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Upper and Lower Bounds for the First and Second Zagreb Indices of Quasi Bicyclic Graphs

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ABSTRACT

The aim of this paper is to give an upper and lower bounds for the first and second Zagreb indices of quasi bicyclic graphs. For a simple graph G, we denote $M_1(G)$ and $M_2(G)$, as the sum of $\deg^2(u)$ overall vertices u in G and the sum of $\deg(u)\deg(v)$ of all edges uv of G, respectively. The graph G is called quasi bicyclic graph if there exists a vertex $x \in V(G)$ such that $G - x$ is a connected bicyclic graph. The results mentioned in this paper, are mostly new or an important of result given by authors for quasi unicyclic graphs in [1].

1. INTRODUCTION

During the last decades a large number of numerical graph invariants (topological indices) have been defined and used for correlation analysis in theoretical chemistry and mathematical chemistry that is calculated based on the molecular graph of a chemical compound. Topological indices are numerical parameters of a graph which characterize its

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topology and are usually graph invariant. The Hosoya index is the first topological index recognized in chemical graph theory. Other famous examples include the Wiener index, Randić's molecular connectivity index, Balaban's J index and Zagreb indices.

In this paper, We review the important properties of the Zagreb group indices on quasi bicyclic graphs. The first and the second Zagreb indices are among the oldest topological indices defined in 1972 by Gutman and Trinajstić [3]. These numbers have been used to study the molecular complexity, chirality and some other chemical quantities. The *first Zagreb index* is defined as the sum of the squares of the degrees of the vertices, i.e. $M_1(G) = \sum_{u \in V(G)} \deg^2(u)$ and the *second Zagreb index* is the sum of $\deg(u)\deg(v)$ overall edges uv of G. This means that $M_2(G) = \sum_{uv \in E(G)} \deg(u)\deg(v)$. Das and Gutman provided some identities for Zagreb indices by which the authors obtained some bounds for the second Zagreb index and in [11], the author established some bound for the first Zagreb index. Qiao [14] gave sharp lower and upper bounds for the Zagreb group indices of $n-$vertex quasi-tree graphs and the corresponding extremal graphs were characterized (see [4-10] and also [12-13] for more results). We continue this work for quasi unicyclic graphs in [1] and now is investigated quasi bicyclic graphs in this paper.

Now, let us remind some graph theorical concepts here. The notations and terminology are standard and we refer to [2] and other authored papers on the indices related to mathematical chemistry for more details and proofs.

An undirected graph in which each edge connects two different vertices and where no two edges connect the same pair of vertices is called a Simple graph. For a simple graph, an unordered pair of vertices u and v that specify a line joining these two nodes are said to form an edge and denote by uv or $\{u, v\}$. Suppose G is a simple graph and $\Delta(G)$ and $\delta(G)$ denote the maximum and minimum degrees of vertices in G. For each $u \in V(G)$, the set of all neighbors of the vertex u is denoted by $N_G(u) = \{v \in V(G) | uv \in E(G)\}$. The vetrex $v \in V(G)$ is said to be pendant vertex if $N_G(u) = 1$ and the edge $uv \in E(G)$ is said to be pendant edge if u or v to be pendant vertex. For a subset W of the vertex set $V(G)$, let $G - W$ be the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, for a subset E of the edge set $E(G)$, $G - E$ denotes the subgraph of G obtained by deleting the edges of $E(G)$. If $W = \{v\}$ and $E = \{xy\}$, the subgraphs $G - W$ and $G - E$ will be simply written as $G - v$ and $G - xy$, respectively. For any two non-adjacent vertices x and y of G, we let $G + xy$ be the graph obtained from G by adding an edge xy, and also for any two adjacent vertices u and v of G, we let $G - uv$ be the graph obtained from G by deleting an edge uv. The *cycle* C_n for $n \geq 3$, is a path of n edges and n vertices where starting and ending at the same vertex. The wheel graph W_n for $n \geq 4$, is a graph formed by connecting a single universal vertex x to all vertices of a cycle graph C_{n-1}. The *complete graph* K_n for $n \geq 2$, is a graph in which each pair u and v of vertices are adjacent.

