Zagreb, Multiplicative Zagreb Indices And Coindices Of $NC_n(k)$ And $Ca_3(C_6)$ Graphs

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ABSTRACT: Let $G=(V,E)$ be a simple connected graph with vertex set $V$ and edge set $E$. The first, second and third Zagreb indices of $G$ are defined, respectively by:

$M_1(G) = \sum_{u \in V} d(u)^2$, $M_2(G) = \sum_{uv \in E} d(u).d(v)$ and $M_3(G) = \sum_{uv \in E} |d(u) − d(v)|$, where $d(u)$ is the degree of vertex $u$ in $G$ and $uv$ is an edge of $G$, connecting the vertices $u$ and $v$. Recently, the first and second multiplicative Zagreb indices of the graph are defined by: $PM_1(G) = \prod_{u \in V} d(u)^2$ and $PM_2(G) = \prod_{uv \in E} d(u)^{d(u)}$. The first and second Zagreb coindices of the graph are defined by: $M_1(G) = \sum_{uv / \in E} (d(u) + d(v))$ and $M_2(G) = \sum_{uv / \in E} d(u).d(v)$. $PM_1(G) = \prod_{uv / \in E} d(u)^{d(u)}$ and $PM_2(G) = \prod_{uv / \in E} d(u)^d(u)$, named as multiplicative Zagreb coindices. In this article, we compute the first, second and third Zagreb indices and the first and second multiplicative Zagreb indices of $NC_n(k)$ and $Ca_3(C_6)$ graphs. The first and second Zagreb coindices and the first and second multiplicative Zagreb coindices of these graphs are also computed.

Key Words: Zagreb Indices, Multiplicative Zagreb Indices, Zagreb Coindices, Multiplicative Zagreb Coindices.

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1. Introduction

The graphs considered in this paper are simple and connected. Let $G=(V,E)$ be a simple connected graph with vertex set $V$ and edge set $E$. A topological index is a fixed number under graph automorphisms. Gutman and Trinajstić [4], defined the first and second Zagreb indices. Zagreb indices are defined as follows:

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

The alternative expression of $M_1(G)$ is $\sum_{u \in V}(d(u) + d(v))$.

G.H.Fath-Tabar [3], defines the third Zagreb index, by:

$M_3(G) = \sum_{uv \in E} |d(u) − d(v)|$

Todeschini et al. [5,6], have recently proposed to consider multiplicative variants of additive graph invariants, applied to the Zagreb indices, lead to:

$PM_1(G) = \prod_{u \in V} d(u)^2$, $PM_2(G) = \prod_{uv \in E} d(u)^{d(u)}$

The alternative expression of $PM_2(G)$ is $\prod_{uv \in E} d(u)^d(u)$.

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Recently, Ashrafi, Došlić and Hamzeh [1,2], define the first and second Zagreb coindices by:
\[
M_1(G) = \sum_{u\in E}(d(u) + d(v)), \quad M_2(G) = \sum_{u\in E} d(u) d(v)
\]
In 2013 Xu, Das and Tang [7], defined multiplicative Zagreb coindices by:
\[
PM_1(G) = \prod_{u\in E} d(u) + d(v), \quad PM_2(G) = \prod_{u\in E} d(u) d(v)
\]
They defined multiplicative sum Zagreb index and the total multiplicative sum Zagreb index by:
\[
PM_i^T(G) = \prod_{u\in E} d(u) + d(v), \quad PM_T(G) = \prod_{u\in V} d(u) + d(v)
\]
The goal of this article is to compute Zagreb indices, multiplicative Zagreb indices and Coindices of NCa₃(C₄), the third member of Capra-designed planar benzenoid series, graphs.

The Harmonic index of NCa₃(k) nanocones are equal to:
\[
\text{Harmonic index} = \frac{2}{\text{number of paths that connect the vertex of degree i with a vertex of degree j}},
\]
In [8], Xu, Das and Tang defined multiplicative sum Zagreb index and the total multiplicative sum Zagreb index of NCa₃(k) nanocones and Cn₃(n), the third member of Capra-designed planar benzenoid series, graphs. We use the above formula to obtain Zagreb and multiplicative Zagreb coindices.

2. Preliminaries

We define \(d_i\) to be the number of vertices with degrees i and \(x_{ij}, i \neq j\), to be the number of edges connecting the vertex of degree i with a vertex of degree j and \(x_{ii}\) to be the number of edges connecting two vertices of degree i. We define \(x_{ij}\) to be the number of paths connecting the vertex of degree i with a vertex of degree j, so that \(x_{ij}\) does not include the number of edges that connect vertices i, j. We define \(x_{ii}\) to be the number of paths connecting two vertices of degree i, so that \(x_{ii}\) does not include the number of edges which connect two vertices of degree i.

