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Reduced Forgotten Topological Indices of some Dendrimers Structures

A. Subhashini and J. Baskar Babujee
Department of Mathematics, MIT Campus
Anna University, Chennai - 600 044
E-mail : subhachelvan2015@gmail.com, baskarbabujee@yahoo.com

Abstract : In computational chemistry, the molecular structures are modeled as graphs which are called the molecular graphs.A massive of early drug tests implies that there exist strong inner relationships between the bio-medical and pharmacology characteristics of drugs and their molecular structures. Dendrimers are highly branched nanostructures and are considered a building block in nanotechnology with a variety of suitable applications. Chemical graph theory is a branch of mathematical chemistry in which different tools from graph theory are used to model chemical phenomena mathematically. Dendrimers have a very well-defined chemical structure with three major architectural components. Dendrimers are considered one of the most important, commercially available building blocks in nanotechnology. A topological index can be considered as the transformation of chemical structure into a real number. Dendrimers are highly-branched star-shaped macromolecules with nanometer-scale dimensions. Dendrimers are defined by three components: a central core, an interior dendritic structure (the branches), and an exterior surface with functional surface groups. In this paper, we determine Reduced Forgotten Topological indices of poly(propyl) ether imine, porphyrin, and zinc-porphyrin dendrimers.

Keywords and phrases : Topological index, Molecular graph, Degree Dendrimers.

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Introduction : Molecules and molecular compounds are often modeled by molecular graphs. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. In the chemical literature, several dozens of vertex-degree-based topological indices have been and are currently considered and applied in QSPR/QSAR studies. Graph theory is used to model molecules mathematically in order to gain insight into the physical properties of these

chemical compounds. The basic idea of chemical graph theory is that physico-chemical properties of molecules can be studied by using the information encoded in their corresponding chemical graphs.

A graph invariant is any function on a graph that does not depend on a labeling of its vertices. Such quantities are called topological indices. Zagreb indices belongs among the best investigated topological indices, but their properties and chemical applications were always studied for case of ordinary chemical graphs. A topological index for a(chemical) graph G is a numerical quantity invariant under automorphisms of G and it does not depend on the labeling or pictorial representation of the graph. A topological index is a real number associated with a graph which characterizes the topology of the graph and is invariant under graph isomorphism. There are many distance or degree based topological indices. Degree based topological indices are of great importance and play a vital role in chemical graph theory [3-13].

Let G be a molecular graph with vertex set $V(G)$ and edge set $E(G)$. If u and v are two adjacent vertices of G, then the edge connecting them will be denoted by uv.

By $\deg(v)$ we denote the degree (=number of first neighbors) of the vertex v of the graph G.

There are two Zagreb indices [1,2]: the first M_1 and the second M_2, defined as

$$M_1 = M_1(G) = \sum_{v \in V(G)} \deg(v)^2 \text{ and } M_2 = M_2(G) = \sum_{uv \in E(G)} \deg(u)\deg(v) \text{ respectively.}$$

The first Zagreb index can be rewritten also as $M_1 = M_1(G) = \sum_{uv \in E(G)} [\deg(u) + \deg(v)]$.

With this notation, the Forgotten Topological index is defined as [14]

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

The Forgotten topological index involving the number of vertices, edges, and maximum and minimum vertex degree.They named this index as "Forgotten Topological index" or "F-index"[15-17]. Topological indices are abundantly being used in the QSPR and QSAR researches. So far, many various types of topological indices have been described.

The Reduced Second Zagreb index is defined as [22]

$$RM_2 = RM_2(G) = \sum_{ij \in E(G)} (d_i - 1)(d_j - 1).$$

Because of the identity $RM_2(G) = M_2(G) - M_1(G) + m$.

In [23] A.Subhashini and J. Baskar Babujee introduced ,

Reduced forgotten topological index as $RF = RF(G) = \sum_{uv \in E(G)} [(d(u)-1)^2 + (d(v)-1)^2]$

Analogous to other topological polynomials, the RF-polynomial of graph G is also defined as: $RF(G,x) = \sum_{uv \in E(G)} x^{[(d(u)-1)^2 + (d(v)-1)^2]}$

In this paper, we determine RF-index and polynomial of poly(propyl) ether imine, porphyrin, and zinc–porphyrin dendrimers.

