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Research Article

Minimum Detour Index of Tricyclic Graphs

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The detour index of a connected graph is defined as the sum of the detour distances (lengths of longest paths) between unordered pairs of vertices of the graph. The detour index is used in various quantitative structure-property relationship and quantitative structure-activity relationship studies. In this paper, we characterize the minimum detour index among all tricyclic graphs, which attain the bounds.

1. Introduction

Let G be a simple and connected graph with $|V(G)| = n$ and $|E(G)| = m$ and $N_G(u)$ be the neighbor vertex set of vertex u, then $d_G(u) = |N_G(u)|$ is called the degree of u. If $m = n - 1 + c$, then G is called a c-cyclic graph. If $c = 0, 1, 2$, and 3, then G is a tree, unicyclic graph, bicyclic graph, and tricyclic graph, respectively. Denote by $\mathcal{T}_n$ the set of all tricyclic graphs of order n.

Let $\widehat{\mathcal{T}} = \left\{\widehat{\mathcal{T}}^i \mid 1 \le i \le 15\right\}$, where graphs $\widehat{\mathcal{T}}^i$ for $i = 1, 2, \ldots, 15$ are defined in Figure 1. By [1, 2], we know that for any $\mathcal{T}^i \in \mathcal{T}_n$, $\mathcal{T}^i$ can be obtained from $\widehat{\mathcal{T}}^i$ $(1 \le i \le 15)$ by attaching trees to some of its vertices. We call $\widehat{\mathcal{T}}^i$ the base of $\mathcal{T}^i$.

A block of the graph G is a maximal 2-connected subgraph of G. A cactus is a connected graph in which no edge lies in more than one cycle, such that each block of a cactus is either an edge or a cycle. A vertex shared by two or more cycles is called a cut vertex. In this paper, denote $\mathcal{C}_n^l$ be the set of all cacti of order n and l cycles, where $l \ge 1$. The length of the cycles may be different and the length of each cycle is at least 3.

The concept of "topological index" was first proposed by Haruo Hosoya for characterizing the topological nature of a graph. Such graph invariants are usually related to the distance function $d(-,-)$.

The detour distance [3, 4] (also known under the name elongation) between vertices u and v in G is the length of a longest path between them, denoted by $l(u, v \mid G)$. Note that $l(u, u \mid G) = 0$ for any $u \in V(G)$; see [5] for a discussion. The detour index of the graph G is defined as [4–9]

$$\omega(G) = \frac{1}{2} \sum_{u,v \in V(G)} l(u, v \mid G). \tag{1}$$

For a connected graph G with $u \in V(G)$, let $L(u \mid G) = \sum_{v \in V(G)} l(u, v \mid G)$, then

$$\omega(G) = \frac{1}{2} \sum_{u \in V(G)} L(u \mid G). \tag{2}$$

If we use the notion of the detour matrix [4], which is an $n \times n$ matrix whose (i, j)-element is $l(v_i, v_j \mid G)$ with $V(G) = \{v_1, v_2, \ldots, v_n\}$, then the detour index is equal to the half-sum of the (off diagonal) elements of the detour matrix. The detour index has been applied to chemistry, especially in quantitative structure-activity relationship (QSAR) studies; see [7, 10] for more details. A new branch cheminformatics is a combination of mathematics and chemistry. This branch studies QSAR/QSPR study, physicochemical properties and topological indices such as Zagreb Indices [11], Kirchhoff index [12], Hosoya index [13] and so on to predict

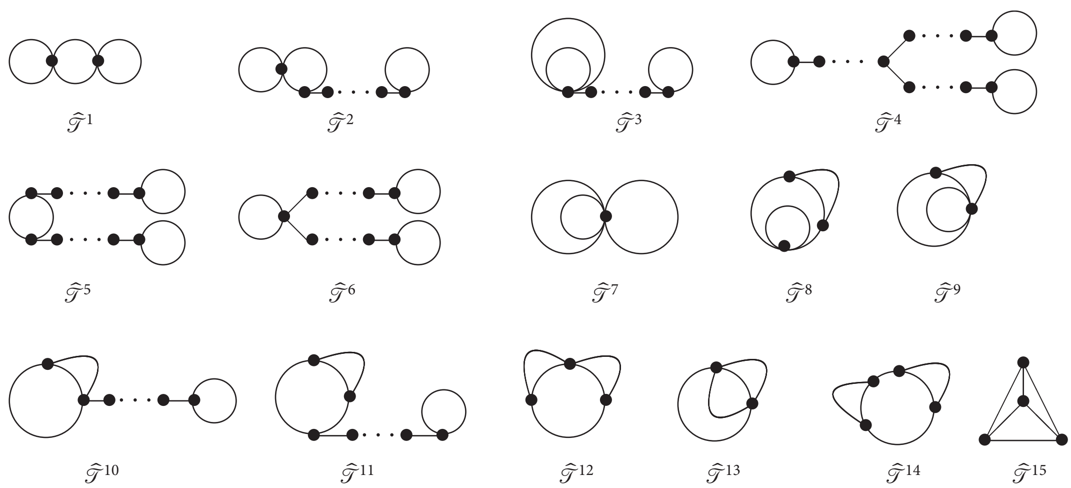

Figure 1: The fifteen types of bases for tricyclic graphs.

physicochemical properties and biological activities of the chemical compounds theoretically.