**Lemma 2.1.** The values of \(x_{ij}, x_{ii}\) are equal to:
\[
x_{ij} = \left( \frac{d_i}{1} \right) \left( \frac{d_j}{1} \right) - x_{ij} = d_i d_j - x_{ij}
\]
\[
x_{ii} = \left( \frac{d_i}{2} \right) - x_{ii} = \frac{d_i(d_i-1)}{2} - x_{ii}
\]
**Proof.** Straight forward. □

We use the above formula to obtain Zagreb and multiplicative Zagreb coindices.

**Lemma 2.2.** The number of paths that connect two vertices of degree i as well as the number of paths that connect the vertex of degree i with a vertex of degree j, are equal to:
\[
\left( \frac{d_i}{2} \right) = \frac{d_i(d_i-1)}{2}
\]
\[
\left( \frac{d_j}{1} \right) = d_j d_i
\]
**Proof.** Straight forward. □

We use these formula to obtain \(PM_T(G)\).

We compute these indices for the figures 1-5.

3. Results and discussions

**Theorem 3.1.** Zagreb, multiplicative Zagreb indices and Coindices of NCa₃(k) nanocones (see Figures 1-5) are computed as follows:
\[
M_1 = 9k^2n + 13kn + 4n, M_2 = 2\frac{kn^2}{2} + \frac{3kn}{2} + 4n, M_3 = 2kn,
\]
\[
PM_1 = 2^{2k+2} n^3 + 3^{2k+2} n^2 + 2kn, PM_2 = 2^{2k+2} n^3 + 3^{2k+2} n^2 + 2kn,
\]
\[
M_3 = 3n^2 k^4 + 11n^2 k^3 (15n^2 - 12n)k^2 + (9n^2 - 18n)k + (2n^2 - 6n),
\]
\[
PM_3 = 2^{\frac{k^2}{2}} n^4 + 15n^2 k^3 (15n^2 - 12n)k^2 + (10n^2 - 23n)k + 2n^2 - 2n,
\]
\[
PM_1 = 2^{\frac{\alpha}{2}} (\frac{2n^2}{2} + 2n^2 + 2n^2 + 2n^2 - 6n) - 2^{\frac{\alpha}{2}} + 2n^2 + 2n^2 - 2n.
\]
5n^2k^3+2n^2k^2+(n^2-2n)k.

\[ \frac{P M_2}{P M_1} = 2^{n^2k^3+3n^2k^2+(3n^2-3n)k} + 3n^2k^4+3n^2k^3+(3n^2-4n)k^2+(n^2-4n)k. \]

**Proof.** We suppose \( NC_n(k) \) denote a nanocone where \( n \) denotes the number of edges in the single triangle, square, pentagon, etc. and \( k \) denotes the number of layers in the nanocone. See Figures 1-5 for examples of this type of nanocones.

First, we obtain the number of vertices and edges of nanocone, calculations show that:

\[ |V(G)| = k^2n+2kn+n, \quad |E(G)| = \frac{3k^2n}{2} + \frac{5kn}{2} + n, \text{ also: } d_2 = kn+n, d_3 = k^2n+kn. \]

Elementary computation gives:

\[ M_1 = 9k^2n+13kn+4n, \quad PM_1 = 2^{2kn+2n}.2^{3k^2n+2kn}, \quad PM_2 = 2^{2kn+2n}.3^{3k^2n+3kn}. \]

Calculations show that: \( x_{22} = n, x_{23} = 2kn, x_{33} = \frac{3k^2n}{2} + kn/2. \)

Elementary computation gives: \( M_2 = 3^{3k^2n} + \frac{3k^2n}{2} + 4n, M_3 = 2kn. \)
Similar calculation shows that:

\[
M_1 = 3n^2k^4 + 11n^2k^3 + (15n^2 - 12n)k^2 + (9n^2 - 18n)k + (2n^2 - 6n),
\]
\[
M_2 = \frac{9n^2}{2}k^4 + 15n^2k^3 + \left(\frac{37n^2}{2} - 18n\right)k^2 + (10n^2 - 23n)k + 2n^2 - 6n,
\]
\[
P M_1 = 2^n k^2 + (3n^2 - 4n)k^2 - 2n^2 - 2n,
\]
\[
P M_2 = 2^n k^2 + 3n^2k^2 + (3n^2 - 3n)k + n^2 - 3n.
\]

Theorem 3.2. Zagreb, multiplicative Zagreb indices and Coindices of \(C_{n3}(C_6)\), the third member of Capra- designed planar benzenoid series (see Figure 6) are computed as follows:

