

# On $ev$ -degree and $ve$ -degree topological indices

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## Abstract

Recently two new degree concepts have been defined in graph theory:  $ev$ -degree and  $ve$ -degree. Also the  $ev$ -degree and  $ve$ -degree Zagreb and Randić indices have been defined very recently as parallel of the classical definitions of Zagreb and Randić indices. It was shown that  $ev$ -degree and  $ve$ -degree topological indices can be used as possible tools in QSPR researches. In this paper we define the  $ve$ -degree and  $ev$ -degree Narumi–Katayama indices, investigate the predicting power of these novel indices and extremal graphs with respect to these novel topological indices. Also we give some basic mathematical properties of  $ev$ -degree and  $ve$ -degree Narumi–Katayama and Zagreb indices.

**Keywords:**  $ev$ -degree,  $ve$ -degree,  $ev$ -degree topological indices,  $ve$ -degree topological indices

**MSC:** 05C07, 05C90, 92E10

## 1. Introduction

Topological indices have important place in theoretical chemistry. Many topological indices were defined by using vertex degree concept. The Zagreb and Randić indices are the most used degree based topological indices so far in mathematical and chemical literature among the all topological indices. Very recently, Chellali, Haynes, Hedetniemi and Lewis have published a seminal study: On  $ve$ -degrees and  $ev$ -degrees in graphs [1]. The authors defined two novel degree concepts in graph theory;  $ev$ -degrees and  $ve$ -degrees and investigate some basic mathematical properties of both novel graph invariants with regard to graph regularity and irregularity [1]. After given the equality of the total  $ev$ -degree and total  $ve$ -degree for any graph, also the total  $ev$ -degree and the total  $ve$ -degree were stated as in relation to the first Zagreb index. It was proposed in the article that the chemical applicability of the total  $ev$ -degree (and the total  $ve$ -degree) could be an interesting problem in view of chemistry and chemical graph theory. In the light of this suggestion, one of the present author has carried these novel degree concepts to chemical graph theory by defining the  $ev$ -degree and  $ve$ -degree Zagreb and Randić indices [2]. It was compared these new group  $ev$ -degree and  $ve$ -degree indices with the other well-known and most used topological indices in literature such as; Wiener, Zagreb and Randić indices by modelling some physicochemical properties of octane isomers [2]. It was shown that the  $ev$ -degree Zagreb index, the  $ve$ -degree Zagreb and the  $ve$ -degree Randić indices give better correlation than Wiener, Zagreb and Randić indices to predict the some specific physicochemical properties of octanes [2]. Also it was given the relations between the second Zagreb index and  $ev$ -degree and  $ve$ -degree Zagreb indices and some mathematical properties of  $ev$ -degree and  $ve$ -degree Zagreb indices [2]. In this paper we define the  $ve$ -degree and  $ev$ -degree Narumi–Katayama indices, investigate the

predicting power of these novel indices and extremal graphs with respect to these topological indices. Also we give some basic mathematical properties of  $ev$ -degree and  $ve$ -degree Zagreb indices.

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  $v$ ,  $N[v]$ .

The first and second Zagreb indices [3] defined as follows: The first Zagreb index of a connected graph  $G$ , defined as;

$$M_1 = M_1(G) = \sum_{u \in V(G)} \deg(u)^2 = \sum_{uv \in E(G)} (\deg(u) + \deg(v)).$$

And the second Zagreb index of a connected graph  $G$ , defined as;

$$M_2 = M_2(G) = \sum_{uv \in E(G)} \deg(u) \cdot \deg(v) .$$

The authors investigated the relationship between the total  $\pi$ -electron energy on molecules and Zagreb indices [3]. For the details see the references [4-6]. Randić investigated the measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons via Randić index [7]. The Randić index of a connected graph  $G$  defined as;

$$R = R(G) = \sum_{uv \in E(G)} (\deg(u) \cdot \deg(v))^{-1/2}.$$

We refer the interested reader to [8-10] and the references therein for the up to date arguments about the Randić index.

The forgotten topological index for a connected graph  $G$  defined as;

$$F = F(G) = \sum_{v \in V(G)} \deg(v)^3 = \sum_{uv \in E(G)} (\deg(u)^2 + \deg(v)^2).$$

It was showed in [11] that the predictive power of the forgotten topological index is very close to the first Zagreb index for the entropy and acentric factor. For further studies about the forgotten topological index we refer to the interested reader [11-13] and references therein.

