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Ordering Tricyclic Connected Graphs Having Minimum Degree Distance

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Abstract

Degree distance $D'(G)$ is an important molecular descriptor which provides valuable insights into the connectivity and properties of molecular graphs, making it a powerful tool in diverse areas of chemical graph theory. This descriptor has attained much attention in the recent past for its broad range of applicability in different problems of 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 behavior accordingly. In this paper, the first sixteen tricyclic graphs are presented which have minimum degree distances (in ascending order) if $n \geq 31$.

1 Introduction

In this paper, simple, finite and undirected graphs are considered. The order and size of a graph represent the number of vertices and edges in it, respectively. In chemical compounds, atoms may be regarded as vertices and their covalent bonds can be visualized as the edges of a graph. The degree of a vertex u refers to number of edges incident to it and is usually denoted by d_u. If $d_u = 1$ then u is said to be a pendent vertex. The minimum and maximum degree in the graph G are usually denoted by $\delta(G)$ and $\Delta(G)$, respectively. Let ρ denote the number of non-pendent vertices in a graph and let $d(u, v)$ denote 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 the eccentricity of v (written as $ecc(v)$) and maximum eccentricity among the vertices of the graph is known as diameter of the graph, denoted by diam(G).
Suppose $\mathcal{G}_n$ is a connected graph of order n. $\mathcal{G}_n$ is considered a tricyclic graphs (written as $\mathcal{G}_n^3$) if the deletion of three appropriate edges produces an acyclic graph of order n. Similar

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definitions hold for unicyclic ($\mathcal{G}_n^1$) and bicyclic ($\mathcal{G}_n^2$) graphs. In the class of $\mathcal{G}_n^3$, the number of edges is $n+2$.

A graph invariant I associates a real number with a graph $\mathcal{G}$, which satisfies the equation $I(\mathcal{G})$ = I($\mathcal{G}^*$) for every graph $\mathcal{G}^*$ isomorphic (structurally equivalent) to $\mathcal{G}$. Molecular descriptors, also known as topological indices, are graph invariant which have many applications in chemical graph theory. The Degree distance is one of the several well-known molecular descriptors that has shown significant better results compared to other degree-based molecular descriptors. It is the tailored form of well-known Wiener index. It was introduced 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 $D'(\mathcal{G})$. The ordering of connected graphs is an important concept which characterizes a sequence of graphs having minimum (or maximum) values of a topological index along with its values (usually in ascending order). Through ordering, chemists can make several connections between chemical properties and reaction behavior of a chemical compound. Tomescu [2] presented the first three graphs having minimum $D'(\mathcal{G})$ if $\mathcal{G} \in \mathcal{G}_n$ with $n \geq 4$ (these graphs are $K_{1,n-1}, BS(n-3,1)$ and $K_{1,n-1}+e$). In [3], Tomescu and Kanwal presented the next six graphs satisfying $n \geq 15$ having different diameters (two of diam($\mathcal{G}$)=2, three of diam($\mathcal{G}$)=3 and one of diam($\mathcal{G}$)=4) and hence completed a series of nine graphs having smallest $D'(\mathcal{G})$. In [4], Tomescu and Kanwal ordered four graphs that belong to $\mathcal{G}_n^1$ having minimum $D'(\mathcal{G})$, provided $n \geq 15$ (one has diam($\mathcal{G}$)=2 and three has diam($\mathcal{G}$)=3). In the class of $\mathcal{G}_n^2$ graphs, Dragan and Tomescu [5] determined ordering of seven graphs having minimum values of $D'(\mathcal{G})$ provided that $n \geq 19$ and having diam($\mathcal{G}$) equal to 2 or 3.

Zhu et al. [6] determined two graphs having smallest $D'(\mathcal{G})$ in the class of $\mathcal{G}_n^3$ provided $n \geq 5$ and both have the same value of $D'(\mathcal{G})$. In this paper, the next fourteen graphs (making a series of sixteen) in the class of $\mathcal{G}_n^3$ are characterized along with their values which have minimum values of $D'(\mathcal{G})$.