A graph G of order n is called a *bicyclic graph*, if is connected and the number of edges of G is $n+1$. Let $B(n)$ be the set of all bicyclic graphs on vertices. If the graph G has the property that $G-x$ induces a bicyclic graph for a suitable vertex x, then G is called a *quasi bicyclic graph*.

Let $B(p,q)$ be the bicyclic graph obtained from two vertex-disjoint cycles C_p and C_q by identifying vertices u of C_p and v of C_q(See Figure 1.) It is clear that the bicycle $B(p,q)$ with some pendant edges is quasi bicyclic graph.

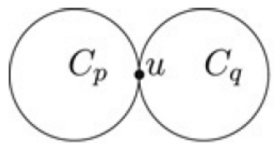


Figure 1: The graph $B(p,q)$.

Throughout this paper, the set of all bicyclic and quasi bicyclic graphs with n vertices will be denoted by $B(n)$ and $QB(n)$, respectively. The purpose of this paper is to prove the following two main theorems that we will prove them in future sections.

Theorem A. Let $G \in QB(n)$ and $n \geq 5$. Then $4n+12 \leq M_1(G) \leq 2n^2+16$. The equality holds in right or left inequality if and only if $G \cong \Omega(n)$ or $G \cong \Gamma(n)$, respectively.

Theorem B. Suppose that $G \in QB(n)$ for every $n \geq 5$. Then $4n+20 \leq M_2(G) \leq 5n^2-6n+25$. The equality holds in right inequality if and only if $G \cong \Omega(n)$ and holds in left inequality if and only if $G \cong \Gamma(n)$ for $n \geq 7$.

2. PROOF OF THEOREMS A AND B

We start by the following simple lemma which plays an important role in the proof of our main theorems.

Lemma 2.1 *Let G be an n −vertex graph, $xy \in E(G)$ and $uv \notin E(G)$. Then,*

1. $M_1(G) \leq M_1(G+uv)$,
2. $M_1(G-xy) \leq M_1(G)$,
3. $M_2(G) \leq M_2(G+uv)$,
4. $M_2(G-xy) \leq M_2(G)$.

Proof. Since the proof of the part (ii) is similar to the proof of the part (i) and the proof of (iv) is similar to the proof of (iii), it is enough to prove (i) and (iii).

- $uv \notin E(G)$. By connecting the vertices u and v, we can see that $M_1(G+uv) - M_1(G) = (\deg(u)+1)^2 + (\deg(v)+1)^2 - \deg^2(u) - \deg^2(v) = 2(1+\deg(u)\deg(v)) > 0$. Hence, $M_1(G) \leq M_1(G+uv)$.

- $uv \notin E(G)$, $N_G(v) = \{x_1, \dots, x_s\}$ and $N_G(v) = \{y_1, \dots, y_r\}$. Therefore, $M_2(G+uv) - M_2(G) = (\deg(u)+1)(\deg(v)+1) + \sum_{i=1}^{r} (\deg(u)+1)(\deg(y_i)) + \sum_{i=1}^{s} (\deg(v)+1)(\deg(x_i)) - \sum_{i=1}^{r} (\deg(u))(\deg(y_i)) - \sum_{i=1}^{s} (\deg(v))(\deg(x_i)) = (\deg(u)+1)(\deg(v)+1) + \sum_{i=1}^{r} \deg(y_i) + \sum_{i=1}^{s} \deg(x_i) > 0$. As a consequence, $M_2(G) \leq M_2(G+uv)$.

This proves the lemma. □

In the following lemma, we give a class of graphs which are not quasi bicyclic.

