Nano-Zagreb Index and Multiplicative Nano-Zagreb Index of Some Graph Operations

Akbar Jahanbani and Hajar Shooshtary

***Abstract*—Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The Nano-Zagreb and multiplicative Nano-Zagreb indices of G are $\mathscr{N}Z(G) = \sum_{uv\in E(G)}(d^2(u) - d^2(v))$ and $\mathscr{N}^*Z(G) = \prod_{uv\in E(G)}(d^2(u) - d^2(v))$, respectively, where $d(v)$ is the degree of the vertex v. In this paper, we define two types of Zagreb indices based on degrees of vertices. Also the Nano-Zagreb index and multiplicative Nano-Zagreb index of the Cartesian product, symmetric difference, composition and disjunction of graphs are computed.**

***Index Terms*—Graph operations, Nano-Zagreb index, Multiplicative Nano-Zagreb index, Zagreb index.**

I. Introduction

THROUGHOUT this paper, all graphs are simple. Let G be a (molecular) graph with vertex set $V(G) = \{v_1, v_2, ..., v_n\}$ and edge set $E(G)$. Denote by uv the edge of G, connecting the vertices u and v. For any vertex u of G, the degree of u is denoted by $d(u)$. We consider only simple connected graphs, i.e. connected graphs without loops and multiple edges. Suppose Σ denotes the class of all graphs, then a function $\Lambda : \Sigma \to R^+$ is called a topological index if $G \cong H$ implies $\Lambda(G) = \Lambda(H)$. Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, the *Wiener* index, and used it to determine physical properties of types of alkanes known as paraffin. The **Cartesian product** $G_1 \times G_2$ of graphs G_1 and G_2 has the vertex set $V(G_1 \times G_2) = V(G_1) \times V(G_2)$ and $(a,x)(b,y)$ is an edge of $G_1 \times G_2$ if $a = b$ and $xy \in E(G_1)$, or $ab \in E(G_1)$ and $x = y$. If (a,x) is a vertex of $G_1 \times G_2$, then

$$d_{G_1\times G_2}((a,x)) = d_{G_1}(a) + d_{G_2}(x).$$

The **corona product** $G_1 \circ G_2$ is defined as the graph obtained from G_1 and G_2 by taking one copy of G_1 and $|V(G_1)|$ copies of G_2 and then by joining with an edge each vertex of the i^{th} copy of G_2 which is named (G_2, i) with the i^{th} vertex of G_1 for $i = 1, 2..., |V(G_1)|$. If u is a vertex of $G_1 \circ G_2$, then

$$d_{G_1\circ G_2}(u) = \begin{cases} d_{G_1}(u) + |V(G_2)| & \text{if} \quad u \in V(G_1) \\ d_{G_2}(u) + 1 & \text{if} \quad u \in (G_2, i). \end{cases}$$

The **tensor product** $G_1 \otimes G_2$ of two graphs G_1 and G_2 is the graph with vertex set $V(G_1) \times V(G_2)$ and $E(G_1 \otimes G_2) = \{(u_1,u_2)(v_1,v_2) \mid u_1v_1 \in E(G_1), u_2v_2 \in E(G_2)\}$.

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The **tensor product** $G_1 \otimes G_2$ of graphs G_1 and G_2 is the graph with a vertex set $V(G_1) \times V(G_2)$ and (u_i, v_j) is adjacent to (u_k, v_l) whenever $u_iu_k \in E(G_1)$ or $v_jv_l \in E(G_2)$. The degree of a vertex (u_i, v_j) of $G_1 \otimes G_2$ is given by

$$d_{G_1\otimes G_2}(u_i,v_j) = n_2d_{G_1}(u_i) + n_1d_{G_2}(v_j) - d_{G_1}(u_i)d_{G_2}(v_j).$$

For two given graphs G_1 and G_2 the **disjunction** $G_1 \vee G_2$ is the graph with vertex set $V(G_1) \times V(G_2)$ in which $(u,v),(x,y) \in G_1 \times G_2$ are adjacent whenever u is adjacent with x in G_1 or v is adjacent with y in G_2. If $|V(G_1)| = n_1, |E(G_1)| = m_1, |V(G_2)| = n_2, |E(G_2)| = m_2$, the degree of a vertex (u,v) of $G_1 \vee G_2$ is given by

$$d_{G_1\vee G_2}(u,v) = n_2d_{G_1}(u) + n_1d_{G_2}(v) - d_{G_1}(u)d_{G_2}(v).$$

The **symmetric difference** $G_1 \oplus G_2$ of two graphs G_1 and G_2 is the graph with vertex set $V(G_1) \times V(G_2)$ in which $(u,v),(x,y) \in G_1 \times G_2$ are adjacent whenever u is adjacent with x in G or v is adjacent with y in G_2, but not both. It follows from the definition that the degree of a vertex (u,v) of $G_1 \oplus G_2$ is given by

$$d_{G_1\oplus G_2}(u,v) = n_2d_{G_1}(u) + n_1d_{G_2}(v) - 2d_{G_1}(u)d_{G_2}(v).$$

The **join** $G = G_1 + G_2$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph union $G_1 \cup G_2$ together with all the edges joining V_1 and V_2. The **composition** $G = G_1[G_2]$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 such that $|V_1| = n_1, |V_2| = n_2$ and edge sets E_1 and E_2 such that $|E_1| = m_1$ and $|E_2| = m_2$ is the graph with vertex set $V_1 \times V_2$ and $u = (u_1,u_2)$ is adjacent with $v = (v_1,v_2)$ whenever u_1 is adjacent with v_1 or $u_1 = v_1$ and u_2 is adjacent with v_2. It follows from the definition for a vertex (u_1,u_2) of $G_1[G_2]$ is given by

$$d_{G_1[G_2]}(u_1,u_2) = n_2d_{G_1}(u_1) + d_{G_2}(u_2).$$

This paper is organized as follows. In Section 2, we present some previously known results. In Section 3, we introduce and investigate the Nano-Zagreb index of a graph also the Cartesian product, composition, join and disjunction of graphs are computed. Moreover, we apply some of our results to compute it. In Section 4, we define the multiplicative Nano-Zagreb index of a graph also we give some upper bounds for various graph operations such as corona product, Cartesian product, composition, disjunction. Moreover, computations are conducted for some well-known graphs.

II. Preliminaries and Known Results

In this section, we shall list some previously known results that will be needed in the next sections. In mathematical chemistry, there is a large number of topological indices of the form

$$TI = TI(G) = \sum_{v_i,v_j \in E(G)} \mathbb{F}(d_i, d_j)$$

and

$$TI = TI(G) = \prod_{v_i,v_j \in E(G)} \mathscr{F}(d_i, d_j).$$

In 1972, within a study of the structure-dependency of total π-electron energy ($\mathscr{E}$), it was shown that $\mathscr{E}$ depends on the sum of squares of the vertex degrees of the molecular graph (later named first Zagreb index), and thus provides a measure of the branching of the carbon-atom skeleton. In the same paper, also the sum of cubes of degrees of vertices of the molecular graph was shown to influence $\mathscr{E}$, but this topological index was never again investigated and was left to oblivion. We now establish a few basic properties of this Nano-Zagreb index and multiplicative Nano-Zagreb index. The *Zagreb* indices are widely studied degree-based topological indices and were introduced by *Gutman* and *Trinajstić* [1] in 1972. In Chemical Science, the physico-chemical properties of chemical compounds are often modeled by means of molecular graph based structure descriptors, which are referred to as topological indices. Recently, Todeschini et al. [2], [3], have proposed the multiplicative variants of ordinary Zagreb indices, which are defined as follows:

$$\prod_1 = \prod_1(G) = \prod_{u \in V(G)} d_G(u)^2,$$
$$\prod_2 = \prod_2(G) = \prod_{uv \in E(G)} d_G(u) d_G(v).$$

Mathematical properties and applications of multiplicative Zagreb indices are reported in [4], [5], [2], [3]. Mathematical properties and applications of multiplicative sum Zagreb indices are reported in [6].

