MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **60** (2008) 585-600

ISSN 0340 - 6253

Bicyclic Graphs with Minimum General Randić Index

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(Received March 4, 2008)

Abstract

The general Randić index $R_\alpha(G)$ of a graph G is defined as the sum of the weights $(d(u)d(v))^\alpha$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G. In this paper, we consider bicyclic graphs with n vertices and give the structure of graphs with minimum general Randić index for $\alpha \le -2$.

1 Introduction

In 1975, M. Randić proposed a pair of chemical indices $R(G)$ and $R_{-1}(G)$ for a (chemical) graph G, i.e.,

$$R(G) = \sum_{uv\in E(G)} (d(u)d(v))^{-1/2}, \quad R_{-1}(G) = \sum_{uv\in E(G)} (d(u)d(v))^{-1},$$

where $d(u)$ denotes the degree of a vertex u in G. Randić himself demonstrated that his index was well correlated with a variety of physico-chemical properties of alkanes, such as boiling point, enthalpy of formation, parameters in the Antoine equation (for vapor pressure), surface area, and solubility in water. Eventually, this structure-descriptor becomes one of the most popular topological indices, and scores of its chemical and pharmacological applications have been reported. Like other successful chemical indices, these two indices have received considerable attention from both chemists and mathematicians. For a comprehensive survey of its mathematical properties see the recent book of Li and Gutman on Mathematical Aspects of Randić-Type Molecular Structure Descriptors [8].

In 1998 Bollobás and Erdös [1] generalized this index by replacing $-\frac{1}{2}$ by any real number α, which is called the general Randić index. Hu, Li and Yuan [6, 7] characterized the trees with extremal general Randić index. And there are also many results on the unicyclic graphs. For $n \geq 3$, let S_n^+ denote the unicyclic graph obtained from the star S_n on n vertices by joining its two vertices of degree one. For $\alpha = -\frac{1}{2}$, Gao and Lu [5] showed that for a unicyclic graph G, $R_{-\frac{1}{2}}(G) \geq (n-3)(n-1)^{-\frac{1}{2}} + 2(2n-2)^{-\frac{1}{2}} + \frac{1}{2}$, and the equality holds if and only if $G \cong S_n^+$. For general α, Wu and Zhang [12], Li, Wang and Zhang [10] gave the structure description of the unicyclic graphs with the minimum general Randić index. Li, Shi and Xu [9] investigated the unicyclic graphs with maximum general Randić index for $\alpha > 0$. Caporossi *et al.* [4] characterized the bicyclic graphs with maximum Randić index. Liu and Huang [11] investigated the bicyclic graphs with the minimum value for $\alpha > 0$. In this paper, we focus on investigating the bicyclic graphs with minimum general Randić index.

For convenience, we need some additional notations and terminologies. A vertex of degree 1 in a graph is called a *leaf vertex* (or simply, a *leaf*). The class $\mathcal{G}$ of graphs is defined as follows: a bicyclic graph G belongs to $\mathcal{G}$, if and only if, G has three cycles whose induced subgraph is $K_4 \backslash e$ (is also called *kite*), and the vertices not on the cycle are leaves. The class $\mathcal{H}$ of graphs is defined as follows: a bicyclic graph H belongs to

$\mathcal{H}$, if and only if, H has three cycles whose induced subgraph is obtained from $K_4\backslash e$ by subdividing an edge whose two end vertices are degree 3, and the vertices not on the cycle are leaves. The class $\mathcal{K}$ of graphs is defined as follows: a bicyclic graph K belongs to $\mathcal{K}$, if and only if, K has two triangles with a common vertex, and the vertices not on the cycle are leaves. The class $\mathcal{K}'$ ($\mathcal{K}''$) of graphs is defined as follows: a bicyclic graph K' (K'') belongs to $\mathcal{K}'$ ($\mathcal{K}''$), if and only if, K' (K'') has two triangles which are connected by one path P_1 (P_2), and the vertices not on the cycle are leaves. We give an example for each class of graphs in Figure 1.1. Undefined notations and terminologies can be found in [2].

