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On *ve*-Degree Irregularity Indices

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Abstract: In this paper, vertex-edge degrees (or simply, *ve*-degrees) of vertices in a graph are considered. The *ve*-degree of a vertex *v* in a graph equals to the number of different edges which are incident to a vertex from the closed neighborhood of *v*. The author introduces the *ve*-degree total irregularity index here and calculates this index for paths and double star graphs. Finally, the maximal trees are characterized with respect to the *ve*-degree total irregularity index.

Keywords: *ve*-degree, Albertson index, *ve*-degree irregularity, *ve*-degree total irregularity.

INTRODUCTION

THE examination of molecular structures expressed through graphs is one of the important pillars of graph applications. In an undirected graph, the degree sequence is a uniform sequence of the degrees of its vertices that does not increase. Invariants belonging to graphs are most commonly referred to as topological indices and they are often stated using the degrees of vertices, distances between vertices, eigenvalues, symmetries, and many other properties of the graphs. The term topological index first appeared in a study by Wiener.[1] Topological indices lead us to foretell particular physico-chemical properties such as boiling point, melting point, enthalpy of evaporation, stability etc. There are more than 150 topological indices currently known and used. Among these indices, degree-based topological indices are more remarkable and they are quite handy tools for chemists. For more information on degree-based topological indices, I refer to the paper,[2] which is a detailed review article on this. Graphs are one of the basic tools used in the studies conducted in many mathematical sciences.[3–5]

An organic compound and its molecular structure are usually indicated by a molecular graph. Here, atoms imply vertices, and bonds between atoms imply edges. Thus, an idea about the physical properties of these chemical compounds is obtained. Today, chemical graph theory studies are a discipline that has an important place in the fields of chemistry, biology, electrical networks and drug designs. Investigation of compounds with the same chemical formula, even if their chemical structures are different, is the field of study of this discipline. There are many important and remarkable conclusions regarding chemical indices for the studies of computational complexity and chemical graph theory.[6]

Albertson index is one of the most important topological indices and it was introduced in 1997.[7] Consider a simple and finite graph. Let G be this graph with the set of vertices $V(G)$ and the set of edges $E(G)$. The degree of a vertex u of the graph G is the number of adjacent vertices with u in G and it is indicated by $\deg(u)$. A graph G is called regular if all its vertices have the same degree. A graph that is not regular is called irregular. Albertson stated the graph invariant as $irr(G)=\sum_{uv\in E(G)}\left|\deg(u)-\deg(v)\right|$ and named it as irregularity of the graph G. In other words, the Albertson index and irregularity mean the same thing. He obtained some upper bounds for trees, bipartite graphs and triangle-free graphs in his study.[7] Graphs with the maximal irregularity were characterized by Abdo *et al*. They took a different approach than Albertson and found a sharp upper bound for graphs with n vertices and some lower bounds on the maximal irregularity of graphs.[8] Also, the total version of the Albertson index was recently defined by Abdo *et al*. They determined all graphs with maximal total irregularity.[9] A comparison between the irregularity and total irregularity was made in[10] and some inequalities were obtained for connected graphs and trees. Moreover, some well-known irregularity measures were compared[11] and it was shown that any two of these irregularity indices are mutually inconsistent. This means that it is difficult to decide definitively which is more and which is less irregular. Gutman demonstrated the calculations of the irregularity measures on molecular graphs and made comparisons between these results.[12] The trees which were the most and least irregular were characterized according to the Albertson index.[13] The irregularity measure based on eigenvalues of graphs described by Collatz and Sinogowitz[14] has been the oldest known numerical irregularity measure. Bell introduced a second such measure based on the variance of the vertex degrees of a graph, another irregularity measure.[15] He determined the most irregular graphs with respect to these two measures. More details about the irregularity of the graphs can be found in the book.[16]

Domination is one of the most important graph invariants. A subset $D \subseteq V(G)$ is a dominating set, if every vertex in *G* either is an element of *D* or is adjacent to at least one member of *D*. The domination number is the number of vertices in a smallest dominating set for *G*.[17] Domination has been shown to be a very sensitive graph theoretical invariant to even the slightest changes in a graph.[18] Domination was studied for chemical materials in the past. For example, the domination number of benzenoid chains and hexagonal grid was obtained by Vukičević and Klobučar.[18]

