

Research Article

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On distance-based indices of regular dendrimers using automorphism group action

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Abstract: The various topological indices are helpful in predicting the bioactivity of molecular compounds in quantitative structure–activity relationship/quantitative structure–property relationship study. The Balaban index and Harary index are the distance-based indices. The sum-Balaban index is another variant of Balaban index. Harary index can be used to indicate the decay of interaction between any two atoms of molecules. Whereas, the Balaban and sum-Balaban indices can be linked with some physico-chemical properties of octanes and lower benzenoids. In this work, the closed expression of Balaban index, sum-Balaban index, and Harary index of some regular dendrimers in the form of parameter m are computed using the action of automorphism group of these dendrimers.

Keywords: graph automorphism, Balaban index, sum-Balaban index, regular dendrimer

1 Introduction

Cheminformatics elegantly linked three disciplines i.e., chemistry, mathematics, and information science. It deals with quantitative structure–activity relationship (QSAR) and structure–property relationship (QSPR) which are used in predicting the biological and chemical behaviors and characteristics of different chemical compounds.

In chemical graph theory, a graph Γ of molecular structure is formed by associating two sets, one is vertex

set $V(\Gamma)$ which represents the atoms in the molecular structure and the other is edge set $E(\Gamma)$ which represents the covalent bond between the atoms.

A topological index is a real number that can be associated with a chemical graph Γ which can be used to indicate the chemical properties and the molecular topology of a chemical compound.

Dendrimers introduced by Buhleier et al. (1978) are macromolecules having star shape. They have a central core from where they expand iteratively so that each succeeding phase represents a new generation and its molecular weight is almost twice that of the preceding generation. Because of its rapidly growing structure, it has different sizes and shapes which helps in protecting inner cores. Moreover, it is useful in conjugating other chemical compounds to its surface, e.g., targeting components, dying agents, imaging agents, or pharmaceutically active compounds (Noriega-Luna et al., 2014). The dendrimers are significantly used in nanotechnology, gene transfection, drug delivery, catalysis, energy harvesting, etc. Although by representing the chemical compounds using topological indices, there is a considerable loss of chemical information, but still these indices give useful information in predicting various chemical properties, in particular, for those chemical compounds which are either difficult to investigate or may be having health risk or in the situation when chemical compound is not in the range.

A molecular graph in chemistry is a graphical and relational description of a molecule such that the atoms in a molecule corresponds to nodes, whereas edges indicate the chemical bonds between the atoms. The study of topological indices of these molecular graphs is useful in establishing the relation between the physicochemical properties of molecule and topological properties of underlying molecular graph. The first such index named as Wiener index was proposed by Wiener (1947) who used this to study the boiling point of alkanes. It is purely a distance-based index. Other distance-based topological indices include Harary index (Plavšić et al., 1993), Balaban index (Balaban, 1982), Schultz index (Schultz, 1989), Gutman index (Gutman, 1994), degree-distance index (Dobrynin and

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Kochetova, 1994), etc. For recent development on topological indices, refer (Ashrafi and Yousefi, 2006; Aslam et al., 2021; Dobrynin et al., 2002; Entringer et al., 1976; Gutman and Zhang, 2006; Hameed et al., 2022; Hong et al., 2020; Imran et al., 2022; Liu et al., 2019; Xu et al., 2019).

The Harary index is a distance-based topological index that was first investigated by Plavšić et al. (1993) and by Ivanciuc et al. (1993). It is defined as follows:

$$H(\Gamma) = \sum_{v \in V(\Gamma)} [d_G(u_1, u_2)]^{-1}$$

where $u_1 \neq u_2$. It can be used to indicate the decay of interaction between any two distinct atoms of a molecule. Alikhani et al. (2014) studied the Harary index of a class of dendrimer nanostars. Heydari (2010) investigated Harary index of regular dendrimers. For more details on Harary index, refer Das et al., 2009; Diudea, 1997; Dobrynin et al. (2001); and Feng and Ilic, 2010.

The Balaban index $J(\Gamma)$ (Balaban, 1982, 1983) and sum-Balaban index $SJ(\Gamma)$ (Balaban et al., 1985) are defined as follows:

$$J(\Gamma) = \frac{|E(\Gamma)|}{\mu + 1} \sum_{u_1 u_2 \in E(\Gamma)} (d(u_1)d(u_2))^{-\frac{1}{2}}$$

$$SJ(\Gamma) = \frac{|E(\Gamma)|}{\mu + 1} \sum_{u_1 u_2 \in E(\Gamma)} (d(u_1) + d(u_2))^{-\frac{1}{2}}$$

where μ is the cyclomatic number of Γ , $d(u) = \sum_{x \in V(\Gamma)} d(u, x)$. The Balaban index can be related with the behavior of melting and glass transition temperatures of linear macromolecules. Zhou and Trinajstić (2008) presented certain bounds of Balaban index. Ashrafi, Shabania and Diudea (2013) studied the Balaban index for various families of Dendrimers. More details and applications of Balaban index can be found in Balaban (2002), Bermudez et al. (1999), Grassy et al. (1998), and Thakur et al. (2004).

In this study, the closed expressions of Balaban index, sum-Balaban index, and Harary index of dendrimers $G[m]$ and $H[m]$ in terms of m are computed by making use of action of automorphism group of dendrimers. In this study, the graph Γ represents a chemical network having $V(\Gamma)$ as vertex set, $E(\Gamma)$ as edge set, and $d(u_1, u_2)$ denotes the shortest distance between the vertices u_1 and u_2 .

2 Methodology and main results

In this work, we formulate the closed expression of the Balaban index, sum-Balaban index, and Harary index of an infinite class of regular dendrimers.

For achieving the required results, we used the group theoretical methods as discussed in Ahmad et al. (2017) and Fazlollahi and Shabani (2014). In particular, we use the idea of automorphism group of a graph and investigate the structure of graphs of dendrimers under the action of its corresponding automorphism group. We then split the graph vertices and edges according to the orbits. Moreover, Matlab programming have been utilized for the numerical computations. Let $S_t(w)$ be the collection of vertices which are at the distance t from w where $0 \leq t \leq e(w)$ and $w \in V(\Gamma)$. Then we can write

$$V(\Gamma) = S_0(w) \cup S_1(w) \cup \dots \cup S_{e(w)}(w)$$

Now define

$$RD(w) = |S_1(w)| + \frac{|S_2(w)|}{2} + \dots + \frac{|S_{e(w)}(w)|}{e(w)}$$

Then, the Harary index can be rewritten as follows:

$$H(\Gamma) = \frac{1}{2} \sum_{w \in V(\Gamma)} RD(w)$$

We will use the following lemmas in proving our main results.

