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$\mathcal{S}$-INDEX OF CERTAIN LINE GRAPH OF SUBDIVISION GRAPHS

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Abstract: There are numerous applications of graph theory in the field of structural chemistry. In this paper, we compute the Sanskruti index $\mathcal{S}(G)$ of the Line graph of Subdivision Graph of cyclic hexagonal-square chain and nanocones $CNC_k[n]$ respectively.

Keywords and Phrases: Topological indices, Sanskruti index, Derived graph, Line graph.

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1. Introduction and Preliminaries

A graph $G = (V, E)$ be a finite, undirected graph, without loops or multiple edges having $p = |V|$ and $q = |E|$ specifies the total number of vertices and edges of a graph G, respectively. Any undefined term in this paper may be found in Harary [11]. Further, Let G be a simple graph, with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, N_u denotes the set of its neighbors in G, the degree of vertex u is $d_u = |N_u|$ and $S_u = \sum_{v\in N_u} d_v$. The subdivision graph $S(G)$ is the graph obtained from G by replacing each of its edge by a path of length 2. The line graph $L(G)$ of graph G is the graph whose vertices are the edges of G, two vertices e and f are incident if and only if they have a common end vertex in G.

A molecular graph is a set of points representing the atoms in the molecule and collection of lines representing the covalent bonds. For example, consider the Hydrocarbon C_2H_6, its molecular structure and molecular graph is shown in Fig. 1 (a) and (b) and Line graph of Subdivision Graphs of molecular graph of Hydrocarbon C_2H_6, is shown in Fig. 1 (c).

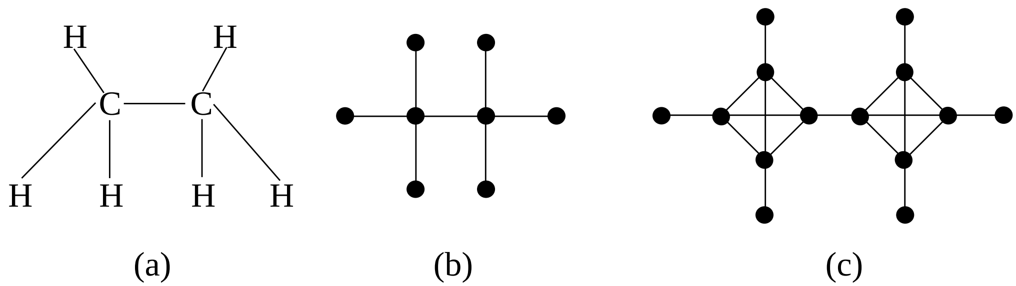

Figure 1

Topological indices are numerical parameters of a graph which are invariant under graph isomorphisms. Nowadays, there are many such indices that have found applications in Mathematical Chemistry especially in the quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (Q S A R) [4, 19]. A large number of such indices depend only on vertex degree of the molecular graph. One of them is the atom-bond connectivity(ABC) index, proposed by Estrada et al. [6] and is defined as:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)d_G(v)}} \tag{1}$$

This index provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes [6, 7]. Details about this index can be found in [2, 3, 10, 23]. For a collection of recent results on topological indices, we refer the interested reader to the articles [1, 5, 8, 12, 15, 16, 18, 20, 21, 22, 13, 14].

Inspired by work on the ABC index, Furtula et al. [9] proposed the following modified version of the ABC index and called it as augmented Zagreb index (AZI):

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_G(u) d_G(v)}{d_G(u) + d_G(v) - 2} \right)^3 \tag{2}$$

The prediction power is better than the ABC index in the study of heat of formation for heptanes and octanes ([9]).

Motivated by the previous research on topological descriptors and their applications, Hosamani [17] put forwarded Sanskruti index $\mathcal{S}(G)$ of a molecular graph G as follows:

$$\mathcal{S}(G) = \sum_{uv \in E(G)} \left(\frac{s_G(u) s_G(v)}{s_G(u) + s_G(v) - 2} \right)^3, \tag{3}$$

in which $s_G(u) = \sum\limits_{v \in N_G(u)} d_G(v)$ and $N_G(u) = \{v \in V(G) \backslash uv \in E(G)\}$. The $\mathcal{S}$-index was correlated with each of these properties and surprisingly, we can see that the $\mathcal{S}$-index has a good correlation with the entropy of octane isomers.

1.1. $\mathcal{S}-$Index of the Line graph of Subdivision Graph of cyclic hexagonal-square chain.

