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Study of Cycle-Path Connected graph by applying degree-based Topological Indices

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Abstract:

Topological indices are tremendously advantageous for assaying colorful physicochemical stress parcels connected with a chemical emulsion. A topological index describes molecular structures by covering them into certain real figures. By converting chemical structures into numerical descriptors, these indices facilitate the development of quantitative structure-activity relationships (QSARs), which is the natural exertion of patches identified with their arrangements of chemical components. In this composition, we will cipher the topological indicators of the cycle-path connected graph. In addition, comparisons of the cycle-path connected graph dispense numerically and graphically.

Keywords: Cycle-Path linked graphs, Topological Indices, First-Zagreb index, sum-connectivity index, Randic connectivity index.
AMS Subject Classification: 05C15, 05C69.

1. Introduction

Consider a molecular graph $G = (V, E)$, such a graph with vertex set $V(G)$ indicates the atoms and edges set $E(G)$ indicates chemical bonds. A degree is represented by $\{d_\theta, \theta \in V(G)\}$ which is defined as the number of edges incident with θ.[For unspecified terminologies and more details, see [1]).

Graph theory is the field of study of mathematics, and it has been applied in almost every academic discipline. Recently, topological indices have garnered significant attention in Quantitative Structure-Property Relationship (QSPR) and Quantitative Structure-Activity Relationship (QSAR) studies. Graph Theory is used to assess the linkage among several topological indices of certain graphs such as cycle-path connected graph, star-path connected graph, wheel-path connected graph, etc.,

Topological indices numerically describe a graph molecule's topology, characterizing its structural properties[2]. Graph Theory assesses relationships among indices in various graphs, such as Cycle-path-connected graphs, Star-path-connected graphs, and wheel-path-connected graphs. Topological indices in chemistry were first established by Harold Wiener in 1947 with the Wiener Index. Initially, it predicted the physical properties of paraffins[3].

The symmetric division degree index (SD) of connected graph (G)[4] is defined as follows:

$SD(G) = \sum_{\sigma\tau \in E(G)} \frac{{d_\sigma}^2 + {d_\tau}^2}{d_\sigma d_\tau}$ ------(1) Where, d_σ and d_τ are the degrees of vertex σ and τ in G.

The sum-connectivity index [5] is defined as follows: $SC(G) = \sum_{\sigma\tau \in E(G)} \frac{1}{\sqrt{d_\sigma + d_\tau}}$ ------(2)

Randic connectivity index is widely used in mathematical chemistry, due to its wide applications in both mathematics and chemistry. It is defined[6] in the following equation: $RC(G) = \sum_{\sigma\tau \in E(G)} \frac{1}{\sqrt{d_\sigma d_\tau}}$ -------(3)

The First-Zagreb index[7] is defined as: $M_1(G) = \sum_{\sigma\tau \in E(G)} (d_\sigma + d_\tau)$ -----(4)

The Second-Zagreb index[7] is defined as: $M_2(G) = \sum_{\sigma\tau \in E(G)} (d_\sigma d_\tau)$ -----(5)

Zhong introduced the harmonic index in 2012 which is defined [8] as follows:

$H(G) = \sum_{\sigma\tau \in E(G)} \frac{2}{(d_\sigma + d_\tau)}$------(6)

For more wide-ranging and comprehensive details, we offer the readers to follow the following articles. [9-13,17-40].

Definition:1.1 A path connected graph $P(G, P_m, k)$ of G is obtained by taking k copies of G, say $G_1, G_2, \dots, G_k, G_i$ is connected with G_{i+1} by a path P_m (calling it as, binding path), such that left and right end vertices of P_m is joined by an edge to a vertex of G_i and $G_{i+1,}$ $1 \leq i \leq k-1$, respectively.Moreover, the distance between two consecutive binding paths must be three.

Definition:1.2 A cycle-path connected graph $P(C_s, P_t, k), s \geq 3, t \geq 1, k \geq 2$ of $C_s, s \geq 3$ is obtained by taking k copies of C_s, say $C_1, C_2, \dots, C_k, C_i$ is connected with C_{i+1} by a path P_t (calling it as, binding path), such that left and right end vertices of P_t is joined by an edge to a vertex of C_i and $C_{i+1,}$ $1 \leq i \leq k-1$, respectively.Moreover, the distance between two consecutive binding paths must be three.

