On the edge version of topological indices for certain networks

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Abstract. In QSPR/QSAR study, topological indices such as Shultz index, generalized Randić index, Zagreb index, general sum-connectivity index, atom-bond connectivity (ABC) index and geometric-arithmetic (GA) index are utilized to guess the physico-chemical and bioactivity of chemical compounds. They can be classified based on the structural properties of graphs used for calculation. There is numerous applications of graph theory in this field of research. The aims of this paper is to investigate the generalize on the edge version Randić, GA, ABC, multiplicative ABC, Zagreb and inverse sum indices for certain graph networks by using the concept of line graphs.

Keywords: line graphs, topological indices, networks.

1. Introduction

Chemical graph theory is a branch of mathematical chemistry which has an important effect on the development of the chemical sciences. Every individual number used to characterize some properties of a graph is known as a topological index of a related (molecular) graph. Topological indices are the numerical quantities which represent the structure of any simple finite graph. It's apparent that the numbers of vertices and edges are topological variants. The first graph invariant reported as (distance based) topological index, Wiener index, is denoted as half of distances between all the pairs of vertices in a graph [1]. Meanwhile, on the basis of the distance between edges, the edge version of Wiener index was proposed by Iranmanesh et al. [6]. Several recent results on various types of Wiener indices (such as Wiener polarity index) can be referred to Ma et al. [7,8]. The meaningful of topological indices is generally

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related with quantitative structure activity (QSAR) and quantitative structures property relationship (QSPR), see [2, 4, 5].

In this article, we will consider only simple graphs, as an unweighted, undirected graph who has no loop and multiple edges attached. As the concept in theoretical and applies areas, a graph is represented by a collection points and lines, we can be separately called vertices and edges. Suppose e is an edge of G, which connects the u and v, then we denote $e = uv$ and state that u and v are adjacent. The degree d_u of a vertex u is the number of edges that are incident to it.

The first and oldest degree based topological index was introduced by Milan Randić in 1975 named Randić index [15]. The Randić index of graph G is defined as

$$R(G) = \sum_{u,v \in G} (d_u d_v)^{-1/2}, \tag{1}$$

where d_u and d_v represent the degree of the vertices u and v, respectively.

In 1998, Bollobas and Erdos [16] generalized this Randić index for any real number α, and known as the generalized Randić index $R_\alpha(G)$:

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha. \tag{2}$$

For further study of Randić index of various graph families, see [2, 13, 18, 32]. Referring to the end vertex degree d_e and d_f of the edges e and f in a line graph of G, Gao et al. [22] proposed the edge version Randić index. This idea is expressed as follows:

$$_eR_\alpha(G) = \sum_{ef \in E(L(G))} (d_e \bullet d_f)^{-1/2}. \tag{3}$$

Furthermore, Randić [14] raised one of the most important topological indices as branching index, that is, the sum of certain bond contributions calculated from the vertex degree of the hydrogen suppressed molecular graphs.

With the reference to Randić connectivity index, Vukicevic and Furtula [33] put forward the geometric-arithmetic index (briefly, GA), a topological index, and it is designed on the ground of the end-vertex degrees of edges in a graph connected G with the vertex set $V(G)$ and the edge set $E(G)$. To be specific, this index can be described as

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u \bullet d_v}}{d_u + d_v}, \tag{4}$$

where d_u states the degree of the vertex u in G . All the information about geometric-arithmetic index is wanted, please refer to Fath-Tabar et al. [19] and Yuan et al. [34]. If more results on topological index computation are in need, please refer to Gao and Farahani [25], Vukicevic and Furtula [29], Gao and Wang [26] and [27], Asadpour [35] and [14, 33, 37-41].

Iranmanesh et al. [36] proposed the edge version of geometric arithmetic index, referring to the end-vertex degrees of edges in a line graph of G. This idea is described in the following:

$$GA_e(G) = \sum_{ef \in E(L(G))} \frac{2\sqrt{d_e \bullet d_f}}{d_e + d_f} \tag{5}$$

where d_e represents the degree of the edge e in G. Recently, Nadeem et al. [42] also studied GA_e index of nanocones.