2 Preliminary results

In this section, some basic results are presented, which are used to prove the results in the next section. The symmetric function

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

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

Lemma 2.1. *([2]). Let a vertex $v \in \mathcal{G}_n$ have 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 2.2. *([5]). Let $V(\mathcal{G}) = \{v_i |\ 1 \leq i \leq n\}$ represent vertex set of $\mathcal{G}_n$ then*

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

Lemma 2.3. *([5]). 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 $ecc(v_p) \geq 3$.*

Lemma 2.4. *If $\mathcal{G} \in \mathcal{G}_n^3$ with order $n \geq 4$ then there are at least four vertices of minimum degree 2.*

Proof. K_4 is the minimal graph in the class of $\mathcal{G}_n^3$ which has four vertices of degree 2. The condition holds for all other graphs in the class of $\mathcal{G}_n^3$. ■

Lemma 2.5. *Sixteen graphs are presented in Figure 1. By direct computations,the values of $D'(\mathcal{G})$ of these graphs are as follows:*
$D'(G_1) = D'(G_2) = 3n^2 + 5n - 32$, $D'(G_3) = 3n^2 + 5n - 30$,
$D'(G_4) = 3n^2+5n-28$, $D'(G_5) = 3n^2+5n-26$, $D'(G_6) = 3n^2+9n-52$, $D'(G_7) = 3n^2+9n-46$,
$D'(G_8) = 3n^2+9n-43$, $D'(G_9) = 3n^2+9n-40$, $D'(G_{10}) = D'(G_{11}) = D'(G_{12}) = 3n^2+9n-38$,
$D'(G_{13}) = 3n^2 + 9n - 36$, $D'(G_{14}) = D'(G_{15}) = 3n^2 + 9n - 34$, $D'(G_{16}) = 3n^2 + 9n - 32$.

3 Main results

In this section, the first sixteen graphs in the class of $\mathcal{G}_n^3$ are presented which have minimum values of $D'(\mathcal{G})$ along with their values. To prove the main result, a few lemmas are useful.

Lemma 3.1. *In the class of $\mathcal{G}_n^3$, the graphs having $\Delta = n - 1$ and $D'(\mathcal{G}) < 3n^2 + 9n - 32$ are $G_1 - G_5$, depicted in Figure 1, provided that $n \geq 7$.*

Proof. Let $\mathcal{G} \in \mathcal{G}_n^3$ satisfying the hypothesis of the lemma. We will prove it using different values of ρ.
If $\rho = 4$, then the degree sequence will be $(n-1, \epsilon, \zeta, \eta, 1, ..., 1)$, where $\epsilon \geq \zeta \geq \eta \geq 2$ and $\epsilon + \zeta + \eta = 9$. It results that the only graphical degree sequence will be $(n-1, 3, 3, 3, 1, ..., 1)$ which has a unique graphical realization characterized as G_1 in Figure 1.
If $\rho = 5$, then the degree sequence will be $(n-1, \epsilon, \zeta, \eta, \theta, 1, ..., 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq 2$ and $\epsilon + \zeta + \eta + \theta = 10$. Only graphical degree sequences will be $(n-1, 4, 2, 2, 2, 1, ..., 1)$ and $(n-1, 3, 3, 2, 2, 1, ..., 1)$ 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 $(n-1, \epsilon, \zeta, \eta, \theta, \iota, 1, ..., 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota = 11$. It results that the only graphical degree sequence will be $(n-1, 3, 2, 2, 2, 2, 1, ..., 1)$. This sequence has a unique graphical realization characterized as G_4 in Figure 1.
If $\rho = 7$, then the degree sequence will be $(n-1, \epsilon, \zeta, \eta, \theta, \iota, \kappa, 1, ..., 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq \kappa \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota + \kappa = 12$. Only graphical degree sequence will be $(n-1, 2, 2, 2, 2, 2, 2, 1, ..., 1)$. This sequence has a unique graphical realization characterized as G_5 in Figure 1.
There is no such graph in $\mathcal{G}_n^3$ fulfilling the conditions of the lemma if $\rho \geq 8$. ■

