Electronic Journal of Mathematics
www.shahindp.com/locate/ejm

Electron. J. Math. **6** (2023) 33–55
DOI: 10.47443/ejm.2023.041

Research Article

Minimum Wiener index of unicyclic chemical graphs with girth 3

Junxiu Wu, Yubin Gao*

School of Mathematics, North University of China, Taiyuan, Shanxi 030051, P. R. China

(Received: 11 September 2023. Received in revised form: 23 October 2023. Accepted: 30 October 2023. Published online: 2 November 2023.)

Abstract

The Wiener index of a connected graph G is defined as the sum of distances between all unordered pairs of vertices of G. It is one of the most-studied topological indices in mathematical chemistry. Determining the minimum Wiener index among all connected graphs of order n with a given girth and maximum degree is an open problem proposed by Chen and Li in the paper [*MATCH Commun. Math. Comput. Chem.* **88** (2022) 683–703]. The main goal of the present paper is to provide a partial solution to this open problem by characterizing the graphs attaining the minimum Wiener index among all unicyclic graphs of order n with girth 3 and maximum degree 4.

Keywords: chemical graph; Wiener index; extremal graph.

2020 Mathematics Subject Classification: 05C50, 05C09, 05C92.

1. Introduction

Let G be a graph with the vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex $v \in V(G)$ is the number of vertices adjacent to v. The maximum degree of G, denoted by $\Delta(G)$ or Δ for short, is the maximum degree of its vertices. The distance $d_G(u, v)$ between the vertices u and v in a connected graph G is the length of any shortest path in G connecting u and v. The girth $g(G)$ of a graph G with at least one cycle is equal to the length of any shortest cycle in G. As usual, we denote the complete graph, path, and star of order n by K_n, P_n, and S_n, respectively.

The Wiener index $W(G)$ of a connected graph G is defined by

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u, v). \tag{1}$$

The Wiener index is one of the most-studied topological indices in mathematical chemistry. It was introduced by Wiener in 1947 to analyze some aspects of branching by fitting experimental data for several properties of alkane compounds. It is known that the star S_n and path P_n have the minimum and maximum Wiener indices, respectively, among all trees of order n. Also, the complete graph K_n and path P_n have the minimum and maximum Wiener indices, respectively, among all connected graphs of order n. There are many known results of this type for more specific classes of graphs; for example, see [1–11]. Particularly, the readers interested in known mathematical properties of this index are referred to the surveys [2, 5, 10].

In [1], Chen and Li determined the graphs that have the maximum Wiener index among all connected graphs of order n with girth g and maximum degree Δ, and proposed the following open problem:

Problem 1.1 (see [1]). *Determine the minimum Wiener index among all connected graphs of order n with given girth and maximum degree.*

In this paper, we attempt to solve Problem 1.1 for unicyclic chemical graphs with girth 3. A connected graph G is a unicyclic graph if G has a unique cycle. The graph G is said to be a chemical graph if $\Delta(G) \le 4$. Let $\mathcal{CG}(n, 3)$ be the set of all unicyclic chemical graphs of order n and girth 3. A graph $G \in \mathcal{CG}(n, 3)$ is said to be a Wiener-minimal graph of $\mathcal{CG}(n, 3)$ if G has the minimum Wiener index in $\mathcal{CG}(n, 3)$. A characterization of Wiener-minimal graphs of $\mathcal{CG}(n, 3)$ is given in this paper.

*Corresponding author (ybgao@nuc.edu.cn).

2. Preliminaries

Lemma 2.1 (see [7]). *Let G_0 be a connected graph and $u_1, u_2 \in V(G_0)$. Let G be the graph obtained from G_0 by attaching k_1, k_2 pendant edges to u_1, u_2, respectively. Let G_i be the graph obtained from G_0 by attaching $k_1 + k_2$ pendant edges to u_i $(i = 1, 2)$. Then, either $W(G_1) < W(G)$ or $W(G_2) < W(G)$.*

Let $T = T_n(d, \Delta)$ be a tree of order n and maximum degree Δ as shown in Figure 1, which is defined in [3], where $\Delta \geq 3$, $d \leq \Delta$,

(1) all vertices of T lie on some line R_i for $0 \leq i \leq k + 1$;

(2) the vertex w is the root of T and $d_T(w) = d$;

(3) if $V(R_i)$ is used to denote the set of the vertices on line R_i, then $|V(R_0)| = |\{w\}| = 1$, $|V(R_i)| = d(\Delta - 1)^{i-1}$ for $i = 1, 2, \ldots, k$, and $|V(R_{k+1})| = n - 1 - d\sum_{i=1}^{k}(\Delta - 1)^{i-1}$; and

(4) if $|V(R_{k+1})| = m(\Delta - 1) + r$ for some $0 \leq r < \Delta - 1$, and $V(R_k) = \{v_1, v_2, \ldots, v_{d(\Delta-1)^{k-1}}\}$ such that v_i lies left of v_j on line R_k for $i < j$, then $d_T(v_i) = \Delta$ for $1 \leq i \leq m$, $d_T(v_{m+1}) = r + 1$, and $d_T(v_i) = 1$ for $m + 2 \leq i \leq d(\Delta - 1)^{k-1}$.

For convenience, we say that $k+1$ is the height of $T_n(d, \Delta)$ and the vertices of $V(R_{k+1})$ are the last-layer vertices of $T_n(d, \Delta)$. We also say that $T_n(d, \Delta)$ is a (d, Δ)-tree of height $k + 1$.

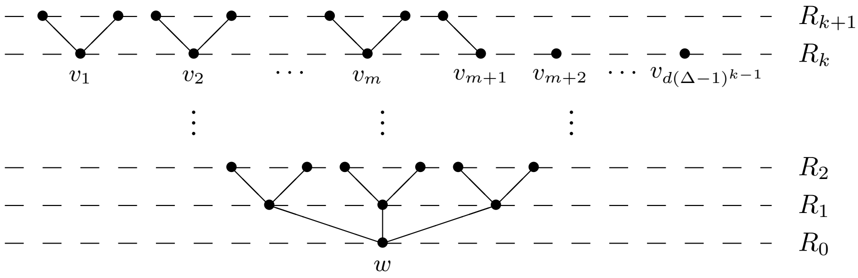

Figure 1: The tree $T = T_n(d, \Delta)$.

Lemma 2.2 (see [3]). *Let T be a tree of order n and maximum degree at most Δ $(\Delta \geq 3)$. Then*

$$W(T) \geq W(T_n(\Delta, \Delta)),$$

where the equality holds if and only if $T \cong T_n(\Delta, \Delta)$.

Now, let us consider the $(2, 4)$-tree $T_n(2, 4)$ of height $k + 1$ as depicted in Figure 1 with $d = 2$ and $\Delta = 4$. Note that

$$\sum_{i=0}^{k} |V(R_i)| = 1 + \sum_{i=1}^{k} 2 \cdot 3^{i-1} = 3^k, \; |V(R_{k+1})| = n - 3^k, \; \text{ and } 3^k < n \leq 3^{k+1}.$$

If $n = 3^{k+1}$, then we say that $T_n(2, 4)$ is saturated; otherwise, we say that it is unsaturated. Let us use $T^{k+1}(2, 4)$ to denote a saturated $(2, 4)$-tree of height $k + 1$.

Lemma 2.3. *Let $T = T^{k+1}(2, 4)$ be a saturated $(2, 4)$-tree of height $k + 1$ with root w as depicted in Figure 1, and let $x \in V(R_{k+1})$. Then*

$$\sum_{y \in V(T)} d_T(w, y) = \frac{1}{2}\left(3^{k+1}(2k + 1) + 1\right), \tag{2}$$

$$\sum_{y \in V(T)} d_T(x, y) = 2k \cdot 3^{k+1} + k + 3. \tag{3}$$

Proof. Note that $|V(R_i)| = 2 \cdot 3^{i-1}$ for $i = 1, 2, \ldots, k + 1$. Then

$$\sum_{y \in V(T)} d_T(w, y) = \sum_{i=1}^{k+1} i \cdot |V(R_i)| = \frac{1}{2}\left(3^{k+1}(2k + 1) + 1\right).$$

Thus, (2) holds.

Take $x \in V(R_{k+1})$. Let $P = wx_1x_2\dots x_kx$ be the path of T from the root w to x, where $x_i \in V(R_i)$ for $i = 1, 2, \dots, k$. Then $T - E(P)$ has $k+2$ components $T_0, T_1, \dots, T_{k+1}$, where $w \in V(T_0)$, $x_i \in V(T_i)$ for $i = 1, 2, \dots, k$, and $x \in V(T_{k+1})$. It is easy to see that $T_0 = T^{k+1}(1,4)$ with the root w, $T_i = T^{k-i+1}(2,4)$ with the root x_i for $i = 1, 2, \dots, k$, and $T_{k+1} = \{x\}$. Let us take $x_0 = w$. Then

$$\begin{aligned}\sum_{y\in V(T)} d_T(x,y) &= \sum_{i=0}^{k}\sum_{y\in V(T_i)} d_T(x,y) = \sum_{i=0}^{k}\sum_{y\in V(T_i)} \left(d_T(x,x_i) + d_T(x_i,y)\right)\\ &= \sum_{i=0}^{k}\left((k+1-i)|V(T_i)| + \sum_{y\in V(T_i)} d_T(x_i,y)\right).\end{aligned}$$

Note that

$$|V(T_0)| = \frac{1}{2}(3^{k+1}+1),\quad |V(T_i)| = 3^{k-i+1},\ i = 1, 2, \dots, k,$$

and by (2),

$$\sum_{y\in V(T_0)} d_T(x_0,y) = \frac{1}{4}\left(3^{k+1}(2k+1)+1\right),$$

$$\sum_{y\in V(T_i)} d_T(x_i,y) = \frac{1}{2}\left(3^{k-i+1}(2k-2i+1)+1\right),\ i = 1, 2, \dots, k.$$

Thus,

$$\begin{aligned}\sum_{y\in V(T)} d_T(x,y) =& \frac{1}{2}(k+1)(3^{k+1}+1) + \frac{1}{4}\left(3^{k+1}(2k+1)+1\right)\\ &+ \sum_{i=1}^{k}\left((k+1-i)\cdot 3^{k-i+1} + \frac{1}{2}\left(3^{k-i+1}(2k-2i+1)+1\right)\right)\\ =& 2k\cdot 3^{k+1} + k + 3.\end{aligned}$$

Hence, (3) holds. □

Lemma 2.4. *Let $T = T_n(2,4)$ be a $(2,4)$-tree of height $k+1$ with root w as depicted in Figure 1. Let x be the right-most vertex on line R_{k+1}. Then*

(1).

$$\sum_{y\in V(T)} d_T(w,y) = \frac{1}{2}\left(3^k(2k-1)+1\right) + (k+1)(n-3^k). \tag{4}$$

(2). *The equation $|V(R_{k+1}) \setminus \{x\}| = n - 3^k - 1$ can be rewritten as*

$$n - 3^k - 1 = \sum_{i=1}^{s} p_i \cdot 3^{k+1-i}, \tag{5}$$

where $0 \le s \le k+1$, $0 \le p_1 \le 1$, $0 \le p_i \le 2$ for $i = 2, \dots, s-1$, and $1 \le p_s \le 2$. Also

$$\sum_{y\in V(T)\setminus V(R_{k+1})} d_T(x,y) = 3^k(2k-1) + k + 2, \tag{6}$$

$$\sum_{y\in V(T)} d_T(x,y) = \sum_{i=1}^{s} 2(k-i+2)p_i\cdot 3^{k+1-i} + 3^k(2k-1) + k + 2. \tag{7}$$

Proof. (1). Note that $|V(R_i)| = 2\cdot 3^{i-1}$ for $i = 1, 2, \dots, k$, and $|V(R_{k+1})| = n - 3^k$. Then

$$\sum_{y\in V(T)} d_T(w,y) = \sum_{i=1}^{k+1} i\cdot |V(R_i)| = \frac{1}{2}\left(3^k(2k-1)+1\right) + (k+1)(n-3^k).$$

(2). Let x be the right-most vertex on line R_{k+1} and x^* be the neighbor of x. Take $V_1 = V(R_{k+1})\setminus\{x\}$. Since $|V(R_{k+1})| = n - 3^k$ and $3^k < n \le 3^{k+1}$, we have $0 \le |V_1| = n - 3^k - 1 < 2\cdot 3^k$, and so there are $0 \le s \le k+1$, $0 \le p_1 \le 1$, $0 \le p_i \le 2$ for $i = 2, \dots, s-1$, and $1 \le p_s \le 2$ such that (5) holds. Note that $s = 0$ only if $|V_1| = 0$.

By (5), there are $p_i \cdot 3^{k+1-i}$ vertices in V_1 such that the distance between x and these vertices is $2(k-i+2)$ for $i = 1, \dots, s$. Then

$$\sum_{y\in V_1} d_T(x,y) = \sum_{i=1}^{s} 2(k-i+2)p_i \cdot 3^{k+1-i}.$$

Note that $|V(T) \setminus V(R_{k+1})| = 3^k$. By (3), replacing k with $k-1$, we get

$$\sum_{y\in V(T)\setminus V(R_{k+1})} d_T(x^*,y) = 2(k-1)\cdot 3^k + k + 2,$$

and so,

$$\sum_{y\in V(T)\setminus V(R_{k+1})} d_T(x,y) = |V(T) \setminus V(R_{k+1})| + \sum_{y\in V(T)\setminus V(R_{k+1})} d_T(x^*,y) = 3^k(2k-1) + k + 2.$$

Thus,

$$\begin{aligned}\sum_{y\in V(T)} d_T(x,y) &= \sum_{y\in V_1} d_T(x,y) + \sum_{y\in V(T)\setminus V(R_{k+1})} d_T(x,y)\\ &= \sum_{i=1}^{s} 2(k-i+2)p_i \cdot 3^{k+1-i} + 3^k(2k-1) + k + 2.\end{aligned}$$

Hence, the lemma follows. □

3. Some basic properties of Wiener-minimal graphs of $\mathcal{CG}(n, 3)$

In this section, we give some basic properties of Wiener-minimal graphs of $\mathcal{CG}(n, 3)$. For any $G \in \mathcal{CG}(n, 3)$, it is easy to see that G is a graph as depicted in Figure 2, where $C_3 = w_1w_2w_3$ is the only cycle of length 3, G_i is a chemical tree of order n_i, $w_i \in V(G_i)$, and $d_{G_i}(w_i) \leq 2$ for $i = 1, 2, 3$, and $n_1 + n_2 + n_3 = n$.

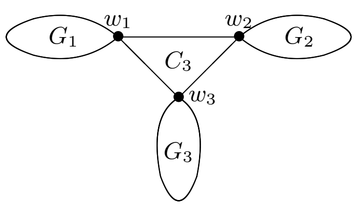

Figure 2: A graph $G \in \mathcal{CG}(n, 3)$.

Lemma 3.1. *Let $G \in \mathcal{CG}(n, 3)$ be a graph as depicted in Figure 2, with $n \geq 25$. If G is a Wiener-minimal graph of $\mathcal{CG}(n, 3)$, then $G_i = T_{n_i}(2, 4)$ with $n_i \geq 3$ for $i = 1, 2, 3$.*

Proof. By Lemma 2.2, we only need to prove that $n_i \geq 3$ for $i = 1, 2, 3$. Suppose to the contrary that there is $1 \leq i \leq 3$ such that $n_i \leq 2$. Without loss of generality, assume that $n_2 \leq 2$. Then, $n_1 + n_3 = n - n_2 \geq 23$. So, we assume that $n_3 \geq n_2$ and $3^k < n_1 \leq 3^{k+1}$, where $k \geq 2$.

