

ORDERING TETRACYCLIC CONNECTED GRAPHS HAVING MINIMUM DEGREE DISTANCE

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ABSTRACT. Degree distance is an important molecular descriptor which has gained much attention in the recent past. It provides valuable insights into the connectivity and properties of molecular graphs, making it a powerful tool in chemical graph theory. Ordering of graphs with certain parameters allows chemists to identify patterns and trends of different chemical compounds and as a result, predict their reaction behaviour accordingly. In this paper, first ten graphs are presented which have minimum degree distance in the class of tetracyclic connected graphs provided $n \geq 15$, along with their values (in ascending order).

Keywords: Degree sequence, Molecular descriptor, Cyclic graphs, Ordering.

AMS Subject Classification: 05C10, 05C12, 05C35, 05C38

1. INTRODUCTION

Consider simple, finite and undirected graphs. The number of vertices and edges in a graph G are called its order and size, respectively. Number of edges incident to a vertex v refers to its degree and usually denoted by d_v . If $d_v = 1$, then v is called a pendent vertex. Minimum and maximum degree in the graph G is usually denoted by $\delta(G)$ and $\Delta(G)$ respectively. Let ρ denotes the number of non-pendent vertices in a graph and $d(u, v)$ is the distance between two vertices u and v . The maximum distance from a vertex v to all other vertices of a graph is known as eccentricity of v (written as $ecc(v)$) and maximum ecc among the vertices of a graph is known as diameter of the graph ($Diam(G)$).

Suppose $\mathcal{G}_n$ be a connected graph having order n . If the deletion of four appropriate edges produce an acyclic graph of order n then $\mathcal{G}_n$ is considered among tetracyclic graphs (will be written as $\mathcal{G}_n^4$). Similarly, unicyclic ($\mathcal{G}_n^1$), bicyclic ($\mathcal{G}_n^2$) and tricyclic ($\mathcal{G}_n^3$) graphs can be defined. In the class of $\mathcal{G}_n^4$, number of edges are $n + 3$.

Let I be a graph invariant which associates a graph $\mathcal{G}$ with a real number and satisfies

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the equation $I(\mathcal{G}) = I(\mathcal{G}^*)$, where the graph $\mathcal{G}^*$ is isomorphic to $\mathcal{G}$. Molecular descriptors are graph invariant which have many applications. Degree distance is one of the several well-known molecular descriptor which has shown significant better results as compare to other degree-based molecular descriptors. It is the tailored form of well-known Wiener index. It was devised by Dobrynin and Kochetova [1] in 1994 to characterize alkanes by an integer. It is described as under:-

$$D'(\mathcal{G}) = \sum_{u \in V} d_u \sum_{v \in V} d(u, v)$$

Since then a lot of work has been done on $D'(\mathcal{G})$. Ordering of connected graphs is an important concept which characterizes a sequence of graphs having minimum (or maximum) values of a molecular descriptor along with its values (usually in ascending order). Through ordering, chemists can make several connections between chemical properties and reaction behaviour of a chemical compound.

Tomescu [2] used a novel technique to determine minimum value of $D'(\mathcal{G})$ in the class of $\mathcal{G}_n$ provided that $n \geq 2$. In [3], Tomescu gave an idea to order some graphs using extremal values of a topological index. He presented first three connected graphs which had minimum values of $D'(\mathcal{G})$ if $\mathcal{G} \in \mathcal{G}_n$ with $n \geq 4$ (these graphs were $K_{1,n-1}$, $BS(n-3, 1)$ and $K_{1,n-1} + e$, in this order). In the same class of graphs, Tomescu and Kanwal [4] determined next six graphs having different diameters (two of $\text{Diam}(\mathcal{G})=2$, three of $\text{Diam}(\mathcal{G})=3$ and 1 of $\text{Diam}(\mathcal{G})=4$) and satisfying $n \geq 15$, hence completed a series of nine graphs which had smallest $D'(\mathcal{G})$ in the class of $\mathcal{G}_n$.