III. Nano-Zagreb index of some Graph Operations

In this section, we define the Nano-Zagreb index of a graph also Nano-Zagreb index of the Cartesian product, composition, symmetric difference and disjunction of graphs are computed. Moreover, we apply some of our results to compute the Nano-Zagreb index.

A topological index is a graph invariant applicable in chemistry. The Wiener index is the first topological index introduced by chemist Harold Wiener [7], [8], [9], [10]. There are some topological indices based on degrees such as the first and second Zagreb indices of molecular graphs. There are some topological indices [11], [7] based on degrees such as: the first M_1, the second M_2 and third Zagreb index M_3 defined as respectively

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2, \quad M_2(G) = \sum_{uv \in E(G)} \Big(d_G(u) d_G(v) \Big),$$

$$M_3(G) = \sum_{uv \in E(G)} \Big| d_G(u) - d_G(v) \Big|.$$

We now define a new graph invariant, named the Nano-Zagreb index. This new graph invariant is denoted by $\mathscr{N}Z(G)$ and defined as follows: The Nano-Zagreb index of a graph G is defined as

$$\mathscr{N}Z(G) = \sum_{uv \in E(G)} (d_G^2(u) - d_G^2(v)).$$

Throughout this paper, $d_G(u) \geqslant d_G(v)$. Recently, there was a vast research on comparing *Zagreb* indices see [12], [13], [14]. A survey on the first *Zagreb* index can be seen in [15]. Usage of topological indices in *chemistry* began in 1947 when *chemist Harold Wiener* developed the most widely known topological descriptor, the *Wiener* index, and used it to determine physical properties of types of *alkanes* known as paraffin. We begin this section with Propositions as follows:

Proposition 3.1: Let G be a regular graph. Then $\mathscr{N}Z(G) = 0$.

Therefore, by Proposition 3.1, we have the following propositions.

Proposition 3.2: Let C_n be a cycle with $n \geqslant 3$ vertices. Then $\mathscr{N}Z(C_n) = 0$.

Proposition 3.3: Let K_n be a complete graph with n vertices. Then $\mathscr{N}Z(K_n) = 0$.

Proposition 3.4: Let $K_{n,n}$ be a complete bipartite graph with $2n$ vertices. Then $\mathscr{N}Z(K_{n,n}) = 0$.

Now, we compute the Nano-Zagreb index for a complete bipartite graph.

Proposition 3.5: Let $K_{n,m}$ be a complete bipartite graph with $1 < m < n$ vertices. Then $\mathscr{N}Z(K_{n,m}) = mn(m^2 - n^2)$.

Proof: Let $K_{n,m}$ be a complete bipartite graph with $1 < m < n$ vertices and nm edges. Consider.

$$\begin{aligned} \mathscr{N}Z(K_{n,m}) &= \sum_{uv \in E(K_{n,m})} [d^2(u) - d^2(v)] \\ &= \underbrace{(m^2 - n^2) + (m^2 - n^2) + \ldots + (m^2 - n^2)}_{mn} \\ &= mn(m^2 - n^2). \end{aligned}$$

■

Proposition 3.6: Let P_n be a path with $n > 3$ vertices. Then $\mathscr{N}Z(P_n) = 6$.

Proof: Let P_n be a path with $n > 3$ vertices. Consider

$$\mathscr{N}Z(P_n) = \sum_{uv \in E(P_n)} [d^2(u) - d^2(v)]^n = 3 + \underbrace{0 + 0 \ldots + 0 \times 0}_{n-2} + 3 = 6$$

. ■

Proposition 3.7: Let W_n be a wheel with $n > 4$ vertices. Then

$$\mathscr{N}Z(W_n) = (n-1)((n-1)^2 - 9).$$

Proof: Let W_n be a wheel with $n > 4$ vertices. Consider

$$\begin{aligned} \mathscr{N}Z(W_n) &= \sum_{uv \in E(W_n)} [d^2(u) - d^2(v)] \\ &= \underbrace{(3^2 - 3^2) + (3^2 - 3^2) + \ldots (3^2 - 3^2)}_{n-1} + \end{aligned}$$

$$\underbrace{((n-1)^2-3^2)+((n-1)^2-3^2)+\ldots((n-1)^2-3^2)}_{n-1}$$
$$=(n-1)((n-1)^2-3^2).$$

■

Lemma 3.8: [16] Let G_1 and G_2 be two connected graphs, then we have:

(a)

$$\begin{aligned}|V(G_1\times G_2)| &= |V(G_1\vee G_2)| = |V(G_1[G_2])|\\ &= |V(G_1\oplus G_2)| = |V(G_1)||V(G_2)|,\\ |E(G_1\times G_2)| &= |E(G_1)||V(G_2)|+|V(G_1)||E(G_2)|,\\ |E(G_1+G_2)| &= |E(G_1)|+|E(G_2)|+|V(G_1)V(G_2)|,\\ |E(G_1[G_2])| &= |E(G_1)||V(G_2)|^2+|E(G_1)||V(G_2)|,\\ |E(G_1\vee G_2)| &= |V(G_1)||V(G_2)|^2+|E(G_1)||V(G_1)|^2\\ &\quad -2|E(G_1)||E(G_2)|,\\ |E(G_1\oplus G_2)| &= |E(G_1)||V(G_2)|^2+|E(G_2)||V(G_1)|^2\\ &\quad -42|E(G_1)||E(G_2)|.\end{aligned}$$

(b) $G_1\times G_2$ is connected if and only if G_1 and G_2 are connected.
(c) If (a,b) is a vertex of $G_1\times G_2$, then $d_{G_1\times G_2}\big((a,b)\big)=d_{G_1}(a)+d_{G_2}(b)$.
(d) If (a,b) is a vertex of $G_1[G_2]$ then $d_{G_1[G_2]}\big((a,b)\big)=|V(G_1)|d_{G_2}(a)+d_{G_2}(b)$.
(e) If (a,b) is a vertex of $G_1\oplus G_2$ or $G_1\otimes G_2$, we have:

$$\begin{aligned}d_{G_1\oplus G_2}\big((a,b)\big) &= |V(G_1)|d_{G_1}(a)+|V(G_1)|d_{G_2}(b)\\ &\quad -2d_{G_1}(a)d_{G_2}(b).\\ d_{G_1\otimes G_2}\big((a,b)\big) &= |V(G_2)|d_{G_1}(a)+|V(G_1)|d_{G_2}(b)\\ &\quad -d_{G_1}(a)d_{G_2}(b).\end{aligned}$$

