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Graphs that Minimizing Symmetric Division Deg Index

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Abstract

Recently, Furtula et al. found that the symmetric division deg (SDD) index is a potentially useful molecular descriptor in structure-property and structure-activity relationships studies. In this paper, we determine the *n*-vertex trees with the second and the third for $n \ge 7$, and the fourth for $n \ge 11$ minimum SDD indices, unicyclic graphs with the first for $n \ge 3$, the second and the third for $n \ge 5$, and the fourth for $n \ge 8$ minimum SDD indices, and bicyclic graphs with the first for $n \ge 4$, the second for $n \ge 6$, and the third for $n \ge 7$ minimum SDD indices. In addition, we establish an upper bound for the *n*-vertex chemical trees (the trees with maximum degree no more than four).

1 Introduction

Let G be a simple connected graph with vertex set V(G) and edge set E(G), where |V(G)| = n and |E(G)| = m. A graph G is said to be a tree, a unicyclic graph, and a bicyclic graph if and only if m = n - 1, n, and n + 1, respectively. For each vertex $u \in V(G)$, let d_u be the degree of vertex u. The maximum degree of G is denoted by $\Delta(G)$.

Topological indices play an important role in mathematical chemistry especially in the QSPR/QSAR investigations [1,4,9,10,12,13]. Various topological indices are introduced

to characterize the physical-chemical properties of molecules [12]. In 2010, Vukičević and Gašperov [16] proposed 148 discrete Adriatic indices and evaluated their predictive properties against the benchmark dataset of the International Academy of Mathematical Chemistry [11]. Among them, just 20 indices were selected as significant predictors of physical-chemical properties.

The symmetric division deg index, which was selected in [16] as a significant predictor of total surface area of polychlorobiphenyls and for which the extremal graphs obtained with the help of MathChem [15] have a particularly simple and elegant structure, is defined as

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

In 2014, Vasilyev [14] gave some lower and upper bounds of this index in some classes of graphs and determined the corresponding extremal graphs. Recently, Furtula et al. [6] found that SDD index deserves to be considered as a viable and applicable topological index, whose quality exceeds that of some popular topological indices. For some mathematically oriented investigations, the readers are referred to the works [7,8,14].

Recall that a pendent edge is an edge incident with a vertex of degree one, whereas a path $u_1u_2...u_l$ is said to be a pendent path at u_1 if $d_{u_1} \ge 3$, $d_{u_i} = 2$ for i = 2, ..., l - 1, and $d_{u_l} = 1$. It should be stressed that the number of pendent paths is an important graph invariant in studying the extremal graphs [2,3]. For convenience, we use k to denote the number of pendent paths in G.

In this paper, we determine the *n*-vertex trees with the second and the third for $n \ge 7$, and the fourth for $n \ge 11$ minimum SDD indices, unicyclic graphs with the first for $n \ge 3$, the second and the third for $n \ge 5$, and the fourth for $n \ge 8$ minimum SDD indices, and bicyclic graphs with the first for $n \ge 4$, the second for $n \ge 6$, and the third for $n \ge 7$ minimum SDD indices. Besides, we establish an upper bound for the *n*-vertex chemical trees.

2 Preliminaries

For any edge uv of G, $\frac{d_u}{d_v} + \frac{d_v}{d_u} \ge 2$ with equality if and only if $d_u = d_v$. In our following proof, we will use this fact frequently.

Lemma 1. If there are k pendent paths in a graph G, then

$$SDD(G) \ge \frac{2}{3}k + 2|E(G)|$$

Proof. For any edge uv of G, when d_u is fixed, as a function on d_v , $\frac{d_u}{d_v} + \frac{d_v}{d_u}$ is increasing for $d_u \leq d_v \leq \Delta(G)$. Then the edge of a path with length 1 contributes to SDD(G) at least $\frac{1}{3} + 3 > \frac{2}{3} + 2$, and the edges of a pendent path with length $m \geq 2$ contributes to SDD(G) at least $(\frac{1}{2} + 2) + (\frac{2}{2} + \frac{2}{2})(m - 2) + (\frac{2}{3} + \frac{3}{2}) = \frac{2}{3} + 2m$. Therefore, the edges of a pendent path with length $m \geq 1$ contributes to SDD(G) at least $\frac{2}{3} + 2m$. Note that there are k pendent paths in G, then we have $SDD(G) \geq \frac{2}{3}k + 2|E(G)|$.