Lemma 2.2 *Let G be an n −vertex graph such that $n \geq 6$. If the number of vertices of degree $n-1$ is greater than 3, then G is not a quasi bicyclic graph.*

Proof. Since $|V(G)| = n$, when $n \geq 6$, there are 6 distinct vertices x_1, x_2, x_3, x_4, x_5 and x_6 such that $\deg(x_1) = \deg(x_2) = \deg(x_3) = \deg(x_4) = n-1$. It is clear that x_1, x_2, x_3, x_4 are adjacent to each other and so the subgraph of G induced by the above sex vertices is not quasi bicyclic, because the graph constructed from G by removing any of these six vertices has at least three cycles. Hence G can not be a quasi bicyclic graph. □

The following corollary is a direct consequence of Lemma 2.3.

Corollary 2.3 *If $G \in QB(n)$, then G has at most three vertices of degree $n-1$.*

Lemma 2.4 *Let $G \in QB(n)$, for every $n \geq 5$ and $m = |E(G)|$. Then*

- $n+1 \leq m \leq 2n-1$,
- $1 \leq \delta(G) \leq 3$.

Proof. Suppose that $G \in QB(n)$ and $n \geq 5$. Since G is connected and is a bicycle, $m \geq n+1$. By our assumption, G has a suitable vertex x such that $G - x \in B(n)$. Thus, $|E(G-x)| = |V(G-x)| = n-1$. Since $\deg(x) \leq n-1$, $m = |E(G)| \leq |E(G-x)| + n - 1 = 2n-2$.

If $G \in QB(n)$ has a pendant vertex, then $\delta(G) = 1$. Suppose G has no pendant vertex. Then $\delta(G) \geq 2$ and for a suitable vertex x, we have $G - x \in B(n-1)$ which implies that $G - x$ has a vertex y of degree 2. If y is adjacent to x, then the minimum degree of G can be at most 3. Hence $1 \leq \delta(G) \leq 3$, as desired. □

Lemma 2.5 *Suppose that K_n be complete graph of order $n \geq 6$. Then $K_n \notin QB(n)$ for every $n \geq 6$.*

Proof. Since the number of vertices of order $n-1$ in complete graph K_n for $n \geq 6$ is more than 3, So K_n is not quasi bicyclic graph by Corollary 2.3. □

We can obtain quasi bicyclic graphs without pendant vertex by $\delta = 3$ and $\Delta = n-1$ by Lemmas 2.3, 2.4, 2.5 and the fact that $\sum_{x\in V(G)} \deg(x) = 2|E(V)|$. Therefore, each quasi bicyclic graph has one of the sequence of degrees of vertices $A = (n-1,4,4,\underbrace{3,\ldots,3}_{n-3})$ or $B = (n-1,5,\underbrace{3,\ldots,3}_{n-2})$.

Apply Lemmas 2.2 and 2.4 to find lower and upper bounds for the Zagreb indices of an arbitrary quasi bicycle graph. We first define a class $\Omega(n)$ of $n-$vertex quasi bicyclic graphs that plays an important role in our results. Let $\Omega(n)$ be the set of all quasi bicyclic graphs with exactly n vertices that contains two vertices of degree $n-1$, one vetex of degree 4, two vertices of degree 3 and the rest of vertices have degree 2 (see Figure 2).

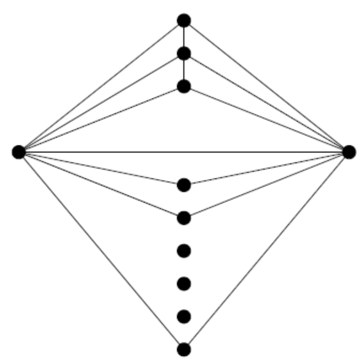


Figure 2: The Graph Structure of a Member of $\Omega(n)$.

Let us now state another class of quasi bicyclic graphs. Define $\Gamma(n)$ to be a quasi bicyclic graph that contains a cycle of length $n-2$, a cycle of length 3 and a pendant vertex that is attached to C_{n-2} (see Figure 3).

