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The Third Leap Zagreb Index of Some Graph Operations

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Abstract: Recently introducing leap Zagreb indices are a generalization of classical Zagreb indices of chemical graph theory. The third leap Zagreb index is equal to the sum of products of first and second degrees of vertices of G, where the first and second degrees of a vertex v in a graph G are equal to the number of their first and second neighbors and denoted by $d(v/G)$ and $d_2(v/G)$, respectively. In this paper, exact expression for third leap Zagreb index of some graph operations will be presented.

Key Words: Distance-degrees (of vertices), third leap Zagreb index, graph operations.

AMS(2010): 05C07, 05C12, 05C76.

§1. Introduction and Preliminaries

In this paper, we are concerned with simple graphs, i.e., finite graphs having no loops, multiple and directed edges. Let $G = (V, E)$ be such a graph with vertex set $V(G)$ and edges set $E(G)$. As usual, we denote by $n = |V|$ and $m = |E|$ to the number of vertices and edges in a graph G, respectively. The distance $d_G(u, v)$ between any two vertices u and v of a graph G is equal to the length of (number of edges in) a shortest path connecting them. For a vertex $v \in V(G)$ and a positive integer k, the open k-neighborhood of v in a graph G is denoted by $N_k(v/G)$ and is defined as $N_k(v/G) = \{u \in V(G) : d_G(u, v) = k\}$. The k-distance degree of a vertex v in G is denoted by $d_k(v/G)$ (or simply $d_k(v)$, if no misunderstanding) and is defined as the number of k-neighbors of the vertex v in G, i.e., $d_k(v/G) = |N_k(v/G)|$. It is clearly that $d_1(v/G) = d(v/G)$ for every $v \in V(G)$.

The complement $\overline{G}$ of a graph G is a graph with vertex set $V(G)$ and two vertices of $\overline{G}$ are adjacent if and only if they are not adjacent in G. For a vertex v of G, the eccentricity $e(v) = \max\{d_G(v, u) : u \in V(G)\}$. The diameter of G is $diam(G) = \max\{e(v) : v \in V(G)\}$ and the radius of G is $rad(G) = \min\{e(v) : v \in V(G)\}$. Let $H \subseteq V(G)$ be any subset of vertices of G. Then the induced subgraph $\langle H\rangle$ of G is the graph whose vertex set is H and whose edge set consists of all of the edges in $E(G)$ that have both endpoints in H. A graph G is called F-free graph if no induced subgraph of G is isomorphic to F.

We follow [9] for unexplained graph theoretic terminologies and notations.

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In the interdisciplinary area where chemistry, physics and mathematics meet, molecular graph based structure descriptors, usually referred to as topological indices, are of significant importance. A topological index of a graph is a graph invariant number calculated from a graph representing a molecule. Among the most important such structure descriptors are the classical first and second Zagreb indices, which introduced, more than forty four years ago, by Gutman and Trinajestic [8], in 1972, and elaborated in [7]. They are defined as:

$$M_1(G) = \sum_{v \in V(G)} d_1^2(v/G) \qquad \text{and} \qquad M_2(G) = \sum_{uv \in E(G)} d_1(u/G) d_1(v/G).$$

For properties of the two Zagreb indices see [5, 7, 13, 18] for details of the theory of Zagreb indices see the survey [4] and the references cited therein. Recently the eccentric harmonic index is established as an eccentric version of the harmonic index, which has a huge area of applications, for more details see [14,17]. After most of the results on Zagreb indices were established, the inevitable occurred, their various modifications have been proposed, thus opening the possibility to do analogous research and publish numerous additional papers. For these modifications see the recent survey [6].

In (2017), Naji et al. [11] have been introduced a new distance-degree-based topological indices conceived depending on the second degrees of vertices, and are so-called leap Zagreb indices of a graph G and are defined as

$$\begin{aligned} LM_1(G) &= \sum_{v \in V(G)} d_2^2(v/G), \\ LM_2(G) &= \sum_{uv \in E(G)} d_2(u/G) d_2(v/G), \\ LM_3(G) &= \sum_{v \in V(G)} d(v/G) d_2(v/G). \end{aligned}$$

The leap Zagreb indices have several chemical applications. Surprisingly, the first leap Zagreb index has very good correlation with physical properties of chemical compounds like boiling point, entropy, DHVAP, HVAP and accentric factor [3].

