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On the Reformulated Zagreb Indices of Certain Nanostructures

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Abstract

The Zagreb indices are the best known and widely used topological indices for a molecular graph in chemical graph theory, the first and second reformulated Zagreb indices of a graph are obtained from the Zagreb indices by replacing vertex degree with edge degree defined as, $EM_1(G) = \sum_{e \in E(G)} \deg(e)^2$ and $EM_2(G) = \sum_{(e \sim f) \in E(G)} \deg(e) \cdot \deg(f)$, where *deg(e)* denotes the degree of the edge '*e*' and '*e~f*' means that edges '*e*' and '*f*' are adjacent. In this article, we give explicit formula for the first and second reformulated Zagreb indices for the nanostructures.

AMS Subject Classification: 05C99

Keywords: Reformulated Zagreb indices, Nanostar Dendrimer, 2D-Lattice, Nanotube, Nanotorus.

1. INTRODUCTION

Let *G=(V,E)* be a connected simple graph with $n = |V|$ vertices and $m = |E|$ edges. The degree of a vertex '*v*' is denoted as *deg(v)* or *d(v)*. We follow[5] for terminologies and notations. A chemical graph or a molecular graph is a graph related to the structure of a chemical compound. Each vertex of this graph represent an atom of the molecule and covalent bonds between atoms are represented by edges between the corresponding vertices. In theoretical chemistry, the physio chemical properties of chemical compounds are often modeled by the molecular graph based molecular structure descriptors which are also refered to as topological indices[4]. Such among the variety of those indices, Zagreb indices are very important and they have prominent role in chemistry, especially in QSPR and QSAR study.

The first Zagreb index $M_1(G)$ equals to the sum of squares of the vertex degrees and the second Zagreb index $M_2(G)$ equals to the sum of product of degrees of pairs of adjacent vertices[4].

$$M_1 = M_1(G) = \sum_{v \in V(G)} d_G(v)^2$$

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

Properties of the Zagreb indices may be found in the number of reports[1,2,3,8,13,14,15]. In 2004 Miličevič, Nikolic and Trinajstić reformulated the Zagreb indices in terms of edge degree instead of vertex degrees[10].

$$EM_1 = EM_1(G) = \sum_{e \in E(G)} d_G(e)^2$$

and

$$EM_2 = EM_2(G) = \sum_{e \sim f \in E(G)} d_G(e) \cdot d_G(f)$$

Where *deg(e)* denoted the degree of the edge e in G and $(e \sim f)$ implies that the edges 'e' and 'f' are adjacent and share a common vertex in G. Degree of an edge 'e' is defined by *deg(e) = deg(u) + deg(v) - 2* with $e = uv$ and share a common vertex in G. Where $EM_1(G)$ is the first reformulated Zagreb index and $EM_2(G)$ is the second reformulated Zagreb index.

2. NANOSTRUCTURE

In this section we compute reformulated Zagreb indices for an infinite family of nanostar dendrimer $D_3[n]$, 2*D*-lattices, nanotube and nanotorus of $T \cup C_4C_8[p,q]$. Dendrimers are hyper-branched macromolecules with a rigorously tailored architecture and are one of the main objects of Nano biotechnology. They can be synthesized, in a controlled manner, either by a divergent or a convergent procedure. Dendrimers have gained a wide range of application in supra-molecular chemistry, particularly in host guest reactions and self assembly process. Their applications in chemistry, biology and nanoscience are unlimited. In this article we denote the n^{th} growth of nanostar dendrimer by $D_3[n]$, $\forall n \in N$. It has $|V(D_3[n])|=2|2n+1|$ number of vertices or atoms because in the structure of dendrimer nanostar $D_3[n]$ there are $3(2^n)$ vertices or atoms with degree 1, $12(2^{n+1}-1)$ vertices of $D_3[n]$ with degree 2 and $15(2^n)-8$ vertices with degree 3. And also there are $|E(D_3[n])|= 12\ [1 \cdot 3(2^n) + 2 \cdot 12(2^{n+1}-1) + 3 \cdot 15(2^n)] = 24(2^{n+1}-1)$ edges or bonds in the Nanostar dendrimer

$D_3[n]$. Recently, the topological indices of some dendrimer nanostars have been investigated in [7,9,12].