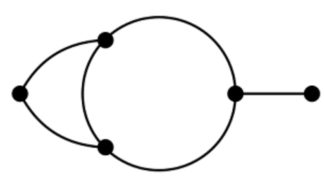


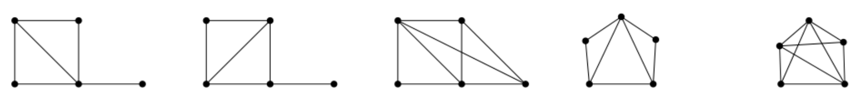
Figure 3: The Graph Structure of a Member of $\Gamma(n)$.

Now, we are ready to prove Theorems A and B.

Proof of Theorem A. Suppose $G \in QB(n)$ for every $n \geq 5$, and x is a vertex of G such that $G - x \in B(n-1)$. We prove the theorem in two parts.

Part 1. Right inequality: In this part, we have the following two cases:

- *G has no pendant vertex*. By Lemma 2.4, $\delta(G) = 2$ or 3. Suppose $\delta(G) = 2$. We proceed by induction on n. If $n = 5$, then it is clear that $M_1(G) \leq 66 = 2n^2 + 16$(see Figure 4).



M_1	34	32	54	42	66
M_2	44	42	89	71	120

Figure 4: The Zagreb Indices of Members on QB(5).

We now assume that $n \geq 6$ and the result holds for $n-1$. If $\deg(x) < n-1$, then we construct a graph G' from G by adding some new edges to G to obtain $\deg(x) = n-1$. By Lemma 2.1, $M_1(G) \leq M_1(G')$. Let u be a vertex adjacent to x and v such that $\deg(u) = 2$, $\deg(x) = n-1$ and $2 \leq \deg(v) \leq n-1$. If we remove the vertex u, then by inductive assumption $M_1(G' - u) \leq 2(n-1)^2 + 16$. Therefore, $M_1(G') - M_1(G' - u) = 4 + [(n-1)^2 - (n-2)^2] + [(\deg(v))^2 - (\deg(v) - 1)^2] = 2 + 2[(n-1) + \deg(v)]$. On the other hand, we have

$$\begin{aligned} M_1(G) \leq M_1(G') &= M_1(G' - u) + 2 + 2[(n-1) + \deg(v)] \\ &\leq 2(n-1)^2 + 16 + 2 + 2[(n-1) + \deg(v)] \\ &\leq 2(n-1)^2 + 18 + 2(2n-2) = 2n^2 + 16. \end{aligned}$$

If $\delta(G) = 3$, then G has one of the sequence of degrees of vertices A or B that zagreb index for them is $n^2 + 7n + 6$ or $n^2 + 7n + 8$. Therefore, $M_1(A) < M_1(B) < 2n^2 + 16$ as required.

- *G has a pendant vertex x*. In this case, we can see that x is not adjacent to other pendant vertices of G. Again we obtain a new graph G' by connecting all pendant vertices to x and Lemma 2.4, $M_1(G) \leq M_1(G')$. So, the proof is completed by using the previous case.

For the second part, we first note that if $G \in \Omega(n)$, then $M_1(G) = \sum_{u \in V(G)} \deg^2(u) = 2n^2 + 16$. Conversely, if $M_1(G) = \sum_{u \in V(G)} \deg^2(u) = 2n^2 + 16$, then we can see that the vertex v has degree $n-1$. This shows that we have two vertices x and v of degree $n-1$. Moreover, we have only three distinct vertices $y, u, w \notin \{x, v\}$ such that x and v are adjacent to y, u and w and $\deg(y) = \deg(u) = 3, \deg(w) = 4$. If for instance y is adjacent to a vertex different from x and v then we will have a new cycle which is a contradiction. Thus $\deg(y) = \deg(u) = 3$. For the rest of vertices as $z \notin \{x, y, u, v, w\}$, we should have $\deg(z) = 2$. Otherwise, a new cycle will be appeared. Hence $G \in \Omega(n)$.