A.I. Tomescu [5] determined the minimum values of $D'(\mathcal{G})$ in the classes of $\mathcal{G}_n^1$ and $\mathcal{G}_n^2$ provided that $n \geq 3$ and $n \geq 4$ respectively. For chemical trees, ordering by Wiener polarity index was determined by Ashrafi and Ghalavand [6]. Same authors also established [7] an ordering in chemical trees having $n \geq 13$, chemical unicyclic graphs having $n \geq 7$, chemical bicyclic graphs having $n \geq 6$ and chemical tricyclic graphs having $n \geq 8$ using Randić and sum-connectivity numbers.

In the class of $\mathcal{G}_n^1$, Tomescu and Kanwal [8] determined ordering by characterizing four graphs having minimum $D'(\mathcal{G})$, provided $n \geq 15$ (one has $\text{Diam}(\mathcal{G})=2$ and three has $\text{Diam}(\mathcal{G})=3$). Ghalavand and Ashrafi [9] presented ordering of unicyclic (chemical) graphs with the help of Wiener polarity index. Same authors also devised [10] ordering of c-cyclic graphs (simply connected and connected chemical graphs with c as cyclomatic number) by considering total irregularity in the graph.

In the class of $\mathcal{G}_n^2$ graphs, Dragan and Tomescu [11] devised ordering of seven graphs having minimum values of $D'(\mathcal{G})$ provided that $n \geq 19$ and having $\text{Diam}(\mathcal{G})$ equal to 2 or 3. Wei Zhu et al. [12] determined two graphs having smallest $D'(\mathcal{G})$ in the class of $\mathcal{G}_n^3$ provided $n \geq 5$ and both had the same value of $D'(\mathcal{G})$. In [13], authors have determined ordering of the graphs in the class of $\mathcal{G}_n^3$ by characterizing first sixteen graphs in this class which have minimum values of $D'(\mathcal{G})$ and determined their values.

In the class of $\mathcal{G}_n^4$, N. Khan et al. [14] characterized an extremal graph which had minimum value of $D'(\mathcal{G})$ and determined its value i.e. $D'(\mathcal{G}) = 3n^2 + 9n - 48$ provided that $n \geq 6$. In this article, by getting enough motivation from all referred research articles, we are presenting a possible ordering in the class of $\mathcal{G}_n^4$ by characterizing first ten graphs which have minimum values of $D'(\mathcal{G})$ along with their values of $D'(\mathcal{G})$.

2. PRELIMINARY RESULTS

This section presents basic results that are used to prove the main results. The symmetric function

$$S(y_1, y_2, \dots, y_r) = \sum_{i=1}^r y_i(2n - 2 - y_i)$$

was defined in [3] $\forall (y_1, y_2, \dots, y_r) \in \mathcal{D}_{r,s,w,z}$, where $\mathcal{D}_{r,s,w,z} = \{y_j \mid 1 \leq y_j \leq s \text{ for } 1 \leq j \leq r, y_1 \geq y_2 \geq \dots \geq y_r \geq 1, y_1 \geq y_2 \geq \dots \geq y_z \geq 2 \text{ and } \sum_{j=1}^r y_j = w \text{ whenever } s \leq n-1 \text{ and } 4 \leq z \leq r\}$. Considering the transformation $\mathcal{T}$ over the vectors in $\mathcal{D}_{r,s,w,z}$, defined as follows: If $1 \leq j < k \leq r, y_j \leq s-1$ and $y_k \geq 2$ (or $y_k \geq 3$ if $k \leq z$) then replace $(y_1, y_2, \dots, y_r)$ by $(y_1, y_2, \dots, y_{j+1}, \dots, y_{k-1}, \dots, y_r)$. We will get $(y_1^*, y_2^*, \dots, y_r^*) \in \mathcal{D}_{r,s,w,z}$ which results $S(y_1, y_2, \dots, y_r) - S(y_1^*, y_2^*, \dots, y_r^*) = 2(1 + y_j - y_k) > 0$ which shows that $S(y_1, y_2, \dots, y_r)$ can be strictly decreased over $\mathcal{D}_{r,s,w,z}$.

