Research Article

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Some topological indices of dendrimers determined by their Banhatti polynomials

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Abstract: Several properties of chemical compounds in a molecular structure can be determined with the aid of mathematical languages provided by various types of topological indices. In this paper, we consider eight dendrimer structures in the context of valency based topological indices. We define four Banhatti polynomials for general (molecular) graphs, and compute them for underline dendrimers. We use these polynomials to determine four Banhatti indices. We also determine Zagreb (first, second and hyper) and forgotten indices by developing their relationships with Banhatti indices.

Keywords: Valency, topological index, Banhatti indices, Banhatti polynomials, dendrimers

AMS: 05C09; 05C92

Introduction

The structural formula of molecules and molecular compounds is represented as a molecular graph $\mathcal{M}$ in chem-

ical graph theory, where nodes (vertices) are atoms and links (edges) between atoms are atom-bonds. We denote the collection of all the atoms in $\mathcal{M}$ by $A(\mathcal{M})$ and the collection of all the atom-bonds in $\mathcal{M}$ by $B(\mathcal{M})$. The number of atom-bonds in $\mathcal{M}$ is called the size of $\mathcal{M}$, and we denote it by $S(\mathcal{M})$. An atom-bond $\epsilon = ab$ between two atoms a and b of $\mathcal{M}$ is said to be incident with both the atoms and vice-versa, and this incidence is written as $a\epsilon$ (or $b\epsilon$). The valency (degree) of an atom a in $\mathcal{M}$ is the number of atom-bonds incident with a , and we symbolize it as v_a . The valency of an atom-bond $\epsilon = ab \in B(\mathcal{M})$ can be computed by the formula $v_\epsilon = v_a + v_b - 2$. Throughout this paper, the notation $\alpha \sim \beta$ will represent the type of an atom-bond whose incident atoms have valencies α and β , and therefore the valency of that atom-bond should be $\alpha + \beta - 2$ accordingly. Whenever the size, $S(\mathcal{M})$, of a molecular graph $\mathcal{M}$ is to be found, we use the following formula provided by the well known hand shake lemma. [10]

$$\sum_{a \in A(\mathcal{M})} v_a = 2S(\mathcal{M}). \quad (1)$$

Combinatorics and chemical graph theory play a significant role to study and characterize molecular structures, spectroscopy, and quantum chemistry [4, 7]. In a newly developed field, called cheminformatics (a combination of chemistry, information and mathematics), qualitative structure activity/property relationships (QSAR) together with topological indices play a vital role for studying molecular compounds with chemical properties of their bioactivities. For such kind of studies, mathematicians and chemists are using several types of topological indices defined on the base of valency of atoms/atom-bonds, and defined on the base of distance (the number of atom-bonds lying in a shortest path) between atoms of a molecular graph. A numerical quantity which captures the symmetry of a molecular structure is known as a topological index. In fact, a topological index is a numerical characterization of a chemical graph and provides a mathematical function of the structure in QSAR studies. There are several valency based topological indices introduced to test the properties of compounds and drugs; such as

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viscosity, the gyration radius, boiling point and many more [27]. In this paper, our aim is to study some valency based topological indices with the correlation of Banhatti indices. The valency based topological indices, which we consider, are defined as follows: In 1972, Gutman and Trinajstić [14] defined first and second Zagreb indices by the following formulae:

$$Z_1(\mathcal{M}) = \sum_{ab \in B(\mathcal{M})} (v_a + v_b) \text{ and } Z_2(\mathcal{M}) = \sum_{ab \in B(\mathcal{M})} (v_a \times v_b). \quad (2)$$

Another novel form of Zagreb indices, called the hyper Zagreb index, were defined by Shirdel et al. [25] as follows:

$$HZ(\mathcal{M}) = \sum_{ab \in B(\mathcal{M})} (v_a + v_b)^2. \quad (3)$$

A few years ago, in 2015, another important valency based topological index, called the forgotten index, was introduced and studied by Furtula and Gutman [12]. It can be computed by the formula

$$F(\mathcal{M}) = \sum_{ab \in B(\mathcal{M})} (v_a^2 + v_b^2). \quad (4)$$

In 2016, the computation of valency based topological indices with the aid of valency of atom-bonds (edges) was initiated by Kulli [17]. He introduced four Banhatti indices, which are defined as follows:

- First and second K Banhatti indices, respectively, are:

$$B_1(\mathcal{M}) = \sum_{a\epsilon} (v_a + v_\epsilon) \text{ and } B_2(\mathcal{M}) = \sum_{a\epsilon} (v_a \times v_\epsilon). \quad (5)$$

- First and second K hyper Banhatti indices, respectively, are:

$$HB_1(\mathcal{M}) = \sum_{a\epsilon} (v_a + v_\epsilon)^2 \text{ and } HB_2(\mathcal{M}) = \sum_{a\epsilon} (v_a \times v_\epsilon)^2. \quad (6)$$

An extension in the theory of Banhatti indices was initiated when, in the same year 2016, Kulli defined and determined multiplicative K Banhatti indices [20]. Further extension to this theory was made in 2017 when Kulli et al. defined and computed connectivity K Banhatti indices including K harmonic Banhatti and multiplicative K harmonic Banhatti indices [16]. For more detail and theory about Banhatti indices, we refer the articles in [2, 5, 16–20, 24].

A huge amount of valency based topological indices and polynomials, defined and studied by various researchers, can be found in the literature (see [1, 3, 6, 8, 13, 21, 22, 26] and the references therein). In this paper, our first aim is to further extend the theory of Banhatti indices

by defining four Banhatti polynomials. Moreover, we establish a few relationships of Banhatti indices, defined in (5) and (6), with the indices provided in (2), (3) and (4). Our second aim is to compute those valency based topological indices which can be determined by using the established relationships. Accordingly, we determine four Banhatti indices together with Zagreb (first, second and hyper) and forgotten indices for a few dendrimer structures with their exact values.

Banhatti polynomials and some relationships

Similar to other topological polynomials such as M-polynomial, Zagreb polynomials, forgotten polynomial, Hosoya polynomials and many more, we define K Banhatti polynomials as follows:

- First and second K Banhatti polynomials with variable x , respectively, are:

$$B_1(\mathcal{M}, x) = \sum_{a\epsilon} x^{(v_a + v_\epsilon)} \text{ and } B_2(\mathcal{M}, x) = \sum_{a\epsilon} x^{(v_a \times v_\epsilon)}. \quad (7)$$

- First and second K hyper Banhatti polynomials with variable x , respectively, are:

$$HB_1(\mathcal{M}, x) = \sum_{a\epsilon} x^{(v_a + v_\epsilon)^2} \text{ and } HB_2(\mathcal{M}, x) = \sum_{a\epsilon} x^{(v_a \times v_\epsilon)^2}. \quad (8)$$

Clearly, by taking the first derivative of these polynomials at $x = 1$, we get the corresponding Banhatti indices. Now, for a molecular graph $\mathcal{M}$, the relationships of Banhatti indices with Zagreb and forgotten indices are established as follows:

$$\blacktriangleright 3Z_1(\mathcal{M}) = B_1(\mathcal{M}) + 4S(\mathcal{M}) \quad (9)$$

According to the formula of the first K Banhatti index from (5), we have

$$\begin{aligned} B_1(\mathcal{M}) &= \sum_{\epsilon=ab \in B(\mathcal{M})} [(v_a + v_\epsilon) + (v_b + v_\epsilon)] \\ &= \sum_{ab \in B(\mathcal{M})} [v_a + v_b + 2(v_a + v_b - 2)] \\ &= \sum_{ab \in B(\mathcal{M})} [3(v_a + v_b) - 4] \\ &= 3Z_1(\mathcal{M}) - 4S(\mathcal{M}) \quad \text{by using (2)} \end{aligned}$$

