INVERSE SUM INDEG INDEX OF THE LINE GRAPHS OF SUBDIVISION GRAPHS OF SOME CHEMICAL STRUCTURES

Wei GAO[1*], Muhammad K. JAMIL[2], Aisha JAVED[3], Mohammad R. FARAHANI[4], Muhammad IMRAN[5]

The degree-based topological indices correlate physico-chemical properties such as stability, strain energy, boiling point etc. of certain chemical compounds. Among the degree based topological indices inverse sum indeg index is a significant predictor of total surface area of some chemical compounds. In this paper, we compute the inverse sum indeg index of some chemical structure by using the line graphs of subdivision of these chemical graphs.

Keywords: Molecular Graph, Chemical Structures, Inverse Sum Indeg Index, Line Graphs, Subdivision Graphs

1. Introduction

Mathematical chemistry is a branch of theoretical chemistry in which we predict and discuss the chemical structures by using mathematical tools. Chemical graph theory is a branch of mathematical chemistry in which we apply tools from graph theory to model the chemical phenomenon mathematically. A structural formula of a chemical compounds is represented by a molecular graph in terms of graph theory, where the vertices and edges of molecular graphs are corresponding to the atoms of the compounds and chemical bonds, respectively.

Let $G=(E(G),V(G))$ be a simple connected graph, where $E(G)$ and $V(G)$ are the sets of vertices and edges, respectively. The number of vertices in the set $V(G)$, $|V(G)|$, is called the order and the number of edges in the set $E(G)$, $|E(G)|$, is

[1] School of Information Science and Technology, Yunnan Normal University, Kunming, PR China, e-mail: gaowei@ynnu.edu.cn
[2] Department of Mathematics, Riphah Institute of Computing and Applied Sciences (RICAS), Riphah International University, Lahore, Pakistan, e-mail: m.kamran.sms@gmail.com
[3] Department of Mathematics, Riphah Institute of Computing and Applied Sciences (RICAS), Riphah International University, Lahore, Pakistan, e-mail: aaishajaved@gmail.com
[4] Department of Applied Mathematics, Iran University of Science and Technology, Narmak, Tehran, Islamic Republic of Iran, e-mail: MRFarahani88@gmail.com
[5] Department of Mathematical Sciences, United Arab Emirates University, Al Ain, United Arab Emirates, e-mail: imrandhab@gmail.com

called the size of the graph *G*. Two vertices in a graph G are adjacent if and only if they are connected with an edge. The degree of a vertex $v \in V(G)$ is the number of adjacent vertices to *v*, it is denoted as *d(v)*. The subdivision graph, *S(G)*, is the graph obtained from graph *G* by replacing each of its edges by a path of length two. The line graph, *L(G)*, of a graph *G* is the graph whose vertices are the edges of existing graph *G*, where two vertices *e* and *f* are incident if and only if they have a common end vertex in *G*.

Graph theory has provided to the theoretical chemists with a variety of useful tools, such as topological matrices, topological polynomials and topological indices. A topological index is an invariant number associated to a graph with the property that topological index of any two graphs *G* and *H* are equal if they are isomorphic.

In 1972, Gutman and Trinajstić introduced the oldest topological indices the Zagreb indices [3]. These topological indices have been used to study boiling point, melting point, molecular complexity, chirality and hetero-systems. The first (M_1) and second (M_2) Zagreb indices are defines as

$$M_1(G) = \sum_{v \in V(G)} (d_v)^2 = \sum_{e=uv \in E(G)} (d_u + d_v)$$

$$M_2(G) = \sum_{e=uv \in E(G)} (d_u d_v)$$

In 1975, Randić [4] proposed a structural descriptor called the branching index that later named as famous Randić index. The Randić index is one of the most successful molecular descriptors in QSPR and QSAR studies. It is suitable for measuring the extent of branching of carbon-atom skeleton of saturated hydrocarbons. It is defined as

$$R(G) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

Sum connectivity index is a closely related variant of the Randić index. Sum connectivity index is proposed by Zhou [11] and it is defined as

$$X(G) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}$$

Recently, Vukičević et. al [10] introduced the inverse sum indeg index. It is defined as

$$ISI(G) = \sum_{e=uv \in E(G)} \frac{d_u d_v}{d_u + d_v}$$

ISI index is used to predict of total surface area for octane isomers.

For further study of these topological indices, we refer [1, 2, 5].

In 2011, Ranjini et. al. [8] calculated the Zagreb indices of the line graph of the tadpole, wheel and ladder graphs with subdivision technique. Su and it Xu [9] computed the general sum-connectivity indices and co-indices of the same graphs. Nadeem et. al [6, 7] computed certain topological indices of the line graphs of subdivision graphs of the tadpole, wheel, ladder graphs and certain nanostructures. In this paper, we computed the inverse sum indeg index of the line graph of subdivision graph of certain structures.

