MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **83** (2020) 205-220

ISSN 0340 - 6253

On the Symmetric Division Deg Index of Molecular Graphs

Akbar Ali[1,*], **Suresh Elumalai**[2], **Toufik Mansour**[2]

[1]*Knowledge Unit of Science, University of Management & Technology, Sialkot 51310, Pakistan*
akbarali.maths@gmail.com

[2]*Department of Mathematics, University of Haifa, 3498838 Haifa, Israel*
sureshkako@gmail.com, tmansour@univ.haifa.ac.il

(Received July 9, 2019)

Abstract

The symmetric division deg (SDD) index is one the 148 discrete Adriatic indices, introduced several years ago. The SDD index has already been proved a valuable index in the QSPR/QSAR (quantitative structure-property/activity relationships) studies. In the present paper, we firstly correct an upper bound on the SDD index of molecular trees, reported in the recent paper [MATCH Commun. Math. Comput. Chem. 82 (2019) 43–55], by giving the best possible upper bound on the SDD index of any molecular (n, m)-graph (a molecular graph with order n and size m). We then establish a lower bound on the SDD index of any molecular (n, m)-graph. Finally, by extending a theorem of the aforementioned paper, we characterize the graphs with fifth to ninth minimum SDD indices from the class of all molecular trees having a fixed, but sufficiently large, order.

1 Introduction

Predicting physicochemical properties of chemical compounds and seeking combinatorial libraries to find molecular structures that are generally comparative to a target structure, can be considered some of the important issues in chemistry. Among the various existing techniques for handling such issues, the method involving molecular descriptors is one of the simplest and most widely used such techniques [1, 3, 17, 18]. Following Todeschini and Consonni [14], we define the molecular descriptor as "the final result of a logical and

*Corresponding author

mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment".

Several years ago, Vukičević and Gašperov [16] considered a new class of molecular descriptors, consisting of one hundred and forty eight descriptors, namely the "discrete Adriatic indices" for improving the various QSPR/QSAR (quantitative structure-property/activity relationships) studies and they found that only a few descriptors from this class are useful. One of these useful discrete Adriatic indices is the symmetric division deg (SDD) index, which is defined as

$$\mathrm{SDD}(G) = \sum_{uv \in E(G)} \left(\frac{d_u}{d_v} + \frac{d_v}{d_u} \right),$$

where $E(G)$ is the edge set of a molecular graph G (a graph in which vertices correspond to atoms of a (hydrogen-suppressed) molecule and edges correspond to bonds between the atoms) and d_u, d_v denote the degrees of the vertices $u, v \in V(G)$, respectively.

Among all the existing molecular descriptors, SDD index has the best correlating ability for predicting the total surface area of polychlorobiphenyls (PCB) [16]. Recently, Furtula, Das and Gutman [7] conducted a thorough multifaceted analysis of the SDD index and they concluded that it deserves to be considered as a viable and applicable molecular descriptor, whose quality exceeds that of some more popular existing molecular descriptors. Thus, it is meaningful to establish mathematical properties of the SDD index, particularly for the molecular graphs. Several papers have been appeared in literature addressing the mathematical aspects of this descriptor; for example see [2, 5–7, 9–13].

The terminology not defined here can be found in some standard book of (chemical) graph theory, like [4,15]. All the graphs considered in this paper are simple and connected. By an n-vertex graph we mean a graph of order n and by an (n, m)-graph we mean an n-vertex graph of size m. Recently, Pan and Li [13] establish the upper bound on the SDD index, given in the following theorem.

Theorem 1. (Theorem 3 of [13]) *For $n \geq 4$, if T is an n-vertex molecular tree then*

$$\mathrm{SDD}(T) \leq \frac{27n + 1}{8}.$$

It can be easily checked that if T is an n-vertex tree, with $n \geq 8$, consisting of only vertices of degrees 1 and 4 then $\mathrm{SDD}(T) = (7n - 1)/2$, which is greater than the bound given in Theorem 1. Thus, Theorem 1 is not generally correct. The current paper can be considered as an extension of [13]. We firstly correct Theorem 1, by giving the best possible upper bound on the SDD index of any molecular (n, m)-graph (a molecular graph with order n and size m). We then establish a lower bound on the SDD index of any molecular (n, m)-graph. Finally, by extending a theorem of [13], we characterize the graphs with fifth to ninth minimum SDD indices from the class of all molecular trees having a fixed but sufficiently large number of vertices.