Hence, we get the required relation.

$$\blacktriangleright F(\mathcal{M}) = B_2(\mathcal{M}) + 2(Z_1(\mathcal{M}) - Z_2(\mathcal{M})) \quad (10)$$

According to the formula of second K Banhatti index from (5), we have

$$\begin{aligned} B_2(\mathcal{M}) &= \sum_{\epsilon=ab \in B(\mathcal{M})} [(v_a \times v_\epsilon) + (v_a \times v_\epsilon)] \\ &= \sum_{ab \in B(\mathcal{M})} [v_a \times (v_a + v_b - 2) + v_b \times (v_a + v_b - 2)] \\ B_2(\mathcal{M}) &= \sum_{ab \in B(\mathcal{M})} [v_a^2 + v_b^2 + 2(v_a \times v_b) - 2(v_a + v_b)] \quad (11) \\ B_2(\mathcal{M}) &= F(\mathcal{M}) + 2Z_2(\mathcal{M}) - 2Z_1(\mathcal{M}) \quad \text{by using (2) \& (4)} \quad (12) \end{aligned}$$

Hence, we get the required relation.

$$\blacktriangleright HZ(\mathcal{M}) = B_2(\mathcal{M}) + 2Z_1(\mathcal{M}) \quad (13)$$

From Equation (11), we have

$$\begin{aligned} B_2(\mathcal{M}) &= \sum_{ab \in B(\mathcal{M})} [(v_a + v_b)^2 - 2(v_a + v_b)] \\ &= HZ(\mathcal{M}) - 2Z_1(\mathcal{M}) \quad \text{by using (2) \& (3)} \end{aligned}$$

Hence, we get the required relation.

$$\blacktriangleright 2(Z_1(\mathcal{M}) + Z_2(\mathcal{M})) = 5B_2(\mathcal{M}) - HB_1(\mathcal{M}) + 8S(\mathcal{M}) \quad (14)$$

According to the formula of the first K hyper Banhatti index from (6), we have

$$\begin{aligned} HB_1(\mathcal{M}) &= \sum_{\epsilon=ab \in B(\mathcal{M})} [(v_a + v_\epsilon)^2 + (v_b + v_\epsilon)^2] \\ &= \sum_{ab \in B(\mathcal{M})} [(v_a + (v_a + v_b - 2))^2 + (v_b + (v_a + v_b - 2))^2] \\ &= \sum_{ab \in B(\mathcal{M})} [v_a^2 + v_b^2 + 8(v_a \times v_b) - 12(v_a + v_b) + 8] \\ HB_1(\mathcal{M}) &= 5F(\mathcal{M}) + 8Z_2(\mathcal{M}) - 12Z_1(\mathcal{M}) + 8S(\mathcal{M}) \\ &\quad \text{by using (2) \& (4)} \quad (15) \end{aligned}$$

By performing the operation “Equation (15)–5×Equation (12)”, we get the required relation.

Dendrimers

Dendrimers are molecular structures which are built symmetrically by attaching to a central core the layers of macromolecules branches with successive increments. In 1978, Buhleier et al. constructed the first dendrimers structure using the approach of synthesis divergence [9]. It has been found in the literature that dendrimers play a significant role in the fields of chemistry, biology and

nanosciences [11]. Due to wide range of expediency, dendrimers attracted many researchers to investigate remarkable foundations upon them. In the context of topological indices, researchers dealt with dendrimers in the following ways (listed few): Szeged topological indices were determined by Ashrafi et al. [6]; atom-bond connectivity index was computed by Alikhani et al. [1]; M-polynomial and related indices were investigated by Munir et al. [23]; computation of forgotten polynomial and index was due to the work done by Bashir et al. [8]; and some novel valency based indices were computed by Kang et al. [15]. Attracted by these remarkable works done for dendrimers, we consider eight dendrimers, from a huge family of various types of dendrimers, in the context of valency based topological polynomials and indices defined in sections 1 and 2. The intention to consider only these eight dendrimers is their structural symmetry and simplicity. Moreover, generations growth in these dendrimers is easily understandable to partition the atom-bonds into different parts according to their valency types, which is a necessary part to compute the underline topological indices.

Poly(propyl) ether imine dendrimer

Our first molecular graph $\mathcal{M}_1$ is the poly (propyl) ether imine (PETIM) dendrimer of generation G_η with $\eta \geq 1$ growth stage. $\mathcal{M}_1$ consists of 4 branches and one central core. The central core contains 7 atoms of valency 2, 2 atoms of valency 3 and 8 atom-bonds as shown in Figure 1. In one branch of $\mathcal{M}_1$, there are $8 + 2 \cdot 8 + 2^2 \cdot 8 + \dots + 2^{\eta-2} \cdot 8 + 2^{\eta-1} \cdot 4 = 12 \cdot 2^{\eta-1} - 8$ atoms, among them $2^{\eta-1}$ atoms are of valency 1; $2^0 + 2^1 + 2^2 + \dots + 2^{\eta-1} + 2^\eta = 2 \cdot 2^\eta - 1$ atoms are of valency 3; and the remaining $12 \cdot 2^{\eta-1} - 8 - 2^{\eta-1} - 2^{\eta-1} + 1 = 7 \cdot 2^{\eta-1} - 7$ atoms are of valency 2. Therefore, in $\mathcal{M}_1$, there are total $24 \cdot 2^\eta - 23$ atoms; among them $2 \cdot 2^\eta$ atoms are of valency 1; $20 \cdot 2^\eta - 21$ atoms are of valency 2; and $2 \cdot 2^\eta - 2$ atoms are of valency 3. The number of atom-bonds in $\mathcal{M}_1$ is $24 \cdot 2^\eta - 24$, by formula (1). According to the valencies of atoms incident with each atom-bond, there are three types $1 \sim 2$, $2 \sim 2$ and $2 \sim 3$ of atom-bonds in $\mathcal{M}_1$. Equivalently, the atom-bonds set of $\mathcal{M}_1$ is partitioned as $B(\mathcal{M}_1) = B_{1 \sim 2} \cup B_{2 \sim 2} \cup B_{2 \sim 3}$, where $B_{1 \sim 2} = \{\epsilon = ab \in B(\mathcal{M}_1) \mid v_a = 1, v_b = 2 \wedge v_\epsilon = 1\}$ with $|B_{1 \sim 2}| = 2 \cdot 2^\eta$, $B_{2 \sim 2} = \{\epsilon = ab \in B(\mathcal{M}_1) \mid v_a = 2, v_b = 2 \wedge v_\epsilon = 2\}$ with $|B_{2 \sim 2}| = 16 \cdot 2^\eta - 18$, $B_{2 \sim 3} = \{\epsilon = ab \in B(\mathcal{M}_1) \mid v_a = 2, v_b = 3 \wedge v_\epsilon = 3\}$ with $|B_{2 \sim 3}| = 6 \cdot 2^\eta - 6$.

