On Harmonic and Ev-Degree Molecular Topological Properties of DOX, RTOX and DSL Networks

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Abstract: Topological indices enable to gather information for the underlying topology of chemical structures and networks. Novel harmonic indices have been defined recently. All degree based topological indices are defined by using the classical degree concept. Recently two novel degree concept have been defined in graph theory: ve-degree and ev-degree. Ve-degree Zagreb indices have been defined by using ve-degree concept. The prediction power of the ve-degree Zagreb indices is stronger than the classical Zagreb indices. Dominating oxide, silicate and oxygen networks are important network models in view of chemistry, physics and information science. Physical and mathematical properties of dominating oxide, silicate and oxygen networks have been considerably studied in graph theory and network theory. Topological properties of the dominating oxide, silicate and oxygen networks have been intensively investigated for the last few years period. In this study we examined, the first, the fifth harmonic and ev-degree topological indices of dominating oxide (DOX), regular triangulene oxide network (RTOX) and dominating silicate network (DSL).

Keywords: Dominating oxide network, dominating silicate network, ev-degree topological indices, harmonic indices, regular triangulene oxide network.

1 Introduction

Graph theory has many applications for science, technology and social sciences. Graph theory enables suitable toys to researches to model real world problems. Chemical graph theory is one of the branch of graph theory. Chemical graph theory is considered the intersection of graph theory, chemistry and information science. In chemistry, pharmacology, medicine and physics molecular graphs has been used to model atomic and molecular substances. Topological indices have been derived from the molecular graphs of chemical compounds. Topological indices are important tools to analyze the underlying topology of networks. Many topological indices have been used to understand and to investigate mathematical properties of real world network models. Topological indices enable to gather information for the underlying topology of chemical structures and networks. Zagreb and Randic indices are the most used indices among the all topological indices in this regard [Gutman and Trinajstić (1972); Randic (1975)]. Harmonic index was defined by Zhong [Zhong (2012)]. Novel harmonic indices have been defined by Ediz et

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al. [Ediz, Farahani and Imran (2017)]. All degree based topological indices are defined by using the classical degree concept. Recently two novel degree concept have been defined in graph theory: ve-degree and ev-degree [Chellali, Haynes, Hedetniemi et al. (2017)]. On mathematical properties of these novel concepts we referred the interested reader to the reference [Horoldagva, Das, Selenge (2019)]. Ev-degree and Ve-degree Zagreb indices and Ev-degree and Ve-degree Randic indices have been defined by using ve-degree concept in Ediz et al. [Ediz (2017a, 2017b, 2018); Şahin and Ediz (2018)]. The prediction power of the ve-degree Zagreb indices is stronger than the classical Zagreb indices. Dominating oxide network is important toll in view of chemistry, physics and information science. Physical and mathematical properties of dominating oxide network have been considerably studied in graph theory and network theory. Topological properties of the dominating oxide network have been intensively investigated for the last five years period see in Arockiaraj et al. [Arockiaraj, Kavitha, Balasubramanian et al. (2018); Baig, Imran and Ali (2015); Gao and Siddiqui (2017); Sarkar, De, Cangül et al. (2019); Simonraj and George (2013)].

The ve-degree topological properties of dominating oxide network have been investigated by [Kulli (2018a)); Kulli (2018b)]. As a continuation of these studies, in this study we examined, ev-degree Zagreb, ev-degree Randic and the first, the fifth harmonic topological indices of DOX, RTOX and DSL networks.

2 Preliminaries

In this section we give some basic and preliminary concepts which we shall use later. A graph *G=(V,E)* consists of two nonempty sets *V* and 2-element subsets of *V* namely *E*. The elements of *V* are called vertices and the elements of *E* are called edges. For a vertex *v*, *deg(v)* show the number of edges that incident to *v*. The set of all vertices which adjacent to v is called the open neighborhood of *v* and denoted by *N(v)*. If we add the vertex *v* to *N(v)*, then we get the closed neighborhood of *v*, *N[v]*. For the vertices u and v, $d(u,v)$ denotes the distance between u and v which means that minimum number of edges between u and v. The largest distance from the vertex v to any other vertex u called the eccentricity of v and denoted by e_v.