Vertex-edge domination (*ve*-domination) and edge-vertex domination (*ev*-domination) are two mixed type domination invariants. An edge *e* dominates a vertex *v*, if *e* is incident to *v* or *e* is incident to a vertex which is adjacent to *v*. A subset $D \subseteq E(G)$ is an edge-vertex dominating set of a graph *G*, if every vertex of *G* is *ev*-dominated by at least one edge of *D*. The minimum cardinality of an *ev*-dominating set is called the *ev*-domination number. A vertex *v* *ve*-dominates an edge *e* which is incident to *v* and any edge which is adjacent to *e*. A set $D \subseteq V(G)$ is a *ve*-dominating set if every edge of a graph *G* is *ve*-dominated by at least one vertex of *D*. The minimum cardinality of a *ve*-dominating set is called the *ve*-domination number. The *ve*-domination and *ev*-domination concepts were introduced by Peters.[19] The lower and upper bounds on the *ve*-domination and *ev*-domination numbers in different graphs were studied.[20] Also, total edge-vertex domination was introduced recently.[17]

Chellali *et al*. introduced two degree concepts: *ve*-degree and *ev*-degree of the graphs based on *ve*-domination and *ev*-domination.[21] The *ve*-degree of a vertex $v \in V(G)$ equals the number of edges *ve*-dominated by *v*. The *ev*-degree of an edge $e = uv$ equals the number of vertices *ev*-dominated by *e*. The regularity and irregularity of graphs about *ve*-degree and *ev*-degree were studied by Horoldagva *et al*.[22] A graph is *ve*-regular if all its vertices have the same *ve*-degree. A graph is *ev*-regular if all its edges have the same *ev*-degree. A graph *G* is called *ve*-irregular if no two vertices in *V*(*G*) have the same *ve*-degree. A graph *G* is called *ev*-irregular if no two edges in *E*(*G*) have the same *ev*-degree.

The *ve*-degree and *ev*-degree concepts of graphs were widely applied to Chemical Graph Theory.[23,24] Many papers were written about the modified versions of the various topological indices with respect to *ve*-degree and *ev*-degree. Some chemical materials were investigated with these modified versions of the topological indices. For example, the *ve*-degree and *ev*-degree based topological properties of single walled titanium dioxide nanotube,[25] *h*-naphtalenic nanotube,[26] silicon carbide Si_2C_3–II[*p*,*g*],[27] two carbon nanotubes,[28] polycyclic graphite carbon nitride[29] and crystallographic structure of cuprite Cu_2O[30] were studied. It has been seen that *ve*-degree and *ev*-degree topological indices can be used as possible tools in QSPR researches.

The *ve*-degree irregularity index was defined recently.[31] The definition of this concept is presented in the second section. Moreover, the maximal trees were characterized with respect to this index.[31] In this paper, I define the *ve*-degree total irregularity index and compute this index for paths and double star graphs. Finally, I obtain the maximal trees with respect to the *ve*-degree total irregularity index.

PRELIMINARIES

Let *G* be a simple graph with the vertex set *V*(*G*) and the edge set *E*(*G*) such that $|V(G)| = n$ and $|E(G)| = m$. For a vertex $u \in V(G)$, the open neighborhood of *u* is defined as $N_G(u) = \{v \mid uv \in E(G)\}$ and the closed neighborhood of *u* is defined as $N_G[u] = \{u\} \cup N_G(u)$.

The degree of a vertex *u* is the cardinality of $N_G(u)$ and it is denoted by $\deg(u)$. A vertex which has degree one is called a leaf. The *ve*-degree of a vertex *v* equals to the number of different edges which are incident to a vertex from the closed neighborhood of *v* and it is denoted by $\deg_{ve}(v)$. Moreover, the *ev*-degree of an edge *e* = *ab* equals to the number of vertices of the union of the closed neighborhoods of *a* and *b*, it is denoted by $\deg_{ev}(v)$.

A graph *G* is *ve*-regular if all its vertices have the same *ve*-degree. The paths, cycles, complete graphs and stars of order *n* are denoted by P_n, C_n, K_n, and $S_{1,n-1}$, respectively. The double star graphs $DS_{p,q}$ are consisted of the stars $S_{1,p}$ and $S_{1,q}$ such that $n = p + q + 2$. The subdivided star S_k^* is obtained from a star $S_{1,k}$ by adding a vertex to every leaf of the star.