Figure 1 Poly (propyl) ether imine dendrimer

Using this partition in the formula of the first K Banhatti polynomial from (7), we have:

$$B_1(\mathcal{M}_1, x) = \left(\sum_{\epsilon=ab \in B_{1 \sim 2}} + \sum_{\epsilon=ab \in B_{2 \sim 2}} + \sum_{\epsilon=ab \in B_{2 \sim 3}} \right) x^{(v_a + v_\epsilon)}$$

$$= 2 \cdot 2^\eta x^5 + (16 \cdot 2^\eta - 18)x^8 + (6 \cdot 2^\eta - 6)x^{11}.$$

Analogously, using the atom-bonds partition in formulae of the other three Banhatti polynomials from (7) and (8), it can be found that

$$B_2(\mathcal{M}_1, x) = 2 \cdot 2^\eta x^3 + (16 \cdot 2^\eta - 18)x^8 + (6 \cdot 2^\eta - 6)x^{15},$$

$$HB_1(\mathcal{M}_1, x) = 2 \cdot 2^\eta x^{13} + (16 \cdot 2^\eta - 18)x^{32} + (6 \cdot 2^\eta - 6)x^{61},$$

$$HB_2(\mathcal{M}_1, x) = 2 \cdot 2^\eta x^5 + (16 \cdot 2^\eta - 18)x^{32} + (6 \cdot 2^\eta - 6)x^{117}.$$

With respect to x , by taking the first derivative of these polynomials at $x = 1$, we get the following K Banhatti indices of $\mathcal{M}_1$.

$$TI(\mathcal{M}_1) = \begin{cases} 204 \cdot 2^\eta - 210 & , \text{ when } TI \text{ is } B_1, \\ 224 \cdot 2^\eta - 234 & , \text{ when } TI \text{ is } B_2, \\ 904 \cdot 2^\eta - 942 & , \text{ when } TI \text{ is } HB_1, \\ 1224 \cdot 2^\eta - 1278 & , \text{ when } TI \text{ is } HB_2. \end{cases}$$

Using relationships (9), (10), (13) and (14), we get the following Zagreb and forgotten indices of $\mathcal{M}_1$.

$$TI(\mathcal{M}_1) = \begin{cases} 100 \cdot 2^\eta - 102 & , \text{ when } TI \text{ is } Z_1, \\ 104 \cdot 2^\eta - 108 & , \text{ when } TI \text{ is } Z_2, \\ 424 \cdot 2^\eta - 438 & , \text{ when } TI \text{ is } HZ, \\ 216 \cdot 2^\eta - 222 & , \text{ when } TI \text{ is } F. \end{cases}$$

The value for the forgotten index F is similar with its value found by Bashir et al. in [8].

Poly ethylene amido amine dendrimer

Our second molecular graph $\mathcal{M}_2$ is the poly ethylene amido amine (PETAA) dendrimer of generation G_η with $\eta \geq 1$ growth stage. $\mathcal{M}_2$ consists of 4 branches and one central core. The central core contains 2 atoms of valency 1, 8 atoms of valency 2, 4 atoms of valency 3, and 13 atom-bonds as depicted in Figure 2. In one branch of $\mathcal{M}_2$, there are $8 + 2 \cdot 8 + 2^2 \cdot 8 + \dots + 2^{\eta-1} \cdot 8 + 2^\eta \cdot 3 = 11 \cdot 2^\eta - 8$ atoms, among them $2^0 + 2^1 + 2^2 + \dots + 2^{\eta-1} + 2^\eta = 2 \cdot 2^\eta - 1$ are leaves (atoms with valency 1); $5 + 2 \cdot 5 + 2^2 \cdot 5 + \dots + 2^{\eta-1} \cdot 5 + 2^{\eta+1} = 7 \cdot 2^\eta - 5$ atoms are of valency 2; and the remaining $11 \cdot 2^\eta - 8 - 2 \cdot 2^\eta + 1 - 7 \cdot 2^\eta + 5 = 2 \cdot 2^\eta - 2$ atoms are of valency 3. Thus $\mathcal{M}_2$ has total $44 \cdot 2^\eta - 18$ atoms, among them $8 \cdot 2^\eta - 2$ atoms are of valency 1; $28 \cdot 2^\eta - 12$ atoms are of valency 2; and $8 \cdot 2^\eta - 4$ atoms are of valency 3.

Figure 2 poly ethylene amido amine dendrimer

The number of atom-bonds in $\mathcal{M}_2$ is $44 \cdot 2^\eta - 19$, by formula (1). With respect to the valencies of atoms incident with each atom-bond, there are four types $1 \sim 2$, $1 \sim 3$, $2 \sim 2$ and $2 \sim 3$ of atom-bonds in $\mathcal{M}_2$. Equivalently, the atom-bonds set of $\mathcal{M}_2$ is partitioned as $B(\mathcal{M}_2) = B_{1 \sim 2} \cup B_{1 \sim 3} \cup B_{2 \sim 2} \cup B_{2 \sim 3}$, where

$$B_{1 \sim 2} = \{\epsilon = ab \in B(\mathcal{M}_2) \mid v_a = 1, v_b = 2 \wedge v_\epsilon = 1\} \text{ with } |B_{1 \sim 2}| = 4 \cdot 2^\eta,$$

$$B_{1 \sim 3} = \{\epsilon = ab \in B(\mathcal{M}_2) \mid v_a = 1, v_b = 3 \wedge v_\epsilon = 2\} \text{ with } |B_{1 \sim 3}| = 4 \cdot 2^\eta - 2,$$

$$B_{2 \sim 2} = \{\epsilon = ab \in B(\mathcal{M}_2) \mid v_a = 2, v_b = 2 \wedge v_\epsilon = 2\} \text{ with } |B_{2 \sim 2}| = 16 \cdot 2^\eta - 7,$$

$$B_{2 \sim 3} = \{\epsilon = ab \in B(\mathcal{M}_2) \mid v_a = 2, v_b = 3 \wedge v_\epsilon = 3\} \text{ with } |B_{2 \sim 3}| = 20 \cdot 2^\eta - 10.$$

Using this partition in the formula of the first K Banhatti

polynomial from (7), we have:

$$B_1(\mathcal{M}_2, x) = \left(\sum_{\epsilon=ab \in B_{1 \sim 2}} + \sum_{\epsilon=ab \in B_{1 \sim 3}} + \sum_{\epsilon=ab \in B_{2 \sim 2}} + \sum_{\epsilon=ab \in B_{2 \sim 3}} \right) x^{(v_a+v_e)} \\ = 4 \cdot 2^\eta x^5 + (20 \cdot 2^\eta - 9)x^8 + (20 \cdot 2^\eta - 10)x^{11}.$$

Equivalently, using the atom-bonds partition in formulae of the other three Banhatti polynomials from (7) and (8), it can be found that

$$B_2(\mathcal{M}_2, x) = 4 \cdot 2^\eta x^3 + (20 \cdot 2^\eta - 9)x^8 \\ + (20 \cdot 2^\eta - 10)x^{15}, \\ HB_1(\mathcal{M}_2, x) = 4 \cdot 2^\eta x^{13} + (4 \cdot 2^\eta - 2)x^{34} + (16 \cdot 2^\eta - 7)x^{32} \\ + (20 \cdot 2^\eta - 10)x^{61}, \\ HB_2(\mathcal{M}_2, x) = 4 \cdot 2^\eta x^5 + (4 \cdot 2^\eta - 2)x^{40} + (16 \cdot 2^\eta - 7)x^{32} \\ + (20 \cdot 2^\eta - 10)x^{117}.$$

With respect to x , by taking the first derivative of these polynomials at $x = 1$, we get the following K Banhatti indices of $\mathcal{M}_2$.

$$TI(\mathcal{M}_2) = \begin{cases} 400 \cdot 2^\eta - 182 & , \text{ when } TI \text{ is } B_1, \\ 472 \cdot 2^\eta - 222 & , \text{ when } TI \text{ is } B_2, \\ 1920 \cdot 2^\eta - 902 & , \text{ when } TI \text{ is } HB_1, \\ 3032 \cdot 2^\eta - 1474 & , \text{ when } TI \text{ is } HB_2. \end{cases}$$