3 SDD indices of trees

It follows from [14] that the path P_n is the unique tree with the minimum *SDD* index among the *n*-vertex trees. In this section, we will determine the *n*-vertex trees with the second and the third for $n \ge 7$, and the fourth for $n \ge 11$ minimum *SDD* indices. Finally, we will give an upper bound for the *n*-vertex chemical trees.

Theorem 2. Among the set of n-vertex trees,

- (i) for n ≥ 7, the trees with a single vertex of maximum degree three, adjacent to three vertices of degree two are the unique trees with the second minimum SDD index, which is equal to 2n.
- (ii) the trees of order n ≥ 7 with a single vertex of maximum degree three, adjacent to one vertex of degree one and two vertices of degree two, and the trees of order n ≥ 10 with exactly two adjacent vertices of maximum degree three, each adjacent to two vertices of degree two are the unique trees with the third minimum SDD index, which is equal to 2n + ²/₃.
- (iii) for n ≥ 11, the trees with exactly two vertices of maximum degree three, each adjacent to three vertices of degree two are the unique trees with the fourth minimum SDD index, which is equal to 2n + 1.

Proof. Let G be an n-vertex tree different from P_n , where $n \ge 7$. Then there are at least three pendent paths in G, that is, $k \ge 3$.



Figure 1. Examples of the trees in Theorem 2 (i)-(iii) with smallest numbers of vertices.

If k = 3, then there is only one vertex with maximum degree three in G. In this case, if G is a tree with a single vertex of maximum degree three, adjacent to two vertices of degree one and one vertex of degree two, then $SDD(G) = (\frac{1}{3} + 3) \times 2 + (\frac{2}{3} + \frac{3}{2}) + (\frac{1}{2} + 2) + 2(n - 5) = 2n + \frac{4}{3} > 2n + 1$. If G is a tree with a single vertex of maximum degree three, adjacent to one vertex of degree one and two vertices of degree two, then $SDD(G) = (\frac{1}{3} + 3) + (\frac{2}{3} + \frac{3}{2}) \times 2 + (\frac{1}{2} + 2) \times 2 + 2(n - 6) = 2n + \frac{2}{3}$. If G is a tree with a single vertex of maximum degree three, adjacent to three vertices of degree two, then $SDD(G) = (\frac{1}{3} + 3) + (\frac{2}{3} + \frac{3}{2}) \times 2 + (\frac{1}{2} + 2) \times 2 + 2(n - 6) = 2n + \frac{2}{3}$. If G is a tree with a single vertex of maximum degree three, adjacent to three vertices of degree two, then $SDD(G) = (\frac{2}{3} + \frac{3}{2}) \times 3 + (\frac{1}{2} + 2) \times 3 + 2(n - 7) = 2n$.

If k = 4, then we need to consider the following two cases: (1) there is only one vertex of maximum degree four and other vertices are of degree one or two in G; (2) there are exactly two vertices of maximum degree three in G. If (1) is true, note that $(\frac{1}{4}+4) + (\frac{2}{2}+\frac{2}{2}) > (\frac{2}{4}+\frac{4}{2}) + (\frac{1}{2}+2)$, then we obtain

$$SDD(G) \ge \left(\frac{2}{4} + \frac{4}{2} + \frac{1}{2} + 2\right) \times 4 + 2(n-9) = 2n+2 > 2n+1.$$

Next, we assume that (2) is true. For convenience, the two vertices of degree three in G are denoted by u and v, respectively. Note that $\left(\frac{1}{3}+3\right)+\left(\frac{2}{2}+\frac{2}{2}\right)>\left(\frac{2}{3}+\frac{3}{2}\right)+\left(\frac{1}{2}+2\right)$. If there is at least one pendent path of length one in G, then we have

$$SDD(G) \ge \left(\frac{2}{3} + \frac{3}{2} + \frac{1}{2} + 2\right) \times 3 + \left(\frac{1}{3} + 3\right) + 2(n-8) = 2n + \frac{4}{3} > 2n + 1$$

If all the four pendent paths of G are of length at least two, then we need to consider the relation between u and v. If u and v are adjacent, then $n \ge 10$ and SDD(G) = $\left(\frac{2}{3} + \frac{3}{2} + \frac{1}{2} + 2\right) \times 4 + 2(n-9) = 2n + \frac{2}{3}$. If u and v are non-adjacent, then $n \ge 11$ and $SDD(G) = \left(\frac{2}{3} + \frac{3}{2}\right) \times 6 + \left(\frac{1}{2} + 2\right) \times 4 + 2(n-11) = 2n+1$.