2. RF-Index and Polynomial of Poly (Propyl) Ether Inline Dendrimer :

Polynomial of Poly(Propyl) Ether Imine (PETIM) dendrimer starts growing three dimensionally from the oxygen as the core and branches out at each tertiary nitrogen, which is separated by eight-bond spacer for each generation of the dendrimer. Consider the molecular graph G of PETIM dendrimer of generation G_n with n growth stages,

where $n \geq 1$ (see Figure 1). The graph of PETIM dendrimer consists of four branches and a central core consisting of eight edges. In each branch, we have $8 + 2\times 8 + 2^2 \times 8 + ... + 2^{n-2} \times 8 + 4\times 2^{n-1} = 6\times 2^n - 8$ edges. The total number of edges in G are $24\times 2^n - 24$. Since G is a tree, it follows directly that the number of vertices of G are $24\times 2^n - 23$.

In G, the total number of vertices of degree 1 are the leaves, which are $4\times 2^{n-1} = 2^{n+1}$ in number. The vertices of degree 3 are $4(1 + 1\times 2 + 1\times 2^2 + ... + 1\times 2^{n-2}) + 2 = 2^{n+1} - 2$. The remaining $24\times 2^n - 23 - (2^{n+1} - 2) - 2^{n+1} = 20\times 2^n - 21$ vertices are of degree 2.

Let e_{ij} denote the number of edges of G connecting vertices of degrees i and j. Clearly, $e_{ij} = e_{ji}$. Let us denote the number of edges connecting vertices of degrees i and j in each branch of the dendrimer by e'_{ij}. The central core consists of six edges e_{ij} with $i = j = 2$ and two edges e_{ij} with $i = 2$ and $j = 3$. Then, we have $e_{12} = 4e'_{12}, e_{22} = 4e'_{22} + 6$ and $e_{23} = e'_{23} + 2$. For $n > 1$,

We can calculate $e'_{12} = 2^{n-1}, e'_{22} = (6 + 2\times 6 + ... + 2^{n-2} \times 6) + 2\times 2^{n-1} - 4\times 2^n - 6$,

$e'_{23} = 6\times 2^n - 8 - 2^{n-1} - (4\times 2^n - 6) = 3\times 2^{n-1} - 2$.

Therefore, we have, $e_{12} = 2^{n-1}, e_{22} = 16\times 2^n - 18, e_{23} = 6\times 2^n - 6$. Now, we compute Reduced Forgotten index and polynomial for the poly(propyl) ether imine (PETIM) dendrimer in the following theorem.

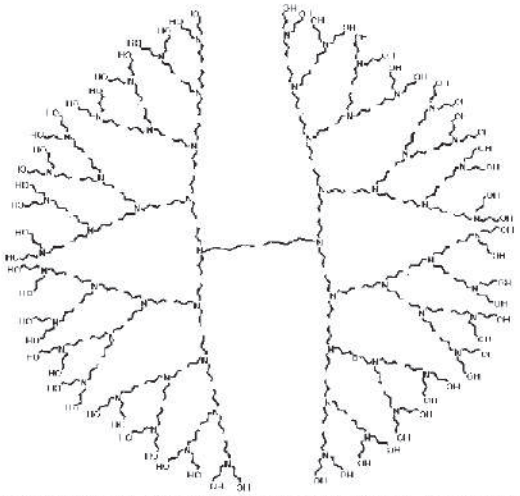

Figure 1. Molecular structure of poly(propyl) ether imine (PETIM) dendrimer with n = 5.

Dendrimers are constructed by hyper branched macromolecules with a fully-tailored architecture. They can be arranged in a composed manner by either convergent or divergent form. Dendrimers have a huge range of applications in all branches of chemistry, especially in host-guest reactions and self-assembly procedures. Dendrimers are used in the formation of nanotubes, nanolatex, chemical sensors, micro/macro capsules, coloured glass, modified electrodes, and photon funnels such as artificial antennas [18]. Because dendrimers are widely used in different applied fields, the study of nanostar dendrimers has received a great deal of attention in both chemical and mathematical literature. For other different applications regarding dendrimers, we refer to [19,20]. Thus, we have been attracted to studying the mathematical properties of the RF-index and its polynomial version of some dendrimers. In order to find the number of edges of the arbitrary graph, the following lemma is used.