In this paper, we consider the minimum detour index among all tricyclic graphs.

2. Preliminaries

In this section, we will introduce some useful lemmas and graph transformations.

2.1. Edge-Lifting Transformation [14, 15]. Let G_1 and G_2 be two graphs with $n_1 \geq 2$ and $n_2 \geq 2$ vertices, respectively. If G is the graph obtained from G_1 and G_2 by adding an edge between a vertex u_0 of G_1 and a vertex v_0 of G_2, G' is the graph obtained by identifying u_0 of G_1 to v_0 of G_2 and adding a pendant edge to $u_0 (v_0)$, then G' is called the edge-lifting transformation of G (see Figure 2).

Lemma 1 (see [16]). *Let G be defined as in Figure 2, and G' is obtained from G by the edge-lifting transformation (see Figure 2). Then, $\omega(G) > \omega(G')$.*

Denote $\mathscr{T}_n^{(1)} = \{\mathscr{T}^1, \mathscr{T}^7, \mathscr{T}^8, \mathscr{T}^9, \mathscr{T}^{12}, \mathscr{T}^{13}, \mathscr{T}^{14}, \mathscr{T}^{15}\}$ (see Figure 1).

By Lemma 1, we can verify that if $\mathscr{T} \in \mathscr{T}_n$ attains the minimum detour index of all graphs in $\mathscr{T}_n$, then the following two conditions hold:

(i) The base $\widehat{\mathscr{T}}$ of $\mathscr{T}$ is one of $\widehat{\mathscr{T}}_n^{(1)}$

(ii) The graph $\mathscr{T}$ is obtained from $\widehat{\mathscr{T}}$ by attaching some pendant edges

Remark 1. In order to determine the tricyclic graphs which attain the minimum detour index of all graphs in $\mathscr{T}_n$, we just need to discuss the tricyclic graphs in $\mathscr{T}$, where $\widehat{\mathscr{T}} \in \mathscr{T}_n^{(1)}$.

2.2. Cycle-Edge Transformation. Let $\mathscr{C} \in \mathscr{C}_n^l$ be a cactus as shown in Figure 3, where $C_r = v_1 v_2 \ldots v_r v_1$ is the biggest cycle of $\mathscr{C}$, $r \geq 4$. Denote the vertex set $W_{v_i} = N_{G_i}(v_i) = N_G(v_i) \cap V(G_i)$, $1 \leq i \leq r$. $\mathscr{C}'$ is the graph obtained from $\mathscr{C}$ by deleting the edges $v_2 v_3$ and v_2 to W_{v_2}, meanwhile adding the edges $v_1 v_3$ and v_1 to W_{v_2}.

We say that $\mathscr{C}'$ is obtained from $\mathscr{C}$ by the cycle-edge transformation (see Figure 3).

Lemma 2 (see [16]). *Let $\mathscr{C} \in \mathscr{C}_n^l$ be a cactus as shown in Figure 3 with $r \geq 4$, and $\mathscr{C}'$ be the cycle-edge transformation of $\mathscr{C}$ (see Figure 3). Then, $\omega(\mathscr{C}) > \omega(\mathscr{C}')$.*

2.3. Cycle-Lifting Transformation. Let $\mathscr{C}_1 \in \mathscr{C}_n^l$ be a cactus as shown in Figure 4. Denote $W_{v_i} = N_{G_i}(v_i) = N_G(v_i) \cap V(G_i)$ for $1 \leq i \leq 3$. Let $\mathscr{C}_1'$ be the graph obtained from $\mathscr{C}_1$ by deleting the edges $v_2 v_x$ for $v_x \in W_{v_2}$ and adding the edges $v_1 v_x$ for $v_x \in W_{v_2}$.

We say that $\mathscr{C}_1'$ is the cycle-lifting transformation of $\mathscr{C}_1$ (see Figure 4).

Lemma 3 (see [16]). *Let $\mathscr{C}_1'$ be the cycle-lifting transformation of $\mathscr{C}_1$ (see Figure 4). Then, $\omega(\mathscr{C}_1) > \omega(\mathscr{C}_1')$.*

2.4. Operation I. We define Operation I as follows. Let G and G' be a simple and connected graph as shown in Figure 5. $v_1 v_2 \ldots v_p$ be the path in a cycle. Denote $W_{v_i} = \{w \mid w v_i \in E(G) \text{ and } d(w) = 1, 1 \leq i \leq p, p \geq 3\}$, and G' be the graph obtained from G by deleting the edges $v_2 v_3$, $v_2 w$ for $w \in W_{v_2}$ and adding the edges $v_1 v_3, v_1 w$ for $w \in W_{v_2}$ (see Figure 5).