Using relationships (9), (10), (13) and (14), we have the following Zagreb and forgotten indices of $\mathcal{M}_2$.

$$TI(\mathcal{M}_2) = \begin{cases} 192 \cdot 2^\eta - 86 & , \text{ when } TI \text{ is } Z_1, \\ 204 \cdot 2^\eta - 94 & , \text{ when } TI \text{ is } Z_2, \\ 856 \cdot 2^\eta - 394 & , \text{ when } TI \text{ is } HZ, \\ 448 \cdot 2^\eta - 206 & , \text{ when } TI \text{ is } F. \end{cases}$$

Porphyrim dendrimer

Our third molecular graph $\mathcal{M}_3$ is the porphyrin dendrimer ($D_\kappa P_\kappa$) of generation G_κ with $\kappa = 2^\eta$ growth stage for $\eta \geq 2$. The structure of $\mathcal{M}_3$ consists of 4 branches and one central core. The central core contains 4 atoms of valency 2, 2 atoms of valency 3, and 5 atom-bonds as shown in Figure 3. In one branch of $\mathcal{M}_3$, there are $4 + 2 \cdot 4 + 2^2 \cdot 4 + \dots + 2^{\eta-3} \cdot 4 + 2^{\eta-2} \cdot 92 = 96 \cdot 2^{\eta-2} - 4$ atoms, among them $26 \cdot 2^{\eta-2}$ atoms are of valency 1; $3 + 2 \cdot 3 + 2^2 \cdot 3 + \dots + 2^{\eta-3} \cdot 3 + 2^{\eta-2} \cdot 31 = 34 \cdot 2^{\eta-2} - 3$ atoms are of valency 2; $8 \cdot 2^{\eta-2}$ atoms are of valency 4; and the remaining $96 \cdot 2^{\eta-2} - 4 - 26 \cdot 2^{\eta-2} - 34 \cdot 2^{\eta-2} + 3 - 8 \cdot 2^{\eta-2} = 28 \cdot 2^{\eta-2} - 1$ atoms are of valency 3. So $\mathcal{M}_3$ keeps total $96 \cdot 2^\eta - 10$ atoms, among them $26 \cdot 2^\eta$ atoms are of valency 1; $34 \cdot 2^\eta - 8$ atoms

are of valency 2; $28 \cdot 2^\eta - 2$ atoms are of valency 3; and the remaining $8 \cdot 2^\eta$ atoms are of valency 4.

The number of atom-bonds in $\mathcal{M}_3$ is $105 \cdot 2^\eta - 11$, by formula (1). According to the valencies of atoms incident with each atom-bond, there are six types $1 \sim 3$, $1 \sim 4$, $2 \sim 2$, $2 \sim 3$, $3 \sim 3$, and $3 \sim 4$ of atom-bonds in $\mathcal{M}_3$. Equivalently, the partition of atom-bonds set of $\mathcal{M}_3$ is $B(\mathcal{M}_3) = B_{1 \sim 3} \cup B_{1 \sim 4} \cup B_{2 \sim 2} \cup B_{2 \sim 3} \cup B_{3 \sim 3} \cup B_{3 \sim 4}$, where $B_{1 \sim 3} = \{\epsilon = ab \in B(\mathcal{M}_3) \mid v_a = 1, v_b = 3 \wedge v_e = 2\}$ with $|B_{1 \sim 3}| = 2 \cdot 2^\eta$, $B_{1 \sim 4} = \{\epsilon = ab \in B(\mathcal{M}_3) \mid v_a = 1, v_b = 4 \wedge v_e = 3\}$ with $|B_{1 \sim 4}| = 24 \cdot 2^\eta$, $B_{2 \sim 2} = \{\epsilon = ab \in B(\mathcal{M}_3) \mid v_a = 2, v_b = 2 \wedge v_e = 2\}$ with $|B_{2 \sim 2}| = 10 \cdot 2^\eta - 5$, $B_{2 \sim 3} = \{\epsilon = ab \in B(\mathcal{M}_3) \mid v_a = 2, v_b = 3 \wedge v_e = 3\}$ with $|B_{2 \sim 3}| = 48 \cdot 2^\eta - 6$, $B_{3 \sim 3} = \{\epsilon = ab \in B(\mathcal{M}_3) \mid v_a = 3, v_b = 3 \wedge v_e = 4\}$ with $|B_{3 \sim 3}| = 13 \cdot 2^\eta$, $B_{3 \sim 4} = \{\epsilon = ab \in B(\mathcal{M}_3) \mid v_a = 3, v_b = 4 \wedge v_e = 5\}$ with $|B_{3 \sim 4}| = 8 \cdot 2^\eta$.

Using this partition in the formula of the first K Banhatti polynomial from (7), we have:

Figure 3 Porphyrin dendrimer

$$B_1(\mathcal{M}_3, x) = \left(\sum_{\epsilon=ab \in B_{1 \sim 3}} + \sum_{\epsilon=ab \in B_{1 \sim 4}} + \sum_{\epsilon=ab \in B_{2 \sim 2}} \right. \\ \left. + \sum_{\epsilon=ab \in B_{2 \sim 3}} + \sum_{\epsilon=ab \in B_{3 \sim 3}} + \sum_{\epsilon=ab \in B_{3 \sim 4}} \right) x^{(v_a+v_e)}$$

$$=(12 \cdot 2^\eta - 5)x^8 + (72 \cdot 2^\eta - 6)x^{11} + 13 \cdot 2^\eta x^{14} + 8 \cdot 2^\eta x^{17}.$$

Similarly, using the atom-bonds partition in formulae of the other three Banhatti polynomials from (7) and (8), it can be found that

$$\begin{aligned} B_2(\mathcal{M}_3, x) &= (12 \cdot 2^\eta - 5)x^8 + (72 \cdot 2^\eta - 6)x^{15} \\ &\quad + 13 \cdot 2^\eta x^{24} + 8 \cdot 2^\eta x^{35}, \\ HB_1(\mathcal{M}_3, x) &= (10 \cdot 2^\eta - 5)x^{32} + 2 \cdot 2^\eta x^{34} + (48 \cdot 2^\eta - 6)x^{61} \\ &\quad + 8 \cdot 2^\eta x^{65} + 13 \cdot 2^\eta x^{98} + 8 \cdot 2^\eta x^{145}, \\ HB_2(\mathcal{M}_3, x) &= (10 \cdot 2^\eta - 5)x^{32} + 2 \cdot 2^\eta x^{40} + (48 \cdot 2^\eta - 6)x^{117} \\ &\quad + 24 \cdot 2^\eta x^{153} + 13 \cdot 2^\eta x^{288} + 8 \cdot 2^\eta x^{625}. \end{aligned}$$

With respect to x , by taking the first derivative of these polynomials at $x = 1$, we get the following K Banhatti indices of $\mathcal{M}_3$.

$$TI(\mathcal{M}_3) = \begin{cases} 1206 \cdot 2^\eta - 106 & , \text{ when } TI \text{ is } B_1, \\ 1768 \cdot 2^\eta - 130 & , \text{ when } TI \text{ is } B_2, \\ 7470 \cdot 2^\eta - 526 & , \text{ when } TI \text{ is } HB_1, \\ 19218 \cdot 2^\eta - 862 & , \text{ when } TI \text{ is } HB_2. \end{cases}$$

Using relationships (9), (10), (13) and (14), Zagreb and forgotten indices of $\mathcal{M}_3$ are:

$$TI(\mathcal{M}_3) = \begin{cases} 542 \cdot 2^\eta - 50 & , \text{ when } TI \text{ is } Z_1, \\ 643 \cdot 2^\eta - 56 & , \text{ when } TI \text{ is } Z_2, \\ 2852 \cdot 2^\eta - 230 & , \text{ when } TI \text{ is } HZ, \\ 1566 \cdot 2^\eta - 118 & , \text{ when } TI \text{ is } F. \end{cases}$$

The value for the forgotten index is similar with its value determined by Bashir et al. in [8].