In the 1980s, Narumi and Katayama considered the production of the degrees of vertices

$$NK = NK(G) = \prod_{v \in V(G)} \deg(v)$$

and named it the “simple topological index” [14]. Later for this graph invariant, the name “Narumi-Katayama index” was used in [15-17]. The extremal graphs with respect to  $NK$  was studied by Gutman and Ghorbani [15], Zolfi and Ashrafi [20]. Some relations between the Narumi-Katayama index and the first Zagreb index were introduced in the more recent paper [21].

Multiplicative versions of first Zagreb index of a connected graph was defined by Eliasi *et al.* in [22] as;

$$\prod_1^* = \prod_1^*(G) = \prod_{uv \in E(G)} [\deg(u) + \deg(v)].$$

For detailed discussions of the multiplicative version of Zagreb indices, we refer the interested reader to [23] and the references cited therein.

In the following section, we will give basic definitions of  $ev$ -degree and  $ve$ -degree concepts,  $ve$ -degree and  $ev$ -degree Zagreb indices and as well as the basic mathematical properties of these novel topological indices. And also we give the definitions of  $ev$ -degree and  $ve$ -degree Narumi-Katayama indices.

## 2. $ve$ -degree and $ev$ -degree concepts and corresponding topological indices

In this section we give the definitions of  $ev$ -degree and  $ve$ -degree concepts which were given by Chellali *et al.* in [1] and the definitions and properties of  $ev$ -degree and  $ve$ -degree topological indices.

**Definition 2.1** [1] Let  $G$  be a connected 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  $v$ . For convenience we prefer to show the  $ve$ -degree of the vertex  $v$ , by  $c_v$ .

**Definition 2.2** [1] 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  $v$ . For convenience we prefer to show the  $ev$ -degree of the edge  $e = uv$ , by  $c_e$  or  $c_{uv}$ .

**Definition 2.4** [1] Let  $G$  be a connected graph and  $v \in V(G)$ . The total  $ev$ -degree of the graph  $G$  is defined as;

$$T_e = T_e(G) = \sum_{e \in E(G)} c_e.$$

And the total  $ve$ -degree of the graph  $G$  is defined as;

$$T_v = T_v(G) = \sum_{v \in V(G)} c_v.$$

**Observation 2.5** [1] For any connected graph  $G$ ,

$$T_e(G) = T_v(G).$$

**Observation 2.6** [1] For any triangle free connected graph  $G$ ,

$$c_e = c_{uv} = \deg(u) + \deg(v).$$

The following theorem states the relationship between the first Zagreb index and the total  $ve$ -degree of a connected graph  $G$ .

**Theorem 2.7** [1] For any connected graph  $G$ ,

$$T_e(G) = T_v(G) = M_1(G) - 3n(G).$$

where  $n(G)$  denotes the total number of triangles in  $G$ .

In [1], the authors suggested the idea that to carry these novel degree concepts to mathematical chemistry. One of the present author following this suggestion defined  $ev$ -degree and  $ve$ -degree Zagreb indices and showed that these novel group Zagreb and Randić indices give better correlation than well-known topological indices such as; Wiener, Zagreb and Randić indices to modelling some physicochemical properties of octane isomers [2]. And now, we give the definitions and some basic mathematical properties of  $ev$ -degree and  $ve$ -degree Zagreb indices which were given in [2].

**Definition 2.8** [2] Let  $G$  be a connected graph and  $e \in E(G)$ . The  $ev$ -degree Zagreb index of the graph  $G$  is defined as;

$$S = S(G) = \sum_{e \in E(G)} c_e^2.$$

**Definition 2.9** [2] Let  $G$  be a connected graph and  $v \in V(G)$ . The first  $ve$ -degree Zagreb alpha index of the graph  $G$  is defined as;

$$S^\alpha = S^\alpha(G) = \sum_{v \in V(G)} c_v^2.$$

**Definition 2.10** [2] Let  $G$  be a connected graph and  $uv \in E(G)$ . The first  $ve$ -degree Zagreb beta index of the graph  $G$  is defined as;

$$S^\beta = S^\beta(G) = \sum_{uv \in E(G)} (c_u + c_v).$$

**Definition 2.11** [2] Let  $G$  be a connected graph and  $uv \in E(G)$ . The second  $ve$ -degree Zagreb index of the graph  $G$  is defined as;

$$S^\mu = S^\mu(G) = \sum_{uv \in E(G)} c_u c_v.$$

**Definition 2.12** [2] Let  $G$  be a connected graph and  $uv \in E(G)$ . The  $ve$ -degree Randić index of the graph  $G$  is defined as;

$$R^\alpha(G) = \sum_{uv \in E(G)} (c_u c_v)^{-1/2}.$$

And now we restate the some basic properties of  $ev$ -degree and  $ve$ -degree Zagreb indices which were given in [2].