Example:1.1

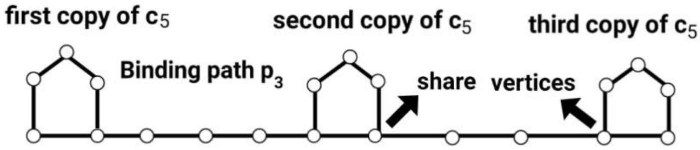
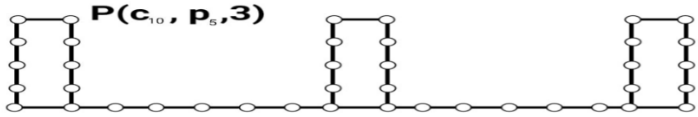


***Figure*: 1. 1** $P(C_5, P_3, 3)$

Note:1.1 Two cycles, say C_n and C_n' are said to be distinct if they don't share a vertex in common. A vertex u of C_n in G is called a share vertex if $N(u)$ has a member outside C_n.

Example: 1.2



$\boldsymbol{Figure}$: **1. 2** $P(C_{10}, P_5, 3)$

2. Results

Observation:2.1 General Form: $P(C_s, P_t, k), s \geq 3, t \geq 1, k \geq 2$.

1. $E(2,2) = k(s-3) + (t-1)(k-1) + 2$.
2. $E(3,3) = k - 2$.
3. $E(2,3) = 4k - 2$.
4. $No\ of\ vertices = ks + t(k-1)$.
5. $No\ of\ Edges = ks + (t+1)(k-1)$
6. Totally $k(s+t-2) - t + 2$ vertices having degree two.
7. $2k - 2$ vertices having degree three.

Theorem:2.2 Let $P(C_s, P_t, k), s \geq 3, t \geq 1, k \geq 2$ be the cycle-path connected graph. Then,
$(i) SD[P(C_s, P_t, k)] = 2(k(s-3) + \big((t-1)(k-1) + 2\big) + 2(k-2) + \frac{13}{3}(2k-1)$.

$(ii)\ SC[P(C_s, P_t, k)] = \frac{1}{2}(k(s-3) + (t-1)(k-1) + 2) + \frac{1}{\sqrt{6}}(k-2) + \frac{1}{\sqrt{5}}(4k-2)$.

$(iii) RC[P(C_s, P_t, k)] = \frac{(k(s-3)+(t-1)(k-1)+2)}{2} + \frac{1}{3}(k-2) + \frac{(4k-2)}{\sqrt{6}}$.

$(iv)\ M_1[P(C_s, P_t, k)] = 4ks + 4tk - 4t + 10k - 10$.

$(v)\ M_2\big(P(C_s, P_t, k)\big) = 4ks + 4tk + 17k - 4t - 18$.

$(vi)\ H[P(C_s, P_t, k)] = \frac{1}{2}(k(s-3) + (t-1)(k-1) + 2) + \frac{1}{3}(k-2) + \frac{2}{5}(4k-2)$.

Proof. The cycle – path connected graph has $2k-2$ vertices of degree3 and $k(s+t-2) - t + 2$ vertices of degree 2.In $P(C_s, P_t, k)$, we get edges of type $E(2,2), E(3,3), E(2,3)$. The number of edges of these types are given in Table 2.1.

Table:2.1 Edge Division

$E(d_u\ d_v)$	$E(2,2)$	$E(3,3)$	$E(2,3)$
Number of Edges	$k(s-3) + (t-1)(k-1) + 2$	$k-2$	$4k-2$

By using Table 2.1 and the Equation [1] we get the desired results, i.e.,

$(i) SD\big(P(C_s, P_t, k)\big) = \sum_{\sigma\tau \in E(P(C_s,P_t,k))} \frac{{d_\sigma}^2 + {d_\tau}^2}{d_\sigma d_\tau} = E(2,2) \sum_{\sigma\tau \in E(P(C_s,P_t,k))} \frac{{d_\sigma}^2 + {d_\tau}^2}{d_\sigma d_\tau} +$
$E(3,3) \sum_{\sigma\tau \in E(P(C_s,P_t,k))} \frac{{d_\sigma}^2 + {d_\tau}^2}{d_\sigma d_\tau} + E(2,3) \sum_{\sigma\tau \in E(P(C_s,P_t,k))} \frac{{d_\sigma}^2 + {d_\tau}^2}{d_\sigma d_\tau}$.