(f) If u is a vertex of $G_1\vee G_2$ then we have:

$$d_{G_1\vee G_2}(u)=\begin{cases}d_{G_1}(u)+|V(G_2)| & \text{if} \quad u\in V(G_1)\\ d_{G_2}(u)+|V(G_1)| & \text{if} \quad u\in V(G_2).\end{cases}$$

Proof: The parts (a) and (b) are consequence of definitions and some famous results of the book of Imrich and Klavzar [16]. For the proof of (c-f) we refer to [17]. ■

Theorem 3.9: Let G_1 and G_2 be two graphs with n_1 and n_2 vertices, m_1 and m_2 edges respectively. Then

$$\mathcal{N}Z(G_1\times G_2)=n_1\Big(\mathcal{N}Z(G_2)+2M_3(G_2)\Big)+n_2\Big(\mathcal{N}Z(G_1)+2M_3(G_1)\Big).$$

Proof: From the definition of the Cartesian product of graphs, we have:

$$E(G_1\times G_2)=\{(a,x)(b,y): ab\in E(G_1), x=y \text{ or } xy\in E(G_2), a=b\}$$

therefore we can write:

$$\begin{aligned}&\mathcal{N}Z(G_1\times G_2)\\ &=\sum_{(ax)(by)\in E(G_1\times G_2)}[d_{G_1\times G_2}((a,x))]^2-[d_{G_1\times G_2}((b,y))]^2\\ &=\sum_{a\in V(G_1)}\sum_{(xy)\in E(G_2)}[d_{G_1}(a)+d_{G_2}(x)]^2-[d_{G_1}(a)+d_{G_2}(y)]^2\\ &+\sum_{x\in V(G_2)}\sum_{(ab)\in E(G_1)}[d_{G_2}(x)+d_{G_1}(a)]^2-[d_{G_2}(x)+d_{G_1}(b)]^2\\ &=\sum_{a\in V(G_1)}\sum_{(xy)\in E(G_2)}[d^2_{G_2}(x)-d^2_{G_2}(y)]+2d_{G_1}(a)\big(d_{G_2}(x)-d_{G_2}(y)\big)\\ &+\sum_{x\in V(G_2)}\sum_{(ab)\in E(G_1)}[d^2_{G_1}(a)-d^2_{G_1}(b)]+2d_{G_2}(x)\big(d_{G_1}(a)-d_{G_1}(b)\big)\\ &=n_1\Big(\mathcal{N}Z(G_2)+2M_3(G_2)\Big)+n_2\Big(\mathcal{N}Z(G_1)+2M_3(G_1)\Big).\end{aligned}$$

■

As an application of Theorem 3.9, we list explicit formulae for the third Zagreb index of the rectangular grid $P_r\times P_s$, C_4-nanotube $P_r\times C_q$ and C_4-nanotorus $P_r\times W_s$. The formulae follow from Theorem 3.9 by using the expressions [18],

$$M_1(P_n)=4n-6,$$
$$M_1(C_n)=4n.$$

Example 3.10: For any graphs $P_r\times P_s$, $P_r\times C_q$ and $P_r\times K_4$, we have the following results:

1) $\mathcal{N}Z(P_r\times P_s)=12(r+s), \quad r,s>3,$
2) $\mathcal{N}Z(P_r\times C_q)=6q,$
3) $\mathcal{N}Z(P_r\times K_4)=24.$

Theorem 3.11: Let G_1 and G_2 be two graphs with n_1 and n_2 vertices, m_1 and m_2 edges respectively. Then

$$\mathcal{N}Z(G_1[G_2])=[2n_2m_1M_3(G_2)+n_1\mathcal{N}Z(G_2)]+[2n_2m_2M_3(G_1)+n_2\mathcal{N}Z(G_1)].$$

Proof: From the definition of the composition $G_1[G_2]$ we have:

$$\begin{aligned}&\mathcal{N}Z(G_1[G_2])\\ &=\sum_{(u_iv_j)(u_pv_q)\in E(G_1[G_2])}[d_{G_1[G_2]}(u_i,v_j)]^2-[d_{G_1[G_2]}(u_p,v_q)]^2\\ &=\sum_{u_i\in V(G_1)}\sum_{(v_jv_q)\in E(G_2)}[d_{G_1}(u_i)n_2+d_{G_2}(v_j)]^2\\ &\quad -[d_{G_1}(u_i)n_2+d_{G_2}(v_q)]^2\\ &+\sum_{(u_iu_p)\in E(G_1)}\sum_{v_j\in V(G_2)}[d_{G_1}(u_i)n_2+d_{G_2}(v_j)]^2\\ &\quad -[d_{G_1}(u_p)n_2+d_{G_2}(v_j)]^2\\ &=\sum_{u_i\in V(G_1)}\sum_{(v_jv_q)\in E(G_2)}n_2d_{G_1}(u_i)[d_{G_2}(v_j)-d_{G_2}(v_q)]\\ &\quad +[d^2_{G_2}(v_j)-d^2_{G_2}(v_q)]\\ &+\sum_{(u_iu_p)\in E(G_1)}\sum_{v_j\in V(G_2)}n_2d_{G_2}(v_j)[d_{G_1}(u_i)-d_{G_1}(u_p)]\\ &\quad +n_2^2[d^2_{G_1}(u_i)-d^2_{G_1}(u_p)]\\ &=[2n_2m_1M_3(G_2)+n_1\mathcal{N}Z(G_2)]\\ &\quad +[2n_2m_2M_3(G_1)+n_2\mathcal{N}Z(G_1)].\end{aligned}$$

■

As an application of Theorem 3.11, we present formulae for the Nano-Zagreb index of the fence graph $C_q[P_r]$ and the closed fence graph $P_r[C_q]$.

Example 3.12: $(C_q[P_r]) = 6q, \quad (P_r[C_q]) = 6q.$

Theorem 3.13: Let G_1 and G_2 be two graphs with n_1 and n_2 vertices, m_1 and m_2 edges respectively. Then

$$\begin{aligned}\mathcal{N}Z(G_1 \circ G_2) = {} & \mathcal{N}Z(G_1) + 2n_2M_3(G_1) + n_1\mathcal{N}Z(G_2) \\ & - 2n_1M_3(G_2) + 2M_1(G_1)n_2 + n_1n_2^3 \\ & + 4n_2m_1 - 2M_1(G_2)n_1 - n_1n_2 - 4m_2n_1.\end{aligned}$$