Lemma 1. (Fazlollahi and Shabani, 2014)

Let the automorphism group of Γ ($\text{Aut}(\Gamma)$) acts on $E(\Gamma)$ so that orbits of this action be $E_1, E_2, \dots, E_l$. Then, we have

$$J(\Gamma) = \frac{|E(\Gamma)|}{\mu + 1} \sum_{j=1}^l \frac{|E_j|}{\sqrt{d(y_{j-1})d(y_j)}}$$

$$SJ(\Gamma) = \frac{|E(\Gamma)|}{\mu + 1} \sum_{j=1}^l \frac{|E_j|}{\sqrt{d(y_{j-1}) + d(y_j)}}$$

where $e_j = y_{j-1}y_j \in E_j$.

Lemma 2. If under the action of $\text{Aut}(\Gamma)$ on $V(\Gamma)$, the orbits are $W_1, W_2, \dots, W_k$, then,

$$H(\Gamma) = \frac{1}{2} \sum_{i=1}^k |W_i| RD(w_i)$$

where w_i is any vertex of W_i .

3 Balaban and sum-Balaban indices of dendrimer $G[n]$

Let the graph of regular dendrimer having precisely m generations and the core isomorphic to P_6 is denoted by $G[m]$. Figure 1 exhibits the graph $G[5]$.

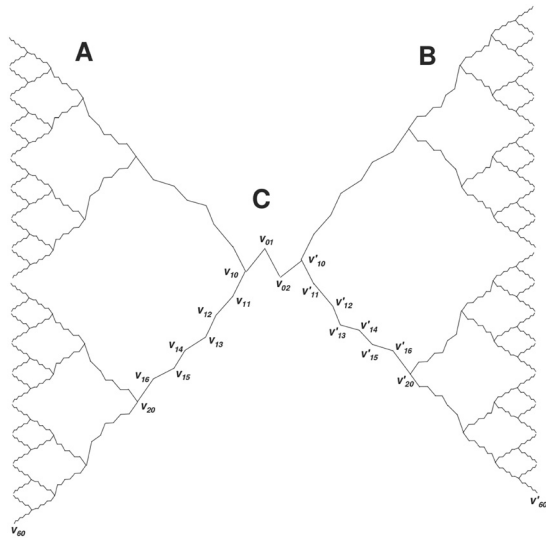


Figure 1: The graph $G[5]$.

Now, the Balaban index of $G[m]$ is calculated using the action of the automorphism group on $E(G[m])$. Since $G[m]$ is a tree, we have $\mu + 1 = 1$. Now, $G[m]$ can be partitioned into three subgraphs G_1 , G_2 , and G_3 , where G_3 is the core. This is depicted in Figure 2. It can be easily seen that both subgraphs G_1 and G_2 consist of $m + 1$ stages where the first m stages contain four levels and the last stage has one level. Therefore, both G_1 and G_2 have $4m + 1$ levels each. Let W_j and W'_j be the collection of vertices of j th stage of G_1 and G_2 , respectively. Let W_{js} and W'_{js} represent the s th level of j th stage in G_1 and G_2 , respectively. Then,

$$W_j = \bigcup_{s=0}^3 W_{js} \text{ and } W'_j = \bigcup_{s=0}^3 W'_{js}$$

We can see that $\text{Aut}(G[m]) \cong Z_2 \sim V_4$, where V_4 acts on the vertices of $\bigcup_{j=1}^{m+1} (W_{j0} \cup W'_{j0})$ and $\sim$ is the wreath

product. Now under this action, the orbits O_{js} , O_1 , and O_2 of $V(G[m])$ are given as follows:

$O_{js} = \{W_{js} \cup W'_{js}\}$, where $0 \leq s \leq 3$, for $1 \leq j \leq m$, and $s = 0$ for $j = m + 1$.

$O_1 = \{v_{01}, v_{04}\}$ and $O_2 = \{v_{02}, v_{03}\}$. Thus $|O_{js}| = 2^{j+1-\delta_{0s}}$ and $|O_1| = |O_2| = 2$, where δ_{0s} is given as follows:

$$\delta_{js} = \begin{cases} 1, & \text{if } j = s \\ 0, & \text{if } j \neq s \end{cases} \quad (1)$$

Hence, $V(G[m])$ can be rewritten as follows:

$$V(G) = O_1 \cup O_2 \bigcup_{j=1}^{m+1} \bigcup_{s=0}^3 O_{js}(1 - \delta_{(m+1)j}(1 - \delta_{0s}))$$

And $|E(G[m])| = 16 \cdot 2^m - 11$. The following notations are used from here onward in this work.

- $\nabla_{lk} = l - k$
- $\varphi = \varphi(l, k) = \min\{l, k\}$
- $\theta = \theta(l, k) = \max\{k - l, 0\}$
-

$$A_m(a_0, d, p) = \sum_{j=1}^m [a_0 + (j-1)d]p^{j-1} = \frac{a_0 - [a_0 + (m-1)d]p^m}{1-p} + \frac{pd(1-p^{m-1})}{(1-p)^2}$$

- $\kappa(j) = 2^{m+4}(1 - 2^j) - 2$
- $\vartheta(j) = 2^{m+7}2^{-j} + (4m + 4j - 11)2^{m+4} + 4j + 59$
- $\sigma(j) = 2\delta_{2j} + 6\delta_{3j}$
- $\tau(m) = 2^n(64m - 48) + 57$