Let *G* be a simple connected graph *G=(V,E)*. Harmonic indices may be defined as;

$$H_{general}(G) = \sum_{uv\in E(G)} \frac{2}{Q_u+Q_v} \tag{1}$$

where Q_u is a unique parameter which is acquired from the vertex $u \in V(G)$.

Definition 1 (**First Harmonic Index**)The first kind of this Harmonic indices was studied by [Zhong, L. (2012)] by considering Q_u to be the degree of the vertex *u*:

$$H_1(G) = \sum_{uv\in E(G)} \frac{2}{d_u+d_v} \tag{2}$$

Definition 2 (**Second Harmonic Index**)The second kind of this class can be defined by considering Q_u to be the number n_u of vertices of *G* lying closer to the vertex *u* than to the vertex *v* for the edge *uv* of the graph *G*:

$$H_2(G) = \sum_{uv\in E(G)} \frac{2}{n_u+n_v} \tag{3}$$

Definition 3 (**Third Harmonic Index**)The third type of this class can be defined by considering Q_u to be the number m_u of edges of *G* lying closer to the vertex *u* than to the vertex *v* for the edge *uv* of the graph *G*:

$$H_3(G) = \sum_{uv\in E(G)} \frac{2}{m_u+m_v} \tag{4}$$

Definition 4 (**Fourth Harmonic Index**)The fourth type of this class can be defined by considering Q_u to be the eccentricity of the vertex *u*:

$$H_4(G) = \sum_{uv\in E(G)} \frac{2}{e_u+e_v} \tag{5}$$

Definiton 5 (**Fifth Harmonic Index**) The fifth type of this class can be defined by considering Q_u to be the $S_u = \sum_{v\in N(u)} d_v$:

$$H_5(G) = \sum_{uv\in E(G)} \frac{2}{S_u+S_v} \tag{6}$$

Definition 6 (**Sixth Harmonic Index**) And the sixth type of this class can be defined by considering Q_u to be the $M_u = \prod_{v\in N(u)} d_v$:

$$H_6(G) = \sum_{uv\in E(G)} \frac{2}{M_u+M_v} \tag{7}$$

And now we give the definitions of ev-degree concept which were given by Chellali et al. [Chellali, Haynes, Hedetniemi et al. (2017)].

Definition 7 **(ve-degree)** Let *G* be a connected simple graph and $v\in V(G)$. The ve-degree of the vertex *v*, $deg_{ve}(v)$, equals the number of different edges that incident to any vertex from the closed neighborhood of *v*.

We also can restate the Definition 7 as follows: Let *G* be a connected simple graph and $v\in V(G)$. The ve-degree of the vertex *v* is the number of different edges between the other vertices with a maximum distance of two from the vertex *v*.

Definition 8 **(ev-degree)** Let *G* be a connected graph and $e=uv\in E(G)$. The ev-degree of the edge *e*, $deg_{ev}(e)$, equals the number of vertices of the union of the closed neighborhoods of *u* and *v*.

The authors in Chellali et al. [Chellali, Haynes, Hedetniemi et al. (2017)] also can give the Definition 8 as follows: Let *G* be a connected graph and $e=uv\in E(G)$. The ev-degree of the edge *e*, $deg_{uv}(e)=degu+degv-n_e$, where n_e means the number of triangles in which the edge *e* lies in.