2 Bounds on the SDD index of molecular (n,m)-graphs

Before giving a correct and more general version of Theorem 1, we point out an error made in the proof of this theorem. The main problem in the aforementioned proof, lies in Equation (3.6) of [13], where it is wrongly claimed that

$$\max_{2\le i\le j\le 4} \frac{\alpha_{i,j} + 2\alpha_{1,4}\left(\frac{i-2}{i} + \frac{j-2}{j}\right)}{\frac{\frac{5}{2}i-4}{i} + \frac{\frac{5}{2}j-4}{j}} = \frac{\alpha_{2,4} + 2\alpha_{1,4}\left(\frac{2-2}{2} + \frac{4-2}{4}\right)}{\frac{\frac{5}{2}\cdot 2-4}{2} + \frac{\frac{5}{2}\cdot 4-4}{4}}$$

where

$$\alpha_{i,j} = \frac{i}{j} + \frac{j}{i} - \frac{5}{2}.$$

The correct version of this equation is

$$\max_{2\le i\le j\le 4} \frac{\alpha_{i,j} + 2\alpha_{1,4}\left(\frac{i-2}{i} + \frac{j-2}{j}\right)}{\frac{\frac{5}{2}i-4}{i} + \frac{\frac{5}{2}j-4}{j}} = \frac{\alpha_{4,4} + 2\alpha_{1,4}\left(\frac{4-2}{4} + \frac{4-2}{4}\right)}{\frac{\frac{5}{2}\cdot 4-4}{4} + \frac{\frac{5}{2}\cdot 4-4}{4}}.$$

Thus, the correct version of the inequality, given just after Equation (3.6) of [13], is $f(H_n) \le n+2$. But, the inequality $n+2 \le \frac{7(n+3)}{8}$ holds if and only if $n \le 5$. Hence, Theorem 1 holds for $n \le 5$.

Next, for establishing the bounds on the SDD index of molecular (n, m)-graphs, we consider the following system of equations which hold for any non-trivial molecular (n, m)-graph G:

$$\sum_{i=1}^{4} n_i = n, \tag{1}$$

$$\sum_{i=1}^{4} i \cdot n_i = 2m, \tag{2}$$

$$\sum_{\substack{1\le i\le 4\\ i\neq j}} x_{j,i} + 2x_{j,j} = j\cdot n_j \tag{3}$$

where $j = 1,2,3,4$; n_i is the number of vertices of G with degree i and $x_{j,i}$ denotes the number of those edges of G whose one end vertex has degree j and the other one has degree i. Clearly, $x_{j,i} = x_{i,j}$. The SDD index for the graph G can be rewritten as

$$\mathrm{SDD}(G) = \sum_{\delta(G)\le i\le j\le \Delta(G)} x_{i,j}(G)\left(\frac{i}{j}+\frac{j}{i}\right). \tag{4}$$

The following values of $x_{1,4}$ and $x_{4,4}$ can be obtained (see also [8]) by solving the system of Equations (1)-(3):

$$x_{1,4} = \frac{4n}{3} - \frac{2m}{3} - \frac{4}{3}x_{1,2} - \frac{10}{9}x_{1,3} - \frac{2}{3}x_{2,2} - \frac{4}{9}x_{2,3} - \frac{1}{3}x_{2,4} - \frac{2}{9}x_{3,3} - \frac{1}{9}x_{3,4},$$
$$x_{4,4} = -\frac{4n}{3} + \frac{5m}{3} + \frac{1}{3}x_{1,2} + \frac{1}{9}x_{1,3} - \frac{1}{3}x_{2,2} - \frac{5}{9}x_{2,3} - \frac{2}{3}x_{2,4} - \frac{7}{9}x_{3,3} - \frac{8}{9}x_{3,4}.$$

After substituting the values of $x_{1,4}$ and $x_{4,4}$ in Equation (4), we have

$$\mathrm{SDD}(G) = 3n + \frac{m}{2} - \frac{5}{2}x_{1,2} - \frac{7}{6}x_{1,3} - \frac{3}{2}x_{2,2} - \frac{5}{6}x_{2,3} - \frac{1}{4}x_{2,4} - \frac{1}{2}x_{3,3} - \frac{1}{6}x_{3,4}. \tag{5}$$

The setting

$$\Gamma_{\mathrm{SDD}}(G) = -\frac{5}{2}x_{1,2} - \frac{7}{6}x_{1,3} - \frac{3}{2}x_{2,2} - \frac{5}{6}x_{2,3} - \frac{1}{4}x_{2,4} - \frac{1}{2}x_{3,3} - \frac{1}{6}x_{3,4} \tag{6}$$

in Equation (5) yields

$$\mathrm{SDD}(G) = 3n + \frac{m}{2} + \Gamma_{\mathrm{SDD}}(G). \tag{7}$$

Theorem 2. *Let G be a molecular (n,m)-graph, where $n-1\le m\le 2n$ and $n\ge 5$.*

(*i*) *If $m+n\equiv 0$ (mod 3) then*

$$\mathrm{SDD}(G) \le 3n + \frac{m}{2}$$

with equality if and only if G contains no vertices of degrees 2 and 3.

(*ii*) *If $m+n\equiv 1$ or 2 (mod 3) then*

$$\mathrm{SDD}(G) \le 3n + \frac{m}{2} - \frac{1}{2}$$

with equality if and only if either G contains no vertex of degree 2 and contains exactly one vertex of degree 3, which is adjacent to three vertices of degree 4; or G contains no vertex of degree 3 and contains exactly one vertex of degree 2, which is adjacent to two vertices of degree 4.

