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EXACT FORMULAE FOR THE FIRST REVERSE ZAGREB BETA INDEX AND SECOND REVERSE ZAGREB INDEX OF STANDARD GRAPHS

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Abstract. The First Reverse Zagreb Beta Index and the Second Reverse Zagreb Index are important degree-based topological indices in chemical graph theory that are widely used to characterize the structural properties of molecular graphs. These indices are defined using the reverse vertex degree of a vertex (v) in a graph (G), given by $(c_v = \Delta(G) + 1 - d_G(v))$, where $(\Delta(G))$ denotes the maximum degree of (G). In this paper, we derive closed-form expressions for the First Reverse Zagreb Beta Index and the Second Reverse Zagreb Index of several standard graph families, namely the tadpole graph, wheel graph, ladder graph, and their line graphs. The results are obtained by partitioning the edge sets according to the reverse vertex degrees of their end vertices, leading to simple and systematic computations of the required indices. The derived formulae provide efficient methods for evaluating these indices and contribute to the theoretical study of reverse Zagreb indices and their applications in chemical graph theory.

1. Introduction

Let $G = (V(G), E(G))$ be a finite, simple, and connected graph, where $V(G)$ and $E(G)$ denote the vertex set and edge set of G, respectively. The degree of a vertex $v \in V(G)$, denoted by $d_G(v)$, is the number of vertices adjacent to v. The maximum degree of G is denoted by $\Delta(G)$. The reverse vertex degree of a vertex v in G is defined as

$$c_v = \Delta(G) + 1 - d_G(v).$$

Thus, the reverse degree assigns larger values to vertices of smaller degree and smaller values to vertices of larger degree. Consequently, it provides an alternative perspective for analyzing the structural properties of graphs by emphasizing the relative contribution of low-degree vertices. The reverse edge corresponding to an edge $uv \in E(G)$ is represented by the ordered pair (c_u, c_v), where c_u and c_v are the reverse degrees of the end vertices. Throughout this paper, we use the standard terminology and notation of graph theory. For all undefined terms and notation, the reader is referred to [2].

Chemical graph theory is an important branch of mathematical chemistry that applies graph-theoretical concepts to represent molecular structures and investigate their physicochemical properties. In this framework, atoms of a molecule

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are represented by vertices, while chemical bonds are represented by edges. This mathematical representation enables researchers to study molecular structures using graph invariants known as topological indices. These indices are numerical parameters associated with molecular graphs and have found extensive applications in quantitative structure–property relationship (QSPR) and quantitative structure–activity relationship (QSAR) studies. They play a significant role in predicting physicochemical, biological, and pharmacological properties of chemical compounds without performing expensive laboratory experiments. Due to their wide range of applications in chemistry, pharmacology, material science, and nanotechnology, numerous degree-based, distance-based, and neighborhood-based topological indices have been proposed and extensively investigated; see [2] and the references therein.

Among the various classes of topological descriptors, the Zagreb indices occupy a prominent position because of their simplicity, computational efficiency, and strong correlation with several molecular properties. Originally introduced for studying the total π-electron energy of conjugated hydrocarbons, Zagreb indices have inspired a large number of variants and generalizations. In recent years, researchers have focused on modified degree concepts to develop new graph invariants capable of capturing different structural characteristics of graphs.

Motivated by the concept of reverse vertex degree, Ediz [1, 4, 5] introduced the First Reverse Zagreb Beta Index and the Second Reverse Zagreb Index, which are defined using reverse degrees instead of ordinary vertex degrees. These indices are given by

$$CM_1(G) = \sum_{uv \in E(G)} (c_u + c_v)$$

and

$$CM_2(G) = \sum_{uv \in E(G)} c_u c_v,$$

respectively.