If $k \geq 5$, then it follows immediately by Lemma 1 that

$$SDD(G) \ge \frac{2}{3}k + 2(n-1) \ge \frac{2}{3} \times 5 + 2(n-1) = 2n + \frac{4}{3} > 2n + 1.$$

From the above arguments, the result follows easily (Fig. 1).

Similar to the proof technique used in [5], we will give an upper bound for the *n*-vertex chemical trees.

Theorem 3. Let T_n be a chemical tree with $n \ge 4$ vertices. Then,

$$SDD(T_n) \le \frac{27n+1}{8}.$$
(3.1)

Proof. Let us consider the following function

$$f(T_n) = \sum_{uv \in E(T_n)} \left(\frac{d_u}{d_v} + \frac{d_v}{d_u} - \frac{5}{2} \right).$$
(3.2)

Note that $f(T_n) = SDD(T_n) - \frac{5}{2}(n-1)$, then the following inequality is equivalent to (3.1):

$$f(T_n) \le \frac{7(n+3)}{8}.$$
 (3.3)

Denote $\alpha_{ij} = \frac{i}{j} + \frac{i}{i} - \frac{5}{2}$. If there is some n and some chemical tree H'_n with n vertices such that $f(H'_n) > \frac{7(n+3)}{8}$, then let H_n be the one with the smallest number of vertices among these trees with minimal value of $m_{12}+m_{13}$. First, we will prove that $m_{11}(H_n)+m_{12}(H_n)+m_{13}(H_n)=0$. Since $m_{11}(H_n)=0$, then we just need to prove $m_{12}(H_n)+m_{13}(H_n)=0$. In the opposite case, we consider one of the following two cases:

CASE 1: $m_{12}(H_n) > 0$.

Let u be a vertex of degree two adjacent to the vertex v of degree one and vertex w of degree greater than one. Note that $m_{12}(H_n - v) + m_{13}(H_n - v) \le m_{12}(H_n) + m_{13}(H_n)$ and $n(H_n - v) < n(H_n)$, thus we have

$$f(H_n - v) \le \frac{7[(n-1)+3]}{8} < \frac{7(n+3)}{8} < f(H_n).$$
(3.4)

On the other hand, since $d_w \ge 2$, then

$$f(H_n - v) = f(H_n) - \alpha_{12} - \alpha_{2d_w} + \alpha_{1d_w} = f(H_n) + \frac{d_w}{2} - \frac{1}{d_w} \ge f(H_n) + \frac{1}{2} > f(H_n), \quad (3.5)$$

a contradiction.

CASE 2: $m_{13}(H_n) > 0$.

Let u be a vertex of degree three adjacent to vertex of degree one and vertices v and w. Let H_n^+ be a tree obtained by adding one pendent vertex to u. Note that $m_{12}(H_n^+) + m_{13}(H_n^+) \leq m_{12}(H_n) + m_{13}(H_n)$, but

$$\begin{split} f(H_n^+) &= f(H_n) + \alpha_{14} + (\alpha_{14} - \alpha_{13}) + (\alpha_{4d_v} - \alpha_{3d_v}) + (\alpha_{4d_w} - \alpha_{3d_w}) \\ &\geq \frac{7(n+3)}{8} \alpha_{14} + (\alpha_{14} - \alpha_{13}) + 2\min_{1 \le i \le 4} (\alpha_{4i} - \alpha_{3i}) \\ &= \frac{7n+41}{8} \\ &\geq \frac{7[(n+1)+3]}{8}, \end{split}$$

a contradiction.