Suppose $v_{js} \in O_{js}$ be the first vertex as depicted in Figure 1. Now, we determine the expression for $d(v_{js})$. If $d(x, A) = \sum_{a \in V(A)} d(x, a)$, then we have

$$d(v_{js}) = d(v_{js}, G_1) + d(v_{js}, G_2) + d(v_{js}, G_3) \quad (2)$$

Now,

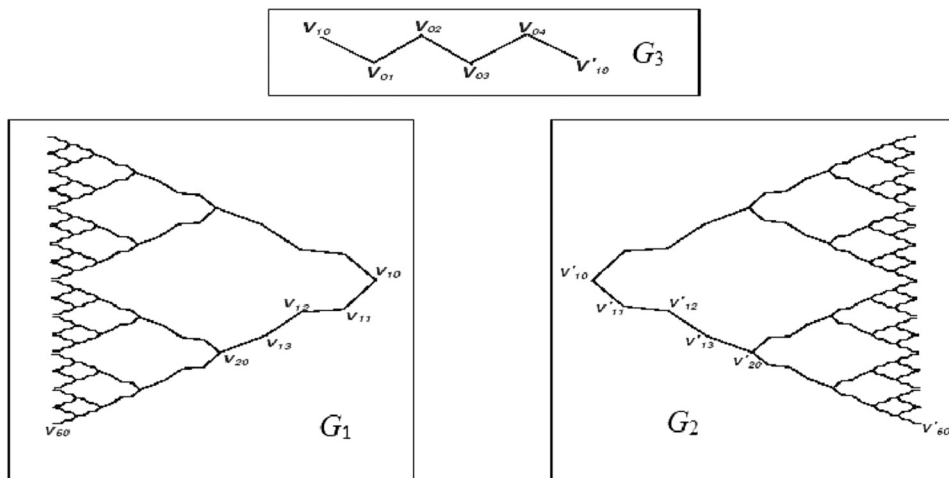


Figure 2: The subgraphs G_1 , G_2 , and G_3 .

$$d(v_{js}, G_1) = \sum_{i=1}^m d(v_{js}, W_i) + d(v_{js}, W_{(m+1)0}) \quad (3)$$

For $1 \leq i \leq j-1$, we get

$$d(v_{js}, W_i) = \sum_{t=0}^3 \frac{1}{2^{\delta_{0t}}} \{4\nabla_{ji} - t + s + A_i(4\nabla_{ji} + t + s, 8)\} \quad (4)$$

Now, for $j \leq i \leq m$, we get

$$d(v_{js}, W_i) = 2^{i-j} \sum_{t=0}^3 \frac{1}{2^{\delta_{0t}}} \{4\nabla_{ji} - t + s + A_j(4\nabla_{ji} + t + s, 8)\} \quad (5)$$

Using Eqs. 3–5, we have

$$d(v_{js}, G_1) = d(v_{js}, W_{(m+1)0}) + \sum_{h=1}^n 2^\theta \sum_{t=0}^3 \frac{1}{2^{\delta_{0t}}} \{4\nabla_{jh} - t + s + A_\varphi(4|\nabla_{jh}| + t + s, 8)\} \quad (6)$$

$$\sum_{t=0}^3 \frac{1}{2^{\delta_{0t}}} A_\varphi(4|\nabla_{ji}| + t + s, 8) = -14|\nabla_{ji}| + 50 - 3 \cdot 5s + (28|\nabla_{ji}| + 7s + 56\varphi - 100)2^{\varphi-1}$$

$$d(v_{js}, W_{(m+1)0}) = 2^{n+1-j}(8-s) + (4m+4j-12+s)2^m$$

Therefore, Eq. 6 becomes

$$d(v_{js}, G_1) = 2^{m+1-i}(8-s) + (4m+4j-12+s)2^m + \sum_{i=1}^m 2^\theta \left\{ -14|\nabla_{ji}| + 50 - 3 \cdot 5s + (28|\nabla_{ji}| + 7s + 56\varphi - 100)2^{\varphi-1} + \sum_{t=0}^3 \frac{|4\nabla_{ji} - t + s|}{2^{\delta_{0t}}} \right\} \quad (7)$$

Now

$$|4\nabla_{ji} - t + s| = \begin{cases} 4\nabla_{ji} - t + s, & \text{if } 1 \leq i \leq j-1 \\ -4\nabla_{ji} + t - s, & \text{if } j+1 \leq i \leq m \\ |s-t|, & \text{if } j=i \end{cases}$$

Thus, using Eq. 7, we have

$$d(v_{js}, G_1) = 2^{m+1-j}(8-s) + (4m+4j-12+s)2^m + 16j + 4s + 22 + |s-1| + |s-2| + |s-3| + 2^{m-j+1}(56-7s) + (28j+28m+7s-128)2^m = 2^{m+1-j}(64-8s) + (32m+32j+8s-140)2^m + (16j+4s+22) + |s-1| + |s-2| + |s-3| \quad (8)$$

Similarly, we have

$$d(v_{js}, G_3) = \sum_{t=0}^3 (4\nabla_{j1} + t + s + 1) = 16\nabla_{j1} + 10 + 4s = 16j - 6 + 4s$$

and

$$d(v_{js}, G_2) = d(v_{js}, W'_{(m+1)0}) + \sum_{i=1}^m \sum_{t=0}^3 2^{i-\delta_{0t}} (4\nabla_{j1} + 4\nabla_{i1} + 5 + t + s) = 2^m(32j+32m-36+8s) + (-28j+37-7s)$$

Thus, Eq. 2 becomes

$$d(v_{js}) = 2^{m+1-j}(64-8s) + (32m+32j+8s-140)2^m + (16j+4s+22) + |s-1| + |s-2| + |s-3| + (16j-6+4s) + 2^m(32j+32m-36+8s) + (-28j+37-7s) = ((2^{m+4}-2) - 2^{m+4-j})s + 2^{m+7}2^{-j} + (4m+4j-11)2^{m+4} + 4j+59+2\delta_{2s}+6\delta_{3s} = ((2^{m+4}-2) - 2^{m+4-j})s + 2^{m+7}2^{-j} + (4m+4j-11)2^{m+4} + 4j+59+2\delta_{2s}+6\delta_{3s} = \kappa(i)t + \vartheta(i) + 2\delta_{2t} + 6\delta_{3t}, = \kappa(j)s + \vartheta(j) + \sigma(s)$$

where $0 \leq s \leq 3$ and $1 \leq j \leq m+1$. Now,

$$d(v_{01}) = 6 + \sum_{i=1}^{m+1} \sum_{t=0}^3 2^{i-\delta_{0t}} \{ (4\nabla_{i1} + 1 + t) + (4\nabla_{i1} + 4 + t) \} = 6 + \sum_{i=1}^{m+1} \sum_{t=0}^3 2^{i-\delta_{0t}} (4i - 4 + 1 + t + 4i - 4 + 4 + t) = 2^m(56m - 56 + 3 + 8m + 5) + (6 + 56 - 3) = 2^m(64m - 48) + 59$$