Let G be a graph. Then $\sum_{v\in V(G)} d_v = 2|E|$

Theorem 2.1:

Let G be the molecular graph of PETIM dendrimer. Then $RF(G) = 64\times 2^n - 66$.

$RF(G,x) = 2^{n+1}x + (16\times 2^n - 18)x^2 + (6\times 2^n - 6)x^5$.

Theorem 2.1:

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$RF(G,x) = 2^{n+1}x + (16\times 2^n - 18)x^2 + (6\times 2^n - 6)x^5$.

Proof:

Let G be a graph of PET IM dendrimer. The vertex set $V(G)$ is divided into three sets based on the degree of the vertices.

The first vertex set $V_1(G)$ consists of 2^{n+1} vertices of degree 1.

The second vertex set $V_2(G)$ consists of $20\times 2^n - 21$ vertices of degree 2.

The third vertex set $V_3(G)$ consists of $2^{n+1} - 2$ vertices of degree 3.

From (1), The RF-index of G is given by

$$RF = RF(G) = \sum_{uv\in E(G)} [(d(u)-1)^2 + (d(v)-1)^2].$$

$$= \sum_{uv\in E_1(G)} [(d(u)-1)^2 + (d(v)-1)^2] + \sum_{uv\in E_2(G)} [(d(u)-1)^2 + (d(v)-1)^2] + \sum_{uv\in E_3(G)} [(d(u)-1)^2 + (d(v)-1)^2]$$

Similarly, the edge partitions of G, based on the degree of end vertices, are defined as
$E_1(G) = \{e = uv \in E(G) : d_u = 1, d_v = 2\}$,
$E_2(G) = \{e = uv \in E(G) : d_u = d_v = 2\} and$
$E_3(G) = \{e = uv \in E(G) : d_u = 2, d_v = 3\}$.

Therefore, we have $|E_1(G)| = 2^{n+1}, |E_2(G)| = 16\times 2^n - 18, |E_3(G)| = 6\times 2^n - 6$.

The RF-polynomial of G is calculated as

$$RF(G,x) = \sum_{uv\in E_1(G)} x + \sum_{uv\in E_2(G)} x^2 + \sum_{uv\in E_3(G)} x^5.$$

$$= 2^{n+1}x + (16\times 2^n - 18)x^2 + (6\times 2^n - 6)x^5.$$

3. RF-Index and Polynomial of Porphyrin Dendrimers

We consider the class of porphyrin dendrimers, denoted by D_nP_n. Note that $n = 2^m$, where $m \geq 2$ is steps of growth (see Figure 2). The molecular graph of D_nP_n has

four similar branches and a central core consisting of five extra edges (Figures 2 and 3). In each branch of D_nP_n, we have $4+2\times4+2^2\times4+...+2^{m-2}\times4+2^{m-2}\times88=24n-4$ vertices, among which $2^{m-2}\times26$ vertices are of degree 1, $3+2\times3+...+2^{m-2}\times3+2^{m-2}\times28=17\times2^{m-1}-3$ vertices are of degree 2, $8\times2^{m-2}$ vertices are of degree 4, and the remaining $24n-4-2^{m-2}\times26-(17\times2^{m-1}-3)-8\times2^{m-2}=7n-1$ vertices are of degree 3. Additionally, the central core contains four vertices of degree 2 and two vertices of degree 3. Therefore, in D_nP_n, there are a total of $96n-10$ vertices, among which $26n$ vertices are of degree 1, $34n-8$ vertices are of degree 2, $28n-2$ vertices are of degree 3, and the remaining $8n$ vertices are of degree 4. It is easy to see from Lemma (1) that the total number of edges of D_nP_n are $105n-11$.