Lemma 2.1. [3] *Let a vertex $v \in \mathcal{G}_n$ having eccentricity e . If $e = 1$ then $D'(v) = (n-1)^2$, if $e = 2$ then $D'(v) = d_v(2n-2-d_v)$ and for $e \geq 3$ we have $D'(v) \geq d_v(2n-d_v + \frac{e^2-3e}{2} - 1)$*

Corollary 2.1. [11] *Let $V(\mathcal{G}) = \{v_i \mid 1 \leq i \leq n\}$ represents vertex set of $\mathcal{G}_n$ then*

$$D'(\mathcal{G}) \geq \sum_{i=1}^n d_{v_i}(2n-2-d_{v_i})$$

Lemma 2.2. [11] *Consider $\mathcal{G} \in \mathcal{G}_n$ with $n \geq 4$ and $\Delta = n-2$ then any pendent vertex v_p of $\mathcal{G}_n$ has $\text{ecc}(v_p) \geq 3$.*

Lemma 2.3. [14] *If $\mathcal{G} \in \mathcal{G}_n^4$ with $n \geq 5$ then the integers $n-1 \geq d_1 \geq d_2 \geq \dots \geq d_n \geq 1$ are the degrees of $V(\mathcal{G})$ iff:*

- i. $\sum_{j=1}^n d_j = 2n+6$
- ii. *The minimum degree of at least five vertices is 2.*

Lemma 2.4. *Ten graphs are presented in figure 1. By direct computations, the values of $D'(\mathcal{G})$ of these graphs are as follows:*

$$D'(G_1) = 3n^2 + 9n - 48, D'(G_2) = 3n^2 + 9n - 46, D'(G_3) = D'(G_4) = 3n^2 + 9n - 44, \\ D'(G_5) = D'(G_6) = 3n^2 + 9n - 42, D'(G_7) = D'(G_8) = 3n^2 + 9n - 40, D'(G_9) = \\ 3n^2 + 9n - 38, D'(G_{10}) = 3n^2 + 9n - 36.$$

3. MAIN RESULTS

In this section, first ten graphs in the class of $\mathcal{G}_n^4$ are presented which have minimum values of $D'(\mathcal{G})$ along with its values.

Theorem 3.1. *If $\mathcal{G} \in \mathcal{G}_n^4$ then the graphs which have minimum values of $D'(\mathcal{G})$ are $G_1 - G_{10}$ (in this order) shown in the Figure 1, provided that $n \geq 15$. All these graphs have $\text{Diam}(\mathcal{G})$ equal to 2 or 3.*

We present some lemmas that are useful to prove the main theorem.

Lemma 3.1. *In the class of $\mathcal{G}_n^4$, the graphs satisfying $\Delta = n-1$ and $D'(\mathcal{G}) \leq 3n^2 + 9n - 36$ are $G_1 - G_{10}$, provided that $n \geq 9$.*

Proof. Let $\mathcal{G} \in \mathcal{G}_n^4$ is satisfying the hypothesis of the lemma. We will prove the lemma using different values of ρ .

If $\rho = 5$, then the degree sequence will be $(n-1, \epsilon, \zeta, \eta, \theta, 1, \dots, 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq 2$