Above all, we have $m_{11}(H_n) + m_{12}(H_n) + m_{13}(H_n) = 0$. Note that

$$\max_{2 \le i \le j \le 4} \frac{\alpha_{ij} + 2 \cdot \left(\frac{i-2}{2} + \frac{j-2}{j}\right) \cdot \alpha_{14}}{\frac{5}{2}i-4} = \frac{\alpha_{24} + 2 \cdot \left(\frac{2-2}{2} + \frac{4-2}{2}\right) \cdot \alpha_{14}}{\frac{5}{2}\cdot2-4} = \frac{\alpha_{24} + \alpha_{14}}{2} = \frac{\alpha_{14}}{2}.$$
(3.6)

Similar to the proof of the theorem in [5], we have

$$\begin{split} f(H_n) &\leq \frac{\alpha_{14}}{2} (n_1(H_n) + n_2(H_n) + n_3(H_n) + n_4(H_n) - 5) + 4\alpha_{14} \\ &= \frac{\alpha_{14}}{2} (n - 5) + 4\alpha_{14} \\ &= \frac{n + 3}{2} \alpha_{14} \\ &= \frac{7(n + 3)}{8}. \end{split}$$

This proves the theorem.

It should be noted that this upper bound is tight. For the families of trees given in Fig. 2, one can easily calculate that $SDD(T'_{4k+5}) = \frac{17}{4}(2k+4) + \frac{5}{2} \cdot 2k = \frac{27}{2}k + 17 = \frac{27n+1}{8}$.



Figure 2. Tree $T'_{4k+5}, k \ge 1$.

SDD indices of unicyclic graphs

In this section, we will determine the *n*-vertex unicyclic graphs with the first for $n \ge 3$, the second and the third for $n \ge 5$, and the fourth for $n \ge 8$ minimum *SDD* indices.

Theorem 4. Among the set of n-vertex unicyclic graphs,

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- (i) for n ≥ 3, the cycle C_n is the unique graph with the minimum SDD index, which is equal to 2n.
- (ii) for n ≥ 5, the graphs with a single vertex of maximum degree three, adjacent to three vertices of degree two are the unique graphs with the second minimum SDD index, which is equal to 2n + 1.
- (iii) the graphs of order n ≥ 5 with a single vertex of maximum degree three, adjacent to one vertex of degree one and two vertices of degree two, and the graphs of order n ≥ 7 with exactly two adjacent vertices of maximum degree three, each adjacent to two vertices of degree two are the unique graphs with the third minimum SDD index, which is equal to 2n + ⁵/₃.
- (iv) the graphs of order n ≥ 8 with exactly two vertices of maximum degree three, each adjacent to three vertices of degree two, and the graphs of order n ≥ 9 obtained by attaching a path on at least two vertices to every vertex of a triangle are the graphs with the fourth minimum SDD index, which is equal to 2n + 2.

Proof. Let G be an n-vertex unicyclic graph, where $n \ge 3$. If k = 0, then $G = C_n$ and SDD(G) = 2n.

If k = 1, then there is only a vertex of maximum three. In this case, if G is a graph with a single vertex of maximum degree three, adjacent to three vertices of degree two, then $n \ge 5$ and $SDD(G) = \left(\frac{2}{3} + \frac{3}{2}\right) \times 3 + \left(\frac{1}{2} + 2\right) + 2(n-4) = 2n+1$. If G is a graph with a single vertex of maximum degree three, adjacent to one vertex of degree one and two vertices of degree two, then $n \ge 4$ and $SDD(G) = \left(\frac{2}{3} + \frac{3}{2}\right) \times 2 + \left(\frac{1}{3} + 3\right) + 2(n-3) = 2n + \frac{5}{3}$.

If k = 2, then we need to consider the following two cases: (I) there is only one vertex on the cycle of G with maximum degree four and other vertices of G are of degree one or two. (II) there are exactly two vertices with maximum degree three in G. Note that $(\frac{1}{4} + 4) + (\frac{2}{2} + \frac{2}{2}) > (\frac{2}{4} + \frac{4}{2}) + (\frac{1}{2} + 2)$. If (I) is satisfied, then we have

$$SDD(G) \ge \left(\frac{2}{4} + \frac{4}{2} + \frac{1}{2} + 2\right) \times 2 + \left(\frac{2}{4} + \frac{4}{2}\right) \times 2 + 2(n-6) = 2n+3 > 2n+2.$$