Zinc porphyrin dendrimer

Our fourth molecular graph $\mathcal{M}_4$ is the zinc porphyrin dendrimer (DPZ_m) of generation G_η with $\eta \geq 1$ growth stage. $\mathcal{M}_4$ consists of 4 branches and one central core. The central core contains 24 atoms of valencies 2 and 3, 1 atom of valency 4, and 60 atom-bonds as displayed in Figure 4. In one branch of $\mathcal{M}_4$, we have $14 + 2 \cdot 14 + 2^2 \cdot 14 + \dots + 2^{\eta-1} \cdot 14 = 14(2^\eta - 1)$ atoms, among them $9 + 2 \cdot 9 + 2^2 \cdot 9 + \dots + 2^{\eta-1} \cdot 9 + 2^{\eta-1} \cdot 11 = 20 \cdot 2^{\eta-1} - 9$ atoms are of valency 2, and the remaining $14(2^\eta - 1) - 20 \cdot 2^{\eta-1} + 9 = 4 \cdot 2^\eta - 5$ atoms are of valency 3. Therefore, there are total $56 \cdot 2^\eta - 7$ atoms in $\mathcal{M}_4$, among them $40 \cdot 2^\eta - 12$ atoms are of valency 2, $16 \cdot 2^\eta + 4$ atoms are of valency 3, and one atom is of valency 4. The number of atom-bonds in $\mathcal{M}_4$ is $64 \cdot 2^\eta - 4$, by formula (1). According to the valencies of atoms incident with each atom-bond, there are four types

Figure 4 Zinc porphyrin dendrimer

$2 \sim 2$, $2 \sim 3$, $3 \sim 3$, and $3 \sim 4$ of atom-bonds in $\mathcal{M}_4$. Accordingly, the atom-bonds set of $\mathcal{M}_4$ is partitioned as $B(\mathcal{M}_4) = B_{2 \sim 2} \cup B_{2 \sim 3} \cup B_{3 \sim 3} \cup B_{3 \sim 4}$, where

$$\begin{aligned} B_{2 \sim 2} &= \{\epsilon = ab \in B(\mathcal{M}_4) \mid v_a = 2, v_b = 2 \wedge v_\epsilon = 2\} \text{ with } |B_{2 \sim 2}| = 16 \cdot 2^\eta - 4, \\ B_{2 \sim 3} &= \{\epsilon = ab \in B(\mathcal{M}_4) \mid v_a = 2, v_b = 3 \wedge v_\epsilon = 3\} \text{ with } |B_{2 \sim 3}| = 40 \cdot 2^\eta - 16, \\ B_{3 \sim 3} &= \{\epsilon = ab \in B(\mathcal{M}_4) \mid v_a = 3, v_b = 3 \wedge v_\epsilon = 4\} \text{ with } |B_{3 \sim 3}| = 8 \cdot 2^\eta + 12, \\ B_{3 \sim 4} &= \{\epsilon = ab \in B(\mathcal{M}_4) \mid v_a = 3, v_b = 4 \wedge v_\epsilon = 5\} \text{ with } |B_{3 \sim 4}| = 4. \end{aligned}$$

Using this partition in the formula of the first K Banhatti polynomial from (7), we have:

$$\begin{aligned} B_1(\mathcal{M}_4, x) &= \left(\sum_{\epsilon=ab \in B_{2 \sim 2}} + \sum_{\epsilon=ab \in B_{2 \sim 3}} + \sum_{\epsilon=ab \in B_{3 \sim 3}} \right. \\ &\quad \left. + \sum_{\epsilon=ab \in B_{3 \sim 4}} \right) x^{(v_a+v_\epsilon)} \\ &= (16 \cdot 2^\eta - 4)x^8 + (40 \cdot 2^\eta - 16)x^{11} \\ &\quad + (8 \cdot 2^\eta + 12)x^{12} + 4x^{17}. \end{aligned}$$

On the same way, using the atom-bonds partition in formulae of the other Banhatti polynomials align (7) and (8), it can be found that

$$\begin{aligned} B_2(\mathcal{M}_4, x) &= (16 \cdot 2^\eta - 4)x^8 + (40 \cdot 2^\eta - 16)x^{15} \\ &\quad + (8 \cdot 2^\eta + 12)x^{18} + 4x^{35}, \\ HB_1(\mathcal{M}_4, x) &= (16 \cdot 2^\eta - 4)x^{32} + (40 \cdot 2^\eta - 16)x^{61} \\ &\quad + (8 \cdot 2^\eta + 12)x^{72} + 4x^{145}, \end{aligned}$$

$$HB_2(\mathcal{M}_4, x) = (16 \cdot 2^\eta - 4)x^{32} + (40 \cdot 2^\eta - 16)x^{117} \\ + (8 \cdot 2^\eta + 12)x^{162} + 4x^{625}.$$

With respect to x , by taking the first derivative of these polynomials at $x = 1$, we get the following K Banhatti indices of $\mathcal{M}_4$.

$$TI(\mathcal{M}_4) = \begin{cases} 664 \cdot 2^\eta + 4 & , \text{ when } TI \text{ is } B_1, \\ 872 \cdot 2^\eta + 84 & , \text{ when } TI \text{ is } B_2, \\ 3528 \cdot 2^\eta + 340 & , \text{ when } TI \text{ is } HB_1, \\ 6488 \cdot 2^\eta + 2444 & , \text{ when } TI \text{ is } HB_2. \end{cases}$$

Using relationships (9), (10), (13) and (14), we receive the Zagreb and forgotten indices of $\mathcal{M}_4$ as follows:

$$TI(\mathcal{M}_4) = \begin{cases} 307 \cdot 2^\eta - 4 & , \text{ when } TI \text{ is } Z_1, \\ 341 \cdot 2^\eta - 7 & , \text{ when } TI \text{ is } Z_2, \\ 260 \cdot 2^\eta + 108 & , \text{ when } TI \text{ is } HZ, \\ 756 \cdot 2^\eta + 20 & , \text{ when } TI \text{ is } F. \end{cases}$$

Porphyrin cored dendrimers

Porphyrin cored dendrimers are of four types. Accordingly, we consider four subsections.

Figure 5 Porphyrin cored dendrimer-I

Figure 6 Porphyrin cored dendrimer-II

Figure 7 Porphyrin cored dendrimer-III

Figure 8 Porphyrin cored dendrimer-IV

Porphyrim cored dendrimers-I

Fifth molecular graph $\mathcal{M}_{51}$ considered in this paper is the porphyrim cored dendrimer-I (PCD-I) of generation G_η with $\eta \geq 1$ growth stage. $\mathcal{M}_{51}$ consists of two similar branches and one central core. The central core contains 10 atoms of valency 2, 14 atoms of valency 3, 1 atom of valency 4, and 34 atom-bonds as shown in Figure 5. In one branch of $\mathcal{M}_{51}$, there are $2^0 + 2^1 + 2^2 + \dots + 2^\eta = 2^{\eta+1} - 1$ atoms, among them 2^η atoms are of valency 1, and $2^0 + 2^1 + 2^2 + \dots + 2^{\eta-1} = 2^\eta - 1$ atoms are of valency 3. Therefore, in $\mathcal{M}_{51}$, there are total $4 \cdot 2^\eta + 23$ atoms, among them $2 \cdot 2^\eta$ atoms are of valency 1, $2 \times 2^\eta + 12$ atoms are of valency 3, 10 atoms are of valency 2, and one atom is of valency 4.