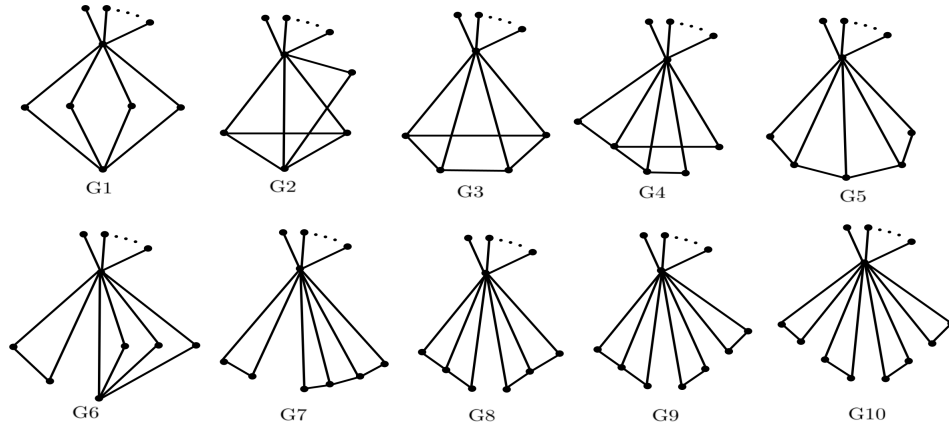


FIGURE 1. First Ten Tetracyclic Graphs having Minimum Degree Distance

and $\epsilon + \zeta + \eta + \theta = 12$. Only graphical degree sequences will be $(n-1, 4, 3, 3, 2, 1, \dots, 1)$ and $(n-1, 3, 3, 3, 3, 1, \dots, 1)$ which have unique graphical realizations characterized as G_2 and G_3 respectively in Figure 1.

If $\rho = 6$, then the degree sequence will be $(n-1, \epsilon, \zeta, \eta, \theta, \iota, 1, \dots, 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota = 13$. It results that the only graphical degree sequences will be $(n-1, 5, 2, 2, 2, 2, 1, \dots, 1)$, $(n-1, 4, 3, 2, 2, 2, 1, \dots, 1)$ and $(n-1, 3, 3, 3, 2, 2, 1, \dots, 1)$. These sequences have unique graphical realizations characterized as G_1 , G_6 and G_4 respectively in Figure 1.

If $\rho = 7$, then the degree sequence will be $(n-1, \epsilon, \zeta, \eta, \theta, \iota, \kappa, 1, \dots, 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq \kappa \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota + \kappa = 14$. Only graphical degree sequences will be $(n-1, 4, 2, 2, 2, 2, 2, 1, \dots, 1)$ and $(n-1, 3, 3, 2, 2, 2, 2, 1, \dots, 1)$. The former sequence has a unique graphical realization characterized as G_5 in Figure 1. In case of the later sequence, there are two graphical realizations characterized as G_7 and G_8 in Figure 1.

If $\rho = 8$, then the degree sequence will be $(n-1, \epsilon, \zeta, \eta, \theta, \iota, \kappa, \lambda, 1, \dots, 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq \kappa \geq \lambda \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota + \kappa + \lambda = 15$. It results that the only graphical degree sequence will be $(n-1, 3, 2, 2, 2, 2, 2, 2, 1, \dots, 1)$ which has a unique graphical realization characterized as G_9 in Figure 1.

If $\rho = 9$, then the degree sequence will be $(n-1, \epsilon, \zeta, \eta, \theta, \iota, \kappa, \lambda, \mu, 1, \dots, 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq \kappa \geq \lambda \geq \mu \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota + \kappa + \lambda + \mu = 16$. The only graphical degree sequence will be $(n-1, 2, 2, 2, 2, 2, 2, 2, 2, 1, \dots, 1)$ which has a unique graphical realization characterized as G_{10} in Figure 1.

There is no such graph in $\mathcal{G}_n^4$ fulfilling the conditions of the lemma if $\rho \geq 9$. □

Lemma 3.2. Let $\mathcal{G} \in \mathcal{G}_n^4$ having $\Delta = n-2$ then $D'(\mathcal{G}) > 3n^2 + 9n - 36$ provided that $n \geq 14$.

Proof. Let $\mathcal{G}$ is a graph fulfilling the hypothesis of this lemma.