Let $x \in V(G_1)$ be the right-most vertex on the line R_{k+1}. Let x^* be the vertex adjacent to x. Let $G' = G - x^*x + w_2x$, $G'_1 = G_1 - x$, $G'_2 = G_2 + w_2x$, and $G'_3 = G_3$. By Lemma 2.4, we assume that

$$n_1 - 3^k - 1 = \sum_{i=1}^{s} p_i \cdot 3^{k+1-i}, \tag{8}$$

where $0 \leq s \leq k+1$, $0 \leq p_1 \leq 1$, $0 \leq p_i \leq 2$ for $i = 2, \dots, s-1$, and $1 \leq p_s \leq 2$, and we have

$$\sum_{y\in V(G_1)} d_G(x,y) = \sum_{i=1}^{s} 2(k-i+2)p_i \cdot 3^{k+1-i} + 3^k(2k-1) + k + 2,$$

$$\begin{aligned}\sum_{y\in V(G_1')} d_{G'}(x,y) = &\sum_{y\in V(G_1')} (2+d_{G'}(w_1,y)) = 2|V(G_1')| + \sum_{y\in V(G_1')} d_{G'}(w_1,y)\\ =&2\,(n_1-1)+\frac{1}{2}\left(3^k(2k-1)+1\right)+(k+1)(n_1-3^k-1)\\ =&(k+3)\sum_{i=1}^{s} p_i\cdot 3^{k+1-i}+\frac{1}{2}\left(3^k(2k+3)+1\right).\end{aligned}$$

Thus,

$$\begin{aligned}W(G)-W(G') =&\sum_{i=1}^{3}\left(\sum_{y\in V(G_i)} d_G(x,y)-\sum_{y\in V(G_i')} d_{G'}(x,y)\right)\\ =&\sum_{i=1}^{s}(k-2i+1)p_i\cdot 3^{k+1-i}+\frac{1}{2}\left(3^k(2k-5)+2k+3\right)+(k+1)n_2+kn_3. \qquad (9)\end{aligned}$$

Case 1. $k\geq 3$.
By (9), we have

$$W(G)-W(G') \geq \frac{1}{2}\left(3^k(2k-5)+2k+3\right)+\sum_{i=3}^{k+1}2(4-2i)\cdot 3^{k+1-i}+2k+1=\frac{1}{2}\left(3^k(2k-7)+10k+7\right)>0,$$

a contradiction.

Case 2. $k=2$.
If $p_1=1$, then by (9), we have

$$W(G)-W(G') \geq \frac{1}{2}\left(3^k(2k-5)+2k+3\right)+3^k+\sum_{i=2}^{3}2(3-2i)\cdot 3^{k+1-i}+2k+1=1.$$

If $p_1=0$, then by (8), $n_1-10\leq 3p_2+p_3\leq 8$, and so $n_1\leq 18$, and $n_2+n_3\geq 7$. By (9), we have

$$W(G)-W(G') \geq \frac{1}{2}\left(3^k(2k-5)+2k+3\right)+\sum_{i=2}^{3}2(3-2i)\cdot 3^{k+1-i}+7k+1=2.$$

Therefore, $W(G)>W(G')$, which again a contradiction. □

In the following, we always assume that $n\geq 25$ and $G\in\mathcal{CG}(n,3)$ is a graph as depicted in Figure 3, where $G_i=T_{n_i}(2,4)$ with $n_i\geq 3$ for $i=1,2,3$, $n_1+n_2+n_3=n$, $3^k<n_1\leq 3^{k+1}$, $3^t<n_2\leq 3^{t+1}$, and $3^\ell<n_3\leq 3^{\ell+1}$. Also, we denote $G=(G_1,n_1,k;\ G_2,n_2,t;\ G_3,n_3,\ell)$, or $G=(G_1;\ G_2;\ G_3)$ or $G=(n_1;\ n_2;\ n_3)$ for short.

Let $T=T_n(2,4)$ be a $(2,4)$-tree of height $k+1$ with root w as depicted in Figure 1. Now, we introduce the concept of a $(2,4)$-subtree of T.

Let $z\in V(R_i)$ $(1\leq i\leq k-1)$ and $N_T(z)=\{z^*,z_1,z_2,z_3\}$, where $z^*\in V(R_{i-1})$ and $z_1,z_2,z_3\in V(R_{i+1})$. Consider $T-z^*z-zz_j$ $(1\leq j\leq 3)$; observe that its component containing the vertex z is a $(2,4)$-tree of height $k-i+1$ or $k-i$ with the root z. We call such a $(2,4)$-tree a $(2,4)$-subtree of T. It is clear that for each vertex $z\in V(R_i)$ with $1\leq i\leq k-1$, T has three different $(2,4)$-subtrees with the root z.

Lemma 3.2. *Let $G\in\mathcal{CG}(n,3)$ be the graph obtained from a unicyclic graph G_0 and two $(2,4)$-trees T_1 and T_2 of height $m+1$, where $m\geq 1$, $V(T_1)\cap V(G_0)=\{w_1\}$, $V(T_2)\cap V(G_0)=\{w_2\}$, and $V(T_1)\cap V(T_2)=\phi$; see Figure 4. If both T_1 and T_2 are unsaturated, then G is not a Wiener-minimal graph of $\mathcal{CG}(n,3)$.*

Proof. Suppose that both T_1 and T_2 are unsaturated $(2,4)$-trees of height $m+1$. Let V_i be the set of all vertices on line ℓ_{m+1} of T_i for $i=1,2$. Then $0<|V_i|<2\cdot 3^m$ for $i=1,2$. Take $V_0=V(G)\setminus(V_1\cup V_2)$. Note that for any $x_1,x_2\in V_1$ and $y_1,y_2\in V_2$, we have $d_G(x_1,y_1)=d_G(x_2,y_2)$ and

$$\sum_{z\in V_0} d_G(x_1,z)=\sum_{z\in V_0} d_G(x_2,z),\quad \sum_{z\in V_0} d_G(y_1,z)=\sum_{z\in V_0} d_G(y_2,z).$$

For simplicity, let us take $d=d_G(x,y)$, $D_1=\sum_{z\in V_0} d_G(x,z)$, and $D_2=\sum_{z\in V_0} d_G(y,z)$ for any $x\in V_1$ and $y\in V_2$. Then $d>2(m+1)$. Without loss of generality, we assume that $D_1\geq D_2$.

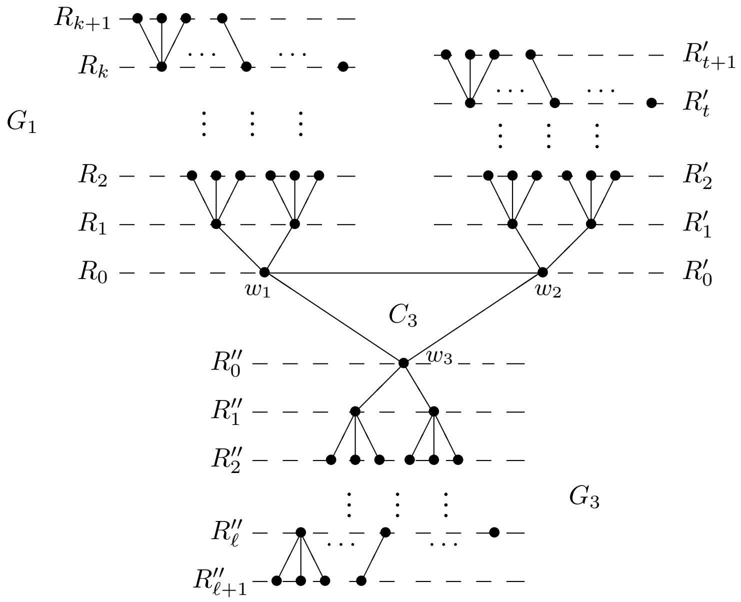

Figure 3: A graph $G \in \mathcal{CG}(n, 3)$.

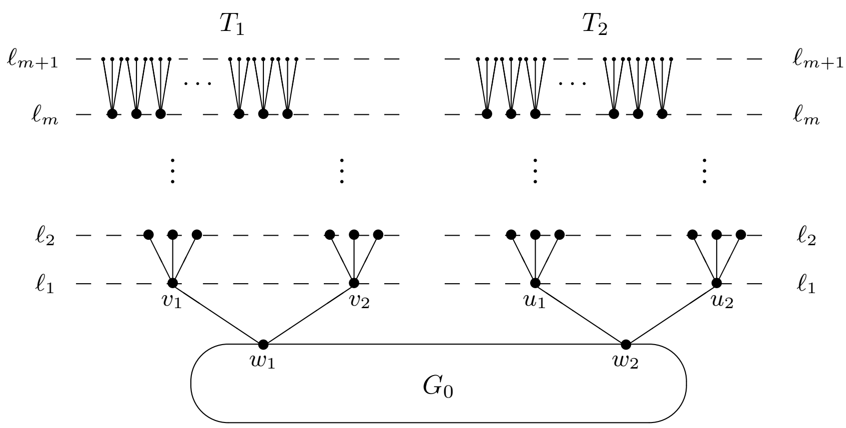

Figure 4: The graph $G \in \mathcal{CG}(n, 3)$ used in Lemma 3.2.

We will prove that there is a graph $G' \in \mathcal{CG}(n, 3)$ such that $W(G) > W(G')$. We prove it by induction on the height of T_1 and T_2.

If the height of T_1 and T_2 is 2 (that is, $m = 1$), then by Lemma 2.1, we assume that $3 \mid |V_1|$ or $3 \mid |V_2|$. Take $G' = G - w_1v_1 - w_2u_2 + w_1u_2 + w_2v_1$, then $G' \in \mathcal{CG}(n, 3)$. If $|V_2| \le 3$ and $|V_1| \le 3$, then

$$W(G) - W(G') = |V_1|\left(D_1 + d|V_2|\right) - |V_1|\left(D_2 + 4|V_2|\right) = |V_1|\left(D_1 - D_2\right) + |V_1||V_2|\left(d - 4\right) > 0.$$

If $|V_2| \le 3$ and $|V_1| > 3$, then $3 \nmid |V_1|$, and so $3 \mid |V_2|$; that is, $|V_2| = 3$. Hence,

$$W(G) - W(G') = 3\left(D_1 + 4(|V_1| - 3) + d|V_2|\right) - 3\left(D_2 + d(|V_1| - 3) + 4|V_2|\right) = 3\left(D_1 - D_2\right) + 3(d-4)\left(|V_2| + 3 - |V_1|\right) > 0.$$

If $3 < |V_2| < 6$, then by Lemma 2.1, $|V_1| = 3$, and hence

$$\begin{aligned} W(G) - W(G') =& |V_1|\left(D_1 + 3d\right) + \left(|V_2| - 3\right)\left(D_2 + 12\right) - |V_1|\left(D_2 + 12\right) - \left(|V_2| - 3\right)\left(D_1 + 3d\right) \\ =& \left(6 - |V_2|\right)\left(D_1 - D_2\right) + \left(6 - |V_2|\right)(3d - 12) > 0. \end{aligned}$$

Thus, the result holds when the height of T_1 and T_2 is 2.

Next, we suppose that $m \ge 1$ and that the result holds when the height of T_1 and T_2 is less than or equal to m. We will prove that the result is true when the height of T_1 and T_2 is $m + 1$.

Consider all the $(2, 4)$-subtrees with the root v_1 or v_2 of T_1 and $(2, 4)$-subtrees with the root u_1 or u_2 of T_2. By the inductive assumption, at most one of these $(2, 4)$-subtrees is unsaturated. This implies that either $3^m \mid |V_1|$ or $3^m \mid |V_2|$. Let

$G' = G - w_1v_1 - w_2u_2 + w_1u_2 + w_2v_1$. Then $G' \in \mathcal{CG}(n,3)$. If $|V_2| \le 3^m$ and $|V_1| \le 3^m$, then

$$W(G) - W(G') = |V_1|\left(D_1 + d|V_2|\right) - |V_1|\left(D_2 + 2(m+1)|V_2|\right) = |V_1|\left(D_1 - D_2\right) + |V_1||V_2|\left(d - 2(m+1)\right) > 0.$$

If $|V_2| \le 3^m$ and $|V_1| > 3^m$, then $3^m \nmid |V_1|$, and so $3^m \mid |V_2|$; that is, $|V_2| = 3^m$ and hence

$$\begin{aligned} W(G) - W(G') =& 3^m\left((2m+1)(|V_1| - 3^m) + D_1 + d|V_2|\right) - 3^m\left(D_2 + (2m+1)|V_2| + d(|V_1| - 3^m)\right) \\ =& 3^m\left(D_1 - D_2\right) + 3^m(d - 2(m+1))\left(|V_2| + 3^m - |V_1|\right) > 0. \end{aligned}$$

If $|V_2| > 3^m$, then $3^m \nmid |V_2|$, and so $3^m \mid |V_1|$; that is, $|V_1| = 3^m$. Thus,

$$\begin{aligned} W(G) - W(G') =& |V_1|\left(D_1 + 3^m d\right) + \left(|V_2| - 3^m\right)\left(D_2 + 2(m+1)3^m\right) - |V_1|\left(D_2 + 2(m+1)3^m\right) - \left(|V_2| - 3^m\right)\left(D_1 + 3^m d\right) \\ =& (2\cdot 3^m - |V_2|)\left(D_1 - D_2\right) + (2\cdot 3^m - |V_2|)3^m(d - 2(m+1)) > 0. \end{aligned}$$

Therefore, the result holds when the height of T_1 and T_2 is $m+1$. □

Lemma 3.3. *Let $G = (G_1, n_1, k;\ G_2, n_2, t;\ G_3, n_3, \ell)$ be a Wiener-minimal graph of $\mathcal{CG}(n,3)$ as depicted in Figure 3 with $3^t < n_2 < 3^{t+1}$.*

(1). *If $k = t$, then $n_1 = 3^{k+1}$.*

(2). *If $k > t$, then $3^{t+1} \mid (n_1 - 3^k)$.*

(3). *If $k = t+1$, then $n_1 = 2\cdot 3^k$ or 3^{k+1}.*

Proof. (1). It follows from Lemma 3.2.

(2). Let $k > t$. If $n_1 = 3^{k+1}$, then $n_1 - 3^k = 2\cdot 3^k$, and so $3^{t+1} \mid (n_1 - 3^k)$. We now assume that $3^k < n_1 < 3^{k+1}$. By Lemma 3.2, for any vertex v on line R_{k-t} of G_1, each $(2,4)$-subtree with the root v of G_1 is saturated. This implies that $3^{t+1} \mid (n_1 - 3^k)$.

(3). If $k = t+1$, then by Part (2), $3^k \mid (n_1 - 3^k)$, and so $n_1 - 3^k = 3^k$ or $2\cdot 3^k$. □

4. Some operations

In this section, we introduce three operations that are very useful to prove the main results.

Operation I

Let $G = (G_1, n_1, k;\ G_2, n_2, t;\ G_3, n_3, \ell) \in \mathcal{CG}(n,3)$ be a graph as depicted in Figure 3 with $3^k < n_1 \le 3^{k+1}$ and $3^t \le n_2 < 3^{t+1}$, and X be the set of m vertices on the line R_{k+1} of G_1 with $1 \le m \le \min\{n_1 - 3^k, 3^{t+1} - n_2\}$. Let G' be the graph obtained from G by moving all vertices of X from G_1 to G_2 such that G' remains in the form of Figure 3. Then, $G' = (G'_1, n_1 - m, k';\ G'_2, n_2 + m, t;\ G'_3, n_3, \ell) \in \mathcal{CG}(n,3)$, where $k' = k$ or $k-1$. We say that G' is obtained from G by **Operation I (moving m vertices from G_1 to G_2)**.