$= (k(s-3)+(t-1)(k-1)+2)\left(\frac{2^2+2^2}{2\times 2}\right)+(k-2)\left(\frac{3^2+3^2}{3\times 3}\right)+(4k-2)(\frac{2^2+3^2}{2\times 3}).$

$= (k(s-3)+(t-1)9k-1)+2)2+(k-2)2+(4k-2)(\frac{3}{6}).$

$= 2(k(s-3)+(t-1)(k-1)+2)+2(k-2)+\frac{13}{3}(2k-1).$

$(ii) SC(G) = \sum_{\sigma\tau\in E(P(C_s,P_t,k))}\frac{1}{\sqrt{d_\sigma+d_\tau}} = E(2,2)\sum_{\sigma\tau\in E(P(C_s,P_t,k))}\frac{1}{\sqrt{d_\sigma+d_\tau}} + E(3,3)\sum_{\sigma\tau\in E(P(C_s,P_t,k))}\frac{1}{\sqrt{d_\sigma+d_\tau}} + \mathrm{E}(2,3)\sum_{\sigma\tau\in E(P(C_s,P_t,k))}\frac{1}{\sqrt{d_\sigma+d_\tau}} = (k(s-3)+(t-1)(k-1)+2)\frac{1}{\sqrt{2+2}}+(k-2)\frac{1}{\sqrt{3+3}}+(4k-2)\frac{1}{\sqrt{2+3}} = \frac{1}{2}(k(s-3)+(t-1)(k-1)+2)+\frac{1}{\sqrt{6}}(k-2)+\frac{1}{\sqrt{5}}(4k-2).$

$(iii)\ RC(P(C_s,P_t,k)) = \sum_{\sigma\tau\in E(P(C_s,P_t,k))}\frac{1}{\sqrt{d_\sigma d_\tau}} =$

$E(2,2)\sum_{\sigma\tau\in E(P(C_s,P_t,k))}\frac{1}{\sqrt{d_\sigma d_\tau}} + E(3,3)\sum_{\sigma\tau\in E(P(C_s,P_t,k))}\frac{1}{\sqrt{d_\sigma d_\tau}} + E(2,3)\sum_{\sigma\tau\in E(P(C_s,P_t,k))}\frac{1}{\sqrt{d_\sigma d_\tau}}$

$$= (k(s-3)+(t-1)(k-1)+2)\ \frac{1}{\sqrt{2\times 2}}+(k-2)\frac{1}{\sqrt{3\times 3}}+(4k-2)\frac{1}{\sqrt{2\times 3}}$$

$= \frac{(k(s-3)+(t-1)(k-1)+2)}{2}+\frac{(k-2)}{3}+\frac{(4k-2)}{\sqrt{6}}.$

$(iv)\ M_1(P(C_s,P_t,k)) = \sum_{\sigma\tau\in E(P(C_s,P_t,k))}(d_\sigma+d_\tau)$

$= E(2,2)\sum_{\sigma\tau\in E(P(C_s,P_t,k))}(d_\sigma+d_\tau) + E(3,3)\sum_{\sigma\tau\in E(P(C_s,P_t,k))}(d_\sigma+d_\tau) + \mathrm{E}(2,3)\sum_{\sigma\tau\in E(P(C_s,P_t,k))}(d_\sigma+d_\tau)$

$= (k(s-3)+(t-1)(k-1)+2)\ (4)+6(k-2)+5(4k-2) = 4ks+4tk-4t+10k-10.$

$(v) M_2(G) = \sum_{\sigma\tau\in E(P(C_s,P_t,k))}(d_\sigma d_\tau) =$

$E(2,2)\sum_{\sigma\tau\in E(P(C_s,P_t,k))}(d_\sigma d_\tau) + E(3,3)\sum_{\sigma\tau\in E(P(C_s,P_t,k))}(d_\sigma d_\tau) + E(2,3)\sum_{\sigma\tau\in E(P(C_s,P_t,k))}(d_\sigma d_\tau).$

$= (k(s-3)+(t-1)(k-1)+2)(4)+(k-2)(9)+(4k-2)(6)$

$= 4ks+4tk+17k-4t-18$

$(vi) H(G) = \sum_{\sigma\tau\in E(G)}\frac{2}{(d_\sigma+d_\tau)}$

$= E(2,2)\sum_{\sigma\tau\in E(G)}\frac{2}{(d_\sigma+d_\tau)} + E(3,3)\sum_{\sigma\tau\in E(G)}\frac{2}{(d_\sigma+d_\tau)} + E(2,3)\sum_{\sigma\tau\in E(G)}\frac{2}{(d_\sigma+d_\tau)}$

$= (k(s-3)+(t-1)(k-1)+2)\frac{2}{4}+(k-2)\frac{2}{6}+(4k-2)\frac{2}{5}$

$= \frac{1}{2}(k(s-3)+(t-1)(k-1)+2)+\frac{1}{3}(k-2)+\frac{2}{5}(4k-2).$

3. Comparison

In this section, we provide the comparison of the above-computed topological indices numerically and the graphically. The numerical comparison of $P(C_s, P_t, k), s \geq 3, t \geq 1, k \geq 2$ where $s = 3,4,5$ and $t = 1,2,3$ are presented in Table 3.1,Table 3.2 and Table 3.3 and the graphical comparison is displayed in the Figure 1 and Figure 2.

