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Topological Indices for Some New Type of Carbon Crystal

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Abstract : In QSAR/QSPR study, topological indices are used to predict the physiochemical and bioactivity of chemical compounds. A large number of such indices depend only on vertex degree of the molecular graph. In this paper, we compute few degree based topological indices for a new type of 2D Carbon Crystal prepared from 1,3,5-trihydroxy benzene and a possible 2D crystal pattern in the 4-6 carbophene family. Also, we compute the Sanskruti index for graphene and its line graph.

Keywords and phrases : Topological index; Molecular graph; Line graph; Graphene; 4-6 Carbophene family.

2000 A.M.S. subject classification : 05C12, 05C25.

Introduction : According to the IUPAC definition [21], a topological index (or molecular structure descriptor) is a numerical value associated with the chemical constitution for the correlation of chemical structure with various physical properties, chemical reactivity or biological activity. There is a strong and natural correspondence between chemical and graph theoretical notions. An atom and bond of a Molecule correspond to vertex and edge of the molecular graph. The significant correlation to topological indices and physiochemical properties of the molecules stimulate to find many topological indices based on distances between pairs of vertices and degree of a vertex. More precisely, given nonnegative numbers $\gamma(i,j)$ a vertex-degree-based topological index is expressed as

$$TI_1(G) = \sum_{1\le i\le j\le n-1} m_{ij}\gamma(i,j) \tag{1}$$

$$TI_2(G) = \prod_{1\le i\le j\le n-1} m_{ij}\mu(i,j) \tag{2}$$

Where G is a molecular graph with n vertices and m_{ij} is the number of edges of G connecting a vertex of degree i with a vertex degree j. For instance, $\gamma(i,j) = i + j$ pertain, to the first Zagreb index [8] $M_1(G)$, $\gamma(i,j) = \frac{2\sqrt{i+j-2}}{ij}$ to the atom-bond connectivity index $ABC(G)$ [19], where as ij, $|i-j|$, $(i+j)^2$, $(\frac{ij}{j+j-2})^3$, $\left(\frac{S_G(u)S_G(v)}{S_G(u)+S_G(v)-2}\right)^3$ respectively, to the second Zagreb $M_2(G)$ [8], third Zagreb $M_3(G)$, Hyper Zagreb $HM(G)$ [19], Augmented Zagreb $AM(G)$ [6] and Sanskruti index $S(G)$ [5]. Similarly, $\mu(i,j) = i + j$ pertain, to first multiple Zagreb index $PM_1(G)$ [4], where as $\mu(i,j) = ij, \frac{2}{i+j}$ respectively into second multiple Zagreb $PM_2(G)$ [20] and harmonic index $H(G)$ [22]. For a collection of degree based topological indices, we refer the following books [5,6,7] and the articles [2,3,7,11,12,16,17,14,20].

2. Modeling of Chemical Compounds:

Graphene as the most stable two-dimensional (2D) form of carbon which exhibits a number of unusual physical and chemical properties, such as spintronics, high electrical and thermal conductivity, huge specific surface area, good optical transparency, high carrier mobility quantum Hall effect. Its honeycomb lattice, which has perfect hexagonal symmetry, plays a prominent role in the formation of the 2D carbon crystal with linear dispersion. Successful preparation of graphene in 2004 has inspired a further search for other 2D carbon crystal. Among the predicted 2D Dirac materials are silicene, silicon germanide monolayer, germanene, graphynes, and so forth, while only Dirac cones in graphene have been actually confirmed experimentally. The stable and robust 2D carbon backbone motivate the searches for other 2D carbon crystal allotropes.

2.1 2D 4-6 Carbophene Family:

Qi-Shi Du et al [18] Prepared a new two dimensional (2D) carbon crystal different from graphene, from 1, 3, 5-trihydroxybenene, consisting of 4-carbon and 6 carbon rings 1:1 ratio, named 4-6 Carbophene in which all carbon atoms possess sp^2 hybrid orbitals with some distortion, forming an extensive conjugated π bonding planar structure. The 4–6 Carbophenes can be synthetized through dehydration and polymerization reactions of 1, 3, 5-trihydroxybenzene or other benzene derivatives. Figure 1(a) shows the

polymerization reaction could happen through intra-molecular dehydration of 1, 3, 5-trihydroxybenzene. Figure 1(b) shows the polymerization reaction also could happen through inter-molecular dehydration between 1, 3, 5-trihydroxybenzene molecules.