It is known that $S_{1,n-1}$ is *ve*-regular tree such that all its vertices have same *ve*-degree $n-1$.[21] The cycle C_n $(n \geq 4)$ is the unique unicyclic graph which is *ve*-regular.[21]

For simplicity, a *ve*-regular graph, each of whose vertices has *ve*-degree *r*, is called r_{ve}-regular.[22] For example, the cycle graph is 4_{ve}-regular for $n \geq 4$. Furthermore, the complete graph K_n is m_{ve}-regular such that the size $m = n(n-1)/2$.

Definition 2.1. For a connected graph *G*,

$$M_1(G) = \sum_{u \in V(G)} \deg^2(u).$$ [32]

Definition 2.2. For a connected graph *G*,

$$\sum_{v \in V(G)} \deg_{ve}(v) = \sum_{e \in E(G)} \deg_{ev}(e) = M_1(G) - 3\eta_G$$

such that η_G is the total number of triangles contained in *G*.[21] It implies that for a triangle-free graph *G*,

$$\sum_{v \in V(G)} \deg_{ve}(v) = \sum_{e \in E(G)} \deg_{ev}(e) = M_1(G).$$

Definition 2.3. Let *G* be a triangle-free graph. Then, for a vertex $u \in V(G)$

$$\deg_{ve}(v) = \sum_{u \in N_G(v)} \deg(u).$$ [24]

Definition 2.4. Let *G* be a triangle-free graph. Then, for an edge $e = ab \in E(G)$

$$\deg_{ev}(e) = \deg(a) + \deg(b).$$ [24]

Definition 2.5. Let *G* be a graph of order *n*. Then, the Albertson index of *G* is computed by

$$irr(G) = \sum_{uv \in E(G)} \left|\deg(u) - \deg(v)\right|.$$ [7]

Definition 2.6. Let *G* be a graph of order *n*. Then, the total irregularity index of *G* is computed by

$$irr_t(G) = \tfrac{1}{2}\sum_{u,v \in V(G)} \left|\deg(u) - \deg(v)\right|.$$ [9]

If the degrees of vertices are ordered as $\deg(v_1) \geq \deg(v_2) \geq \ldots \geq \deg(v_n)$, the total irregularity index can be calculated by

$$irr_t(G) = \sum_{i>j} (\deg(v_i) - \deg(v_j)).$$

Lemma 2.7. If *T* is a tree of order *n*, then

i) $irr(T) \leq (n-1)(n-2)$

such that the equality holds if and only if *T* is a star.[13]

ii) $irr_t(T) \leq (n-1)(n-2)$

such that the equality holds if and only if *T* is a star.[9]

The *ve*-degree version of the Albertson index was expressed as in the following definition.

Definition 2.8. Let *G* be a graph of order *n*. Then, the *ve*-degree irregularity of *G* vis computed by

$$irr_{ve}(G) = \sum_{uv \in E(G)} \left|\deg_{ve}(u) - \deg_{ve}(v)\right|.$$

It is clear that $irr_{ve}(G) = 0$ for *ve*-regular graphs. The total *ve*-degree irregularity index can be defined as follows.

Definition 2.9. Let *G* be a graph of order *n*. Then, the *ve*-degree total irregularity index of *G* is computed by

$$irr^t_{ve}(G) = \tfrac{1}{2}\sum_{u,v \in V(G)} \left|\deg_{ve}(u) - \deg_{ve}(v)\right|.$$

If the *ve*-degrees of vertices are ordered as $\deg_{ve}(v_1) \geq \deg_{ve}(v_2) \geq \ldots \geq \deg_{ve}(v_n)$, the *ve*-degree total irregularity index can be calculated by

$$irr^t_{ve}(G) = \sum_{i>j} (\deg_{ve}(v_i) - \deg_{ve}(v_j)).$$

It is denoted the *ve*-degree sequence by the notation $[\deg_{ve}(v_1), \deg_{ve}(v_2), \ldots, \deg_{ve}(v_n)]$ for $\deg_{ve}(v_1) \geq \deg_{ve}(v_2) \geq \ldots \geq \deg_{ve}(v_n)$. The repeated degrees can be shown by exponential numbers.