Since the molecular graph of D_nP_n has four similar branches and five extra edges (Figures 2 and 3) in which we have

$e_{13}=4e_{13}^{'},e_{14}=4e_{14}^{'},e_{22}=4e_{22}^{'}+3,e_{23}^{'}=4e_{23}^{'}+2,e_{33}=4e_{33}^{'},e_{34}=4e_{34}^{'}$.

To compute $e_{13}=2n,e_{14}=24n,e_{22}=10n-5,e_{23}=48n-6,e_{33}=13n,e_{34}=8n$..

Now, we compute the RF-index and polynomial of this type of dendrimer through the following theorem.

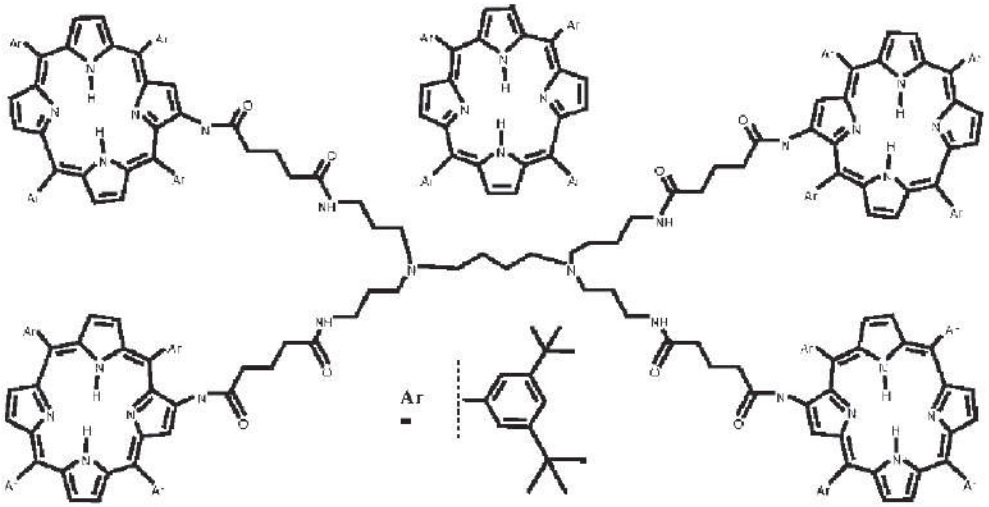

Figure 2. Molecular structure of porphyrin dendrimer D_4P_4 .

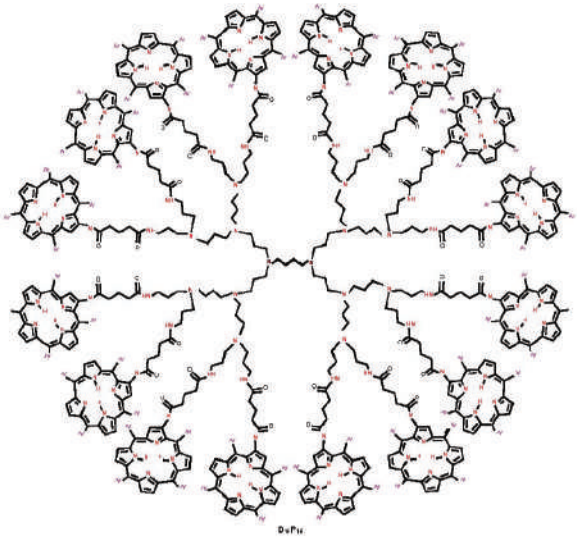

Figure 3. Molecular structure of porphyrin dendrimer $D_{16}P_{16}$.

Theorem 3.1:

Let D_nP_n be a Porphyrin dendrimer. Then $RF(D_nP_n) = 692n - 40.$

$$RF(D_nP_n, x) = 2nx^4 + 24nx^9 + (10n-15)x^2 + (48n-6)x^5 + 13nx^8 + 8nx^{13}.$$

Proof:

Let G be a graph of D_nP_n Porphyrin dendrimer.