Estrada et al. [9] put forward a topological index with the name of the atom-bond connectivity index (briefly, ABC) as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \bullet d_v}}, \tag{6}$$

where d_u and d_v represent the degrees of the vertices u and v, respectively.

Recent advances on ABC index can be referred to Das et al. [10], Lin et al. [11] , Gao and Shao [23] , and Bianchi et al. [12]. Farahani [17] proposed the edge version of atom-bond connectivity index. This idea is expressed as follows: This idea is expressed as follows:

$$ABC_e(G) = \sum_{ef \in E(L(G))} \sqrt{\frac{d_e + d_f - 2}{d_e \bullet d_f}}, \tag{7}$$

where d_e is the degree of the edge e in $L(G)$.

The multiplicative atom-bond connectivity index was introduced by Kulli in 2016 [20]. Later, the edge version of multiplicative atom-bond connectivity index [21] of a graph G was introduced and it is defined as

$$ABCII_e(G) = \prod_{ef \in E(L(G))} \sqrt{\frac{d_e + d_f - 2}{d_e \bullet d_f}}, \tag{8}$$

where d_e is the degree of the edge e in $L(G)$.

Zagreb index is a degree based molecular descriptor that was introduced by Gutman and Trinajstic [12] more than 3 decades ago. Gao et al. [22] proposed the edge version Zagreb index. This idea is expressed as follows:

$${}_eM_1(G) = \sum_{ef \in E(L(G))} (d_e + d_f), \tag{9}$$

where d_e is the degree of the edge e in $L(G)$.

In 2010, Vukicevic and Gasperov [28] introduced the inverse sum indeg index of a graph G. The edge version of inverse sum indeg index of graph G was found by Bhanumathi et al. [30] and is defined as

$$ISI_e(G) = \sum_{ef \in E(L(G))} \frac{d_e \bullet d_f}{d_e + d_f}, \tag{10}$$

where d_e is the degree of the edge e in $L(G)$. For further study of edge version of indices of various graph families, see [20, 30, 32-36].

Now, we define some notations of the graph theory. In graph G, if the corresponding edges share a vertex in G, the line graph $L(G)$ of a graph G is considered as a graph with vertices of the edges in G, and it possesses two adjacent vertices. Similarly, the degree of an edge $e \in E(G)$ is represented by the number of its adjacent vertices in $V(L(G))$.

2. Topological indices of $L(G)$

In 2012, Farahani [17] computed ABC_e index of the circumcoronene series of benzenoid. Recently, Gao et al. [24] studies on the ABC_e and GA_e indices of certain graph operations. They also studied the edge version of Randić, Zagreb, ABC_e and GA_e of $HAC_5C_6C_7[p, q]$ in [22]. In 2018, Kulli [20] computed the edge version of multiplicative ABC index of certain nanotubes and nanotorus. Also, Bhanumathi et al. [30] studied the edge inverse sum indeg index connected graph.

Motivated by the result of [17, 20, 22, 24, 30], we computed close formulae of the edge version of Randić, GA, ABC, multiplicative ABC, Zagreb and inverse sum indices by using the concept of line graphs for chain silicate (CS_n), hexagonal (HX_n) and oxide (OX_n) networks. For more information about these networks see [31].