Now, we assume that (II) is satisfied. For convenience, the two vertices of degree three in G are denoted by u and v, respectively. If the two pendent paths are all of length one in G, then

$$SDD(G) \ge \left(\frac{1}{3} + 3\right) \times 2 + 2(n-2) = 2n + \frac{8}{3} > 2n + 2.$$

If there is only one pendent path of length one in G, then there are at least three edges in G connecting vertices of degree two and three. Together with the two pendent edges in G, we obtain

$$SDD(G) \ge \left(\frac{2}{3} + \frac{3}{2}\right) \times 3 + \left(\frac{1}{2} + 2\right) + \left(\frac{1}{3} + 3\right) + 2(n-5) = 2n + \frac{7}{3} > 2n + 2.$$

Otherwise, the two pendent paths are of length at least two. When u and v are adjacent, we have $n \ge 7$ and $SDD(G) = \left(\frac{2}{3} + \frac{3}{2}\right) \times 4 + \left(\frac{1}{2} + 2\right) \times 2 + \left(\frac{3}{3} + \frac{3}{3}\right) + 2(n-7) = 2n + \frac{5}{3}$. When u and v are non-adjacent, we have $n \ge 8$ and $SDD(G) = \left(\frac{2}{3} + \frac{3}{2}\right) \times 6 + \left(\frac{1}{2} + 2\right) \times 2 + 2(n-8) = 2n+2$.

If k = 3, then we need to consider two cases: (1) there is at least one pendent path of length one in G, then

$$SDD(G) \ge \left(\frac{1}{3}+3\right) + \left(\frac{2}{3}+\frac{3}{2}+\frac{1}{2}+2\right) \times 2 + 2(n-5) = 2n + \frac{8}{3} > 2n + 2.$$

(2) there is no pendent path of length one in G. In this case, if there is a pendent path at the vertex of degree at least four, then

$$SDD(G) \ge \left(\frac{1}{2} + 2 + \frac{4}{2} + \frac{2}{4}\right) + \left(\frac{2}{3} + \frac{3}{2} + \frac{1}{2} + 2\right) \times 2 + 2(n-6) = 2n + \frac{7}{3} > 2n + 2.$$

Otherwise, $\Delta(G) = 3$. Assume that the three pendent paths in G are all at the vertices, say x, y, z, of degree three. If at most two pairs of vertices x, y, z are adjacent, then one can see that there are at least five edges connecting vertices of degree two and three. Note that there are three pendent edges in G, then we have

$$SDD(G) \ge \left(\frac{2}{3} + \frac{3}{2}\right) \times 5 + \left(\frac{1}{2} + 2\right) \times 3 + 2(n-8) = 2n + \frac{7}{3} > 2n + 2.$$
 (4.7)

If x, y, z are pairwise adjacent, then G is a graph formed by attaching a path on at least two vertices to every vertex of a triangle. Hence, $n \ge 9$ and $SDD(G) = \left(\frac{2}{3} + \frac{3}{2}\right) \times 3 + \left(\frac{1}{2} + 2\right) \times 3 + \left(\frac{3}{3} + \frac{3}{3}\right) \times 3 + 2(n-9) = 2n+2.$

If $k \ge 4$, then by Lemma 1, we have

$$SDD(G) \ge \frac{2}{3}k + 2n \ge \frac{2}{3} \times 4 + 2n = 2n + \frac{8}{3} > 2n + 2.$$

From the above arguments, the result follows easily (see Fig. 3).



Figure 3. Examples of the unicyclic graphs in Theorem 4 (i)-(iv) with smallest numbers of vertices.

5 SDD indices of bicyclic graphs

In this section, we will determine the *n*-vertex bicyclic graphs with the first for $n \ge 4$, the second for $n \ge 6$, and the third for $n \ge 7$ minimum *SDD* indices. For convenience, we use some notations to denote some classes of bicyclic graphs as follows:

 $\mathbf{B}_1^1(n)$: the set of bicyclic graphs obtained from C_n by adding an edge, where $n \ge 4$.

 $\mathbf{B}_1^2(n)$: the set of bicyclic graphs obtained by joining two vertex-disjoint cycles C_a and C_b with a + b = n by an edge, where $n \ge 6$.