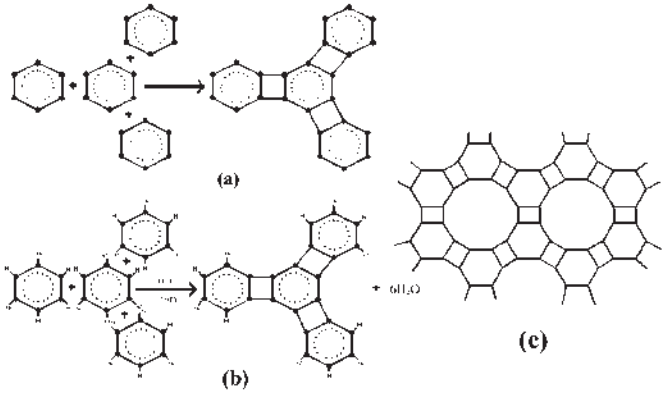

Figure 1. Illustration of chemical reaction mechanism from 1, 3, 5-trihydroxybenzene to 4-6 carbophene 2D crystal.

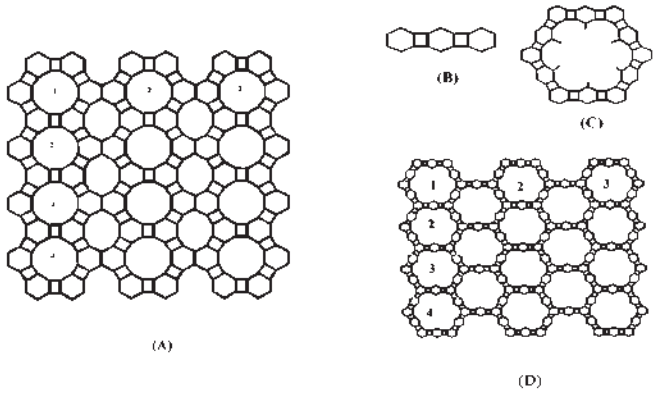

Figure 2. (A) The structural pattern of the new 2D carbon crystal prepared from 1, 3, 5 trihydroxybenzene with 4 rows and 3 columns. (B) Each side of the hexagonal unit is linearly ranged (6C-ring)-(4C-ring)-(6C-ring). (C) In each hexagonal hole, there are six carbon vertexes, on which a single valence atom or an atomic group. (D) The 2D carbon crystal consists of joining hexagonal units is bonded.

2.2 2D Nanotube-Graphene

Graphene is an atomic-scale honeycomb lattice made of carbon atoms. It is one of the most important Nanomaterials because of its unique combination of excellent

properties, which opens a way for its exploitation in a wide spectrum of applications ranging from electronics to optics, sensors, and biodevices. Denoted by $G[s,t]$ and $LG[s,t]$ respectively to 2D graphene and its line graph. Figure 3 shows 2D graphene G[7,7] and its LG[7,7]

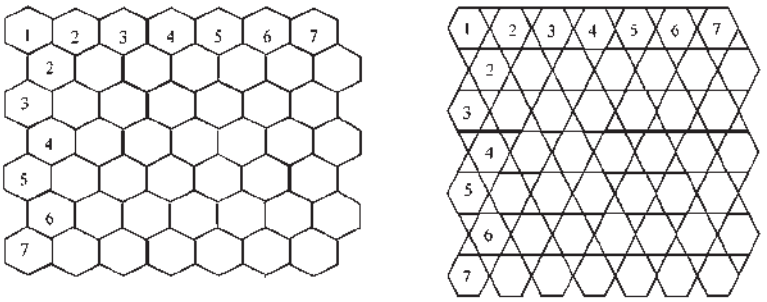

Figure 3. Two-dimensional structure of graphene and its line graph with t rows and s benzene rings in each row.