Part 2. Left inequality: Similar to the right part, two cases can be happened as follows:

- *G has no pendant vertex*. We can proceed by induction on n. Let $n = 5$, then we have several kinds of quasi bicyclic graphs depicted in Figure 4. For the graph depicted on this figure, we can see that $M_1 \geq 32$, as desired. Suppose that $n \geq 6$ and the result holds for $n-1$. Proceed by induction, we assume that $2 \leq \deg(x) = r \leq n-1$ and $N_G(x) = \{x_1, \dots, x_r\}$. If we remove all edges xx_2, xx_3, ..., xx_r and obtain the new graph G', then we can see that $M_1(G) > M_1(G - xx_2) > M_1(G - \{xx_2, xx_3\}) > \cdots > M_1(G - \{xx_2, \dots, xx_r\}) = M_1(G')$.
  If we remove the vertex x from G', then by induction hypothesis, $M_1(G' - x) \geq 4(n-1) + 12$. Therefore, $M_1(G') - M_1(G' - x) = 1 + [\deg^2(x_1) - (\deg(x_1) - 1)^2] = 2\deg(x_1) \geq 4$. Hence, $M_1(G') \geq 4(n-1) + 12 + 2\deg(x_1) \geq 4n + 12$, as desired.

- *G has pendant vertex u adjacent to v, where* $2 \leq \deg(v) \leq n-1$. By removing the vertex u we achieved a new graph G'' that by induction hypothesis satisfies $M_1(G'') > 4(n-1) + 2$. So, $M_1(G) = M_1(G'') + 1 + [(\deg^2(v) - (\deg(v) - 1)^2] \geq 4(n-1) + 12 + 1 + 1 + 2\deg(v) \geq 4n+$
- 12 and the proof is completed.

To prove the second part, we first assume that $G \in \Gamma(n)$. It is clear that $M_1(G) = \sum_{u \in V(G)} \deg^2(u) = 4n + 12$. Conversely one can easily see that the minimum value of $M_1(G)$ occurs when $\deg(x) = 1$, Since $M_1(G) = 4n + 12$, x must be adjacent to only one vertex of C_{n-2}, and C_{n-2} conneceted to C_3 with a common edge, and the result follows. □

As similar as the method for giving lower and upper bounds of $M_1(G)$ in Theorem A, we can state it for $M_2(G)$ in Theorem B.

Proof of Theorem B. Suppose $G \in QB(n)$, when $n \geq 5$, and x is a vertex in G such that $G - x \in B(n-1)$. We prove the theorem in two parts. For the right hand side of the inequality, we may consider two cases as follows:

1. *G has no pendant vertex.* By Lemma 2.4, $\delta(G) = 2 \ or \ 3$. Suppose $\delta(G) = 2$ and apply induction on n. If $n = 5$, then equality holds, see Figure 4. We assume that $n \geq 6$ and the result holds for $n - 1$. If $deg(x) < n - 1$, then there are vertices in the graph that are not adjacent to x. We connect these vertices to x and obtain a new graph G'. By Lemma 2.2, $M_2(G) \leq M_2(G')$. Let u be a vertex adjacent to x and v such that $\deg(u) = 2$, $\deg(x) = n - 1$ and $2 \leq \deg(v) = r \leq n - 1$. Suppose x and v have neighbors $y_1, \ldots, y_{n-1}$ and $w_1, \ldots, w_r$, respectively. If we remove the vertex u, then by induction assumption, $M_2(G - u) \leq 5(n-1)^2 - 6(n-1) + 25$. Therefore, $M_2(G') - M_2(G' - u) = 2(n-1) + 2r + \sum_{i=1}^{n-2} (n-1)\deg(y_i) + \sum_{i=1}^{r-1} r\deg(w_i) \quad - \sum_{i=1}^{n-2} (n-2)\deg(w_i) - \sum_{i=1}^{r-1} (r-1)\deg(w_i)$. According to the above description and the fact that $\sum_{x \in V(G)} \deg(x) = 2|E(V)|$, we have $M_2(G') \leq M_2(G' - u) + 10n - 11 \quad \leq 5(n-1)^2 - 6(n-1) + 25 + 10n - 11 = 5n^2 - 6n + 25$. If $\delta(G) = 3$, then G has one of the sequence of degrees of vertices A or B that second zagreb index for them is less than $5n^2 - 6n + 25$ as required.

