Computation on Zagreb Polynomial of Some Families of Dendrimers

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Abstract
In mathematical chemistry, a particular attention is given to degree-based graph invariant. The Zagreb polynomial is one of the degree based polynomials considered in chemical graph theory. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this note, the first, second and third Zagreb polynomials of some nanostar dendrimers are determined.
Keywords: *Zagreb polynomial, Dendrimer, Graph.*

1. INRODUCTION

In this paper, we consider only simple and connected graph G with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex $v \in G$ is the number of edges incident to v and denoted by $\deg_G(v)$ or d_v. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds.

A graphical invariant is a number related to a graph which is structural invariant, that is to say it is fixed under graph automorphism. In chemistry and for chemical graphs, these invariant numbers are known as the topological indices [1,2].

A topological index $Top(G)$ of a graph G, is a number with this property that every graph H isomorphic to G, $Top(G) = Top(G)$. The Wiener index is the first and most studied topological indices, both from theoretical point of view and application [3-5].

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajstic [6] and they are defined as $ZG_1(G) = \sum_{uv\in E(G)} d_u + d_v$ and $ZG_2(G) = \sum_{uv\in E(G)} d_u\, d_v$, where $ZG_1(G)$ and $ZG_2(G)$ denotes the first and second Zagreb indices of G, respectively. We encourage the reader to consult [7-13] for historical background and mathematical properties of Zagreb indices. In 2011, Fath-Tabar [14] introduced a new graph invariant, namely the third Zagreb index and defined as $ZG_3(G) = \sum_{uv\in E(G)} |d_u - d_v|$.

Recently, Fath-Tabar [15] has put forward the concept of the first and the second Zagreb polynomial of the graph G, defined respectively as

$$ZG_1(G,x) = \sum_{uv\in E(G)} x^{d_u + d_v},$$

$$ZG_2(G,x) = \sum_{uv\in E(G)} x^{d_u d_v}.$$

where x is a dummy variable. The third Zagreb polynomial was first studied in [16] and defined as follows.

$$ZG_3(G,x) = \sum_{uv\in E(G)} x^{|d_u - d_v|}.$$

The nanostars dendrimers is a part of a new group of macromolecules that seem photon funnels just like artificial antennas and also is a great resistant of photo bleaching [17]. Recently some researchers investigated the mathematical properties of this nanostructures in [18-25]. Some applications of nanoscience and nanostructures can be referred in [26,27]

It is well-known that a graph can be described by a connection table, a sequence of numbers, a matrix, a polynomial or a derived number called a topological index, in this paper, we apply a polynomial approach to study the molecular graphs. In Refs. [15,16,28-30], the authors investigated the Zagreb polynomial of dendrimers, Cartesian product of graphs, thorn graphs, nanotubes and hydrocarbon structure. Motivated by these works, in this paper, we continue this program to compute a closed formulae for Zagreb polynomials of some nanostar dendrimers.

2. MAIN RESULTS

In this section, we shall compute the first, second and third Zagreb polynomial of some dendrimer nanostars. First, we compute the first, second and third Zagreb polynomial of type of dendrimer nanostars known as PAMAM dendrimer with trifunctional core unit by construction of dendrimers generations G_n with n growth stages. We denote simply this graph by $PD_1[n]$. Figure 1 shows PAMAM dendrimer $PD_1[n]$ of the generations G_n with three growth stages.

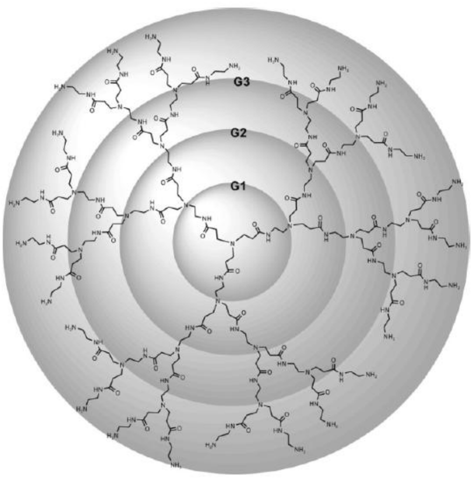

Figure 1. *PAMAM dendrimer of generations G_n with 3-growth stages, $PD_1[3]$.*

Let $D_{i,j}$ be the set of all edges connecting the vertices of degrees i and j, and define $D_{i,j} = \{e = uv \in E(G) | d_u = i$ and $d_v = j\}$. Let d_{ij} denote the number of edges connecting the vertices of degrees i and j, respectively. Thus $d_{i,j} = |D_{i,j}|$. Assume (*m*,*n*)-edge be the edge with end-vertices *m* and *n*.