$$d(v_{02}) = 4 + \sum_{i=1}^{m+1} \sum_{t=0}^3 2^{i-\delta_{0t}} \{ (4\nabla_{i1} + 2 + t) + (4\nabla_{i1} + 3 + t) \} = 2^m(56m - 56 + 3 + 8m + 5) + (4 + 56 - 3) = 2^m(64m - 48) + 57$$

and $d(v_{02}) = d(v_{03})$. This implies that

$$d(v_{01}) = \tau + 2, d(v_{02}) = \tau$$

Now, under $\text{Aut}(G[m])$ on edge set, let E_j and E'_j be the collection of edges of j th stages of G_1 and G_2 , respectively. Let E_{js} and E'_{js} be the collection of edges joining s and $s-1$ levels of j th stage in G_1 and G_2 , respectively. Also, let F_j and F'_j be the collection of edges joining 3rd level of j th stage and 0th level of $(j+1)$ th stage of G_1 and G_2 , respectively. Then,

$$E_j = \left\{ \bigcup_{s=1}^3 E_{js}, F_j \right\} \text{ and } E'_j = \left\{ \bigcup_{s=1}^3 E'_{js}, F'_j \right\}$$

Then, the orbits of this action are as follows:

$$ES_1 = \{v_{01}v_{10}, v'_{10}v_{04}\},$$

$$ES_2 = \{v_{02}v_{01}, v_{04}v_{03}\}, ES_3 = \{v_{02}v_{03}\}, ES_{js} = \{E_{js} \cup E'_{js}\} \text{ and } EF_j = \{F_j \cup F'_j\}, \text{ where } 1 \leq s \leq 3 \text{ and } 1 \leq j \leq m.$$

Thus,

$$|ES_{js}| = |EF_j| = 2^{j+1}, \quad |ES_1| = 2, \quad |ES_2| = 2, \quad \text{and} \quad |ES_3| = 1$$

$$d(v_{j(s-1)})d(v_{js}) = (\kappa(j)s + \vartheta(j) + \sigma(s))(\kappa(j)s - \kappa(j) + \vartheta(j) + \sigma(s-1))$$

$$d(v_{j3})d(v_{(j+1)0}) = (3\kappa(j) + \vartheta(j) + 6)\vartheta(j+1)$$

$$d(v_{01})d(v_{10}) = (\tau + 2)\vartheta(1)$$

$$d(v_{02})d(v_{01}) = \tau^2 + 2\tau$$

$$d(v_{03})d(v_{02}) = \tau^2$$

$$\begin{aligned} J(G[m]) &= (162^m - 11) \left[\frac{|ES_1|}{\sqrt{d(v_{01})d(v_{10})}} \right] + \frac{|ES_2|}{\sqrt{d(v_{02})d(v_{01})}} + \frac{|ES_3|}{\sqrt{d(v_{03})d(v_{02})}} + \sum_{j=1}^m \left\{ \sum_{s=1}^3 \frac{|ES_{js}|}{\sqrt{d(v_{j(s-1)})d(v_{js})}} + \frac{|EF_j|}{\sqrt{d(v_{j3})d(v_{(j+1)0})}} \right\} \\ &= (162^m - 11) \left[\frac{2}{\sqrt{(\tau + 2)\vartheta(1)}} \right] + \frac{2}{\sqrt{\tau^2 + 2\tau}} + \frac{1}{\tau} + \sum_{j=1}^m 2^{j+1} \left\{ \frac{1}{\sqrt{(3\kappa(j) + \vartheta(j) + 6)\vartheta(j+1)}} \right. \\ &\quad \left. + \sum_{i=1}^3 \frac{1}{\sqrt{(\kappa(j)s + \vartheta(j) + \sigma(s))(\kappa(j)s - \kappa(j) + \vartheta(j) + \sigma(s-1))}} \right\} \end{aligned}$$

and the sum-Balaban index is given as follows:

$$\begin{aligned} SJ(G[m]) &= (162^m - 11) \left[\frac{|ES_1|}{\sqrt{d(v_{01})d(v_{10})}} \right] + \frac{|ES_2|}{\sqrt{d(v_{02})d(v_{01})}} + \frac{|ES_3|}{\sqrt{d(v_{03})d(v_{02})}} \\ &= (162^m - 11) \left[\frac{2}{\sqrt{\tau + \vartheta(1) + 2}} \right] + \frac{2}{\sqrt{2\tau + 2}} + \frac{1}{\sqrt{2\tau}} + \sum_{j=1}^m 2^{j+1} \left\{ \frac{1}{\sqrt{3\kappa(j) + \vartheta(j) + \vartheta(j+1) + 6}} \right. \\ &\quad \left. + \sum_{i=1}^3 \frac{1}{\sqrt{2\kappa(j)s + 2\vartheta(j) - \kappa(j) + \sigma(s) + \sigma(s-1)}} \right\} \end{aligned}$$

Balaban index and sum-Balaban index of $G[m]$ for different values of m are calculated in Table 1. The behavior of Balaban index of $G[m]$ for $1 \leq m \leq 10$ and $1 \leq m \leq 20$ are shown in Figures 3 and 4, respectively.

4 Harary index of dendrimers $G[m]$ and $H[m]$

Now, we compute the Harary index of the dendrimer $G[m]$ and $H[m]$ using the same technique as used in Section 3.