Proof. From Equations (1) and (2), the following congruence (see also [8]) follows:

$$m + n \equiv n_3 - n_2 \pmod 3. \tag{8}$$

If $m + n \equiv 0 \pmod 3$ then from (8) we have $n_2 \equiv n_3 \pmod 3$. We note from (6) that $\Gamma_{\mathrm{SDD}}(G) \leq 0$ with equality if and only if G contains no vertices of degrees 2 and 3. Hence, from Equations (6) and (7) the first part of the theorem follows. In what follows, we assume that $m + n \equiv 1$ or $2 \pmod 3$. By (8), we have

$$n_3 - n_2 \equiv 1 \text{ or } 2 \pmod 3. \tag{9}$$

But, (9) ensures that either $n_2 \geq 1$ or $n_3 \geq 1$. If either at least one of $x_{1,2}$, $x_{1,3}$, $x_{2,2}$, $x_{2,3}$ is non-zero or $x_{3,3} \geq 2$ then by using (6) and (7), we have $\mathrm{SDD}(G) < 3n + \frac{m}{2} - \frac{1}{2}$. If $x_{1,2} = x_{1,3} = x_{2,2} = x_{2,3} = 0$ and $x_{3,3} = 1$, then $n_3 \geq 2$, which implies (due to (3) for $j = 3$) $x_{3,4} \geq 4$ and hence again from (6) and (7), it follows that $\mathrm{SDD}(G) < 3n + \frac{m}{2} - \frac{1}{2}$.

The final case to be considered is $x_{1,2} = x_{1,3} = x_{2,2} = x_{2,3} = x_{3,3} = 0$. In this case, bearing in mind (3) for $j = 2, 3$, we have $x_{2,4} = 2n_2$ and $x_{3,4} = 3n_3$. If any of n_2 and n_3 is greater than or equal to 2, or $n_2 = n_3 = 1$, then (bearing in mind $x_{2,4} = 2n_2$ and $x_{3,4} = 3n_3$ and) by using (6) and (7), we have $\mathrm{SDD}(G) < 3n + \frac{m}{2} - \frac{1}{2}$. If $n_2 = 0, n_3 = 1$ or $n_2 = 1, n_3 = 0$ then ($x_{2,4} = 0$, $x_{3,4} = 3$ or $x_{2,4} = 2$, $x_{3,4} = 0$, respectively, and) by using (6) and (7), we have $\mathrm{SDD}(G) = 3n + \frac{m}{2} - \frac{1}{2}$. ■

The setting $m = n - 1$ in Theorem 2 gives a corrected (but stronger) version of Theorem 1.

Corollary 1. *For $n \geq 5$, let T be an n-vertex molecular tree.*

(i) If $n \equiv 2$ (mod 3) then

$$\mathrm{SDD}(G) \leq \frac{7n - 1}{2}$$

with equality if and only if G contains no vertices of degrees 2 and 3.

(ii) If $n \equiv 0$ or 1 (mod 3) then

$$\mathrm{SDD}(G) \leq \frac{7n - 2}{2}$$

with equality if and only if either G contains no vertex of degree 2 and contains exactly one vertex of degree 3, which is adjacent to three vertices of degree 4; or G contains no vertex of degree 3 and contains exactly one vertex of degree 2, which is adjacent to two vertices of degree 4.

Next, we derive a lower bound on the SDD index of molecular (n, m)-graphs. The following values of $x_{1,2}$ and $x_{2,2}$ can be obtained (see also [8]) by solving the system of Equations (1)-(3):

$$x_{1,2} = 2n - 2m - \frac{2}{3}x_{1,3} - \frac{1}{2}x_{1,4} + \frac{1}{3}x_{2,3} + \frac{1}{2}x_{2,4} + \frac{2}{3}x_{3,3} + \frac{5}{6}x_{3,4} + x_{4,4},$$
$$x_{2,2} = 3m - 2n - \frac{1}{3}x_{1,3} - \frac{1}{2}x_{1,4} - \frac{4}{3}x_{2,3} - \frac{3}{2}x_{2,4} - \frac{5}{3}x_{3,3} - \frac{11}{6}x_{3,4} - 2x_{4,4}.$$

After substituting the values of $x_{1,2}$ and $x_{2,2}$ in Equation (4), we get

$$\mathrm{SDD}(G) = n + m + x_{1,3} + 2x_{1,4} + \frac{1}{3}x_{2,3} + \frac{3}{4}x_{2,4} + \frac{1}{3}x_{3,3} + \frac{1}{2}x_{3,4} + \frac{1}{2}x_{4,4}. \tag{10}$$

The setting

$$\Gamma'_{\mathrm{SDD}}(G) = x_{1,3} + 2x_{1,4} + \frac{1}{3}x_{2,3} + \frac{3}{4}x_{2,4} + \frac{1}{3}x_{3,3} + \frac{1}{2}x_{3,4} + \frac{1}{2}x_{4,4} \tag{11}$$

in Equation (10) yields

$$\mathrm{SDD}(G) = n + m + \Gamma'_{\mathrm{SDD}}(G). \tag{12}$$

Clearly, it holds that $\Gamma'_{\mathrm{SDD}}(G) \geq 0$ with equality if and only if maximum degree of G is 2 and hence we have the next result.