Lemma 4. *Let G and G' be the graph shown in Figure 5. Then, $\omega(G) > \omega(G')$.*

Proof. Let $V(G) = V(G') = \{v_1, v_2, v_3, \ldots, v_n\}$, and $W_{v_i} = \{w \mid w v_i \in E(G) \text{ and } d(w) = 1, 1 \leq i \leq p\}$. For the vertices $v_i, v_j \in V(G - v_2)$, obviously

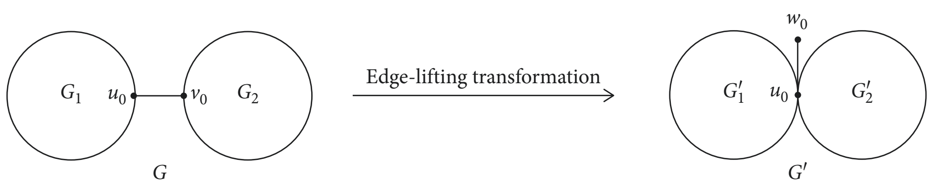

Figure 2: The edge-lifting transformation.

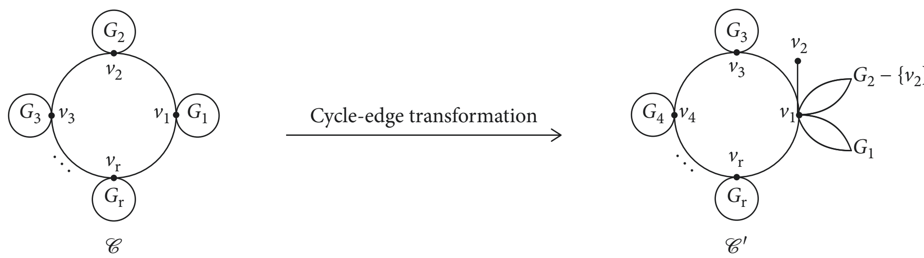

Figure 3: The cycle-edge transformation.

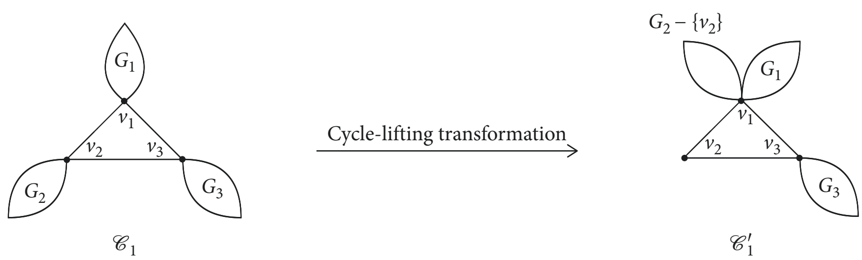

Figure 4: The cycle-lifting transformation.

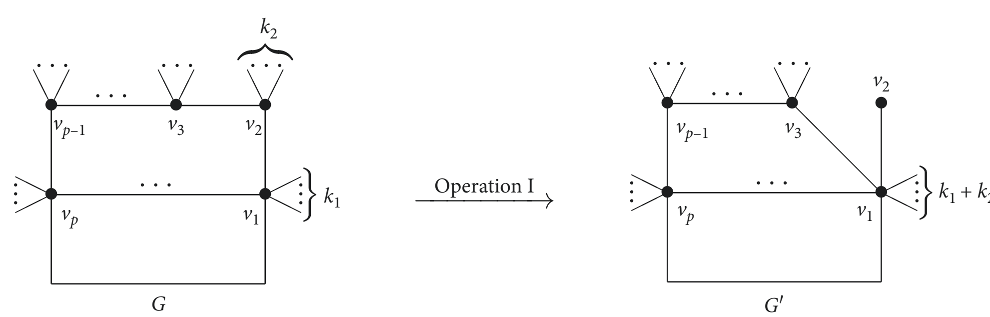

Figure 5: Operation I on graph G.

$$l(v_i, v_j \mid G) \geq l(v_i, v_j \mid G'), \tag{3}$$

$$l(v_1, v_2 \mid G) > l(v_1, v_2 \mid G') = 1. \tag{4}$$

Let P_i be the set of the longest path between v_2 and v_i in G and Q_i be the set of the longest path between v_1 and v_i in G, where $3 \leq i \leq n$.

Case 1. $v_1v_2 \in E(P_i)$ and $v_2v_3 \in E(P_i)$, where $3 \leq i \leq n$.

Obviously, for $3 \leq i \leq n$, $l(v_2, v_i \mid G) = l(v_2, v_i \mid G') - 1$. On the other hand, if $v_1v_2 \in E(P_i)$ and $v_2v_3 \in E(P_i)$, then $v_1v_2, v_2v_3 \in \mathscr{L}_i$, where $\mathscr{L}_i$ be the any one longest path between v_1 and v_i in G. Therefore, $l(v_1, v_i \mid G) = l(v_1, v_i \mid G') + 1$, and

$$\begin{aligned} & l(v_2, v_i \mid G) + l(v_1, v_i \mid G) \\ & \quad = l(v_2, v_i \mid G') + l(v_1, v_i \mid G'), \quad 3 \leq i \leq n. \end{aligned} \tag{5}$$

Case 2. $v_1v_2 \notin E(P_i)$ and $v_2v_3 \in E(P_i)$.

Obviously, for $3 \leq i \leq n$, we have

$$\begin{aligned} l(v_2, v_i \mid G) &= l(v_3, v_i \mid G) + 1 \\ &> l(v_1, v_i \mid G) + 1 \\ &\geq l(v_1, v_i \mid G') + 1 \\ &= l(v_2, v_i \mid G'). \end{aligned} \tag{6}$$

Case 3. $v_1v_2 \in E(P_i)$ and $v_2v_3 \notin E(P_i)$.