Theorem 1. Let $PD_1[n]$ be PAMAM dendrimers with n growth of stages and $n = \{0,1,2,...\}$. Then, the first, second and third Zagreb polynomial of $PD_1[n]$ are given by

$$Z_1(PD_1[n],x) = (21 \times 2^n - 12)x^5 + (24 \times 2^n - 12)x^4 + (3 \times 2^n)x^3,$$

$$Z_2(PD_1[n],x) = (21 \times 2^n - 12)x^6 + (18 \times 2^n - 9)x^4 + (6 \times 2^n - 3)x^3 + (3 \times 2^n)x^2,$$

$$Z_3(PD_1[n],x) = (6 \times 2^n - 3)x^2 + (24 \times 2^n - 12)x + (18 \times 2^n - 9).$$

Proof. For nanostar $PD_1[n]$ which contributed (1,2), (1,3), (2,2) and (2,3)-edge, the formula of first, second and third of Zagreb polynomial is reduced to

$Z_1(PD_1[n],x) = d_{23}x^5 + [d_{13} +$ *d22x4+d12x3*,

$$Z_2(PD_1[n],x) = d_{23}x^6 + d_{22}x^4 + d_{13}x^3 + d_{12}x^2,$$

$$Z_3(PD_1[n],x) = d_{13}x^2 + [d_{12} + d_{23}]x + d_{22}.$$

Using simple calculation, one can show that $|V(PD_1[n])| = 12 \times 2^{n+2} - 23$ and $|E(PD_1[n])| = 12 \times 2^{n+2} - 24$. The edge set of the PAMAM dendrimers $PD_1[n]$ can be divided to four partitions in each step. So we have four types of edges d_{12}, d_{13}, d_{22} and d_{23}. The core of $PD_1[n]$ indicates the graph of the first stage, that is, $PD_1[n]$ $(n = 0)$ as depicted in Figure 2.

There are 3×2^n, $6 \times 2^n - 3$, $18 \times 2^n - 9$ and $21 \times 2^n - 12$ edges of types d_{12}, d_{13}, d_{22} and d_{23}, respectively. Table 1 shows the values of d_{ij} where $(i,j) = (1,2), (1,3), (2,2)$ and $(2,3)$ and $n = 0,1,2$. Therefore, we obtain

$Z_1(PD_1[n],x) = (21 \times 2^n - 12)x^5 + (24 \times 2^n - 12)x^4 + (3 \times 2^n)x^3$,
$Z_2(PD_1[n],x) = (21 \times 2^n - 12)x^6 + (18 \times 2^n - 9)x^4 + (6 \times 2^n - 3)x^3 + (3 \times 2^n)x^2$,
$Z_3(PD_1[n],x) = (6 \times 2^n - 3)x^2 + (24 \times 2^n - 12)x + (18 \times 2^n - 9)$.

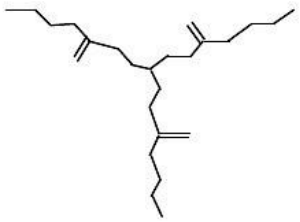

Figure 2. *The core of* $PD_1[0]$

Table 1. *The value of* d_{ij} *in* $PD_1[n]$ *where* $(i,j) = (1,2),(1,3),(2,2)$ *and* $(2,3)$ *and steps* $n = 0,1,2$.

Stage / $d_{i,j}$	0	1	2	3
$d_{1,2}$	3	6	12	24
$d_{1,3}$	3	9	21	45
$d_{2,2}$	9	27	63	135
$d_{2,3}$	9	30	72	156

This completes the proof. □

Now we shall consider the second type of PAMAM dendrimers with different core, denoted by $PD_2[n]$. The graph $PD_2[3]$ is shown in Figure 3.

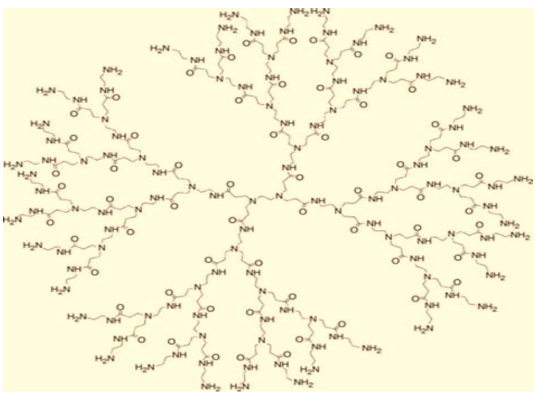

Figure 3. *PAMAM dendrimers with 3-growth stages,* $PD_2[3]$.