 $\mathbf{B}_2(n)$: the set of bicyclic graphs obtained from $C_a = v_0 v_1 \dots v_{a-1}$ with $4 \le a \le n-2$ by joining v_0 and v_2 by an edge, and attaching a path on n-a vertices to v_1 .

 $\mathbf{B}_{3}^{1}(n)$: the set of bicyclic graphs obtained by joining two non-adjacent vertices of C_{a} with $4 \leq a \leq n-1$ by a path of length n-a+1, where $n \geq 5$.

 $\mathbf{B}_{3}^{2}(n)$: the set of bicyclic graphs obtained by joining two non-adjacent cycles C_{a} and C_{b} with a + b < n by a path of length n - a - b + 1, where $n \geq 7$.

 $\mathbf{B}_4(n)$: the set of bicyclic graphs obtained by attaching a path on at least two vertices to the two vertices of degree two of the unique 4-vertex bicyclic graph, where $n \ge 8$.

 $\mathbf{B}_{5}^{1}(n)$: the set of bicyclic graphs obtained from a graph in $\mathbf{B}_{1}^{1}(k)$ with $k \geq 5$ or $\mathbf{B}_{1}^{2}(k)$ with $k \geq 6$ by attaching a path on $n - k \geq 2$ vertices to a vertex of degree two, whose two neighbors are of degree two and three, where $n \geq 7$.

 $\mathbf{B}_{5}^{2}(n)$: the set of bicyclic graphs obtained from a graph in $\mathbf{B}_{3}^{1}(k)$ with $k \geq 5$ or $\mathbf{B}_{3}^{2}(k)$ with $k \geq 7$ by attaching a path on $n - k \geq 2$ vertices to a vertex of degree two, whose two neighbors are both of degree three, where $n \geq 7$.

 $\mathbf{B}_6(n)$: the set of bicyclic graphs obtained from $C_{n-1} = v_0 v_1 \dots v_{n-2}$ by joining v_0 and

 v_2 by an edge, and attaching a vertex of degree one to v_1 , where $n \ge 5$.

Theorem 5. Among the set of n-vertex bicyclic graphs,

- (i) the graphs in B¹₁(n) for n ≥ 4 and the graphs in B²₁(n) for n ≥ 6 are the unique graphs with the minimum SDD index, which is equal to 2n + ⁸/₃.
- (ii) the graphs in $B_2(n) \cup B_3^1(n)$ for $n \ge 6$ and the graphs in $B_3^2(n)$ for $n \ge 7$ are the unique graphs with the second minimum SDD index, which is equal to 2n + 3.
- (iii) the graphs in $\mathbf{B}_5^1(n) \cup \mathbf{B}_5^2(n)$ for $n \ge 7$ and the graphs in $\mathbf{B}_4(n)$ for $n \ge 8$ are the unique graphs with the third minimum SDD index, which is equal to $2n + \frac{10}{3}$.

Proof. Let G be an n-vertex bicyclic graph, where $n \ge 4$.

If k = 0, then $3 \le \Delta \le 4$. If $G \in \mathbf{B}_1^1(n)$ or $G \in \mathbf{B}_1^2(n)$ with $n \ge 6$, then $SDD(G) = \left(\frac{2}{3} + \frac{3}{2}\right) \times 4 + 2(n-3) = 2n + \frac{8}{3}$. If $G \in \mathbf{B}_3^1(n)$ with $n \ge 5$ or $G \in \mathbf{B}_3^2(n)$ with $n \ge 7$, then $SDD(G) = \left(\frac{2}{3} + \frac{3}{2}\right) \times 6 + 2(n-5) = 2n + 3$. If G is a graph obtained by identifying one vertex of two cycles, then $SDD(G) = \left(\frac{2}{4} + \frac{4}{2}\right) \times 4 + 2(n-3) = 2n + 4 > 2n + \frac{10}{3}$.