If $\rho = 5$, then the degree sequence will be $(n-2, \epsilon, \zeta, \eta, \theta, 1, \dots, 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq 2$ and $\epsilon + \zeta + \eta + \theta = 13$. It results that the only graphical degree sequences will be $(n-2, 5, 3, 3, 2, 1, \dots, 1)$, $(n-2, 4, 4, 3, 2, 1, \dots, 1)$ and $(n-2, 4, 3, 3, 3, 1, \dots, 1)$. In case of $(n-2, 5, 3, 3, 2, 1, \dots, 1)$, there is a unique graphical realization which is characterized as G_{16} in Figure 2. Furthermore, using Lemmas 2.1 and 2.2, we have $D'(\mathcal{G}) \geq S(n-2, 5, 3, 3, 2) + (n-5)(2n-3) = 3n^2 + 11n - 58 > 3n^2 + 9n - 36$ for $n \geq 12$. In case of

$(n-2, 4, 4, 3, 2, 1, \dots, 1)$, there are two graphical realizations which are characterized as G_{14} and G_{15} in Figure 2. Furthermore, we have $D'(\mathcal{G}) \geq S(n-2, 4, 4, 3, 2) + (n-5)(2n-3) = 3n^2 + 11n - 56 > 3n^2 + 9n - 36$ for $n \geq 11$. Now for $(n-2, 4, 3, 3, 3, 1, \dots, 1)$, there are three graphical realizations which are characterized as G_{11} , G_{12} and G_{13} in Figure 2. We also have $D'(\mathcal{G}) \geq S(n-2, 4, 3, 3, 3) + (n-5)(2n-3) = 3n^2 + 11n - 54 > 3n^2 + 9n - 36$ for $n \geq 10$.

If $\rho = 6$, then the degree sequence will be $(n-2, \epsilon, \zeta, \eta, \theta, \iota, 1, \dots, 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota = 14$. This corresponds to following graphical sequences: $(n-2, 6, 2, 2, 2, 2, 1, \dots, 1)$, $(n-2, 5, 3, 2, 2, 2, 1, \dots, 1)$, $(n-2, 4, 4, 2, 2, 2, 1, \dots, 1)$, $(n-2, 4, 3, 3, 2, 2, 1, \dots, 1)$ and $(n-2, 3, 3, 3, 3, 2, 1, \dots, 1)$. In case of $(n-2, 6, 2, 2, 2, 2, 1, \dots, 1)$, there is a unique graphical realization which is characterized as G_{17} in Figure 2. Furthermore, using Lemma 2.1 and 2.2, we have $D'(\mathcal{G}) \geq S(n-2, 6, 2, 2, 2, 2) + (n-6)(2n-3) = 3n^2 + 11n - 62 > 3n^2 + 9n - 36$ for $n \geq 14$. In case of $(n-2, 5, 3, 2, 2, 2, 1, \dots, 1)$, a unique graphical realization is characterized as G_{18} in Figure 2. Furthermore, we have $D'(\mathcal{G}) \geq S(n-2, 5, 3, 2, 2, 2) + (n-6)(2n-3) = 3n^2 + 11n - 56 > 3n^2 + 9n - 36$ for $n \geq 11$. For $(n-2, 4, 4, 2, 2, 2, 1, \dots, 1)$, there are many graphical realizations but we have (using Lemma 2.1 and 2.2), $D'(\mathcal{G}) \geq S(n-2, 4, 4, 2, 2, 2) + (n-6)(2n-3) = 3n^2 + 11n - 54 > 3n^2 + 9n - 36$ for $n \geq 10$.

In case of $(n-2, 4, 3, 3, 2, 2, 1, \dots, 1)$, G_{19} in Figure 2 is a unique graphical realization. We also have $D'(\mathcal{G}) \geq S(n-2, 4, 3, 3, 2, 2) + (n-6)(2n-3) = 3n^2 + 11n - 62 > 3n^2 + 9n - 36$ for $n \geq 14$. Next for $(n-2, 3, 3, 3, 3, 2, 1, \dots, 1)$, there are many graphical realizations. But we have $D'(\mathcal{G}) \geq S(n-2, 3, 3, 3, 3, 2) + (n-6)(2n-3) = 3n^2 + 11n - 50 > 3n^2 + 9n - 36$ for $n \geq 8$.