MAIN RESULTS

Theorem 3.1. For paths,

$$irr^t_{ve}(P_n) = \begin{cases} 0, & n = 2,3 \\ 6(n-4)+4 & n \geq 4 \end{cases}.$$

Proof. If a path has two or three vertices, their *ve*-degrees are equal. Then, the total *ve*-degree irregularity index equals to zero. Consider a path graph $P_n : v_1 v_2 \ldots v_n$ with $n \geq 4$. it is obtained that $\deg_{ve}(v_1) = \deg_{ve}(v_n) = 2$, $\deg_{ve}(v_2) = \deg_{ve}(v_{n-1}) = 3$ and $\deg_{ve}(v_i) = 4$ for $3 \leq i \leq n-2$. Therefore, I have the *ve*-degree sequence of paths as $[4^{n-4}, 3^2, 2^2]$. The *ve*-degree total irregularity index can be obtained by

$$\begin{aligned} irr^t_{ve}(P_n) &= 2(n-4)(4-3) + 2(n-4)(4-2) + 4(3-2) \\ &= 6(n-4)+4. \end{aligned}$$

Theorem 3.2. Let $DS_{p,q}$ be a double star graph of order $n = p + q + 2$. Then,

i) $irr_{ve}(DS_{p,q}) = 2pq$

ii) $irr^t_{ve}(DS_{p,q}) = pq(p-q+4)$.

Proof. It is known that a double star graph $DS_{p,q}$ consists of two stars $S_{1,p}$ and $S_{1,q}$. Assume that $p \geq q$. It means that there are $p+q$ vertices having degree one and two central vertices of stars having degree $p+1$ and $q+1$, respectively. Now the *ve*-degrees of the vertices in $DS_{p,q}$ are determined. The central vertices of stars *ve*-dominate all edges. Then, the *ve*-degrees of central vertices are $p+q+1$.

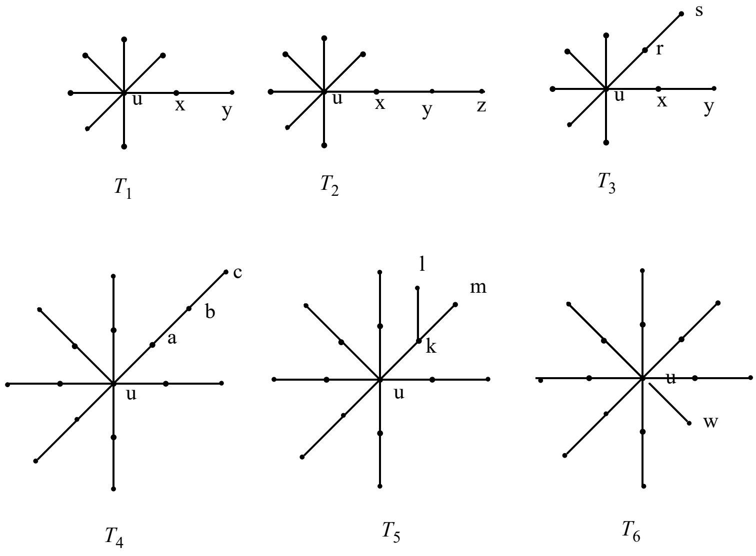

Figure 1. The trees T_1, T_2, T_3, T_4, T_5, T_6.

The *ve*-degree of the leaves of $S_{1,p}$ is $p+1$ and the *ve*-degree of the leaves of $S_{1,q}$ is $q+1$. Then, I obtain the *ve*-degree sequence of $DS_{p,q}$ as $[(p+q+1)^2,(p+1)^p,(q+1)^q]$.

$$i)\quad irr_{ve}(DS_{p,q}) = p[p+q+1-(p+1)] + q[p+q+1-(q+1)] = 2pq.$$

$$\begin{aligned} ii)\quad irr_{ve}^t(DS_{p,q}) &= 2p[p+q+1-(p+1)] \\ &+ 2q[p+q+1-(q+1)] \\ &+ pq[p+1-(q+1)] \\ &= 2pq+2pq+pq(p-q) \\ &= pq(p-q+4). \end{aligned}$$

Theorem 3.3. Let *T* be a simple tree with order *n*, then

$$i)\quad irr_{ve}^t(T) \le \frac{n^3+n^2-17n+15}{8},$$

if $n=2k+1$ and the equality holds if and only if $T \cong S_k^*$.

$$ii)\quad irr_{ve}^t(T) \le \frac{n^3+5n^2-17n+11}{8},$$

if $n=2k+2$ and the equality holds if and only if $T \cong T_6$, which is indicated in Figure 1.