**Lemma 2.13** [2] Let  $T$  be a tree and  $v \in V(T)$  then,

$$c_v = \sum_{u \in N(v)} \deg(u).$$

**Theorem 2.14** [2] Let  $T$  be a tree with the vertex set  $V(T) = \{v_1, v_2, \dots, v_n\}$  then

$$S^\beta(T) = 2M_2(T).$$

**Theorem 2.15** [2] Let  $G$  be a triangle free connected graph, then;

$$S(G) = F(G) + 2M_2(G).$$

**Corollary 2.16** Let  $T$  be a tree then;

$$S(T) = F(T) + S^\beta(T).$$

And now we give the definitions of  $ev$ -degree and  $ve$ -degree Narumi-Katayama indices for a graph  $G$ .

**Definition 2.17** The  $ve$ -Narumi-Katayama index of a graph  $G$  is defined with the following equation

$$NK_{ve} = NK_{ve}(G) = \prod_{v \in V(G)} c_v.$$

If a graph has an isolated vertex, its  $NK_{ve} = 0$  which is the minimal value of  $NK_{ve}$ . We take the graphs without isolated vertices in the following results which will be introduced in the section four.

**Definition 2.18** The  $ev$ -Narumi-Katayama index of a graph  $G$  is defined with the following equation

$$NK_{ev} = NK_{ev}(G) = \prod_{e \in E(G)} c_e.$$

In the next section we investigate the predicting power of these novel topological indices and after that we investigate some mathematical properties of these novel indices.

**3 New tools for QSPR researches: the  $ev$ -Narumi-Katayama index and the  $ve$ -Narumi-Katayama index**

In this section we compare the Narumi-Katayama index and its corresponding versions of the *ev*-Narumi-Katayama and *ve*-Narumi-Katayama indices with each other by using strong correlation coefficients acquired from the chemical graphs of octane isomers. We get the experimental results at the [www.moleculardescriptors.eu](http://www.moleculardescriptors.eu) (see Table 1). The following physicochemical features have been modeled:

- Entropy,
- Acentric factor (AcenFac),
- Enthalpy of vaporization (HVAP),
- Standard enthalpy of vaporization (DHVAP).

We select those physicochemical properties of octane isomers for which give reasonably good correlations, i.e. the absolute value of correlation coefficients are larger than 0.8959 (see Table 2). Also we find the Narumi-Katayama index of octane isomers values at the [www.moleculardescriptors.eu](http://www.moleculardescriptors.eu) (see Table 3). We also calculate and show the *ev*-Narumi-Katayama and the *ve*-Narumi-Katayama indices of octane isomers values in Table 3.

**Table 1.** Some physicochemical properties of octane isomers

Molecule	Entropy	AcenFac	HVAP	DHVAP
n-octane	111.70	0.39790	73.19	9.915
2-methyl-heptane	109.80	0.37792	70.30	9.484
3-methyl-heptane	111.30	0.37100	71.30	9.521
4-methyl-heptane	109.30	0.37150	70.91	9.483
3-ethyl-hexane	109.40	0.36247	71.70	9.476
2,2-dimethyl-hexane	103.40	0.33943	67.70	8.915
2,3-dimethyl-hexane	108.00	0.34825	70.20	9.272
2,4-dimethyl-hexane	107.00	0.34422	68.50	9.029
2,5-dimethyl-hexane	105.70	0.35683	68.60	9.051
3,3-dimethyl-hexane	104.70	0.32260	68.50	8.973
3,4-dimethyl-hexane	106.60	0.34035	70.20	9.316
2-methyl-3-ethyl-pentane	106.10	0.33243	69.70	9.209
3-methyl-3-ethyl-pentane	101.50	0.30690	69.30	9.081
2,2,3-trimethyl-pentane	101.30	0.30082	67.30	8.826
2,2,4-trimethyl-pentane	104.10	0.30537	64.87	8.402
2,3,3-trimethyl-pentane	102.10	0.29318	68.10	8.897
2,3,4-trimethyl-pentane	102.40	0.31742	68.37	9.014
2,2,3,3-tetramethylbutane	93.06	0.25529	66.20	8.410