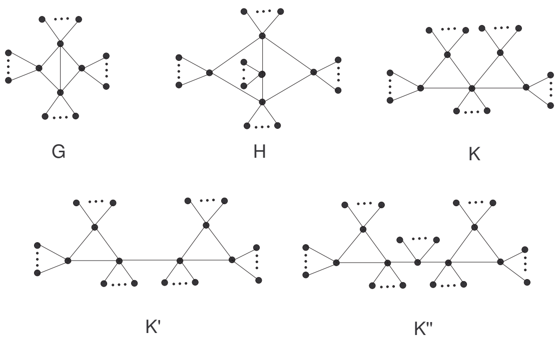

Figure 1.1

2 Some Lemmas

Since the problem is trivial if the graphs under consideration have fewer than 8 vertices, we only consider bicyclic graphs with at least 8 vertices in the following.

If G is a bicyclic graph with three cycles, denote u and v the only two common vertices of the three cycles. Denote $P_{uv}^{(1)}$, $P_{uv}^{(2)}$ and $P_{uv}^{(3)}$ the three paths connected u and v on the cycles. If G is a bicyclic graph with two cycles, there must be a path connecting the two cycles. Denote u and v the two common vertices of the path and two cycles, respectively, and C_u (C_v) the cycle which contains the vertex u (v).

Lemma 2.1 *(Theorem 3.1 of [12]) Suppose the star S_n, $n \geq 2$, is disjoint from a graph G and v is its center. For a vertex $u \in V(G)$, let $G_1 = G \cup S_n + uv$, and G_2 be the graph obtained from G by attaching a star S_{n+1} to the vertex u with u as its center, as shown in Figure 2.1. If u is not an isolated vertex, then $R_\alpha(G_1) > R_\alpha(G_2)$ for $\alpha < 0$.* ∎

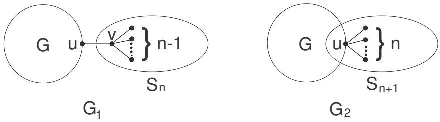

Figure 2.1

Lemma 2.2 *(i) If $ax \geq 2$, then for $\alpha < 0$, the function*

$$g(x,a) = x(x+3)^\alpha + (x+3)^\alpha(a+2)^\alpha + a(a+2)^\alpha - (x+a+1)(x+a+4)^\alpha > 0.$$

(ii) If $xy \geq 4$, then for $\alpha < 0$, the function

$$f(x,y) = x(x+3)^\alpha + y(y+3)^\alpha + (x+3)^\alpha(y+3)^\alpha - (x+y+1)(x+y+5)^\alpha > 0.$$

(iii) If $x \geq 0$ and $a \geq 1$, then for $\alpha < 0$, the function

$$h(x,a) = x(x+3)^\alpha + a(a+2)^\alpha + (2x+6)^\alpha + (2a+4)^\alpha - (x+a+2)(x+a+5)^\alpha > 0.$$

Proof. (i) Since $ax \geq 2$ and $\alpha < 0$, we have

$$\begin{aligned} g(x,a) &= x(x+3)^\alpha + (x+3)^\alpha(a+2)^\alpha + a(a+2)^\alpha - (x+a+1)(x+a+4)^\alpha \\ &= x\left[(x+3)^\alpha - (x+a+4)^\alpha\right] + a\left[(a+2)^\alpha - (x+a+4)^\alpha\right] \\ &\quad + \left[(ax+2x+3a+6)^a - (x+a+4)^a\right] \\ &= -\alpha\left[\xi_1^{\alpha-1}x(a+1) + \xi_2^{\alpha-1}a(x+2) - \xi_3^{\alpha-1}(ax+x+2a+2)\right] \\ &> -\alpha\xi_3^{\alpha-1}(ax-2) \geq 0, \end{aligned}$$

where $\xi_1 \in (x+3, x+a+4)$, $\xi_2 \in (a+2, x+a+4)$, $\xi_3 \in (x+a+4, ax+2x+3a+6)$ and $\xi_1, \xi_2 < \xi_3$.

(ii) Similar to the proof of (i).

(iii) We have $h(x,a) = x[(x+3)^\alpha - (x+a+5)^\alpha] + a[(a+2)^\alpha - (x+a+5)^\alpha] + [(2x+6)^\alpha - (x+a+5)^\alpha] + [(2a+4)^\alpha - (x+a+5)^\alpha]$.