If k = 1, then $3 \le \Delta \le 5$ and we need to consider the following two cases: (a) this pendent path is of length one, (b) the pendent path is of length at least two. If (a) holds and $\Delta = 4, 5$, then there are at least two edges in G connecting vertices of degree two and Δ . Together with the single pendent edge in G, we have

$$SDD(G) \ge \left(\frac{2}{\Delta} + \frac{\Delta}{2}\right) \times 2 + \left(\frac{1}{3} + 3\right) + 2(n-2)$$
$$\ge \left(\frac{2}{4} + \frac{4}{2}\right) \times 2 + \left(\frac{1}{3} + 3\right) + 2(n-2)$$
$$= 2n + \frac{13}{3}$$
$$> 2n + \frac{10}{3}.$$

If (a) holds and $\Delta = 3$, then there are exactly three vertices, say x, y, z, of degree three in G. Suppose that at most two pairs of vertices x, y, z are adjacent, then there are at least four edges in G connecting vertices of degree two and three. Together with the unique pendent edge in G, we obtain

$$SDD(G) \ge \left(\frac{2}{3} + \frac{3}{2}\right) \times 4 + \left(\frac{1}{3} + 3\right) + 2(n-4) = 2n+4 > 2n + \frac{10}{3}.$$

Suppose that x, y, z are pairwise adjacent, then $G = \mathbf{B}_6(n)$ with $n \ge 5$ and

$$SDD(G) \ge \left(\frac{2}{3} + \frac{3}{2}\right) \times 2 + \left(\frac{1}{3} + 3\right) + 2(n-2) = 2n + \frac{11}{3} > 2n + \frac{10}{3}$$

If (b) holds and $\Delta = 4, 5$, then there are at least three edges in G connecting of degree two and Δ . Consider the single pendent edge in G, then we have

$$SDD(G) \ge \left(\frac{2}{\Delta} + \frac{\Delta}{2}\right) \times 3 + \left(\frac{1}{2} + 2\right) + 2(n-3)$$
$$\ge \left(\frac{2}{4} + \frac{4}{2}\right) \times 3 + \left(\frac{1}{2} + 2\right) + 2(n-3)$$
$$= 2n + 4$$
$$> 2n + \frac{10}{3}.$$

If (b) holds and $\Delta = 3$, then there are three vertices, say u_1, u_2, u_3 , of degree three in G. Assume that at most one pair of vertices u_1, u_2, u_3 is adjacent, then one can see that there are at least seven edges connecting vertices of degree two and three. Note that there is a pendent edge in G, we have

$$SDD(G) \ge \left(\frac{2}{3} + \frac{3}{2}\right) \times 7 + \left(\frac{1}{2} + 2\right) + 2(n-7) = 2n + \frac{11}{3} > 2n + \frac{10}{3}$$

Assume that there are two pairs of vertices u_1 , u_2 , u_3 are adjacent, then $G \in \mathbf{B}_5^1(n)$ or $G \in \mathbf{B}_5^2(n)$ with $n \ge 7$, and

$$SDD(G) = \left(\frac{2}{3} + \frac{3}{2}\right) \times 5 + \left(\frac{1}{2} + 2\right) + 2(n-5) = 2n + \frac{10}{3}.$$

Suppose that u_1, u_2, u_3 are pairwise adjacent, then $G \in \mathbf{B}_2(n)$ with $n \ge 6$, and

$$SDD(G) = \left(\frac{2}{3} + \frac{3}{2}\right) \times 3 + \left(\frac{1}{2} + 2\right) + 2(n-3) = 2n+3.$$

If k = 2, then $3 \le \Delta \le 6$. Suppose that $4 \le \Delta \le 6$, then there are at least two edges in G connecting vertices of degree two and Δ . Note that there are two pendent paths in G, then we have

$$SDD(G) \ge \left(\frac{2}{\Delta} + \frac{\Delta}{2}\right) \times 2 + \left(\frac{1}{2} + 2 + \frac{2}{3} + \frac{3}{2}\right) \times 2 + 2(n-5)$$
$$\ge \left(\frac{2}{4} + \frac{4}{2}\right) \times 2 + \left(\frac{1}{2} + 2 + \frac{2}{3} + \frac{3}{2}\right) \times 2 + 2(n-5)$$
$$= 2n + \frac{13}{3}$$
$$> 2n + \frac{10}{3}.$$