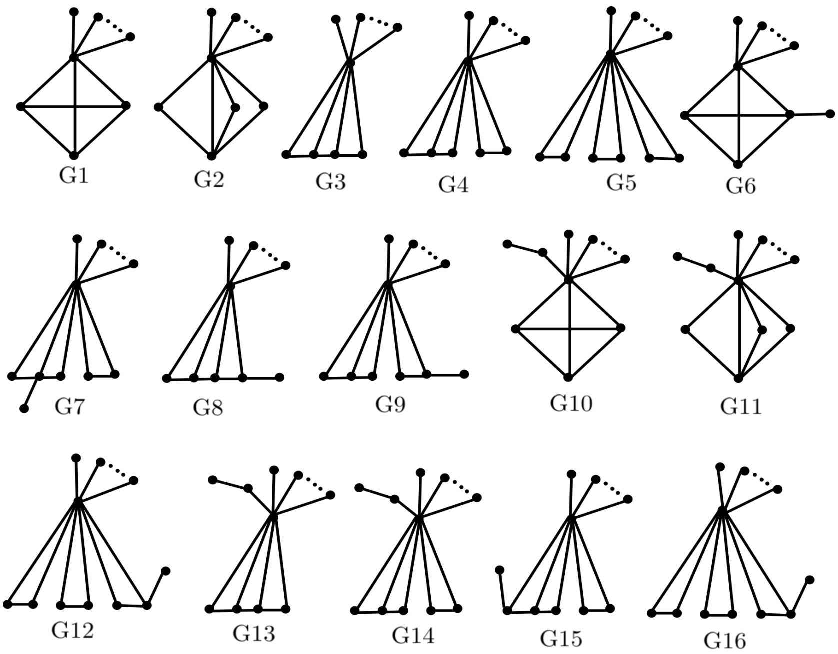

Figure 1: The first sixteen graphs having minimum degree distance.

Lemma 3.2. *Let $\mathcal{G} \in \mathcal{G}_n^3$, the graphs having $\Delta = n-2$ and $D'(\mathcal{G}) \leq 3n^2+9n-32$ are $G_6 - G_{16}$, depicted in Figure 1, provided that $n \geq 24$.*

Proof. Let $\mathcal{G} \in \mathcal{G}_n^3$ having $\Delta = n-2$. When $\rho = 4$, the degree sequence will be $(n-2, \epsilon, \zeta, \eta, 1, ..., 1)$, where $\epsilon \geq \zeta \geq \eta \geq 2$ and $\epsilon + \zeta + \eta = 10$. This results that the only graphical degree sequence will be $(n-2, 4, 3, 3, 1, ..., 1)$ which has a unique graphical realization characterized as G_6 in Figure 1.

If $\rho = 5$, then the degree sequence will be $(n-2, \epsilon, \zeta, \eta, \theta, 1, ..., 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq 2$ and $\epsilon + \zeta + \eta + \theta = 11$. It results that the only graphical degree sequences will be $(n-2, 4, 3, 2, 2, 1, ..., 1)$ and $(n-2, 3, 3, 3, 2, 1, ..., 1)$. In case of $(n-2, 4, 3, 2, 2, 1, ..., 1)$, there are two graphical realizations which are characterized as G_{17} and G_{18} in Figure 2. Furthermore, $D'(G_{17}) = 3n^2 + 19n - 49 > 3n^2 + 9n - 32$ for $n \geq 2$ and $D'(G_{18}) = 3n^2 + 10n - 55 > 3n^2 + 9n - 32$ for $n \geq 24$. In case of $(n-2, 3, 3, 3, 2, 1, ..., 1)$, there are four graphical realizations which are characterized as G_8, G_{10} in Figure 1 and G_{19}, G_{20} in Figure 2. Moreover, $D'(G_{19}) = 3n^2+10n-53 > 3n^2+9n-32$ for $n \geq 22$ and $D'(G_{20}) = 3n^2+11n-55 > 3n^2+9n-32$ for $n \geq 12$.