Unlike the classical Zagreb indices, which depend directly on the vertex degrees, the reverse Zagreb indices measure graph structures through reverse degrees. This approach assigns greater importance to vertices with relatively smaller degrees and therefore offers a complementary structural characterization of graphs. These indices have attracted considerable attention due to their mathematical properties and potential applications in chemical graph theory. In particular, they provide useful descriptors for investigating molecular structures, comparing graph families, and establishing quantitative relationships between graph topology and molecular characteristics.

The computation of reverse Zagreb indices for standard graph classes and graph operations is an active area of research in chemical graph theory. Explicit formulae for these indices not only facilitate efficient computation but also provide valuable insights into the influence of graph structure on reverse degree-based descriptors. In this paper, we derive closed-form expressions for the First Reverse Zagreb Beta Index and the Second Reverse Zagreb Index of several important graph families by partitioning their edge sets according to the reverse degrees of the end vertices. The obtained results contribute to the growing literature on reverse degree-based topological indices and provide useful formulae for further theoretical investigations and chemical applications.

2. $CM_1(G)$ and $CM_2(G)$ of well known graphs and their line graphs.

In this paper, we investigate the First Reverse Zagreb Beta Index and the Second Reverse Zagreb Index for several standard graph families. In particular, we derive explicit formulae for the tadpole graph, wheel graph, ladder graph, and their subdivision graphs. To obtain these results, the edge sets of the considered graphs are partitioned according to the reverse degrees of the end vertices. The resulting expressions provide convenient and efficient formulae for computing the proposed indices and contribute to the further study of reverse Zagreb indices for standard graph families [3, 6].

2.1. Tadpole Graph. Let C_n be a cycle on n vertices ($n \geq 3$) and P_k be a path on k vertices ($k \geq 1$). The *tadpole graph*, denoted by $T_{n,k}$, is the graph obtained by joining one vertex of the cycle C_n to an end vertex of the path P_k by a single edge.

Theorem 2.1. *For a tadpole graph $T_{n,k}$, $(n \geq 3, k \geq 1)$*

$$\begin{aligned} CM_1(T_{n,k}) &= 4k + 4n - 2 \\ CM_2(T_{n,k}) &= 4k + 4n - 4. \end{aligned}$$

Proof. A tadpole graph $T_{n,k}$ has $n+k$ vertices and $n+k$ edges with $\Delta(T_{n,k}) = 3$. The edge partition of the tadpole graph $T_{n,k}$ based on the reverse vertex degree is given in table 1. By definition of $CM_1(G)$, $CM_2(G)$ and from table 1, for $(n \geq 3, k \geq 1)$, we get

(c_u, c_v) where $uv \in E(T_{n,k})$	(1, 2)	(2, 2)	(2 3)
No. of edges	3	n+k-4	1

TABLE 1. Edge partition of $T_{n,k}$ using reverse vertex degree

$$\begin{aligned} C_1(T_{n,k}) &= 3 \cdot (1+2) + (n+k-4) \cdot (2+2) + 1 \cdot (2+3) \\ &= 4k + 4n - 2 \end{aligned}$$

$$\begin{aligned} C_2(T_{n,k}) &= 3 \cdot (1 \cdot 2) + (n+k-4) \cdot (2 \cdot 2) + 1 \cdot (2 \cdot 3) \\ &= 4k + 4n - 4. \end{aligned}$$

□

Theorem 2.2. *For a line graph of a tadpole graph $L(T_{n,k})$, $(n \geq 3, k \geq 1)$*

$$\begin{aligned} C_1(L(T_{n,k})) &= 4k + 4n - 2 \\ C_2(L(T_{n,k})) &= 4k + 4n - 9. \end{aligned}$$

Proof. A line graph of a tadpole graph $L(T_{n,k})$ has $n+k$ vertices and $n+k+1$ edges with $\Delta(T_{n,k}) = 3$. The edge partition of the line graph of a tadpole graph $L(T_{n,k})$ based on the reverse vertex degree is given in table 3. By definition of $CM_1(G)$, $CM_2(G)$ and from table 3, for $(n \geq 3, k \geq 1)$, we get

