S−INDEX OF CERTAIN PARA-LINE GRAPHS

BALACHANDRA P.[1], PADMAJA VENUGOPAL[1], SHANMUKHA B[2], AND MANJUNATH N[3]*

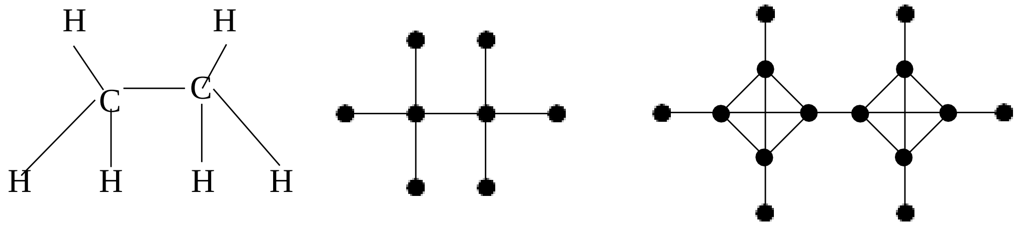
ABSTRACT. Recently Hosamani [14] has put forward a novel topological index namely the Sanskruti index $S(tt)$ of a molecular graph tt. Topological indices are valuable in the study of QSAR/QSPR. There are numerous applications of graph theory in the field of structural chemistry. In this paper, we computed the Sanskruti index $S(tt)$ of the para-line graph of cyclic hexagonal-square chain and nanocones $CNC_k[n]$ respectively.

1. Introduction and Preliminaries

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. The para-line graph of G is the line graph of the subdivision graph of 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 Para-line graph of molecular graph of Hydrocarbon C_2H_6, is shown in Fig. 1 (c).

Key words and phrases. Topological indices, para-line graph.



(a) (b) (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 (QSAR) [4, 16]. 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:

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

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, 20]. For a collection of recent results on topological indices, we refer the interested reader to the articles [1, 5, 8, 11, 12, 13, 15, 17, 18, 19].

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):

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

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 [14] put forwarded Sanskruti index $S(G)$ of a molecular graph G as follows:

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

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

1.1. $S-$**Index of the para-line 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 $C_{m,n}$.