2.1 The edge version of topological indices for $L(CS_n)$

Lemma 2.1. *Let G be the line graph CS_n with dimension of $n = 1, 2$ and 3.*

1. *For n=1. Then the edge version of topological indices is given by*
   (a) ${}_eR_{-1/2}(G) = 3$;
   (b) $GA_e(G) = 12$;
   (c) $ABC_e(G) = 3\sqrt{6}$;
   (d) $ABCII_e(G) = 3\sqrt{6}$;
   (e) ${}_eM_1(G) = 96$;
   (f) $ISI_e(G) = 24$.
2. *For $n = 2$. Then the edge version of topological indices is given by*

(a) ${}_eR_{-1/2}(G) = \frac{3}{2} + \frac{6}{\sqrt{7}} + \frac{15}{7}$;

(b) $GA_e(G) = 27 + \frac{48\sqrt{7}}{11}$;

(c) $ABC_e(G) = \frac{3\sqrt{6}}{2} + \frac{18\sqrt{7}+30\sqrt{3}}{7}$;

(d) $ABCII_e(G) = \frac{2430\sqrt{14}}{49}$;

(e) ${}_eM_1(G) = 390$;

(f) $ISI_e(G) = \frac{2091}{22}$.

3. *For n=3. Then the edge version of topological indices is given by*

(a) ${}_eR_{-1/2}(G) = \sqrt{\frac{10}{7}} + \frac{66}{14} + \frac{8\sqrt{7}}{7}$;

(b) $GA_e(G) = 28 + \frac{64\sqrt{7}}{11} + \frac{20\sqrt{70}}{17}$;

(c) $ABC_e(G) = \frac{3\sqrt{6}}{2} + \frac{24\sqrt{7}+44\sqrt{3}}{7} + 10\sqrt{\frac{3}{14}}$;

(d) $ABCII_e(G) = \frac{47520\sqrt{3}}{49}$;

(e) ${}_eM_1(G) = 720$;

(f) $ISI_e(G) = \frac{31959}{187}$.

Proof. First consider the line graph $L(CS_n)$ with $n = 1$ as shown in Fig. 1(b). In this graph there are total 6 vertices, consisting 6 vertices of degree 4. Hence, we get the edge partition, based on the degree of an edge e and f as shown in Table 1. We apply Formulas $(3), (5), (7) - (10)$ to Table 1 and obtain the required results. By similar arguments we can obtain the expression of the edge version of topological indices for $n = 2$ and 3 by viewing edge partition in Tables 2 and 3. □

Figure 1: (a) A chain silicate network CS_1 ; (b) the line graph $L(CS_1)$.

Table 1: The edge partition of $L(CS_n)$ for $n = 1$

(d_e, d_f) where $ef \in E(L(G))$	Number of edges
$(4, 4)$	12

Table 2: The edge partition of $L(CS_n)$ for $n = 2$

(d_e, d_f) where $ef \in E(L(G))$	Number of edges
$(4, 4)$	6
$(4, 7)$	12
$(7, 7)$	15

Table 3: The edge partition of $L(CS_n)$ for $n = 3$

(d_e, d_f) where $ef \in E(L(G))$	Number of edges
$(4, 4)$	6
$(4, 7)$	16
$(7, 7)$	22
$(7, 10)$	10

Theorem 2.1. *Let G be the line graph CS_n with dimension of $n \geq 4$, then*

1. ${}_eR_{-1/2}(G) = \left(28\sqrt{\frac{2}{5}} + \frac{16}{\sqrt{7}} + 8\sqrt{7} + \sqrt{10}\right) n + 12 - 49\sqrt{\frac{2}{5}} + \frac{16}{\sqrt{7}} - 2\sqrt{7} - 3\sqrt{10}$;
2. $GA_e(G) = \left(9 + \frac{16\sqrt{7}}{11} + \frac{16\sqrt{70}}{17}\right) n + 1 + \frac{16\sqrt{7}}{11} - \frac{28\sqrt{70}}{17}$;
3. $ABC_e(G) = \left(4\sqrt{\frac{6}{7}} + \frac{3}{5\sqrt{2}} + \frac{16\sqrt{3}}{7} + \frac{6}{\sqrt{7}}\right) n + 3\sqrt{\frac{3}{2}} - \frac{9}{5\sqrt{2}} - \frac{4\sqrt{3}}{7} + \frac{6}{\sqrt{7}} - \sqrt{42}$;
4. $ABCII_e(G) = \sqrt{6}\left(\frac{5184n^4 - 20736n^3 + 7452n^2 + 26568n}{245} - \frac{972}{35}\right)$;
5. ${}_eM_1(G) = 312n - 234$;
6. $ISI_e(G) = \frac{14235}{187}n - \frac{10746}{187}$.