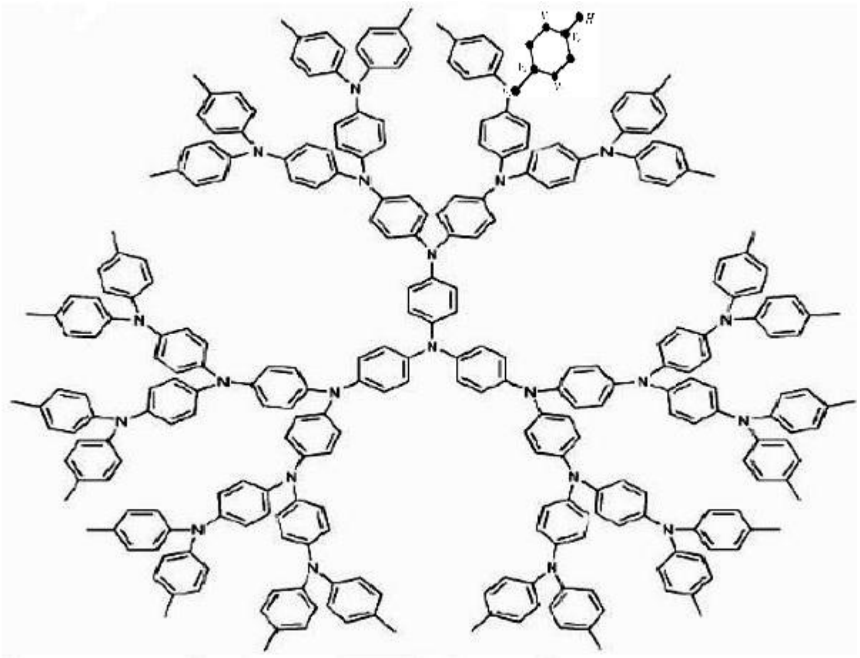

Figure.1 Nanostar dendrimer $D_3[n]$

From the structure of dendrimer nanostar $D_3[n]$ in the n^{th} growth of nanostar dendrimer in figure 1, we see that an element as figure 2 (called Leaf) is added to $D_3[n-1]$in the n^{th} growth of nanostar dendrimer.

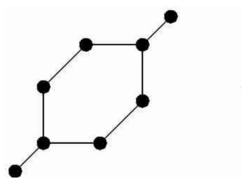

Figure : 2 Leaf of Nanostar Dendrimer $D_3[n]$

Note 1. In $D_3[n]$, the leaves are connected with vertices/atoms N, to construct the proof we consider central vertex/atom as N and the remaining vertices/atoms as N'. Recently Nadeem et.al.[11] and S.M.Hosamani et.al.[6] obtained expressions for certain topological indices of nanostructures. In this paper we study the 2D-Lattice, nanotube and nanotorus of $T \cup C_4C_8[p,q]$, where p and q denote the number of squares in a row and the number of rows of squares, respectively.

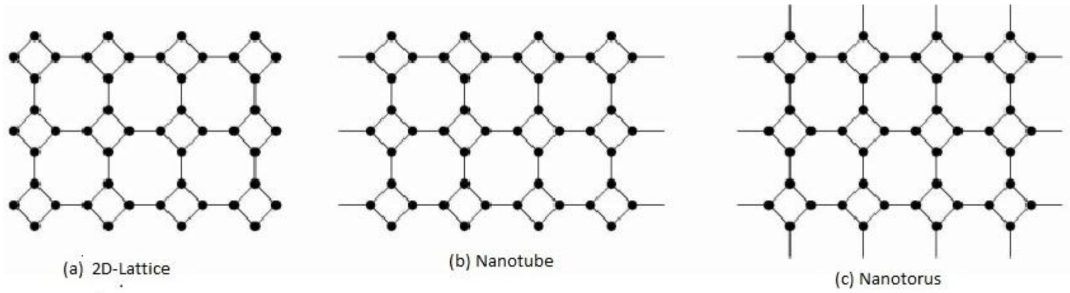

Figure : 3 (a) 2D − Lattice, (b) Nanotube, (C) Nanotorus of $T \cup C_4C_8[p,q]$

In figure 3, 2*D*-lattice, nanotube and nanotorus of $T \cup C_4C_8[p,q]$ are depicted. The order and size of 2*D*-lattice, nanotube and nanotorus of $T \cup C_4C_8[p,q]$ are 4*pq* and 6*pq* − *p* − *q*, 4*pq* and 6*pq* − *q*, 4*pq* and 6*pq* respectively.