Definition 9 (**ev-degree Zagreb index**) Let *G* be a connected graph and $e=uv\in E(G)$. The ev-degree Zagreb index of the graph *G* defined as;

$$M^{ev}(G) = \sum_{e\in E(G)} deg_{ev}e^2 \tag{8}$$

Definition 10 (**the first ve-degree Zagreb alpha index**) Let *G* be a connected graph and $v\in V(G)$. The first ve-degree Zagreb alpha index of the graph *G* defined as;

$$M_1^{\alpha ve}(G) = \sum_{v\in V(G)} deg_{ve}v^2 \tag{9}$$

Definition 11 (**the first ve-degree Zagreb beta index**) Let *G* be a connected graph and $uv\in E(G)$. The first ve-degree Zagreb beta index of the graph *G* defined as;

$$M_1^{\beta ve}(G) = \sum_{uv\in E(G)} (deg_{ve}u + deg_{ve}v) \tag{10}$$

Definition 12 (**the second ve-degree Zagreb index**) Let *G* be a connected graph and $uv\in E(G)$. The second ve-degree Zagreb index of the graph *G* defined as;

$$M_2^{ve}(G)=\sum_{uv\in E(G)} deg_{ve}u deg_{ve}v \tag{11}$$

Definition 13 (**ve-degree Randic index**) Let *G* be a connected graph and $uv\in E(G)$. The ve-degree Randic index of the graph *G* defined as;

$$R^{ve}(G)=\sum_{uv\in E(G)}(deg_{ve}u deg_{ve}v)^{-1/2} \tag{12}$$

Definition 14 (**ev-degree Randic index)**) Let *G* be a connected graph and $e=uv\in E(G)$. The ev-degree Randic index of the graph *G* defined as;

$$R^{ev}(G)=\sum_{e\in E(G)} deg_{ev}e^{-1/2} \tag{13}$$

After these definitions, we calculate the first and the fifth harmonic and ev-degree indices for the DOX, DSL and RTOX networks in the following sections.

3 Harmonic, ev-degree Zagreb and ev-degree Randic indices of dominating oxide network (DOX)

The structure of a DOX network is depicted in Fig. 1. Before we calculate the ev-degree and the first and the fifth harmonic topological indices of DOX network we have to determine the ev-degrees of end vertices of the all edges for an arbitrary DOX network.

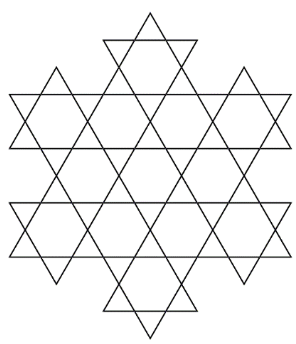

Figure 1: A dominating oxide DOX(2) network model

Observe that from Fig. 1, every edge of dominating oxide network lies in only one triangle. In this regard, the ev-degree of the each edge of dominating oxide network is equal to the degree of sum of end vertices minus one. The following Tab. 1, shows the partition of the edges with respect to their ev-degree of end vertices for an arbitrary DOX network.

Table 1: The ev-degrees of the end vertices of edges for DOX networks

$(degu, degv)$	$deg_{ev}uv$	Number of Edges
(2,4)	5	$24n-12$
(4,4)	7	$54n^2-78n+30$

Table 2: The sum degrees of the end vertices of edges for DOX networks

(S_u,S_v)	Number of edges ($e=uv$)
(8,12)	$12n$
(8,14)	$12n-12$
(12,12)	6
(12,14)	$12n-12$
(14,16)	$24n-24$
(16,16)	$54n^2-114n+60$

And now, we begin to compute ev-degree and harmonic topological indices for DOX networks.

Theorem 1 The ev-degree Zagreb index of an arbitrary dominating oxide network is equal to $2646n^2-3222n+1170$.

Proof From the definition of the ev-degree Zagreb index and Tab. 1, we can directly write;

$$M^{ev}(\mathrm{DOX})=\sum_{e\in E(\mathrm{DOX})} deg_{ev}e^2=(24n-12)x5^2+(54n^2-78n+30)x7^2$$
$$=25x24n-25x12+54x49n^2-78x49n+30x49$$
$$=600n-300+2646n^2-3822n+1470$$
$$=2646n^2-3222n+1170$$

Theorem 2 The ev-degree Randic index of an arbitrary dominating oxide network is equal to $\frac{24n-12}{\sqrt{5}}+\frac{54n^2-78n+30}{\sqrt{7}}$