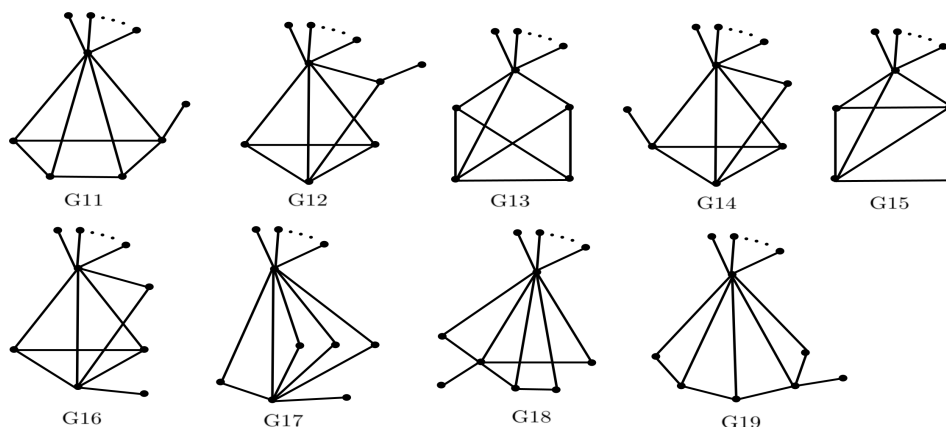
If $\rho = 7$, then the degree sequence will be $(n-2, \epsilon, \zeta, \eta, \theta, \iota, \kappa, 1, \dots, 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq \kappa \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota + \kappa = 15$. This corresponds to following graphical sequences: $(n-2, 5, 2, 2, 2, 2, 2, 1, \dots, 1)$, $(n-2, 4, 3, 2, 2, 2, 2, 1, \dots, 1)$ and $(n-2, 3, 3, 3, 2, 2, 2, 1, \dots, 1)$. In these cases, there are multiple graphical realizations but we have following calculations:

$D'(\mathcal{G}) \geq S(n-2, 5, 2, 2, 2, 2, 2) + (n-7)(2n-3) = 3n^2 + 11n - 54 > 3n^2 + 9n - 36$ for $n \geq 10$,
 $D'(\mathcal{G}) \geq S(n-2, 4, 3, 2, 2, 2, 2) + (n-7)(2n-3) = 3n^2 + 11n - 50 > 3n^2 + 9n - 36$ for $n \geq 8$
and $D'(\mathcal{G}) \geq S(n-2, 3, 3, 3, 2, 2, 2) + (n-7)(2n-3) = 3n^2 + 11n - 48 > 3n^2 + 9n - 36$ for $n \geq 7$.

If $\rho = 8$, then the degree sequence will be $(n-2, \epsilon, \zeta, \eta, \theta, \iota, \kappa, \lambda, 1, \dots, 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq \kappa \geq \lambda \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota + \kappa + \lambda = 16$. It results that the only graphical degree sequences are $(n-2, 4, 2, 2, 2, 2, 2, 2, 1, \dots, 1)$ and $(n-2, 3, 3, 2, 2, 2, 2, 2, 1, \dots, 1)$ which have many graphical realizations. We have $D'(\mathcal{G}) \geq S(n-2, 4, 2, 2, 2, 2, 2, 2) + (n-8)(2n-3) = 3n^2 + 11n - 48 > 3n^2 + 9n - 36$ for $n \geq 7$ and $D'(\mathcal{G}) \geq S(n-2, 3, 3, 2, 2, 2, 2, 2) + (n-8)(2n-3) = 3n^2 + 11n - 46 > 3n^2 + 9n - 36$ for $n \geq 6$.

If $\rho = 9$, then the degree sequence will be $(n-2, \epsilon, \zeta, \eta, \theta, \iota, \kappa, \lambda, \mu, 1, \dots, 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq \kappa \geq \lambda \geq \mu \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota + \kappa + \lambda + \mu = 17$. The only graphical degree sequence is $(n-2, 3, 2, 2, 2, 2, 2, 2, 2, 1, \dots, 1)$ which has many graphical realizations. We have, $D'(\mathcal{G}) \geq S(n-2, 3, 2, 2, 2, 2, 2, 2, 2) + (n-9)(2n-3) = 3n^2 + 11n - 52 > 3n^2 + 9n - 36$ for $n \geq 9$.