If $x \geq a-1$, then $2x+6 \geq x+a+5$, $2a+4 \leq x+a+5$. So

$$\begin{aligned} h(x,a) &\geq x[(x+3)^\alpha - (x+a+5)^\alpha] + a[(a+2)^\alpha - (x+a+5)^\alpha] \\ &\quad +[(2x+6)^\alpha - (x+a+5)^\alpha] \\ &= -\alpha[\xi_1^{\alpha-1}x(a+2) + \xi_2^{\alpha-1}a(x+3) - \xi_3^{\alpha-1}(x-a+1)] \\ &> -\alpha\xi_3^{\alpha-1}[x(a+2) + a(x+3) - x + a - 1] > 0, \end{aligned}$$

where $\xi_1 \in (x+3, x+a+5)$, $\xi_2 \in (a+2, x+a+5)$, $\xi_3 \in (x+a+5, 2x+6)$ and $\xi_1, \xi_2 < \xi_3$. If $x < a-1$, then $2x+6 < x+a+5$, $2a+4 > x+a+5$. We have

$$\begin{aligned} h(x,a) &> x[(x+3)^\alpha - (x+a+5)^\alpha] + a[(a+2)^\alpha - (x+a+5)^\alpha] \\ &\quad +[(2a+4)^\alpha - (x+a+5)^\alpha] \\ &= -\alpha[\xi_1^{\alpha-1}x(a+2) + \xi_2^{\alpha-1}a(x+3) - \xi_3^{\alpha-1}(a-x-1)] \\ &> -\alpha\xi_3^{\alpha-1}[x(a+2) + a(x+3) - a + x + 1] > 0, \end{aligned}$$

where $\xi_1 \in (x+3, x+a+5)$, $\xi_2 \in (a+2, x+a+5)$, $\xi_3 \in (x+a+5, 2a+4)$ and $\xi_1, \xi_2 < \xi_3$. ∎

Lemma 2.3 *For $\alpha \leq -2$,*

(i) $(x+2^\alpha)(x+3)^\alpha - (x+1)(x+4)^\alpha > 0$ for $x \geq 3$;

(ii) $(x+2\cdot 3^\alpha)(x+2)^\alpha - (x+1+3^\alpha)(x+4)^\alpha > 0$ for $x \geq 1$;

(iii) $(x+3^\alpha)(x+3)^\alpha - (x+1)(x+5)^\alpha > 0$ for $x \geq 1$;

(iv)$(x+3^\alpha)(x+2)^\alpha - (x+1+3^\alpha)(x+3)^\alpha > 0$ for $x \geq 2$.

Proof. (1).We have $(\frac{x+3}{x+4})^\alpha > (\frac{x+3}{x+4})^{-2} > \frac{x+1}{x}$, since $x(x+4)^2 - (x+1)(x+3)^2 = x^2 + x - 9 > 0$ for $x \geq 3$. That implies $(x+2^\alpha)(x+3)^\alpha - (x+1)(x+4)^\alpha > x(x+3)^\alpha - (x+1)(x+4)^\alpha > 0$.

(ii), (iii), (iv) can be proved similarly to the proof of (i). ∎

3 The main results for $\alpha \leq -2$

From Lemma 2.1, we have the following result:

Lemma 3.1 *For $\alpha < 0$, assume G is the minimum bicyclic graph with order n. If T is a tree attached to a vertex w, which is in some cycle of G, then T must be a star with w as its center.* ∎

Lemma 3.2 *Let G be a bicyclic graph with order n. If G has three cycles and $G \notin \mathcal{G}\bigcup\mathcal{H}$, then there exists a graph $G' \in \mathcal{G}\bigcup\mathcal{H}$ with the same order of G, satisfying that $R_\alpha(G) \geq R_\alpha(G')$ for $\alpha < 0$.*

Proof. Let G be a bicyclic graph with order n, having three cycles, but $G \notin \mathcal{G}\bigcup\mathcal{H}$. In the following, we will find a graph $G' \in \mathcal{G}\bigcup\mathcal{H}$ with the same order of G satisfying $R_\alpha(G) > R_\alpha(G')$. By Lemma 3.1, we only consider the following three cases.

Case 1. In path $P_{uv}^{(i)}$ (for some $i \in \{1,2,3\}$), there are two vertices w_1 and w_2 ($w_1, w_2 \notin \{u,v\}$), such that S_{a+1}, S_{b+1} ($a, b \geq 1$) are the two stars attached to w_1, w_2, respectively.