Theorem 3. *For $n \geq 3$ and $n - 1 \leq m \leq 2n$, if G is a molecular (n, m)-graph then*

$$\mathrm{SDD}(G) \geq n + m$$

with equality if and only if G is isomorphic to either the path graph P_n or the cycle graph C_n.

The following result is due to Pan and Li [13].

Proposition 2. [13] *If G is a graph with k pendant paths and m edges then it holds that*

$$\mathrm{SDD}\,(G) \geq 2m + \frac{2k}{3}\,. \tag{13}$$

Remark 3. *It is easy to see that*

$$\mathrm{SDD}(G) = 2m + f(G), \tag{14}$$

where $f(G) = \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u d_v}$. Combining (13) and (14), we get

$$f(G) \geq \frac{2k}{3}\,. \tag{15}$$

If G is either a regular graph or it has maximum degree 3 with $x_{1,2} = k = x_{2,3}$ and $x_{1,3} = 0$, then equality sign in (15), and hence in (13), holds.

3 The (molecular) trees with fifth to ninth minimum SDD indices

The problem of characterizing the graphs, with minimum SDD index, from the class of all n-vertex (molecular) trees was solved in [2].

Theorem 4. [2] *The path graph P_n is the unique graph with minimum* SDD *index among all (molecular) trees for $n \geq 4$.*

A vertex $v \in V(G)$ with degree 1 or degree greater than 2 is called pendant vertex or branching vertex, respectively. A path $P: \; v_1v_2\cdots v_r$ (of length $r-1$) in a graph is called pendant path if and only if one of the vertices v_1, v_r is pendant and the other is branching, and the remaining vertex/vertices (if exist(s)) of P has/have degree 2. A path $P: \; v_1v_2\cdots v_r$ in a graph is called internal path if and only if both the vertices v_1, v_r are branching and the remaining vertex/vertices (if exist(s)) of P has/have degree 2. A tree containing exactly one branching vertex is called a *starlike tree*. Denote by $S_n(r_1, r_2, \ldots, r_k)$ the n-vertex starlike tree whose pendant paths have lengths $r_1, r_2, \ldots, r_k$, where $r_1 \geq r_2 \geq \cdots \geq r_k \geq 1$ and $r_1 + r_2 + \cdots + r_k + 1 = n$. Denote by $S_{\alpha,\beta}(r_1, r_2, \ldots, r_\alpha; s_1, s_2, \ldots, s_\beta)$ the n-vertex double starlike tree, that is the tree obtained from the 2-vertex path graph P_2 by attaching α pendant paths of lengths $r_1, r_2, \ldots, r_\alpha$ to one vertex of P_2 and β pendant paths of lengths $s_1, s_2, \ldots, s_\beta$ to its other vertex, where $r_1 \geq r_2 \geq \cdots \geq r_\alpha \geq 1$, $r_1+r_2+\cdots+r_\alpha+s_1+s_2+\cdots+s_\beta+2 = n$, $s_1 \geq s_2 \geq \cdots \geq s_\beta \geq 1$ and $\alpha \geq \beta \geq 2$. Let $S_{\alpha,\beta} = S_{\alpha,\beta}(1, 1, \ldots, 1; 1, 1, \ldots, 1)$, that is the double star on $\alpha+\beta+2$ vertices.

Recently, Pan and Li [13] extended Theorem 4 by characterizing the graphs, with second to fourth minimum SDD indices, from the class of all n-vertex (molecular) trees for sufficiently large n.

Theorem 5. [13] *Let $r_1 \geq r_2 \geq r_3 \geq 2$ and $s_1 \geq s_2 \geq 2$ (for $i = 1, 2$, the values of r_i may vary in different parts of this theorem). Among all n-vertex (molecular) trees,*

1. *only the starlike tree(s) $S_n(r_1, r_2, r_3)$ has/have the second minimum* SDD *index, which is equal to $2n$, for $n \geq 7$;*
2. *only the following trees attain the third minimum* SDD *index, which is equal to $2n + \frac{2}{3}$:*

(a) *starlike trees* $S_n(r_1, r_2, 1)$ *for* $n \geq 7$*,*

(b) *double starlike tree(s)* $S_{2,2}(r_1, r_2; s_1, s_2)$ *for* $n \geq 10$*;*

3. *only the trees with exactly two vertices of maximum degree 3, each adjacent to three vertices of degree 2, have the fourth minimum* SDD *index, which is equal to* $2n+1$*, for* $n \geq 11$.