Proof. The graph $L(CS_n)$ for $n \geq 4$ as shown in Fig. 2(b) and contain the number vertices and edges in $L(G)$ are $|V(L(G))| = 6n$ and $|E(L(G))| = 21n - 9$. It also consists of five partitions as given in Table 4. Apply Formulas $(3), (5), (7) - (10)$ to the edge partition shown in Table 4 to get the required results. □

Table 4: The edge partition of $L(CS_n)$ for $n = 4$

(d_e, d_f) where $ef \in E(L(G))$	Number of edges
$(4, 4)$	6
$(4, 7)$	$4n + 4$
$(7, 7)$	$8n - 2$
$(7, 10)$	$8n - 14$
$(10, 10)$	$n - 3$

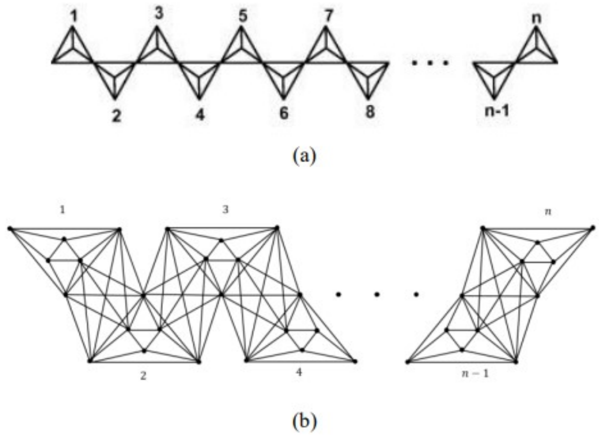

Figure 2: (a) A chain silicate network CS_n ; (b) the line graph $L(CS_n)$.

2.2 The edge version of topological indices for $L(HX_n)$

Lemma 2.2. *Let H be the line graph HX_n with dimension of $n = 2$, 3 and 4.*

1. *For n=2. Then the edge version of topological indices is given by*
   (a) ${}_eR_{-1/2}(H) = \frac{3}{2} + \frac{6}{\sqrt{7}} + \frac{15}{7}$;
   (b) $GA_e(H) = 27 + \frac{48\sqrt{7}}{11}$;
   (c) $ABC_e(H) = \frac{3\sqrt{6}}{2} + \frac{18\sqrt{7}+30\sqrt{3}}{7}$;
   (d) $ABCII_e(H) = \frac{2430\sqrt{14}}{49}$;
   (e) ${}_eM_1(H) = 390$;
   (f) $ISI_e(H) = \frac{2091}{22}$.
2. *For n=3.Then the edge version of topological indices is given by*
   (a) ${}_eR_{-1/2}(H) = \frac{36}{5} + \frac{15\sqrt{14}+63\sqrt{5}+42\sqrt{10}+12\sqrt{35}+9\sqrt{70}}{35}$;
   (b) $GA_e(H) = 57 + 2\sqrt{35} + 16\sqrt{5} + \frac{16\sqrt{14}}{5} + \frac{96\sqrt{10}}{13} + \frac{36\sqrt{70}}{17}$;
   (c) $ABC_e(H) = 12\sqrt{\frac{2}{7}} + 18\sqrt{\frac{3}{14}} + 35\sqrt{\frac{1}{5}} + \frac{3(343\sqrt{2}+28\sqrt{100}+10\sqrt{182}+35\sqrt{14})}{70}$;
   (d) $ABCII_e(H) = \frac{997691904\sqrt{858}}{875}$;
   (e) ${}_eM_1(H) = 2562$;
   (f) $ISI_e(H) = \frac{696994}{1105}$.
3. *For n=4.Then the edge version of topological indices is given by*
   (a) ${}_eR_{-1/2}(H) = 2\sqrt{3} + \frac{201}{10} + \frac{147\sqrt{5}+14\sqrt{30}+42\sqrt{10}+12\sqrt{35}+9\sqrt{70}+15\sqrt{14}}{35}$;