3. RESULTS

Theorem 3.1. Let G be a graph of nanostar dendrimer $D_3[n]$, then the first reformulated Zagreb index is,

$$EM_1(G) = 12\left[15 + 2^n + 12\sum_{k=1}^{n} 2^{(k-1)} + 11\sum_{k=1}^{n} 2^k\right]$$

Proof. Let $G = D_3[n]$ be a graph of nanostar dendrimer, $\forall\, n \geq 1$.

We construct the proof considering the following steps.

Step I. Consider the degree of the edges in $D_3[n]$ which are incident with central vertex *N* which is 4. Then the first reformulated Zagreb index is $4^2 \cdot 3 = 16 \cdot 3 = 48$.

And the first reformulated Zagreb index of remaining edges incident with *N′* is,

$$\sum_{e \in E(G) \in N} \deg(e)^2 = 144\sum_{k=2}^{n} 2^{k-1}$$

Step II. Consider the degree of the edges in leaves of $D_3[n]$ which are not adjacent with edges incident with central vertex *N* is 2, then the first reformulated Zagreb index is $2 \cdot 2^2 \cdot 3 = 24$.

And the first reformulated Zagreb index of remaining edges of leaves in $D_3[n]$ which are adjacent to the vertex *N′* is,

$$\sum_{e \in E(G) \in N} \deg(e)^2 = 24\sum_{k=1}^{n} 2^k$$

Step III. Now we consider the degree of the edges in leaves which are adjacent to the edges incident with central vertex N which is 3, then the first reformulated Zagreb index is, $9 \cdot 2^2 \cdot 3 = 108$.

And the first reformulated Zagreb index of remaining edges of leaves in $D_3[n]$ which are adjacent to the vertex N' is,

$$\sum_{e \in E(G) \in N} \deg(e)^2 = 108 \sum_{k=1}^{n} 2^k$$

Step IV. Consider the degree of the edges containing pendent vertex in $D_3[n]$ which is 2, then the first reformulated Zagreb index is $2^2 \cdot 3 \cdot 2^n = 12 \cdot 2^n$.

From the above steps I, II, III and IV, the first reformulated Zagreb index of $D_3[n]$ is,

$$\begin{aligned} EM_1(G) &= EM_1(D_3[G]) \\ &= \sum_{e \in E(G) \in N} \deg(e)^2 \\ &= 48 + 24 + 108 + 144 \sum_{k=1}^{n} 2^{k-1} + 108 \sum_{k=1}^{n} 2^k + 24 \sum_{k=1}^{n} 2^k + 12 \cdot 2^n \\ &= 12 \left[15 + 2^n + 12 \sum_{k=1}^{n} 2^{(k-1)} + 11 \sum_{k=1}^{n} 2^k \right]. \end{aligned}$$

Theorem 3.2. Let G be a graph of nanostar dendrimer $D_3[n]$, then the second reformulated Zagreb index is,

$$EM_2(G) = 264 + 36 \left[4 \sum_{k=1}^{n} 2^{(k-1)} + 6 \sum_{k=1}^{n} 2^k - 2^n \right]$$

Proof. Let $G = D_3[n]$ be a graph of nanostar dendrimer, $\forall\ n \geq 1$.

We use the following steps to prove the theorem.

Step I. Let us consider the structure of $D_3[n]$ with central vertex N and the leaves which are incident with central vertex N. There are three edges incident with each vertex N.

Consider the leaves, in each leaf, there are 4-edges adjacent with edges of degree 3 and 2-edges adjacent with edges of degree 3. Therefore the second reformulated Zagreb index of this structure is,

$$\sum_{e \sim f \in E(G)} d_G(e) \cdot d_G(f) = (4 \cdot 4)3 + (4 \cdot 3)(4 \cdot 3) + (2 \cdot 3)(4 \cdot 3) = 264$$