Proof From the definition of the ev-degree Randic index and Tab. 1, we can directly write;

$$R^{ev}(DOX)=\sum_{e\in E(DOX)} deg_{ev}e^{-1/2}=\frac{24n-12}{\sqrt{5}}+\frac{54n^2-78n+30}{\sqrt{7}}$$

Theorem 3 The first harmonic index of an arbitrary dominating oxide network is equal to $\frac{27}{2}n^2+\frac{55}{2}n+\frac{7}{2}$

Proof From the definition of the first harmonic index and Tab. 1, we can directly write;

$$H_1(\mathrm{DOX})=\sum_{uv\in E(\mathrm{DOX})}\frac{2}{d_u+d_v}=(24n-12)\frac{2}{6}+(54n^2-78n+30)\frac{2}{8}=\frac{1}{2}(27n^2-39n+15)+8n-4=\frac{27}{2}n^2+\frac{55}{2}n+\frac{7}{2}$$

Theorem 4 The fifth harmonic index of an arbitrary dominating oxide network is equal to $\frac{27n^2}{8}-\frac{13219n}{5720}+\frac{32913}{8580}$

Proof From the definition of the first harmonic index and Tab. 2, we can directly write;

$$H_5(\mathrm{DOX})=\sum_{uv\in E(\mathrm{DOX})}\frac{2}{S_u+S_v}=12n\frac{2}{20}+(12n-12)\frac{2}{22}+6\frac{2}{24}+(12n-12)\frac{2}{26}+(24n-24)\frac{2}{30}+\left(54n^2-114n+60\right)\frac{2}{32}=\frac{6n}{5}+\frac{12n}{11}-\frac{12}{11}+\frac{1}{2}+\frac{12n}{13}-\frac{12}{13}+\frac{24n}{15}-\frac{24}{15}+\frac{27n^2}{8}-\frac{57n}{8}+\frac{15}{4}=\frac{27n^2}{8}-\frac{13219n}{5720}+\frac{32913}{8580}$$

4 Harmonic, ev-degree Zagreb and ev-degree Randic indices of regular triangulene oxide network (RTOX)

The structure of a RTOX network is depicted in Fig. 2. Before we calculate the ev-degree and the first and the fifth harmonic topological indices of RTOX network we have to determine the ev-degrees of the all edges for an arbitrary RTOX network.

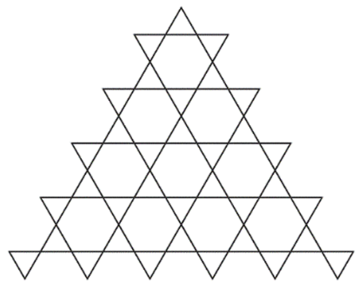

Figure 2: Regular triangulate oxide network RTOX(5)

Table 3: Edge partition of the regular triangulene oxide network RTOX(n) ($n \geq 3$)

$(degu, degv)$	$deg_{ev}uv$	Number of edges (e=uv)
(2,2)	3	2
(2,4)	5	$6n$
(4,4)	7	$3n^2 - 2$

The following Tab. 4, shows the partition of the edges with respect to their sum degree of end vertices an arbitrary RTOX network.

Table 4: The sum degrees of the end vertices of edges for RTOX(n) ($n \geq 3$) networks

(S_u,S_v)	Number of edges (e=uv)
(6,6)	2
(6,12)	4
(8,12)	4
(8,14)	$6n - 8$
(12,12)	1
(12,14)	6
(14,14)	$6n - 9$
(14,16)	$6n - 12$
(16,16)	$3n^2 - 12n + 12$

And now, we begin to compute ev-degree and harmonic topological indices for RTOX networks.

Theorem 5 The ev-degree Zagreb index of an arbitrary triangulene oxide network (RTOX) is equal to $247n^2 + 150n - 80$.