In a later work [12], the first leap Zagreb index of graph operations was studied. In [2], the expressions for these three leap Zagreb indices of generalized xyz point line transformation graphs $T^{xyz}(G)$, when $z = 1$ are obtained. The authors in [15], generalized the results of [11], pertaining to trees and unicyclic graphs. They determined upper and lower bounds on leap Zagreb indices and characterized the extremal graphs. Leap Zagreb indices are considered in a recent survey [6].

In this paper, we present the exact expressions for the third leap Zagreb index of some graph operations containing cartesian product, composition, disjunction, symmetric difference and corona product of graphs. The following fundamental results which will be required for many of our arguments in this paper are found in Yamaguchi [19] and Soner and Naji [16].

Theorem 1.1([16,19]) *Let G be a connected graph with n vertices and m edges. Then*

$$d_2(v/G) \leq (\sum_{u\in N_1(v/G)} d_1(u/G)) - d_1(v/G).$$

and equality holds if and only if G is a $\{C_3, C_4\}$-free graph.

§2. Main Results

2.1 Cartesian Product

Definition 2.1([10]) *For given graphs G and H their cartesian product, denoted $G\Box H$, is defined as the graph on the vertex set $V(G)\times V(H)$, and vertices $u=(u_1,u_2)$ and $v=(v_1,v_2)$ of $V(G)\times V(H)$ are connected by an edge if and only if either ($u_1=v_1$ and $u_2v_2\in E(H)$) or ($u_2=v_2$ and $u_1v_1\in E(G)$).*

It is a well known fact that the cartesian product of graphs is commutative and associative up to isomorphism. $|V(G\Box H)| = |V(G)||V(H)|$, the distance between any two vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ in $G\Box H$ is given by

$$d_{G\Box H}(u,v) = d_G(u_1,v_1) + d_H(u_2,v_2).$$

Lemma 2.2([12]) *Let G and H be connected graphs of orders n_1 and n_2, respectively. Then for any vertex $(u,v)\in V(G\Box H)$,*

(1) $d_1((u,v)/G\Box H) = d_1(u/G) + d_1(v/H)$;

(2) $d_2((u,v)/G\Box H) = d_2(u/G) + d_1(u/G)d_1(v/H) + d_2(v/H)$.

Theorem 2.3 *Let G and H be two nontrivial connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively. Then*

$$\begin{aligned} LM_3(G\Box H) &= n_2LM_3(G) + 2m_2(M_1(G) \\ &\quad + \sum_{u\in V(G)} d_2(u/G)) + n_1LM_3(H) + 2m_1(M_1(H) + \sum_{v\in V(H)} d_2(v/H)). \end{aligned}$$

Proof Let G and H be two nontrivial connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively. Then by Lemma 2.2, we obtain

$$\begin{aligned} LM_3(G\Box H) &= \sum_{(u,v)\in V(G\Box H)} d_1((u,v)/G\Box H)d_2((u,v)/G\Box H) \\ &= \sum_{u\in V(G)}\sum_{v\in V(H)} \Big[(d_1(u/G)+d_1(v/H))(d_2(u/G)+d_1(u/G)d_1(v/H)+d_2(v/H))\Big] \end{aligned}$$