Without loss of generality, suppose the degrees of all vertices in the path $P_{w_1w_2}$ are two (if there exists such vertex) in G and $|E(P_{w_1w_2})| = c$. Now transform G into a new bicyclic graph G' as follows: contracting the path $P_{w_1w_2}$ into one vertex $w_1(w_2)$, and attaching a star $S_{a+b+c+1}$ to it (see Figure 3.1). Similarly to the proof of Lemma 3.5 of [12], we can prove $R_\alpha(G) > R_\alpha(G')$ for $\alpha < 0$.

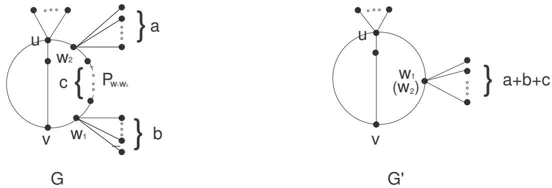

Figure 3.1

Case 2. In path $P_{uv}^{(i)}$ (for some $i \in \{1, 2, 3\}$, without loss of generality, assume $i = 3$), there is only one vertex $w \notin \{u, v\}$, such that S_{a+1} $(a \geq 1)$ is a star attached to w.

Suppose $|E(P_{uv}^{(i)})| \geq 3$ and $|P_{wv}| \geq |P_{uw}| = c$. Let u_1, u_2, u_3 be the only three neighbors of u on cycles and $d(u_i) = y_i \geq 2$. Let $d(u) = x + 3$. Now transform G into a new bicyclic graph G' as follows: contracting the path P_{uw} into one vertex $u(w)$, and attaching a star S_{x+a+c} to it (see Figure 3.2).

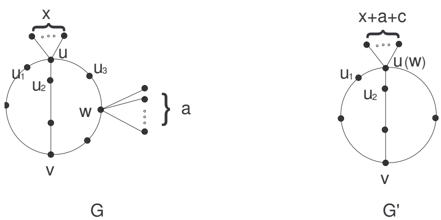

Figure 3.2

If $c = 1$, that is $uw \in E(G)$, then

$$\begin{aligned} & R_\alpha(G) - R_\alpha(G') \\ = \; & x(x+3)^\alpha + (x+3)^\alpha(a+2)^\alpha + a(a+2)^\alpha + (y_1^\alpha + y_2^\alpha)(x+3)^\alpha + 2^\alpha(a+2)^\alpha \\ & -[(x+a+1)(x+a+4)^\alpha + (y_1^\alpha + y_2^\alpha)(x+a+4)^\alpha + 2^\alpha(x+a+4)^\alpha]. \end{aligned}$$

If $ax \geq 2$, by Lemma 2.2 (i), we have $R_\alpha(G) - R_\alpha(G') > g(x,a) > 0$.
If $a = x = 1$, we have

$$\begin{aligned} R_\alpha(G) - R_\alpha(G') &> 4^\alpha + 12^\alpha + 3^\alpha - 3 \cdot 6^\alpha \\ &= (3^\alpha - 6^\alpha) + (4^\alpha - 6^\alpha) - (6^\alpha - 12^\alpha) \\ &= (3^\alpha - 6^\alpha)(1 - 2^\alpha) + (4^\alpha - 6^\alpha) > 0. \end{aligned}$$

If $x = 0$ and $a \geq 2$, we have

$$\begin{aligned} & R_\alpha(G) - R_\alpha(G') \\ > \; & 3^\alpha(a+2)^\alpha + a(a+2)^\alpha + 2^\alpha(a+2)^\alpha - (a+1)(a+4)^\alpha - 2^\alpha(a+4)^\alpha \\ = \; & a[(a+2)^\alpha - (a+4)^\alpha] + [(2a+4)^a - (a+4)^a] + [(3a+6)^a - (2a+8)^a] \\ = \; & -\alpha[2a\xi_1^{\alpha-1} - a\xi_2^{\alpha-1} - (a-2)\xi_3^{\alpha-1}] > -\alpha\xi_2^{\alpha-1}[2a - a - (a-2)] > 0, \end{aligned}$$

where $\xi_1 \in (a+2, a+4)$, $\xi_2 \in (a+4, 2a+4)$, $\xi_3 \in (2a+8, 3a+6)$ and $\xi_1 < \xi_2 < \xi_3$.
If $x = 0$ and $a = 1$, we have $R_\alpha(G) - R_\alpha(G') > 9^\alpha + 3^\alpha + 6^\alpha - 2 \cdot 5^\alpha - 10^\alpha > 0$.