**Table 2.** Topological indices of octane isomers

Molecule	Nar	evNar	veNar
n-octane	4.159	9.129	9.129
2-methyl-heptane	3.871	9.640	9.757
3-methyl-heptane	3.871	9.575	9.575
4-methyl-heptane	3.871	9.575	9.510
3-ethyl-hexane	3.871	9.510	9.352
2,2-dimethyl-hexane	3.466	10.491	10.738
2,3-dimethyl-hexane	3.584	10.045	10.098
2,4-dimethyl-hexane	3.584	10.085	10.163
2,5-dimethyl-hexane	3.584	10.150	10.386
3,3-dimethyl-hexane	3.466	10.386	10.450
3,4-dimethyl-hexane	3.584	9.980	9.940
2-methyl-3-ethyl-pentane	3.584	9.980	9.911
3-methyl-3-ethyl-pentane	3.466	10.281	10.240
2,2,3-trimethyl-pentane	3.178	10.869	11.075
2,2,4-trimethyl-pentane	3.178	11.002	11.298
2,3,3-trimethyl-pentane	3.178	10.828	11.010
2,3,4-trimethyl-pentane	3.296	10.515	10.658
2,2,3,3-tetramethylbutane	2.773	11.736	12.210

**Table 3.** The correlation coefficients between new and old topological indices and some physicochemical properties of octane isomers

Index	Entropy	AcenFac	HVAP	DHVAP
Nar	0.9398	0.9700	0.8959	0.9410
ve-Nar	-0.9192	-0.9092	-0.9236	-0.9490
ev-Nar	-0.9369	-0.9486	-0.9202	-0.9568

**Table 4.** The squares of correlation coefficients between topological indices and some physicochemical properties of octane isomers

Index	Entropy	AcenFac	HVAP	DHVAP
Nar	0.8832	0.9409	0.8026	0.8854
ve-Nar	0.8449	0.8266	0.8530	0.9006
ev-Nar	0.8778	0.8998	0.8468	0.9154

Note that the all values in Table 2 are given by using natural logarithm. It can be seen from the Table 2 that the most convenient indices which are modelling the Entropy, Enthalpy of vaporization (HVAP), Standard enthalpy

of vaporization (DHVAP) and Acentric factor (AcenFac) are Narumi-Katayama index ( $S$ ) for entropy and Acentric Factor,  $ve$ -Narumi-Katayama index for the Enthalpy of vaporization (HVAP) and  $ev$ -Narumi-Katayama index for the Standard enthalpy of vaporization (DHVAP), respectively. But notice that the Narumi-Katayama index show the positive strong correlation and the  $ve$ -Narumi-Katayama and the  $ev$ -Narumi-Katayama indices show the negative strong correlation. Because of this fact we can compare these graph invariants with each other by using the squares of correlation coefficients for ensure the compliance between the positive and negative correlation coefficients (see Table 4).

The cross-correlation matrix of the indices are given in Table 5.

**Table 5.** The cross-correlation matrix of the topological indices

Index	Nar	$ve$ -Nar	$ev$ -Nar
Nar	1.0000		
$ve$ -Nar	-0.9901	1.0000	
$ev$ -Nar	-0.9715	0.9931	1.0000

It can be shown from the value of the minimum

among the indices is 0.9715 which is indicate strong correlation among all these indices. From the above arguments, we can say that the  $ve$ -Narumi-Katayama index and  $ev$ -Narumi-Katayama index are possible tools for QSPR researches.

Table 5 that the absolute correlation efficient

#### 4. Main results

In this section, we firstly give some basic mathematical properties of  $ve$ -degree,  $ev$ -Narumi-Katayama and  $ve$ -Narumi-Katayama indices. And secondly we investigate certain mathematical properties of  $ev$ -degree and  $ve$ -degree Zagreb indices.

**Lemma 4.1.** *Let  $G$  be a connected graph then;*

$$\sum_{v \in V(G)} n_v = \sum_{e \in E(G)} n_e = 3n(G)$$

where  $n_v$ ,  $n_e$ ,  $n(G)$  denote the number of triangles in  $G$  containing the vertex  $v$ , the number of triangles in  $G$  containing the edge  $e$  and the total number of triangles in  $G$ , respectively.