$$d(v_{j(s-1)}) + d(v_{js}) = (\kappa(j)s + \vartheta(j) + \sigma(s)) + (\kappa(j)s - \kappa(j) + \vartheta(j) + \sigma(s-1))$$

$$= 2\kappa(j)s + 2\vartheta(j) - \kappa(j) + \sigma(s) + \sigma(s-1)$$

$$d(v_{j3}) + d(v_{(j+1)0}) = 3\kappa(j) + \vartheta(j) + \vartheta(j+1) + 6$$

$$d(v_{01}) + d(v_{10}) = \tau + \vartheta(1) + 2$$

$$d(v_{02}) + d(v_{01}) = 2\tau + 2$$

$$d(v_{03}) + d(v_{02}) = 2\tau$$

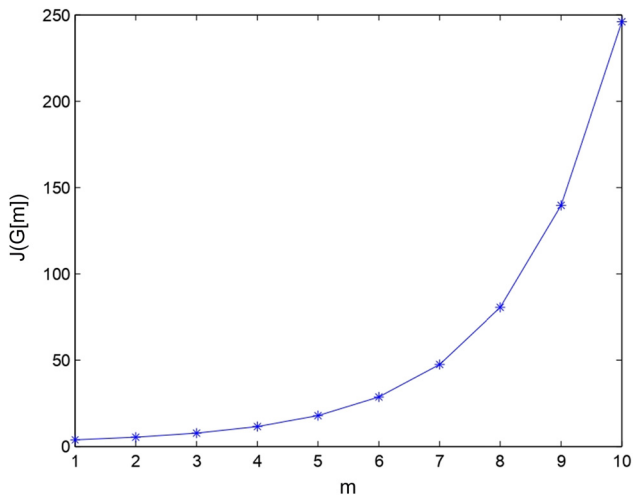
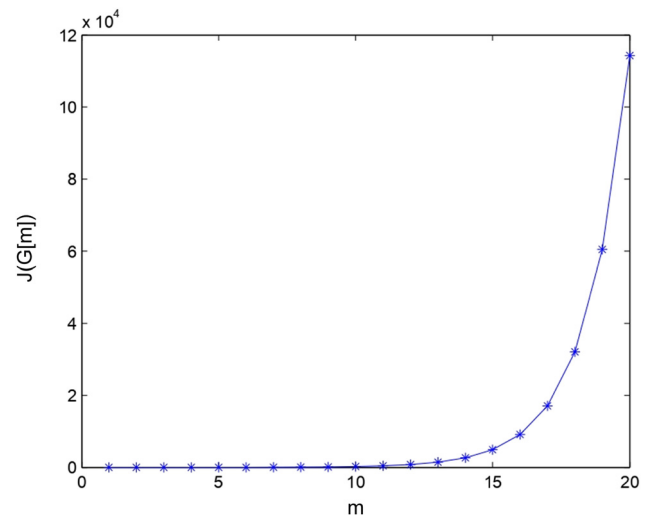
where $1 \leq s \leq 3$ and $1 \leq j \leq m$.

Hence, using all the discussions and calculations, the Balaban index and sum-Balaban index of $G[m]$ are given in the following theorem.

Theorem 1. The Balaban and sum-Balaban index of $G[m]$ are computed as follows:

Table 1: Balaban index of $G[m]$, for different values of m

m	$J(G[m])$	m	$J(G[m])$
1	3.87277102310468	2	5.41500541558913
3	7.74234307673819	4	11.5251445157719
5	17.859614874861	6	28.6833076938857
7	47.4843449495098	8	80.6034322171595
9	139.652150501735	10	246.028563012556
11	439.383541115064	12	793.55089136859
13	1,446.61736307702	14	2,657.84853621665
15	4,915.74184281229	16	9,143.62361453381
17	17,091.7183685288	18	32,086.3482723475
19	60,464.2721123531	20	114,323.517498065

Figure 3: Behavior of Balaban index for $1 \leq m \leq 10$.Figure 4: Behavior of Balaban index for $1 \leq m \leq 20$.

Let $RD(u, A) = \sum_{a \in A} |d(u, a)|^{-1}$ and $v_{js} \in W_{js}$ be the vertex of orbit O_{js} as shown in Figure 2. Then,

$$RD(v_{js}, W_j) = \sum_{t=0}^3 RD(v_{jt}, W_{jt})$$

Theorem 2. The Harary index of $G[m]$ is computed as follows:

$$H(G[m]) = \frac{11}{3} + \frac{1}{2} \sum_{i=1}^{m+1} \sum_{t=0}^3 \left\{ 2^{i-\delta_{0t}+2} \left(\frac{1}{4\nabla_{i1} + 1 + t} + \frac{1}{4\nabla_{i1} + 4 + t} \right) \right\} + \sum_{k=1}^{m+1} \sum_{r=0}^3 \left\{ 2^{i+1-\delta_{0r}} \left(\frac{2^{\theta(k,i)-\delta_{0r}}(1-\delta_{0r})(1-\delta_{ki}\delta_{tr})}{|4\nabla_{ki} - t + r| + \delta_{ki}\delta_{tr}} \right. \right. \\ \left. \left. + \frac{2^{i-\delta_{0t}}}{4\nabla_{k1} + 4\nabla_{i1} + 5 + t + r} + \sum_{q=\delta_{0r}\delta_{0t}}^{\varphi(k,i)-1} \frac{2^{\theta(k,i)+q-\delta_{0t}}}{4|\nabla_{ki}| + 8q + t + r} \right) (1 - \delta_{(m+1)k}(1 - \delta_{0r})) + \sum_{p=0}^3 \frac{2^{i+1-\delta_{0p}}}{4\nabla_{i1} + t + 1 + p} \right\} \\ \times (1 - \delta_{(m+1)i}(1 - \delta_{0t}))$$

Proof. First, we compute the form for $RD(v_{j0}, W_i)$. Now either $i < j$ or $i \geq j$. $\square$

Case 1. Suppose $i < j$

$$RD(v_{j0}, W_{i0}) = \frac{1}{4\nabla_{ji}} + \frac{1}{4\nabla_{ji} + 8(i)} + \cdots + \frac{2^{i-2}}{4\nabla_{ji} + 8(i-1)} \\ = \frac{1}{4\nabla_{ji}} + \sum_{q=1}^{i-1} \frac{2^{q-1}}{4\nabla_{ji} + 8q}.$$

Similarly,

$$RD(v_{j0}, W_{i1}) = \frac{1}{4\nabla_{ji} - 1} + \sum_{q=0}^{i-1} \frac{2^q}{4\nabla_{ji} + 8q + 1}$$

$$RD(v_{j0}, W_{i2}) = \frac{1}{4\nabla_{ji} - 2} + \sum_{q=0}^{i-1} \frac{2^q}{4\nabla_{ji} + 8q + 2}$$

$$RD(v_{j0}, W_{i3}) = \frac{1}{4\nabla_{ji} - 3} + \sum_{q=0}^{i-1} \frac{2^q}{4\nabla_{ji} + 8q + 3}$$