Lemma 4.1. *Let $G' = (G'_1, n_1 - m, k';\ G'_2, n_2 + m, t';\ G'_3, n_3, \ell) \in \mathcal{CG}(n,3)$ be the graph obtained from G by Operation I (moving m vertices from G_1 to G_2). Then*

$$\begin{aligned} W(G) - W(G') =& m\left(\frac{1}{2}\left(3^k(4k+1) - 3^t(4t+1)\right) + (k+t+3)(n_2 - n_1 + m) + (k-t)(n_3+1)\right) \\ &+ \sum_{x,y \in V(R_{k+1})\setminus X} \left(d_G(x,y) - d_{G'}(x,y)\right) + \sum_{x,y \in V(R'_{t+1})} \left(d_G(x,y) - d_{G'}(x,y)\right) \\ &+ \sum_{x,y \in X} \left(d_G(x,y) - d_{G'}(x,y)\right) + \sum_{\substack{x\in X \\ y \in V(R_{k+1})\setminus X}} d_G(x,y) - \sum_{\substack{x \in X \\ y \in V(R'_{t+1})}} d_{G'}(x,y). \qquad (10) \end{aligned}$$

Proof. For any vertex $x \in X$, by Lemmas 2.3 and 2.4, we have

$$\sum_{z \in V(G_1)\setminus V(R_{k+1})} d_G(x,z) = 3^k(2k-1) + k + 2,$$

$$\begin{aligned}
\sum_{z\in V(G_2)} d_G(x,z) =& \sum_{z\in V(G_2)} \left(d_G(x,w_2)+d_G(w_2,z)\right)\\
=&(k+2)|V(G_2)|+\sum_{z\in V(G_2)} d_G(w_2,z)\\
=&(k+2)n_2+\frac{1}{2}\left(3^t(2t-1)+1\right)+(t+1)(n_2-3^t)\\
=&(k+t+3)(n_2-3^t)+\frac{1}{2}\left(3^t(2k+2t+3)+1\right),\\
\sum_{z\in V(G_1')} d_{G'}(x,z) =& \sum_{z\in V(G_1')} \left(d_{G'}(x,w_1)+d_{G'}(w_1,z)\right)\\
=&(t+2)|V(G_1')|+\sum_{z\in V(G_1')} d_{G'}(w_1,z)\\
=&(t+2)(n_1-m)+\frac{1}{2}\left(3^k(2k-1)+1\right)+(k+1)(n_1-3^k-m)\\
=&(k+t+3)(n_1-3^k-m)+\frac{1}{2}\left(3^k(2k+2t+3)+1\right),\\
\sum_{z\in V(G_2')\setminus(V(R_{t+1}')\cup X)} d_{G'}(x,z) =&3^t(2t-1)+t+2,
\end{aligned}$$

and for any $u\in V(G_3)$, we have $d_G(x,u)-d_{G'}(x,u)=k-t$. Thus,

$$\begin{aligned}
W(G)-W(G') =& \sum_{x\in X,z\in V(G)} d_G(x,z)-\sum_{x\in X,z\in V(G')} d_{G'}(x,z)\\
=&\sum_{x\in X}\left(\sum_{z\in V(G_1)\setminus V(R_{k+1})} d_G(x,z)+\sum_{z\in V(G_2)} d_G(x,z)-\sum_{z\in V(G_1')} d_{G'}(x,z)-\sum_{z\in V(G_2')\setminus(V(R_{t+1}')\cup X)} d_{G'}(x,z)\right)\\
&+\sum_{x\in X,z\in V(G_3)}(k-t)+\sum_{x,y\in V(R_{k+1})\setminus X}\left(d_G(x,y)-d_{G'}(x,y)\right)+\sum_{x,y\in V(R_{t+1}')}\left(d_G(x,y)-d_{G'}(x,y)\right)\\
&+\sum_{x,y\in X}\left(d_G(x,y)-d_{G'}(x,y)\right)+\sum_{\substack{x\in X\\ y\in V(R_{k+1})\setminus X}} d_G(x,y)-\sum_{\substack{x\in X\\ y\in V(R_{t+1}')}} d_{G'}(x,y)\\
=&m\left(\frac{1}{2}\left(3^k(4k+1)-3^t(4t+1)\right)+(k+t+3)(n_2-n_1+m)+(k-t)(n_3+1)\right)\\
&+\sum_{x,y\in V(R_{k+1})\setminus X}\left(d_G(x,y)-d_{G'}(x,y)\right)+\sum_{x,y\in V(R_{t+1}')}\left(d_G(x,y)-d_{G'}(x,y)\right)\\
&+\sum_{x,y\in X}\left(d_G(x,y)-d_{G'}(x,y)\right)+\sum_{\substack{x\in X\\ y\in V(R_{k+1})\setminus X}} d_G(x,y)-\sum_{\substack{x\in X\\ y\in V(R_{t+1}')}} d_{G'}(x,y).
\end{aligned}$$

□

Operation II

Let $G=(G_1,n_1,k;\ G_2,n_2,t;\ G_3,n_3,\ell)\in\mathcal{CG}(n,3)$ be a graph as depicted in Figure 3 with $3^k<n_1\le 3^{k+1}$, $3^t\le n_2<3^{t+1}$, and $3^\ell<n_3\le 3^{\ell+1}$. Let X be the set of m_1 vertices on the line R_{k+1} of G_1, and Y be the set of m_2 vertices on the line $R''_{\ell+1}$ of G_3 with $1\le m_1\le n_1-3^k$, $1\le m_2\le n_3-3^\ell$, and $m_1+m_2\le 3^{t+1}-n_2$. Let G' be the graph obtained from G by moving all vertices of X from G_1 to G_2 and moving all vertices of Y from G_3 to G_2, respectively, such that G' remains in the form of the graph shown in Figure 3. Then, $G'=(G_1',n_1-m_1,k';\ G_2',n_2+m_1+m_2,t;\ G_3',n_3-m_2,\ell')\in\mathcal{CG}(n,3)$, where $k'=k$ or $k-1$, and $\ell'=\ell$ or $\ell'=\ell-1$. We say that G' is obtained from G by **Operation II (moving m_1 vertices from G_1 to G_2 and moving m_2 vertices from G_3 to G_2, respectively)**.

Lemma 4.2. *Let $G' = (G'_1, n_1 - m_1, k';\ G'_2, n_2 + m_1 + m_2, t;\ G'_3, n_3 - m_2, \ell') \in \mathcal{CG}(n,3)$ be the graph obtained from G by Operation II (moving m_1 vertices from G_1 to G_2 and moving m_2 vertices from G_3 to G_2, respectively). Then*

$$\begin{aligned} W(G) - W(G') = {} & m_1 \left(\frac{1}{2}\left(3^k(4k+1) - 3^t(4t+1)\right) + (k+t+3)(n_2 - n_1 + m_1) + (k-t)(n_3+1) \right) \\ & + m_2 \left(\frac{1}{2}\left(3^\ell(4\ell+1) - 3^t(4t+1)\right) + (\ell+t+3)(n_2 - n_3 + m_1 + m_2) + (\ell-t)(n_1 - m_1 + 1) \right) \\ & + \sum_{x,y \in V(R_{k+1}) \setminus X} (d_G(x,y) - d_{G'}(x,y)) + \sum_{x,y \in V(R'_{t+1})} (d_G(x,y) - d_{G'}(x,y)) \\ & + \sum_{x,y \in V(R''_{\ell+1}) \setminus Y} (d_G(x,y) - d_{G'}(x,y)) + \sum_{\substack{x \in X \\ y \in V(R_{k+1}) \setminus X}} d_G(x,y) + \sum_{\substack{x \in Y \\ y \in V(R''_{\ell+1}) \setminus Y}} d_G(x,y) \\ & + \sum_{x,y \in X} (d_G(x,y) - d_{G'}(x,y)) + \sum_{x,y \in Y} (d_G(x,y) - d_{G'}(x,y)) \\ & - \sum_{\substack{x \in X \\ y \in V(R'_{t+1})}} d_{G'}(x,y) - \sum_{\substack{x \in Y \\ y \in V(R'_{t+1})}} d_{G'}(x,y) - \sum_{\substack{x \in X \\ y \in Y}} d_{G'}(x,y). \end{aligned} \tag{11}$$

Proof. Let H be the graph obtained from G by Operation I (moving m_1 vertices from G_1 to G_2). Take $H = (H_1;\ H_2;\ H_3)$. Then, G' can be obtained from H by Operation I (moving m_2 vertices from H_3 to H_2). By Lemma 4.1, we have

$$\begin{aligned} W(G) - W(H) = {} & m_1 \left(\frac{1}{2}\left(3^k(4k+1) - 3^t(4t+1)\right) + (k+t+3)(n_2 - n_1 + m_1) + (k-t)(n_3+1) \right) \\ & + \sum_{x,y \in V(R_{k+1}) \setminus X} (d_G(x,y) - d_H(x,y)) + \sum_{x,y \in V(R'_{t+1})} (d_G(x,y) - d_H(x,y)) \\ & + \sum_{x,y \in X} (d_G(x,y) - d_H(x,y)) + \sum_{\substack{x \in X \\ y \in V(R_{k+1}) \setminus X}} d_G(x,y) - \sum_{\substack{x \in X \\ y \in V(R'_{t+1})}} d_H(x,y) \\ = {} & m_1 \left(\frac{1}{2}\left(3^k(4k+1) - 3^t(4t+1)\right) + (k+t+3)(n_2 - n_1 + m_1) + (k-t)(n_3+1) \right) \\ & + \sum_{x,y \in V(R_{k+1}) \setminus X} (d_G(x,y) - d_{G'}(x,y)) + \sum_{x,y \in V(R'_{t+1})} (d_G(x,y) - d_H(x,y)) \\ & + \sum_{x,y \in X} (d_G(x,y) - d_H(x,y)) + \sum_{\substack{x \in X \\ y \in V(R_{k+1}) \setminus X}} d_G(x,y) - \sum_{\substack{x \in X \\ y \in V(R'_{t+1})}} d_H(x,y) \quad \text{and} \end{aligned}$$

$$\begin{aligned} W(H) - W(G') = {} & m_2 \left(\frac{1}{2}\left(3^\ell(4\ell+1) - 3^t(4t+1)\right) + (\ell+t+3)(n_2 + m_1 - n_3 + m_2) + (\ell-t)(n_1 - m_1 + 1) \right) \\ & + \sum_{x,y \in V(R''_{\ell+1}) \setminus Y} (d_H(x,y) - d_{G'}(x,y)) + \sum_{x,y \in V(R'_{t+1}) \cup X} (d_H(x,y) - d_{G'}(x,y)) \\ & + \sum_{x,y \in Y} (d_H(x,y) - d_{G'}(x,y)) + \sum_{\substack{x \in Y \\ y \in V(R''_{\ell+1}) \setminus Y}} d_H(x,y) - \sum_{\substack{x \in Y \\ y \in V(R'_{t+1}) \cup X}} d_{G'}(x,y) \\ = {} & m_2 \left(\frac{1}{2}\left(3^\ell(4\ell+1) - 3^t(4t+1)\right) + (\ell+t+3)(n_2 - n_3 + m_1 + m_2) + (\ell-t)(n_1 - m_1 + 1) \right) \\ & + \sum_{x,y \in V(R''_{\ell+1}) \setminus Y} (d_G(x,y) - d_{G'}(x,y)) + \sum_{x,y \in V(R'_{t+1})} (d_H(x,y) - d_{G'}(x,y)) \\ & + \sum_{x,y \in X} (d_H(x,y) - d_{G'}(x,y)) + \sum_{\substack{x \in X \\ y \in V(R'_{t+1})}} (d_H(x,y) - d_{G'}(x,y)) \\ & + \sum_{x,y \in Y} (d_G(x,y) - d_{G'}(x,y)) + \sum_{\substack{x \in Y \\ y \in V(R''_{\ell+1}) \setminus Y}} d_G(x,y) - \sum_{\substack{x \in Y \\ y \in V(R'_{t+1})}} d_{G'}(x,y) - \sum_{\substack{x \in Y \\ y \in X}} d_{G'}(x,y). \end{aligned}$$

By adding the last two equations, we get (11). □

Operation III

Let $G = (G_1, n_1, k;\ G_2, n_2, t;\ G_3, n_3, \ell) \in \mathcal{CG}(n, 3)$ be a graph as depicted in Figure 3 with $3^k < n_1 \le 3^{k+1}$, $n_2 = 3^{t+1}$, and $3^\ell \le n_3 < 3^{\ell+1}$. Let X and Y be the sets of m_1 and m_2 vertices on the line R_{k+1} of G_1, respectively, with $1 \le m_1 \le 2 \cdot 3^{t+1}$, $1 \le m_2 \le 3^{\ell+1} - n_3$, and $m_1 + m_2 \le n_1 - 3^k$. Let G' be the graph obtained from G by moving all vertices of X from G_1 to G_2 and moving all vertices of Y from G_1 to G_3, respectively. Then, $G' = (G'_1, n_1 - m_1 - m_2, k';\ G'_2, n_2 + m_1, t+1;\ G'_3, n_3 + m_2, \ell) \in \mathcal{CG}(n, 3)$, where $k' = k$ or $k - 1$. We say that G' is obtained from G by **Operation III (moving m_1 and m_2 vertices from G_1 to G_2 and G_3, respectively)**.

Lemma 4.3. *Let $G' = (G'_1, n_1 - m_1 - m_2, k';\ G'_2, n_2 + m_1, t + 1;\ G'_3, n_3 + m_2, \ell) \in \mathcal{CG}(n, 3)$ be the graph obtained from G by Operation III (moving m_1 and m_2 vertices from G_1 to G_2 and G_3, respectively). Then*

$$\begin{aligned}
W(G) - W(G') = {} & m_1 \left(\frac{1}{2} \left(3^k(4k+1) + 3^{t+1}(2k - 2t + 3) \right) - (k+t+4)(n_1 - m_1) + (k - t - 1)(n_3 + 1) \right) \\
& + m_2 \left(\frac{1}{2} \left(3^k(4k+1) - 3^\ell(4\ell+1) + 3^{t+1}(2k - 2\ell) \right) + (k+\ell+3)(n_3 - n_1 + m_1 + m_2) + (k - \ell)(m_1 + 1) \right) \\
& + \sum_{x,y \in V(R_{k+1}) \setminus (X \cup Y)} (d_G(x,y) - d_{G'}(x,y)) + \sum_{x,y \in V(R''_{\ell+1})} (d_G(x,y) - d_{G'}(x,y)) \\
& + \sum_{x,y \in X} (d_G(x,y) - d_{G'}(x,y)) + \sum_{x,y \in Y} (d_G(x,y) - d_{G'}(x,y)) + \sum_{\substack{x \in X \\ y \in V(R_{k+1}) \setminus X}} d_G(x,y) \\
& + \sum_{\substack{x \in Y \\ y \in V(R_{k+1}) \setminus (X \cup Y)}} d_G(x,y) - \sum_{\substack{x \in Y \\ y \in V(R''_{\ell+1})}} d_{G'}(x,y).
\end{aligned} \tag{12}$$

Proof. Let H be the graph obtained from G by Operation I (moving m_1 vertices from G_1 to G_2). Take $H = (H_1;\ H_2;\ H_3)$. Then G' can be obtained from H by Operation I (moving m_2 vertices from H_1 to H_3). By Lemma 4.1, we have

$$\begin{aligned}
W(G) - W(H) = {} & m_1 \left(\frac{1}{2} \left(3^k(4k+1) - 3^{t+1}(4t+5) \right) + (k+t+4)(3^{t+1} - n_1 + m_1) + (k - t - 1)(n_3 + 1) \right) \\
& + \sum_{x,y \in V(R_{k+1}) \setminus X} (d_G(x,y) - d_H(x,y)) + \sum_{x,y \in X} (d_G(x,y) - d_H(x,y)) + \sum_{\substack{x \in X \\ y \in V(R_{k+1}) \setminus X}} d_G(x,y) \\
= {} & m_1 \left(\frac{1}{2} \left(3^k(4k+1) + 3^{t+1}(2k - 2t + 3) \right) - (k+t+4)(n_1 - m_1) + (k - t - 1)(n_3 + 1) \right) \\
& + \sum_{x,y \in V(R_{k+1}) \setminus (X \cup Y)} (d_G(x,y) - d_H(x,y)) + \sum_{x,y \in Y} (d_G(x,y) - d_H(x,y)) \\
& + \sum_{\substack{x \in Y \\ y \in V(R_{k+1}) \setminus (X \cup Y)}} (d_G(x,y) - d_H(x,y)) + \sum_{x,y \in X} (d_G(x,y) - d_{G'}(x,y)) + \sum_{\substack{x \in X \\ y \in V(R_{k+1}) \setminus X}} d_G(x,y) \quad \text{and}
\end{aligned}$$

$$\begin{aligned}
W(H) - W(G') = {} & m_2 \left(\frac{1}{2} \left(3^k(4k+1) - 3^\ell(4\ell+1) + 3^{t+1}(2k - 2\ell) \right) + (k+\ell+3)(n_3 - n_1 + m_1 + m_2) + (k - \ell)(m_1 + 1) \right) \\
& + \sum_{x,y \in V(R_{k+1}) \setminus (X \cup Y)} (d_H(x,y) - d_{G'}(x,y)) + \sum_{x,y \in V(R''_{\ell+1})} (d_H(x,y) - d_{G'}(x,y)) \\
& + \sum_{x,y \in Y} (d_H(x,y) - d_{G'}(x,y)) + \sum_{\substack{x \in Y \\ y \in V(R_{k+1}) \setminus (X \cup Y)}} d_H(x,y) - \sum_{\substack{x \in Y \\ y \in V(R''_{\ell+1})}} d_{G'}(x,y) \\
= {} & m_2 \left(\frac{1}{2} \left(3^k(4k+1) - 3^\ell(4\ell+1) + 3^{t+1}(2k - 2\ell) \right) + (k+\ell+3)(n_3 - n_1 + m_1 + m_2) + (k - \ell)(m_1 + 1) \right) \\
& + \sum_{x,y \in V(R_{k+1}) \setminus (X \cup Y)} (d_H(x,y) - d_{G'}(x,y)) + \sum_{x,y \in V(R''_{\ell+1})} (d_G(x,y) - d_{G'}(x,y)) \\
& + \sum_{x,y \in Y} (d_H(x,y) - d_{G'}(x,y)) + \sum_{\substack{x \in Y \\ y \in V(R_{k+1}) \setminus (X \cup Y)}} d_H(x,y) - \sum_{\substack{x \in Y \\ y \in V(R''_{\ell+1})}} d_{G'}(x,y).
\end{aligned}$$

By adding the last two equations, we get (12). □

5. Some auxiliary lemmas

Let $G = (G_1, n_1, k;\ G_2, n_2, t;\ G_3, n_3, \ell) \in \mathcal{CG}(n, 3)$ be the graph as depicted in Figure 3. If not specifically stated, we say that moving m vertices from G_1 to G_2 always mean that we move the right-most m vertices on the last layer of G_1 to G_2, and then arrange these m vertices on the last layer of G_2 on top of the original vertices (if G_2 is unsaturated) or on a new layer of G_2 (if G_2 is saturated), such that the obtained graph remains in the form of the graph shown in Figure 3.