**Proof.** The second part of this equality were given in [1]. The first part comes from that since every triangle consists of three vertices and edges, we count every triangle exactly three times for each vertex. Since the total number of triangles in the graph  $G$  will not be changed, the desired result acquired easily.  $\square$



**Lemma 4.2.** Let  $G$  be a connected graph and  $v \in V(G)$ , then;

$$c_v = \sum_{u \in N(v)} \deg(u) - n_v.$$

**Proof.** From the Definition 2.1, we know that  $c_v$  equals the number of different edges incident to any vertex of  $N(v)$ . Therefore  $c_v = \sum_{u \in N(v)} \deg(u)$  if  $v$  does not lie in a triangle. But if  $v$  belongs a triangle then the edge that does not incident to  $v$  of this triangle must be counted twice in the sum  $\sum_{u \in N(v)} \deg(u)$ . Therefore we must minus one from the sum  $\sum_{u \in N(v)} \deg(u)$  for we find the exact number of different edges incident to  $N(v)$ . Thus if  $v$  lies in more than one triangle then we must minus  $n_v$  from the the sum  $\sum_{u \in N(v)} \deg(u)$  for we find the exact number of different edges incident to  $N(v)$ .  $\square$

**Corollary 4.3.** For the  $n$ -vertex triangle free graph  $G$  the  $ve$ -degree Narumi-Katayama index  $NK_{ve}(G)$  is calculated by the next equation;

$$NK_{ve}(G) = \prod_{v \in V} (\sum_{u \in N(v)} \deg(u)).$$

**Example 4.4.** Consider the  $P_2$  path graph  $c_{v_1} = c_{v_2} = 1$  and  $NK_{ve}(P_2) = 1$ . For  $P_3$  path graph  $c_{v_1} = c_{v_2} = c_{v_3} = 2$  and  $NK_{ve}(P_3) = 8$ . For  $P_4$ ,  $c_{v_1} = c_{v_4} = 2$  and  $c_{v_2} = c_{v_3} = 3$  so that  $NK_{ve}(P_4) = 36$ . We take the  $P_n$  such that  $n \geq 5$ .  $c_{v_1} = c_{v_n} = 2$  and  $c_{v_2} = c_{v_{n-1}} = 3$  and the  $ve$ -degree of the other vertices are 4. Therefore

$$NK_{ve}(P_n) = 9 \cdot 4^{n-3}.$$

**Example 4.5.** Consider the  $C_3$  cycle  $c_{v_1} = c_{v_2} = c_{v_3} = 3$  and  $NK_{ve}(C_3) = 27$ . For  $n \geq 4$  every cycle  $4_{ve}$ -regular and

$$NK_{ve}(C_n) = 4^n.$$

**Example 4.6.** Consider the  $S_n$  star graph on  $n$  vertices. Every vertices have the same  $ve$ -degree such that  $(n-1)$ . This means;

$$NK_{ve}(S_n) = (n-1)^n.$$

**Example 4.7.** Consider the  $K_n$  complete graph with  $n$  vertices.  $K_n$  is a  $m_{ve}$ -regular graph with the size  $m = n(n-1)/2$ . Therefore,

$$NK_{ve}(K_n) = m^n.$$

**Proposition 4.8.** Let  $G$  be a graph with  $n$  vertices, then

$$NK_{ve}(G) \leq NK_{ve}(K_n).$$

**Proof.** Note that contribution each edge is positive. Hence,  $NK_{ve}(G)$  reaches its maximum value for the complete graphs.  $\square$

**Proposition 4.9.** For the  $P_n$  path graph with  $n$  vertices such that  $n \geq 4$ ,

$$NK_{ve}(P_n) = NK_{ev}(P_n) = 9 \cdot 4^{n-3}.$$

**Proof.** We have already known that  $NK_{ve}(P_n) = 9 \cdot 4^{n-3}$  from the Example 4.4. There are  $n - 3$  edges with their  $ev$ -degrees equal 4 and 2 edges with their  $ev$ -degrees equal 3 for the  $n$ -vertex path. Therefore the proof is completed.  $\square$