Theorem 2. Let $PD_2[n]$ be the PAMAM dendrimers with n growth of stages and $n = \{1,2,\dots\}$. Then, the first, second and third Zagreb polynomial of $PD_2[n]$ are given by

$$Z_1(PD_2[n],x) = (28 \times 2^n - 14\,)x^5 + (32 \times 2^n - 15)x^4 + (4 \times 2^n)x^3,$$
$$Z_2(PD_2[n],x) = (28 \times 2^n - 14)x^6 + (24 \times 2^n - 11)x^4 + (8 \times 2^n - 4)x^3 + (4 \times 2^n)x^2,$$
$$Z_3(PD_2[n],x) = (8 \times 2^n - 4)x^2 + (32 \times 2^n - 14)x + (24 \times 2^n - 11).$$

Proof. For nanostar $PD_2[n]$ which contributed (1,2), (1,3), (2,2) and (2,3)-edge, the formula of first, second and third of Zagreb polynomial is reduced to

$$Z_1(PD_2[n],x) = d_{23}x^5 + [d_{13} +$$
d22x4+d12x3,
$$Z_2(PD_2[n],x) = d_{23}x^6 + d_{22}x^4 + d_{13}x^3 + d_{12}x^2,$$
$$Z_3(PD_2[n],x) = d_{13}x^2 + [d_{12} + d_{23}]x + d_{22}.$$

Using simple calculation, one can show that $|V(PD_2[n])| = 16 \times 2^{n+2} - 28$ and $|E(PD_2[n])| = 16 \times 2^{n+2} - 29$. The edge set of the PAMAM dendrimers $PD_2[n]$ can be divided to four partitions in each step. So we have four types of edges d_{12}, d_{13}, d_{22} and d_{23}.
In general, there are 4×2^n, $8 \times 2^n - 4$, $24 \times 2^n - 11$ and $28 \times 2^n - 14$ edges of types d_{12}, d_{13}, d_{22} and d_{23}, respectively. Table 2 shows the values of d_{ij} where $(i,j) = (1,2),(1,3),(2,2)$ and $(2,3)$ and $n = 0,1,2$. Therefore, we obtain the result first, second and third Zagreb polynomial of $PD_2[n]$ as follows.
$Z_1(PD_2[n],x) = (28 \times 2^n - 14\,)x^5 + (32 \times 2^n - 15)x^4 + (4 \times 2^n)x^3$,
$Z_2(PD_2[n],x) = (28 \times 2^n - 14)x^6 + (24 \times 2^n - 11)x^4 + (8 \times 2^n - 4)x^3 + (4 \times 2^n)x^2$,
$Z_3(PD_2[n],x) = (8 \times 2^n - 4)x^2 + (32 \times 2^n - 14)x + (24 \times 2^n - 11)$.

Table 2. *The value of* d_{ij} *in* $PD_2[n]$ *where* $(i,j) = (1,2),(1,3),(2,2)$ *and* $(2,3)$ *and steps* $n = 1,2,3$.

$Stage$ \ $d_{i,j}$	1	2	3
$d_{1,2}$	8	16	32
$d_{1,3}$	12	28	60
$d_{2,2}$	37	85	181
$d_{2,3}$	42	98	210

This completes the proof. □

Now we consider another kind of dendrimer nanostars, namely tetrathiafulvalene dendrimer, denoted by $TD_2[n]$. The graph $TD_2[n]$ is shown in Figure 4.

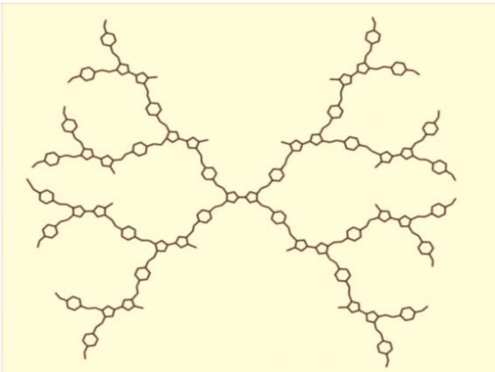

Figure 4. *Tetrathiafulvalene dendrimer with 2-growth stages,* $TD_2[2]$.