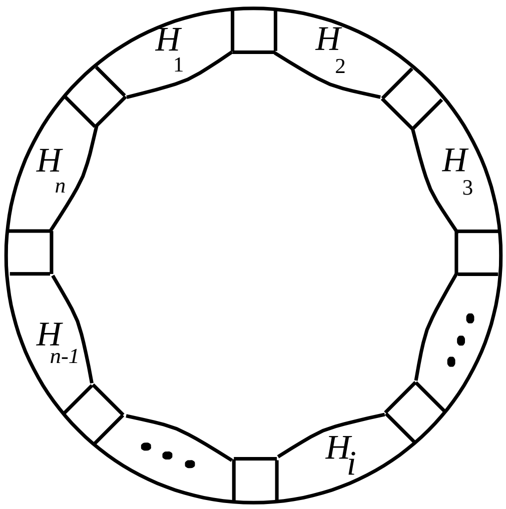


FIGURE 2. Cyclic hexagonal-square chain $C_{m,n}$

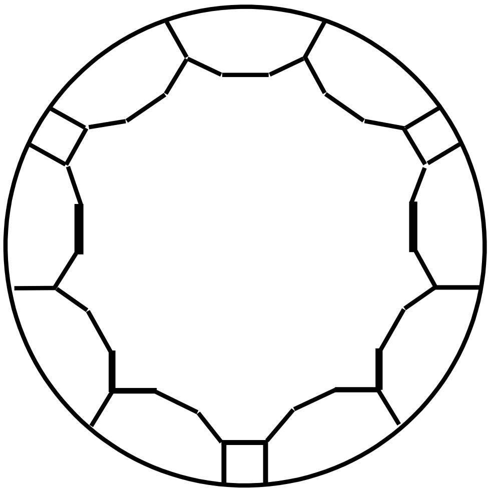


FIGURE 3. The graph $C_{3,3}$

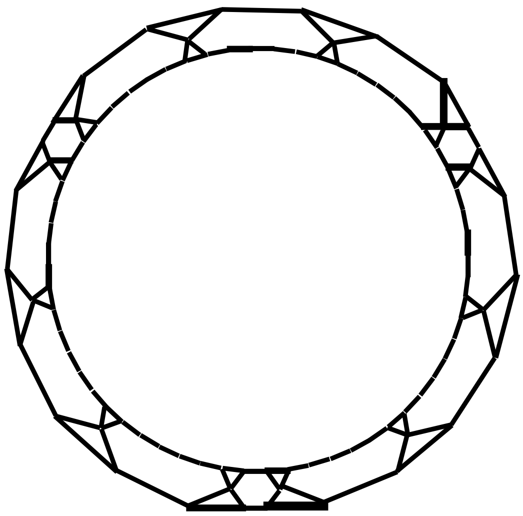


FIGURE 4. Line graph of subdivision of $C_{3,3}$.

Theorem 1.1. *Let G^* be the para-line graph of $C_{m,n}$.*

$$S(G^*) = (1127.217)mn + (1163.6158)n.$$

Proof. The edge partition of G^* based on the sum of neighborhood degrees can be divided into seven edge partitions $E_i(G^*)$, $i = 4, 5, \ldots, 9$, 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

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

Q

1.2. **S−Index of the para-line 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 para-line graphs are shown in Fig. 5 and Fig. 6 respectively.

Theorem 1.2. *Let G^* be the para-line graph of $CNC_k[n]$.*

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

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 $2kn$

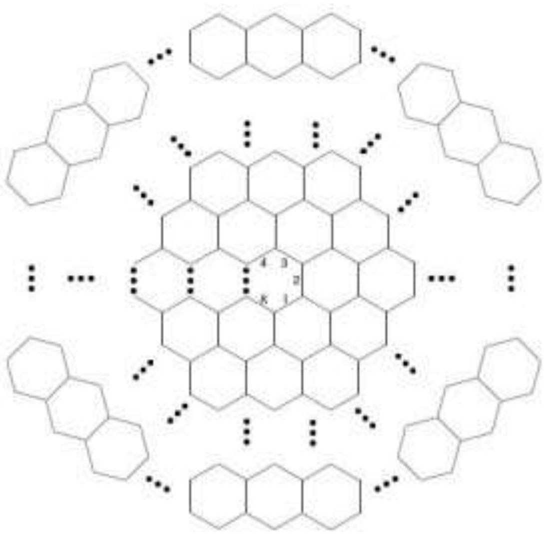


FIGURE 5. A graph $CNC_k[n]$.

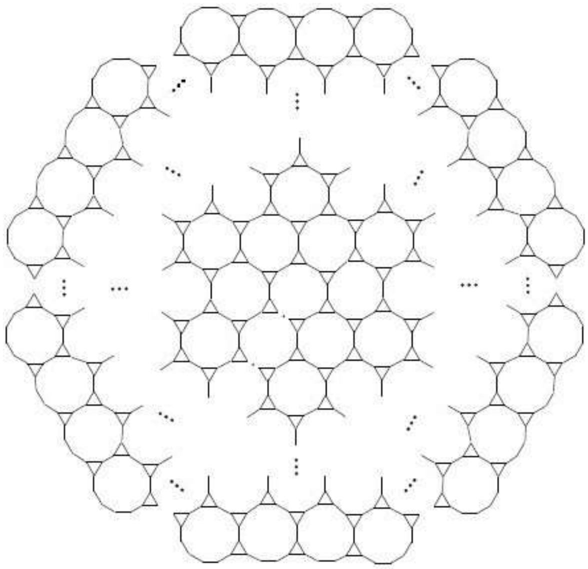


FIGURE 6. Line graph of subdivision of $CNC_k[n]$.

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 $k \times \left(\frac{9}{2}n^2 + \frac{1}{2}n\right)$ edges uv, where

$S_u = 9$ and $S_v = 9$ Thus

$$S(G) = \sum_{uv\in E(tt)} \left(\frac{S_G(u)S_G(v)}{S_G(u)+S_G(v)-2} \right)^3$$

$$= k\left(\frac{4\times 4}{4+4-2}\right)^3 + 2k\left(\frac{4\times 5}{4+5-2}\right)^3 + k(n-1)\left(\frac{5\times 5}{5+5-2}\right)^3$$

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

$$+ 2kn\left(\frac{8\times 9}{8+9-2}\right)^3 + \left(k\times\frac{9}{2}n^2+\frac{1}{2}n\right)\left(\frac{9\times 9}{9+9-2}\right)^3$$

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

Q

References

[1] G. Caporossi, P. Hansen, D. Vukičević, Comparing Zagreb indices of cyclic graphs, MATCH Commun. Math. Comput. Chem. 63 (2010), 441–451.