The number of atom-bonds in $\mathcal{M}_{51}$ is $4 \cdot 2^\eta + 30$, by formula (1). According to the valencies of atoms incident with each atom-bond, there are five types $1 \sim 3$, $2 \sim 2$, $2 \sim 3$, $3 \sim 3$, and $3 \sim 4$ of atom-bonds in $\mathcal{M}_{51}$. Equivalently, the atom-bonds set of $\mathcal{M}_{51}$ is partitioned as $B(\mathcal{M}_{51}) = B_{1\sim 3} \cup B_{2\sim 2} \cup B_{2\sim 3} \cup B_{3\sim 3} \cup B_{3\sim 4}$, where $B_{1\sim 3} = \{\epsilon = ab \in B(\mathcal{M}_{51}) \mid v_a = 1, v_b = 3 \wedge v_\epsilon = 2\}$ with $|B_{1\sim 3}| = 2 \cdot 2^\eta$, $B_{2\sim 2} = \{\epsilon = ab \in B(\mathcal{M}_{51}) \mid v_a = 2, v_b = 2 \wedge v_\epsilon = 2\}$ with $|B_{2\sim 2}| = 4$, $B_{2\sim 3} = \{\epsilon = ab \in B(\mathcal{M}_{51}) \mid v_a = 2, v_b = 3 \wedge v_\epsilon = 3\}$ with $|B_{2\sim 3}| = 12$, $B_{3\sim 3} = \{\epsilon = ab \in B(\mathcal{M}_{51}) \mid v_a = 3, v_b = 3 \wedge v_\epsilon = 4\}$ with $|B_{3\sim 3}| = 2 \cdot 2^\eta + 10$, $B_{3\sim 4} = \{\epsilon = ab \in B(\mathcal{M}_{51}) \mid v_a = 3, v_b = 4 \wedge v_\epsilon = 5\}$ with $|B_{3\sim 4}| = 4$.

Using this partition in the formula of the first K Banhatti polynomial from (7), we have:

$$B_1(\mathcal{M}_{51}, x) = \left(\sum_{\epsilon=ab \in B_{1\sim 3}} + \sum_{\epsilon=ab \in B_{2\sim 2}} + \sum_{\epsilon=ab \in B_{2\sim 3}} + \sum_{\epsilon=ab \in B_{3\sim 3}} + \sum_{\epsilon=ab \in B_{3\sim 4}} \right) x^{(v_a+v_b)} \\ = (2 \cdot 2^\eta + 4)x^8 + 12x^{11} + (2 \cdot 2^\eta + 10)x^{14} + 4x^{17}.$$

Analogously, using the atom-bonds partition in formulae of the other three Banhatti polynomials from (7) and (8), it can be found that

$$B_2(\mathcal{M}_{51}, x) = 2 \cdot 2^\eta x^8 + 4x^8 + 12x^{15} \\ + (2 \cdot 2^\eta + 10)x^{24} + 4x^{35}, \\ HB_1(\mathcal{M}_{51}, x) = 2 \cdot 2^\eta x^{34} + 8x^{16} + 12x^{61} \\ + (2 \cdot 2^\eta + 10)x^{98} + 4x^{145}, \\ HB_2(\mathcal{M}_{51}, x) = 2 \cdot 2^\eta x^{40} + 8x^{16} + 12x^{117}$$

$$+ (2 \cdot 2^\eta + 10)x^{288} + 4x^{625}.$$

With respect to x , by taking the first derivative of these polynomials at $x = 1$, we get the following K Banhatti indices of $\mathcal{M}_{51}$.

$$TI(\mathcal{M}_{51}) = \begin{cases} 44 \cdot 2^\eta + 372 & , \text{ when } TI \text{ is } B_1, \\ 64 \cdot 2^\eta + 430 & , \text{ when } TI \text{ is } B_2, \\ 264 \cdot 2^\eta + 2420 & , \text{ when } TI \text{ is } HB_1, \\ 656 \cdot 2^\eta + 6912 & , \text{ when } TI \text{ is } HB_2. \end{cases}$$

Using relationships (9), (10), (13) and (14), Zagreb and forgotten indices of $\mathcal{M}_{51}$ have the following values:

$$TI(\mathcal{M}_{51}) = \begin{cases} 20 \cdot 2^\eta + 164 & , \text{ when } TI \text{ is } Z_1, \\ 24 \cdot 2^\eta + 226 & , \text{ when } TI \text{ is } Z_2, \\ 104 \cdot 2^\eta + 920 & , \text{ when } TI \text{ is } HZ, \\ 56 \cdot 2^\eta + 468 & , \text{ when } TI \text{ is } F. \end{cases}$$

Porphyrim cored dendrimer-II

Our sixth molecular graph $\mathcal{M}_{52}$ is the porphyrim cored dendrimer-II (PCD-II) of generation G_η with $\eta \geq 1$ growth stage. $\mathcal{M}_{52}$ consists of four similar branches and one central core. The central core contains 8 atoms of valency 2, 16 atoms of valency 3, 1 atom of valency 4, and 36 atom-bonds as shown in Figure 6. In one branch of $\mathcal{M}_{52}$, there are $2^0 + 2^1 + 2^2 + \dots + 2^\eta = 2^{\eta+1} - 1$ atoms, among them 2^η atoms are of valency 1, and $2^0 + 2^1 + 2^2 + \dots + 2^{\eta-1} = 2^\eta - 1$ atoms are of valency 3. Therefore, in $\mathcal{M}_{52}$, there are total $8 \cdot 2^\eta + 21$ atoms, among them $4 \cdot 2^\eta$ atoms are of valency 1, $4 \times 2^\eta + 12$ atoms are of valency 3, 8 atoms are of valency 2, and one atom is of valency 4.

The number of atom-bonds in $\mathcal{M}_{52}$ is $8 \cdot 2^\eta + 28$, by formula (1). According to the valencies of atoms incident with each atom-bond, there are five types $1 \sim 3$, $2 \sim 2$, $2 \sim 3$, $3 \sim 3$, and $3 \sim 4$ of atom-bonds in $\mathcal{M}_{52}$. Equivalently, the atom-bonds set of $\mathcal{M}_{52}$ is partitioned as $B(\mathcal{M}_{52}) = B_{1\sim 3} \cup B_{2\sim 2} \cup B_{2\sim 3} \cup B_{3\sim 3} \cup B_{3\sim 4}$, where $B_{1\sim 3} = \{\epsilon = ab \in B(\mathcal{M}_{52}) \mid v_a = 1, v_b = 3 \wedge v_\epsilon = 2\}$ with $|B_{1\sim 3}| = 4 \cdot 2^\eta$, $B_{2\sim 2} = \{\epsilon = ab \in B(\mathcal{M}_{52}) \mid v_a = 2, v_b = 2 \wedge v_\epsilon = 2\}$ with $|B_{2\sim 2}| = 4$, $B_{2\sim 3} = \{\epsilon = ab \in B(\mathcal{M}_{52}) \mid v_a = 2, v_b = 3 \wedge v_\epsilon = 3\}$ with $|B_{2\sim 3}| = 8$, $B_{3\sim 3} = \{\epsilon = ab \in B(\mathcal{M}_{52}) \mid v_a = 3, v_b = 3 \wedge v_\epsilon = 4\}$ with $|B_{3\sim 3}| = 4 \cdot 2^\eta + 12$, $B_{3\sim 4} = \{\epsilon = ab \in B(\mathcal{M}_{52}) \mid v_a = 3, v_b = 4 \wedge v_\epsilon = 5\}$ with $|B_{3\sim 4}| = 4$.