Obviously, for $3 \leq i \leq n$, we have

$$l(v_2, v_i \mid G) = l(v_2, v_i \mid G'). \tag{7}$$

Case 4. $v_1v_2 \notin E(P_i)$ and $v_2v_3 \notin E(P_i)$.

Obviously, $v_i \in W_{v_2} \subset V(G)$, and

$$l(v_2, v_i \mid G) = l(v_1, v_i \mid G') = 1, \quad (8)$$

$$l(v_1, v_i \mid G) > l(v_2, v_i \mid G') = 2. \quad (9)$$

By (5)–(9), we have

$$\begin{aligned} &l(v_2, v_i \mid G) + l(v_1, v_i \mid G) \\ &\geq l(v_2, v_i \mid G') + l(v_1, v_i \mid G'), \quad 3 \leq i \leq n. \end{aligned} \quad (10)$$

By (3), (4), and (10), we have $\omega(G) > \omega(G')$. □

2.5. Operation II. We define Operation II as follows. Let G and G' be a simple and connected graph as shown in Figure 6. Denote $v_1v_2v_3v_1$ be a cycle with length 3, $W_{v_i} = \{w \mid wv_i \in E(G) \text{ and } d(w) = 1, i = 1, 2\}$, and G' be the graph obtained from G by deleting the edges v_2w for $w \in W_{v_2}$ and adding the edges v_1w for $w \in W_{v_2}$ (see Figure 6).

Lemma 5. *Let G and G' be the graph shown in Figure 6. Then, $\omega(G) > \omega(G')$, and the equality holds if and only if $G \cong G'$.*

Proof. Let $V(G) = V(G') = \{v_1, v_2, v_3, \ldots, v_n\}$. For the vertices $v_i, v_j \in V(G) - W_{v_2}$, $v_x, v_y \in W_{v_2}$, we have

$$l(v_i, v_j \mid G) = l(v_i, v_j \mid G'), \quad (11)$$

$$l(v_x, v_y \mid G) = l(v_x, v_y \mid G') = 2. \quad (12)$$

For the vertices $v_i \in V(G) - W_{v_2} - \{v_1, v_2\}$, $w \in W_{v_2}$, we have

$$\begin{aligned} &l(w, v_i \mid G) \\ &= \max\{3 + l(v_1, v_i \mid G), 3 + l(v_3, v_i \mid G)\} \\ &\geq \max\{1 + l(v_1, v_i \mid G), 3 + l(v_3, v_i \mid G)\} \\ &= \max\{1 + l(v_1, v_i \mid G'), 3 + l(v_3, v_i \mid G')\} \\ &= l(w, v_i \mid G'), \end{aligned} \quad (13)$$

especially, if $G \ncong G'$, then

$$l(w, v_3 \mid G) > l(w, v_3 \mid G'), \quad (14)$$

$$\begin{aligned} l(w, v_1 \mid G) &= l(v_1, v_2 \mid G) + 1 \\ &= l(v_1, v_2 \mid G') + 1 \\ &= l(w, v_2 \mid G'), \end{aligned} \quad (15)$$

$$l(w, v_2 \mid G) = l(w, v_1 \mid G') = 1. \quad (16)$$

By (11)–(16), we have $\omega(G) \geq \omega(G')$, and the equality holds if and only if $G \cong G'$. □

Denote $\mathcal{T}_n^{(2)} = \{\mathcal{T}^{16}, \mathcal{T}^{17}, \mathcal{T}^{18}, \mathcal{T}^{19}, \mathcal{T}^{20}, \mathcal{T}^{21}\}$; see Figure 7.

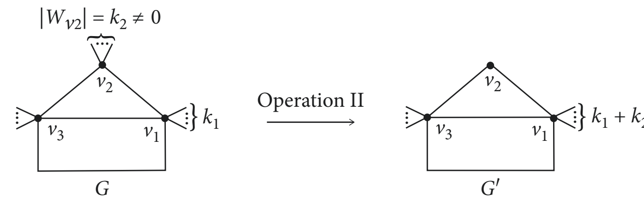

Figure 6: Operation II on graph G.

By Lemma 2–5, we can verify that if $\mathcal{T} \in \mathcal{T}_n$ attains the minimum detour index of all graphs in $\mathcal{T}_n$, then $\mathcal{T} \in \mathcal{T}_n^{(2)}$.

Remark 2. In order to determine the tricyclic graphs which attain the minimum detour index of all graphs in $\mathcal{T}_n$, we just need to discuss the tricyclic graphs in $\mathcal{T}$, where $\widehat{\mathcal{T}} \in \mathcal{T}_n^{(2)} = \{\mathcal{T}^{16}, \mathcal{T}^{17}, \mathcal{T}^{18}, \mathcal{T}^{19}, \mathcal{T}^{20}, \mathcal{T}^{21}\}$; see Figure 7.

2.6. Operation III. We define Operation III as follows. Let $G \in \mathcal{T}^{17} \cup \mathcal{T}^{18} \cup \mathcal{T}^{20} \cup \mathcal{T}^{21}$ as shown in Figure 7. Denote $W_{v_i} = \{w \mid wv_i \in E(G) \text{ and } d(w) = 1\}$ and G' be the graph obtained from G by deleting the edges v_3w for $w \in W_{v_3}$ and adding the edges v_1w for $w \in W_{v_3}$ (see Figures 8–11).