Proof From the definition of the ev-degree Zagreb index and Tab. 3, we can directly write;

$$M^{ev}(\text{RTOX}) = \sum_{e\in E(\text{RTOX})} deg_{ev}e^2 = 2\,x3^2 + 6nx5^2 + (3n^2 - 2)x7^2$$
$$= 18 + 150n + 247n^2 - 98 = 247n^2 + 150n - 80$$

Theorem 6 The ev-degree Randic index of an arbitrary triangulene oxide network (RTOX) is equal to $\frac{2}{\sqrt{3}} + \frac{6n}{\sqrt{5}} + \frac{3n^2-7}{\sqrt{7}}$

Proof From the definition of the ev-degree Randic index and Tab. 3, we can directly write;

$$R^{ev}(\text{RTOX}) = \sum_{e\in E(\text{RTOX})} deg_{ev}e^{-1/2} = \frac{2}{\sqrt{3}} + \frac{6n}{\sqrt{5}} + \frac{3n^2 - 7}{\sqrt{7}}$$

Theorem 7 The first harmonic index of an arbitrary triangulene oxide network (RTOX) is equal to $\frac{3}{4}n^2 + 2n + \frac{1}{2}$

Proof From the definition of the first harmonic index and Tab. 3, we can directly write;

$$H_1(\text{RTOX}) = \sum_{uv\in E(\text{RTOX})} \frac{2}{d_u + d_v} = 3x\frac{2}{4} + 6nx\frac{2}{6} + (3n^2 - 7)x\frac{2}{8} = \frac{3}{2} + 2n + \frac{3}{4}n^2 - \frac{7}{4} = \frac{3}{4}n^2 + 2n + \frac{1}{2}$$

Theorem 8 The fifth harmonic index of an arbitrary triangulene oxide network (RTOX) is equal to $\frac{n^2}{5} + \frac{231n}{385} + \frac{105097}{180180}$

Proof From the definition of the first harmonic index and Tab. 4, we can directly write;

$$H_5(\text{RTOX}) = \sum_{uv\in E(\text{RTOX})} \frac{2}{S_u + S_v} = 2x\frac{2}{12} + 4x\frac{2}{18} + 4x\frac{2}{20} + (6n - 8)x\frac{2}{22} + 1x\frac{2}{24} + 6x\frac{2}{26} + (6n - 9)x\frac{2}{28} + (6n - 12)x\frac{2}{30} + (3n^2 - 12n + 12)x\frac{2}{30} = \frac{1}{3} + \frac{4}{9} + \frac{2}{5} + \frac{6n}{11} - \frac{8}{11} + \frac{1}{12} + \frac{9}{13} + \frac{3n}{7} - \frac{18}{28} + \frac{2n}{5} - \frac{4}{5} + \frac{n^2}{5} - \frac{4n}{5} + \frac{4}{5} = \frac{n^2}{5} + \frac{231n}{385} + \frac{105097}{180180}$$

5 Harmonic, ev-degree Zagreb and ev-degree Randic indices of dominating silicate network (DSL)

The structure of a DSL network is depicted in Fig. 3. Before we calculate the ve-degree topological indices of DSL network we have to determine the ev-degrees of all the edges for an arbitrary DSL network. The following Tab. 5, shows the partition of the edges with respect to their sum degree of end vertices of an arbitrary DSL network.

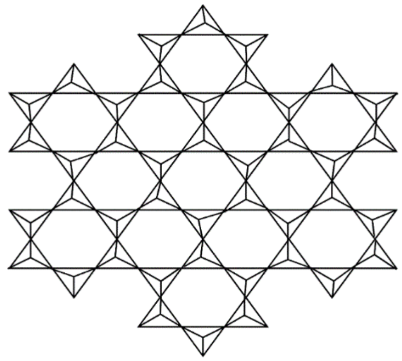

Figure 3: Dominating silicate network DSL(2)

Table 5: Edge partition of the dominating silicate network DSL(n)

$(degu, degv)$	$deg_{ev}uv$	Number of edges (*e*=*uv*)
(2,3)	4	$12n-6$
(2,6)	7	$24n-12$
(3,6)	7	$54n^2-66n+24$
(6,6)	11	$54n^2-78n+30$

Table 6: The sum degrees of the end vertices of edges for DSL(n) networks

(S_u, S_v)	Number of edges (*e*=*uv*)
(15,15)	$12n-6$
(15,24)	$24n$
(15,27)	$24n-24$
(18,27)	$12n-12$
(18,30)	$54n^2-102n+48$
(24,24)	6
(24,27)	$12n-12$
(27,30)	$24n-24$
(30,30)	$54n^2-114n+60$

Theorem 9 The ev-degree Zagreb index of an arbitrary dominating silicate network (DSL) is equal to $9180n^2-11304n+4122$.