**Proposition 4.10.** For the cycle  $C_n$  on  $n$  vertices such that  $n \geq 4$ ,

$$NK_{ve}(C_n) = NK_{ev}(C_n) = 4^n.$$

**Proof.** From the Example 4.5 we can directly write that  $NK_{ve}(C_n) = 4^n$ . And clearly from the definition of  $ev$ -degree, every edge of  $C_n$  is  $4_{ev}$ -regular. The proof comes from this fact.  $\square$

**Proposition 4.11.** For the  $S_n$  star graph with  $n$  vertices such that  $n \geq 4$ ,

$$NK_{ev}(S_n) = n^{n-1} < NK_{ve}(S_n) = (n-1)^n.$$

**Proof.** We make the proof by induction on  $n$ . For  $n = 4$ ,

$$NK_{ev}(S_4) = 4^3 = 64 < NK_{ve}(S_4) = 3^4 = 81$$

as desired. We assume that the claim is true for  $n = k$  and we will show that it is true  $n = k + 1$ .

For  $n = k$ ,  $k^{k-1} < (k-1)^k$  is equivalent to,

$$\left(1 + \frac{1}{k-1}\right)^{k-1} < (k-1)$$

and for  $n = k + 1$ ,  $(k+1)^k < k^{k+1}$ . Thus we want to show that

$$\left(1 + \frac{1}{k}\right)^k < k.$$

$$\begin{aligned} \left(1 + \frac{1}{k}\right)^k &< \left(1 + \frac{1}{k-1}\right)^k = \left(1 + \frac{1}{k-1}\right)^{k-1} \left(1 + \frac{1}{k-1}\right) \\ &< (k-1) \frac{k}{(k-1)} = k. \text{ So the proof ends. } \square \end{aligned}$$

**Theorem 4.12.**

(a) The  $n$ -vertex tree with maximal  $NK_{ve}$  is the  $S_n$  such that  $NK_{ve}(S_n) = (n-1)^n$ .

(b) The  $n$ -vertex unicyclic graph with the maximal  $NK_{ve}$  is the  $S_n + e$  (depicted in Fig.1) such that  $NK_{ve}(S_n + e) = n^3(n-1)^{n-3}$ .

(c) The  $n$ -vertex bicyclic graph with the maximal  $NK_{ve}$  is  $Z_n$  (depicted in Fig.1) such that  $NK_{ve}(Z_n) = (n+1)^4(n-1)^{n-4}$ .

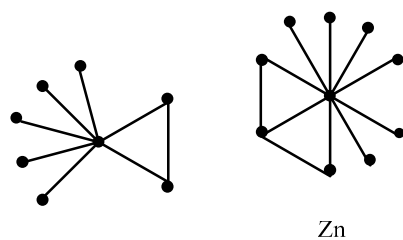


Figure 1. The graphs  $S_n + e$  and  $Z_n$ .

**Theorem 4.13.**

(a) The  $n$ -vertex tree with minimal  $NK_{ve}$  is the  $P_n$  ( $n \geq 4$ ) such that  $NK_{ve}(P_n) = 9 \cdot 4^{n-3}$ .

(b) The  $n$ -vertex unicyclic graph with the minimal  $NK_{ve}$  is the  $R_n$  (depicted in Fig. 2) such that

$$NK_{ve}(R_n) = 2 \cdot 3 \cdot 5^2 \cdot 4^{n-4}.$$

(c) The  $n$ -vertex bicyclic graph with the minimal  $NK_{ve}$  is the  $T_n$  (depicted in Fig. 2) such that

$$NK_{ve}(T_n) = 5^4 \cdot 4^{n-4}.$$

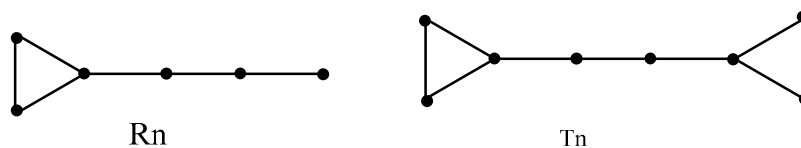


Figure 2. Graphs which are used for Theorem 2.