Theorem 3. Let $TD_2[n]$ be the tetrathiafulvalene dendrimer with n growth stages and $n = \{0,1,2,\dots\}$. Then, the first, second and third Zagreb polynomial of $TD_2[n]$ are given by

$Z_1(TD_2[n],x) = (8 \times 2^n - 5)x^6 + (96 \times 2^n -$

60x5+32×2n−20x4+4×2nx3,

$$Z_2(TD_2[n],x) = (8 \times 2^n - 5)x^9 + (96 \times 2^n - 60)x^6 + (28 \times 2^n - 16)x^4 + (4 \times 2^n - 4)x^3 + (4 \times 2^n)x^2,$$

$Z_3(TD_2[n],x) = (4 \times 2^n - 4)x^2 + (100 \times 2^n -$

60x+36×2n−21.

Proof. From the graph $TD_2[n]$ which contributes (1,2), (1,3), (2,2), (2,3) and (3,3)-edge, the formula of first, second and third of Zagreb polynomial is reduced to

$$Z_1(TD_2[n],x) = d_{33}x^6 + d_{23}x^5 + [d_{13} + d_{22}]x^4 + d_{12}x^3,$$
$$Z_2(TD_2[n],x) = d_{33}x^9 + d_{23}x^6 + d_{22}x^4 + d_{13}x^3 + d_{12}x^2,$$
$$Z_3(TD_2[n],x) = d_{13}x^2 + [d_{12} + d_{23}]x + d_{22} + d_{33}.$$

Using simple calculation, one can show that $|V(TD_2[n])| = 31 \times 2^{n+2} - 74$ and $|E(TD_2[n])| = 35 \times 2^{n+2} - 85$. The edge set of graph $TD_2[n]$ can be divided to three partitions in each step. So we have five types of edges d_{12}, d_{13}, d_{22}, d_{23} and d_{33}. The core of $TD_2[n]$ indicates the graph of the first stage, that is, $TD_2[n]$ $(n = 0)$ as depicted in Figure 5.
In general, there are 4×2^n, $4 \times 2^n - 4$, $28 \times 2^n - 16$, $96 \times 2^n - 60$ and $8 \times 2^n - 5$ edges of types d_{12}, d_{13}, d_{22}, d_{23} and d_{33}, respectively. Table 3 shows the values of d_{ij} where $(i,j) = (1,2), (1,3), (2,2), (2,3)$ and $(3,3)$ and $n = 0,1,2$. Therefore, we obtain the result for first, second and third Zagreb polynomial of $TD_2[n]$ as follows.

$Z_1(TD_2[n],x) = (8 \times 2^n - 5)x^6 + (96 \times 2^n -$

60x5+32×2n−20x4+4×2nx3,

$$Z_2(TD_2[n],x) = (8 \times 2^n - 5)x^9 + (96 \times 2^n - 60)x^6 + (28 \times 2^n - 16)x^4 + (4 \times 2^n - 4)x^3 + (4 \times 2^n)x^2,$$

$Z_3(TD_2[n],x) = (4 \times 2^n - 4)x^2 + (100 \times 2^n -$

60x+36×2n−21.

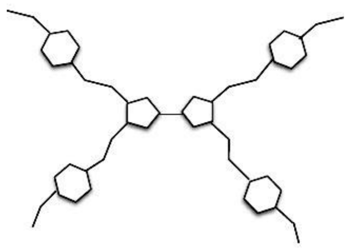

Figure 5. *The core of* $TD_2[0]$

Table 3. *The value of d_{ij} in $TD_2[n]$ where $(i,j) = (1,2), (1,3), (2,2), (2,3)$ and $(3,3)$ and steps $n = 0,1,2$.*

$Stage$ / $d_{i,j}$	0	1	2
$d_{1,2}$	4	8	16
$d_{1,3}$	0	4	12
$d_{2,2}$	12	40	96
$d_{2,3}$	36	132	324
$d_{3,3}$	3	11	27

Now the proof is complete. □

Let consider another type of dendrimer nanostars, denoted by $DS_1[n]$. Figure 6 shows that the graph $DS_1[n]$ of generation G_n with three growth stages.