In what follows, we extend Theorem 5 by characterizing the graphs, with fifth to ninth minimum SDD indices, from the class of all n-vertex (molecular) trees for sufficiently large n.

Theorem 6. *(In the statement of this theorem, by a "path" in a graph, we mean a "pendant path" unless otherwise stated. For* $i = 1, 2, 3$*, the values of* r_i *as well as of* s_1 *may vary in different parts of this theorem.) Let* $r_1 \geq r_2 \geq r_3 \geq r_4 \geq 2$ *and* $s_1 \geq s_2 \geq 2$*. Among all* n*-vertex (molecular) trees,*

1. *only the following trees attain the fifth minimum* SDD *index, which is equal to* $2n + \frac{4}{3}$*:*

   (a) *starlike tree* $S_n(r_1, 1, 1)$ *for* $n \geq 11$*,*

   (b) *double starlike trees* $S_{2,2}(r_1, r_2; s_1, 1)$ *for* $n \geq 11$*,*

   (c) *trees obtained from the 3-vertex path graph* P_3 *by attaching two paths to every pendant vertex and one path to the unique non-pendant vertex such that all the attached five paths have lengths at least 2, for* $n \geq 13$*;*

2. *only the following trees attain the sixth minimum* SDD *index, which is equal to* $2n + \frac{5}{3}$*:*

   (a) *trees obtained from a path graph of order at least 3, by attaching two paths to each pendant vertex such that among the attached four paths, exactly one has length 1, for* $n \geq 11$*,*

   (b) *trees obtained from a path graph of order at least 4, by attaching two paths to every pendant vertex and one path to the neighbor of a pendant vertex, such that all the attached five paths have lengths at least 2, for* $n \geq 14$*;*

3. only the following trees attain the seventh minimum SDD *index, which is equal to* $2n + 2$*:*

   (a) starlike trees $S_n(r_1, r_2, r_3, r_4)$ *for* $n \geq 11$*,*

   (b) double starlike trees $S_{2,2}(r_1, r_2; 1, 1)$ *and* $S_{2,2}(r_1, 1; s_1, 1)$ *for* $n \geq 11$*,*

   (c) trees obtained from a path graph of order at least 5, by attaching two paths to every pendant vertex and one path to that vertex of degree 2 whose both neighbors have also degree 2, such that all the attached five paths have lengths at least 2, for $n \geq 15$*,*

   (d) trees obtained from the 3-vertex path graph P_3 *by attaching two paths to every pendant vertex and one path to the unique non-pendant vertex such that among the attached five paths, exactly one has length 1, for* $n \geq 12$*,*

   (e) trees of the form, shown in Figure 1, such that every internal path has length 1 and all the pendant paths have length at least 2, for $n \geq 16$*;*

4. only the following trees attain the eighth minimum SDD *index, which is equal to* $2n + \frac{7}{3}$*:*

   (a) trees obtained from a path graph, on at least 3 vertices, by attaching two paths to each pendant vertex such that among the attached four paths, exactly two have length 1, for $n \geq 11$*;*

   (b) trees obtained from a path graph, on at least 4 vertices, by attaching two paths to every pendant vertex and one path to the neighbor of a pendant vertex such that among the attached five paths, exactly one has length 1, for $n \geq 13$*,*

   (c) trees of the form, shown in Figure 1, such that exactly two internal paths have length 1 and all the pendant paths have length at least 2, for $n \geq 17$*;*

5. only the double starlike tree(s) $S_{3,2}(r_1, r_2, r_3; s_1, s_2)$ *attain(s) the ninth minimum* SDD *index, which is equal to* $2n + \frac{29}{12}$*, for* $n \geq 12$*.*

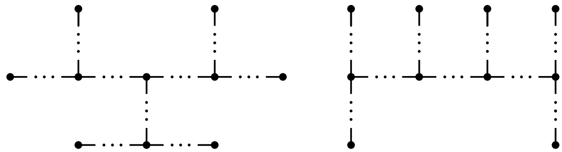

Figure 1. Two general structures of a tree having maximum degree 3 and containing exactly four vertices of degree 3.

Proof. Let T be an n-vertex tree different from the extremal trees specified in Theorems 4 and 5, with $n \geq 11$. It is clear that

$$\mathrm{SDD}(T) = 2n - 2 + \sum_{uv \in E(T)} \frac{(d_u - d_v)^2}{d_u d_v} = 2n - 2 + f(T)\,. \tag{16}$$