Lemma 5.1. *Let $G = (G_1, n_1, k;\ G_2, n_2, t;\ G_3, n_3, \ell) \in \mathcal{CG}(n, 3)$ be the graph as depicted in Figure 3, where $k \geq t + 1$, $3^k < n_1 \leq 3^{k+1}$, and $3^t < n_2 < 3^{t+1}$. If G is a Wiener-minimal graph of $\mathcal{CG}(n, 3)$, then the following statements hold:*

(1). *The inequality $k \leq t + 2$ holds.*

(2). *If $k = t + 1$, then $n_3 < 3^{t+1}$.*

(3). *If $k = t + 2$, then $n_3 < 2 \cdot 3^{t+1}$.*

(4). *If $k = t + 2$, then $n_1 \neq 2 \cdot 3^k + r \cdot 3^{k-1}$ with $r = 1$, 2 or 3.*

(5). *If $k = t + 2$, $n_3 \geq 3^{t+1}$, then $n_1 \neq 3^k + r \cdot 3^{k-1}$ with $r = 1$ or 2.*

Proof. By Lemma 3.3(2), $3^{t+1} \mid (n_1 - 3^k)$. Thus, $n_1 - 3^k \geq 3^{t+1}$ and n_1 can be written as

$$n_1 = 3^k + 2 \cdot 3^t + \sum_{i=1}^{k-t+1} p_i \cdot 3^{k+1-i}, \tag{13}$$

where $0 \leq p_1 \leq 1$, $0 \leq p_i \leq 2$ for $i = 2, \ldots, k - t$, and $p_{k-t+1} = 1$.

Take $m = 3^{t+1} - n_2$. Let X be the set of the right-most m vertices on the line R_{k+1} of G_1 and Y be the set of the right-most $n_2 - 3^t$ vertices, except for X, on the line R_{k+1} of G_1. Let $G' = (n_1 - m;\ n_2 + m;\ n_3) \in \mathcal{CG}(n, 3)$ be the graph obtained from G by Operation I (moving m vertices from G_1 to G_2). Then

$$\begin{aligned}
\sum_{\substack{x \in X \\ y \in V(R_{k+1}) \setminus X}} d_G(x, y) - \sum_{\substack{x \in X \\ y \in V(R'_{t+1})}} d_{G'}(x, y) &= \sum_{\substack{x \in X \\ y \in V(R_{k+1}) \setminus (X \cup Y)}} d_G(x, y) + \sum_{\substack{x \in X \\ y \in Y}} d_G(x, y) - \sum_{\substack{x \in X \\ y \in V(R'_{t+1})}} d_{G'}(x, y) \\
&= \sum_{\substack{x \in X \\ y \in V(R_{k+1}) \setminus (X \cup Y)}} d_G(x, y) = |X| \sum_{i=1}^{k-t+1} 2(k - i + 2) p_i \cdot 3^{k+1-i}.
\end{aligned}$$

By Lemma 4.1, we have

$$\begin{aligned}
W(G) - W(G') &= m \left(\frac{1}{2} \left(3^k(4k + 1) - 3^t(4t + 1) \right) + (k + t + 3)(n_2 - n_1 + m) + (k - t)(n_3 + 1) \right) \\
&\quad + \sum_{\substack{x \in X \\ y \in V(R_{k+1}) \setminus X}} d_G(x, y) - \sum_{\substack{x \in X \\ y \in V(R'_{t+1})}} d_{G'}(x, y) \\
&= \left(3^{t+1} - n_2 \right) \left(\frac{1}{2} \left(3^k(2k - 2t - 5) + 3^t(2k - 2t + 5) \right) + (k - t)(n_3 + 1) \right. \\
&\quad \left. + \sum_{i=1}^{k-t} (k - t - 2i + 1) p_i \cdot 3^{k+1-i} - 3^t(k - t + 1) \right).
\end{aligned} \tag{14}$$

(1). If $k \geq t + 3$, then $\sum_{i=1}^{k-t} (k - t - 2i + 1) p_i \cdot 3^{k+1-i} \geq \sum_{i=3}^{k-t} 2(4 - 2i) \cdot 3^{k+1-i}$. Thus, by (14), we have

$$W(G) - W(G') \geq \frac{1}{2} \left(3^{t+1} - n_2 \right) \left(3^k(2k - 2t - 7) + 3^t(12k - 12t - 3) + 2(k - t)(n_3 + 1) \right) > 0,$$

a contradiction.

(2). If $k = t + 1$ and $n_3 \geq 3^{t+1}$, then by (14), we have $W(G) - W(G') = \left(3^{t+1} - n_2 \right) \left(1 - 3^{t+1} + n_3 \right) > 0$, a contradiction.

(3). If $k = t + 2$ and $n_3 \geq 2 \cdot 3^{t+1}$, then

$$\sum_{i=1}^{k-t}(k-t-2i+1)p_i \cdot 3^{k+1-i} \geq -2 \cdot 3^{k-1}.$$

By (14), we have

$$W(G) - W(G') \geq \left(3^{t+1} - n_2\right)\left(3^{t+1} + 2\right) > 0,$$

a contradiction.

(4). If $k = t + 2$ and $n_1 = 2 \cdot 3^k + r \cdot 3^{k-1}$ with $r = 1$, 2 or 3, then $p_1 = 1$ and $p_2 = r - 1$ in (13), and hence

$$\sum_{i=1}^{k-t}(k-t-2i+1)p_i \cdot 3^{k+1-i} = 3^k - (r-1) \cdot 3^{k-1}.$$

By (14), we have $W(G) - W(G') = \left(3^{t+1} - n_2\right)\left(2 + (3-r) \cdot 3^{t+1} + 2n_3\right) > 0$, a contradiction.

(5). If $k = t + 2$, $n_3 \geq 3^{t+1}$, and $n_1 = 3^k + r \cdot 3^{k-1}$ with $r = 1$ or 2, then $p_1 = 0$ and $p_2 = r - 1$ in (13), and thus

$$\sum_{i=1}^{k-t}(k-t-2i+1)p_i \cdot 3^{k+1-i} = -(r-1) \cdot 3^{k-1}.$$

By (14), we have $W(G) - W(G') \geq \left(3^{t+1} - n_2\right)\left(2 + (2-r) \cdot 3^{t+1}\right) > 0$, a contradiction. □

Lemma 5.2. *Let $G = (G_1, n_1, k;\ G_2, n_2, t;\ G_3, n_3, \ell) \in \mathcal{CG}(n, 3)$ be the graph as depicted in Figure 3, where $k \geq t + 2$, $3^k < n_1 \leq 3^{k+1}$, and $n_2 = 3^{t+1}$. If G is a Wiener-minimal graph of $\mathcal{CG}(n, 3)$, then the following statements hold:*

(1). *The inequality $k \leq t + 3$ is valid.*

(2). *The inequality $n_3 < 3^k$ is valid.*

(3). *If $k = t + 2$ and $n_3 \geq 3^{t+1}$, then either $3^k + 2 \cdot 3^{k-1} < n_1 \leq 2 \cdot 3^k$ or $n_1 > 2 \cdot 3^k + 2 \cdot 3^{k-1}$.*

(4). *If $k = t + 3$, then $3^k + 2 \cdot 3^{k-2} < n_1 \leq 2 \cdot 3^k$.*

(5). *If $k = t + 3$ and $n_3 \geq 3^{t+2}$, then either $n_1 \leq 3^k + 2 \cdot 3^{k-2}$ or $n_1 > 3^k + 2 \cdot 3^{k-1}$.*

Proof. Suppose that m is a positive integer such that $0 < m \leq 2 \cdot 3^{t+1}$ and $3^{t+1} \mid (n_1 - 3^k - m)$. Then $n_1 - 3^k - m$ can be written as

$$n_1 - 3^k - m = \sum_{i=1}^{k-t} p_i \cdot 3^{k+1-i}, \tag{15}$$

where $0 < m \leq 2 \cdot 3^{t+1}$, $0 \leq p_1 \leq 1$, $0 \leq p_i \leq 2$ for $i = 2, \ldots, k-t-1$, and $p_{k-t} \leq 1$. Let X be the set of right-most m vertices on the line R_{k+1} of G_1. Let $G' = (n_1 - m;\ n_2 + m;\ n_3)$ be the graph obtained from G by Operation I (moving m vertices from G_1 to G_2). Note that

$$\sum_{\substack{x \in X \\ y \in V(R_{k+1}) \setminus X}} d_G(x, y) = m \sum_{i=1}^{k-t} 2(k-i+2)p_i \cdot 3^{k+1-i}.$$

Then, by Lemma 4.1, replacing t with $t + 1$, we have

$$\begin{aligned}
&W(G) - W(G') \\
&= m\left(\frac{1}{2}\left(3^k(4k+1) - 3^{t+1}(4t+5)\right) + (k+t+4)(3^{t+1} - n_1 + m) + (k-t-1)(n_3+1)\right) + \sum_{\substack{x \in X \\ y \in V(R_{k+1}) \setminus X}} d_G(x, y) \\
&= m\left(\frac{1}{2}\left(3^k(2k-2t-7) + 3^{t+1}(2k-2t+3)\right) + \sum_{i=1}^{k-t}(k-t-2i)p_i \cdot 3^{k+1-i} + (k-t-1)(n_3+1)\right) &(16) \\
&\geq m\left(\frac{1}{2}\left(3^k(2k-2t-7) + 3^{t+1}(2k-2t+3)\right) + \sum_{i=1}^{k-t-1}(k-t-2i)p_i \cdot 3^{k+1-i} - (k-t) \cdot 3^{t+1} + (k-t-1)(n_3+1)\right). &(17)
\end{aligned}$$

(1). If $k \geq t+4$, then $\sum_{i=1}^{k-t-1}(k-t-2i)p_i \cdot 3^{k+1-i} \geq \sum_{i=3}^{k-t-1} 2(4-2i) \cdot 3^{k+1-i}$. By (17), we have

$$W(G) - W(G') \geq \frac{m}{2}\left(3^k(2k-2t-9) + 3^{t+2}(4k-4t-5) + 2(k-t-1)(n_3+1)\right) > 0, \quad \text{a contradiction.}$$

(2). If $n_3 \geq 3^k$, then

$$\sum_{i=1}^{k-t-1}(k-t-2i)p_i \cdot 3^{k+1-i} \geq \sum_{i=2}^{k-t-1} 2(2-2i) \cdot 3^{k+1-i},$$

because $t+2 \leq k \leq t+3$ by Part (1). From (17), it follows that

$$W(G) - W(G') \geq \frac{m}{2}\left(3^k(4k-4t-15) + 3^{t+2}(4k-4t-1) + 2k-2t-2\right) > 0,$$

which yields a contradiction.

(3). If $k = t+2$, $n_3 \geq 3^{t+1}$, and $r \cdot 3^k < n_1 \leq r \cdot 3^k + 2 \cdot 3^{k-1}$ with $r = 1$ or 2, then we choose m such that $p_1 = r-1$ and $p_2 = 0$ in (15). By (16), we have $W(G) - W(G') \geq m > 0$, a contradiction.

(4). If $k = t+3$, then (15) becomes

$$n_1 - 3^k - m = p_1 \cdot 3^k + p_2 \cdot 3^{k-1} + p_3 \cdot 3^{k-2}, \tag{18}$$

where $0 < m \leq 2 \cdot 3^{k-2}$, $0 \leq p_1 \leq 1$, $0 \leq p_2 \leq 2$, and $p_3 \leq 1$. If $3^k < n_1 \leq 3^k + 2 \cdot 3^{k-2}$, then $p_1 = p_2 = p_3 = 0$ in (18), and hence by (16), we have $W(G) - W(G') = m\,(2 + (k-t-1)n_3) > 0$, a contradiction. If $n_1 > 2 \cdot 3^k$, then $p_1 = 1$ in (18), and thus

$$\sum_{i=1}^{k-t}(k-t-2i)p_i \cdot 3^{k+1-i} \geq (k-t-2) \cdot 3^k + 2(k-t-4) \cdot 3^{k-1} - (k-t) \cdot 3^{k-2}.$$

By (16), we have $W(G) - W(G') \geq m\,(2 + (k-t-1)n_3) > 0$, a contradiction.

(5). If $k = t+3$, $n_3 \geq 3^{t+2}$, and $3^k + 2 \cdot 3^{k-2} < n_1 \leq 3^k + 2 \cdot 3^{k-1}$, then we choose m such that $p_1 = 0$ and $p_2 + p_3 \leq 2$ in (18), and hence $\sum_{i=1}^{k-t}(k-t-2i)p_i \cdot 3^{k+1-i} = -p_2 \cdot 3^{k-1} - 3p_3 \cdot 3^{k-2} = -(p_2+p_3) \cdot 3^{k-1} \geq -2 \cdot 3^{k-1}$. By (16), we have $W(G) - W(G') \geq 2m > 0$, a contradiction. □

Lemma 5.3. *Let* $G = (G_1, n_1, k;\ G_2, n_2, t;\ G_3, n_3, \ell) \in \mathcal{CG}(n,3)$ *be the graph as depicted in Figure 3, where* $k = t = \ell + 1$, $3^k + 3^{k-1} + 2 \cdot 3^{k-2} + 1 < n_1 \leq 3^{k+1}$, $n_2 = 3^{t+1}$, *and* $n_3 = 3^{\ell+1}$. *Take*

$$m = \begin{cases} 2 \cdot 3^{k-1}, & \text{if } 3^k + 3^{k-1} + 2 \cdot 3^{k-2} + 1 < n_1 \leq 2 \cdot 3^k + 2 \cdot 3^{k-1}, \\ 3^{k+1} - n_1 + 3^{k-1}, & \text{if } 2 \cdot 3^k + 2 \cdot 3^{k-1} < n_1 \leq 3^{k+1}. \end{cases}$$

Let $G' = (G'_1, 3^k - m, k';\ G'_2, 3^{t+1} + n_1 - 3^k + m + 2 \cdot 3^\ell, t+1;\ G'_3, 3^\ell, \ell - 1) \in \mathcal{CG}(n,3)$ *where* $k' = k-2$ *or* $k' = k-1$. *Then*

(1). *If* $\ell \geq 2$, *then* $W(G) > W(G')$.

(2). *If* $\ell = 1$ *and* $2 \cdot 3^k < n_1 \leq 3^{k+1}$, *then* $W(G) > W(G')$.

(3). *If* $\ell = 1$ *and* $3^k + 3^{k-1} + 2 \cdot 3^{k-2} + 1 < n_1 \leq 2 \cdot 3^k$, *then* $W(G) < W(G')$.