If $c \geq 2$, then by Lemma 2.2 (iii), we have

$$\begin{aligned} & R_\alpha(G) - R_\alpha(G') \\ = \; & x(x+3)^\alpha + 2^\alpha(x+3)^\alpha + a(a+2)^\alpha + 2 \cdot (2a+4)^\alpha + (c-2)4^\alpha \\ & +(y_1^\alpha + y_2^\alpha)(x+3)^\alpha - (x+a+c)(x+a+c+3)^\alpha - (y_1^\alpha + y_2^\alpha)(x+a+c+3)^\alpha \\ & -2^\alpha(x+a+c+3)^\alpha \\ > \; & x(x+3)^\alpha + a(a+2)^\alpha + (2x+6)^\alpha + (2a+4)^\alpha + (c-2)4^\alpha \\ & -(x+a+c)(x+a+c+3)^\alpha \\ > \; & x(x+3)^\alpha + a(a+2)^\alpha + (2x+6)^\alpha + (2a+4)^\alpha - (x+a+2)(x+a+5)^\alpha \\ = \; & h(x,a) > 0. \end{aligned}$$

Case 3. In path $P_{uv}^{(i)}$ (for some $i \in \{1,2,3\}$, without loss of generality, suppose $i = 3$), each vertex except u and v has degree two.

Let u_1, u_2, u_3 be the only three neighbors of u on cycles and $d(u_i) = y_i \geq 2$. Let $d(u) = x + 3$. Now transform G into a new bicyclic graph G' as follows: contracting the path uu_3 into one vertex $u(u_3)$, and attaching a star S_{x+1} to it.

We have

$$\begin{aligned} R_\alpha(G) - R_\alpha(G') &= x(x+3)^\alpha + (y_1^\alpha + y_2^\alpha + 2^\alpha)(x+3)^\alpha + 4^\alpha \\ &\quad -[(x+1)(x+4)^\alpha + (y_1^\alpha + y_2^\alpha + 2^\alpha)(x+4)^\alpha] \\ &= x[(x+3)^\alpha - (x+4)^\alpha] + [4^\alpha - (x+4)^\alpha] > 0. \end{aligned}$$

Thus, we complete the proof. ∎

By the same method, we have

Lemma 3.3 *Let G be a bicyclic graph with order n. If G has two cycles and $G \notin \mathcal{K} \bigcup \mathcal{K}' \bigcup \mathcal{K}''$, then there exists a graph $G' \in \mathcal{K} \bigcup \mathcal{K}' \bigcup \mathcal{K}''$ with the same order of G, satisfying that $R_\alpha(G) > R_\alpha(G')$ for $\alpha < 0$.* ∎

Lemma 3.4 *If $G \in \mathcal{H}$ is a bicyclic graph with order n, then there exists a graph $G' \in \mathcal{G}$ with the same order of G, satisfying that $R_\alpha(G) \geq R_\alpha(G')$ for $\alpha \leq -2$.*

Proof. Let $G \in \mathcal{H}$ be a bicyclic graph with order n. Set $d(v) = x + 3$ and $d(u) = y + 3$. Without loss of generality, we suppose $y \geq x \geq 0$. Let u_1, u_2 and u_3 be the only three neighbors of u on cycles with degree $a + 2$, $b + 2$ and $c + 2$, respectively (see Figure 3.3).

Case 1. $y \geq 1$

Now transform G into a new bicyclic graph G' as follows: contracting edge uu_3 into one vertex $u(u_3)$, and attaching a star S_{y+c+1} to it (see Figure 3.3). We have

$$\begin{aligned} & R_\alpha(G) - R_\alpha(G') \\ = \; & c(c+2)^\alpha + y(y+3)^\alpha + (c+2)^\alpha(x+3)^\alpha + [(a+2)^\alpha + (b+2)^\alpha + (c+2)^\alpha](y+3)^\alpha \\ & -(y+c+1)(y+c+4)^\alpha - [(x+3)^\alpha + (a+2)^\alpha + (b+2)^\alpha](y+c+4)^\alpha. \qquad (3.1) \end{aligned}$$

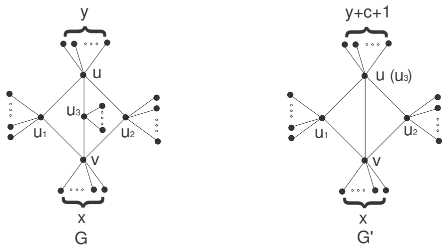

Figure 3.3

Subcase 1.1. $cy \geq 2$

Since $cy \geq 2$, by Lemma 2.2 (i), $R_\alpha(G) - R_\alpha(G') \geq g(y, c) > 0$.