It can be easily verified that the tree(s) specified in each part of the theorem has/have SDD index given in that part. Consequently, bearing in mind Theorems 4 and 5, we deduce that any tree having SDD index greater than $2n + \frac{29}{12}$ (which is claimed to be the ninth minimum SDD index) must have kth minimum SDD index, for some $k \geq 10$, among all n-vertex trees. Hence, we have to find all those n-vertex trees whose SDD index is at most $2n + \frac{29}{12}$. But, from Equation (16), it is clear that the SDD index of an n-vertex tree T is at most $2n + \frac{29}{12}$ if and only if $f(T) \leq \frac{53}{12}$. Thereby, we have to find all those trees which satisfy the inequality

$$f(T) \leq \frac{53}{12}\,. \tag{17}$$

Certainly, the functions g and h, defined by

$$g(x) = \frac{(1-x)^2}{(1)(x)} \quad \text{and} \quad h(x) = \frac{(1-2)^2}{(1)(2)} + \frac{(2-x)^2}{(2)(x)}\,,$$

are increasing for $x \geq 3$. This implies that a pendant path of length 1 and a pendant path of length at least 2 in T contributes to $f(T)$ at least $\frac{(1-3)^2}{(1)(3)} = \frac{4}{3}$ and $\frac{(1-2)^2}{(1)(2)} + \frac{(2-3)^2}{(2)(3)} = \left(\frac{1}{2} + \frac{1}{6}\right) = \frac{2}{3}$, respectively. Consequently, if T has at least seven pendant paths, then (17) does not hold because $f(T) \geq 7 \times \frac{2}{3} > \frac{53}{12}$. Hence, we need only to consider the cases when T has at most 6 pendant paths. Let p be the number of pendant paths of length 1 in T.

Case 1. T has exactly three pendant paths.

Since we have assumed that T is different from the extremal trees specified in Theorem 5, so $p = 2$ and hence (17) holds in this case.

Case 2. T has exactly four pendant paths.

We consider two subcases.

Subcase 2.1. Maximum degree of T is 3.

We note that, in this subcase, T contains exactly two vertices of degree 3. Since we have assumed that T is different from the extremal trees specified in Theorem 5, so $p \geq 1$. Let u and v be the vertices of degree 3. If u and v are adjacent, then we have $f(T) = \frac{8}{3} + \frac{2p}{3}$ and if u and v are nonadjacent, then it holds that $f(T) = 3 + \frac{2p}{3}$. Clearly, whether the vertices u and v are adjacent or not, Inequality (17) holds only for $p = 1, 2$ in this subcase.

Subcase 2.2. Maximum degree of T is 4.

In this subcase, T contains exactly one vertex of degree greater than 2 and hence $f(T) = 4 + \frac{5p}{4}$. Thus, Inequality (17) holds only for $p = 0$ in this subcase.

Case 3. The tree T has exactly five pendant paths.

Here, we consider three subcases.

Subcase 3.1. Maximum degree of T is 3.

In this subcase, T contains exactly three vertices of degree 3. We have following three possibilities.

i) T has exactly two pairs of adjacent vertices of degree 3.

For this possibility, Inequality (17) holds only for $p = 0, 1$, because $f(T) = \frac{10}{3} + \frac{2p}{3}$.

ii) T has exactly one pair of adjacent vertices of degree 3.

For this possibility, (17) holds only for $p = 0, 1$, because $f(T) = \frac{11}{3} + \frac{2p}{3}$.

iii) T has no pair of adjacent vertices of degree 3.

For this possibility, (17) holds only for $p = 0$ because $f(T) = 4 + \frac{2p}{3}$.

Subcase 3.2. Maximum degree of T is 4.

We note that T contains exactly one vertex of degree 4 and exactly one vertex of degree 3. Let u and v be the vertices of degrees 3 and 4, respectively. Let p_1 and p_2 be the number of pendant vertices adjacent to u and v, respectively. Evidently, $0 \leq p_1 \leq 2$ and

$0 \leq p_2 \leq 3$. There are two possibilities.

i) The vertices u and v are adjacent.

For this possibility, Inequality (17) holds only for $p_1 = 0$ and $p_2 = 0$ because

$$f(T) = \frac{53}{12} + \frac{2p_1}{3} + \frac{5p_2}{4}.$$

ii) The vertices u and v are nonadjacent.

For this possibility, (17) does not hold because

$$f(T) = 5 + \frac{2p_1}{3} + \frac{5p_2}{4} > \frac{53}{12}.$$

Subcase 3.3. Maximum degree of T is 5.

In this subcase, T contains exactly one vertex of degree greater than 2 and hence (17) does not hold because

$$f(T) = 7 + \frac{9p}{5} > \frac{53}{12}.$$

Case 4. T has exactly six pendant paths.

We consider five subcases.

Subcase 4.1. Maximum degree of T is 3.

We note that T contains exactly four vertices of degree 3 and it has one of the forms depicted in Figure 1. We consider following four possibilities.

i) T has exactly three pairs of adjacent vertices of degree 3.

For this possibility, Inequality (17) holds only for $p = 0$ because $f(T) = 4 + \frac{2p}{3}$.

ii) T has exactly two pairs of adjacent vertices of degree 3.

Also for this possibility, (17) holds only for $p = 0$ because $f(T) = \frac{13}{3} + \frac{2p}{3}$.

iii) T has exactly one pair of adjacent vertices of degree 3.