Proof. Let X be the set of the right-most m vertices on the line R_k of G_1. Let $H = (H_1;\ H_2;\ H_3)$ be the graph obtained from G by Operation II (moving all vertices of $V(R_{k+1})$ from G_1 to G_2 and moving all vertices of $V(R''_{\ell+1})$ from G_3 to G_2, respectively). Here the last layer vertices of H_2 are the vertices of $V(R''_{\ell+1}) \cup V(R_{k+1})$. In the sequence of the last layer vertices of H_2, we arrange the vertices of $V(R''_{\ell+1})$ first and then the vertices of $V(R_{k+1})$. The graph G' then can be obtained from H by Operation I (moving all vertices of X from H_1 to H_2). The last layer vertices of G'_2 are the vertices of $V(R''_{\ell+1}) \cup X \cup V(R_{k+1})$. For the sake of calculations, in the sequence of the last layer vertices of G'_2, we arrange the vertices of $V(R''_{\ell+1})$ first, then the vertices of X, and finally the vertices of $V(R_{k+1})$. By Lemmas 4.1 and 4.2, we have

$$\begin{aligned} W(G) - W(H) =& (n_1 - 3^k)\left(\frac{1}{2}\left(3^k(4k+1) - 3^{t+1}(4t+5)\right) + (k+t+4)(3^{t+1} - 3^k) + (k-t-1)(3^{\ell+1}+1)\right) \\ &+ 2 \cdot 3^\ell\left(\frac{1}{2}\left(3^\ell(4\ell+1) - 3^{t+1}(4t+5)\right) + (\ell+t+4)(3^{t+1} - 3^{\ell+1} + n_1 - 3^k + 2 \cdot 3^\ell)\right. \\ &\left. + (\ell-t-1)(3^k+1)\right) + \sum_{x,y \in V(R_{k+1})}(d_G(x,y) - d_H(x,y)) - \sum_{\substack{x \in V(R_{k+1}) \\ y \in V(R''_{\ell+1})}} d_H(x,y), \end{aligned}$$

and

$$\begin{aligned} W(H)-W(G') &= m\left(\frac{1}{2}\left(3^{k-1}(4k-3)-3^{t+1}(4t+5)\right)+(k+t+3)(3^{t+1}+n_1-3^k+2\cdot 3^\ell-3^k+m)\right.\\ &\quad\left.+(k-t-2)(3^\ell+1)\right)+\sum_{x,y\in V(R_{k+1})\cup V(R''_{\ell+1})}(d_H(x,y)-d_{G'}(x,y))+\sum_{x,y\in X}(d_H(x,y)-d_{G'}(x,y))\\ &\quad+\sum_{\substack{x\in X\\ y\in V(R_k)\setminus X}}d_H(x,y)-\sum_{\substack{x\in X\\ y\in V(R_{k+1})\cup V(R''_{\ell+1})}}d_{G'}(x,y)\\ &= m\left(\frac{1}{2}\left(3^{k-1}(4k-3)-3^{t+1}(4t+5)\right)+(k+t+3)(3^{t+1}+n_1-3^k+2\cdot 3^\ell-3^k+m)\right.\\ &\quad\left.+(k-t-2)(3^\ell+1)\right)+\sum_{x,y\in V(R_{k+1})}(d_H(x,y)-d_{G'}(x,y))+\sum_{\substack{x\in V(R_{k+1})\\ y\in V(R''_{\ell+1})}}(d_H(x,y)-d_{G'}(x,y))\\ &\quad+\sum_{x,y\in X}(d_G(x,y)-d_{G'}(x,y))+\sum_{\substack{x\in X\\ y\in V(R_k)\setminus X}}d_G(x,y)-\sum_{\substack{x\in X\\ y\in V(R_{k+1})}}d_{G'}(x,y)-\sum_{\substack{x\in X\\ y\in V(R''_{\ell+1})}}d_{G'}(x,y). \end{aligned}$$

Note that $3^{k-1}\le m<2\cdot 3^{k-1}$ and $|V(R''_{\ell+1})|+|X|+|V(R_{k+1})|=2\cdot 3^\ell+m+n_1-3^{k-1}\le 3^{k+1}$. Then

$$\begin{aligned} \sum_{\substack{x\in V(R_{k+1})\\ y\in V(R''_{\ell+1})}}d_{G'}(x,y) &=|V(R''_{\ell+1})||V(R_{k+1})|\cdot 2(k+1)=3^\ell(n_1-3^k)(4k+4),\\ \sum_{x,y\in X}(d_G(x,y)-d_{G'}(x,y)) &=3^{k-1}\left(m-3^{k-1}\right)(2k-2(t+1))=-2\cdot 3^{k-1}\left(m-3^{k-1}\right),\\ \sum_{\substack{x\in X\\ y\in V(R''_{\ell+1})}}d_{G'}(x,y) &=2\cdot 3^\ell\left(3^{k-1}\cdot 2t+\left(m-3^{k-1}\right)\cdot 2(t+1)\right). \end{aligned}$$

Thus,

$$\begin{aligned} W(G)-W(G') &=(W(G)-W(H))+(W(H)-W(G'))\\ &=n_1\left(2\cdot 3^{k-1}-1\right)-m\left(3^{k-1}(10k+17)+2\right)+m(n_1+m)(2k+3)-4\cdot 3^{2k-1}-3^{k-1}\\ &\quad+\sum_{x,y\in V(R_{k+1})}(d_G(x,y)-d_{G'}(x,y))+\sum_{\substack{x\in X\\ y\in V(R_k)\setminus X}}d_G(x,y)-\sum_{\substack{x\in X\\ y\in V(R_{k+1})}}d_{G'}(x,y). \end{aligned}$$

Case 1. $3^k+3^{k-1}+2\cdot 3^{k-2}+1<n_1\le 2\cdot 3^k+2\cdot 3^{k-1}$.
In this case, we have $|X|=m=2\cdot 3^{k-1}$ and $\sum_{x\in X,y\in V(R_k)\setminus X}d_G(x,y)=0$. Thus,

$$W(G)-W(G')=n_1\left(3^{k-1}(4k+8)-1\right)-3^{2k-2}(12k+34)-5\cdot 3^{k-1}+\sum_{x,y\in V(R_{k+1})}(d_G(x,y)-d_{G'}(x,y))-\sum_{\substack{x\in X\\ y\in V(R_{k+1})}}d_{G'}(x,y).$$

Subcase 1.1 $3^k+3^{k-1}+2\cdot 3^{k-2}+1<n_1\le 3^k+2\cdot 3^{k-1}$.
Note that if $\ell=1$ then $3^k+3^{k-1}+2\cdot 3^{k-2}+1=3^k+2\cdot 3^{k-1}$. Hence $\ell\ge 2$. Since

$$\begin{aligned} \sum_{\substack{x\in X\\ y\in V(R_{k+1})}}d_{G'}(x,y) &=|V(R_{k+1})|\left(3^{k-1}\cdot 2t+3^{k-1}\cdot 2(t+1)\right)=\left(n_1-3^k\right)3^{k-1}(4t+2),\\ \sum_{x,y\in V(R_{k+1})}(d_G(x,y)-d_{G'}(x,y)) &=0, \end{aligned}$$

we have

$$\begin{aligned} W(G)-W(G') &=n_1\left(2\cdot 3^k-1\right)-28\cdot 3^{2k-2}-5\cdot 3^{k-1}\\ &\ge\left(3^k+3^{k-1}+2\cdot 3^{k-2}+2\right)\left(2\cdot 3^k-1\right)-28\cdot 3^{2k-2}-5\cdot 3^{k-1}\\ &=7\cdot 3^{k-2}-2>0. \end{aligned}$$

Subcase 1.2 $3^k + 2\cdot 3^{k-1} < n_1 \le 2\cdot 3^k$.
Note that

$$\begin{aligned}\sum_{\substack{x\in X\\ y\in V(R_{k+1})}} d_{G'}(x,y) =& 3^{k-1}|V(R_{k+1})|\cdot 2(t+1) + 3^{k-1}\cdot 2\cdot 3^{k-1}\cdot 2t + 3^{k-1}\left(|V(R_{k+1})| - 2\cdot 3^{k-1}\right)\cdot 2(t+1)\\ =& \left(n_1 - 3^k\right)3^{k-1}(4k+4) - 4\cdot 3^{2k-2},\\ \sum_{x,y\in V(R_{k+1})}\left(d_G(x,y) - d_{G'}(x,y)\right) =& 2\cdot 3^{k-1}\left(|V(R_{k+1})| - 2\cdot 3^{k-1}\right)(2k - 2(t+1)) = 20\cdot 3^{2k-2} - 4n_1\cdot 3^{k-1}.\end{aligned}$$

Thus,

$$W(G) - W(G') = 2\cdot 3^{2k-2} - 5\cdot 3^{k-1} - n_1.$$

If $\ell = 1$, then $k = 2$ and $W(G) - W(G') \le 2\cdot 3^{2k-2} - 5\cdot 3^{k-1} - \left(3^k + 2\cdot 3^{k-1} + 1\right) = 3^{k-1}\left(2\cdot 3^{k-1} - 10\right) - 1 < 0$. If $\ell \ge 2$, then $k \ge 3$ and $W(G) - W(G') \ge 2\cdot 3^{2k-2} - 5\cdot 3^{k-1} - 2\cdot 3^k = 3^{k-1}\left(2\cdot 3^{k-1} - 11\right) - 1 > 0$.

Subcase 1.3 $2\cdot 3^k < n_1 \le 2\cdot 3^k + 2\cdot 3^{k-1}$.
Note that

$$\begin{aligned}\sum_{\substack{x\in X\\ y\in V(R_{k+1})}} d_{G'}(x,y) =& 3^{k-1}|V(R_{k+1})|\cdot 2(t+1) + 3^{k-1}\cdot 2\cdot 3^{k-1}\cdot 2t + 3^{k-1}\left(|V(R_{k+1})| - 2\cdot 3^{k-1}\right)\cdot 2(t+1)\\ =& \left(n_1 - 3^k\right)3^{k-1}(4k+4) - 4\cdot 3^{2k-2},\\ \sum_{x,y\in V(R_{k+1})}\left(d_G(x,y) - d_{G'}(x,y)\right) =& 2\cdot 3^{k-1}\cdot 3^{k-1}(2k - 2(t+1)) + 3^{k-1}\left(|V(R_{k+1})| - 3^k\right)(2(k+1) - 2t)\\ =& -16\cdot 3^{2k-2} + 2n_1\cdot 3^{k-1}.\end{aligned}$$

Thus, $W(G) - W(G') = n_1\left(2\cdot 3^k - 1\right) - 34\cdot 3^{2k-2} - 5\cdot 3^{k-1} \ge 3^{k-1}\left(2\cdot 3^{k-1} - 5\right) - 1 > 0$.

Case 2. $2\cdot 3^k + 2\cdot 3^{k-1} < n_1 \le 3^{k+1}$.
In this case, $|X| = m = 10\cdot 3^{k-1} - n_1$. Let S be the set of the left-most $n_1 - 2\cdot 3^k - 2\cdot 3^{k-1}$ vertices on the line R_{k+1} of G_1. Then, $|S| = n_1 - 8\cdot 3^{k-1} \le 3^{k-1}$, $|V(R_{k+1})\setminus S| = 5\cdot 3^{k-1}$, and $|S| + |X| = 2\cdot 3^{k-1} = |V(R_k)\setminus X| + |X|$; that is, $|S| = |V(R_k)\setminus X|$. Note that

$$\begin{aligned}\sum_{\substack{x\in X\\ y\in V(R_{k+1})}} d_{G'}(x,y) =& \sum_{x\in X, y\in S} d_{G'}(x,y) + 3^{k-1}\cdot 5\cdot 3^{k-1}\cdot 2(t+1) + \left(m - 3^{k-1}\right)\left(3^k\cdot 2(t+1) + 2\cdot 3^{k-1}\cdot 2t\right)\\ =& \sum_{x\in X, y\in S} d_{G'}(x,y) + 3^{2k-2}(10k+10) + \left(3^{k+1} - n_1\right)\cdot 3^{k-1}(10k+6),\end{aligned}$$

$$\sum_{\substack{x\in X\\ y\in V(R_k)\setminus X}} d_G(x,y) - \sum_{x\in X, y\in S} d_{G'}(x,y) = |S|\cdot 3^{k-1}(2k - 2(t+1)) = -2\cdot 3^{k-1}\left(n_1 - 8\cdot 3^{k-1}\right),$$

$$\sum_{x,y\in V(R_{k+1})}\left(d_G(x,y) - d_{G'}(x,y)\right) = 0.$$

Therefore, $W(G) - W(G') = 70\cdot 3^{2(k-1)} - 7\cdot 3^k - n_1\left(7\cdot 3^{k-1} - 1\right) \ge 7\cdot 3^{2(k-1)} - 4\cdot 3^k > 0$. □

Lemma 5.4. *Let $G = (G_1, n_1, k;\ G_2, n_2, t;\ G_3, n_3, \ell) \in \mathcal{CG}(n,3)$ be the graph as depicted in Figure 3, where $k = t+1$, $t = \ell+1$, $n_1 = 2\cdot 3^k$, $3^t < n_2 < 3^{t+1}$ and $n_3 = 3^{\ell+1}$. If G is a Wiener-minimal graph of $\mathcal{CG}(n,3)$, then $3^t < n_2 < \frac{1}{2}\cdot 3^{t+1} - \frac{1}{2}$.*

Proof. Suppose to the contrary that $\frac{1}{2}\cdot 3^{t+1} - \frac{1}{2} \le n_2 < 3^{t+1}$. Let X be the set of the right-most $2\cdot 3^{\ell+1}$ vertices on the line R_{k+1} of G_1 and Y be the set of the right-most m vertices, except for X, on the line R_{k+1} of G_1, where

$$m = \begin{cases} 3^t, & \text{if } \frac{1}{2}\cdot 3^{t+1} - \frac{1}{2} \le n_2 \le 2\cdot 3^t,\\ 3^{t+1} - n_2, & \text{if } 2\cdot 3^t < n_2 < 3^{t+1}.\end{cases}$$

Let $G' = (G_1', n_1 - 2\cdot 3^{\ell+1} - m, k';\ G_2', n_2 + m, t;\ G_3', 3^{\ell+2}, \ell+1) \in \mathcal{CG}(n,3)$ be the graph obtained from G by Operation III (moving $2\cdot 3^{\ell+1}$ and m vertices from G_1 to G_3 and G_2, respectively), where $k' = k$ or $k-1$. Here, the last layer vertices of

G_2' are the vertices of $Y \cup V(R_{t+1}')$. For the sake of calculations, in the sequence of the last layer vertices of G_2', we arrange the vertices of Y first and then the vertices of $V(R_{t+1}')$. Note that

$$\sum_{\substack{x\in X\\ y\in V(R_{k+1})\setminus X}} d_G(x,y) = 3^t \cdot 2 \cdot 3^t \cdot 2(t+1) = 3^{2t}(4t+4).$$

By Lemma 4.3, replacing $t, \ell, m_1, m_2, n_1, n_3$ with $\ell, t, 2\cdot 3^{\ell+1}, m, 2\cdot 3^k, n_2$, respectively, we have

$$\begin{aligned} W(G) - W(G') =& -2\cdot 3^{2t+1} + 2n_2 \cdot 3^t + 2\cdot 3^t + m\left(3^t(-4t-6) + (2t+4)(n_2+m) + 1\right) \\ &+ \sum_{\substack{x\in Y\\ y\in V(R_{k+1})\setminus(X\cup Y)}} d_G(x,y) - \sum_{\substack{x\in Y\\ y\in V(R_{t+1}')}} d_{G'}(x,y). \end{aligned}$$

Case 1. $\frac{1}{2}\cdot 3^{t+1} - \frac{1}{2} \le n_2 \le 2\cdot 3^t$.
In this case, $|Y| = m = 3^t$ and $V(R_{k+1}) \setminus (X\cup Y) = \phi$. Hence,

$$\sum_{x\in Y, y\in V(R_{t+1}')} d_{G'}(x,y) = 3^t\left(n_2 - 3^t\right)\cdot 2(t+1)$$

and thus, we have $W(G) - W(G') = -2\cdot 3^{2t+1} + 4n_2\cdot 3^t + 3^{t+1} \ge -2\cdot 3^{2t+1} + 2\left(3^{t+1}-1\right)\cdot 3^t + 3^{t+1} = 3^t > 0$, a contradiction.