In this paper we use $LC[mC_6: 2e]$, $C[s,t]$, and $CC[s,t]$ respectively to denote the molecular graph of each side of the hexagonal unit is linearly ranged (6C-ring)-(4C-ring)-(6C-ring) as shown in Figure 2(B) , 2D carbon crystal prepared from 1, 3, 5 trihydroxybenzene with s rows and t columns, shown in Figure 1 and the 2D carbon crystal consists of joining hexagonal units is bonded as shown Figure 2 (D) later, we compute the First Zagreb indices, Second Zagreb indices, Third Zagreb indices, hyper Zagreb index, First multiple Zagreb indices, Second multiple Zagreb indices, Harmonic index, Atom bond connectivity index, Augmented Zagreb index and Sanskruti index of 2D crystal pattern of 4, 6 Carbophene family and line graph of graphene.

3. Results and discussions:

Let G be a simple, finite and undirected graph. For a graph G, the vertex set and edge set of G will be denoted by $V(G)$ and $E(G)$ respectively. The degree of a vertex $u \in V(G)$ will be denoted by d, while the edge connecting the vertices u and v will be denoted by uv. Let $N_G(u)$ be the set of all neighbors of $u \in V(G)$. For any d, define $V_d = \{u \in V(G) | S_G(u) = d\}$, in which $S_G(u) = \sum_{v \in N_G(u)} d_G(v)$ and $N_G(u) = \{v \in V(G) \mid uv \in E(G)\}$. We introduce the following definition to interpret the linearly ranged molecules.

Definition: Linearly ranged cycles $LC[mC_6: 2e]$is obtained from m copies of cycles $C_n^1, C_n^2, \dots, C_n^m$ by joining C_n^i and C_n^{i+1} by two non-adjacent edges. (i.e) If $xy \in E(C_n^i)$ and $uv \in E(C_n^{i+1})$ then $(xu, yv) \in E(LC[C_n^i, C_n^{i+1}: 2e]$.

For example a linearly ranged cycles $LC[3C_6: 2e]$ is the molecular graph of each side of the hexagonal unit is linearly ranged (6C-ring)-(4C-ring)-(6C-ring) as shown in Figure 3 (A).

Theorem 1 Let $G = LC[mC_n: 2e]$ be the linearly ranged cycles obtained from m copies of cycles $C_n^1, C_n^2, \dots, C_n^m$ by joining C_n^i and C_n^{i+1} by two non-adjacent edges then,

$$M_1(G) = 4nm + 16m - 84$$

$$M_2(G) = 4nm + 26m - 94$$

$$M_3(G) = 4(m-1)$$

$$ABC(G) = (nm - 17)\sqrt{\frac{1}{2}} + \frac{4}{3}(2m-1)$$

$$AZ(G) = 8(nm) + \frac{729}{32}[m-1] - 136$$

$$HM(G) = 16nm + 108m - 380$$

$$PM_1(G) = 4^{nm-4m-13} \times 22500^{(m-1)}$$

$$PM_2(G) = 4^{nm-4m-13} \times 104976^{(m-1)}$$

$$H(G) = 2^{8m-nm+9} \times 5625^{(-m+1)}$$

Proof. We noticed that in structure of mC_n vertices have degree two or three. Hence we can partite the edge set $E_1 = \{uv | d_u = 2; d_v = 2\}$, $E_2 = \{uv | d_u = 2\ ;\ d_v = 3\}, E_3 = \{uv | d_u = 3; d_v = 3\}$ which is shown in the Table 1. From $TI_1(G) = \sum_{uv \in E(G)} m_{ij}\gamma(u,v)$, $TI_2(G) = \sum_{uv \in E(G)} m_{ij}\mu(u,v)$ where $\gamma(u,v)$ and $\mu(u,v)$ are respective topological indices of G and m_{ij} is equal to $|E_1|, |E_2|$ and $|E_3|$.