Suppose that $\Delta = 3$, then there are exactly four vertices, say v_1 , v_2 , v_3 , v_4 , of degree three in G. If there is at least one pendent path of length one, then

$$SDD(G) \ge \left(\frac{1}{3}+3\right) + \left(\frac{1}{2}+2+\frac{2}{3}+\frac{3}{2}\right) + 2(n-2) = 2n+4 > 2n+\frac{10}{3}.$$

Otherwise, the two pendent paths are of length at least two. Since G is a bicyclic graph, then at most five pairs of vertices v_1 , v_2 , v_3 , v_4 are adjacent. Suppose that at most four pairs of v_1 , v_2 , v_3 , v_4 are adjacent, then there are at least four edges in G connecting vertices of degree two and three. Consider the two pendent edges in G, then we have

$$SDD(G) \ge \left(\frac{2}{3} + \frac{3}{2}\right) \times 4 + \left(\frac{1}{2} + 2\right) \times 2 + 2(n-5) = 2n + \frac{11}{3} > 2n + \frac{10}{3}$$

Suppose that there are five pairs of vertices of v_1 , v_2 , v_3 , v_4 are adjacent, then $G \in \mathbf{B}_4(n)$ with $n \ge 8$, and

$$SDD(G) = \left(\frac{2}{3} + \frac{3}{2}\right) \times 2 + \left(\frac{1}{2} + 2\right) \times 2 + 2(n-3) = 2n + \frac{10}{3}.$$

If $k \geq 3$, then by Lemma 1, we have

$$SDD(G) \ge \frac{2}{3}k + 2(n+1) \ge \frac{2}{3} \times 3 + 2(n+1) = 2n + 4 > 2n + \frac{10}{3}$$

From the above arguments, the result follows easily (see Fig. 4).



Figure 4. Examples of the bicyclic graphs in Theorem 5 (i)-(iii) with smallest numbers of vertices.

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References

- J. Devillers, A. T. Balaban (Eds.), Topological Indices and Related Descriptors in QSAR and QSPR, Gordon & Brench, Amsterdam, 1999.
- [2] Z. Du, B. Zhou, N. Trinajstić, On geometric–arithemetic indices of (molecular) trees, unicyclic graphs and bicyclic graphs, MATCH Commun. Math. Comput. Chem. 66 (2011) 681–697.
- [3] Z. Du, B. Zhou, On Randić indices of trees, unicyclic graphs, and bicyclic graphs, Int J. Quantum Chem. 111 (2011) 2760–2770.
- [4] M. Dehmer, K. Varmuza, D. Bonchev (Eds.), Statistical Modeling of Molecular Descriptors in QSAR/QSPR, Wiley, New York, 2012.
- [5] B. Furtula, A. Graovac, D. Vukičević, Atom-bond connectivity index of trees, *Discr. Appl. Math.* 157 (2009) 2828–2835.
- [6] 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) #e25659.
- [7] C. K. Gupta, V. Lokesha, S. B. Shwetha, On the symmetric division deg index of graph, *Southeast Asian Bull. Math.* 40 (2016) 59–80.
- [8] C. K. Gupta, V. Lokesha, S. B. Shwetha, P. S. Ranjini, Graph operations on the symmetric division deg index of graphs, *Palest. J. Math.* 6 (2017) 280–286.
- [9] I. Gutman, Degree-based topological indices, Croat. Chem. Acta. 86 (2013) 351-361.
- [10] M. Karelson, Molecular Descriptors in QSAR/QSPR, Wiley, New York, 2000.
- Milano chemometrics and QSAR research group, molecular descriptors dataset, http://www.moleculardescriptors.eu/dataset/dataset.htm.
- [12] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley–VCH, Weinheim, 2000.
- [13] R. Todeschini, V. Consonni, Molecular Descriptors for Chemoinformatics, Wiley, New York, 2009.
- [14] A. Vasilyev, Upper and lower bounds of symmetric division deg index, Iran. J. Math. Chem. 2 (2014) 91–98.
- [15] A. Vasilyev, D. Stevanović, MathChem: a Python package for calculating topological indices, MATCH Commun. Math. Comput. Chem. 71 (2014) 657–680.
- [16] D. Vukičević, M. Gašperov, Bond addictive modeling 1. Adriatic indices, Croat. Chem. Acta. 83 (2010) 243–260.