Proof: Using the definition of the Nano-Zagreb index, we have

$$\begin{aligned}& \mathcal{N}Z(G_1 \circ G_2) \\ & = \sum_{uv \in (G_1 \circ G_2)} [d_{(G_1 \circ G_2)}(u)]^2 - [d_{(G_1 \circ G_2)}(v)]^2 \\ & + \sum_{uv \in E(G_2)} \sum_{i=1}^{n_1} [d^2_{(G_2)}(u) - d^2_{(G_2)}(v)] - 2[d_{(G_2)}(u) - d_{(G_2)}(v)] \\ & + \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [d^2_{(G_1)}(u) + n_2^2 + 2n_2d_{(G_1)}(u) - d^2_{(G_2)}(v) \\ & \quad - 1 - 2d_{(G_2)}(v)] \\ & = \mathcal{N}Z(G_1) + 2n_2M_3(G_1) + n_1\mathcal{N}Z(G_2) - 2n_1M_3(G_2) \\ & \quad + 2M_1(G_1)n_2 + n_1n_2^3 + 4n_2m_1 - 2M_1(G_2)n_1 - n_1n_2 \\ & \quad - 4m_2n_1.\end{aligned}$$

■

Example 3.14: $\mathcal{N}Z(P_r \circ C_q) = rq^3 - rq - 28q + 6.$

Theorem 3.15: Let G_1 and G_2 be two graphs with n_1 and n_2 vertices, m_1 and m_2 edges respectively. Then

$$\begin{aligned}\mathcal{N}Z(G_1 + G_2) = {} & \mathcal{N}Z(G_1) - 2n_2M_3(G_1) + \mathcal{N}Z(G_2) \\ & - 2n_1M_3(G_2) + n_2M_1(G_1) + n_2^3n_1 + 4n_2^2m_1 \\ & - n_1M_1(G_2) - n_1^3n_2 - 4n_1^2m_2.\end{aligned}$$

Proof: From the definition, we know that:

$$E(G_1 + G_2) = E(G_1) \cup E(G_2) \cup \{uv : u \in V(G_1), v \in V(G_2)\}.$$

So, we have:

$$\begin{aligned}\mathcal{N}Z(G_1 + G_2) & = \sum_{uv \in (G_1 + G_2)} [d_{(G_1+G_2)}(u)]^2 - [d_{(G_1+G_2)}(v)]^2 \\ & = \sum_{uv \in E(G_2)} [d_{(G_1+G_2)}(u)]^2 - [d_{(G_1+G_2)}(v)]^2 \\ & + \sum_{uv \in E(G_1)} [d_{(G_1+G_2)}(u)]^2 - [d_{(G_1+G_2)}(v)]^2 \\ & + \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [d_{(G_1+G_2)}(u)]^2 - [d_{(G_1+G_2)}(v)]^2.\end{aligned}$$

It is easy to see that:

$$\begin{aligned}& \sum_{uv \in E(G_1)} [d_{(G_1+G_2)}(u)]^2 - d_{(G_1+G_2)}(v)]^2 \\ & = \sum_{uv \in E(G_1)} [d^2_{(G_1)}(u) - d^2_{(G_1)}(v)] - 2n_2\big(d_{(G_1)}(u) - d_{(G_1)}(v)\big) \\ & = \mathcal{N}Z(G_1) - 2n_2M_3(G_1). \qquad (1)\end{aligned}$$

and similarly we have:

$$\begin{aligned}& \sum_{uv \in E(G_2)} [d_{(G_1+G_2)}(u) - d_{(G_1+G_2)}(v)]^2 \\ & = \sum_{uv \in E(G_2)} [d^2_{(G_2)}(u) - d^2_{(G_2)}(v)] - 2n_1\big(d_{(G_2)}(u) - d_{(G_2)}(v)\big) \\ & = \mathcal{N}Z(G_2) - 2n_1M_3(G_2). \qquad (2)\end{aligned}$$

Finally, we can write:

$$\begin{aligned}& \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [d_{(G_1+G_2)}(u)]^2 - [d_{(G_1+G_2)}(v)]^2 \\ & = \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [d_{(G_1)}(u) + n_2]^2 - [d_{(G_2)}(v) - n_1]^2 \\ & = \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \Big[d^2_{(G_1)}(u) + n_2^2 + 2n_2d_{(G_1)}(u) - d^2_{(G_2)}(v) \\ & \quad - n_1^2 - 2n_1d_{(G_2)}(v)\Big] \qquad (3) \\ & = n_2M_1(G_1) + n_2^3n_1 + 4n_2^2m_1 - n_1M_1(G_2) - n_1^3n_2 - 4n_1^2m_2. \qquad (4)\end{aligned}$$

Combining those three equations (1), (2), (4) will complete the proof. ■

Example 3.16: $\mathcal{N}Z(P_r + C_q) = q^3r - qr^3 - 4r^2q - 4q^2 + 4q^2r - 4qr + 36r - 48.4q^2 - qr - 2q - 2.$

Theorem 3.17: Let G_1 and G_2 be two graphs with n_1 and n_2 vertices, m_1 and m_2 edges respectively. Then

$$\begin{aligned}\mathcal{N}Z(G_1 \vee G_2) = {} & NZ(G_1) + 2n_2M_3(G_1) + NZ(G_2) + 2n_1M_3(G_2) \\ & + n_2M_1(G_1) + n_2^3n_1 + 4n_2m_1 - n_1M_1(G_2) - n_1^3n_2 \\ & - 4n_1m_2.\end{aligned}$$

Proof: By the definition of the Nano-Zagreb index and from the above partition of the edge set in $G_1 \vee G_2$, we have

$$\begin{aligned}& \mathcal{N}Z(G_1 \vee G_2) \\ & = \sum_{(u_iv_j)(u_pv_q) \in E(G_1 \vee G_2)} [d_{G_1 \vee G_2}(u_i, v_j)]^2 - [d_{G_1 \vee G_2}(u_p, v_q)]^2 \\ & = \sum_{(u_iu_p) \in E(G_1)} [\big(d_{G_1}(u_i) + n_2]^2 - [d_{G_1}(u_p) + n_2]^2 \\ & \sum_{(v_jv_q) \in E(G_2)} [(d_{G_2}(v_j) + n_1]^2 - [d_{G_2}(v_q) + n_1]^2 \\ & + \sum_{u_i \in V(G_1)} \sum_{v_j \in V(G_2)} [d_{G_1}(u_i) + n_2] - [d_{G_2}(v_j) + n_1]^2 \\ & = \sum_{(u_iu_p) \in E(G_1)} [d^2_{G_1}(u_i) - d^2_{G_1}(u_p)] + 2n_2[d_{G_1}(u_i) - d_{G_1}(u_p)] \\ & \sum_{(v_jv_q) \in E(G_2)} [d^2_{G_2}(v_j) - d^2_{G_2}(v_q)] + 2n_1[d_{G_2}(v_j) - d_{G_1}(v_q)] \\ & + \sum_{u_i \in V(G_1)} \sum_{v_j \in V(G_2)} [d^2_{G_1}(u_i) + n_2^2 + 2n_2d_{G_1}(u_i)] \\ & \quad - [d^2_{G_2}(v_j) + n_1^2 + 2n_1d_{G_1}(v_j)] \\ & = NZ(G_1) + 2n_2M_3(G_1) + NZ(G_2) + 2n_1M_3(G_2) \\ & + n_2M_1(G_1) + n_2^3n_1 + 4n_2m_1 - n_1M_1(G_2) - n_1^3n_2 - 4n_1m_2.\end{aligned}$$