**Theorem 4. 14.**

(a) The  $n$ -vertex tree with second maximal  $NK_{ve}$  is the  $X_n$  (depicted in Fig. 3) such that

$$NK_{ve}(X_n) = 2(n-1)^2(n-2)^{n-3}.$$

(b) The  $n$ -vertex unicyclic graph with second maximal  $NK_{ve}$  is the  $S_n + e + e'$  (depicted in Fig.4) such that

$$NK_{ve}(S_n + e + e') = 4 \cdot n^3 \cdot (n-2)^{n-4}.$$

(c) The  $n$ -vertex bicyclic graph with second maximal  $NK_{ve}$  is  $L_n$  (depicted in Fig. 3 ) such that

$$NK_{ve}(L_n) = 5 \cdot (n+1)^2 n^2 (n-2)^{n-5}.$$

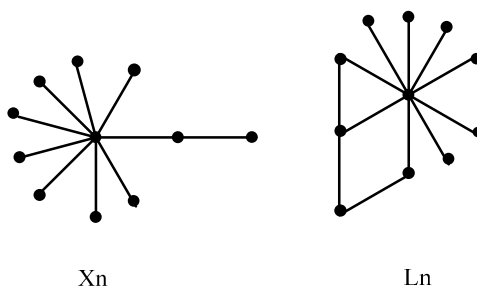


Figure 3. The graph  $X_n$  and  $L_n$ .

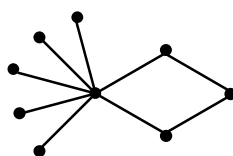


Figure 4. The graph  $S_n + e + e'$ .

**Theorem 4.15.**

(a) The  $n$ -vertex tree with second minimal  $NK_{ve}$  is the  $Q$  graph (depicted in Fig. 5) such that

$$NK_{ve}(Q) = 2^2 \cdot 3^3 \cdot 5^3 \cdot 4^{n-8}$$

(b) The  $n$ -vertex unicyclic graph with second minimal  $NK_{ve}$  is the  $R$  graph (depicted in Fig. 6) such that

$$NK_{ve}(R) = 2 \cdot 3^2 \cdot 5^5 \cdot 4^{n-8}$$

(c) The  $n$ -vertex bicyclic graph with second minimal  $NK_{ve}$  is the  $S$  graph (depicted in Fig. 7) such that

$$NK_{ve}(S) = 3 \cdot 5^7 \cdot 4^{n-8}$$

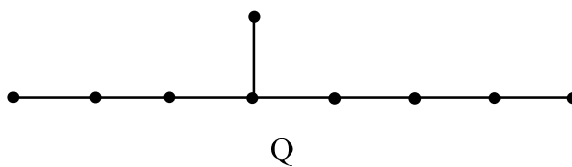
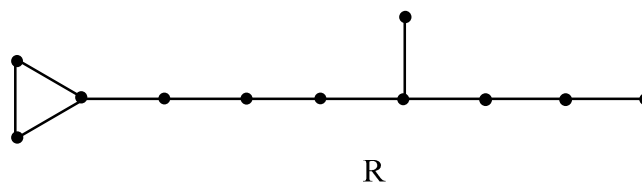
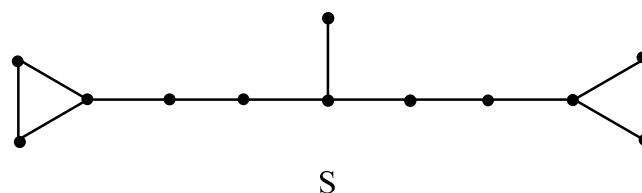


Fig 5. The graph  $Q$ .

Fig 6. The graph  $R$ .Fig 7. The graph  $S$ .

**Corollary 4.16.** For any triangle-free graph  $G$ ,

$$NK_{ev}(G) = \prod_1^*(G).$$

**Proof.** The proof directly comes from the Observation 2.6, the Definition 2.18 and the definition of multiplicative version of the first Zagreb index.  $\square$

And now we give some mathematical properties of  $ev$ -degree and  $ve$ -degree Zagreb indices in terms of the forgotten topological index and the total number of the triangles  $n(G)$  of a connected graph  $G$ . Before giving propositions, we give following terminologies which be used

**Theorem 4.17.** Let  $G$  be a connected graph then;

$$S(G) = F(G) + 2M_2(G) - 2 \sum_{e=uv \in E(G)} (\deg(u) + \deg(v))n_e + \sum_{e=uv \in E(G)} n_e^2.$$