$$
\begin{aligned}
&= \sum_{u\in V(G)}\sum_{v\in V(H)}\Big[(d_1(u/G)d_2(u/G)+d_1^2(u/G)d_1(v/H)+d_1(u/G)d_2(v/H)\\
&\quad + d_2(u/G)d_1(v/H)+d_1(u/G)d_1^2(v/H)+d_1(v/H)d_2(v/H))\Big]\\
&= \sum_{u\in V(G)}\Big[n_2d_1(u/G)d_2(u/G)+2m_2d_1^2(u/G)+d_1(u/G)\sum_{v\in V(H)}d_2(v/H)\\
&\quad + 2m_2d_2(u/G)+M_1(H)d_1(u/G)+LM_3(H)\Big]\\
&= n_2LM_3(G)+2m_2M_1(G)+2m_1\sum_{v\in V(H)}d_2(v/H)+2m_2\sum_{u\in V(G)}d_2(u/G)\\
&\quad + 2m_1M_1(H)+n_1LM_3(H)\\
&= n_2LM_3(G)+2m_2\Big(M_1(G)+\sum_{u\in V(G)}d_2(u/G)\Big)+n_1LM_3(H)\\
&\quad + 2m_1\Big(M_1(H)+\sum_{v\in V(H)}d_2(v/H)\Big).
\end{aligned}
$$

This completes the proof. □

From Theorem 1.1, the following result follows.

Corollary 2.4 *If G and H are nontrivial connected (C_3, C_4)-free graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively. Then*

$$LM_3(G\Box H) = n_2LM_3(G)+4m_2M_1(G)+n_1LM_3(H)+4m_1M_1(H)-8m_1m_2.$$

2.2 Composition

Definition 2.5([10]) *The composition $G[H]$ of graphs G and H with disjoint vertex sets and edge sets is a graph on vertex set $V(G)\times V(H)$ in which (u_1,v_1) is adjacent with (u_2,v_2) whenever [u_1 is adjacent with u_2] or [$u_1=u_2$ and v_1 is adjacent with v_2].*

The composition is not commutative. The easiest way to visualize the composition $G[H]$ is to expand each vertex of G into a copy of H, with each edge of G replaced by the set of all possible edges between the corresponding copies of H. Hence, by letting $\mathfrak{N}_1 = |E(G[H])|$, then

$$\mathfrak{N}_1 = n_1m_2 + n_2^2m_1. \tag{1}$$

Lemma 2.6([12]) *Let G and H be two graphs with disjoint vertex sets with n_1 and n_2 vertices and edges sets with m_1 and m_2 edges, respectively. Then*

(1) it $d_1((u,v)/G[H]) = n_2d_1(u/G)+d_1(v/H)$;

(2) $d_2((u,v)/G[H])) = n_2d_2(u/G)+d_1(v/\overline{H})$.

Theorem 2.7 *Let G and H be two graphs with disjoint vertex sets with n_1 and n_2 vertices and* *edges sets with m_1 and m_2 edges, respectively. Then*

$$\begin{aligned} LM_3(G[H]) &= n_2^3 LM_3(G) - n_1 M_1(H) \\ &\quad -4n_2 m_1 m_2 + 2\mathfrak{N}_1(n_2-1) + 2n_2 m_2 \sum_{u\in V(G)} d_2(u/G). \end{aligned}$$

Proof Let G and H be two graphs with disjoint vertex sets with n_1 and n_2 vertices and edges sets with m_1 and m_2 edges, respectively. Then by Lemma 2.6, we obtain

$$\begin{aligned} LM_3(G[H]) &= \sum_{(u,v)\in V(G\Box H)} d_1((u,v)/G[H]) d_2((u,v)/G[H]) \\ &= \sum_{v\in V(H)} \sum_{u\in V(G)} \Big[\Big(n_2 d_1(u/G) + d_1(v/H)\Big)\Big(n_2 d_2(u/G) + d_1(v/\overline{H})\Big)\Big] \\ &= \sum_{v\in V(H)} \sum_{u\in V(G)} \Big[n_2^2 d_1(u/G) d_2(u/G) + n_2 d_1(u/G) d_1(v/\overline{H}) + n_2 d_2(u/G) d_1(v/H) \\ &\quad + d_1(v/H) d_1(v/\overline{H})\Big] \\ &= \sum_{v\in V(H)} \Big[n_2^2 LM_3(G) + 2n_2 m_1 d_1(v/\overline{H}) + n_2 d_1(v/H) \sum_{u\in V(G)} d_2(u/G) \\ &\quad + n_1 d_1(v/H) d_1(v/\overline{H})\Big] \end{aligned}$$