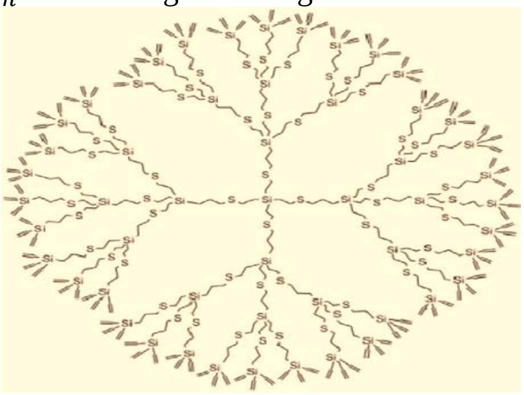

Figure 6. *Dendrimers nanostars $DS_1[n]$ of generation G_n with 3-growth stages*

Lastly, we consider POPAM dendrimers, denoted by $POD_2[n]$. Figure 7 shows that POPAM dendrimers $POD_2[n]$ of generation G_n with two growth stages.

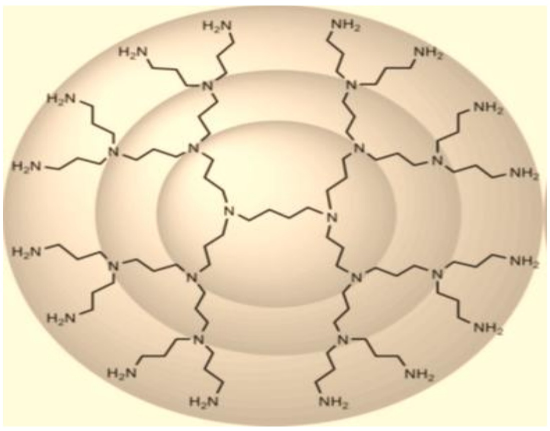

Figure 7. *POPAM dendrimer of generations G_n with 2-growth stages, $POD_2[2]$*

We can obtain the following results.

Theorem 4. Let $DS_1[n]$ be the dendrimer nanostars with n growth of stages and $n = \{0,1,2,\ldots\}$. Then, the first, second and third Zagreb polynomial of $DS_1[n]$ are given by

$$Z_1(DS_1[n], x) = (4 \times 3^n - 4)x^6 + (4 \times 3^n)x^5 + (10 \times 3^n - 10)x^4,$$
$$Z_2(DS_1[n], x) = (4 \times 3^n - 4)x^8 + (14 \times 3^n - 10)x^4,$$
$$Z_3(DS_1[n], x) = (4 \times 3^n)x^3 + (4 \times 3^n - 4)x^2 + (10 \times 3^n - 10).$$

Proof. Similar to the proofs of Theorems 1, 2 and 3. □

Theorem 5. Let $POD_2[n]$ be the dendrimer nanostars with n growth of stages and $n = \{0,1,2,\ldots\}$. Then, the first, second and third Zagreb polynomial of $POD_2[n]$ are given by

$$Z_1(POD_2[n], x) = (12 \times 2^n - 6)x^5 + (16 \times 2^n - 5)x^4 + (4 \times 2^n)x^3,$$

$$Z_2(POD_2[n], x) = (12 \times 2^n - 6)x^6 + (16 \times 2^n - 5)x^4 + (4 \times 2^n)x^2,$$

$$Z_3(POD_2[n], x) = (16 \times 2^n - 6)x + 16 \times 2^n - 5.$$

Proof. Similar to the proofs of Theorems 1, 2 and 3. □

3. CONCLUSION

In summary, in this paper, we have considered some families of dendrimers, namely, PAMAM, tetrathiafulvalene and POPAM dendrimers, and studied their topological polynomial. The closed formulas of the first, second and third Zagreb polynomial of these families of dendrimers are determined. In the future, we are interested to study and compute topological indices and polynomial of various families of dendrimers or nanostructures, in general.