For $1 \leq i \leq j-1$, we get

$$RD(v_{j0}, W_i) = \sum_{i=0}^3 \left(\frac{1}{4\nabla_{ji} - i} + \sum_{q=\delta_{0i}}^{i-1} \frac{2^{q-\delta_{0i}}}{4\nabla_{ji} + 8q + i} \right) \quad (9)$$

Case 2. If $j \geq i$, then,

$$\begin{aligned} \text{RD}(v_{j0}, W_{i0}) &= \frac{2^{i-j}}{4\nabla_{ji}} + \frac{2^{i-j}}{4\nabla_{ji} + 8} \\ &\quad + \dots + \frac{2^{i-2}}{4\nabla_{ji} + 8(j-1)} \\ &= \frac{2^{i-j}}{4\nabla_{ji}} + \sum_{q=0}^{i-1} \frac{2^{i-j+q-1}}{4\nabla_{ji} + 8q} \end{aligned} \quad (10)$$

Similarly,

$$\text{RD}(v_{j0}, W_{i1}) = \frac{2^{i-j}}{4\nabla_{ji} + 1} + \sum_{q=0}^{i-1} \frac{2^{i-j+q}}{4\nabla_{ji} + 8q + 1} \quad (11)$$

$$\text{RD}(v_{j0}, W_{i2}) = \frac{2^{i-j}}{4\nabla_{ji} + 2} + \sum_{q=0}^{i-1} \frac{2^{i-j+q}}{4\nabla_{ji} + 8q + 2} \quad (12)$$

$$\text{RD}(v_{j0}, W_{i3}) = \frac{2^{i-j}}{4\nabla_{ji} - 3} + \sum_{q=0}^{i-1} \frac{2^{i-j+q}}{4\nabla_{ji} + 8q + 3} \quad (13)$$

Since the first term of Eq. 10 is not needed when $i = j$ and Eqs. 11–13 are not required for $i = m + 1$ and also $\nabla_{ji} = -\nabla_{ij}$, for $j \leq i \leq m + 1$, we have

$$\begin{aligned} \text{RD}(v_{j0}, W_i) &= \sum_{t=0}^3 \left(\frac{2^{i-j}(1\delta_{ji}\delta_{t0})}{|4\nabla_{ji} - t| + \delta_{ji}\delta_{t0}} \right. \\ &\quad \left. + \sum_{q=\delta_{0t}}^{j-1} \frac{2^{i-j+q-\delta_{0t}}}{4|\nabla_{ji}| + 8q + t} \right) (1 \\ &\quad - \delta_{(m+1)i}(1 - \delta_{0t})) \end{aligned} \quad (14)$$

From Eqs. 9 and 14, we have

$$\begin{aligned} \text{RD}(v_{i0}, G_1) &= \sum_{i=1}^{j-1} \text{RD}(v_{j0}, W_i) + \sum_{i=j}^{m+1} \text{RD}(v_{j0}, W_i) \\ &= \sum_{i=1}^{m+1} \sum_{t=0}^3 \left(\frac{2^{\theta(j,i)}(1 - \delta_{ji}\delta_{t0})}{|4\nabla_{ji} - t| + \delta_{ji}\delta_{t0}} \right. \\ &\quad \left. + \sum_{q=\delta_{0t}}^{\varphi(j,i)-1} \frac{2^{\theta(j,i)+q-\delta_{0t}}}{|4\nabla_{ji} - t| + 8q + t + \delta_{ji}\delta_{t0}} \right) \\ &\quad \times (1 - \delta_{(m+1)i}(1 - \delta_{0t})) \end{aligned}$$

Now,

$$\text{RD}(v_{j0}, G_3) = \sum_{t=0}^3 \frac{1}{4\nabla_{j1} + t + 1}$$

and

$$\text{RD}(v_{j0}, G_2) = \sum_{i=1}^m \sum_{t=0}^3 \frac{2^{i-\delta_{0t}}(1 - \delta_{(m+1)i}(1 - \delta_{0t}))}{4\nabla_{j1} + 4\nabla_{i1} + 5 + t}$$

Therefore,

$$\text{RD}(v_{j0}) = \text{RD}(v_{j0}, G_1) + \text{RD}(v_{i0}, G_2) + \text{RD}(v_{i0}, G_3)$$

$$\begin{aligned} \text{RD}(v_{j0}) &= \sum_{i=1}^{m+1} \left[\sum_{t=0}^3 \left(\frac{2^{\theta(j,i)}(1\delta_{ji}\delta_{t0})}{|4\nabla_{ji} - s| + \delta_{ji}\delta_{t0}} \right. \right. \\ &\quad \left. \left. + \frac{2^{i-\delta_{0t}}}{4\nabla_{j1} + 4\nabla_{i1} + 5 + t} \sum_{q=\delta_{0t}}^{\varphi(j,i)-1} \frac{2^{\theta(j,i)+q-\delta_{0t}}}{4|\nabla_{ji}| + 8q + t} \right) (1 \right. \\ &\quad \left. - \delta_{(m+1)i}(1 - \delta_{0t})) \right] + \sum_{t=0}^3 \frac{1}{4\nabla_{j1} + t + 1} \end{aligned}$$