$$\begin{aligned} LM_3(G[H]) &= \sum_{v\in V(H)} \Big[n_2^2 LM_3(G) + 2n_2 m_1 (n_2 - 1 - d_1(v/H)) + n_2 d_1(v/H) \sum_{u\in V(G)} d_2(u/G) \\ &\quad + n_1 d_1(v/H)(n_2 - 1 - d_1(v/H))\Big] \\ &= n_2^3 LM_3(G) + 2n_2 m_1 (n_2(n_2-1) - 2m_2) + 2n_2 m_2 \sum_{u\in V(G)} d_2(u/G) \\ &\quad + 2m_2 n_1 (n_2 - 1) - n_1 M_1(H)\Big] \\ &= n_2^3 LM_3(G) - n_1 M_1(H) + 2n_2^2 m_1 (n_2 - 1) - 4n_2 m_1 m_2 \\ &\quad + 2n_1 m_2 (n_2 - 1) + 2n_2 m_2 \sum_{u\in V(G)} d_2(u/G). \end{aligned}$$

By using equation 1, we get

$$\begin{aligned} LM_3(G[H]) &= n_2^3 LM_3(G) - n_1 M_1(H) \\ &\quad -4n_2 m_1 m_2 + 2\mathfrak{N}_1(n_2-1) + 2n_2 m_2 \sum_{u\in V(G)} d_2(u/G). \end{aligned}$$

This completes the proof. □

From Theorem 1.1, the following result follows.

Corollary 2.8 *If G and H are nontrivial connected (C_3, C_4)-free graphs with n_1, n_2 vertices* *and m_1, m_2 edges, respectively. Then,*

$$\begin{aligned} LM_3(G[H]) &= n_2^3 LM_3(G) + 2n_2m_2M_1(G) \\ &\quad -n_1M_1(H) + 2n_2^2m_1(n_2-1) + 2n_1m_2(n_2-1) - 8n_2m_1m_2. \end{aligned}$$

2.3 Disjunction

Definition 2.9([10]) *The disjunction $G \vee H$ of two graphs G and H with disjoint vertex sets and edge sets is the graph with vertex set $V(G) \times V(H)$ in which (u_1, v_1) is adjacent with (u_2, v_2) whenever u_1 is adjacent with u_2 in G or v_1 is adjacent with v_2 in H.*

The disjunction is commutative and the number of edges of $G \vee H$ is $\mathfrak{M}_1$ ([1]) and equal to

$$\mathfrak{M}_1 = n_1^2 m_2 + n_2^2 m_1 - 2m_1m_2. \tag{2}$$

Lemma 2.10([12]) *Let G and H be two graphs with n_1 and n_2 vertices and m_1 and m_2 edges, respectively. Then,*

(1) $d_1((u,v)/G \vee H) = n_2d_1(u/G) + n_1d_1(v/H) - d_1(u/G)d_1(v/H)$;
(2) $d_2((u,v)/G \vee H) = (n_1n_2 - 1) - n_2d_1(u/G) - n_1d_1(v/H) + d_1(u/G)d_1(v/H)$.

Theorem 2.11 *Let G and H be two graphs with n_1 and n_2 vertices and m_1 and m_2 edges, respectively, such that G or H not a complete graph. Then,*

$$\begin{aligned} LM_3(G \vee H) &= (4n_2m_2 - n_2^3)M_1(G) + (4n_1m_1 - n_1^3)M_1(H) \\ &\quad -M_1(G)M_1(H) + 2\mathfrak{M}_1(n_1n_2 - 1) - 2m_1m_2(4n_1n_2 - 1). \end{aligned}$$