2. Main Results

In this section, we extend the study of computation of certain topological indices of the line graphs of subdivision graphs. We computed the inverse sum indeg index of the line graph of hexagonal parallelogram *P(m,n)* nanotube, triangle Benzenoid G_n, zigzag- edge coronoid fused with starphene *ZCS(k,l,m)* and 2D-lattics, nanotube and nanotorus of $TUC_4C_8[m,n]$ by using the concept of subdivision.

2.1. Hexagonal Parallelogram *P(m,n)* Nanotube

Hexagonal parallelogram, *P(m,n)*; $\forall m,n \in$ □, consists of a hexagons arranged in parallelogram shape. In *P(m;n)*, m denotes the number of hexagons in any row and *n* is the number of hexagons in any column. The order and the size of the hexagonal parallelogram structure is *2(m+n+mn)* and *3mn+2m+2n*+1, respectively.

The number of vertices in the line graph of the subdivision graph of *P(m;n)* are *2(3mn+2m+2n 1)* and the number of edges are *9mn+4m+4n 5*, respectively. Fig. 1 shows the parallelogram and its subdivision and Fig. 2 shows the line graph of subdivision graph of *P(m,n)*.

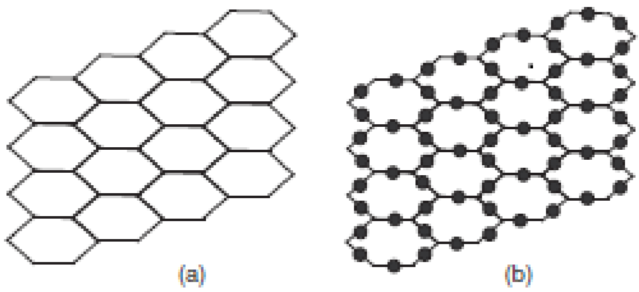

Fig. 1: (a) A hexagonal parallelogram *P(4,4)*. (b) A subdivision of hexagonal parallelogram *P(4,4)*.

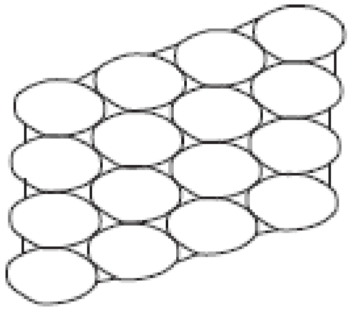

Fig. 2: A line graph of subdivision graph of hexagonal parallelogram *P(4,4)*.

Theorem 1. Let *G* denotes the line graph of subdivision graph of the hexagonal parallelogram, then the inverse sum indeg index of the graph *G* is equal to

$$ISI(G)=\frac{1}{10}\ (135mn+38m+38n-91).$$

Table 1:
Edge partition of the line graph of the subdivision graph of hexagonal parallelogram *P(m,n)* based on degree of end vertices of each edge.

Row	$E_{2,2}$	$E_{2,3}$	$E_{3,3}$
1	m+6	2m	9m-5
2	2	4	9m-2
3	2	4	9m-2
.	.	.	.
.	.	.	.
.	.	.	.
n	m+6	2m	7m-4
Total	2(m+n+4)	4(m+n-2)	9mn-2m-2n-5

Proof. To find the inverse sum indeg index of hexagonal parallelogram *P(m,n)*, we partition the edge set of the line graph of the subdivision graph of hexagonal parallelogram structure based on degree of end vertices in Table1. With the help of Table 1 we can find the inverse sum indeg index of line graph of subdivision graph of hexagonal parallelogram *P(m;n)*, as follows:

$$ISI(G)=\sum_{uv\in G)}\frac{d(u)d(v)}{d(u)+d(v)}$$

$$= \sum_{uv\in E_{2,2}} \frac{d(u)d(v)}{d(u)+d(v)} + \sum_{uv\in E_{2,3}} \frac{d(u)d(v)}{d(u)+d(v)} + \sum_{uv\in E_{3,3}} \frac{d(u)d(v)}{d(u)+d(v)}$$

$$= 2(m+n+4)\frac{2\times 2}{2+2} + 4(m+n-2)\frac{2\times 3}{2+3} + (9mn-2m-2n-5)\frac{3\times 3}{3+3}$$

$$= \frac{1}{10}(135mn+38m+38n-91).$$

2.2. Triangular Benzenoid G_n

The triangular Benzenoid, G_n $(\forall n \in \mathbb{N})$,, is the generalizations of benzene molecule C_6H_6 in which benzene rings form a triangular shape. The benzene molecule is a very useful to synthesize aromatic compounds. The graphical structures of triangular Benzenoid G_n, subdivision of triangular Benzenoid $S(G_n)$ and line graph of subdivision graph of triangular Benzenoid $L(S(G_n))$ are shown in Figs. 3 and 4. The graph of triangular Benzenoid contain n^2+4n+1 vertices and $\frac{3}{2}n(n+3)$ edges, and the line graph of subdivision graph of triangular Benzenoid contain $3n(n+3)$ vertices and $\frac{3}{2}(3n^2+7n+2)$.