Proof. In order to prove the equalities, I apply some operations to $S_{1,n-1}$ graphs. It is clear that the star graphs are *ve*-regular graphs. Then, the *ve*-degree irregularity index and *ve*-degree total irregularity index of stars equal to 0.

i) Assume that $n=2k+1$. If I remove a leaf from a star $S_{1,n-1}$ and attach it to another leaf, I obtain double star graph $T_1 = DS_{n-3,1}$, which is indicated in Figure 1. Then, T_1 is a double star graph which consists of a star graph $S_{1,n-3}$ with the central vertex *u* and a path P_2 *xy* such that *u* is joined to *x*. Thus, $\deg_{ve}(y)=2$, $\deg_{ve}(x)=\deg_{ve}(u)=n-1$ and the remaining $(n-3)$ vertices have *ve*-degree $(n-2)$. Then, its *ve*-degree sequence is $[(n-1)^2,(n-2)^{n-3},2]$. So, $irr_{ve}^t(T_1) = 2(n-3)+2(n-3)+(n-3)(n-4) = n^2-3n$.

If I remove a leaf and attach it (say that *z*) to the vertex *y* on T_1, I obtain the tree T_2, which is indicated in Figure 1. It is obtained that $\deg_{ve}(z)=2$, $\deg_{ve}(y)=3$, $\deg_{ve}(x)=n-1$, $\deg_{ve}(u)=n-2$ and the remaining $(n-4)$ vertices have *ve*-degree $(n-3)$ for T_2. Then, the *ve*-degree sequence of T_2 is $[n-1,n-2,(n-3)^{(n-4)},3,2]$. So,

$$\begin{aligned} irr_{ve}^t(T_2) &= 1+2(n-4)+n-4+n-3+n-4+n-5 \\ &+ n-4+(n-4)(n-6)+(n-4)(n-5)+1 \\ irr_{ve}^t(T_2) &= 2n^2-12n+18. \end{aligned}$$

Then, it can be seen that $irr_{ve}^t(T_2) - irr_{ve}^t(T_1) = n^2 - 9n+18 > 0$ for $n \ge 7$. If the operation which is used in the transformation from T_1 to T_2 is used $(n-3)$-times to a star, I obtain a path at the end.

Now I remove a leaf *s* and attach it to a vertex (*r*) which is incident to the central vertex *u* on T_1. Thus, I obtain the tree T_3, which is indicated in Figure 1. For the tree T_3, $\deg_{ve}(y)=\deg_{ve}(s)=2$, $\deg_{ve}(x)=\deg_{ve}(r)=n-2$, $\deg_{ve}(u)=n-1$ and the remaining $(n-5)$ vertices have *ve*-degree $(n-3)$. Then, the *ve*-degree sequence of T_3 is $[n-1,(n-2)^2,(n-3)^{(n-5)},2^2]$. So,

$$\begin{aligned} irr_{ve}^t(T_3) &= 2+2(n-5)+2(n-3)+2(n-5) \\ &+ 4(n-4)+2(n-5)^2 \\ irr_{ve}^t(T_3) &= 2n^2-10n+10 \end{aligned}$$

Consequently, $irr_{ve}^t(T_3) - irr_{ve}^t(T_2) = 2n-8 \ge 0$ for $n \ge 4$. It is seen that the difference of the *ve*-degree total irregularity index between T_3 and T_1 is greater than the difference of the *ve*-degree total irregularity index between T_2 and T_1. By this way, I obtain the subdivided star graph S_k^* which is the maximal tree with respect to the *ve*-degree total irregularity index with order $n=2k+1$. For S_k^*, the *ve*-degree of the central vertex *u* is 2*k*, the *ve*-degree of the vertices at distance 1 from *u* is $(k+1)$ and the *ve*-degree of the vertices at distance 2 from *u* is 2. Therefore, the *ve*-degree sequence of S_k^* is $[2k,(k+1)^k,2^k]$. So,

$$irr_{ve}^t(S_k^*) = k(k-1)+k(2k-2)+k^2(k-1)$$
$$irr_{ve}^t(S_k^*) = k(k-1)(k+3)$$
$$irr_{ve}^t(S_k^*) = \frac{n-1}{2}\times\frac{n-3}{2}\times\frac{n+5}{2}$$
$$irr_{ve}^t(S_k^*) = \frac{n^3+n^2-17n+15}{8}.$$

ii) I investigate the second case for $n=2k+2$. It means that a vertex of degree should be attached to a subdivided star graph S_k^*. Thus, I should investigate the trees T_4, T_5, T_6.