■

Example 3.18: $\mathcal{N}Z(P_r \vee K_4) = 4r^3 - 36r + 34.$

IV. The Multiplicative Nano-Zagreb index of some Graph Operations

In this section, we define the multiplicative Nano-Zagreb index of a graph also we give some upper bounds for the multiplicative Nano-Zagreb index of various graph operations such as corona product, Cartesian product, composition, disjunction and symmetric difference. Moreover, computations are conducted for some well-known graphs. Eliasi et al. [4] considered a new multiplicative version of the first Zagreb index as

$$II_1^*(G) = \prod_{uv\in E(G)} [d_G(u) + d_G(v)].$$

Recently many other multiplicative indices and coindices of graphs were studied, for example, in [19], [20], [21]. In this paper, we initiate a study of the multiplicative Nano-Zagreb indices of graphs. We define the multiplicative Nano-Zagreb index of a graph G as follows

$$\mathcal{N}^*Z(G) = \prod_{uv\in E(G)} [d_G^2(u) - d_G^2(v)].$$

We begin this section with standard inequality as follows:

Lemma 4.1 (Arithmetic Mean-Geometric Mean Inequality): [22] Let $x_1, x_2, \dots, x_n$ be non-negative numbers. Then

$$\frac{x_1 + x_2 + \ldots + x_n}{n} \geqslant \sqrt[n]{x_1 x_2 \ldots x_n} \tag{5}$$

holds with equality if and only if all the x_k's are equal.

Proposition 4.2: Let G be a regular graph. Then $\mathcal{N}^*Z(G) = 0$.

Therefore, by Proposition 4.2 we have the following propositions.

Proposition 4.3: Let C_n be a cycle with $n \geqslant 3$ vertices. Then $\mathcal{N}^*Z(C_n) = 0$.

Proposition 4.4: Let K_n be a complete graph with n vertices. Then $\mathcal{N}^*Z(K_n) = 0$.

Proposition 4.5: Let $K_{n,n}$ be a complete bipartite graph with $2n$ vertices. Then $\mathcal{N}^*Z(K_{n,n}) = 0$.

Now, we compute the Multiplicative Nano-Zagreb index for a complete bipartite graph.

Proposition 4.6: Let $K_{n,m}$ be a complete bipartite graph with $m+n$ vertices. Then $\mathcal{N}^*Z(K_{n,m}) = [m^2 - n^2]^{mn}$.

Proof: Let $K_{n,m}$ be a complete bipartite graph with $m+n$ vertices and nm edges. Consider.

$$\begin{aligned}\mathcal{N}^*Z(K_{n,m}) &= \prod_{uv\in E(K_{n,m})} [d^2(u) - d^2(v)] \\ &= \underbrace{(m^2-n^2)\times\ldots\times(m^2-n^2)(m^2-n^2)}_{mn} \\ &= [m^2-n^2]^{mn}.\end{aligned}$$

■

Proposition 4.7: Let P_n be a path with $n > 3$ vertices. Then $\mathcal{N}^*Z(P_n) = 0$.

Proof: Let P_n be a path with $n > 3$ vertices. Consider

$$\begin{aligned}\mathcal{N}^*Z(P_n) &= \prod_{uv\in E(P_n)} [d^2(u) - d^2(v)] \\ &= 3\times\underbrace{0\times 0\ldots\times 0\times 0}_{n-2}\times 3 = 0.\end{aligned}$$

■

Proposition 4.8: Let W_n be a wheel with $n > 4$ vertices. Then $\mathcal{N}^*Z(W_n) = 0$.

Proof: Let W_n be a wheel with $n > 4$ vertices. Consider

$$\begin{aligned}&\mathcal{N}^*Z(W_n) \\ &= \prod_{uv\in E(W_n)} [d^2(u) - d^2(v)] \\ &= (3^2-3^2)\times(3^2-3^2)\times\ldots\times(3^2-3^2) \\ &\times\left((n-1)^2-3^2\right)\times\left((n-1)^2-3^2\right)\times\ldots\times\left((n-1)^2-3^2\right) = 0.\end{aligned}$$

■

Theorem 4.9: Let G_1 and G_2 be two graphs with n_1 and n_2 vertices, m_1 and m_2 edges respectively. Then

$$\begin{aligned}&\mathcal{N}^*Z(G_1\times G_2) \\ &\leqslant \left[\frac{n_1\mathcal{N}^*Z(G_2) + 4m_1 M_3(G_2)}{n_1 m_2}\right]^{n_1 m_2} \\ &\quad\times\left[\frac{n_2\mathcal{N}^*Z(G_1) + 4m_2 M_3(G_1)}{n_2 m_1}\right]^{n_2 m_1}.\end{aligned}$$

Proof: By the definition of the multiplicative Nano-Zagreb index and from the above partition of the edge set in $G_1\times G_2$, we have

$$\begin{aligned}&\mathcal{N}^*Z(G_1\times G_2) \\ &= \prod_{(u_iv_j)(u_pv_q)\in E(G_1\times G_2)} [d_{G_1\times G_2}(u_i,v_j)]^2 - [d_{G_1\times G_2}(u_p,v_q)]^2.\end{aligned}$$

This actually can be written as

$$\begin{aligned}&= \prod_{u_i\in V(G_1)}\prod_{(v_jv_q)\in E(G_2)} [d_{G_1}(u_i)+d_{G_2}(v_j)]^2 - [d_{G_1}(u_i)+d_{G_2}(v_q)]^2 \\ &\times\prod_{v_j\in V(G_2)}\prod_{(u_iu_p)\in E(G_1)} [d_{G_1}(u_i)+d_{G_2}(v_j)]^2 - [d_{G_1}(u_p)+d_{G_2}(v_j)]^2.\end{aligned}$$

However, from the inequality (5), we get

$$\begin{aligned}&\leqslant\Bigg[\sum_{u_i\in V(G_1)}\sum_{(v_jv_q)\in E(G_2)} [d_{G_1}^2(u_i)+d_{G_2}^2(v_j)+2_{G_1}(u_i)d_{G_2}(v_j)] \\ &-[d_{G_1}^2(u_i)+d_{G_2}^2(v_q)+2d_{G_1}(u_i)d_{G_2}(v_q)]\Bigg]^{n_1m_2} \\ &\times\Bigg[\sum_{v_j\in V(G_2)}\sum_{(u_iu_p)\in E(G_1)} [d_{G_1}^2(u_i)+d_{G_2}^2(v_j)+2_{G_1}(u_i)d_{G_2}(v_j)] \\ &-[d_{G_1}^2(u_p)+d_{G_2}^2(v_j)+2d_{G_1}(u_p)d_{G_2}(v_j)]\Bigg]^{n_2m_1} \\ &=\Bigg[\sum_{u_i\in V(G_1)}\sum_{(v_jv_q)\in E(G_2)} [d_{G_2}^2(v_j)-d_{G_2}^2(v_q)] \\ &\quad+2d_{G_1}(u_i)[d_{G_2}(v_j)-d_{G_2}(v_q)]\Bigg]^{n_1m_2} \\ &\times\Bigg[\sum_{v_j\in V(G_2)}\sum_{(u_iu_p)\in E(G_1)} [d_{G_1}^2(u_i)-d_{G_1}^2(u_p)] \\ &\quad+2d_{G_2}(v_j)[d_{G_1}(u_i)-d_{G_1}(u_p)]\Bigg]^{n_2m_2} \\ &\leqslant\left[\frac{n_1\mathcal{N}^*Z(G_2)+4m_1M_3(G_2)}{n_1m_2}\right]^{n_1m_2}\end{aligned}$$

$$\times\left[\frac{n_2\mathcal{N}^*Z(G_1)+4m_2M_3(G_1)}{n_2m_1}\right]^{n_2m_1}.$$