Similarly,

$$\begin{aligned} \text{RD}(v_{j1}) &= \sum_{i=1}^{m+1} \left[\sum_{t=0}^3 \left(\frac{2^{\theta(j,i)-\delta_{0t}}(1 - \delta_{ji}\delta_{t1})}{|4\nabla_{ji} - s + 1| + \delta_{ji}\delta_{t1}} \right. \right. \\ &\quad \left. \left. + \frac{2^{i-\delta_{0t}}}{4\nabla_{j1} + 4\nabla_{i1} + 5 + t + 1} \right. \right. \\ &\quad \left. \left. + \sum_{q=0}^{\varphi(j,i)-1} \frac{2^{\theta(j,i)+q-\delta_{0t}}}{4|\nabla_{ji}| + 8q + t + 1} \right) (1 - \delta_{(m+1)i}(1 - \delta_{0t})) \right] \\ &\quad + \sum_{t=0}^3 \frac{1}{4\nabla_{j1} + t + 2} \\ \text{RD}(v_{j2}) &= \sum_{i=1}^{m+1} \left[\sum_{t=0}^3 \left(\frac{2^{\theta(j,i)-\delta_{0t}}(1 - \delta_{ji}\delta_{t2})}{|4\nabla_{ji} - t + 1| + \delta_{ji}\delta_{t2}} \right. \right. \\ &\quad \left. \left. + \frac{2^{i-\delta_{0t}}}{4\nabla_{j1} + 4\nabla_{i1} + 5 + t + 2} \right. \right. \\ &\quad \left. \left. + \sum_{q=0}^{\varphi(j,i)-1} \frac{2^{\theta(j,i)+q-\delta_{0t}}}{4|\nabla_{ji}| + 8q + t + 2} \right) (1 - \delta_{(m+1)i}(1 - \delta_{0t})) \right] \\ &\quad + \sum_{t=0}^3 \frac{1}{4\nabla_{j1} + t + 3} \\ \text{RD}(v_{j3}) &= \sum_{i=1}^{m+1} \left[\sum_{t=0}^3 \left(\frac{2^{\theta(j,i)-\delta_{0t}}(1 - \delta_{ji}\delta_{t3})}{|4\nabla_{ji} - s + 1| + \delta_{ji}\delta_{t3}} \right. \right. \\ &\quad \left. \left. + \frac{2^{i-\delta_{0t}}}{4\nabla_{j1} + 4\nabla_{i1} + 5 + t + 3} \right. \right. \\ &\quad \left. \left. + \sum_{q=0}^{\varphi(j,i)-1} \frac{2^{\theta(j,i)+r-\delta_{0t}}}{4|\nabla_{ji}| + 8q + t + 3} \right) (1 - \delta_{(m+1)i}(1 - \delta_{0t})) \right] \\ &\quad + \sum_{t=0}^3 \frac{1}{4\nabla_{j1} + t + 4} \end{aligned}$$

This implies that

$$\begin{aligned} \text{RD}(v_{js}) = & \sum_{i=1}^{m+1} \left[\sum_{t=0}^3 \left(\frac{2^{\theta(j,i)-\delta_{0t}(1-\delta_{0s})(1-\delta_{ji}\delta_{s1})}}{|4\nabla_{ji}-t+s|+\delta_{ji}\delta_{ts}} \right. \right. \\ & + \frac{2^{i-\delta_{0t}}}{4\nabla_{j1}+4\nabla_{i1}+5+t+s} \\ & \left. \left. + \sum_{q=\delta_{0s}\delta_{0t}}^{\varphi(j,i)-1} \frac{2^{\theta(j,i)+q-\delta_{0t}}}{4|\nabla_{ji}|+8q+t+s} \right) (1-\delta_{(m+1)i}(1-\delta_{0t})) \right] \\ & + \sum_{t=0}^3 \frac{1}{4\nabla_{j1}+t+1+s} \end{aligned}$$

where $0 \leq s \leq 3$ when $1 \leq j \leq m$ and $s = 0$ when $j = m+1$. Also,

$$\begin{aligned} \text{RD}(v_{01}) = & \sum_{i=1}^{m+1} \left[\sum_{t=0}^3 (2^{j-\delta_{0t}}) \left\{ \frac{1}{4\nabla_{j1}+1+s} + \frac{1}{4\nabla_{j1}+4+s} \right\} \right] (1 \\ & - \delta_{(m+1)j}(1-\delta_{0s})) + \frac{11}{6} \end{aligned}$$

$$\begin{aligned} \text{RD}(v_{02}) = & \sum_{i=1}^{m+1} \left[\sum_{s=0}^3 (2^{j-\delta_{0s}}) \left\{ \frac{1}{4\nabla_{j1}+2+s} + \frac{1}{4\nabla_{j1}+3+s} \right\} \right] (1 \\ & - \delta_{(m+1)j}(1-\delta_{0s})) + \frac{5}{2} \end{aligned}$$

Thus,

$$\begin{aligned} H(G[m]) = & \frac{1}{2}|O_1|\text{RD}(v_{01}) + \frac{1}{2}|O_2|\text{RD}(v_{02}) \\ & + \frac{1}{2} \sum_{j=1}^{m+1} \sum_{s=0}^3 |O_{js}|\text{RD}(v_{js})(1-\delta_{(m+1)j}(1-\delta_{0s})) \end{aligned}$$

Hence,

$$\begin{aligned} (G[m]) = & \frac{13}{3} + \frac{1}{2} \sum_{i=1}^{m+1} \left[\sum_{t=0}^3 \left\{ \sum_{m=1}^4 \frac{2^{i-\delta_{0t}+1}}{4\nabla_{j1}+m+t} \right. \right. \\ & + \sum_{k=1}^{m+1} \sum_{r=0}^3 2^{k+1-\delta_{0r}} \left(\frac{2^{\theta(k,i)-\delta_{0t}(1-\delta_{0r})(1-\delta_{ki}\delta_{tr})}}{4|\nabla_{ki}-t+r|+\delta_{ki}\delta_{tr}} \right. \\ & + \frac{2^{i-\delta_{0t}}}{4\nabla_{k1}+4\nabla_{i1}+5+t+r} \\ & \left. \left. + \sum_{q=\delta_{0r}\delta_{0t}}^{\varphi(k,i)-1} \frac{2^{\theta(k,i)+q-\delta_{0t}}}{4|\nabla_{ki}|+8q+t+r} \right) (1-\delta_{(m+1)k}(1 \right. \\ & \left. - \delta_{0r})) \right\} (1-\delta_{(m+1)i}(1-\delta_{0t})) \right] \\ & + \frac{1}{2} \sum_{i=1}^{m+1} \sum_{t=0}^3 \sum_{s=0}^3 \frac{2^{i+1-\delta_{0t}}}{4\nabla_{i1}+s+1+t} (1-\delta_{(m+1)i}(1-\delta_{0t})) \end{aligned}$$