The molecular graph of a cyclic hexagonal-square chain consisting of n mutually isomorphic hexagonal chains $H_1, H_2, \ldots, H_n$, cyclically concatenated by cycle of length 4, in which the each H_i is a chain containing m hexagons as shown in Fig. 2, it is denoted by $C_{m,n}$. There are $4mn + 2n$ vertices and $5mn + 3n$ edges in $C_{m,n}$.

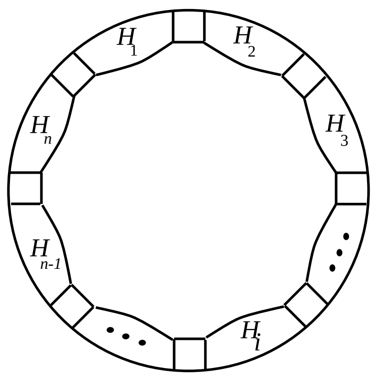

Figure 2: Cyclic hexagonal-square chain $C_{m,n}$

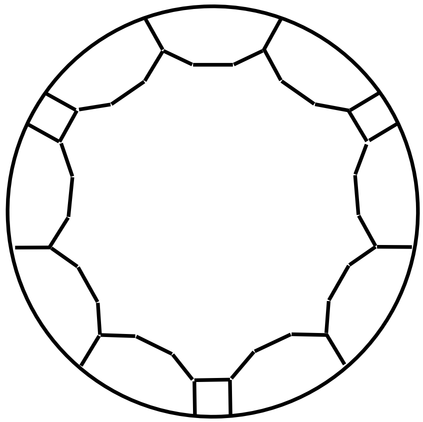

Figure 3: The graph $C_{3,3}$

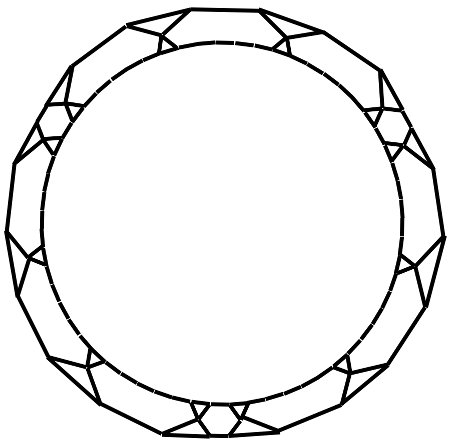

Figure 4: Line graph of subdivision of $C_{3,3}$.

Theorem 1.1. *Let G^* be the Line graph of Subdivision Graph of $C_{m,n}$.*

$$\mathcal{S}(G^*) = (1127.217)mn + (1163.6158)n.$$

Proof. The edge partition of G^* based on the sum of neighborhood degrees can be divided into seven edge partitions $E_i(G^*)$, $i = 4, 5, \dots, 9$, i.e. $E(G^*) = \cup_{i=4}^{9} E_i(G^*)$. The edge partition $E_4(G^*)$ contains mn edges uv, where $S_u = S_v = 4$, the edge partition $E_5(G^*)$ contains $2mn$ edges uv, where $S_u = 4$ and $S_v = 5$, the edge partition $E_6(G^*)$ contains $2mn$ edges uv, where $S_u = 5$ and $S_v = 8$, the edge partition $E_7(G^*)$ contains $mn-n$ edges uv, where $S_u = S_v = 8$, the edge partition $E_8(G^*)$ contains $2mn+2n$ edges uv, where $S_u = 8$ and $S_v = 9$, and the edge partition $E_9(G^*)$ contains $5mn+8n$ edges uv, where $S_u = S_v = 9$. Thus

$$\begin{aligned}
\mathcal{S}(G) &= \sum_{uv\in E(G)}\left(\frac{s_G(u)s_G(v)}{s_G(u)+s_G(v)-2}\right)^3 \\
&= mn\left(\frac{4\times 4}{4+4-2}\right)^3 + 2mn\left(\frac{4\times 5}{4+5-2}\right)^3 + 2mn\left(\frac{5\times 8}{5+8-2}\right)^3 \\
&+ (mn-n)\left(\frac{8\times 8}{8+8-2}\right)^3 + (2mn+2n)\left(\frac{8\times 9}{8+9-2}\right)^3 \\
&+ (5mn+8n)\left(\frac{9\times 9}{9+9-2}\right)^3 \\
&= (1127.217)mn + (1163.6158)n.
\end{aligned}$$

1.2. $\mathcal{S}-$Index of the Line graph of Subdivision Graph of nanocones $CNC_k[n]$

The graphical structure of $CNC_k[n]$ nanocones have a cycle of $k-$lenght at its central part and n levels of hexagons positioned at the conical exterior around its central part. The graph of $CNC_k[n]$ and its Line graph of Subdivision Graph are shown in Fig. 5 and Fig. 6 respectively.