(b) $GA_e(H) = 189+2\sqrt{35}+\frac{96\sqrt{3}}{7}+\frac{16\sqrt{14}}{5}+\frac{112\sqrt{5}}{3}+\frac{24\sqrt{30}}{11}+\frac{96\sqrt{10}}{13}+\frac{36\sqrt{70}}{17}$;

(c) $ABC_e(H) = 12\sqrt{\frac{3}{10}}+12\sqrt{\frac{2}{7}}+18\sqrt{\frac{3}{14}}+3\sqrt{14}$
$+84\sqrt{\frac{1}{5}}+\frac{3(1169\sqrt{2}+28\sqrt{110}+10\sqrt{182})}{70}+12$;

(d) $ABCII_e(H) = \frac{692216782848\sqrt{\frac{143}{5}}}{125}$;

(e) ${}_eM_1(H) = 6546$;

(f) $ISI_e(H) = \frac{414051719}{255255}$.

Proof. The graph $L(HX_n)$ for $n = 2$ as shown in Fig. 3(b). It contains 12 vertices among which 6 vertices are of degree 4 and remaining all are of degree 7. Hence, we get the edge partition, based on the degree of an edge e and f as shown in Table 5. We apply Formulas (3), (5), (7) – (10) to Table 5 and obtain the required results. By similar arguments we can obtain the expression of the edge version of topological indices for $n = 3$ and 4 (see Fig. 4(b) and 5(b)) by viewing edge partition in Tables 6 and 7. □

Figure 3: (a) A hexagonal network HX_2 ; (b) the line graph $L(HX_2)$.

Table 5: The edge partition of $L(HX_2)$

(d_e, d_f) where $ef \in E(L(G))$	Number of edges
$(4, 4)$	6
$(4, 7)$	12
$(7, 7)$	15

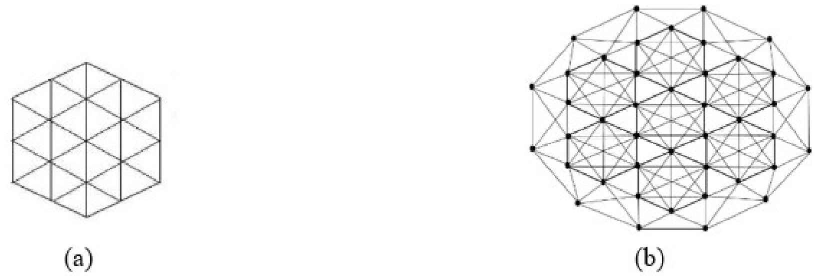

Figure 4: (a) A hexagonal network HX_3 ; (b) the line graph $L(HX_3)$.

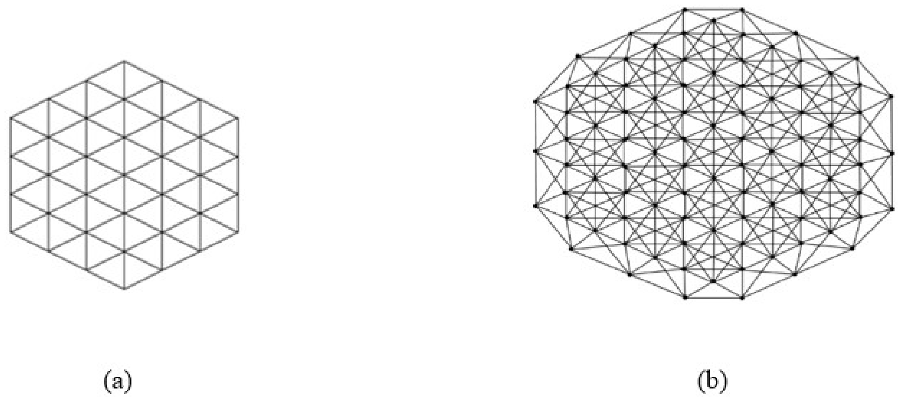

Figure 5: (a) A hexagonal network HX_4 ; (b) the line graph $L(HX_4)$.