Step II. Since there are $3 \sum_{k=1}^{n} 2^{(k-1)}$ number of N' vertices/atoms containing 3-pairs of mutually adjacent edges with degree 4. Then the second reformulated Zagreb index is,

$$\sum_{e\sim f\in E(G)} \deg(e)\cdot\deg(f) = (4\cdot 4)\ \cdot 3\cdot 3\sum_{k=1}^{n} 2^{(k-1)} = 144\sum_{k=1}^{n} 2^{(k-1)}$$

Step III. Now we consider $3\left(4\sum_{k=2}^{n} 2^{(k-1)} - 2\cdot 2^{n}\right)$ pairs of adjacent edges with degree 3 and degree 4 of all the leaves in *D*3*[n]*. Then the second reformulated Zagreb index is,

$$\sum_{`e\sim f\in E(G)} \deg(e)\cdot\deg(f) = (3\cdot 4)\cdot 3\left(4\cdot\sum_{k=1}^{n} 2^{k} - 2\cdot 2^{n}\right) = 36\left(4\cdot\sum_{k=1}^{n} 2^{k} - 2\cdot 2^{n}\right)$$

Step IV. Now we consider the 4 - pair of adjacent edges of each leaf with degree 2and degree 3 which is $3\sum_{k=1}^{n} 2^{k}$ times. Then the second reformulated Zagreb index is,

$$\sum_{e\sim f\in E(G)} \deg(e)\cdot\deg(f) = (3\cdot 4)\cdot(4\cdot 3)\sum_{k=1}^{n} 2^{k} = 72\sum_{k=1}^{n} 2^{k}$$

Step V. Finally consider the pendent edges with degree 2 which are adjacent with edges of degree 3. Since there are 3(2^n) pendent edges in *D*3*[n],* then the second reformulated Zagreb index is,

$$\sum_{e\sim f\in E(G)} \deg(e)\cdot\deg(f) = (3\cdot 2)\cdot(2\cdot 3)\cdot 2^{n} = 36\cdot 2^{n}$$

From the above steps I, II, III, IV and V, the second reformulated Zagreb index of *D*3*[n]* is,

$$\begin{aligned} EM_2(G) &= EM_2(D_3[G]) \\ &= \sum_{e\sim f\in E(G)} \deg(e)\cdot\deg(f) \\ &= 264 + 144\sum_{k=1}^{n} 2^{k-1} + 36\left(4\sum_{k=1}^{n} 2^{k} - 2\cdot 2^{n}\right) + 72\sum_{k=1}^{n} 2^{k} + 36\cdot 2^{n} \\ &= 264 + 36\left[4\sum_{k=1}^{n} 2^{(k-1)} + 6\sum_{k=1}^{n} 2^{k} - 2^{n}\right]. \end{aligned}$$

Theorem 3.3. Let *G* be a graph of 2*D*-lattice of $T\bigcup C_4C_8[p,q]$ then the first reformulated Zagreb index is,

$$EM_1(G) = 96pq - 44(p+q) + 8$$

Proof. Let *G* be 2*D*-lattice of $T\bigcup C_4C_8[p,q]$ graph with 6*pq – p - q* number of edges.

In 2*D*-lattice of $T \cup C_4C_8[p,q]$, 4-edges are of degree 2, 2[2*p*-2*q*-4] edges are of degree 3 and remaining 6*pq*-5(*p*+*q*)+4 edges are of degree 4.

Then the first reformulated Zagreb index of 2*D*-lattice is,

$$\begin{aligned} EM_1(G) &= EM_1(D_3[G]) \\ &= \sum_{e \in E(G) \in N} \deg(e)^2 \\ &= 2^n \cdot 4 + 3^2 \cdot 4(p+q-2) + 4^2(6pq - 5(p+q)+4) \\ &= 96pq - 44(p+q) + 8 \end{aligned}$$

Theorem 3.4. Let G be a graph of 2D-lattice of $T \cup C_4C_8[p,q]$ then the second reformulated Zagreb index is,

$$EM_2(G) = 16pq[8pq - 2p - 2q + 7]$$

Proof. Let *G* be 2*D*-lattice of $T \cup C_4C_8[p,q]$ graph with edges.

We use the following steps to construct the proof.