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REFERENCES

1. Todeschini, R., Consonni, V., (2000). "*Handbook of Molecular Descriptor*", Wiley-VCH, Weinheim.
2. Trinajtic, N., (1992). "*Chemical Graph Theory*", CRC Press, Boca Raton, FL.
3. Dobrynin, A.A., Entringer, R., Gutman, I., (2011). "Wiener index of trees: Theory and applications", *Acta Appl.. Math.*, 66: 211-249.
4. Dobrynin, A.A., Gutman, I., Klavzar, S., Zigert, P., (2002). "Wiener index of hexagonal systems*", Acta Appl. Math*., 72: 247-294.
5. Wiener, H., (1947). "Structural determination of the paraffin boiling points", *J. Am. Chem. Soc*., 69: 17-20.
6. Gutman, I., Trijnastic, N., (1972). "Graph theory and molecular orbitals, Total π electron energy of alternant hydricarbons", *Chem. Phys. Lett.* 17: 535-538.
7. Braun, J., Kerber, A., Meringer, M., Rucker, C., (2005). "Similarity of molecular descriptors: the equivalent of Zagreb indices and walk counts", *MATCH Commun. Math. Comput. Chem*., 54(9): 163-176.
8. Das, K.C., Gutman, I., (2004). "Some properties of the second Zagreb index", *MATCH Commun. Math. Comput. Chem.*, 52: 103-112.
9. Gutman, I., Das, K.C., (2004). "The first Zagreb index 30 years after", *MATCH Commun. Math. Comput. Chem*., 50: 83-92.
10. Nikolic, S., Kovacevic, G., Milicevic, A., Trijnastic, N., (2003). "The Zagreb indices 30 years after", *Croat. Chem. Acta*., 76: 113-124.
11. Zhou, B., Gutman, I., (2004). "Relations between Wiener, hyper-Wiener and Zagreb indices", *Chem. Phys. Lett*., 394: 93-95.
12. Zhou, B., (2004). "Zagreb indices", *MATCH Commun. Math. Comput. Chem*., 52: 113-118.
13. Zhou, B., Gutman, I., (2005). "Further properties of Zagreb indices", *MATCH Commun. Math. Comput. Chem*., 54: 233-239.
14. Fath-Tabar, G.H., (2011). " Old and new Zagreb indices of graphs", *MATCH Commun. Math. Comput. Chem*., 65: 79-84.
15. Fath-Tabar, G.H., (2009). "Zagreb polynomial and PI indices of some nano-structure", *Dig. J. Nanomater. Bios*., 4: 189-191.
16. Astanesh-Asl, A., Fath-Tabar, G., (2011). "Computing the first and third Zagreb polynomial of Cartesian product of graphs", *Iranian J. Math. Chem* 2(2): 73-78.
17. Klajnert, B., Bryszewska, M., (2001), "Dendrimers: properties and applications", *Acta Biochim. Polonica*, 48: 199-208.
18. Ahmadi, M. B., Sadeghimehr, M., (2009). "Second order connectivity index of an infinite class of dendrimers nanostars", *Dig. J. Nanomater. Bios*. 4: 639-643.
19. Alikhani, S., Iranmanesh, M.A., (2010). "Chromatic polynomial of some dendrimers", *J. Comput. Theor. Nanosci.*, 7: 2314-2316.
20. Arif, N.E., Hasni, R., Alikhani, S., (2011). "Chromatic polynomials of certain families of dendrimer nanostars", *Dig. J. Nano. Biostr*., 6:1551-1556.
21. Ashrafi, A.R., Mirzargar, M., (2008). "PI Szeged and edge Szeged indices of an infinite family of nanostars dendrimers", *Indian J. Chem*., 47A: 538-541.
22. Dorostic, N., Iranmanesh, A., Diudea, M.V., (2009). "Computing the Cluj index of dendrimer nanostars", *MATCH Commun. Math. Comput. Chem*., 62: 389-395.
23. Iranmanesh, A., Gholami, N.A., (2009). "Computing the Szeged index of styrylbenzene dendrimer and triarilamine dendrimer of generation 1-3", *MATCH Commun. Math. Comput. Chem*. 62: 371-379.
24. Mirzagar, M., (2009). "PI, Szeged and edge Szeged polynomials of a dendrimers nanostars", *MATCH Commun. Math. Comput. Chem*., 62: 363-370.
25. Yousefi-Azari, H., Ashrafi, A.R., Baharin, A., Yazdani, Y., (2008). "Computing topological indices of some types of benzenoid systems and nanostars", *Asian J. Chem*. 20: 15-20.
26. Rahmani, S., Mahmooudifard, M., Safi, M., (2014). "Protecting surfaces using one-dimensional nanostructures", *Int. J. Nanosci. Naotechnol*., 10(1): 61-66.
27. Jafarbeglou, M., Abdouss, M., Ramezanianpour, A.A., (2015). "Nanoscience and nano engineering in concrete advances a review", *Int. J. Nanosci. Naotechnol*., 11(4): 263-273.

28. Farahani, M.R., (2014). "First and second Zagreb polynomial of VC_5C_7[p,q] and HC_5C_7[p,q] nanotubes", *Int. Lett. Chem. Phys. Astr.*, 12: 56-62.
29. Farahani, M.R., (2013). "Zagreb indices and Zagreb polynomial of polycyclic aromatic hydrocarbona PAHs, *J. Chem. Acta*, 2: 70-72.
30. Li, S., (2011). "Zagreb polynomial of thorn graphs", *Kragujevac J. Sci*., 33: 33-38.