Table 6: The edge partition of $L(HX_3)$

(d_e, d_f) where $ef \in E(L(G))$	Number of edges
$(5,5)$	12
$(5,7)$	12
$(5,8)$	24
$(7,8)$	12
$(7,10)$	18
$(8,8)$	12
$(8,10)$	36
$(10,10)$	33

Table 7: The edge partition of $L(HX_4)$

(d_e, d_f) where $ef \in E(L(G))$	Number of edges
$(5,5)$	6
$(5,6)$	12
$(5,7)$	12
$(5,8)$	24
$(6,8)$	24
$(7,8)$	12
$(7,10)$	18
$(8,8)$	24
$(8,10)$	84
$(10,10)$	159

Theorem 2.2. *Let H be the line graph HX_n with dimension of $n \geq 5$, then*

1. ${}_eR_{-1/2}(H) = \frac{9}{2}n^2 + \left(2\sqrt{3} + \frac{12}{\sqrt{5}} - \frac{82}{5}\right)n + \frac{137}{10} + 9\sqrt{\frac{2}{35}} + 3\sqrt{\frac{2}{7}} + 6\sqrt{\frac{2}{5}} + 2\sqrt{\frac{6}{5}} - 6\sqrt{3} - \frac{27}{\sqrt{5}} + \frac{12}{\sqrt{35}}$;
2. $GA_e(H) = 45^2 + \left(\frac{96\sqrt{3}}{7} + \frac{64\sqrt{5}}{3} - 171\right)n + 153 - \frac{288\sqrt{3}}{7} - 48\sqrt{5} + \frac{96\sqrt{10}}{13} + \frac{16\sqrt{14}}{5} + \frac{24\sqrt{30}}{11} + 2\sqrt{35} + \frac{36\sqrt{70}}{17}$;
3. $ABC_e(H) = \frac{27}{\sqrt{2}}n^2 + \left(12 - \frac{567}{5\sqrt{2}} + 3\sqrt{\frac{7}{2}} + \frac{48}{\sqrt{5}} + \sqrt{10}\right)n - 36 - 12\sqrt{\frac{2}{7}} + 9\sqrt{\frac{6}{7}} + 6\sqrt{\frac{6}{5}} + \frac{117}{\sqrt{2}} + \frac{12\sqrt{2}}{5} + 3\sqrt{\frac{26}{7}} + 6\sqrt{\frac{22}{5}} - \frac{108}{\sqrt{5}} - 4\sqrt{10} - 3\sqrt{14}$;
4. $ABCII_e(H) = \frac{104976}{875}\sqrt{286}(6n-24)(12n-24)(24n-72)(48n-108)(45n^2-189n+195)$;
5. ${}_eM_1(H) = 900n^2 - 1500n - 1038$;
6. $ISI_e(H) = 225n^2 - \frac{12251}{21}n + \frac{30259113}{85085}$.