(u,v)	(2,2)	(2,3)	(3,3)
No. of edges	nm-4m-13	4(m-1)	2(m-1)

Table 1. Edge partition of $G = mC_n + 2e$ based on vertex degree

Hence,

$$\sum_{uv \in E(G)} \gamma(u,v) = \sum_{uv \in E_1} \gamma(u,v) + \sum_{uv \in E_2} \gamma(u,v) + \sum_{uv \in E_3} \gamma(u,v)$$

$$= |E_1|\,\gamma(u,v) + |E_2|\,\gamma(u,v) + |E_3|\,\gamma(u,v) \quad (3)$$

Similarly,

$$\prod_{uv\in E(G)} \mu(u,v) = \prod_{uv\in E_1} \mu(u,v) \times \prod_{uv\in E_2} \mu(u,v) \times \prod_{uv\in E_3} \mu(u,v)$$

$$= \mu(u,v)^{|E_1|} \times \mu(u,v)^{|E_2|} \times \mu(u,v)^{|E_3|} \quad (4)$$

By using Table 1 and substituting respective function for $\gamma(u,v)$, $\mu(u,v)$ of topological index in (3) and (4) one can compute the topological index.

Theorem 2: Let $G = LC[mC_n; 2e]\ n > 6, m > 2$ be the linearly ranged cycles obtained from m copies of cycles $C_n^1, C_n^2, \ldots, C_n^m$ by joining C_n^i and C_n^{i+1} by two non-adjacent edges then, Sanskruti index $S(G) = 18.96296mn + 516.0615m - 478.1335$

Proof. We observed that in structure of $LC[mC_n; 2e]$ vertices have degree two or three. we denote the set of vertices with degree two and three as $V_4 = \{v \in V(G) | s_G(v) = 4\}$, $V_5 = \{v \in V(G) | s_G(v) = 5\}, V_6 = \{v \in V(G) | s_G(v) = 6\}, V_8 = \{v \in V(G) | s_G(v) = 8$, From V_4, V_5, V_6, V_8 we can partite the edge set based on V_4, V_5, V_6, V_8 such as $E_{45} = \{uv | u \in V_4, v \in V_4 ; u \neq v\}$, $E_{45} = \{uv | u \in V_4; v \in V_5\}$, $E_{58} = \{uv | u \in V_5; v \in V_8\}, E_{68} = \{uv | u \in V_6; v \in V_8\}, E_{88} = \{uv | u \in V_8; v \in V_8\ u \neq v\}$.

$S_G(u,v)$	(4,4)	(4,5)	(5,8)	(8,8)
No. of Edges	mn-10m+10	4(m-1)	4(m-1)	4(m-1)

Table 2. Edge partition of $G = mC_n + 2e$ based on $S_G(u)$.

Table 2 shows the cardinality of E_{44}, E_{45} ,E_{58}, E_{68}, E_{88}.

Hence,

$$S(G) = (mn - 8m + 10)\left(\frac{4\times 4}{4+4-2}\right)^3 + 4(m-1)\left(\frac{5\times 4}{5+4-2}\right)^3$$

$$+4(m-1)\left(\frac{5\times 8}{5+8-2}\right)^3 + 4(m-1)\left(\frac{8\times 8}{8+8-2}\right)^3$$

$$= 18.96296mn + 516.0615m - 478.1335$$

Which complete the proof.

Corollary 3: Let $LC[mC_6; 2e]$, $m > 3$ Each side of the hexagonal unit is linearly ranged (6C-ring)-(4C-ring)-(6C-ring), then,

$$M_1(G) = 40m - 84$$

$$M_2(G) = 50m - 94$$

$$M_3(G) = 4(m-1)$$

$$ABC(G) = (6m-17)\sqrt{\frac{1}{2}} + \frac{4}{3}(2m-1)$$

$$AZ(G) = 48m + \frac{729}{32}[m-1] - 136$$

$$HM(G) = 204m - 380$$

$$PM_1(G) = 4^{2m-13} \times 22500^{(m-1)}$$

$$PM_2(G) = 4^{2m-13} \times 104976^{(m-1)}$$

$$H(G) = 2^{2m+9} \times 5625^{(-m+1)}$$

By substituting $n = 6$ in Theorem 1 we get the result.