Subcase 1.2. $c = y = 1$

By (3.1), we have

$$\begin{aligned} R_\alpha(G) - R_\alpha(G') &> 4^\alpha + 3^\alpha + 12^\alpha + 3^\alpha(x+3)^\alpha + [(a+2)^\alpha + (b+2)^\alpha]4^\alpha \\ &\quad -3 \cdot 6^\alpha - [(x+3)^\alpha + (a+2)^\alpha + (b+2)^\alpha]6^\alpha \\ &> 4^\alpha + 3^\alpha + 12^\alpha - 3 \cdot 6^\alpha > 0 \end{aligned}$$

Subcase 1.3. $c = 0$, $y \geq 1$

We only consider the case of $a = b = c = 0$. Since otherwise, if $a \neq 0$, we can construct G' by contracting the edge uu_1 and do as above. Then by (3.1), we have

$$\begin{aligned} & R_\alpha(G) - R_\alpha(G') \\ = \;& y(y+3)^\alpha + 2^\alpha(x+3)^\alpha + 3 \cdot 2^\alpha(y+3)^\alpha - (y+1)(y+4)^\alpha \\ & -2 \cdot 2^\alpha(y+4)^\alpha - (y+4)^\alpha(x+3)^\alpha \\ > \;& [y(y+3)^\alpha + 2^\alpha(y+3)^\alpha - (y+1)(y+4)^\alpha] + [2^\alpha - (y+4)^\alpha](x+3)^\alpha \\ > \;& (y+2^\alpha)(y+3)^\alpha - (y+1)(y+4)^\alpha. \end{aligned}$$

By Lemma 2.3 (i), we have $R_\alpha(G) - R_\alpha(G') > 0$ for $y \geq 3$. For $y = 1, 2$, we can verify $R_\alpha(G) - R_\alpha(G') > 0$ by simple calculation.

Case 2. $y = 0$

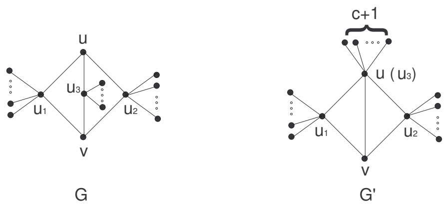

Figure 3.4

Since $y \geq x \geq 0$, $x = 0$. By our assumption, the order of G is at least 8, then one of a, b and c is not zero. Without loss of generality, assume $c \geq 1$. Now transform G into a new bicyclic graph G' as follows: contracting edge uu_3 into one vertex $u(u_3)$, and attaching a star S_{c+1} to it (see Figure 3.4). Then, by Lemma 2.3 (ii), we have

$$\begin{aligned} & R_\alpha(G) - R_\alpha(G') \\ = \;& c(c+2)^\alpha + 2 \cdot 3^\alpha (c+2)^\alpha + [(a+2)^\alpha + (b+2)^\alpha] \cdot 3^\alpha \\ & -(c+1)(c+4)^\alpha - [3^\alpha + (a+2)^\alpha + (b+2)^\alpha](c+4)^\alpha \\ > \;& (c + 2 \cdot 3^\alpha)(c+2)^\alpha - (c+1+3^\alpha)(c+4)^\alpha > 0. \end{aligned}$$

We complete the proof. ∎

Lemma 3.5 *If $G \in \mathcal{K}' \bigcup \mathcal{K}''$ is a bicyclic graph with order n, then there exists a graph $G' \in \mathcal{K}$ with the same order of G, satisfying that $R_\alpha(G) > R_\alpha(G')$ for $\alpha \leq -2$.*

Proof. Suppose G be a bicyclic graph with order n and $G \in \mathcal{K}' \bigcup \mathcal{K}''$. Let $d(u) = x + 3$, $d(v) = y + 3$ and suppose $x \geq y \geq 0$.