If $\rho = 6$, then the degree sequence will be $(n-2, \epsilon, \zeta, \eta, \theta, \iota, 1, ..., 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota = 12$. Only graphical degree sequences will be $(n-2, 4, 2, 2, 2, 2, 1, ..., 1)$ and $(n-2, 3, 3, 2, 2, 2, 1, ..., 1)$. In case of $(n-2, 4, 2, 2, 2, 2, 1, ..., 1)$, there are three graphical realizations which are characterized as G_7, G_{11} in Figure 1 and G_{21} in Figure 2. Furthermore, $D'(G_{21}) = 3n^2+12n-68 > 3n^2+9n-32$ for $n \geq 13$. In case of $(n-2, 3, 3, 2, 2, 2, 1, ..., 1)$, there are seven graphical realizations which are characterized as G_9, G_{13} and G_{15} in Figure 1 and G_{22}, G_{23}, G_{24} and G_{25} in Figure 2. Moreover, $D'(G_{22}) = 3n^2+10n-46 > 3n^2+9n-32$ for $n \geq 15$, $D'(G_{23}) = 3n^2+11n-60 > 3n^2+9n-32$ for $n \geq 15$, $D'(G_{24}) = 3n^2+10n-54 > 3n^2+9n-32$ for $n \geq 23$ and $D'(G_{25}) = 3n^2 + 10n - 53 > 3n^2 + 10n - 50$ for $n \geq 19$

If $\rho = 7$, then the degree sequence will be $(n-2, \epsilon, \zeta, \eta, \theta, \iota, \kappa, 1, ..., 1)$, where $\epsilon \geq \zeta \geq \eta \geq$

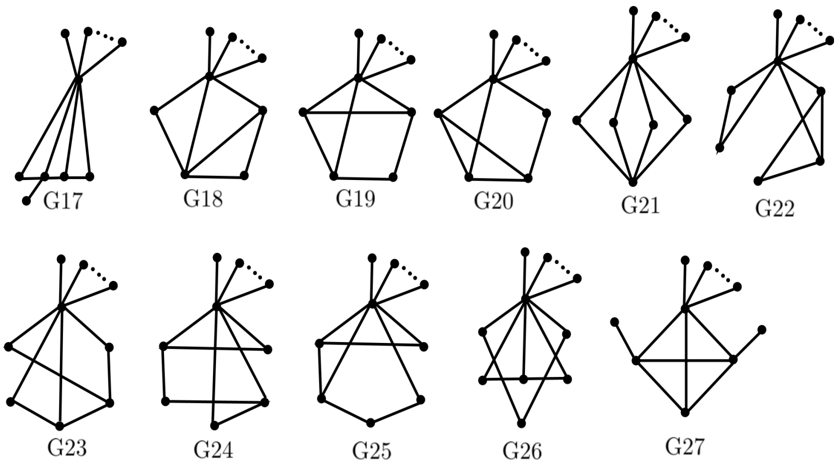

Figure 2: Graphs G_{17}-G_{27}.

$\theta \geq \iota \geq \kappa \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota + \kappa = 13$. Only graphical degree sequence will be $(n-2, 3, 2, 2, 2, 2, 2, 1, ..., 1)$ which has three graphical realizations characterized as G_{12} and G_{14} in Figure 1 and G_{26} in Figure 2. Moreover, $D'(G_{26}) = 3n^2 + 10n - 42 > 3n^2 + 9n - 32$ for $n \geq 11$

If $\rho = 8$, then the degree sequence will be $(n-2, \epsilon, \zeta, \eta, \theta, \iota, \kappa, \lambda, 1, ..., 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq \kappa \geq \lambda \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota + \kappa + \lambda = 14$. It results that the only graphical degree sequence will be $(n-2, 2, 2, 2, 2, 2, 2, 2, 1, ..., 1)$, which has a unique graphical realization characterized as G_{16} in Figure 1.