Using definitions of RF index and RF-Polynomial, We have

$$RF(D_nP_n) = 2n\times 4 + 24n\times 9 + (10n-5)2 + (48n-6)5 + 13n\times 8 + 8n\times 13.$$
$$= 8n + 216n + 20n - 10 + 240n - 30 + 104n + 104n.$$
$$= 692n - 40.$$

The RF-polynomial of G is calculated as
$RF(D_nP_n, x) = 2nx^4 + 24nx^9 + (10n-15)x^2 + (48n-6)x^5 + 13nx^8 + 8nx^{13}.$

4 . RF-Index and Polynomial of Zinc–Porphyrin Dendrimer

We consider the class of dendrimer zinc–porphyrin DPZ_n (see Figure 4), where n is the steps of growth and $n \geq 1$. The molecular graph of DPZ_n consists of four similar branches and a central core. It is easy to see that the central core of DPZ_n consists of 49

vertices among which 24 vertices are of degree two and three respectively, and one vertex of degree four. In each branch of DPZ_n, we have

$14+2\times14+...+2^{n-1}\times14=14(2^n-1)$ vertices, among which

$9+2\times+...+2^{n-2}\times9+2^{n-1}\times11=11\times2^n-9$ vertices are of degree two and the remaining $14(2^n-1)-(11\times2^n-9)=3\times2^n-5$ vertices are of degree three. Therefore, in DPZ_n there are a total of $56\times2^n-7$ vertices, among which $44\times2^n-12$ vertices are of degree 2, $12\times2^n+4$ vertices are of degree 3, and the remaining 1 vertex is of degree 4.From Lemma (1) that the total number of edges of DPZ_n are $64\times2^n-4$. Additionally, we can calculate $e_{22}=16\times2^n-4, e_{23}=40\times2^n-16, e_{33}=8\times2^n+12$ and $e_{34}=4$.Now, we compute the RF-index and polynomial of zinc–porphyrin dendrimer as shown in Figure 4.

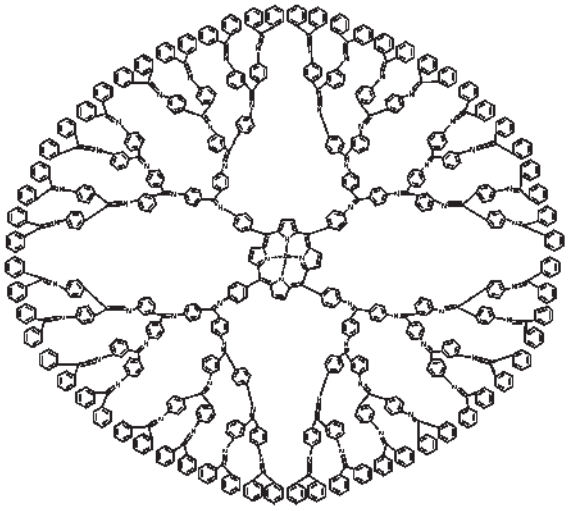

Figure 4. Molecular structure of dendrimer zinc porphyrin DPZ4.

Theorem 4.1:

Let DPZ_n be a zinc–porphyrin dendrimer. Then $RF(DPZ_n)=304\times2^n-4$.

$RF(DPZ_n,x)=(16\times2^n-4)x^4+(40\times2^n-16)x^5+(8\times2^n+12)x^4+4x^{13}$.

Proof:

Let G be a graph of DPZ_n be a zinc–porphyrin dendrimer.

Using definitions of RF index and RF-Polynomial, We have

$$RF(DPZ_n) = 2^n[32+240+32]-96-8+48+52.$$

$$= 304\times 2^n - 4.$$

$$RF(DPZ_n, x) = (16\times 2^n - 4)x^4 + (40\times 2^n - 16)x^5 + (8\times 2^n + 12)x^4 + 4x^{13}.$$

5. Conclusion

In this paper, we find with three dendrimer families and studied RF-index and RF-polynomial on these molecular structures which will be helpful in computational chemistry. Moreover, we have also computed the edge partition of each dendrimer structure based on end vertices of each edge, which can be used to compute many other topological indices, as computed in [18].

Abbreviations

The following abbreviations are used in this manuscript:

PETIM Poly(Propyl) Ether Imine

D_nP_n Porphyrin dendrimers

DPZ dendrimer Zinc-Porphyrin

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