If $\rho = 10$, then the degree sequence will be $(n-2, \epsilon, \zeta, \eta, \theta, \iota, \kappa, \lambda, \mu, \nu, 1, \dots, 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq \kappa \geq \lambda \geq \mu \geq \nu \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota + \kappa + \lambda + \mu + \nu = 18$. The only graphical degree sequence is $(n-2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 1, \dots, 1)$ which has many graphical realizations. We have, $D'(\mathcal{G}) \geq S(n-2, 2, 2, 2, 2, 2, 2, 2, 2, 2) + (n-10)(2n-3) = 3n^2 + 11n - 42 > 3n^2 + 9n - 36$ for $n \geq 4$.

FIGURE 2. Graphs G_{11} - G_{19}

In case of $\rho = 11$, $\sum_{i=1}^{10} d_i = 19$ which is not possible (where $d_i \geq 2$ for $i = 1, \dots, 10$). Hence there is no further graph which fulfils the conditions of the lemma if $\rho \geq 11$. $\square$

Lemma 3.3. *If $\mathcal{G} \in \mathcal{G}_n^4$ having $\Delta \leq n - 3$ and $n \geq 15$ then $D'(\mathcal{G}) > 3n^2 + 9n - 36$*

Proof. Let $\mathcal{G}$ is a graph fulfilling the conditions of this lemma. Consider the symmetric function S and set of vectors $\mathcal{D}_{r,s,w,z}$. By incorporating the conditions of the lemma leads to $\mathcal{D}_{n,s,2n+6,z}$ with $s \leq n-3$ (which contains all graphs satisfying conditions of the lemma). Using corollary 2.1, we get $D'(\mathcal{G}) \geq \min S(y_1, y_2, \dots, y_r)$ where $(y_1, y_2, \dots, y_r) \in \mathcal{D}_{n,s,2n+6,z}$ with $s \leq n-4$ and $z \geq 5$. Consider this minimum as $g(n, s, 2n+6, z)$. Suppose $z_2 \geq z_1 \geq 5$ and $s_1 \geq s_2$ then we have $g(n, s, 2n+6, z_1) \leq g(n, s, 2n+6, z_2)$ and $g(n, s_1, 2n+6, 5) \leq g(n, s_2, 2n+6, 5)$. It results $\min g(n, s, 2n+6, z)$ is reached for $s = n-3$ and $z = 5$. Thus, $\min S(y_1, y_2, \dots, y_r)$ over $\mathcal{D}_{n,n-3,2n+6,5}$ is realized for $(n-3, 8, 2, 2, 1, \dots, 1)$ which leads to $S(n-3, 8, 2, 2, 1, \dots, 1) = 3n^2 + 13n - 92 > 3n^2 + 9n - 36$ for $n \geq 15$. Hence the result follows. $\square$

Proof of Theorem 3.1 By using lemmas 3.1-3.3, the result follows.

4. CONCLUSION

In this paper, we have determined the first ten graphs in the class of $\mathcal{G}_n^4$ which have minimum values of $D'(\mathcal{G})$ along with their values. Although ordering of graphs is generally challenging, the authors have tried to achieve ordering on the basis of degree distance of graphs. It is expected that this research article will help chemists in a number of ways such as identifying the most reactive and stable conformations of a molecule, predicting a biological activity by observing different changes in the molecular structure, preparing more accurate QSAR models, and determining the most efficient pathways for synthesizing target compounds. The authors feel that this work can be further extended in the following directions:

- i. Explore the ordering in the class of k -cyclic graphs ($k \geq 5$) with respect to the degree distance.
- ii. Explore the ordering in some classes of graphs with a fixed diameter.
- iii. Ordering k -cyclic ($k \geq 1$) graphs having a fixed girth.

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