Case 2. $2\cdot 3^t < n_2 < 3^{t+1}$.
Note that $|Y| = m = 3^{t+1} - n_2 < 3^t$. Let H be the set of the left-most $3^t - m$ vertices on the line R_{t+1}' of G_2. Then $|H| = 3^t - m = |V(R_{k+1})\setminus(X\cup Y)|$ and

$$\sum_{x\in Y, y\in V(R_{t+1}')} d_{G'}(x,y) = m\cdot 3^t\cdot 2(t+1) + \sum_{x\in Y, y\in H} d_{G'}(x,y).$$

Hence, we have $W(G) - W(G') = 2\cdot 3^{2t+1} + 5\cdot 3^t - n_2(2\cdot 3^t+1) > 2\cdot 3^{2t+1} + 5\cdot 3^t - 3^{t+1}(2\cdot 3^t+1) = 2\cdot 3^t > 0$, a contradiction. □

Lemma 5.5. *Let $G = (G_1, n_1, k;\ G_2, n_2, t;\ G_3, n_3, \ell) \in \mathcal{CG}(n,3)$ be the graph as depicted in Figure 3, where $k = t+2$, $n_1 = 3^k + p\cdot 3^{k-1}$ $(1\le p\le 2)$, and $3^t < n_2 < 3^{t+1}$. If G is a Wiener-minimal graph of $\mathcal{CG}(n,3)$, then $n_3 \ne 3^t$.*

Proof. Suppose to the contrary that $n_3 = 3^t$. Let $G' = (n_1 + n_2 - 3^t;\ 3^t;\ n_3) \in \mathcal{CG}(n,3)$ be the graph obtained from G by Operation I (moving all vertices of $V(R_{t+1}')$ from G_2 to G_1). Note that

$$\sum_{\substack{x\in V(R_{t+1}')\\ y\in V(R_{k+1})}} d_{G'}(x,y) = \left(n_2 - 3^t\right)\cdot 2kp\cdot 3^{k-1}.$$

By Lemma 4.1, replacing m, k, t, n_2, n_1 with $(n_2 - 3^t), t, k, n_1, n_2$, respectively, we have

$$W(G) - W(G') = (n_2 - 3^t)\left(p\cdot 3^{t+1} - 2 - 2n_3\right) = (n_2 - 3^t)\left((3p-2)\cdot 3^t - 2\right) > 0,$$

a contradiction. □

Lemma 5.6. *Let $G = (G_1, n_1, k;\ G_2, n_2, t;\ G_3, n_3, \ell) \in \mathcal{CG}(n,3)$ be the graph as depicted in Figure 3, where $k = t = \ell$, and $3^k < n_1 < 3^{k+1}$, $n_2 = 3^{t+1}$, $n_3 = 3^{\ell+1}$. If G is a Wiener-minimal graph of $\mathcal{CG}(n,3)$, then either $n_1 = 3^k + 1$ or $n_1 > \frac{5}{2}\cdot 3^k - \frac{3}{2}$.*

Proof. Suppose to the contrary that $3^k + 2 \le n_1 \le \frac{5}{2}\cdot 3^k - \frac{3}{2}$. Take $X = V(R_{\ell+1}'')$. Let Y be the set of the left-most m vertices on line R_{k+1} of G_1, where

$$m = \begin{cases} n_1 - 3^k, & \text{if } 3^k + 2 \le n_1 \le 2\cdot 3^k, \\ 3^k, & \text{if } 2\cdot 3^k < n_1 \le \frac{5}{2}\cdot 3^k - \frac{3}{2}. \end{cases}$$

Then $|X| = 2\cdot 3^\ell = 2\cdot 3^t$, and $|Y| = m \le 3^t$. Let $G' = (G_1', n_1 - m, k';\ G_2', 3^{t+1} + 2\cdot 3^\ell + m, t+1;\ G_3', 3^\ell, \ell - 1) \in \mathcal{CG}(n,3)$ be the graph obtained from G by Operation II (moving moving all vertices of X from G_3 to G_2, and all vertices of Y from G_1 to G_2, respectively), where $k' = k$ or $k-1$. Here, the last layer vertices of G_2' are the vertices of $X\cup Y$. In the sequence of the last layer vertices of G_2', we arrange the vertices of X first and then the vertices of Y. Then

$$\sum_{x\in X, y\in Y} d_{G'}(x,y) = 2m\cdot 3^t\cdot 2(t+1).$$

By Lemma 4.2, replacing $t, k, \ell, m_1, m_2, n_1, n_2, n_3$ with $t+1, \ell, k, 2\cdot 3^\ell, m, 3^{\ell+1}, 3^{t+1}, n_1$, respectively, we have

$$W(G) - W(G') = 2\cdot 3^\ell\left(3^\ell - n_1 - 1\right) + m\left(3^\ell(2\ell+8) + (2\ell+4)(m-n_1) - 1\right) + \sum_{\substack{x\in Y\\ y\in V(R_{k+1})\setminus Y}} d_G(x,y).$$

Case 1. $3^k + 2 \le n_1 \le 2 \cdot 3^k$.
In this case, $m = n_1 - 3^k$ and $V(R_{k+1}) \setminus Y = \phi$. Thus, we have $W(G) - W(G') = (n_1 - 3^\ell)(2 \cdot 3^\ell - 1) - 2 \cdot 3^\ell > 0$, a contradiction.

Case 2. $2 \cdot 3^k \le n_1 \le \frac{5}{2} \cdot 3^k - \frac{3}{2}$.
Note that $m = 3^k$ and

$$\sum_{\substack{x \in Y \\ y \in V(R_{k+1}) \setminus Y}} d_G(x,y) = 3^k \left(n_1 - 2 \cdot 3^k\right) \cdot 2(k+1).$$

Thus, we have $W(G) - W(G') = 3^\ell \left(10 \cdot 3^\ell - 4n_1 - 3\right) \ge 3^{\ell+1} > 0$, a contradiction. □

Lemma 5.7. *Let $G = (G_1, n_1, k;\ G_2, n_2, t;\ G_3, n_3, \ell) \in \mathcal{CG}(n,3)$ be the graph as depicted in Figure 3, where $k = \ell = t$, $\ell \ge 2$, $n_2 = 3^{t+1}$, and $n_3 = 3^{\ell+1}$. If G is a Wiener-minimal graph of $\mathcal{CG}(n,3)$, then $n_1 \ne 3^k + 1$.*

Proof. Suppose to the contrary that $n_1 = 3^k + 1$. Let X be the set of the right-most $3^{t-1} - 1$ vertices on the line $V(R'_t)$ of G_2, $Y = V(R_k)$, $V(R_{k+1}) = \{v\}$, and suppose that the $(3^{t-1}+1)$-th vertex on the line $V(R'_t)$ of G_2 is u.

Let $H = (H_1;\ H_2;\ H_3)$ be the graph obtained from G by Operation II (moving all vertices of $V(R'_{t+1})$ from G_2 to G_3 and moving the vertex v from G_1 to G_3, respectively). Here, the last layer vertices of H_3 are the vertices of $V(R'_{t+1}) \cup \{v\}$. In the sequence of the last layer vertices of H_3, we arrange the vertices of $V(R'_{t+1})$ first and then the vertex v. Let $G' = (G'_1;\ G'_2;\ G'_3)$ be the graph obtained from H by Operation II (moving all vertices of Y from H_1 to H_3 and moving all vertices of X from H_2 to H_3, respectively). Then $G' = (3^{k-1};\ 2 \cdot 3^{t-1} + 1;\ 3^{\ell+1} + 2 \cdot 3^t + 3^{t-1} + 2 \cdot 3^{k-1}) \in \mathcal{CG}(n,3)$. The last layer vertices of G'_3 are the vertices of $V(R'_{t+1}) \cup \{v\} \cup X \cup Y$. For the sake of calculations, in the sequence of the last layer vertices of G'_3, we arrange the vertices of $V(R'_{t+1})$ first, then the vertex v, then the vertices of X, and finally the vertices of Y. Note that $V(R'_{t+1}) = 2 \cdot 3^t$, $|X| = 3^{t-1} - 1$, and $|Y| = 2 \cdot 3^{k-1}$. Thus,

$$\sum_{x \in V(R'_{t+1})} d_H(v,x) = \sum_{x \in V(R'_{t+1})} d_{G'}(v,x) = 2 \cdot 3^t \cdot 2(t+1) = 3^t(4t+4),$$

$$\sum_{\substack{x \in X \\ y \in V(R'_t) \setminus X}} d_H(x,y) = \sum_{\substack{x \in X \\ y \in V(R'_t) \setminus X}} d_G(x,y) = 3^{t-1}\left(3^{t-1} - 1\right) \cdot 2t + \sum_{x \in X} d_G(u,x),$$

$$\sum_{\substack{x \in X \\ y \in V(R'_{t+1}) \cup \{v\}}} d_{G'}(x,y) = 2 \cdot 3^t \left(3^{t-1} - 1\right) \cdot 2(t+1) + \sum_{x \in X} d_{G'}(v,x),$$

$$\sum_{\substack{x \in Y \\ y \in V(R'_{t+1}) \cup \{v\}}} d_{G'}(x,y) = 2 \cdot 3^{k-1}\left(2 \cdot 3^t \cdot 2(t+1) + 2t\right) = 3^{2t-1}(8t+8) + 4t \cdot 3^{t-1},$$

$$\sum_{\substack{x \in X \\ y \in Y}} d_{G'}(x,y) = 2 \cdot 3^{k-1}\left(3^{t-1} - 1\right) \cdot 2t = 4t \cdot 3^{2t-2} - 4t \cdot 3^{t-1},$$

$$\sum_{x \in X} d_G(u,x) = \sum_{x \in X} d_{G'}(v,x).$$

By Lemma 4.2, replacing $X, Y, k, \ell, t, n_1, n_2, n_3, m_1, m_2$ with $V(R'_{t+1}), \{v\}, t, k, \ell+1, 3^{t+1}, 3^{\ell+1}, 3^k+1, 2 \cdot 3^t, 1$, respectively, we have

$$W(G) - W(H) = 3^t(4t+4) - 1 - \sum_{x \in V(R'_{t+1})} d_H(v,x) = -1.$$

By Lemma 4.2, replacing $k, \ell, t, n_1, n_2, n_3, m_1, m_2$ with $t-1, k-1, \ell+1, 3^t, 3^{\ell+1} + 2 \cdot 3^t + 1, 3^k, 3^{t-1} - 1, 2 \cdot 3^{k-1}$, respectively, we have

$$\begin{aligned} W(H) - W(G') =& 3^{2t-2}(38t+43) - 3^{t-1}(10t+19) + 2 + \sum_{\substack{x \in X \\ y \in V(R'_t) \setminus X}} d_H(x,y) - \sum_{\substack{x \in X \\ y \in V(R'_{t+1}) \cup \{v\}}} d_{G'}(x,y) \\ & - \sum_{\substack{x \in Y \\ y \in V(R'_{t+1}) \cup \{v\}}} d_{G'}(x,y) - \sum_{\substack{x \in X \\ y \in Y}} d_{G'}(x,y) \\ =& 7 \cdot 3^{2t-2} - 7 \cdot 3^{t-1} + 2. \end{aligned}$$

By adding the last two equations, we arrive at $W(G) - W(G') = 7 \cdot 3^{2t-2} - 7 \cdot 3^{t-1} + 1 > 0$, a contradiction. □

Lemma 5.8. *Let $G = (G_1, n_1, k;\ G_2, n_2, t;\ G_3, n_3, \ell) \in \mathcal{CG}(n, 3)$ be the graph as depicted in Figure 3, where $k = t + 1$, $\ell = t$, $3^k + 3^{k-1} + 1 \le n_1 \le 2 \cdot 3^k + 3^{k-1}$, $n_2 = 3^{t+1}$, and $n_3 = 3^{\ell+1}$. Take*

$$m = \begin{cases} 2 \cdot 3^\ell, & \text{if } 3^k + 3^{k-1} + 1 \le n_1 \le 3^k + 2 \cdot 3^{k-1}, \\ 3^{k+1} - n_1 - 2 \cdot 3^t, & \text{if } 3^k + 2 \cdot 3^{k-1} < n_1 \le 2 \cdot 3^k + 3^{k-1}. \end{cases}$$

Let $G' = (G_1', n_1 + 2 \cdot 3^t + m, k;\ G_2', 3^t, t-1;\ G_3', n_3 - m, \ell') \in \mathcal{CG}(n, 3)$ be the graph obtained from G by Operation II (moving all vertices on line R_{t+1}' of G_2 to G_1, and moving m vertices on line $R_{\ell+1}''$ of G_3 to G_1, respectively), where $\ell' = \ell$ or $\ell - 1$, such that G' remains in the form of the graph depicted in Figure 3.

(1). *If $n_1 = 3^k + 3^{k-1} + 1$, then $W(G) < W(G')$.*

(2). *If $n_1 = 3^k + 3^{k-1} + 2$, then $W(G) = W(G')$.*

(3). *If $3^k + 3^{k-1} + 2 < n_1 \le 3^k + \frac{5}{2} \cdot 3^{k-1} - \frac{3}{2}$, then $W(G) > W(G')$.*

(4). *If $3^k + \frac{5}{2} \cdot 3^{k-1} - \frac{3}{2} < n_1 \le 2 \cdot 3^k + 3^{k-1}$, then $W(G) < W(G')$.*

Proof. Take $X = V(R_{t+1}')$. Let Y be the set of the right-most m vertices on the line $R_{\ell+1}''$ of G_3. The last layer vertices of G_1' are the vertices of $X \cup Y \cup V(R_{k+1})$. For the sake of calculations, in the sequence of the last layer vertices of G_1', we arrange the vertices of X first, then the vertices of Y, and finally the vertices of $V(R_{k+1})$. By Lemma 4.2, replacing $k, t, n_1, n_2, n_3, m_1, m_2$ with $t, k, 3^{t+1}, n_1, 3^{\ell+1}, 2 \cdot 3^{k-1}, m$, respectively, we have

$$\begin{aligned} W(G) - W(G') =& 3^{2k-2}(-12k - 16) + 3^{k-1}\left((4k+4)n_1 - (6k+6)m - 2\right) + m\left((2k+2)(n_1 + m) - 1\right) \\ &+ \sum_{\substack{x \in Y \\ y \in V(R_{\ell+1}'') \setminus Y}} d_G(x, y) + \sum_{x, y \in Y} \left(d_G(x, y) - d_{G'}(x, y)\right) - \sum_{\substack{x \in X \\ y \in V(R_{k+1})}} d_{G'}(x, y) \\ &- \sum_{\substack{x \in Y \\ y \in V(R_{k+1})}} d_{G'}(x, y) - \sum_{\substack{x \in X \\ y \in Y}} d_{G'}(x, y). \end{aligned}$$

Case 1. $3^k + 3^{k-1} + 1 \le n_1 \le 3^k + 2 \cdot 3^{k-1}$.
In this case, $|Y| = m = 2 \cdot 3^\ell = 2 \cdot 3^{k-1}$. Note that

$$\sum_{x, y \in Y} \left(d_G(x, y) - d_{G'}(x, y)\right) = -\,2 \cdot 3^{2k-2},$$

$$\sum_{\substack{x \in X \\ y \in V(R_{k+1})}} d_{G'}(x, y) = 2 \cdot 3^{k-1}\left(n_1 - 3^k\right) \cdot 2(k+1),$$

$$\sum_{\substack{x \in Y \\ y \in V(R_{k+1})}} d_{G'}(x, y) + \sum_{\substack{x \in X \\ y \in Y}} d_{G'}(x, y) = 3^{k-1}\left(2 \cdot 3^{k-1} + n_1 - 3^k\right)\left(2k + 2(k+1)\right).$$

Therefore, we have

$$W(G) - W(G') = -8 \cdot 3^{2k-2} + 3^{k-1}(2n_1 - 4) = 2 \cdot 3^{k-1}\left(n_1 - 3^k - 3^{k-1} - 2\right).$$

If $n_1 = 3^k + 3^{k-1} + 1$, then $W(G) < W(G')$.
If $n_1 = 3^k + 3^{k-1} + 2$, then $W(G) = W(G')$.
If $3^k + 3^{k-1} + 2 < n_1 \le 3^k + 2 \cdot 3^{k-1}$, then $W(G) > W(G')$.