Table: 3.1 Numerical Result of $P(C_3, P_1, k), k \geq 2$.

k	SD	SC	RC	M_1	M_2	H
2	17	3.68	3.45	38	44	3.4
3	27.67	5.88	5.41	64	77	5.33
4	38.3	8.08	7.39	90	110	7.27
5	49	10.28	9.35	116	143	9.2
6	59.67	12.47	11.31	142	176	11.13
7	70.33	14.67	13.29	168	209	13.07
8	81	16.05	15.25	194	242	15
9	91.67	19.07	17.21	220	275	16.93
10	102.33	21.26	19.18	246	308	18.87

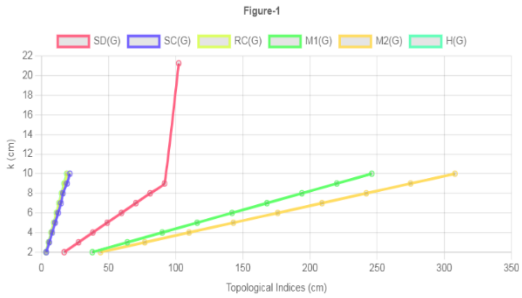
Table: 3.2 Numerical Result of $P(C_3, P_2, k), k \geq 2$.

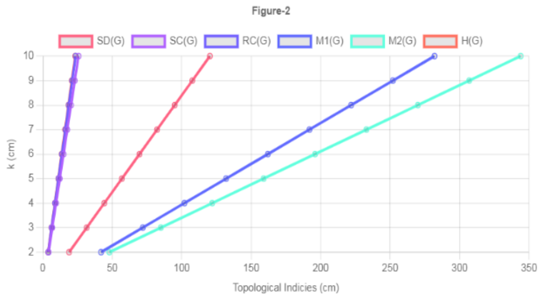
k	SD	SC	RC	M_1	M_2	H
2	19	4.18	3.95	42	48	3.9
3	31.67	6.88	6.42	72	85	6.33
4	44.33	9.58	8.88	102	122	8.77
5	57	12.27	11.35	132	159	11.2
6	69.67	14.97	13.82	162	196	13.63
7	82.33	17.67	16.28	192	233	16.07
8	95	20.36	18.75	222	270	18.5
9	107.67	23.06	21.21	252	307	20.93
10	120.33	25.76	23.68	282	344	23.37

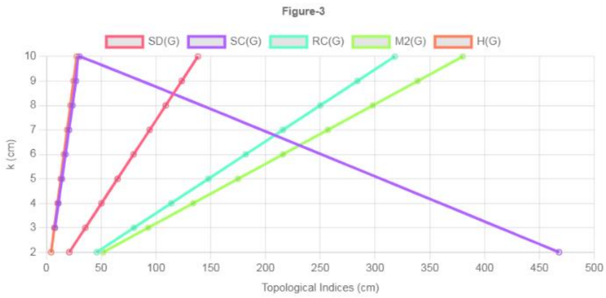
Table: 3.3 Numerical Result of $P(C_3, P_3, k), k \geq 2$.

k	SD	SC	RC	M_1	M_2	H
2	21	4.68	4.45	46	52	4.4
3	35.67	7.88	7.42	80	93	7.33
4	50.33	11.08	10.38	114	134	10.27
5	65	14.28	13.35	148	175	13.2
6	79.67	17.47	16.32	182	216	16.13
7	94.33	20.67	19.28	216	257	19.07
8	109	23.87	22.25	250	298	22

9	123.67	27.06	25.21	284	339	24.93
10	138.33	30.26	28.18	318	380	27.87







4. Conclusion

Topological indices help to understand the information about biological activity, chemical reactivity, and physical characteristics of chemical compounds. We derived the general formulas of some of the topological indices based on the degree of vertex . i.e., sum connectivity index(SC), Randic connectivity index(RC),symmetric division degree index (SD),Harmonic index(H),the first Zagreb index(M_1) and the second Zagreb index(M_2) of cycle path connected graph $P(C_s, P_t, k), s \geq 3, t \geq 1, k \geq 2$. These outcomes can be employed to further understand the topological characteristics of graphs. The comparison of expressed graphically and numerically.

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