Proof. Let H be the line graph $L(HX_n)$ for $n \geq 5$, contains the number of vertices and edges in $L(H)$ are $|V(L(H))| = 9n^2 - 15n + 6$ and $|E(L(H))| = 45n^2 - 99n + 51$. It consists of eleven partitions as given in Table 8. Apply Formulas $(3), (5), (7) - (10)$ to the edge partition shown in Table 8 to get the required results. □

Table 8: The edge partition of $L(HX_n)$ for $n \geq 5$

(d_e, d_f) where $ef \in E(L(G))$	Number of edges
$(5,5)$	6
$(5,6)$	12
$(5,7)$	12
$(5,8)$	24
$(6,6)$	$6n-24$
$(6,8)$	$24n-72$
$(7,8)$	12
$(7,10)$	18
$(8,8)$	$12n-24$
$(8,10)$	$48n-108$
$(10,10)$	$45n^2-189n+195$

2.3 The edge version of topological indices for $L(OX_n)$

Theorem 2.3. *Let K be the line graph HX_n with dimension of $n \geq 1$, then*

1. ${}_eR_{-1/2}(K) = 9n^2 + \left(3\sqrt{6} - \frac{15}{2}\right) n + \frac{5}{2} - \sqrt{6}$;
2. $GA_e(K) = 54n^2 + \left(\frac{72\sqrt{6}}{5} - 48\right) n + 12 - \frac{24\sqrt{6}}{5}$;
3. $ABC_e(K) = 9\sqrt{10}n^2 - \left(3\sqrt{\frac{3}{2}} + 12\sqrt{3} - 9\sqrt{10}\right) n + 3\sqrt{\frac{3}{2}} - 4\sqrt{3} + \sqrt{10}$;
4. $ABCII_e(K) = \sqrt{5}\left(972n^4 - 324n^3 - 864n^2 + 396n - 36\right)$;
5. ${}_eM_1(K) = 648n^2 - 240n$;
6. $ISI_e(K) = 162n^2 - \frac{318}{5}n + \frac{6}{5}$.

Proof. Let K be the line graph $L(OX_n)$ for $n \geq 1$ and the graph K in Fig. 6(b) and 7(b). It contain the number of vertices and edges in $L(K)$ are $|V(L(K))| = 18n^2$ and $|E(L(K))| = 54n^2 - 12n$. Also, it consists of three partitions as given in Table 9. Apply Formulas $(3), (5), (7) - (10)$ to the edge partition shown in Table 9 to get the required results. □

Table 9: The edge partition of $L(OX_n)$ for $n \geq 1$

(d_e, d_f) where $ef \in E(L(G))$	Number of edges
$(4,4)$	$6n+6$
$(4,6)$	$36n-12$
$(6,6)$	$54n^2-54n+6$

Figure 6: (a) An oxide network OX_1 ; (b) the line graph $L(OX_1)$.

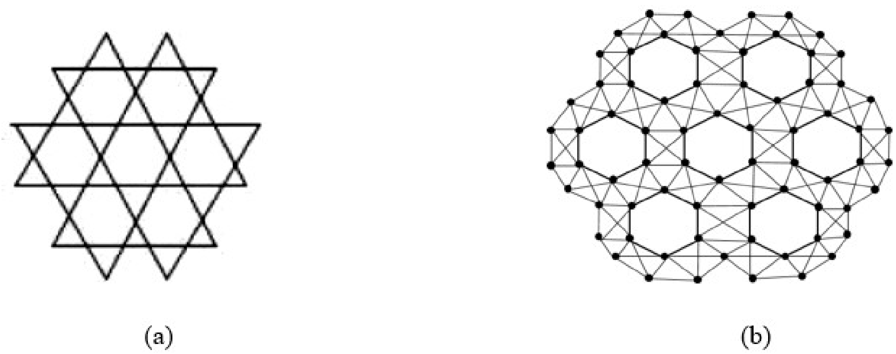

Figure 7: (a) An oxide network OX_2 ; (b) the line graph $L(OX_2)$.

3. Conclusion

In this paper, certain degree based topological indices, namely the edge version of Randić, GA, ABC, multiplicative ABC, Zagreb and inverse sum indices for the line graphs of chains silicate, hexagonal and oxide networks were studied. In future, we will pay attention to some new classes of the line graph and study their topological indices which will be reasonably useful to recognize their underlying topologies.

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