Lemma 6. *Let G_i and G_i' $(1 \leq i \leq 4)$ be the graph in Figures 8–11. Then, $\omega(G) \geq \omega(G')$, and the equality holds if and only if $G \cong G'$.*

Proof. Let $V(G_1) = V(G_1') = \{v_1, v_2, v_3, \ldots, v_n\}$. For the vertices $v_i, v_j \in V(G) - W_{v_3} - \{v_1, v_3\}$; $v_x, v_y \in W_{v_3}$, we have

$$l(v_i, v_j \mid G_1) = l(v_i, v_j \mid G_1'), \quad (17)$$

$$l(v_x, v_y \mid G_1) = l(v_x, v_y \mid G_1') = 2, \quad (18)$$

$$l(v_1, v_i \mid G_1) = l(v_1, v_i \mid G_1'), \quad (19)$$

$$l(v_3, v_x \mid G_1) = l(v_1, v_x \mid G_1'), \quad (20)$$

$$l(v_3, v_i \mid G_1) \geq l(v_1, v_i \mid G_1'), \quad (21)$$

$$\begin{aligned} l(v_x, v_i \mid G_1) &= l(v_3, v_i \mid G_1) + 1 \\ &= l(v_3, v_i \mid G_1') + 1 \\ &\geq l(v_1, v_i \mid G_1') + 1 \\ &= l(v_x, v_i \mid G_1'), \end{aligned} \quad (22)$$

$$l(v_x, v_5 \mid G_1) = 5 > 3 = l(v_x, v_5 \mid G_1'). \quad (23)$$

By (17)–(23), we have $\omega(G_1) > \omega(G_1')$.

Similarly, we have $\omega(G_i) \geq \omega(G_i')$, and the equality holds if and only if $G_i \cong G_i'$ $(i = 2, 3, 4)$. □

2.7. Operation IV. We define Operation IV as follows. Let $G \in \mathcal{T}^{19}$ as shown in Figure 12. Denote $W_{v_i} = \{w \mid wv_i \in E(G) \text{ and } d(w) = 1\}$, and G' be the graph obtained from G

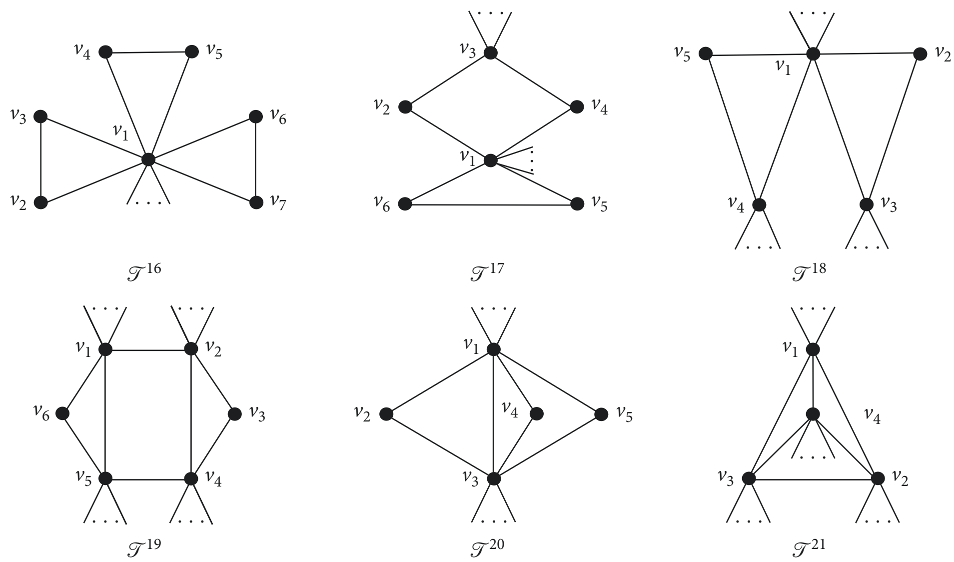

FIGURE 7: Graph $\mathcal{T}_n^{(2)}$.

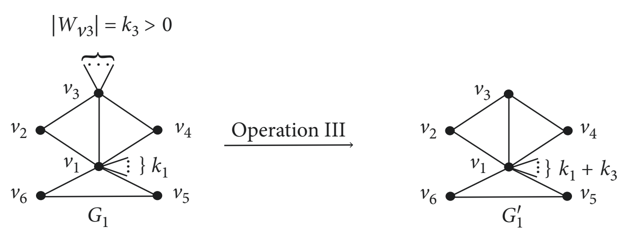

FIGURE 8: Operation III on graph $G_1 \in \mathcal{T}^{17}$.