This implies

$$\begin{aligned} H(G[m]) = & \frac{13}{3} + \frac{1}{2} \sum_{i=1}^{m+1} \sum_{t=0}^3 \left\{ \sum_{m=1}^4 \frac{2^{i-\delta_{0t}+1}}{4\nabla_{j1}+m+t} \right. \\ & + \sum_{k=1}^{m+1} \sum_{r=0}^3 2^{k+1-\delta_{0r}} \left(\frac{2^{\theta(k,i)-\delta_{0t}(1-\delta_{0r})(1-\delta_{ki}\delta_{tr})}}{4|\nabla_{ki}-t+r|+\delta_{ki}\delta_{tr}} \right. \\ & + \frac{2^{i-\delta_{0t}}}{4\nabla_{k1}+4\nabla_{i1}+5+t+r} \\ & \left. \left. + \sum_{q=\delta_{0r}\delta_{0t}}^{\varphi(k,i)-1} \frac{2^{\theta(k,i)+q-\delta_{0t}}}{4|\nabla_{ki}|+8q+t+r} \right) (1 \right. \\ & \left. - \delta_{(m+1)k}(1-\delta_{0r})) + \sum_{s=0}^3 \frac{2^{i+1-\delta_{0t}}}{4\nabla_{i1}+s+1+t} \right\} (1 \\ & - \delta_{(m+1)i}(1-\delta_{0t})) \end{aligned}$$

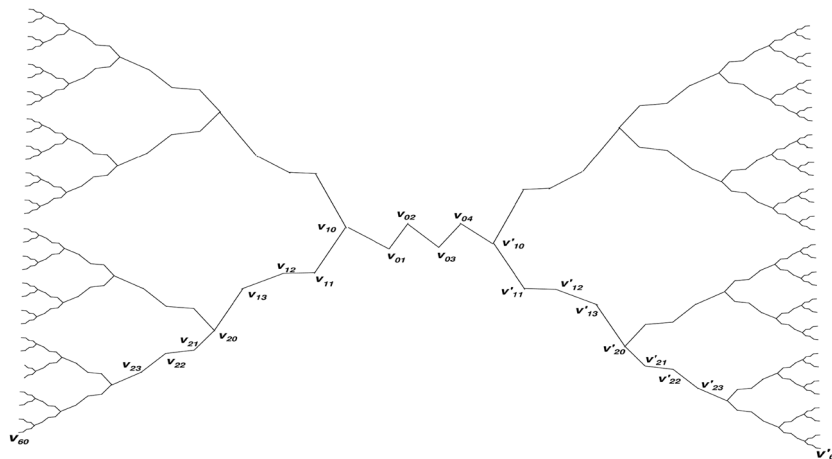


Figure 5: Graph of $H[5]$.

Table 2: Harary index of $G[m]$

m	$pH(G[m])$	m	$H(G[m])$
1	65.0501887001887	2	235.070181400986
3	717.664915085889	4	2,097.48370593313
5	6,160.44405078429	6	18,581.2299007141
7	58,032.2266196311	8	187,775.589218233
9	627,254.506242267	10	2,152,017.49563537
11	7,543,657.67406971	12	26,895,994.0086778
13	97,183,045.2149698	14	354,884,200.296531
15	1,306,990,781.2165	16	4,846,999,362.42041
17	18,079,245,935.2937	18	67,765,356,588.9581
19	255,067,628,544.391	20	963,576,855,504.784

Using similar arguments, the Harary index of dendrimer $H[m]$ as shown in Figure 5 is expressed as Theorem 3.

Theorem 3. *The Harary index of $H[m]$ is given as follows:*

$$\begin{aligned}
 H(G[m]) = & 1 + \frac{1}{2} \sum_{i=1}^{m+1} \sum_{t=0}^6 \left\{ 2^{i-\delta_{0t}+1} \left(\frac{1}{7\nabla_{j1} + 1 + s} + \frac{1}{7\nabla_{j1} + 2 + s} \right) \right\} \\
 & \times \sum_{i=1}^{m+1} \sum_{t=0}^6 2^{i-\delta_{0t}+1} \left(\frac{2^{\theta(i,j)-\delta_{0s}(1-\delta_{0t})}(1-\delta_{ij}\delta_{st})}{|7\nabla_{ij} - s + t| + \delta_{ij}\delta_{st}} \right. \\
 & + \frac{2^{i-\delta_{0s}}}{7\nabla_{i1} + 7\nabla_{j1} + 3 + s + t} \\
 & + \left. \sum_{q=\delta_{0r}\delta_{0s}}^{\varphi(i,j)-1} \frac{2^{\theta(i,j)+r-\delta_{0s}}}{7|\nabla_{ij}| + 14r + s + t} \right) (1 - \delta_{(m+1)i}(1 - \delta_{0t})) \\
 & + \sum_{t=0}^1 \left\{ \frac{2^{j+1-\delta_{0s}}}{7\nabla_{j1} + s + 1 + t} \right\} (1 - \delta_{(m+1)j}(1 - \delta_{0s}))
 \end{aligned}$$

The Harary index of $G[m]$ and $H[m]$, for different values of m are given in Tables 2 and 3, respectively.

Table 3: Harary index of $H[m]$

m	$H(H[m])$	m	$H(H[m])$
1	109.681953014306	2	442.128674473556
3	1,376.61494131809	4	4,008.94771520027
5	11,647.6343663172	6	34,702.6705442988
7	107,165.644080992	8	343,527.457460052
9	1,139,175.67747687	10	3,886,758.65672239
11	13,568,082.9742705	12	48,223,466.2842861
13	173,823,303.433015	14	633,535,445.982603
15	2,329,591,828.97235	16	8,628,126,415.55135
17	32,147,277,446.3993	18	120,380,550,331.966
19	452,730,030,758.554	20	1,709,017,733,128.75

5 Conclusion

Regardless of the restricted number of generations of these dendrimers, the proven expressions to determine Balaban, sum-Balaban, and Harary indices have a useful diagnostic value, specifically, in establishing composition rules of a global property by local contributions of the structural repeat units/monomers. In this way, the Balaban and Harary indices can be used both as an interpreter of information inferred from molecular structure databases and molecular descriptor in QSAR/QSPR. By using the definition of Balaban index and Harary index and action of automorphism group of graphs on the vertices and edges, this distance index is computed for regular dendrimer graph $G[m]$ in this study. The obtained results can be used to study the behavior of melting and glass transition temperatures of these dendrimers. It would be interesting to correlate the values of Balaban index and Harary index of these dendrimers with associated temperatures. As dendrimers have a lot of applications as protein mimics, anticancer or antiviral therapeutics, and delivery agents for drugs, so the obtained results may provide a useful indicator for these investigations. In future, we will develop the closed form of different types of indices with more complexed dendrimers, nanotubes, nanotori, etc. Relatively less work has been done to investigate the correlation of these indices with the chemical properties of molecular structures. It would be noteworthy to explore this part of the study in future.

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