If $G \in \mathcal{K}'$, we will find a new graph $G' \in \mathcal{K}$ with the same order of G, such that $R_\alpha(G) > R_\alpha(G')$. G' is constructed from G by contracting edge uv to a vertex $u(v)$ and attaching a star S_{x+y+1} to the vertex u (see Figure 3.5). We have

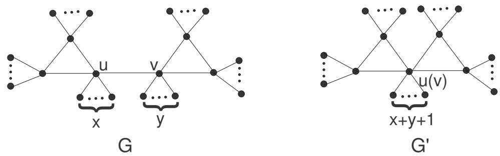

Figure 3.5

$$R_\alpha(G) - R_\alpha(G') > x(x+3)^\alpha + y(y+3)^\alpha + (x+3)^\alpha(y+3)^\alpha - (x+y+1)(x+y+5)^\alpha. \tag{3.2}$$

If $xy \geq 4$, by Lemma 2.2 (ii), $R_\alpha(G) - R_\alpha(G') > f(x,y) > 0$.

Therefore, we only consider the following five cases other than $xy \geq 4$.

(1). if $x = 3$ and $y = 1$,

$$\begin{aligned} R_\alpha(G) - R_\alpha(G') &> 4^\alpha + 24^\alpha + 3 \cdot 6^\alpha - 5 \cdot 9^\alpha \\ &> (4^\alpha - 4 \cdot 8^\alpha) + (6^\alpha - 9^\alpha) + 24^\alpha + 2 \cdot 6^\alpha \\ &> 4^\alpha - 4 \cdot 2^\alpha \cdot 4^\alpha \geq 0; \end{aligned}$$

(2). if $x = 2$ and $y = 1$, similarly, $R_\alpha(G) - R_\alpha(G') > 4^\alpha + 20^\alpha + 2 \cdot 5^\alpha - 4 \cdot 8^\alpha > 0$;

(3). if $x = 1$ and $y = 1$,

$$\begin{aligned} R_\alpha(G) - R_\alpha(G') &> 2 \cdot 4^\alpha + 16^\alpha - 3 \cdot 7^\alpha \\ &= (2 - 3 \cdot (\frac{7}{4})^\alpha) \cdot 4^\alpha + 16^\alpha > 0; \end{aligned}$$

(4). if $y = 0$ and $x > 0$, by Lemma 2.3 (iii), we have

$$R_\alpha(G) - R_\alpha(G') > (x + 3^\alpha)(x+3)^\alpha - (x+1)(x+5)^\alpha > 0;$$

(5). if $x = y = 0$, we find another new graph $G'' \in \mathcal{K}$ with the same order of G (see Figure 3.6). Without loss of generality, we suppose $a = \max\{a, b, c, d\}$. By our assumption, the order of G is at least 8, then we have $a \geq 1$.

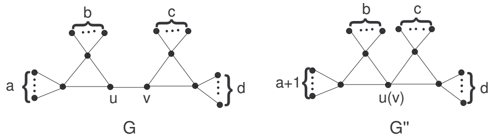

Figure 3.6

$$
\begin{aligned}
& R_\alpha(G) - R_\alpha(G'') \\
= \; & a(a+2)^\alpha + (a+2)^\alpha[3^\alpha + (b+2)^\alpha] + 3^\alpha[(b+2)^\alpha + (c+2)^\alpha + (d+2)^\alpha] + 9^\alpha \\
& -(a+1)(a+3)^\alpha - (a+3)^\alpha[4^\alpha + (b+2)^\alpha] - 4^\alpha[(b+2)^\alpha + (c+2)^\alpha + (d+2)^\alpha] \\
> \; & a(a+2)^\alpha + (a+2)^\alpha[3^\alpha + (b+2)^\alpha] + 3^\alpha(b+2)^\alpha + 9^\alpha \\
& -(a+1)(a+3)^\alpha - (a+3)^\alpha[4^\alpha + (b+2)^\alpha] - 4^\alpha(b+2)^\alpha.
\end{aligned}
$$

If $a \geq 2$, by Lemma 2.3 (iv), we have

$$
\begin{aligned}
R_\alpha(G) - R_\alpha(G'') &> 9^\alpha + (a+3^\alpha)(a+2)^\alpha - (a+1+4^\alpha)(a+3)^\alpha \\
&> (a+3^\alpha)(a+2)^\alpha - (a+1)(a+3)^\alpha > 0.
\end{aligned}
$$

For $a = 1$, we consider all the possible values of b, then we can verify that $R_\alpha(G) - R_\alpha(G'') > 0$.