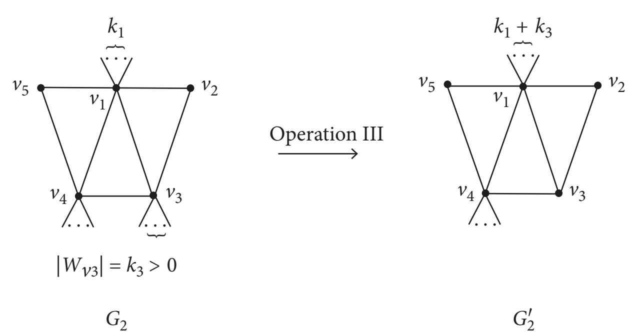

FIGURE 9: Operation III on graph $G_2 \in \mathcal{T}^{18}$.

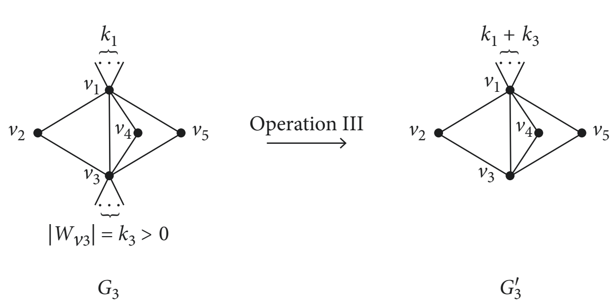

FIGURE 10: Operation III on graph $G_3 \in \mathcal{T}^{20}$.

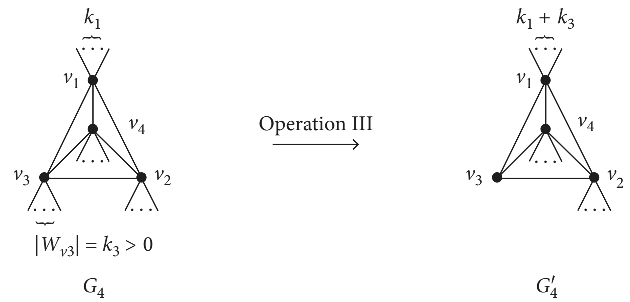

Figure 11: Operation III on graph $G_4 \in \mathcal{T}^{21}$.

by deleting the edges $v_i w$ for $w \in W_{v_i}, i = 2, 4, 5$ and adding the edges $v_1 w$ for $w \in W_{v_i}, i = 2, 4, 5$ (see Figure 12).

Lemma 7. *Let G and G′ be the graph shown in Figure 12. Then, $\omega(G) \geq \omega(G')$ with equality holding if and only if $G \cong G'$.*

Proof. Let $V_1 = \{v_i \mid 1 \leq i \leq 6\}$, $V_2 = V(G) - V_1$, we have

$$\begin{aligned}\omega(G) = &\sum_{v_x, v_y \in V_1} l(v_x, v_y \mid G) \\ &+ \sum_{v_x \in V_1, v_y \in V_2} l(v_x, v_y \mid G) \\ &+ \sum_{v_x, v_y \in V_2} l(v_x, v_y \mid G),\end{aligned} \quad (24)$$

$$\begin{aligned}\omega(G') = &\sum_{v_x, v_y \in V_1} l(v_x, v_y \mid G') \\ &+ \sum_{v_x \in V_1, v_y \in V_2} l(v_x, v_y \mid G') \\ &+ \sum_{v_x, v_y \in V_2} l(v_x, v_y \mid G').\end{aligned} \quad (25)$$

Obviously,

$$\begin{aligned}\sum_{v_x, v_y \in V_1} l(v_x, v_y \mid G) &= \sum_{v_x, v_y \in V_1} l(v_x, v_y \mid G'), \\ \sum_{v_x \in V_1, v_y \in V_2} l(v_x, v_y \mid G) &= + \sum_{v_x \in V_1, v_y \in V_2} l(v_x, v_y \mid G'),\end{aligned} \quad (26)$$

$$\begin{aligned}&l(v_x, v_y \mid G) = l(v_x, v_y \mid G') = 2, \quad v_x, v_y \in W_{v_i}, \\ &l(v_x, v_y \mid G) > 2 = l(v_x, v_y \mid G'), \\ &\qquad v_x \in W_{v_i},\ v_y \in W_{v_j},\ i \neq j.\end{aligned} \quad (27)$$

Therefore,

$$\begin{aligned}&\omega(G) - \omega(G') \\ &\quad = \sum_{v_x, v_y \in V_2} l(v_x, v_y \mid G) - \sum_{v_x, v_y \in V_2} l(v_x, v_y \mid G') \\ &\quad \geq 0,\end{aligned} \quad (28)$$

and the equality holds if and only if $G \cong G'$. □

Denote $\mathcal{T}_n^{(3)} = \{\mathcal{T}^{16} \cup \mathcal{T}^{22} \cup \mathcal{T}^{23} \cup \mathcal{T}^{24} \cup \mathcal{T}^{25} \cup \mathcal{T}^{26}\}$ (see Figure 13).

By Lemma 6-7, we can verify that if $\mathcal{T} \in \mathcal{T}_n$ attains the minimum detour index of all graphs in $\mathcal{T}_n$, then $\widehat{\mathcal{T}} \in \mathcal{T}_n^{(3)}$.

Remark 3. In order to determine the tricyclic graphs which attain the minimum detour index of all graphs in $\mathcal{T}_n$, we just need to discuss the tricyclic graphs in $\mathcal{T}$, where $\widehat{\mathcal{T}} \in \mathcal{T}_n^{(3)} = \{\mathcal{T}^{16}, \mathcal{T}^{22}, \mathcal{T}^{23}, \mathcal{T}^{24}, \mathcal{T}^{25}, \mathcal{T}^{26}\}$ (see Figure 13).