2. *G has a pendant vertex.* If G has a pendant vertex x then we can see that x is not adjacent to other pendant vertices and hence we can obtain a new graph G' by connecting all pendant vertices to x. Again by Lemma 2.2, $M_2(G) \leq M_2(G')$ and the proof can be completed by using the Case 1.

To prove the second part, it's clear that if $G \in \Omega(n)$, then $M_2(G) = \sum_{uv \in E(G)} \deg(u)\deg(v) = 5n^2 - 6n + 25$. Conversely, if $M_2(G) = \sum_{uv \in E(G)} \deg(u)\deg(v) = 5n^2 - 6n + 25$, then we can see that the vertex v should be of degree $n - 1$. Thus, we have two vertices x and v of degree $n - 1$.

Moreover, we have only three distinct vertices $y, u, w \notin \{x, v\}$ such that x and v are adjacent to y, u and w and $\deg(y) = \deg(u) = 3, \deg(w) = 4$. If for instance y is adjacent to a vertex different from x, v and w then we will have a new cycle which is a contradiction. Thus $\deg(y) = \deg(u) = 3$, and $\deg(w) = 4$. For the rest of vertices as $z \notin \{x, y, u, v, w\}$, we should have $\deg(z) = 2$. Otherwise, a new cycle will be appeared. Hence $G \in \Omega(n)$.

For the left hand side inequality, two cases can be arised as follows:

1. *G has no pendant vertex.* Again our proof can be proceed by induction on n. If $n = 5$, then we have five kinds of quasi bicyclic graphs as in Figure 4. For this graphs we have $M_2 \geq 40$ and the inequality holds, as desired. We now assume that $n \geq 6$ and the result holds for $n-1$. To prove the result for n, let $2 \leq \deg(x) = r \leq n-1$ and $N_G(x) = \{x_1, \dots, x_r\}$. If we remove the edges xx_2, xx_3, ..., xx_r then we obtain a new graph G' such that $M_2(G) > M_2(G - xx_2) > M_2(G - \{xx_2, xx_3\}) > \cdots > M_2(G - \{xx_2, \dots, xx_r\}) = M_2(G')$. If we remove the vertex x from G', then by induction hypothesis, we have $M_2(G' - x) \geq 4(n-1) + 20$. Therefore, $M_2(G') \geq M_2(G' - x) + r + \sum_{i=1}^{r-1} (r - (r-1))\deg(y_i) \geq 4n - 4 + 20 + 2 + \sum_{i=1}^{r-1} \deg(y_i) \geq 4n + 20$ that all vertices y_i, $1 \leq i \leq r$, are adjacent to x_1 and $\deg(y_i) \geq 2$. Hence the result follows.

2. *G has pendant vertex u adjacent to v, where* $2 \leq \deg(v) \leq n-1$. By removing vertex u we achieve a new graph G'' such that $M_2(G'') \geq 4(n-1) + 20$. Therefore,

$$\begin{aligned} M_2(G) &\geq M_2(G'') + r + \sum_{i=1}^{r-1} (r - (r-1))\deg(y_i) \\ &\geq 4n - 4 + 20 + 2 + \sum_{i=1}^{r-1} \deg(y_i) \geq 4n + 20, \end{aligned}$$

that all vertices y_i, $1 \leq i \leq r$, are adjacent to v. Since the degree of at least one vertex y_i is greater than or equal to 2, $r \geq 2$ which completes the proof of this case.

To prove the second part, we note that if $G \cong \Gamma(n)$ for $n \geq 7$, then $M_2(G) = \sum_{uv \in E(G)} \deg(u)\deg(v) = 4n + 20$. Conversely, one can easily see that the minimum value of $M_2(G)$ occurs when $\deg(x) = 1$. Since $M_2(G) = 4n + 20$, x has to must be adjacent to only one vertex of C_{n-2}, and C_{n-2} conneceted to C_3 with a common edge, and the result follows. Finally, we may suggest to the reader to continue this kind of computations for quasi n-cyclic graphs where $n \geq 3$. □

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