Proof Let G and H be two graphs with n_1 and n_2 vertices and m_1 and m_2 edges, respectively, such that G or H not a complete graph. Then from Lemma 2.10, we get

$$\begin{aligned} LM_3(G \vee H) = &\sum_{(u,v)\in V(G\vee H)} d_1((u,v)/G \vee H)d_2((u,v)/G \vee H) \\ &= \sum_{v\in V(H)} \sum_{u\in V(G)} \Big[n_2(n_1n_2-1)d_1(u/G) - n_2^2d_1^2(u/G) - n_1n_2d_1(u/G)d_1(v/H) \\ &\quad + n_2d_1^2(u/G)d_1(v/H) + n_1(n_1n_2-1)d_1(v/H) - n_1n_2d_1(u/G)d_1(v/H) \\ &\quad - n_1^2d_1^2(v/H) + n_1d_1(u/G)d_1^2(v/H) - (n_1n_2-1)d_1(u/G)d_1(v/H) \\ &\quad + n_2d_1^2(u/G)d_1(v/H) + n_1d_1(u/G)d_1^2(v/H) - d_1^2(u/G)d_1^2(v/H) \Big] \\ &= 2m_1n_2^2(n_1n_2-1) - n_2^3M_1(G) - 4n_1n_2m_1m_2 + 2m_2n_2M_1(G) \\ &\quad + 2m_2n_1^2(n_1n_2-1) - 4n_1n_2m_1m_2 - n_1^3M_1(H) + 2m_1n_1M_1(H) \\ &\quad - 4m_1m_2(n_1n_2-1) + 2n_2m_2M_1(G) + 2n_1m_1M_1(H) - M_1(G)M_1(H) \\ &= (4n_2m_2 - n_2^3)M_1(G) + (4n_1m_1 - n_1^3)M_1(H) - M_1(G)M_1(H) \\ &\quad + 2(n_1n_2-1)(n_1^2m_2 + n_2^2m_1) - 4m_1m_2(3n_1n_2-1). \end{aligned}$$

By using equation 2, we get

$$\begin{aligned} LM_3(G\vee H) &= (4n_2m_2-n_2^3)M_1(G)+(4n_1m_1-n_1^3)M_1(H) \\ &\quad -M_1(G)M_1(H)+2\mathfrak{M}_1(n_1n_2-1)-2m_1m_2(4n_1n_2-1). \end{aligned}$$

This completes the proof. □

2.4 Symmetric Difference

Definition 2.12([10]) *The symmetric difference $G\oplus H$ of two graphs G and H with disjoint vertex sets and edge sets is the graph with vertex set $V(G)\times V(H)$ in which (u_1,v_1) is adjacent with (u_2,v_2) whenever u_1 is adjacent with u_2 in G or v_1 is adjacent with v_2 in H but not both.*

The symmetric difference is commutative and the number of edges of $G\oplus H$ is $\mathfrak{M}_2$ ([1]) and equal to

$$\mathfrak{M}_2 = n_1^2m_2+n_2^2m_1-4m_1m_2. \tag{3}$$

Lemma 2.13([12]) *Let G and H be two graphs with n_1 and n_2 vertices and m_1 and m_2 edges, respectively. Then,*

(1) $d_1((u,v)/G\oplus H)=n_2d_1(u/G)+n_1d_1(v/H)-2d_1(u/G)d_1(v/H)$;

(2) $d_2((u,v)/G\oplus H)=(n_1n_2-1)-n_2d_1(u/G)-n_1d_1(v/H)+2d_1(u/G)d_1(v/H)$.

Theorem 2.14 *Let G and H be two graphs with n_1 and n_2 vertices and m_1 and m_2 edges, respectively, such that G or H not a complete graph. Then,*

$$\begin{aligned} LM_1(G\oplus H) &= (8n_2m_2-n_2^3)M_1(G) \\ &\quad +(8n_1m_1-n_1^3)M_1(H)-4M_1(G)M_1(H)+2(n_1n_2-1)(\mathfrak{M}_2-4m_1m_2). \end{aligned}$$

Proof The proof is similar to the proof of Theorem 2.11. □

2.5 Corona Product

Definition 2.15([10]) *Let G and H be two graphs on disjoint vertex sets with n_1 and n_2 vertices, respectively. The corona $G\circ H$ of G and H is defined as the graph obtained by taking one copy of G and n_1 copies of H, and then joining the i^{th} vertex of G to every vertex in the i^{th} copy of H.*

It is clear from the definition of $G\circ H$ that $n=|V(G\circ H)|=n_1+n_1n_2$ and $m=|E(G\circ H)|=m_1+n_1(n_2+m_2)$, where m_1 and m_2 are the sizes of G and H, respectively. In the following results, H^j, for $1\le j\le n_1$, denotes the copy of a graph H which joining to a vertex v_j of a graph G. Note that in general this operation is not commutative.