Theorem 4: Let $C[s,t]$ be the structural pattern of the 2D carbon crystal prepared from 1, 3, 5-trihydroxybenzene. Then

$$M_1(C[s,t]) = 104t - 214st + 232$$

$$M_2(C[s,t]) = 153st - 341t + 32s + 333$$

$$M_3(C[s,t]) = 8t + 4s$$

$$ABC(C[s,t]) = (12t+6s)\sqrt{\frac{1}{2}} + \frac{1}{2}[17st - 45st + 37]$$

$$AZ(C[s,t]) = 8(12t+6s) + \frac{729}{64}[17st - 45t + 37]$$

$$HM(C[s,t]) = 612st - 1356t + 132s + 1132$$

$$PM_1(C[s,t]) = 4^{4t+2s} \times 5^{8t+4s} \times 6^{17st-45t+37}$$

$$PM_2(C[s,t]) = 4^{4t+2s} \times 6^{8t+4s} \times 9^{17st-45t+37}$$

$$H(C[s,t]) = 4^{2t-s} \times 5^{-(8t+4s)} \times 3^{45t-17st-37}$$

Proof. We noticed that in the structure of 2D carbon crystal prepared from 1, 3, 5-trihydroxybenzene vertices have degree two or three. Hence we can partite the edge set $E_1 = \{uv | d_u = 2;\ d_v = 2\}$, $E_2 = \{uv | d_u = 2;\ d_v = 3\}$, $E_3 = \{uv | d_u = 3; d_v = 3\}$ which is shown in the Table 3. From $TI_1(G) = \sum_{uv \in E(G)} m_{ij}\gamma(u,v)$, $TI_2(G) =$

$\sum_{uv\in E(G)} m_{ij}\mu(u,v)$ where $\gamma(u,v)$ and $\mu(u,v)$ are respective topological indices of G and m_{ij} is equal to $|E_1|, |E_2|$ and $|E_3|$.

(u,v)	(2,2)	(2,3)	(3,3)
No. of edges	4t+2s	8t+4s	75t+36st-8s+64

Table 3. Edge partition of $C[s,t]$ 2D carbon crystal of prepared from 1, 3, 5-trihydroxybenzene based on vertex degree

$$\sum_{uv\in E(C[s,t])} \gamma(u,v) = \sum_{uv\in E_1} \gamma(u,v) + \sum_{uv\in E_2} \gamma(u,v) + \sum_{uv\in E_1} \gamma(u,v)$$
$$= |E_1|\,\gamma(u,v) + |E_2|\,\gamma(u,v) + |E_3|\,\gamma(u,v) \quad (5)$$

Similarly,

$$\prod_{uv\in E(G)} \mu(u,v) = \prod_{uv\in E_1} \mu(u,v) \times \prod_{uv\in E_2} \mu(u,v) \times \prod_{uv\in E_3} \mu(u,v)$$
$$= \mu(u,v)^{|E_1|} \times \mu(u,v)^{|E_2|} \times \mu(u,v)^{|E_3|} \quad (6)$$

By using Table 3 and substituting respective function for $\gamma(u,v)$, $\mu(u,v)$ of topological index in (5) and (6) one can compute the topological index.

Theorem 5: Let $C[s,t]$ be the structural pattern of the 2D carbon crystal prepared from 1,3,5-trihydroxybenzene. Then Sankruti index $S(C[s,t] = 4670.8668st + 7884.917s + 208.4658t - 11790.5301$.

Proof. We observed that in the structure of 2D carbon crystal prepared from 1, 3, 5-trihydroxybenzene vertices have degree two or three. We denote the set of vertices of degree two and three as $V_5 = \{v \in V(C[s,t])|s_{C[s,t]}(v) = 5\}$, $V_8 = \{v \in V(C[s,t])|s_{C[s,t]}(v) = 8\}$, $V_9 = \{v \in V(C[s,t])|s_{C[s,t]}(v) = 9\}$. We can partite the edge set $E_{55}, E_{58}, E_{88}, E_{89}$ and E_{99} based on V_5, V_8, V_9 and cardinality of the edge set shown in table 4.

$s_{C[s,t]}(u,v)$	(5,5)	(5,8)	(8,8)	(8,9)	(9,9)
No. of Edges	4t+2s	8t+4s	2t+4	12t+8s-8	36st+52s-14t-87

Table 4. Edge partition of $C[s,t]$ 2D carbon crystal of prepared from 1,3,5-trihydroxybenzene based on $s_{C[s,t]}(u)$.