(c_u, c_v) where $uv \in E(L(T_{n,k}))$	(1, 1)	(1, 2)	(2, 2)	(2, 3)
No. of edges	3	3	n+k-6	1

TABLE 2. Edge partition of $L(T_{n,k})$ using reverse vertex degree

$$\begin{aligned} C_1(L(T_{n,k})) &= 3 \cdot (1+1) + 3 \cdot (1+2) + (n+k-6) \cdot (2+2) + 1 \cdot (2+3) \\ &= 4k + 4n - 2 \end{aligned}$$

$$\begin{aligned} C_2(L(T_{n,k})) &= 3 \cdot (1 \cdot 1) + 3 \cdot (1 \cdot 2) + (n+k-6) \cdot (2 \cdot 2) + 1 \cdot (2 \cdot 3) \\ &= 4k + 4n - 9. \end{aligned}$$

□

2.2. Wheel Graph. Let C_{n-1} be a cycle on $n-1$ vertices $(n \geq 4)$. The *wheel graph*, denoted by W_n, is the graph obtained by adding a new vertex, called the *hub*, and joining it to every vertex of the cycle C_{n-1}. Equivalently, W_n is formed by connecting the hub vertex to all vertices of C_{n-1}.

Theorem 2.3. *For a wheel graph W_n, $(n \geq 4)$*

$$CM_1(W_n) = 3n^2 - 11n + 8$$

$$CM_2(W_n) = n^3 - 6n^2 + 11n - 6.$$

Proof. A tadpole graph W_n has n vertices and $2n-2$ edges with $\Delta(W_n) = n-1$. The edge partition of the wheel graph W_n based on the reverse vertex degree is given in table 5. By definition of $CM_1(G)$, $CM_2(G)$ and from table 5, for $(n \geq 4)$, we get

(c_u, c_v) where $uv \in E(W_n)$	(1, n-3)	(n-3, n-3)
No. of edges	n-1	n-1

TABLE 3. Edge partition of W_n using reverse vertex degree

$$\begin{aligned} C_1(W_n) &= (n-1) \cdot (1 + (n-3)) + (n-1) \cdot ((n-3) + (n-3)) \\ &= 3n^2 - 11n + 8 \end{aligned}$$

$$\begin{aligned} C_2(W_n) &= (n-1) \cdot (1 \cdot (n-3)) + (n-1) \cdot ((n-3) \cdot (n-3)) \\ &= n^3 - 6n^2 + 11n - 6. \end{aligned}$$

□

Theorem 2.4. *For a line graph of wheel graph $L(W_n)$, $(n \geq 4)$*

$$\begin{aligned} CM_1(L(W_n)) &= 5n^2 - 17n + 12 \\ CM_2(L(W_n)) &= n^3 - \frac{9n^2}{2} + \frac{11n}{2} - 2. \end{aligned}$$

Proof. A line graph of wheel graph $L(W_n)$ has $2n-2$ vertices and $\frac{(n-1)(n+4)}{2}$ edges with $\Delta(L(W_n)) = n-1$. The edge partition of the line graph of wheel graph $L(W_n)$ based on the reverse vertex degree is given in table 7. By definition of $CM_1(G)$, $CM_2(G)$ and from table 7, for $(n \geq 4)$, we get

(c_u, c_v) where $uv \in E(L(W_n))$	(1, 1)	(1, n-3)	(n-3, n-3)
No. of edges	$\frac{(n-1)(n-2)}{2}$	2(n-1)	(n-1)

Table 4. Edge partition of $L(W_n)$ using reverse vertex degree

$$\begin{aligned} C_1(L(W_n)) &= \frac{(n-1)(n-2)}{2} \cdot (1+1) + (2n-2) \cdot (1 + (n-3)) + (n-1) \cdot ((n-3) + (n-3)) \\ &= 5n^2 - 17n + 12 \\ C_2(L(W_n)) &= \frac{(n-1)(n-2)}{2} \cdot (1 \cdot 1) + (2n-2) \cdot (1 \cdot (n-3)) + (n-1) \cdot ((n-3) \cdot (n-3)) \\ &= n^3 - \frac{9n^2}{2} + \frac{11n}{2} - 2. \end{aligned}$$