Analogously as in the case of porphyrim cored dendrimer-I, $\mathcal{M}_{51}$, using the atom-bonds partition in formulae of the

Banhatti polynomials from (7) and (8), it can be found that

$$\begin{aligned} B_1(\mathcal{M}_{52}, x) &= (4 \cdot 2^\eta + 4)x^8 + 8x^{11} \\ &\quad + (4 \cdot 2^\eta + 12)x^{14} + 4x^{17} \\ B_2(\mathcal{M}_{52}, x) &= 4 \cdot 2^\eta x^8 + 4x^8 + 8x^{15} \\ &\quad + (4 \cdot 2^\eta + 12)x^{24} + 4x^{35}, \\ HB_1(\mathcal{M}_{52}, x) &= 4 \cdot 2^\eta x^{34} + 8x^{16} + 8x^{61} \\ &\quad + (4 \cdot 2^\eta + 12)x^{98} + 4x^{145}, \\ HB_2(\mathcal{M}_{52}, x) &= 4 \cdot 2^\eta x^{40} + 8x^{16} + 8x^{117} \\ &\quad + (4 \cdot 2^\eta + 12)x^{288} + 4x^{625}. \end{aligned}$$

With respect to x , by taking the first derivative of these polynomials at $x = 1$, we get the following K Banhatti indices of $\mathcal{M}_{52}$.

$$TI(\mathcal{M}_{52}) = \begin{cases} 88 \cdot 2^\eta + 356 & , \text{ when } TI \text{ is } B_1, \\ 128 \cdot 2^\eta + 580 & , \text{ when } TI \text{ is } B_2, \\ 528 \cdot 2^\eta + 2372 & , \text{ when } TI \text{ is } HB_1, \\ 1312 \cdot 2^\eta + 7020 & , \text{ when } TI \text{ is } HB_2. \end{cases}$$

Using relationships (9), (10), (13) and (14), Zagreb and forgotten indices of $\mathcal{M}_{52}$ are:

$$TI(\mathcal{M}_{52}) = \begin{cases} 40 \cdot 2^\eta + 156 & , \text{ when } TI \text{ is } Z_1, \\ 48 \cdot 2^\eta + 220 & , \text{ when } TI \text{ is } Z_2, \\ 208 \cdot 2^\eta + 892 & , \text{ when } TI \text{ is } HZ, \\ 112 \cdot 2^\eta + 452 & , \text{ when } TI \text{ is } F. \end{cases}$$

Porphyry cored dendrimer-III

Our seventh molecular graph $\mathcal{M}_{53}$ is the porphyrin cored dendrimer-III (PCD-III) of generation G_η with $\eta \geq 1$ growth stage. $\mathcal{M}_{53}$ consists of eight similar branches and one central core. The central core contains 4 atoms of valency 2, 20 atoms of valency 3, 1 atom of valency 4, and 40 atom-bonds as shown in Figure 7. In one branch of $\mathcal{M}_{53}$, there are $2^0 + 2^1 + 2^2 + \dots + 2^\eta = 2^{\eta+1} - 1$ atoms, among them 2^η atoms are of valency 1, and $2^0 + 2^1 + 2^2 + \dots + 2^{\eta-1} = 2^\eta - 1$ atoms are of valency 3. Therefore, in $\mathcal{M}_{53}$, there are total $16 \cdot 2^\eta + 17$ atoms, among them $8 \cdot 2^\eta$ atoms are of valency 1, $8 \times 2^\eta + 12$ atoms are of valency 3, 4 atoms are of valency 2, and one atom is of valency 4.

The number of atom-bonds in $\mathcal{M}_{53}$ is $16 \cdot 2^\eta + 24$, by formula (1). According to the valencies of atoms incident with each atom-bond, there are four types $1 \sim 3$, $2 \sim 3$, $3 \sim 3$, and $3 \sim 4$ of atom-bonds in $\mathcal{M}_{53}$. Equivalently, the atom-bonds set of $\mathcal{M}_{53}$ is partitioned as $B(\mathcal{M}_{53}) = B_{1 \sim 3} \cup B_{2 \sim 3} \cup B_{3 \sim 3} \cup B_{3 \sim 4}$, where

$$B_{1 \sim 3} = \{\epsilon = ab \in B(\mathcal{M}_{53}) \mid v_a = 1, v_b = 3 \wedge v_\epsilon = 2\} \text{ with } |B_{1 \sim 3}| = 8 \cdot 2^\eta,$$

$$B_{2 \sim 3} = \{\epsilon = ab \in B(\mathcal{M}_{53}) \mid v_a = 2, v_b = 3 \wedge v_\epsilon = 3\} \text{ with } |B_{2 \sim 3}| = 8,$$

$$B_{3 \sim 3} = \{\epsilon = ab \in B(\mathcal{M}_{53}) \mid v_a = 3, v_b = 3 \wedge v_\epsilon = 4\} \text{ with } |B_{3 \sim 3}| = 8 \cdot 2^\eta + 12,$$

$$B_{3 \sim 4} = \{\epsilon = ab \in B(\mathcal{M}_{53}) \mid v_a = 3, v_b = 4 \wedge v_\epsilon = 5\} \text{ with } |B_{3 \sim 4}| = 4.$$

Analogously as in the case of porphyrin cored dendrimer-I, $\mathcal{M}_{51}$, using the atom-bonds partition in formulae of the Banhatti polynomials from (7) and (8), it can be found that

$$\begin{aligned} B_1(\mathcal{M}_{53}, x) &= 8 \cdot 2^\eta x^8 + 8x^{11} \\ &\quad + (8 \cdot 2^\eta + 12)x^{14} + 4x^{17} \\ B_2(\mathcal{M}_{53}, x) &= 8 \cdot 2^\eta x^8 + 8x^{15} \\ &\quad + (8 \cdot 2^\eta + 12)x^{24} + 4x^{35}, \\ HB_1(\mathcal{M}_{53}, x) &= 8 \cdot 2^\eta x^{34} + 8x^{61} \\ &\quad + (8 \cdot 2^\eta + 12)x^{98} + 4x^{145}, \\ HB_2(\mathcal{M}_{53}, x) &= 8 \cdot 2^\eta x^{40} + 8x^{117} \\ &\quad + (8 \cdot 2^\eta + 12)x^{288} + 4x^{625}. \end{aligned}$$

With respect to x , by taking the first derivative of these polynomials at $x = 1$, we get the following K Banhatti indices of $\mathcal{M}_{53}$.

$$TI(\mathcal{M}_{53}) = \begin{cases} 176 \cdot 2^\eta + 324 & , \text{ when } TI \text{ is } B_1, \\ 256 \cdot 2^\eta + 548 & , \text{ when } TI \text{ is } B_2, \\ 1056 \cdot 2^\eta + 2244 & , \text{ when } TI \text{ is } HB_1, \\ 2624 \cdot 2^\eta + 6892 & , \text{ when } TI \text{ is } HB_2. \end{cases}$$

Using relationships (9), (10), (13) and (14), we get Zagreb and forgotten indices of $\mathcal{M}_{53}$.