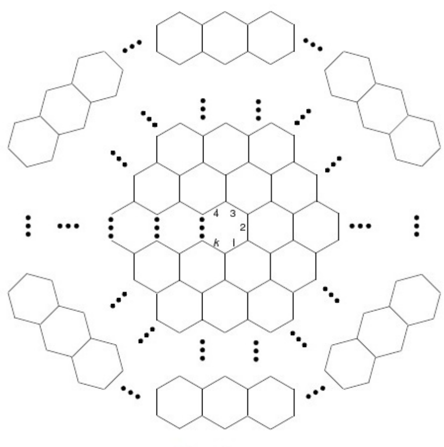

Figure 5: A graph $CNC_k[n]$.

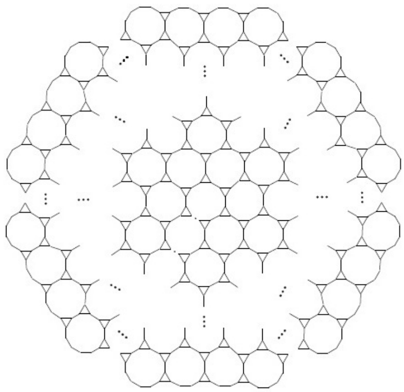

Figure 6: Line graph of subdivision of $CNC_k[n]$.

Theorem 1.2. *Let G^* be the Line graph of Subdivision Graph of $CNC_k[n]$.* $\mathcal{S}(G^*) = (30.0783)k + (30.5175)n + (316.7163)kn + (129.7463)\left(k \times \frac{9}{2}n^2 + \frac{1}{2}n\right)$

Proof. The edge partition of G^* based on the sum of neighborhood degrees can be divided into seven edge partitions $E_i(G^*)$, $i = 4, 5, \ldots, 10$, i.e. $E(G^*) = \cup_{i=4}^{9} E_i(G^*)$. The edge partition $E_4(G^*)$ contains k edges uv, where $S_u = S_v = 4$, the edge partition $E_5(G^*)$ contains $2k$ edges uv, where $S_u = 4$ and $S_v = 5$, the edge partition $E_6(G^*)$ contains $k(n-1)$ edges uv, where $S_u = 5$ and $S_v = 5$, the edge partition $E_7(G^*)$ contains $2kn$ edges uv, where $S_u = 5$ and $S_v = 8$, the edge partition $E_8(G^*)$ contains kn edges uv, where $S_u = 8$ and $S_v = 8$, the edge partition $E_9(G^*)$ contains $2kn$ edges uv, where $S_u = 8$ and $S_v = 9$ and the edge partition $E_{10}(G^*)$ contains $\left(k \times \frac{9}{2}n^2 + \frac{1}{2}n\right)$ edges uv, where $S_u = 9$ and $S_v = 9$ Thus

$$\begin{aligned}
\mathcal{S}(G) &= \sum_{uv \in E(G)} \left(\frac{s_G(u)s_G(v)}{s_G(u) + s_G(v) - 2} \right)^3 \\
&= k\left(\frac{4 \times 4}{4+4-2}\right)^3 + 2k\left(\frac{4 \times 5}{4+5-2}\right)^3 + k(n-1)\left(\frac{5 \times 5}{5+5-2}\right)^3 \\
&+ 2kn\left(\frac{5 \times 8}{5+8-2}\right)^3 + kn\left(\frac{8 \times 8}{8+8-2}\right)^3 \\
&+ 2kn\left(\frac{8 \times 9}{8+9-2}\right)^3 + \left(k \times \frac{9}{2}n^2 + \frac{1}{2}n\right)\left(\frac{9 \times 9}{9+9-2}\right)^3
\end{aligned}$$

$$= (30.0783)k + (30.5175)n + (316.7163)kn + (129.7463)\left(k \times \frac{9}{2}n^2 + \frac{1}{2}n\right).$$

2. Conclusion

The application part of Sanskruti index in chemical nanostructures has been well explained and the detailed description may be found in [17].

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