□

2.3. Ladder Graph. Let P_n be a path on n vertices $(n \geq 2)$. The *ladder graph*, denoted by L_n, is the graph obtained by joining the corresponding vertices of two disjoint copies of the path P_n by edges. Equivalently, the ladder graph L_n is the Cartesian product of the path graphs P_n and P_2, that is,

$$L_n = P_n \square P_2.$$

Theorem 2.5. *For a ladder graph L_n, $(n \geq 2)$*

$$\begin{aligned} CM_1(L_n) &= 6n + 4 \\ CM_2(L_n) &= 3n + 8. \end{aligned}$$

Proof. A ladder graph L_n has $2n$ vertices and $3n-2$ edges with $\Delta(L_n) = 3$. The edge partition of the ladder graph L_n based on the reverse vertex degree is given in table 9. By definition of $CM_1(G)$, $CM_2(G)$ and from table 9, for $(n \geq 2)$, we get

$$\begin{aligned} C_1(W_n) &= 2 \cdot (2+2) + 4 \cdot (2+1) + (3 * n - 8) \cdot (1+1) \\ &= 6n + 4. \end{aligned}$$

(c_u, c_v) where $uv \in E(L_n)$	(2, 2)	(2, 1)	(1, 1)
No. of edges	2	4	3n-8

TABLE 5. Edge partition of L_n using reverse vertex degree

$$\begin{aligned} C_2(W_n) &= 2 \cdot (2 \cdot 2) + 4 \cdot (2 \cdot 1) + (3n - 8) \cdot (1 \cdot 1) \\ &= 3n + 8. \end{aligned}$$

□

Theorem 2.6. *For a line graph of ladder graph $L(L_n)$, $(n \geq 2)$*

$$\begin{aligned} CM_1(L(L_n)) &= 12n + 4; \\ CM_2(L(L_n)) &= 6n + 20. \end{aligned}$$

Proof. A line graph of ladder graph $L(L_n)$ has $3n - 2$ vertices and $6n - 8$ edges with $\Delta(L(L_n)) = 4$. The edge partition of the line graph of ladder graph $L(L_n)$ based on the reverse vertex degree is given in table 11. By definition of $CM_1(G)$, $CM_2(G)$ and from table 11, for $(n \geq 2)$, we get

(c_u, c_v) where $uv \in E(L(L_n))$	(3, 2)	(2, 1)	(1, 1)
No. of edges	4	8	6n-20

TABLE 6. Edge partition of $L(L_n)$ using reverse vertex degree

$$\begin{aligned} C_1(S(L_n)) &= 4 \cdot (3 + 2) + 8 \cdot (2 + 1) + (6n - 20) \cdot (1 + 1) \\ &= 12n + 4 \end{aligned}$$

$$\begin{aligned} C_2(S(L_n)) &= 4 \cdot (3 \cdot 2) + 8 \cdot (2 \cdot 1) + (6n - 20) \cdot (1 \cdot 1) \\ &= 6n + 20. \end{aligned}$$

□

3. Conclusion

In this paper, we derived explicit formulae for the First Reverse Zagreb Beta Index and the Second Reverse Zagreb Index of the tadpole graph, wheel graph, ladder graph, and their line graphs. The computations were performed by partitioning the edge sets according to the reverse vertex degrees of their end vertices, leading to simple and systematic derivations of the required indices. The obtained closed-form expressions provide an efficient approach for computing the First Reverse Zagreb Beta Index and the Second Reverse Zagreb Index and enhance the theoretical understanding of reverse Zagreb indices in graph theory and mathematical chemistry. Moreover, the results presented in this paper may serve as a basis for further investigations of these indices for other graph classes, graph operations, and molecular structures in future research.

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