3. Results and Discussion

From the discussions of Section 2, we can verify that if $\mathcal{T} \in \mathcal{T}_n$ attains the minimum detour index of all graphs in $\mathcal{T}_n$, then $\omega(\mathcal{T}) = \min\{\omega(G)\}$, where $\widehat{G} \in \mathcal{T}_n^{(3)} = \{\mathcal{T}^{16}, \mathcal{T}^{22}, \mathcal{T}^{23}, \mathcal{T}^{24}, \mathcal{T}^{25}, \mathcal{T}^{26}\}$.

Theorem 1. *Let $\mathcal{T}_n^{(3)}$ be defined as in Figure 13.*

(1) *When $n = 4$ or $n \geq 8$, $\mathcal{T}^{26}$ is the unique graph which attains the minimum detour index of all graphs in $\mathcal{T}_n$ and $\omega(\mathcal{T}^{26}) = n^2 + 4n - 14$.*

(2) *When $n = 5$ or $n = 6$, $\mathcal{T}^{25}$ is the unique graph which attains the minimum detour index of all graphs in $\mathcal{T}_n$ and $\omega(\mathcal{T}^{25}) = n^2 + 5n - 21$.*

(3) *When $n = 7$, $\mathcal{T}^{25}$ and $\mathcal{T}^{26}$ are the graphs which attain the minimum detour index of all graphs in $\mathcal{T}_n$ and $\omega(\mathcal{T}^{25}) = \omega(\mathcal{T}^{26}) = 63$.*

Proof. It can be checked directly that

$$\begin{aligned}&L(v_1 \mid \mathcal{T}^{16}) = n + 5; \\ &L(v_i \mid \mathcal{T}^{16}) = 3n - 1, \text{ where } 2 \leq i \leq 7; \\ &L(w \mid \mathcal{T}^{16}) = 2n + 3, \text{ where } w \in W_{v_1}.\end{aligned} \quad (29)$$

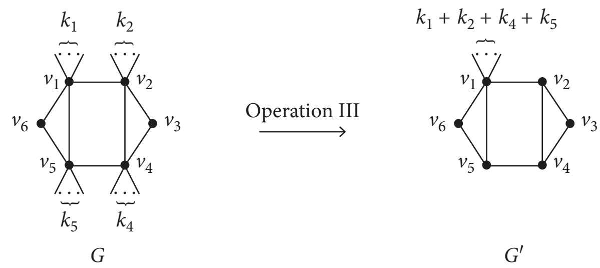

Figure 12: Operation IV on graph $G \in \mathcal{T}^{19}$.

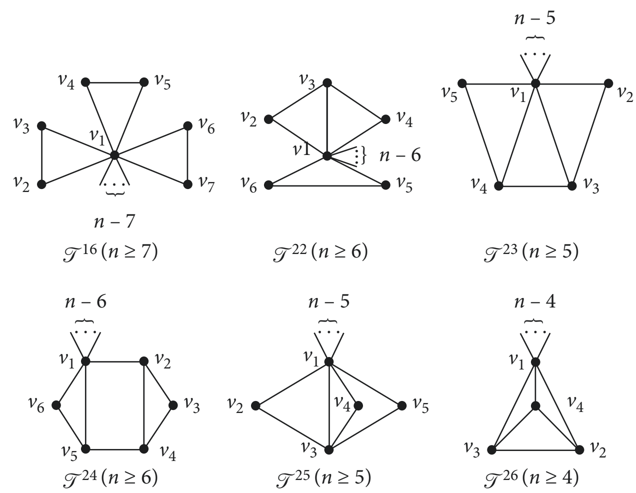

Figure 13: Graph $\mathcal{T}_n^{(3)}$.

Therefore,

$$\begin{aligned}\omega\left(\mathcal{T}^{16}\right) &= \frac{1}{2} \sum_{u \in V\left(\mathcal{T}^{16}\right)} L\left(u \mid \mathcal{T}^{16}\right) \\ &= \frac{1}{2}\left[(n+5) + 6(3n-1) + (2n+3)(n-7)\right] \\ &= n^2 + 4n - 11, \quad n \geq 7.\end{aligned} \tag{30}$$

Similarly, we have

$$\begin{aligned}\omega\left(\mathcal{T}^{22}\right) &= n^2 + 5n - 15 \\ &= n^2 + 4n + (n-15), \quad n \geq 6, \\ \omega\left(\mathcal{T}^{23}\right) &= n^2 + 8n - 27 \\ &= n^2 + 4n + (4n-27), \quad n \geq 5, \\ \omega\left(\mathcal{T}^{24}\right) &= n^2 + 15n - 57 \\ &= n^2 + 4n + (11n-57), \quad n \geq 6, \\ \omega\left(\mathcal{T}^{25}\right) &= n^2 + 5n - 21 \\ &= n^2 + 4n + (n-21), \quad n \geq 5, \\ \omega\left(\mathcal{T}^{26}\right) &= n^2 + 4n - 14, \quad n \geq 4.\end{aligned} \tag{31}$$

(1) When $n = 4$ or $n \geq 8$, obviously, $\mathcal{T}^{26}$ is the unique graph which attains the minimum detour index of all graphs in $\mathcal{T}_n$ and $\omega(\mathcal{T}^{26}) = n^2 + 4n - 14$.