Now,

$$S(G) = (4t + 2s)\left(\frac{5 \times 5}{5 + 5 - 2}\right)^3 + (8t + 4s)\left(\frac{5 \times 8}{5 + 8 - 2}\right)^3 + (2t + 4)\left(\frac{8 \times 8}{8 + 8 - 2}\right)^3$$
$$+ (12t + 8s - 8)\left(\frac{8 \times 9}{8 + 9 - 2}\right)^3 + (36st + 52s - 14t$$
$$- 87)\left(\frac{9 \times 9}{9 + 9 - 2}\right)^3$$
$$= 4670.8668st + 7884.917s + 208.4658t - 11790.5301.$$

Which completes the proof.

Theorem 6: Let $CC[s,t]$ be 2D carbon crystal consists of joining hexagonal units is bonded. Then

$$M_1(CC[s,t]) = 468st - 40s - 2t - 60$$
$$M_2(CC[s,t]) = 666st - 64s - 29t - 90$$
$$M_3(CC[s,t]) = 12t(2s + 1)$$
$$ABC(CC[s,t]) = (12st + 8t + s)\sqrt{2} + \frac{2}{3}[58st - 13t - 8s - 10]$$
$$AZ(CC[s,t]) = 8(24st + 16t + 2s) + \frac{729}{64}[58st - 13t - 8s - 10]$$
$$HM(CC[s,t]) = 8(336st - 13t - 64s - 45)$$
$$PM_1(CC[s,t]) = 4^{4t+2s} \times 5^{12t(2s+1)} \times 6^{58st-13t-8s-10}$$
$$PM_2(CC[s,t]) = 4^{4t+2s} \times 6^{12t(2s+1)} \times 9^{58st-13t-8s-10}$$
$$H(CC[s,t]) = 4^{6st-4t-s} \times 5^{-12t(2s+1)} \times 3^{13t+8s-58st-10}$$

Proof. Consider $CC[s,t]$ be 2D carbon crystal consists of joining hexagonal units is bonded whose vertex degree partition based on vertex degree $E_1 = \{uv | d_u = 2;\ d_v = 2\}$, $E_2 = \{uv | d_u = 2;\ d_v = 3\}$, $E_3 = \{uv | d_u = 3; d_v = 3\}$. From $TI_1(G) = \sum_{uv \in E(G)} m_{ij}\gamma(u,v)$, $TI_2(G) = \sum_{uv \in E(G)} m_{ij}\mu(u,v)$ where $\gamma(u,v)$ and $\mu(u,v)$ are respective topological indices of G and m_{ij} is equal to $|E_1|, |E_2|$ and $|E_3|$.

(u,v)	(2,2)	(2,3)	3,3)
No. of edges	4t+2s	12t(2s+1)	58st-13t-8s-10

Table 5. Edge partition of 2D carbon crystal of prepared from 1,3,5-trihydroxybenzene based on vertex degree.

$$\sum_{uv\in E(C[s,t])} \gamma(u,v) = \sum_{uv\in E_1} \gamma(u,v) + \sum_{uv\in E_2} \gamma(u,v) + \sum_{uv\in E_3} \gamma(u,v)$$
$$= |E_1|\,\gamma(u,v) + |E_2|\,\gamma(u,v) + |E_3|\,\gamma(u,v) \quad (7)$$

Similarly,

$$\prod_{uv\in E(G)} \mu(u,v) = \prod_{uv\in E_1} \mu(u,v) \times \prod_{uv\in E_2} \mu(u,v) \times \prod_{uv\in E_3} \mu(u,v)$$
$$= \mu(u,v)^{|E_1|} \times \mu(u,v)^{|E_2|} \times \mu(u,v)^{|E_3|} \quad (8)$$

By using Table 5 and substituting respective function for $\gamma(u,v)$, $\mu(u,v)$ of topological index in (3) and (4) one can compute the topological index.

Theorem 7: Let $CC[s,t]$ be 2D carbon crystal consists of joining hexagonal units is bonded. Then $S(CC[s,t]) = 1899.837st + 3961.383s + 5689.961t + 3380.644$

Proof. We observed that in the structure of 2D carbon crystal consists of joining hexagonal units is bonded. We denote the set of vertices of degree two and three as $V_5 = \{v \in V(CC[s,t])|s_{CC[s,t]}(v) = 5\}$, $V_8 = \{v \in V(CC[s,t])|s_{CC[s,t]}(v) = 8\}$, $V_9 = \{v \in V(CC[s,t])|s_{CC[s,t]}(v) = 9\}$. We can partite the edge set $E_{55}, E_{58}, E_{58}, E_{68}, E_{89}$ and E_{99} based on V_5, V_8, V_9 and cardinality of the edge set shown in table 6.