If $\rho = 9$, then the degree sequence will be $(n-2, \epsilon, \zeta, \eta, \theta, \iota, \kappa, \lambda, \mu, 1, ..., 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq \kappa \geq \lambda \geq \mu \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota + \kappa + \lambda + \mu = 15$, which is not possible. Similarly, in the case of $\delta = 10$, $\sum_{i=1}^{9} d_i = 16$, which is again not possible (where $d_i \geq 2$ for $i = 1, ..., 9$). Hence there is no further graph fulfilling the conditions of the lemma if $\rho \geq 9$. ■

Lemma 3.3. *If $\mathcal{G} \in \mathcal{G}_n^3$ having $\Delta = n - 3$ and $n \geq 23$, then we have $D'(\mathcal{G}) > 3n^2 + 9n - 32$.*

Proof. Let $\mathcal{G} \in \mathcal{G}_n^3$ having $\Delta = n - 3$. When $\rho = 4$, the degree sequence will be $(n-3, \epsilon, \zeta, \eta, 1, ..., 1)$, where $\epsilon \geq \zeta \geq \eta \geq 2$ and $\epsilon + \zeta + \eta = 11$ which results the only graphical degree sequence is $(n-3, 4, 4, 3, 1, ..., 1)$. This degree sequence has a unique graphical realization characterized as G_{27} in Figure 2 and $D'(G_{27}) = 3n^2 + 13n - 76 > 3n^2 + 9n - 32$ for $n \geq 12$.

If $\rho = 5$, then the degree sequence will be $(n-3, \epsilon, \zeta, \eta, \theta, 1, ..., 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq 2$ and $\epsilon + \zeta + \eta + \theta = 12$. It results that only graphical degree sequences will be $(n-3, 4, 4, 2, 2, 1, ..., 1)$, $(n-3, 4, 3, 3, 2, 1, ..., 1)$ and $(n-3, 3, 3, 3, 3, 1, ..., 1)$. These degree sequences have many graphical realizations. In case of $(n-3, 4, 4, 2, 2, 1, ..., 1)$, using Lemmas 2.1 and 2.3, we have

$D'(\mathcal{G}) \geq S(n-3, 4, 4, 2, 2) + (n-5)(2n-2) = 3n^2 + 10n - 57 > 3n^2 + 9n - 32$ for $n \geq 26$.

Similarly, for $(n-3, 4, 3, 3, 2, 1, ..., 1)$ we have

$D'(\mathcal{G}) \geq S(n-3, 4, 3, 3, 2) + (n-5)(2n-2) = 3n^2 + 10n - 55 > 3n^2 + 9n - 32$ for $n \geq 24$

and for $(n-3, 3, 3, 3, 3, 1, ..., 1)$ we have

$D'(\mathcal{G}) \geq S(n-3, 3, 3, 3, 3) + (n-5)(2n-2) = 3n^2 + 10n - 53 > 3n^2 + 9n - 32$ for $n \geq 22$.