Case 2. $3^k + 2 \cdot 3^{k-1} < n_1 \le 2 \cdot 3^k$.
Note that $3^{k-1} = 3^\ell \le |Y| = m = 7 \cdot 3^{k-1} - n_1 < 2 \cdot 3^{k-1}$. Let H_0 be the set of the right-most 3^ℓ vertices on the line $R_{\ell+1}''$ of G_3. Take $H_1 = Y \setminus H_0$ and $H_2 = V(R_{\ell+1}'') \setminus Y$. Let the vertices of H_3 be the $(3^k + 1)$-th to $(3^k + m - 3^{k-1})$-th vertices in the last layer of G_1'. Let H_4 be the set of the left-most $n_1 - 3^k - 2 \cdot 3^{k-1}$ vertices on the line $V(R_{k+1})$ of G_1. Then $3^{k-1} = 3^\ell = |H_1| + |H_2| = |H_3| + |H_4| = 3^{k-1}$. Hence

$$\sum_{\substack{x \in Y \\ y \in V(R_{\ell+1}'') \setminus Y}} d_G(x, y) = \left(2 \cdot 3^\ell - m\right) 3^\ell \cdot 2(\ell+1) + \sum_{x \in H_1, y \in H_2} d_G(x, y),$$

$$\sum_{x \in X, y \in V(R_{k+1})} d_{G'}(x, y) = 2 \cdot 3^{k-1}\left(n_1 - 3^k\right) \cdot 2(k+1) = 3^{k-1}\left(n_1 - 3^k\right)(4k+4),$$

$$\sum_{x,y\in Y}(d_G(x,y)-d_{G'}(x,y)) = 3^\ell\left(m-3^\ell\right)(2(\ell+1)-2(k+1)) = -2\cdot 3^\ell\left(m-3^\ell\right),$$

$$\sum_{\substack{x\in Y\\ y\in V(R_{k+1})}} d_{G'}(x,y)+\sum_{\substack{x\in X\\ y\in Y}} d_{G'}(x,y)$$

$$= 2m\cdot 3^{k-1}\cdot 2k + 2\cdot 3^{k-1}\left(m-3^{k-1}\right)\cdot 2(k+1) + 3^{k-1}\left(n_1-3^k\right)\cdot 2(k+1) + \sum_{x\in H_3, y\in H_4} d_{G'}(x,y).$$

Thus, we have

$$W(G)-W(G') = 22\cdot 3^{2k-2} - 3^{k+1} - n_1\left(4\cdot 3^{k-1}-1\right).$$

If $3^k+2\cdot 3^{k-1} < n_1 \le 3^k + \frac{5}{2}\cdot 3^{k-1} - \frac{3}{2}$, then

$$W(G)-W(G') \ge \frac{5}{2}\cdot 3^{k-1} - \frac{3}{2} > 0.$$

If $3^k + \frac{5}{2}\cdot 3^{k-1} - \frac{3}{2} < n_1 \le 2\cdot 3^k$, then

$$W(G)-W(G') \le -\frac{3}{2}\cdot 3^{k-1} - \frac{1}{2} < 0.$$

Case 3. $2\cdot 3^k < n_1 \le 2\cdot 3^k + 3^{k-1}$.
In this case, $0 \le |Y| = m = 7\cdot 3^{k-1} - n_1 < 3^{k-1} = 3^\ell$. Let S_0 be the set of the right-most $3^\ell - m$ vertices, except for Y, on the line $R''_{\ell+1}$ of G_3. Let S_1 be the set of the left-most $n_1 - 2\cdot 3^k$ vertices on the line $V(R_{k+1})$ of G_1. Then $3^{k-1} = 3^\ell = |S_0| + |Y| = |Y| + |S_1| = 3^{k-1}$. Thus,

$$\sum_{\substack{x\in Y\\ y\in V(R''_{\ell+1})\setminus Y}} d_G(x,y) = 3^\ell m\cdot 2(\ell+1) + \sum_{\substack{x\in S_0\\ y\in Y}} d_G(x,y),$$

$$\sum_{x\in X, y\in V(R_{k+1})} d_{G'}(x,y) = 2\cdot 3^{k-1}\left(3^k\cdot 2(k+1) + 2k\left(n_1 - 2\cdot 3^k\right)\right),$$

$$\sum_{\substack{x\in Y\\ y\in V(R_{k+1})}} d_{G'}(x,y) + \sum_{\substack{x\in X\\ y\in Y}} d_{G'}(x,y) = m\left(2\cdot 3^{k-1}\cdot 2k + 3^k\cdot 2(k+1)\right) + \sum_{\substack{x\in S_1\\ y\in Y}} d_{G'}(x,y).$$

Consequently, we have $W(G)-W(G') = -14\cdot 3^{2k-2} + n_1\left(2\cdot 3^{k-1}+1\right) - 3^{k+1} \le -2\cdot 3^{k-1} < 0$. □

Lemma 5.9. *Let $G = (G_1, n_1, k;\ G_2, n_2, t;\ G_3, n_3, \ell) \in \mathcal{CG}(n,3)$ be the graph as depicted in Figure 3, where $k = t+2$, $\ell \le t$, $3^k < n_1 < 3^{k+1}$, $n_2 = 3^{t+1}$, and $n_3 = 3^{\ell+1}$. If G is a Wiener-minimal graph of $\mathcal{CG}(n,3)$, then either $3^k < n_1 \le 3^k + 2\cdot 3^{k-1}$ or $n_1 \ge 2\cdot 3^k$.*

Proof. Suppose to the contrary that $3^k + 2\cdot 3^{k-1} < n_1 < 2\cdot 3^k$. Let X be the set of the right-most m vertices on the line R'_{t+1} of G_2, where

$$m = \begin{cases} 2\cdot 3^t, & \text{if } 3^k + 2\cdot 3^{k-1} < n_1 \le 3^k + 2\cdot 3^{k-1} + 3^{k-2}, \\ 2\cdot 3^k - n_1, & \text{if } 3^k + 2\cdot 3^{k-1} + 3^{k-2} < n_1 < 2\cdot 3^k. \end{cases}$$

Let $G' = (G'_1, n_1+m, k;\ G'_2, n_2-m, t';\ G'_3, n_3, \ell) \in \mathcal{CG}(n,3)$ be the graph obtained from G by Operation I (moving m vertices on line R'_{t+1} of G_2 to G_1), where $t' = t$ or $t-1$. By Lemma 4.1, replacing k, t, n_1, n_2, n_3 with $t, k, 3^{t+1}, n_1, 3^{\ell+1}$, respectively, we have

$$\begin{aligned} W(G)-W(G') &= m\left(3^{k-2}(-22k-11) + (2k+1)(n_1+m) - 2\cdot 3^{\ell+1} - 2\right) + \sum_{\substack{x\in X\\ y\in V(R_{t+1})\setminus X}} d_G(x,y) \\ &\quad + \sum_{x,y\in V(R_{k+1})}(d_G(x,y)-d_{G'}(x,y)) + \sum_{x,y\in X}(d_G(x,y)-d_{G'}(x,y)) - \sum_{x\in X, y\in V(R_{k+1})} d_{G'}(x,y) \\ &\ge m\left(3^{k-2}(-22k-11) + (2k+1)(n_1+m) - 2\cdot 3^{t+1} - 2\right) + \sum_{\substack{x\in X\\ y\in V(R_{t+1})\setminus X}} d_G(x,y) \\ &\quad + \sum_{x,y\in V(R_{k+1})}(d_G(x,y)-d_{G'}(x,y)) + \sum_{x,y\in X}(d_G(x,y)-d_{G'}(x,y)) - \sum_{x\in X, y\in V(R_{k+1})} d_{G'}(x,y). \end{aligned}$$

Case 1. $3^k+2\cdot 3^{k-1}<n_1\leq 3^k+2\cdot 3^{k-1}+3^{k-2}$.
Note that $|X|=m=2\cdot 3^t=2\cdot 3^{k-2}$. Suppose that the vertices of X are the $(2\cdot 3^{k-1}+1)$-th to $(2\cdot 3^{k-1}+2\cdot 3^{k-2})$-th vertices in the last layer of G_1'. Let V_1 be the set of the left-most $2\cdot 3^{k-1}$ vertices on the line R_{k+1} of G_1, and take $V_2=V(R_{k+1})\setminus V_1$. Then, we have

$$\sum_{\substack{x\in X\\ y\in V(R_{k+1})}} d_{G'}(x,y)=2\cdot 3^{k-2}\left(2\cdot 3^{k-1}\cdot 2k+\left(n_1-3^k-2\cdot 3^{k-1}\right)\cdot 2(k-1)\right),$$

and hence

$$W(G)-W(G')\geq -10\cdot 3^{2k-2}+2\cdot 3^{k-1}\left(5\cdot 3^{k-1}+1\right)-4\cdot 3^{k-2}=2\cdot 3^{k-2}>0,$$

a contradiction.

Case 2. $3^k+2\cdot 3^{k-1}+3^{k-2}<n_1<2\cdot 3^k$.
In this case, $|X|=m=2\cdot 3^k-n_1<2\cdot 3^k-(3^k+2\cdot 3^{k-1}+3^{k-2})=2\cdot 3^{k-2}$. The last layer vertices of G_1' are the vertices of $V(R_{k+1})\cup X$. In the sequence of the last layer vertices of G_1', we arrange the vertices of $V(R_{k+1})$ first and then the vertices of X. Let V_1 be the set of the left-most $2\cdot 3^{k-1}$ vertices on the line R_{k+1} of G_1. Let V_2 be the set of the left-most 3^{k-2} vertices, except for V_1, on the line R_{k+1} of G_1. Take $V_3=V(R_{k+1})\setminus(V_1\cup V_2)$ and $H_1=V(R'_{t+1})\setminus X$. Then $|V_3|+|X|=2\cdot 3^{k-2}=|H_1|+|X|$; that is, $|V_3|=|H_1|$. thus, we have

$$\sum_{\substack{x\in X\\ y\in V(R_{k+1})}} d_{G'}(x,y)=2m\cdot 3^{k-1}\cdot 2k+3^{k-2}m\cdot 2(k-1)+\sum_{\substack{x\in X\\ y\in V_3}} d_{G'}(x,y),$$

$$\sum_{\substack{x\in X\\ y\in V(R_{t+1})\setminus X}} d_G(x,y)=\sum_{\substack{x\in X\\ y\in H_1}} d_G(x,y).$$

Therefore, we have $W(G)-W(G')\geq\left(2\cdot 3^k-n_1\right)\left(3^{k-1}-2\right)>0$, a contradiction. □

Lemma 5.10. *Let $G=(G_1,n_1,k;\ G_2,n_2,t;\ G_3,n_3,\ell)\in\mathcal{CG}(n,3)$ be the graph as depicted in Figure 3, where $k=t+2$, $\ell=t$, $n_2=3^{t+1}$, and $n_3=3^{\ell+1}$. If G is a Wiener-minimal graph of $\mathcal{CG}(n,3)$, then $n_1\neq 2\cdot 3^k+2\cdot 3^{k-1}+1$.*

Proof. Suppose to the contrary that $n_1=2\cdot 3^k+2\cdot 3^{k-1}+1$. Let $G'=(G_1';\ G_2';\ G_3')\in\mathcal{CG}(n,3)$ be the graph obtained from G by moving $2\cdot 3^{t+1}$ and $2\cdot 3^{\ell+1}$ vertices on the line R_{k+1} of G_1 to G_2 and G_3, respectively. Then $|V(G_1')|=3^k+3^{k-1}+1$. By Lemma 5.8(1), the inequality $W(G)>W(G')$ is obtained, which yields a contradiction. □

Lemma 5.11. *Let $G=(G_1,n_1,k;\ G_2,n_2,t;\ G_3,n_3,\ell)\in\mathcal{CG}(n,3)$ be the graph as depicted in Figure 3, where $k=t+3$, $\ell=t$, $3^k<n_1<3^{k+1}$, $n_2=3^{t+1}$, and $n_3=3^{\ell+1}$. If G is a Wiener-minimal graph of $\mathcal{CG}(n,3)$, then either $3^k<n_1\leq 3^k+2\cdot 3^{k-2}$ or $3^k+3^{k-1}+2\cdot 3^{k-2}+2\cdot 3^{k-3}+1<n_1<3^{k+1}$.*

Proof. Suppose to the contrary that $3^k+2\cdot 3^{k-2}<n_1\leq 3^k+3^{k-1}+2\cdot 3^{k-2}+2\cdot 3^{k-3}+1$. Let X be the set of the left-most $2\cdot 3^{k-2}$ vertices on the line R_{k+1} of G_1. Let Y be the set of the left-most m vertices, except for X, on the line R_{k+1} of G_1, where

$$m=\begin{cases} n_1-3^k-2\cdot 3^{k-2}, & \text{if } n_1\leq 3^k+3^{k-1}+3^{k-2},\\ 2\cdot 3^{k-2}, & \text{if } n_1>3^k+3^{k-1}+3^{k-2}.\end{cases}$$

Let $G'=(G_1';\ G_2';\ G_3')\in\mathcal{CG}(n,3)$ be the graph obtained from G by Operation III (moving $2\cdot 3^{k-2}$ vertices from G_1 to G_2 and moving m vertices from G_1 to G_3, respectively). Note that

$$\sum_{x,y\in V(R_{k+1})\setminus(X\cup Y)}\left(d_G(x,y)-d_{G'}(x,y)\right)=0.$$

By Lemma 4.3, replacing ℓ,m_1,m_2,n_3 with $\ell+1,2\cdot 3^{k-2},m,3^{\ell+1}$, respectively, we have

$$\begin{aligned}W(G)-W(G')=&3^{2k-4}(44k+26)+4\cdot 3^{k-2}-3^{k-2}n_1(4k+2)+m\left(3^{k-2}(22k+17)+(2k+1)(m-n_1)+2\right)\\&+\sum_{\substack{x\in Y\\ y\in V(R_{k+1})\setminus(X\cup Y)}} d_G(x,y)+\sum_{\substack{x\in X\\ y\in V(R_{k+1})\setminus X}} d_G(x,y)+\sum_{x,y\in Y}\left(d_G(x,y)-d_{G'}(x,y)\right).\end{aligned}$$

Case 1. $3^k + 2 \cdot 3^{k-2} < n_1 \leq 3^k + 3^{k-1}$.
In this case, $|Y| = m = n_1 - 3^k - 2 \cdot 3^{k-2} \leq 3^{k-2}$ and $V(R_{k+1}) \setminus (X \cup Y) = \phi$. Thus,

$$\sum_{\substack{x \in X \\ y \in V(R_{k+1}) \setminus X}} d_G(x,y) = 2m \cdot 3^{k-2} \cdot 2(k-1),$$

and hence, we have $W(G) - W(G') = 2\left(n_1 + 3^{k-1}\left(2 \cdot 3^{k-3} - 3\right)\right) > 0$, a contradiction.

Case 2. $3^k + 3^{k-1} < n_1 \leq 3^k + 3^{k-1} + 3^{k-2}$.
Note that $3^{k-2} < |Y| = m = n_1 - 3^k - 2 \cdot 3^{k-2} \leq 2 \cdot 3^{k-2}$ and $V(R_{k+1}) \setminus (X \cup Y) = \phi$. Therefore,

$$\sum_{\substack{x \in X \\ y \in V(R_{k+1}) \setminus X}} d_G(x,y) = 2 \cdot 3^{k-2}\left(3^{k-2} \cdot 2(k-1) + \left(m - 3^{k-2}\right) \cdot 2k\right),$$

$$\sum_{x,y \in Y} \left(d_G(x,y) - d_{G'}(x,y)\right) = 3^{k-2}\left(m - 3^{k-2}\right)\left(2k - 2(\ell+2)\right) = 2 \cdot 3^{k-2}\left(m - 3^{k-2}\right).$$

Thus, we have $W(G) - W(G') = 2 \cdot 3^{k-1}\left(n_1 - 34 \cdot 3^{k-3} - 3\right) + 2n_1 > 0$, a contradiction.