For this possibility, (17) does not hold for any value of p because $f(T) = \frac{14}{3} + \frac{2p}{3}$.

iv) T has no pair of adjacent vertices of degree 3.

Also for this possibility, (17) does not hold for any value of p because $f(T) = 5 + \frac{2p}{3}$.

Subcase 4.2. T contains a single vertex of maximum degree 4 and it contains exactly two vertices of degree 3.

Let $u \in V(T)$ be the vertex of maximum degree 4 and $v, w \in V(T)$ be the vertices of degree 3. Let p_1, p_2, p_3 be the number of pendant vertices adjacent to u, v, w, respectively. We consider two subcases.

Subcase 4.2.1. The vertex u lies on the unique v-w path.

It is clear that $0 \leq p_i \leq 2$ for $i = 1, 2, 3$. We have three possibilities.

i). The vertex u is adjacent to both v and w.

For this possibility, it holds that

$$f(T) = \frac{29}{6} + \frac{5p_1}{4} + \frac{2p_2}{3} + \frac{2p_3}{3} > \frac{53}{12}.$$

ii). The vertex u is adjacent to exactly one of the vertices v, w.

For this possibility, it holds that $f(T) = \frac{65}{12} + \frac{5p_1}{4} + \frac{2p_2}{3} + \frac{2p_3}{3} > \frac{53}{12}$.

iii). The vertex u is neither adjacent to v nor to w.

For this possibility, it holds that $f(T) = 6 + \frac{5p_1}{4} + \frac{2p_2}{3} + \frac{2p_3}{3} > \frac{53}{12}$.

Thus, in this subcase, T does not satisfy (17).

Subcase 4.2.2. Either v lies on the u-w path or w lies on the u-v path.

Without loss of generality, we assume that v lies on the u-w path. Then, it holds that $0 \leq p_1 \leq 3$, $0 \leq p_2 \leq 1$ and $0 \leq p_3 \leq 2$. We have four possibilities.

i). The vertex v is adjacent to both u and w.

For this possibility, it holds that $f(T) = \frac{61}{12} + \frac{5p_1}{4} + \frac{2p_2}{3} + \frac{2p_3}{3} > \frac{53}{12}$.

ii). The vertex v is adjacent to w and but v is not adjacent to u.

For this possibility, it holds that $f(T) = \frac{17}{3} + \frac{5p_1}{4} + \frac{2p_2}{3} + \frac{2p_3}{3} > \frac{53}{12}$.

iii). The vertex v is adjacent to u and but v is not adjacent to w.

For this possibility, it holds that $f(T) = \frac{65}{12} + \frac{5p_1}{4} + \frac{2p_2}{3} + \frac{2p_3}{3} > \frac{53}{12}$.

iv). The vertex v is neither adjacent to u nor adjacent to w.

For this possibility, it holds that $f(T) = 6 + \frac{5p_1}{4} + \frac{2p_2}{3} + \frac{2p_3}{3} > \frac{53}{12}$.

Hence, also for this subcase, T does not satisfy (17).

Subcase 4.3. T has exactly two vertices of degree 4.

Let u and v be the vertices of degree 4. Recall that $0 \leq p \leq 6$. It is clear that all the vertices of T except u and v have degrees less than 3. If u and v are adjacent then $f(T) = 6 + \frac{5p}{4} > \frac{53}{12}$ and if u and v are nonadjacent then $f(T) = 7 + \frac{5p}{4} > \frac{53}{12}$. Thus, for this subcase too, T does not satisfy (17).

Subcase 4.4. Maximum degree of T is 5.

We note that, in this subcase, T has exactly one vertex of degree 5, exactly one vertex of degree 3, and its all other vertices have degrees less than 3. Let u and v be the vertices of degrees 3 and 5, respectively. Let p_1 and p_2 be the number of pendant vertices adjacent to u and v, respectively. Then, $0 \leq p_1 \leq 2$ and $0 \leq p_2 \leq 4$. If u and v are adjacent then $f(T) = \frac{36}{5} + \frac{2p_1}{3} + \frac{9p_2}{5} > \frac{53}{12}$ and if u and v are nonadjacent then we have

$f(T) = 8 + \frac{2p_1}{3} + \frac{9p_2}{5} > \frac{53}{12}$. Therefore, Inequality (17) does not hold also in this subcase.

Subcase 4.5. Maximum degree of T is 6.

Also for this subcase, T does not satisfy (17) because $f(T) = 11 + \frac{7p}{3} > \frac{53}{12}$.