Proof From the definition of the ev-degree Zagreb index and Tab. 5, we can directly write; $M^{ev}(\text{DSL}) = \sum_{e\in E(\text{DSL})} deg_{ev}e^2 = (12n-6)x4^2 + (24n-12)x7^2 + (54n^2-66n+24)x7^2 + (54n^2-78n+30))x11^2 = 192n - 96 + 1176n - 588 + 2646n^2 - 3234n + 1176 + 6534n^2 - 9438n + 3630 = 9180n^2 - 11304n + 4122$

Theorem 10 The ev-degree Randic index of an arbitrary dominating silicate network (DSL) is equal to $\frac{54n^2-42n+12}{\sqrt{7}} + \frac{54n^2-78n+30}{\sqrt{11}} + 6n - 3 + \frac{24n-12}{\sqrt{7}}$

Proof From the definition of the ev-degree Randic index and Tab. 5, we can directly write;

$$R^{ev}(DSL) = \sum_{e\in E(DSL)} deg_{ev}e^{-1/2} = \frac{12n-6}{\sqrt{4}} + \frac{24n-12}{\sqrt{7}} + \frac{54n^2-66n+24}{\sqrt{7}} + \frac{54n^2-78n+30}{\sqrt{11}}$$
$$= \frac{54n^2-42n+12}{\sqrt{7}} + \frac{54n^2-78n+30}{\sqrt{11}} + 6n - 3 + \frac{24n-12}{\sqrt{7}}$$

Theorem 11 The first harmonic index of an arbitrary dominating oxide network is equal to $21n^2 - \frac{121n}{5} + \frac{74}{15}$

Proof From the definition of the first harmonic index and Tab. 5, we can directly write;

$H_1(\text{DSL}) = \sum_{uv\in E(\text{DSL})} \frac{2}{d_u+d_v} = (12n-6)\frac{2}{5} + (24n-12)\frac{2}{8} + (54n^2-66n+24)\frac{2}{9} + (54n^2-78n+30)\frac{2}{12} = \frac{24n}{5} - \frac{12}{5} + 6n - 3 + 12n^2 - 22n + \frac{16}{3} + 9n^2 - 13n + 5 = 21n^2 - \frac{121n}{5} + \frac{74}{15}$

Theorem 12 The fifth harmonic index of an arbitrary dominating silicate network (DSL) is equal to $\frac{33}{10}n^2 + \frac{8227443}{2645370}n + \frac{116819}{135660}$

Proof From the definition of the first harmonic index and Tab. 6, we can directly write;

$H_5(\text{DSL}) = \sum_{uv\in E(\text{DSL})} \frac{2}{S_u+S_v} = (12n-6)x\frac{2}{30} + 24nx\frac{2}{39} + (24n-24)x\frac{2}{42} + (12n-12)x\frac{2}{45} + (54n^2-102n+48)x\frac{2}{48} + 6x\frac{2}{48} + (12n-12)x\frac{2}{51} + (24n-24)x\frac{2}{57} + (54n^2-114n+60)x\frac{2}{60} = \frac{33}{10}n^2 + \frac{8227443}{2645370}n + \frac{116819}{135660}$

6 Conclusion

The ev-degree topological indices have been defined recently. We examined the ev-degree Zagreb indices and ev-degree Randic indices of dominating oxide, silicate and oxygen networks. Also, we calculated the first, the fifth and the sixth harmonic indices of the same networks. The mathematical properties of ev-degree and harmonic indices have not been investigated so far. The mathematical properties of ev-degree and harmonic indices are worth to study for future researches.

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