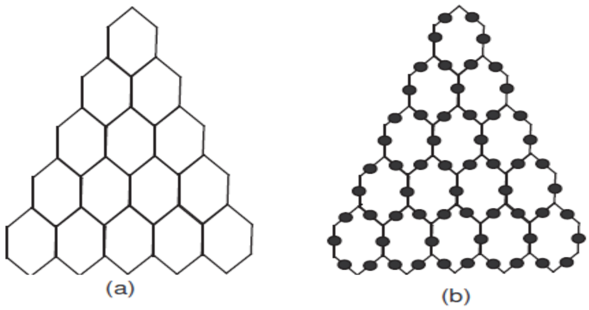

Fig. 3: (a) Triangular Benzenoid G_n for $n=5$. (b) A subdivision of triangular Benzenoid G_n for $n=5$.

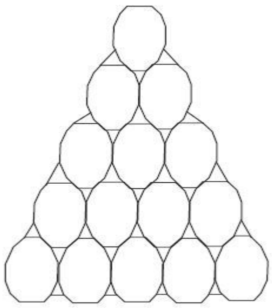

Fig. 4: Line graph of subdivision graph of triangular Benzenoid G_n for $n=5$.

Theorem 2. Let *H* denotes the line graph of the subdivision graph of triangular Benzenoid G_n, then

$$ISI(H)=\frac{3}{20}\ (45n^2+83n+48)$$

Proof. The total number of edges in the structure of the line graph of the subdivision graph of triangular Benzenoid G_n are $^3{}_2$ $(3n^2+7n\ 2)$. To obtain the required result we partitioned the edge set of the line graph of subdivision graph of triangular Benzenoid G_n as show in Table 2. We use Table 2 to obtain the required result.

$$ISI(H)=\sum\nolimits_{uv\in H)}\frac{d(u)d(v)}{d(u)+d(v)}$$

$$=\sum_{uv\in E_{2,2}}\frac{d(u)d(v)}{d(u)+d(v)}+\sum_{uv\in E_{2,3}}\frac{d(u)d(v)}{d(u)+d(v)}+\sum_{uv\in E_{3,3}}\frac{d(u)d(v)}{d(u)+d(v)}$$

$$=3(n+3)\frac{2\times 2}{2+2}+6(n-1)\frac{2\times 3}{2+3}+\frac{3}{2}(3n^2+n-4)\frac{3\times 3}{3+3}$$

$$=\frac{3}{20}(45n^2+83n-48).$$

Table 2:
Edge partition of the line graph of the subdivision graph of triangular Benzenoid G_n based on degree of end vertices of each edge.

E_{d_u,d_v}	$E_{2,2}$	$E_{2,3}$	$E_{3,3}$
Number of edges	3(n+3)	6(n-1)	$\frac{3}{2}(3n^2+n-4)$

2.3. Zigzag-edge coronoid fused with starphene nanotubes *ZCS(k,l,m)* for *k=l=m≥4*

This system is a composite Benzenoid generated by fusing a zigzag-edge coronoid *ZC(k,l,m)* with a starphene *St(k,l,m)*. The graphical structure of zigzag-edge coronoid fused with starphene nanotubes *ZCS(k,l,m)* contain $36k+54$ vertices and $15(k+l+m)-63$ edges. Figs. 5 and 6 shows the graphical structure of zigzag-edge coronoid fused with starphene nanotubes, its subdivision graph and the line graph of subdivision graph. The line graph of subdivision graph of zigzag-edge coronoid fused with starphene nanotubes contain $30(k+l+m\ 126)$ vertices and $39(k+l+m)+153$ edges.