Step I. In 2*D*-lattice of $T \cup C_4C_8[p,q]$, 8-pairs of edges degree 2 and degree 3, therefore the second reformulated Zagreb index is,

$$\sum_{e \sim f \in E(G)} \deg(e) \cdot \deg(f) = (2 \cdot 3) \cdot 8 = 48$$

Step II. Since there are 4[*p*+*q*-2] pairs of edges with degree 3 and degree 4 in a graph of 2*D*-lattice of $T \cup C_4C_8[p,q]$. Therefore the second reformulated Zagreb index is,

$$\sum_{e \sim f \in E(G)} \deg(e) \cdot \deg(f) = (3 \cdot 4) \cdot (2 \cdot 4)[p+q-2] = 96(p+q-2)$$

Step III. Similarly, there are 8[*pq*-*p*-*q*+1] pairs of edges with degree 4 in a graph of 2*D*-lattice of $T \cup C_4C_8[p,q]$. Therefore the second reformulated Zagreb index is,

$$\sum_{e \sim f \in E(G)} \deg(e) \cdot \deg(f) = 4^2 \cdot 8\,[pq - p - q + 1] = 128[pq - p - q + 1]$$

Therefore, from the steps I, II and III, we get

$$\begin{aligned} EM_2(G) &= \sum_{e \sim f \in E(G)} \deg(e) \cdot \deg(f) \\ &= 48 + 96[p+q-2] + 128[pq - p - q + 1] \\ &= 16\,[8pq - 2(p+q) - 1]. \end{aligned}$$

Theorem 3.5. Let G be a graph of nanotube of $T \cup C_4C_8[p,q]$, then the first reformulated Zagreb index is,

$$EM_1(G) = 4p[24q - 11]$$

Proof. Let G be nanotube of $T \cup C_4C_8[p,q]$ graph with 6*pq*-*p* number of edges.

The degree of all the edges of nanotube of $T \cup C_4C_8[p,q]$ are equal to 4 except 4*p* edges which are of degree 3.

Therefore, the first reformulated Zagreb index of nanotube of $T \cup C_4C_8[p,q]$ is,

$$\begin{aligned} EM_1(G) &= \sum_{e \in E(G) \in N} \deg(e)^2 \\ &= 3^2 \cdot 4p + 4^2[6pq - p - 4p] \\ &= 36p + 16(pq - 5p) \\ &= 4p[24q - 11]. \end{aligned}$$

Theorem 3.6. Let G be a graph of nanotube of $T \cup C_4C_8[p,q]$, then the second reformulated Zagreb index is,

$$EM_2(G) = 2p[64q + 25]$$

Proof. Let G be a graph of nanotube of $T \cup C_4C_8[p,q]$ with 6*pq*-*p* number of edges.

We use the following steps to construct the proof.

Step I. There are 2*p*-pairs of edges with degree 3 in graph of nanotube of $T \cup C_4C_8[p,q]$ therefore the second reformulated Zagreb index is,

$$\sum_{e \sim f \in E(G)} \deg(e) \cdot \deg(f) = (3 \cdot 3) \cdot 2p = 18p$$

Step II. Now we consider 8*p*-pairs of edges with degree 3 and degree 4 in graph of nanotube of $T \cup C_4C_8[p,q]$. Therefore the second reformulated Zagreb index is

$$\sum_{e \sim f \in E(G)} \deg(e) \cdot \deg(f) = (3 \cdot 4) \cdot 8p = 96p$$

Step III. Since there are 8*pq*-4*p* pairs of edges with degree 4 in a graph of nanotube of $T \cup C_4C_8[p,q]$. Therefore the second reformulated Zagreb index is,

$$\sum_{e \sim f \in E(G)} \deg(e) \cdot \deg(f) = 4^2 \cdot 4(2pq - p) = 64(2pq - p)$$

Therefore, from the steps I, II, and III, we get

$$\begin{aligned} EM_2(G) &= \sum_{e \sim f \in E(G)} \deg(e) \cdot \deg(f) \\ &= 18p + 96p + 64(2pq - p) \\ &= 2p[64q - 25] \end{aligned}$$

Theorem 3.7. Let G be a graph of nanotorus of $T \cup C_4C_8[p,q]$, then the first reformulated Zagreb index is,

$$EM_1(G) = 96pq$$

Proof. Let G be a graph of nanotorus of $T \cup C_4C_8[p,q]$ with 6*pq* number of edges.

The degree of all the edges in nanotorus of $T \cup C_4C_8[p,q]$ is 4.

