorem 2.4: The neighbourhood versions of Forgotten Index, modified Forgotten Index, Second Zagreb Index & First Hyper Zagreb Index are given by,

a) $F_N(LC_n) = 17016n - 4518$

b) $F_N^*(LC_n) = 5952n - 1386$

c) $M_2^*(LC_n) = 2928n - 701$

d) $HM_N(LC_n) = 11808n - 2788$

Similar methodology followed in calculating twenty *TIs* and seven *NTIs* of the molecular graph of *Dimer*1(0*D*)andtheir results are presented in Tables 7 & 8.

Table 7. Twenty topological indices of molecular graph of *Dimer* 1(0*D* oligomer).

*TI*s	Results of *Dimer* 1(0 *D*)			
R(*Dimer* 1)	17.89898		*S* (*Dimer* 1)	19.93977
R^{α}(*Dimer* 1)	12 (4^{α}) + 12 (6^{α}) + 21 (9^{α})		M_1 (*Dimer* 1)	234
RR (*Dimer* 1)	116.39388		M_2 (*Dimer* 1)	228
RRR (*Dimer* 1)	70.97056		M_3 (*Dimer* 1)	12
Re Z_1(*Dimer* 1)	57.9		*AZ* (*Dimer* 1)	431.20313
ReZ$_2$ (*Dimer* 1)	36		*H* (*Dimer* 1)	17.8
Re Z_3(*Dimer* 1)	1686		*ABC* (*Dimer* 1)	30.97056
RM_2 (*Dimer* 1)	120		*GA* (*Dimer* 1)	33.9798
HM_1 (*Dimer* 1)	1248		*F* (*Dimer* 1)	630
HM_2 (*Dimer* 1)	2325		*SDD*(*Dimer* 1)	105

Table 8. Seven neighbourhood degree sum of topological indices of *Dimer* 1 (0*D* oligomer).

*NTI*s	Results			
ABC_4(*Dimer* 1)	23.18799		F_N^*(*Dimer* 1)	4566
GA_5 (*Dimer* 1)	44.6490		M_2^*(*Dimer* 1)	2227
SK (*Dimer* 1)	3199.06767		HM_N(*Dimer* 1)	9020
F_N (*Dimer* 1)	12498			

4. Conclusion

Twenty numbers degree-based and seven numbers neighborhood degree-based topological indices are computed on the molecular graph of cove type periphery based on 11, 11'-dibromo-5,5'-bis chrysene as a key monomer-dimer 1for 0*D*&1*D* monomers in graphene context. With the help of computed above topological indices, the outstanding properties of *Dimer* 1 in graphene context(0*D*& 1*D*) can be estimated for future new material developments thus helping the engineering industries especially semi-conductors.

This study will open up many new areas to explore all *PAH* materials consideration in the graphene context to explore the future graphene era.

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