■

Theorem 4.10: Let G_1 and G_2 be two graphs with n_1 and n_2 vertices, m_1 and m_2 edges respectively. Then

$$\begin{aligned}&\mathcal{N}^*Z(G_1\circ G_2)\\&\leqslant\left[\frac{\mathcal{N}^*Z(G_1)+2n_2M_3(G_1)}{m_1}\right]^{m_1}\\&\times\left[\frac{n_1\mathcal{N}^*Z(G_2)+2n_1M_3(G_2)}{n_1m_2}\right]^{n_1m_2}\\&\times\left[\frac{n_2M_1(G_1)+n_2^3n_1+4n_2^2m_1-n_1M_1(G_2)-n_1n_2-4m_2n_1}{n_1n_2}\right]^{n_1n_2}.\end{aligned}$$

Proof: By the definition of the multiplicative Nano-Zagreb index and from the above partition of the edge set in $G_1\circ G_2$, we have

$$\begin{aligned}&\mathcal{N}^*Z(G_1\circ G_2)\\&=\prod_{(u_iv_j)(u_pv_q)\in E(G_1\circ G_2)}[d_{G_1\circ G_2}(u_i,v_j)]^2-[d_{G_1\circ G_2}(u_p,v_q)]^2\\&=\prod_{(u_iu_p)\in E(G_1)}[d_{G_1}(u_i)+n_2]^2-[d_{G_1}(u_p)+n_2]^2\\&\times\prod_{u_i\in V(G_1)}\prod_{(v_jv_q)\in E(G_2)}[d_{G_2}(v_j)+1]^2-[d_{G_2}(v_q)+1]^2\\&\times\prod_{u_i\in V(G_1)}\prod_{v_j\in V(G_2)}[d_{G_1}(u_i)+n_2]^2-[d_{G_2}(v_j)+1]^2\\&=\prod_{(u_iu_p)\in E(G_1)}[d^2_{G_1}(u_i)-d^2_{G_1}(u_p)]+2n_2[d_{G_1}(u_i)-d_{G_1}(u_p)]\\&\times\prod_{u_i\in V(G_1)}\prod_{(v_jv_q)\in E(G_2)}[d^2_{G_2}(v_j)-d^2_{G_2}(v_q)]\\&\quad+2[d_{G_2}(v_j)-d_{G_2}(v_q)]\\&\times\prod_{u_i\in V(G_1)}\prod_{v_j\in V(G_2)}[d^2_{G_1}(u_i)+n_2^2+2n_2d_{G_1}(u_i)-d^2_{G_2}(v_j)\\&\quad-1-2d_{G_2}(v_j)].\end{aligned}$$

However, from the inequality (5), we get

$$\begin{aligned}&\leqslant\left[\frac{\mathcal{N}^*Z(G_1)+2n_2M_3(G_1)}{m_1}\right]^{m_1}\\&\times\left[\frac{n_1\mathcal{N}^*Z(G_2)+2n_1M_3(G_2)}{n_1m_2}\right]^{n_1m_2}\\&\times\left[\frac{n_2M_1(G_1)+n_2^3n_1+4n_2^2m_1-n_1M_1(G_2)-n_1n_2-4m_2n_1}{n_1n_2}\right]^{n_1n_2}.\end{aligned}$$

■

Theorem 4.11: Let G_1 and G_2 be two graphs with n_1 and n_2 vertices, m_1 and m_2 edges respectively. Then

$$\begin{aligned}\mathcal{N}^*Z(G_1[G_2])\leqslant&\left[\frac{n_1\mathcal{N}^*Z(G_2)+4n_2m_1M_3(G_2)}{n_1m_2}\right]^{n_1m_2}\\&\times\left[\frac{n_2^3\mathcal{N}^*Z(G_1)+4n_2m_2M_3(G_2)}{m_1n_2}\right]^{m_1n_2^2}.\end{aligned}$$

Proof: By the definition of the multiplicative Nano-Zagreb index and from the above partition of the edge set in $G_1[G_2]$, we have

$$\begin{aligned}&\mathcal{N}^*Z(G_1[G_2])\\&=\prod_{(u_iv_j)(u_pv_q)\in E(G_1[G_2])}[d_{G_1[G_2]}(u_i,v_j)]^2-[d_{G_1[G_2]}(u_p,v_q)]^2\\&=\prod_{u_i\in V(G_1)}\prod_{(v_jv_q)\in E(G_2)}[d_{G_1}(u_i)n_2+d_{G_2}(v_j)]^2\\&\quad-[d_{G_1}(u_i)n_2+d_{G_2}(v_q)]^2\\&\times\prod_{(u_iu_p)\in E(G_1)}\prod_{v_j\in V(G_2)}\Big[[(d_{G_1}(u_i)n_2+d_{G_2}(v_j)]^2\\&\quad-[d_{G_1}(u_p)n_2+d_{G_2}(v_j)]^2\Big]^{n_2}\\&=\prod_{u_i\in V(G_1)}\prod_{(v_jv_q)\in E(G_2)}[d^2_{G_2}(v_j)-d^2_{G_2}(v_q)]\\&\quad+2n_2d_{G_1}(u_i)[d_{G_2}(v_j)-d_{G_2}(v_q)]\\&\times\prod_{(u_iu_p)\in E(G_1)}\prod_{v_j\in V(G_2)}\Big[n_2^2[d^2_{G_1}(u_i)-d^2_{G_1}(u_p)]\\&\quad+2n_2d_{G_2}(v_j)[d_{G_1}(u_i)-d_{G_1}(u_p)]\Big]^{n_2}.\end{aligned}$$

However, from the inequality (5), we get

$$\begin{aligned}&\leqslant\left[\frac{n_1\mathcal{N}^*Z(G_2)+4n_2m_1M_3(G_2)}{n_1m_2}\right]^{n_1m_2}\\&\times\left[\frac{n_2^3\mathcal{N}^*Z(G_1)+4n_2m_2M_3(G_2)}{m_1n_2}\right]^{m_1n_2^2}.\end{aligned}$$