$s_G(u,v$	(5,5)	(5,8)	(6,8)	(8,8)	(8,9)	(9,9)
Total	2s+4t	4s+12t	24st-4s	14st+2s+6t+6	4st+32s+40t+16	24st-6s-6t+8

Table 6. Edge partition of $CC[s,t]$ 2D carbon crystal of prepared from 1,3,5 trihydroxy-benzene based on $s_{CC[s,t]}(u)$.

Hence

$$S(CC[s,t]) = 1899.837st + 3961.383s + 5689.961t + 3380.644$$

Which complete the proof

Theorem 8: Let $G[s,t]$ be the 2D graphene with t rows of benzene rings and s benzene in each row then $S(G) = 389.239st + 649.161s - 383.6373t - 2290.13$.

Proof. The 2D graphene of $G[s,t]$. Further notice that the vertices of degree is two and three only therefore we can partition the edge set of $G[s,t]$based on the degree sum of neighborhood vertices of each vertex is obtained, as shown in Table 7.

$s_{G[s,t]}(u,v)$	(5,4)	(5,5)	(5,7)	(5,8)	(6,7)	(7,9)	(8,8)	(9,9)
No. of edges	4	T	t+2	2t-4	4s-8	2s-1	t-2	3st-2s-5t-10

Table 7. Edge partition of 2D graphene based on $s_{G[s,t]}(u)$.

using table one can deduced that

$$S(G[s,t]) = 389.239st + 649.161s - 383.6373t - 2290.13$$

Which complete the proof.

Theorem 9: Let G be a 2D Line Graph of graphene $LG[s,t]$, then $S(LG[s,t])$=4349.649st-3176.464s+2677.724t-9600.355.

Proof: We observed that in the structure of line graph of graphene $LG[s,t]$ vertices have degree two three and four. We denote the set of vertices with degree two and three as $V_5 = \{v \in V(LG[s,t]) | s_{LG[s,t]}(v) = 5\}$, $V_6 = \{v \in V(LG[s,t]) | s_{LG[s,t]}(v) = 6\}$, $V_9 = \{v \in V(LG[s,t]) | s_{LG[s,t]}(v) = 9\}$. $V_{10} = \{v \in V(LG[s,t]) | s_{LG[s,t]}(v) = 10\}$, $V_{14} = \{v \in V(LG[s,t]) | s_{LG[s,t]}(v) = 14\}$, $V_{15} = \{v \in V(LG[s,t]) | s_{LG[s,t]}(v) = 15\}$, $V_{16} = \{v \in V(LG[s,t]) | s_{LG[s,t]}(v) = 16\}$. We partite the edge set V_5, V_6, V_9, V_{10}, V_{11}, V_{14}, V_{15}, V_{16} based on $s_{LG[s,t]}(u)$ as shown in table 8. Using the same technique as in theorem 1.

$S_{LG[s,t]}(u,v)$	(5,5)	(5,9)	(5,10)	(6,9)	(6,10)	(9,9)	(9,10)
No.of edges	2	2	2	3	2t-6	2	4

$S_{S_{LG[s,t]}}(u,v)$	(10,14)	(10,15)	(14,15)	(14,16)	(15,16)	(16,16)
No.of edges	6s-10	2t-5	2t	4s-5	4t-7	7st-12s-2t

Table 8. Edge partition of 2D line graph of graphene $LG[s,t]$ based on $s_{LG[s,t]}$

Using table one can deduced that,

$$S(LG[s,t]) = 4349.649\text{st} - 3176.464\text{s} + 2677.724\text{t} - 9600.355$$

4. Conclusion :

The results obtained in our study can be applied for predicting certain physiochemical properties of 2D crystal pattern 4, 6 Carbophene. Computing the distance based Topological indices of 2D crystal pattern 4, 6 Carbophene family will be our future work.

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