$$TI(\mathcal{M}_{53}) = \begin{cases} 40 \cdot 2^\eta + 140 & , \text{ when } TI \text{ is } Z_1, \\ 96 \cdot 2^\eta + 204 & , \text{ when } TI \text{ is } Z_2, \\ 416 \cdot 2^\eta + 828 & , \text{ when } TI \text{ is } HZ, \\ 224 \cdot 2^\eta + 420 & , \text{ when } TI \text{ is } F. \end{cases}$$

Porphyry Cored dendrimer-IV

Our eighth and last molecular graph $\mathcal{M}_{54}$ is the porphyrin cored dendrimer-IV (PCD-IV) of generation G_η with $\eta \geq 1$ growth stage. $\mathcal{M}_{54}$ consists of twelve similar branches and one central core. The central core contains 24 atoms of valency 3, 1 atom of valency 4, and 44 atom-bonds as shown in Figure 8. In one branch of $\mathcal{M}_{54}$, there are $2^0 + 2^1 + 2^2 + \dots + 2^\eta = 2^{\eta+1} - 1$ atoms, among them 2^η atoms are of valency 1, and $2^0 + 2^1 + 2^2 + \dots + 2^{\eta-1} = 2^\eta - 1$ atoms are of valency 3. Therefore, in $\mathcal{M}_{54}$, there are total $24 \cdot 2^\eta + 13$ atoms, among them $12 \cdot 2^\eta$ atoms are of valency 1, $12 \times 2^\eta + 12$ atoms are of valency 3, and one atom is of valency 4.

The number of atom-bonds in $\mathcal{M}_{54}$ is $24 \cdot 2^\eta + 20$, by formula (1). According to the valencies of atoms incident

with each atom-bond, there are four types $1 \sim 3$, $3 \sim 3$, and $3 \sim 4$ of atom-bonds in $\mathcal{M}_{54}$. Equivalently, the atom-bonds set of $\mathcal{M}_{54}$ is partitioned as $B(\mathcal{M}_{54}) = B_{1\sim 3} \cup B_{3\sim 3} \cup B_{3\sim 4}$, where

$B_{1\sim 3} = \{e = ab \in B(\mathcal{M}_{54}) \mid v_a = 1, v_b = 3 \wedge v_e = 2\}$ with $|B_{1\sim 3}| = 12 \cdot 2^\eta$,

$B_{3\sim 3} = \{e = ab \in B(\mathcal{M}_{54}) \mid v_a = 3, v_b = 3 \wedge v_e = 4\}$ with $|B_{3\sim 3}| = 12 \cdot 2^\eta + 16$,

$B_{3\sim 4} = \{e = ab \in B(\mathcal{M}_{54}) \mid v_a = 3, v_b = 4 \wedge v_e = 5\}$ with $|B_{3\sim 4}| = 4$.

Analogously as in the case of porphyrin cored dendrimer-I, $\mathcal{M}_{51}$, using the atom-bonds partition in formulae of the Banhatti polynomials from (7) and (8), it can be found that

$$B_1(\mathcal{M}_{54}, x) = 12 \cdot 2^\eta x^8 + (12 \cdot 2^\eta + 16)x^{14} + 4x^{17}$$

$$B_2(\mathcal{M}_{54}, x) = 12 \cdot 2^\eta x^8 + (12 \cdot 2^\eta + 16)x^{24} + 4x^{35},$$

$$HB_1(\mathcal{M}_{54}, x) = 12 \cdot 2^\eta x^{34} + (12 \cdot 2^\eta + 16)x^{98} + 4x^{145},$$

$$HB_2(\mathcal{M}_{54}, x) = 12 \cdot 2^\eta x^{40} + (12 \cdot 2^\eta + 16)x^{288} + 4x^{625}.$$

With respect to x , by taking the first derivative of these polynomials at $x = 1$, we get the following K Banhatti indices of $\mathcal{M}_{54}$.

$$TI(\mathcal{M}_{54}) = \begin{cases} 264 \cdot 2^\eta + 292 & , \text{ when } TI \text{ is } B_1, \\ 384 \cdot 2^\eta + 524 & , \text{ when } TI \text{ is } B_2, \\ 1584 \cdot 2^\eta + 2148 & , \text{ when } TI \text{ is } HB_1, \\ 3936 \cdot 2^\eta + 7108 & , \text{ when } TI \text{ is } HB_2. \end{cases}$$

Using relationships (9), (10), (13) and (14), we have the following values for Zagreb and forgotten indices of $\mathcal{M}_{54}$.

$$TI(\mathcal{M}_{54}) = \begin{cases} 120 \cdot 2^\eta + 124 & , \text{ when } TI \text{ is } Z_1, \\ 144 \cdot 2^\eta + 192 & , \text{ when } TI \text{ is } Z_2, \\ 624 \cdot 2^\eta + 772 & , \text{ when } TI \text{ is } HZ, \\ 336 \cdot 2^\eta + 388 & , \text{ when } TI \text{ is } F. \end{cases}$$

Geometric comparison and conclusion

Topological indices are tools which are extensively useful for chemical analysis of molecular compounds. The results due to topological indices have remarkable significance in chemistry, engineering, bioscience and nanoscience applications. We considered numerous imperative molecular structures and computed their valency based topological indices by defining and computing four Banhatti polynomials. The obtained results are useful in forecasting several molecular properties of chemical compounds such as π -electron energy, medical configuration, boiling point and many more.

Figure 9 First K Banhatti index

Figure 10 Second K Banhatti index

Using the technique of atom-bonds set partition of dendrimers in accordance with valencies and Banhatti polynomials, we investigated exact values for the first and second K Banhatti, K hyper Banhatti and Zagreb indices together with hyper Zagreb and forgotten indices. We separately plot values of each topological index obtained for eight dendrimers in Figure 9–16 to compare them geometrically. In each of these plots,

- thin solid curve is for poly (propyle) ethre imine (PETIM) dendrimer,
- short dotted curve is for poly ethylene amido amine (PETAA) dendrimer,
- short dashed curve is for porphyrin dendrimer ($D_\kappa P_\kappa$),
- dash dotted curve is for zinc porphyrin dendrimer (DPZ_η),

Figure 11 First K hyper Banhatti index

Figure 13 First Zagreb index

Figure 12 Second K hyper Banhatti index

Figure 14 Second Zagreb index

- long dashed curve is for porphyrin cored dendrimer-I (PCD-I),
- space dashed curve is for porphyrin cored dendrimer-II (PCD-II),
- space dotted curve is for porphyrin cored dendrimer-III (PCD-III),
- thick solid curve is for porphyrin cored dendrimer-IV (PCD-IV).

Each plot depicts that the behavior of indices for every dendrimer is same for $\eta < 10$. When η is increasing, then $D_K P_K$ has greatest value of each index, whereas PCD-I has least value of each index. The dendrimer DPZ_η has second greatest value of each index except of hyper Zagreb index, and for this index it preserves third least value as shown in the plot of Figure 15. It can also be observed that some

of the dendrimers have almost coinciding and very nearest values of several indices, for instance:

- Plots in Figures 10, 11 and 14 show that PETIM and PCD-III have very nearest values of second K Banhatti, first K hyper Banhatti and second Zagreb indices;
- The plot in Figure 12 depicts that PETAA and PCD-III have very closest values of second K hyper Banhatti index, while this index receives almost coinciding values for PETIM and PCD-II;
- The plot in Figure 13 provides that the first Zagreb index behaved same for PETIM and PCD-I till $\eta < 15$, and onward it gained very nearest values;
- Plots in Figures 15 and 16 show that the values of both the hyper Zagreb and forgotten indices coincide for PETIM and PCD-III.

Figure 15 Hyper Zagreb index

Figure 16 Forgotten index

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