Lemma 2.16([12]) *Let G and H be two graphs with n_1 and n_2 vertices and m_1 and m_2 edges, respectively. Assume that $1\le j\le n$, then,*

$$(1)\quad d_1(v/(G\circ H))=\begin{cases} d_1(v/G)+n_2, & if\ v\in V(G),\\ d_1(v/H)+1, & if\ v\in V(H).\end{cases};$$

$$(2)\quad d_2(v/(G\circ H))=\begin{cases} d_2(v/G)+n_2d_1(v/G), & if\ v\in V(G),\\ d_1(v_j/G)+n_2-1+d_1(v/H^j), & if\ v\in V(H^j).\end{cases}.$$

Theorem 2.17 *Let G and H be two graphs with n_1 and n_2 vertices and m_1 and m_2 edges, respectively. Assuming that $1\le j\le n$, then*

$$\begin{aligned} LM_3(G\circ H) &= LM_3(G)+n_1(M_1(G)-M_1(H))+2n_1n_2(m_1+m_2)\\ &\quad -4n_1m_2+2n_2m_1+n_1n_2(n_2-1)+4m_1m_2+n_1\sum_{v\in V(G)} d_2(v/G).\end{aligned}$$

Proof Let G and H be two graphs with n_1 and n_2 vertices and m_1 and m_2 edges, respectively. Assuming that $1\le j\le n$, then by Lemma 2.16 we get

$$\begin{aligned} LM_3(G\circ H) &= \sum_{v\in V(G\circ H)} d_1(v/G\circ H)d_2(v/G\circ H)\\ &= \sum_{v\in V(G)} d_1(v/G\circ H)d_2(v/G\circ H)+\sum_{j=1}^{n_1}\sum_{v\in V(H^j)} d_1(v/G\circ H)d_2(v/G\circ H)\end{aligned}$$

$$\begin{aligned} LM_3(G\circ H) &= \sum_{v\in V(G)} \big[(d_1(v/G)+n_2)(d_2(v/G)+n_2d_1(v/G))\big]\\ &\quad +\sum_{j=1}^{n_1}\sum_{v\in V(H^j)} \big[(d_1(v/H)+1)(d_1(v_j/G)+n_2-1-d_1(v/H^j))\big]\\ &= \sum_{v\in V(G)} \big[d_1(v/G)d_2(v/G)+n_2d_1(v/G)^2+n_1(d_2(v/G)+n_1n_2d_1(v/G)\big]\\ &\quad +\sum_{j=1}^{n_1}\sum_{v\in V(H^j)} \big[d_1(v/H)d_1(v_j/G)+(n_2-1)d_1(v/H)+d_1(v/H^2)+d_1(v_j/G)\\ &\quad +n_2-1-d_1(v/H)\big]\\ &= LM_3(G)+n_1M_1(G)+n_1\sum_{v\in V(G)} d_2(v/G)+2n_1n_2m_1+2m_2(n_2-1)\\ &\quad +\sum_{j=1}^{n_1}\big[2m_2d_1(v_j/G)-M_1(H)+n_2d_2(v_j/G)+n_2(n_2-1)-2m_2\big]\\ &= LM_3(G)+n_1M_1(G)+n_1\sum_{v\in V(G)} d_2(v/G)+2n_1n_2m_1+2n_1m_2(n_2-1)\\ &\quad -n_1M_1(H)+2n_2m_1+n_1n_2(n_2-1)-2n_1m_2\\ &= LM_3(G)+n_1(M_1(G)-M_1(H))+2n_1n_2(m_1+m_2)-4n_1m_2+2n_2m_1\\ &\quad +n_1n_2(n_2-1)+4m_1m_2+n_1\sum_{v\in V(G)} d_2(v/G). \qquad\square\end{aligned}$$

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