For the tree T_4, $\deg_{ve}(c)=2$, $\deg_{ve}(b)=3$, $\deg_{ve}(a)=k+2$, $\deg_{ve}(u)=2k$, the *ve*-degree of the $(k-1)$ vertices at distance 1 from *u* is $(k+1)$ and the *ve*-degree of the $(k-1)$ vertices at distance 2 from *u* is 2. Thus, the *ve*-degree sequence of T_4 is $[2k,k+2,(k+1)^{k-1},3,2^k]$. I compute the *ve*-degree total irregularity index of T_4 as follows.

$$irr_{ve}^t(T_4) = k-2+(k-1)^2+2k-3+k(2k-2)+k-1$$
$$+k-1+k^2+(k-2)(k-1)+k(k-1)^2+k$$
$$irr_{ve}^t(T_4) = k^3+3k^2+4$$
$$irr_{ve}^t(T_4) = \left(\frac{n-1}{2}\right)^3+3\left(\frac{n-1}{2}\right)^2+4$$
$$irr_{ve}^t(T_4) = \frac{n^3+3n^2-9n+37}{8}.$$

For the tree T_5, $\deg_{ve}(l)=\deg_{ve}(m)=3$, $\deg_{ve}(k)=k+2$, $\deg_{ve}(u)=2k+1$, the *ve*-degree of the $(k-1)$ vertices at distance 1 from *u* is $(k+1)$ and the *ve*-degree of the $(k-1)$ vertices at distance 2 from *u* is 2. Then, the *ve*-degree sequence of T_5 is $[2k+1,k+2,(k+1)^{k-1},3^2,2^{k-1}]$. I calculate the *ve*-degree total irregularity index of T_5 as follows.

$$irr_{ve}^t(T_5) = k-1+k(k-1)+2(2k-2)+(2k-1)(k-1)$$
$$+k-1+(k-1)^2+k(k-1)+2(k-1)(k-2)$$
$$+(k-1)^3+2(k-1)$$
$$irr_{ve}^t(T_5) = k^3+3k^2-k-3$$
$$irr_{ve}^t(T_5) = \left(\frac{n-1}{2}\right)^3+3\left(\frac{n-1}{2}\right)^2-\frac{n-1}{2}-3$$
$$irr_{ve}^t(T_5) = \frac{n^3+3n^2-13n-15}{8}.$$

For the tree T_6, $\deg_{ve}(w)=k+1$, $\deg_{ve}(u)=2k+1$, the *ve*-degree of the *k* vertices at distance 1 from *u* is $(k+2)$ and the *ve*-degree of the *k* vertices at distance 2 from *u* is 2. Then, the *ve*-degree sequence of T_6 is $[2k+1,(k+2)^k,\ k+1,2^k]$. So,

$$irr_{ve}^t(T_6) = k(k-1)+k+2(2k-1)+k+k^3+k(k-1)$$
$$irr_{ve}^t(T_6) = k^3+4k^2-k$$
$$irr_{ve}^t(T_6) = \left(\frac{n-1}{2}\right)^3+4\left(\frac{n-1}{2}\right)^2-\frac{n-1}{2}$$
$$irr_{ve}^t(T_6) = \frac{n^3+5n^2-17n+11}{8}.$$

It implies that T_6 has the maximal *ve*-degree total irregularity index of even order in the trees.

CONCLUSION

After the introduction of the *ve*-degree irregularity index,[31] the *ve*-degree total irregularity index is defined in this paper. Moreover, the *ve*-degree total irrregularity index of paths and double star graphs are obtained, and the maximal graphs with respect to this index are attained. Consequently, the present paper is a contribution to find the *ve*-degree based topological indices in different sciences. By means of the *ve*-degree based topological indices, the number of tools which are used in the computation of graph irregularity is increased.

As the paralleling of the rapid growing of science and technology, the importance of analysing in networks is increased. Then, the *ve*-degree irregularity indices may be used in the computation of the chemical, biological and other properties of chemical materials.

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