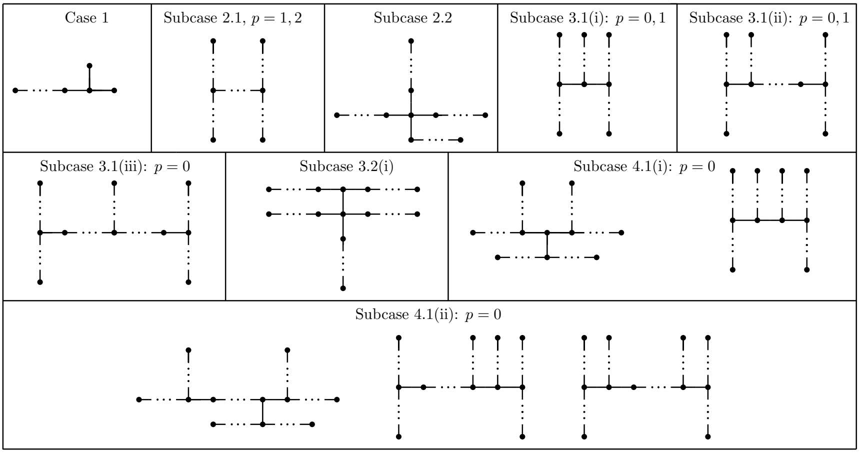

Figure 2. General structures of those trees which satisfy Inequality (17), together with the case numbers where such trees occur. Here, p denotes the number of pendant paths of length 1. Also, the (pendant or internal) path in which a vertex of degree 2 is shown, has length at least 2 otherwise it has length at least 1.

From the above arguments, we deduce that Inequality (17) may holds only if T is the tree specified in either of the following cases: Case 1, Subcase 2.1, Subcase 2.2, Subcase 3.1, Subcase 3.2 (i), Subcase 4.1 (i), Subcase 4.1 (ii). General structures of those trees which satisfy Inequality (17), together with the case numbers where such trees occur, are depicted in Figure 2. We calculate the output values under f for all these aforementioned trees and then obtain the ordering of these values. Finally, by using Equation (16), we get the desired result. ■

Acknowledgement: Suresh Elumalai's research is supported by University of Haifa, Israel, for the Postdoctoral studies and it is gratefully acknowledged.

References

[1] A. Ahlawat, P. Khatkar, V. Singh, S. Asija, Diorganotin(IV) complexes of Schiff bases derived from salicylaldehyde and 2-amino-6-substituted benzothiazoles: synthesis, spectral studies, in vitro antimicrobial evaluation and QSAR studies, *Res. Chem. Intermed.* **44** (2018) 4415–4435.

[2] A. Vasilyev, Upper and lower bounds of symmetric division deg index, *Iranian J. Math. Chem.* **5** (2014) 91–98.

[3] S. C. Basak, Use of graph invariants in quantitative structure–activity relationship studies, *Croat. Chem. Acta* **89** (2016) 419–429.

[4] J. A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, London, 2008.

[5] K. C. Das, M. Matejić, E. Milovanović, I. Milovanović, Bounds for symmetric division deg index of graphs, *Filomat*, in press.

[6] N. De, Topological indices of k-th subdivision and semi total point graphs, *Contemp. Stud. Discr. Math.* **2** (2018) 1–11.

[7] B. Furtula, K. C. Das, I. Gutman, Comparative analysis of symmetric division deg index as potentially useful molecular descriptor, *Int. J. Quantum Chem.* **118** (2018) Art# e25659.

[8] I. Gutman, O. Miljković, Molecules with smallest connectivity indices, *MATCH Commun. Math. Comput. Chem.* **41** (2000) 57–70.

[9] C. K. Gupta, V. Lokesha, B. Shwetha Shetty, P. S. Ranjini, Graph operations on the symmetric division deg index of graphs, *Palestine J. Math* **5** (2016) 1–18.

[10] C. K. Gupta, V. Lokesha, B. Shwetha Shetty, P. S. Ranjini, On the symmetric division deg index of graph, *Southeast Asian Bull. Math.* **41** (2016) 1–23.

[11] V. Lokesha, T. Deepika, Symmetric division deg index of tricyclic and tetracyclic graphs, *Int. J. Sci. Eng. Res.* **7** (2016) 53–55.

[12] G. Mohanappriya, D. Vijayalakshmi, Symmetric division degree index and inverse sum index of transformation graph, *IOP Conf. Ser. J. Phys.* **1139** (2018) #012048.

[13] Y. Pan, J. Li, Graphs that minimizing symmetric division deg index, *MATCH Commun. Math. Comput. Chem.* **82** (2019) 43–55.

[14] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley–VCH, Weinheim, 2009.

[15] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1992.

[16] D. Vukičević, M. Gašperov, Bond additive modeling 1. Adriatic indices, *Croat. Chem. Acta* **83** (2010) 243–260.

[17] Q. Zhang, K. Xiao, M. Chen, L. Xu, Calculation of topological indices from molecular structures and applications, *J. Chemom.* **32** (2018) #e2928.

[18] A. K. Zhokhov, A. Yu. Loskutov, I. V. Rybal'chenko, Methodological approaches to the calculation and prediction of retention indices in capillary gas chromatography, *J. Anal. Chem.* **73** (2018) 207–220.