■

Theorem 4.12: Let G_1 and G_2 be two graphs with n_1 and n_2 vertices, m_1 and m_2 edges respectively. Then

$$\mathcal{N}^*Z(G_1\otimes G_2)=0.$$

Proof: By the definition of the multiplicative Nano-Zagreb index and from the above partition of the edge set in $G_1\otimes G_2$, we have

$$\begin{aligned}&\mathcal{N}^*Z(G_1\otimes G_2)\\&=\prod_{(u_iv_j)(u_pv_q)\in E(G_1\otimes G_2)}[d_{G_1\otimes G_2}(u_i,v_j)]^2-[d_{G_1\otimes G_2}(u_p,v_q)]^2\\&=\prod_{(u_iu_p)\in E(G_1)}\prod_{v_j\in V(G_2)}[n_1d_{G_2}(v_j)+n_2d_{G_1}(u_i)-d_{G_1}(u_i)d_{G_2}(v_j)]^2\\&-[n_1d_{G_2}(v_j)+n_2d_{G_1}(u_p)-d_{G_1}(u_p)d_{G_2}(v_j)]^2\\&\times\prod_{u_i\in V(G_1)}\prod_{v_j\in V(G_2)}[n_1d_{G_2}(v_j)+n_2d_{G_1}(u_i)-d_{G_1}(u_i)d_{G_2}(v_j)]^2\\&-[n_1d_{G_2}(v_j)+n_2d_{G_1}(u_i)-d_{G_1}(u_i)d_{G_2}(v_j)]^2\\&=\prod_{u_i\in V(G_1)}\prod_{(v_j,v_q)\in E(G_2)}\big[n_1^2d^2_{G_2}(v_j)+n_2^2d^2_{G_1}(u_i)-d^2_{G_1}(u_i)d^2_{G_2}(v_j)\\&+2n_1n_2d_{G_1}(u_i)d_{G_2}(v_j)-2n_2d^2_{G_1}(u_i)d_{G_2}(v_j)\\&-2n_1d_{G_1}(u_i)d^2_{G_2}(v_j)\big]\\&-\big[n_1^2d^2_{G_2}(v_j)+n_2^2d^2_{G_1}(u_p)-d^2_{G_1}(u_p)d^2_{G_2}(v_j)\\&+2n_1n_2d_{G_1}(u_p)d_{G_2}(v_j)-2n_2d^2_{G_1}(u_p)d_{G_2}(v_j)\end{aligned}$$

$$- 2n_1 d_{G_1}(u_p) d^2_{G_2}(v_j)\big] \times \prod_{(u_iu_p)\in E(G_1)} \prod_{v_j\in V(G_2)} \Big[n_1^2 d^2_{G_2}(v_j) + n_2^2 d^2_{G_1}(u_i) - d^2_{G_1}(u_i) d^2_{G_2}(v_j) + 2n_1n_2 d_{G_1}(u_i) d_{G_2}(v_j) - 2n_2 d^2_{G_1}(u_i) d_{G_2}(v_j) - 2n_1 d_{G_1}(u_i) d^2_{G_2}(v_j)\big] - \big[n_1^2 d^2_{G_2}(v_j) + n_2^2 d^2_{G_1}(u_i) - d^2_{G_1}(u_i) d^2_{G_2}(v_j) + 2n_1n_2 d_{G_1}(u_i) d_{G_2}(v_j) - 2n_2 d^2_{G_1}(u_i) d_{G_2}(v_j) - 2n_1 d_{G_1}(u_i) d^2_{G_2}(v_j)\big] = 0.$$

■

Theorem 4.13: Let G_1 and G_2 be two graphs with n_1 and n_2 vertices, m_1 and m_2 edges respectively. Then

$$\mathcal{N}^*Z(G_1 \vee G_2) \leqslant \left[\frac{\mathcal{N}^*Z(G_1) + 2n_2 M_3(G_1)}{m_1}\right]^{m_1} \times \left[\frac{\mathcal{N}^*Z(G_2) + 2n_1 M_3(G_2)}{m_2}\right]^{m_2} \times \left[\frac{n_2 M_1(G_1) + n_2^3 n_1 + 4n_2 m_1 - n_1 M_1(G_2) - n_1^3 n_2 - 4n_1 m_2}{n_1 n_2}\right]^{n_1 n_2}.$$

Proof: By the definition of the multiplicative Nano-Zagreb index and from the above partition of the edge set in $G_1 \vee G_2$, we have

$$\begin{aligned}
\mathcal{N}^*Z(G_1 \vee G_2) &= \prod_{(u_iv_j)(u_pv_q)\in E(G_1\vee G_2)} [d_{G_1\vee G_2}(u_i,v_j)]^2 - [d_{G_1\vee G_2}(u_p,v_q)]^2 \\
&= \prod_{(u_iu_p)\in E(G_1)} [(d_{G_1}(u_i) + n_2]^2 - [d_{G_1}(u_p) + n_2]^2 \prod_{(v_jv_q)\in E(G_2)} [(d_{G_2}(v_j) + n_1]^2 - [d_{G_2}(v_q) + n_1]^2 \\
&\times \prod_{u_i\in V(G_1)} \prod_{v_j\in V(G_2)} [d_{G_1}(u_i) + n_2] - [d_{G_2}(v_j) + n_1]^2 \\
&= \prod_{(u_iu_p)\in E(G_1)} [d^2_{G_1}(u_i) - d^2_{G_1}(u_p)] + 2n_2[d_{G_1}(u_i) - d_{G_1}(u_p)] \prod_{(v_jv_q)\in E(G_2)} [d^2_{G_2}(v_j) - d^2_{G_2}(v_q)] + 2n_1[d_{G_2}(v_j) - d_{G_1}(v_q)] \\
&\times \prod_{u_i\in V(G_1)} \prod_{v_j\in V(G_2)} [d^2_{G_1}(u_i) + n_2^2 + 2n_2 d_{G_1}(u_i)] - [d^2_{G_2}(v_j) + n_1^2 + 2n_1 d_{G_1}(v_j)].
\end{aligned}$$

However, from the inequality (5), we get

$$\leqslant \left[\frac{\mathcal{N}^*Z(G_1) + 2n_2 M_3(G_1)}{m_1}\right]^{m_1} \times \left[\frac{\mathcal{N}^*Z(G_2) + 2n_1 M_3(G_2)}{m_2}\right]^{m_2} \times \left[\frac{n_2 M_1(G_1) + n_2^3 n_1 + 4n_2 m_1 - n_1 M_1(G_2) - n_1^3 n_2 - 4n_1 m_2}{n_1 n_2}\right]^{n_1 n_2}.$$

■

Theorem 4.14: Let G_1 and G_2 be two graphs with n_1 and n_2 vertices, m_1 and m_2 edges respectively. Then

$$\mathcal{N}^*Z(G_1 \oplus G_2) = 0.$$

Proof: By the definition of the multiplicative Nano-Zagreb index and from the above partition of the edge set in $G_1 \oplus G_2$, we have