Case 3. $3^k + 3^{k-1} + 3^{k-2} < n_1 \leq 3^k + 3^{k-1} + 2 \cdot 3^{k-2} + 2 \cdot 3^{k-3} + 1$.
In this case, It holds that $|Y| = m = 2 \cdot 3^{k-2} = 2 \cdot 3^{\ell+1}$. So,

$$\sum_{\substack{x \in X \\ y \in V(R_{k+1}) \setminus X}} d_G(x,y) = 2 \cdot 3^{k-2}\left(3^{k-2} \cdot 2(k-1) + 2k\left(n_1 - 3^k - 3^{k-1}\right)\right),$$

$$\sum_{\substack{x \in Y \\ y \in V(R_{k+1}) \setminus (X \cup Y)}} d_G(x,y) = \left(n_1 - 3^k - 3^{k-1} - 3^{k-2}\right)\left(3^{k-2} \cdot 2k + 3^{k-2} \cdot 2(k-1)\right),$$

$$\sum_{x,y \in Y} \left(d_G(x,y) - d_{G'}(x,y)\right) = 3^{2k-4}\left(2k - 2(\ell+2)\right) = 2 \cdot 3^{2k-4}.$$

Therefore, we have $W(G) - W(G') = 2 \cdot 3^{k-2}\left(44 \cdot 3^{k-2} - 3n_1 + 4\right) \geq 2 \cdot 3^{k-2} > 0$, a contradiction. □

Lemma 5.12. *Let $G = (G_1, n_1, k;\ G_2, n_2, t;\ G_3, n_3, \ell) \in \mathcal{CG}(n,3)$ be the graph as depicted in Figure 3, where $k = \ell + 1$, $t = \ell + 2$, $3^k < n_1 < 3^{k+1}$, $n_2 = 3^{t+1}$, and $n_3 = 3^{\ell+1}$. If G is a Wiener-minimal graph of $\mathcal{CG}(n,3)$, then $3^k < n_1 \leq \frac{1}{2} \cdot 3^{k+1} - \frac{3}{2}$.*

Proof. Suppose to the contrary that $\frac{1}{2} \cdot 3^{k+1} - \frac{3}{2} < n_1 < 3^{k+1}$. Let $G' = (G'_1;\ G'_2;\ G'_3) \in \mathcal{CG}(n,3)$ be the graph obtained from G by Operation III (moving $2 \cdot 3^{\ell+1}$ vertices and $3^{k+1} - n_1$ vertices on the line R'_{t+1} of G_2 to G_3 and G_1, respectively). Since $|V(G'_2)| = 3^{t+1} - 2 \cdot 3^{\ell+1} - 3^{k+1} + n_1$, we have

$$3^t + \frac{5}{2} \cdot 3^{t-1} - \frac{3}{2} < |V(G'_2)| < 2 \cdot 3^t + 3^{t-1}.$$

By Lemma 5.8(4), we have $W(G) > W(G')$, a contradiction. □

6. Main result

In this section, we give a characterization of the Wiener-minimal graphs of $\mathcal{CG}(n,3)$.

Theorem 6.1. *Let $G \in \mathcal{CG}(n,3)$ be a Wiener-minimal graph of $\mathcal{CG}(n,3)$ with $n \geq 25$. If $n = 10 \cdot 3^\ell + 2$ with $\ell \geq 1$, then $G \cong (3^{\ell+1} + 3^\ell + 2;\ 3^{\ell+1};\ 3^{\ell+1})$ or $G \cong (2 \cdot 3^{\ell+1} + 2 \cdot 3^\ell + 2;\ 3^\ell;\ 3^\ell)$. If $n \neq 10 \cdot 3^\ell + 2$ for any $\ell \geq 1$, then $G \cong (n_1;\ n_2;\ n_3)$, where $n_1 + n_2 + n_3 = n$, and one of the following holds:*

(1). *$n_1 = 3^{k+1}$, $n_2 = 3^{t+1}$, $n_3 = 3^{\ell+1}$, $t = \ell$, and $t \leq k \leq t+2$.*

(2). *$n_1 = 2 \cdot 3^k$, $3^t < n_2 < \frac{1}{2} \cdot 3^{t+1} - \frac{1}{2}$, $n_3 = 3^{\ell+1}$, $k = t+1$, and $t = \ell + 1$.*

(3). *$n_1 = 2 \cdot 3^k$, $3^t < n_2 < 3^{t+1}$, $n_3 = 3^{\ell+1}$, $k = t+2$, and $\ell \leq t \leq \ell + 1$.*

(4). *$\frac{5}{2} \cdot 3^k - \frac{3}{2} < n_1 < 3^{k+1}$, $n_2 = 3^{t+1}$, $n_3 = 3^{\ell+1}$, and $k = t = \ell$.*

(5). *$3^k < n_1 < 3^k + 3^{k-1} + 2$ or $3^k + \frac{5}{2} \cdot 3^{k-1} - \frac{3}{2} < n_1 < 3^{k+1}$, $n_2 = 3^{t+1}$, $n_3 = 3^{\ell+1}$, $k = t+1$ and $t = \ell$.*

(6). *$n_1 = 2 \cdot 3^k$ or $2 \cdot 3^k + 2 \cdot 3^{k-1} + 1 < n_1 < 3^{k+1}$, $n_2 = 3^{t+1}$, $n_3 = 3^{\ell+1}$, $k = t+2$ and $t = \ell$.*

(7). $3^k + 3^{k-1} + 2 \cdot 3^{k-2} + 2 \cdot 3^{k-3} + 1 < n_1 \leq 2 \cdot 3^k$ *and* $n_1 \neq 46, 47, 48$, $n_2 = 3^{t+1}$, $n_3 = 3^{\ell+1}$, $k = t + 3$ *and* $t = \ell$.

(8). $n_1 = 2 \cdot 3^k$, $n_2 = 3^{t+1}$, $n_3 = 3^{\ell+1}$, $k = \ell + 3$ *and* $t = \ell + 1$.

(9). $3^k < n_1 \leq 2 \cdot 3^k$, $n_2 = 3^{t+1}$, $n_3 = 3^{\ell+1}$, $k = t = 2$ *and* $\ell = 1$.

(10). $3^k < n_1 \leq 3^k + 3^{k-1} + 2 \cdot 3^{k-2} + 1$, $n_2 = 3^{t+1}$, $n_3 = 3^{\ell+1}$, $k = t = \ell + 1$ *and* $\ell \geq 2$.

(11). $3^k < n_1 \leq \frac{1}{2} \cdot 3^{k+1} - \frac{3}{2}$, $n_2 = 3^{t+1}$, $n_3 = 3^{\ell+1}$, $k = \ell + 1$ *and* $t = \ell + 2$.

Proof. Let $G \in \mathcal{CG}(n, 3)$ be a Wiener-minimal graph of $\mathcal{CG}(n, 3)$, where $n \geq 25$. By Lemma 3.1,

$$G = (G_1, n_1, k;\ G_2, n_2, t;\ G_3, n_3, \ell)$$

has the form of the graph shown in Figure 3, where $G_i = T_{n_i}(2, 4)$ with $n_i \geq 3$ for $i = 1, 2, 3$, $n_1 + n_2 + n_3 = n$, $3^k < n_1 \leq 3^{k+1}$, $3^t < n_2 \leq 3^{t+1}$, and $3^\ell < n_3 \leq 3^{\ell+1}$. We consider four cases.

Case 1. $n_1 = 3^{k+1}$, $n_2 = 3^{t+1}$, $n_3 = 3^{\ell+1}$, and $k \geq \ell \geq t$.
By Lemma 5.2(1) and Lemma 5.2(4), $k \leq t + 2$. If $k = t + 2$, then by Lemma 5.2(2), $\ell = k - 2 = t$. If $k = t + 1$, then by Lemma 5.3, $\ell \neq k$; that is, $\ell = t$. consequently, $t = \ell$ and $t \leq k \leq t + 2$.

Case 2. $3^k < n_1 < 3^{k+1}$, $3^t < n_2 < 3^{t+1}$, $3^\ell < n_3 < 3^{\ell+1}$, and $k \geq \ell \geq t$.
By Lemma 3.3(1), the numbers k, t, and ℓ are different. Thus, $k = t + 2$ and $\ell = t + 1$ by Lemma 5.1(1), which contradicts Lemma 5.1(3). Thus, there is no such case.

Case 3. $3^k < n_1 < 3^{k+1}$, $3^t < n_2 < 3^{t+1}$, and $n_3 = 3^{\ell+1}$, and $k \geq t$.
By Lemma 3.3(1), Lemmas 3.3(2), and Lemma 5.1(1), $t + 1 \leq k \leq t + 2$ and $3^{t+1} \mid (n_1 - 3^k)$.

Subcase 3.1. $k = t + 1$.
By Lemma 3.3(3) and Lemma 5.1(2), $n_1 = 2 \cdot 3^k$ and $n_3 = 3^{\ell+1} < 3^{t+1}$. Therefore, $t > \ell$. If $t \geq \ell + 2$, then this contradicts Lemma 5.2(2) because $n_1 > 3^k = 3^{t+1}$. Hence, $t = \ell + 1$. By Lemma 5.4, $3^t < n_2 < \frac{1}{2} \cdot 3^{t+1} - \frac{1}{2}$.

Subcase 3.2. $k = t + 2$.
Note that $3^{k-1} \mid (n_1 - 3^k)$ and $3^k < n_1 < 3^{k+1}$. Then

$$n_1 - 3^k = p_1 \cdot 3^k + p_2 \cdot 3^{k-1}, \tag{19}$$

where $0 \leq p_1 \leq 1$, $0 \leq p_2 \leq 2$, and $p_1 + p_2 \geq 1$. By Lemma 5.1(3), $n_3 < 2 \cdot 3^{t+1}$; that is, $\ell \leq t$. By Lemma 5.2(1), $k \leq \ell + 3$. Hence, $\ell \leq t \leq \ell + 1$. If $t = \ell$, then by (19), Lemma 5.1(4), and Lemma 5.1(5), $n_1 = 2 \cdot 3^k$ because $n_3 = 3^{\ell+1} = 3^{t+1}$. If $t = \ell + 1$, then by Lemma 5.2(4), $3^k + 2 \cdot 3^{k-2} < n_1 \leq 2 \cdot 3^k$. Hence, by (19), either $n_1 = 2 \cdot 3^k$ or $n_1 = 3^k + p_2 \cdot 3^{k-1}$ with $1 \leq p_2 \leq 2$. By Lemma 5.5, $n_1 = 2 \cdot 3^k$.

Case 4. $3^k < n_1 < 3^{k+1}$, $n_2 = 3^{t+1}$, $n_3 = 3^{\ell+1}$, and $t \geq \ell$.
By Lemma 5.2(1) and Lemma 5.2(4), $k \leq \ell + 3$ and $t \leq \ell + 2$. By Lemma 5.1(1) and Lemma 5.1(4), $t \leq k + 1$. Thus, $\ell \leq t \leq \ell + 2$ and $t - 1 \leq k \leq \ell + 3$.

Subcase 4.1. $t = \ell$.
If $k = t - 1$, then it contradicts Lemma 5.1(2).
If $k = t$, then by Lemma 5.6 and Lemma 5.7, $n_1 > \frac{5}{2} \cdot 3^k - \frac{3}{2}$.
If $k = t + 1$, then by Lemma 5.8(2) and Lemma 5.8(3), either $3^k < n_1 \leq 3^k + 3^{k-1} + 2$ or $3^k + \frac{5}{2} \cdot 3^{k-1} - \frac{3}{2} < n_1 < 3^{k+1}$.
If $k = t + 2$, then by Lemma 5.2(3), Lemma 5.9, and Lemma 5.10, either $n_1 = 2 \cdot 3^k$ or $2 \cdot 3^k + 2 \cdot 3^{k-1} + 1 < n_1 < 3^{k+1}$.
If $k = t + 3$, then by Lemma 5.2(4) and Lemma 5.11, $3^k + 3^{k-1} + 2 \cdot 3^{k-2} + 2 \cdot 3^{k-3} + 1 < n_1 \leq 2 \cdot 3^k$. If $t = \ell = 0$ and $n_1 = 3^k + 2 \cdot 3^{k-1} + p = 3^3 + 2 \cdot 3^2 + p$, where $p = 1, 2, 3$; that is, $n_2 = n_3 = 3$ and $n_1 = 46, 47$, or 48, then by Lemma 5.3(3), there is the graph $H = (n_1 - 30;\ 27;\ 9) \in \mathcal{CG}(n, 3)$ such that $W(H) < W(G)$. Therefore, $n_1 \neq 46, 47, 48$.

In particular, by Lemma 5.8(2), the two graphs corresponding to "$k = t + 1$ and $n_1 = 3^k + 3^{k-1} + 2$" and "$k = t + 2$ and $n_1 = 2 \cdot 3^k + 2 \cdot 3^{k-1} + 2$" have the same Wiener index; that is, $W(\widehat{G}) = W(\overline{G})$, where $\widehat{G} = (3^{\ell+1} + 3^\ell + 2;\ 3^{\ell+1};\ 3^{\ell+1})$ and $\overline{G} = (2 \cdot 3^{\ell+1} + 2 \cdot 3^\ell + 2;\ 3^\ell;\ 3^\ell)$. In this case, $n = 10 \cdot 3^\ell + 2$, which implies that for $n = 10 \cdot 3^\ell + 2$, there are two Wiener-minimal graphs $\widehat{G}, \overline{G} \in \mathcal{CG}(n, 3)$.

Subcase 4.2. $t = \ell + 1$.
Note that $\ell \leq k \leq \ell + 3$. By Lemma 5.1(2) and Lemma 5.2(2), $k \neq \ell$ and $k \neq \ell + 2$.

If $k = \ell + 1$ and $\ell = 1$, then by Lemma 5.3(2), $3^k < n_1 \leq 2 \cdot 3^k$. If $k = \ell + 1$ and $\ell \geq 2$, then by Lemma 5.3(1), $3^k < n_1 \leq 3^k + 3^{k-1} + 2 \cdot 3^{k-2} + 1$.

If $k = \ell + 3$, then by Lemma 5.2(4), Lemma 5.2(5), and Lemma 5.9, $n_1 = 2 \cdot 3^k$.

Subcase 4.3. $t = \ell + 2$.
In this subcase, $\ell + 1 \leq k \leq \ell + 3$. By Lemma 5.2(2), $n_1 < 3^t$; that is, $k < t = \ell + 2$. therefore, $k = \ell + 1$. By Lemma 5.12, $3^k < n_1 \leq \frac{1}{2} \cdot 3^{k+1} - \frac{3}{2}$. □

Corollary 6.1. *Let $G \in \mathcal{CG}(n, 3)$ be a Wiener-minimal graph of $\mathcal{CG}(n, 3)$, where $n \geq 25$. The graph G is unique except for $n = 10 \cdot 3^\ell + 2$ with $\ell \geq 1$. For $n = 10 \cdot 3^\ell + 2$ with $\ell \geq 1$, there are exactly two such graphs.*

7. Conclusion

In this paper, the problem of determining the Wiener-minimal graphs is completely solved for unicyclic chemical graphs of order n and girth 3. It turns out that for $n = 10 \cdot 3^\ell + 2$ with $\ell \geq 1$, there are exactly two Wiener-minimal graphs. However, for every $n \geq 25$, satisfying $n \neq 10 \cdot 3^\ell + 2$, there exists exactly one such Wiener-minimal graph. Determining the Wiener-minimal graphs in the case of general graphs of fixed order with given girth and maximum degree remains an open problem.

Acknowledgements

The authors are extremely thankful to the anonymous reviewers for their valuable comments and suggestions. This work was supported by Shanxi Scholarship Council of China (Grant No. 2022-149).

References

[1] H. Chen, C. Li, Wiener index, Kirchhoff index in graphs with given girth and maximum degree, *MATCH Commun. Math. Comput. Chem.* **88** (2022) 683–703.
[2] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.
[3] M. Fischermann, A. Hoffmann, D. Rautenbach, L. Székely, L. Volkmann, Wiener index versus maximum degree in trees, *Discrete Appl. Math.* **122** (2002) 127–137.
[4] Y. Hong, H. Liu, X. Wu, On the Wiener index of unicyclic graphs, *Hacettepe J. Math. Stat.* **40** (2011) 63–68.
[5] M. Knor, R. Škrekovski, A. Tepeh, Mathematical aspects of Wiener index, *Ars Math. Contemp.* **11** (2016) 327–352.
[6] M. Knor, R. Škrekovski, A. Tepeh, Chemical graphs with the minimum value of Wiener index, *MATCH Commun. Math. Comput. Chem.* **81** (2019) 119–132.
[7] H. Liu, M. Lu, A unified approach to extremal cacti for different indices, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 183–194.
[8] P. Luo, C. Q. Zhang, X. D. Zhang, Wiener index of unicycle graphs with given number of even degree vertices, *Discrete Math. Algorithm. Appl.* **12(4)** (2020) 2050054.
[9] S. Tan, The minimum Wiener index of unicyclic graphs with a fixed diameter, *J. Appl. Math. Comput.* **56** (2018) 93–114.
[10] K. Xu, M. Liu, K. C. Das, I. Gutman, B. Furtula, A survey on graphs extremal with respect to distance-based topological indices, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 461–508.
[11] G. Yu, L. Feng, On the Wiener index of unicyclic graphs with given girth, *Ars Combin.* **94** (2010) 361–369.