(2) When $n = 5$ or $n = 6$, obviously, $\mathcal{T}^{25}$ is the unique graph which attains the minimum detour index of all graphs in $\mathcal{T}_n$ and $\omega(\mathcal{T}^{25}) = n^2 + 5n - 21$.

(3) When $n = 7$, obviously, $\mathcal{T}^{25}$ and $\mathcal{T}^{26}$ are the graphs which attain the minimum detour index of all graphs in $\mathcal{T}_n$ and $\omega(\mathcal{T}^{25}) = \omega(\mathcal{T}^{26}) = 63$. □

4. Conclusions

Mathematical chemistry is an area of research in chemistry in which mathematical tools are used to solve problems of chemistry. Chemical graph theory is an important area of research in mathematical chemistry which deals with topology of molecular structures such as the mathematical study of isomerism and the development of topological descriptors or indices. In this paper, we first introduce some useful graph transformations, and then we determine the minimum detour index of all tricyclic graphs. In addition, all the corresponding extremal graphs are characterized.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare no conflicts of interest regarding the content and implications of this manuscript.

Acknowledgments

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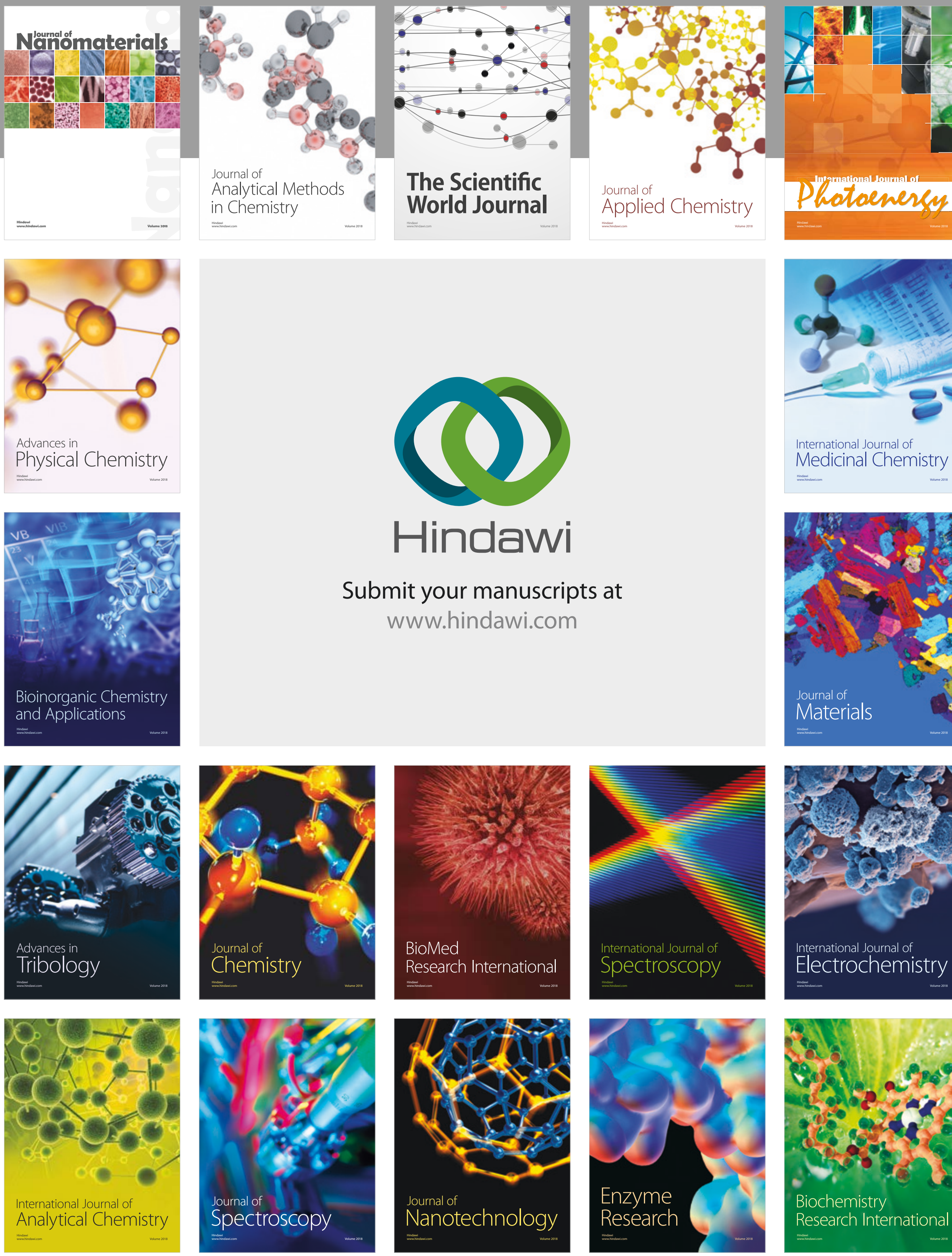
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