If $G \in \mathcal{K}''$, we will find a new graph $G' \in \mathcal{K}'$ with the same order of G, such that $R_\alpha(G) \geq R_\alpha(G')$. Denote w the common neighbor vertex of u and v and $d(w) = t+2$. G' is constructed from G by contracting edge uw to a vertex $u(w)$ and attaching a star S_{x+t+1} to the vertex u (see Figure 3.7). We have

$$
\begin{aligned}
R_\alpha(G) - R_\alpha(G') &> x(x+3)^\alpha + t(t+2)^\alpha + [(x+3)^\alpha + (y+3)^\alpha](t+2)^\alpha \\
&\quad -(x+t+1)(x+t+4)^\alpha - (y+3)^\alpha(x+t+4)^\alpha
\end{aligned}
$$

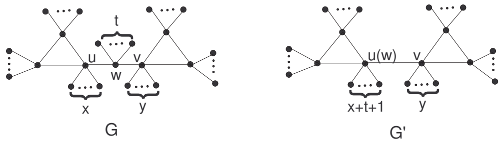

Figure 3.7

If $tx \geq 2$, then by Lemma 2.2 (i), $R_\alpha(G) - R_\alpha(G') \geq g(x,t) > 0$.

If $t = x = 1$, then $R_\alpha(G) - R_\alpha(G') > 4^\alpha + 3^\alpha + 12^\alpha - 3 \cdot 6^\alpha > 0$.

If $t = 0$ and $x > 0$, since $x \geq y$, we have

$$\begin{aligned}
& R_\alpha(G) - R_\alpha(G') \\
> \; & x(x+3)^\alpha + 2^\alpha[(x+3)^\alpha + (y+3)^\alpha] - (x+1)(x+4)^\alpha - (y+3)^\alpha(x+4)^\alpha \\
> \; & (x+2^\alpha)(x+3)^\alpha - (x+1)(x+4)^\alpha + (x+3)^\alpha[2^\alpha - (x+4)^\alpha].
\end{aligned}$$

By Lemma 2.3 (i), $R_\alpha(G) - R_\alpha(G') > 0$ for $x \geq 3$. For $x = 1, 2$, we can verify $R_\alpha(G) - R_\alpha(G') > 0$ by simple calculation.

If $x = 0$ and $t > 0$, then $y = 0$. By Lemma 2.3 (ii), we have

$$R_\alpha(G) - R_\alpha(G') > t(t+2)^\alpha + 2 \cdot 3^\alpha (t+2)^\alpha - (t+1)(t+4)^\alpha - 3^\alpha(t+4)^\alpha > 0.$$

If $t = x = y = 0$, we find another new graph $G'' \in \mathcal{K}'$ with the same order of G (see Figure 3.8). Without loss of generality, we suppose $a = \max\{a, b, c, d\}$. By our assumption, the order of G is at least 8, then we have $a \geq 1$.

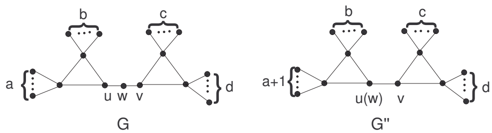

Figure 3.8

$$\begin{aligned} R_\alpha(G) - R_\alpha(G'') &= a(a+2)^\alpha + (a+2)^\alpha[3^\alpha + (b+2)^\alpha] + 2 \times 6^\alpha \\ &\quad -(a+1)(a+3)^\alpha - (a+3)^\alpha[3^\alpha + (b+2)^\alpha] - 9^\alpha. \end{aligned}$$

Since $a \geq b$, we have

$$\begin{aligned} R_\alpha(G) - R_\alpha(G'') &\geq 2 \cdot 6^\alpha - 9^\alpha + (a + 3^\alpha)(a+2)^\alpha - (a + 1 + 3^\alpha)(a+3)^\alpha \\ &\quad +(a+2)^\alpha[(a+2)^\alpha - (a+3)^\alpha] \end{aligned}$$

By Lemma 2.3 (iv), $R_\alpha(G) - R_\alpha(G'') > 0$ for $a \geq 2$. For $a = 1$, we can verify that $R_\alpha(G) - R_\alpha(G'') > 0$ by calculation.

Thus, we complete the proof. ∎

By Lemma 3.2, 3.3, 3.4 and 3.5, we have the following theorem.

Theorem 3.6 *For $\alpha \leq -2$, the minimum bicyclic graph must be in $\mathcal{G}$ or $\mathcal{K}$.* ∎

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