Then first reformulated Zagreb index is,

$$\begin{aligned} EM_1(G) &= \sum_{e \in E(G)} \deg(e)^2 \\ &= 4^2 \cdot 6pq \\ &= 96pq \end{aligned}$$

Theorem 3.8. Let G be a graph of nanotorus of $T \cup C_4C_8[p,q]$, then the second reformulated Zagreb index is,

$$EM_2(G) = 192pq$$

Proof. Let G be a graph of nanotorus of $T \cup C_4C_8[p,q]$ with 6*pq* number of edges.

The degree of all the edges in nanotorus of $T \cup C_4C_8[p,q]$ is 4. Since each pair of edges is repeated twice in $T \cup C_4C_8[p,q]$.

Then second reformulated Zagreb index is,

$$\begin{aligned} EM_2(G) &= \sum_{e \sim f \in E(G)} \deg(e) \cdot \deg(f) \\ &= 4^2 \cdot 2 \cdot 6pq \\ &= 192pq \end{aligned}$$

4. CONCLUSION

In mathematical chemistry, numbers encoding certain structural features of organic molecules and derived from the corresponding molecular graph, are called molecular topology(or topological indices), it has widely demonstrated its high performance in the discovery and design of new drugs. In this paper we studied and computed new results on reformulated Zagreb indices for nanostructures such as nanostar dendrimer $D_3[n]$ and 2D-lattice, nanotube, nanotorus of $T \bigcup C_4C_8[p,q]$ and which are have many chemical applications. Further this study can be extended to compute new results on topological indices of various families of chemical structures.

5. ACKNOWLEDGEMENT

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REFERENCES

[1] Bollobás B., Erdos, P., 1998, "Graph of extremal weight," Ars Combin, 50, pp. 225-233.
[2] Das, K . C., and Gutman, I., 2004, "Some properties of the second Zagreb index," MATCH Commun. Math. Comput. Chem., 52, pp. 103-112.
[3] Gutman, I., and Das. K.C., 2004, "The first Zagreb index 30 years after," MATCH Commun. Math. Comput. Chem., 50, pp. 83-92.
[4] Gutman, I., and Trinajastić, N., 1972, "Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons," Chem. Phys. Lett., 17, pp. 535-538.
[5] Harary, F., 1969, "Graph theory," Addison-Wesely, Reading.
[6] Hosamani, S. M., and Zafar, S., "On topological properties of the line graphs of subdivision graphs of certain nanostructures-II,"(pre-print).
[7] Heydari, A., and Taeri, B., 2007, "Szeged index of nanotubes," MATCH Commun. Math. Comput. Chem., 57, pp. 463-477.
[8] Janežić, D., Miličevič, A., Nikolič, S., Trinajstić, N., and Vukičević, D., 2007, "Zagreb indices: extension to weighted graphs representing molecules contining heteroatoms," Croat Chem Acta, 80, pp. 541-545.
[9] Li, Y., Yan, L., Farahni, M. R., Alkenani, A. N., Pajesh Kanna, M. R., and Pradeep Kumar, R., 2016, "The edge eccentric connectivity index of nanostar Dendrimer $D_3[n]$," International Journal of Biology, Pharmacy and Allied Sciences, 5(7), pp. 1591-1596.
[10] Miličević, A., Nikolić, S., and Trinajastić, N., 2004, "On reformulated Zagreb indices," Mol. Divers., 8, pp. 393-399.
[11] Nadeem, M. F., Zafar, S., and Zahid, Z., 2016, "On topological properties of the line graph of certain nanostructures," Appl. Math. Comput., 273, pp. 125-130.
[12] Newkome, G. R., Moorefield, C.N., and Vogtlen, F., 2002, "Dendrimer and Dendrons concepts, synthesis, Applications," Wiely-VCH verlag Gmbh and Co. Kgaa.
[13] Nikolić, S., Kovačević, G., Miličevič, A., and Trinajstić, N., 2003, "The Zagreb indices 30 years after," Croat. Chem. Acta., 76, pp. 113-124.

[14] Zhou, B., 2004, "Zagreb indices," MATCH Commun. Math. Comput. Chem., 52, pp. 113-118.
[15] Zhou, B., Gutman, I., 2005, "Further properties of Zagreb indices," MATCH Commun. Math. Comput. Chem., 54, pp.233-239.