[2] J. Chen, J. Liu, X. Guo, Some upper bounds for the atom-bond connectivity index of graphs. Applied Mathematics Letters 25(2012) 1077–1081.

[3] K.C. Das,I. Gutman, B. Furtula, On atom-bond connectivity index. Filomat 26(2012) 733–738.

[4] J. Devillers, A. T. Balaban (Eds.) Topological Indices and Related Descriptors in QSAR and QSPR (1999). Gordon and Breach, Amsterdam.

[5] A. A. Dobrynin, A. A. Kochetova, Degre distance of a graph: A degree analogue of the Wiener index, J. Chem. Inf. Comput. Sci., 34 (1994) 1082–1086.

[6] E. Estrada, L. Torres, L. Rodrguez, I. Gutman, An atom-bond connectivity index: modelling the enthalpy of formation of alkanes. Indian Journal of Chemistry-Section A 37(1998) 849–855.

[7] E. Estrada, Atom-bond connectivity and the energetic of branched alkanes. Chemical Physics Letters 463(2008) 422–425.

[8] G. H. Fath-Tabar, Old and new Zagreb indices of graphs, MATCH Commun. Math. Comput. Chem. 65 (2011) 79–84.

[9] B. Furtula, A. Graovac, D. Vukičević, Augmented Zagreb index. Journal of Mathematical Chemistry 48(2010) 370–380.

[10] B. Furtula, I. Gutman, M. Ivanović, D. Vukičević, Computer search for trees with minimal ABC index. Applied Mathematics and Computation 219(2012) 767–772.

[11] I. Gutman, K. C. Das, The first Zagreb index 30 years after, MATCH Commun. Math. Comput.Chem. 50 (2004), 83–92.

[12] S. M. Hosamani and I. Gutman, Zagreb indices of transformation graphs and total transformation graphs, Appl. Math. Comput. 247 (2014) 1156-1160.

[13] S. M. Hosamani, B. Basavanagoud, New upper bounds for the first Zagreb index, MATCH Commun. Math. Comput. Chem. 74(1) (2015) 97–101.

[14] S. M. Hosamani, Computing Sanskruti index of certain nanostructures, Journal of Applied Mathematics and Computing, 1-9 (2016).

[15] S. M. Hosamani, and M. Krzywkowski, On the difference of Zagreb coindices of graph operation, Gulf Journal of Mathematics, 4(3)(2016), 36-41

[16] S. M. Hosamani, D. Perigidad, S. gavade, QSPR Analysis of Certain Degree Based Topological Indices, J. Stat. Appl. Pro. 6, No. 2, 1-11 (2017)

[17] S. M. Hosamani, On topological properties of the line graphs of subdivision graphs of certain nanostructures-II, GJSCR, 17(4), 2017

[18] S. M. Hosamani, S. H. Malghan , P. V. Patil First Zagreb Coindex of Hamiltonian Graphs, Journal of Information and Optimization Sciences, 38:3-4, 417-422

[19] S. M. Hosamani, E. Suresh, T. Mansour, M. A. Rastomi, More on inverse degree and topological indices of graphs, Filomat, 32(1):165-178 (2018)

[20] W. Lin, T. Gao, Q. Chen, X. Lin, On the minimal ABC index of connected graphs with given degree sequence. MATCH Communications in Mathematical and in Computer Chemistry 69(2013) 571–578.

[3*] Department of Mathematics, Christ University, Faculty Of Engineering, Kanminike, Kumbalgodu, Bengaluru.

E-mail address: manjunath.nanjappa@christuniversity.in

[1] Department of Mathematics, S. J. B. I. T. BGS Health and Education City, Ben- galuru.

E-mail address: balachandrapsjbit@gmail.com

[2] Department of Mathematics, P.E.S College of Engineering, Mandya.