**Proof.** We know that  $c_{e=uv} = \deg(u) + \deg(v) - n_e$  and  $S = S(G) = \sum_{e \in E(G)} c_e^2$ . Therefore;

$$\begin{aligned} S &= S(G) = \sum_{e=uv \in E(G)} c_e^2 = (\deg(u) + \deg(v) - n_e)^2 \\ &= \sum_{e=uv \in E(G)} (\deg(u) + \deg(v))^2 - 2 \sum_{e=uv \in E(G)} (\deg(u) + \deg(v))n_e + \sum_{e=uv \in E(G)} n_e^2 \\ &= \sum_{e=uv \in E(G)} (\deg(u)^2 + \deg(v)^2) + 2 \sum_{e=uv \in E(G)} \deg(u) \deg(v) \\ &\quad - 2 \sum_{e=uv \in E(G)} (\deg(u) + \deg(v))n_e + \sum_{e=uv \in E(G)} n_e^2 \\ &= F(G) + 2M_2(G) - 2 \sum_{e=uv \in E(G)} (\deg(u) + \deg(v))n_e + \sum_{e=uv \in E(G)} n_e^2. \quad \square \end{aligned}$$

**Theorem 4.18.** Let  $G$  be a connected graph then;

$$S^{\beta}(G) = 2M_2(G) - 6n(G)$$

$n(G)$  denotes the total number of triangles in  $G$ .

**Proof.** From the definition of the first  $ve$ -degree Zagreb beta index and Lemma 4.2 we get that;

$$\begin{aligned} S^{\beta}(G) &= \sum_{uv \in E(G)} (c_u + c_v) = \sum_{uv \in E(G)} \left[ \left( \sum_{w \in N(u)} \deg(w) - n_u \right) + \left( \sum_{w \in N(v)} \deg(w) - n_v \right) \right] \\ &= \sum_{uv \in E(G)} \left( \sum_{w \in N(u)} \deg(w) + \sum_{w \in N(v)} \deg(w) \right) - \sum_{uv \in E(G)} (n_u + n_v) \\ &= 2M_2(G) - 6n(G). \quad \square \end{aligned}$$

**Theorem 4.19.** Let  $G$  be a connected graph then;

$$S^{\alpha}(G) = F(G) - 2 \sum_{v \in V(G)} \left( \sum_{u \in N(v)} \deg(u) n_v \right) + \sum_{v \in V(G)} n_v^2$$

$n_v$  the number of triangles in  $G$  containing the vertex  $v$ .

**Proof.** From the definition of the first  $ve$ -degree Zagreb alpha index and Lemma 4.2 we get that;

$$\begin{aligned} S^{\alpha}(G) &= \sum_{v \in V(G)} c_v^2 = \sum_{v \in V(G)} \left( \sum_{u \in N(v)} (\deg(u) - n_v) \right)^2 \\ &= \sum_{v \in V(G)} \left[ \left( \sum_{u \in N(v)} \deg(u) \right)^2 - 2 \sum_{u \in N(v)} \deg(u) n_v + n_v^2 \right] \\ &= \sum_{v \in V(G)} \left( \sum_{u \in N(v)} \deg(u) \right)^2 - 2 \sum_{v \in V(G)} \left( \sum_{u \in N(v)} \deg(u) n_v \right) + \sum_{v \in V(G)} n_v^2 \\ &= \sum_{v \in V(G)} \deg(v)^3 - 2 \sum_{v \in V(G)} \left( \sum_{u \in N(v)} \deg(u) n_v \right) + \sum_{v \in V(G)} n_v^2 \\ &= F(G) - 2 \sum_{v \in V(G)} \left( \sum_{u \in N(v)} \deg(u) n_v \right) + \sum_{v \in V(G)} n_v^2. \quad \square \end{aligned}$$

It is very surprisingly to see that for any triangle free graph the forgotten topological index and the first  $ve$ -degree Zagreb alpha index equal each other. The following corollary states this fact.

**Corollary 4.20.** Let  $G$  be a triangle-free connected graph then;

$$S^{\alpha}(G) = F(G).$$

## 5. Conclusion

In this study we defined  $ev$ -degree and  $ve$ -degree Narumi-Katayama indices and showed that these novel degree based topological indices can be used possible tools for QSPR researches. Also we investigated some basic mathematical properties of  $ev$ -degree and  $ve$ -degree Narumi-Katayama and Zagreb indices. It can be interesting to

compute the exact value of  $ev$ -degree and  $ve$ -degree topological indices for some graph operations. It can also be interesting to investigate the  $ev$ -degree and  $ve$ -degree concepts for the other topological indices for further studies.

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