$$\begin{aligned}
&\mathcal{N}^*Z(G_1 \oplus G_2) \\
&= \prod_{(u_iv_j)(u_pv_q)\in E(G_1\oplus G_2)} [d_{G_1\oplus G_2}(u_i,v_j)]^2 - [d_{G_1\oplus G_2}(u_p,v_q)]^2 \\
&= \prod_{u_i\in V(G_1)} \prod_{(v_jv_q)\in E(G_2)} \big[(n_2 d_{G_1}(u_i) + n_1 d_{G_2}(v_j) - 2d_{G_1}(u_i) d_{G_2}(v_j)\big]^2 - \big[n_2 d_{G_1}(u_i) + n_1 d_{G_2}(v_q) - 2d_{G_1}(u_i) d_{G_2}(v_q)\big]^2 \\
&\times \prod_{(u_iu_p)\in E(G_1)} \prod_{v_j\in V(G_2)} \Big[\big[n_2 d_{G_1}(u_i) + n_1 d_{G_2}(v_j) - 2d_{G_1}(u_i) d_{G_2}(v_j)\big]^2 \big[n_2 d_{G_1}(u_p) + n_1 d_{G_2}(v_j) - 2d_{G_1}(u_p) d_{G_2}(v_j)\big]\Big]^{n_2} \\
&\times \prod_{u_i\in V(G_1)} \prod_{v_j\in V(G_2)} \big[n_2 d_{G_1}(u_i) + n_1 d_{G_2}(v_j) - 2d_{G_1}(u_i) d_{G_2}(v_j)\big]^2 - \big[n_2 d_{G_1}(u_i) + n_1 d_{G_2}(v_j) - 2d_{G_1}(u_i) d_{G_2}(v_j)\big]^2 \\
&= \prod_{u_i\in V(G_1)} \prod_{(v_jv_q)\in E(G_2)} \big[n_2^2 d^2_{G_1}(u_i) + n_1^2 d^2_{G_2}(v_j) - 4d^2_{G_1}(u_i) d^2_{G_2}(v_j) + 2n_1n_2 d_{G_1}(u_i) d_{G_2}(v_j) - 4n_2 d^2_{G_1}(u_i) d_{G_2}(v_j) - 4n_1 d_{G_1}(u_i) d^2_{G_2}(v_j)\big] \\
&- \big[n_2^2 d^2_{G_1}(u_i) + n_1^2 d^2_{G_2}(v_q) - 4d^2_{G_1}(u_i) d^2_{G_2}(v_q) + 2n_1n_2 d_{G_1}(u_i) d_{G_2}(v_q) - 4n_2 d^2_{G_1}(u_i) d_{G_2}(v_q) - 4n_1 d_{G_1}(u_i) d^2_{G_2}(v_q)\big] \\
&\prod_{(u_iu_p)\in E(G_1)} \prod_{v_j\in V(G_2)} \Big[\big[n_2^2 d^2_{G_1}(u_i) + n_1^2 d^2_{G_2}(v_j) - 4d^2_{G_1}(u_i) d^2_{G_2}(v_j) + 2n_1n_2 d_{G_1}(u_i) d_{G_2}(v_j) - 4n_2 d^2_{G_1}(u_i) d_{G_2}(v_j) - 4n_1 d_{G_1}(u_i) d^2_{G_2}(v_j)\big] \\
&- \big[n_2^2 d^2_{G_1}(u_p) + n_1^2 d^2_{G_2}(v_j) - 4d^2_{G_1}(u_p) d^2_{G_2}(v_j) + 2n_1n_2 d_{G_1}(u_p) d_{G_2}(v_j) - 4n_2 d^2_{G_1}(u_p) d_{G_2}(v_j) - 4n_1 d_{G_1}(u_p) d^2_{G_2}(v_j)\big]\Big]^{n} \\
&\times \prod_{u_i\in V(G_1)} \prod_{v_j\in V(G_2)} \big[n_2^2 d^2_{G_1}(u_i) + n_1^2 d^2_{G_2}(v_j) - 4d^2_{G_1}(u_i) d^2_{G_2}(v_j) + 2n_1n_2 d_{G_1}(u_i) d_{G_2}(v_j) - 4n_2 d^2_{G_1}(u_i) d_{G_2}(v_j) - 4n_1 d_{G_1}(u_i) d^2_{G_2}(v_j)\big] \\
&- \big[n_2^2 d^2_{G_1}(u_i) + n_1^2 d^2_{G_2}(v_j) - 4d^2_{G_1}(u_i) d^2_{G_2}(v_j) + 2n_1n_2 d_{G_1}(u_i) d_{G_2}(v_j) - 4n_2 d^2_{G_1}(u_i) d_{G_2}(v_j) - 4n_1 d_{G_1}(u_i) d^2_{G_2}(v_j)\big] = 0.
\end{aligned}$$

■

Two graphs are **isomorphic** if there exists a vertex labeling that preserves adjacency, they can be viewed as different geometrical representations of the same abstract graph defined as a set of elements (vertices) $\{v_i\}, i \in 1,2,\ldots,n$ and a set of elements (edges) that are unordered duplets from the former set $\{u_i v j\}, i \notin j \in 1,2,\ldots,n$.

Example 4.15: As an application in Chemistry, shows that in all alkanes on n vertices, we computed the value of $\mathscr{N}Z$ and $\mathscr{N}^*Z$ depends on the respected isomer. For instance, we computed these values for octane isomers as reported in Table I. All isomers of octane are depicted in Figure 1.

TABLE I
$\mathscr{N}Z$ AND $\mathscr{N}^*Z$ OF THE OCTANE ISOMERS.

Molecule	$\mathscr{N}Z$	$\mathscr{N}^*Z$
Octane	6	0
2-methyl-heptane	42	0
3-methyl-heptane	40	0
4-methyl-heptane	24	0
3-ethyl-hexane	32	0
2,2-dimethyl-hexane	68	759375
2,3-dimethyl-hexane	24	0
2,4-dimethyl-hexane	60	0
2,5-dimethyl-hexane	78	12960000
3,3-dimethyl-hexane	24	0
3,4-dimethyl-hexane	60	0
2-methyl-3-ethyl-pentane	68	3628800
3-methyl-3-ethyl-pentane	32	0
2,2,3-trimethyl-pentane	24	0
2,2,4-trimethyl-pentane	60	699840
2,3,3-trimethyl-pentane	42	19200
2,3,4-trimethyl-pentane	90	0
2,2,3,3-tetramethylbutane	32	0

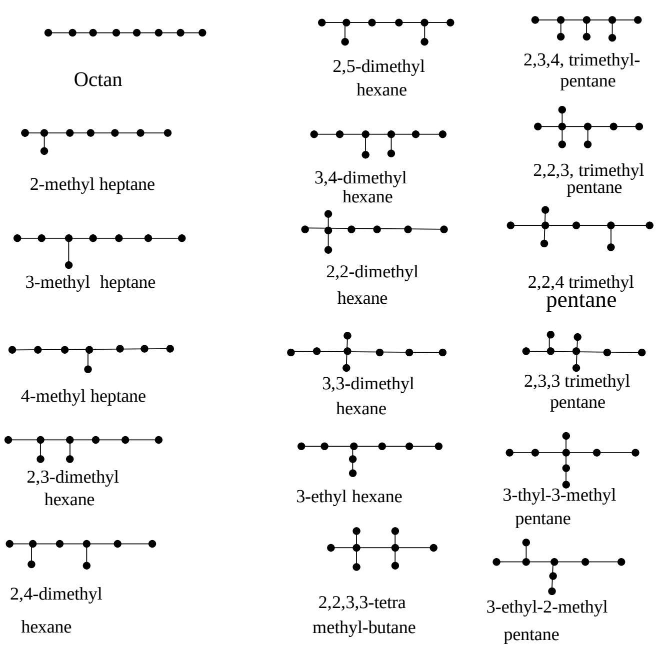

Fig. 1. All octane isomers.

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