If $\rho = 6$, then the degree sequence will be $(n-3, \epsilon, \zeta, \eta, \theta, \iota, 1, ..., 1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq 2$ and $\epsilon + \zeta + \eta + \theta + \iota = 13$. The only graphical degree sequences will be $(n-3, 4, 3, 2, 2, 2, 1, ..., 1)$ and $(n-3, 3, 3, 3, 2, 2, 1, ..., 1)$. These degree sequences have many graphical realizations. In the case of $(n-3, 4, 3, 2, 2, 2, 1, ..., 1)$, we have

$D'(\mathcal{G}) \geq S(n-3,4,3,2,2,2) + (n-6)(2n-2) = 3n^2+10n-54 > 3n^2+9n-32$ for $n \geq 23$.
Similarly, for $(n-3,3,3,3,2,2,1,...,1)$ we have
$D'(\mathcal{G}) \geq S(n-3,3,3,3,2,2) + (n-6)(2n-2) = 3n^2+10n-52 > 3n^2+9n-32$ for $n \geq 21$.
If $\rho = 7$, then the degree sequence will be $(n-3,\epsilon,\zeta,\eta,\theta,\iota,\kappa,1,...,1)$, where $\epsilon \geq \zeta \geq \eta \geq \theta \geq \iota \geq \kappa \geq 2$ and $\epsilon+\zeta+\eta+\theta+\iota+\kappa = 14$. Consequently, the only graphical degree sequence is $(n-3,3,3,2,2,2,2,1,...,1)$ which has many graphical realizations, so we have
$D'(\mathcal{G}) \geq S(n-3,3,3,2,2,2,2) + (n-7)(2n-2) = 3n^2+10n-51 > 3n^2+9n-32$ for $n \geq 20$.
In view of the above, similar results hold for $\rho \geq 8$. Hence, the result follows. ■

Lemma 3.4. *If $\mathcal{G} \in \mathcal{G}_n^3$ having $\Delta \leq n-4$ and $n \geq 31$ then $D'(\mathcal{G}) > 3n^2+9n-32$.*

Proof. Let $\mathcal{G} \in \mathcal{G}_n^3$ having $\Delta \leq n-4$. Consider the symmetric function S and the set of vectors $\mathcal{D}_{r,s,w,z}$. Incorporating the conditions of the lemma leads to $\mathcal{D}_{n,s,2n+4,z}$ with $s \leq n-4$ (which contains all graphs that satisfy the conditions of the lemma). Using Corollary 2.2, we get $D'(\mathcal{G}) \geq min\ S(y_1,y_2,...,y_r)$ where $(y_1,y_2,...,y_r) \in \mathcal{D}_{n,s,2n+4,z}$ with $s \leq n-4$ and $z \geq 4$. Consider this minimum as $g(n,s,2n+4,z)$. Suppose $z_2 \geq z_1 \geq 4$ and $s_1 \geq s_2$ then we have $g(n,s,2n+4,z_1) \leq g(n,s,2n+4,z_2)$ and $g(n,s_1,2n+4,4) \leq g(n,s_2,2n+4,4)$. It results that $min\ g(n,s,2n+4,z)$ is reached for $s = n-4$ and $z = 4$. Thus, $min\ S(y_1,y_2,...,y_r)$ over $\mathcal{D}_{n,n-4,2n+4,4}$ is realized for $(n-4,8,2,2,1,...,1)$, which leads to $S(n-4,8,2,2,1,...,1) = 3n^2+11n-92 > 3n^2+9n-32$ for $n \geq 31$. Hence the result follows. ■

Theorem 3.5. *If $\mathcal{G} \in \mathcal{G}_n^3$ then the graphs that have minimum values of $D'(\mathcal{G})$ are $G_1 - G_{16}$ (in this order), depicted in Figure 1, provided that $n \geq 31$. All these graphs have diam($\mathcal{G}$) equal to 2 or 3.*

Proof. Using Lemmas 3.1 to 3.4, the result follows. ■

4 Concluding remarks

In this paper, we have determined the first sixteen graphs in the class of $\mathcal{G}_n^3$ which have minimum values of $D'(\mathcal{G})$ along with its values. Although, in general, ordering of graphs is difficult to estimate perfectly, however the authors have tried this in the best possible manner. It would be interesting to find the same characterization of $D'(\mathcal{G})$ in the class of connected $k-$cyclic graphs with $k \geq 4$.

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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