Theorem 3. Let *I* be the line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes *ZCS(k,l,m)* for $k=l=m=4$. Then we have

$$ISI(I)=\frac{3}{2}(121(l+m+k)-731)$$

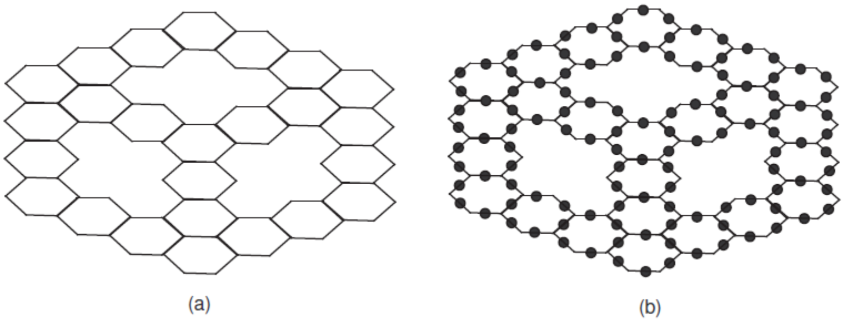

Fig. 5: (a) The Zigzag-edge conronoid fused with starphene nanotubes *ZCS(k,l,m)* for *k=l=m=4*. (b) The subdivision graph of zigzag-edge coronoid fused with starphene nanotubes *ZCS(k,l,m) for k=l=m=4*.

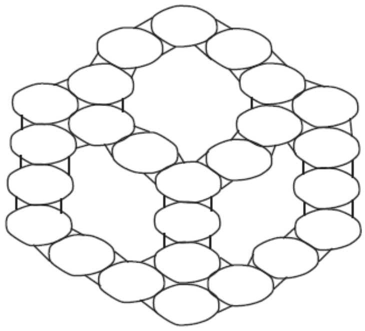

Fig. 6: The line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes *ZCS(k,l,m)* for *k=l=m=4*.

Proof. Zigzag-edge coronoid fused with starphene nanotubes *ZCS(k,l,m)* have *39(k+l+m)+153* edges in its graphical structure. We partitioned these edges based on the degree of the end vertices of each edge as shown in Table 3. Then we use the Table 3 to obtain the required result.

$$ISI(I)=\sum_{uv\in I)}\frac{d(u)d(v)}{d(u)+d(v)}$$

$$=\sum_{uv\in E_{2,2}}\frac{d(u)d(v)}{d(u)+d(v)}+\sum_{uv\in E_{2,3}}\frac{d(u)d(v)}{d(u)+d(v)}+\sum_{uv\in E_{3,3}}\frac{d(u)d(v)}{d(u)+d(v)}$$

$$=6(k+l+m-5)\frac{2\times 2}{2+2}+12(k+l+m-7)\frac{2\times 3}{2+3}+21(k+l+m)-39\frac{3\times 3}{3+3}$$

$$=\frac{3}{2}(121(l+m+k)-731).$$

Table 3:
Edge partition of the line graph of the subdivision graph of zigzag-edge coronoid fused with starphene *ZCS(k,l,m)* based on degree of end vertices of each edge.

E_{d_u,d_v}	$E_{2,2}$	$E_{2,3}$	$E_{3,3}$
Number of edges	6(k+l+m-5)	12(k+l+m-7)	21(k+l+m)-39

3. Conclusion

The inverse sum indeg index is a recently introduced topological index, which play a significant role to predict the surface area of certain molecules. In this paper we discussed the line graph of subdivision graph of certain molecular graph and then found the exact formulas for inverse sum indeg index of the line graph of subdivision graph of hexagonal parallelogram, triangular benzenoid system and Zigzag-edge coronoid fused with starphene nanotubes.

REFERENCES

[1] I. Gutman, Degree-based topological indices, Croat. Chem. Acta 86 (2013) 351-361.
[2] I. Gutman, M.K. Jamil, N. Akhter, Graphs with fixed number of pen-dent vertices and minimalfirst Zagreb index, Transaction on Cobinatorics, 4(1) (2015) 43-48.
[3] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals, Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett., 17 (1972) 535-538.
[4] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc., 97 (1975) 6609-6615.
[5] S. Nikolic, G. Kovacevic, A. Milicevic, N. Trinajstić, The Zagreb indices 30 years after, Croat. Chem. Acta, 76 (2003) 113-124.
[6] M.F. Nadeem, S. Zafar, Z. Zahid, On certain topological indices of the line graph of subdivision graphs, Applied Mathematics and Computation, 271 (2015) 790-794.
[7] M.F. Nadeem, S. Zafar, Z. Zahid, On topological properties of the line graphs of subdivision graphs of certain nanostructures, Applied Mathematics and Computation, 273 (2016) 125-130.
[8] P. S. Ranjini, V. Lokesha, I. N. Cangul, On the Zagreb indices of the line graphs of the subdivision graphs, Applied Mathematics and Computation, 218 (2011) 699-702.
[9] G. Su, L. Xu, Topological indices of the line graph of subdivision graphs and their Schurbounds, Applied Mathematics and Computation, 253 (2015) 395-401.
[10] D. Vukicevic, M. Gasperov, Bond additive modeling 1. Adriatic indices, Croat. Chem. Acta, 83 (2010) 243-260.
[11] B. Zhou, N. Trinajstić, On a novel connectivity index, J. Math. Chem., 46 (2009) 1252-1270.