**Figure 5.** \(NC_7(4)\) Nanocone

\[
M_1 = 4.3^n + 18.7n - 1 - 6,
\]
\[
M_2 = \begin{cases} 
24 & n = 1 \\
27.7n^{-1} + 10.3n^{-1} - 15 & n > 1
\end{cases}
\]
\[
M_3 = \begin{cases} 
0 & n = 1 \\
4.3^{n-1} & n > 1
\end{cases}
\]
\[
P M_1 = 2^3s^3 + 6.3^4 s^{-1} - 4^n,
\]
\[
P M_2 = 2^3s^3 + 6.3^6 s^{-1} - 6^n,
\]
\[
M_1 = \begin{cases} 
36 & n = 1 \\
12.7^{2n} - 2 + 2.3^{2n} + 10.3^n 7^{n-1} - 4.3^n - 18.7^n - 1 + 6 & n > 1
\end{cases}
\]
\[
M_2 = \begin{cases} 
36 & n = 1 \\
18.7^{2n} - 2 + 2.3^{2n} + 12.3^n 7^{n-1} - 16.3^n - 1 - 36.3^n - 1 + 18 & n > 1
\end{cases}
\]
\[
P M_1 = 2^{18} k^2 + 3n^2 + 5.3^n - 8.7^n - 1 + 6.3^2 k^2 + 2.3^n - 8.7^n - 1 + 6, 
\]
\[
P M_2 = \begin{cases} 
2^{18} & n = 1 \\
2^2 s^2 + 3n^2 + 3^n + 6.7^n - 1 - 6 & n > 1
\end{cases}
\]
Proof. We suppose $Ca_3(C_6)$ denotes a planar benzenoid where the first layer has a hexagonal, the second layer has six hexagonal and the third layer has six Figure such as the second layer etc. First, we obtain the number of vertices and edges of $Ca_3(C_6)$. Calculations show that:

$$d_{2,n} = 6\left(\frac{d_{2,n-1} - 2}{2}\right) - 6.$$

Where $d_{2,n}, d_{2,n-1}$ denote the number of vertices with degree two of the last layer and previous the last layer, respectively:

$$d_2 = 3^n + 3.$$

First, we obtain the number of vertices of a layer we compute six times the number of vertices of the previous layer in addition to the number of vertices of previous layer, then we subtract the common part of the six added figure and previous layer from the obtained number.

![Graph Ca_3(C_6)](image)

Figure 6. Graph $Ca_3(C_6)$ is the third member of Capra-designed planar benzenoid series $Ca_k(C_6)$

The number of vertices around the previous layer is equal to:

$$6\left(\frac{d_{2,n-2} - 2}{2} + \frac{d_{2,n-2} - 2}{2} - 1\right) = 6(d_{2,n-2} - 3) = 6(3^{n-2} + 3 - 3) = 2.3^{n-1}.$$

Where $d_{2,n-2}$ denotes the number of vertices with degree two of the two previous layers. Also, to obtain the number of vertices of the common parts of the six added figures. We compute sixtimes of the number of vertices around two previous layers plus one, then we divide it by two. Therefore:

$$6\left[\frac{1}{4}(2.3^{n-2}) + 1\right] = 2.3^{n-1} + 6.$$

So, the number of common vertices is equal to:

$$2.3^{n-1} + 2.3^{n-1} + 6 = 4.3^{n-1} + 6.$$

Therefore:
\[ |V(G)| = 2.7n^{-1} + 7.3n^{-1} + 7 - [4.3n^{-1} + 6] = 2.7n^{-1} + 3n + 1. \]

The amount included in square brackets is the number of vertices of the common parts of the six added figures and around of the previous layer.

Also: \( d_3 = |V(G)| - d_2 = 2.7n^{-1} - 2. \)

Elementary computation gives:

\[
M_1 = 4.3^n + 18.7^n - 6, \\
P M_1 = 2^{2.3^n} + 6.3n^{-1} - 4, \quad PM_2 = 2^{2.3^n} + 6.3n^{-1} - 6.
\]

We obtain the number of edges of the graph as we did for computing the number of vertices of the graph, so:

\[ |E(G)| = 3.7n^{-1} + 7.3n^{-1} - [4.3n^{-1}] = 3.7n^{-1} + 3n. \]

The amount included in square brackets is the number of edges of the common parts of the six added figures and around of the previous layer.

\[
x_{22} = 6\left(\frac{22n^{-1} - 2}{2}\right) = 3x_{22,n-1} - 6 = 3^{n-1} + 3, \\
x_{23} = 6\left(\frac{23n^{-1} - 2}{2}\right) = 3x_{23,n-1} = 4.3^{n-1}
\]

and so, for \( n > 1. \)

Where \( x_{22,n-1}, x_{23,n-1}, \) denote the number of edges \( x_{22}, x_{23} \) of the previous layer, respectively.

Calculations show that:

\[
x_{22} = \begin{cases} 
6 & n = 1 \\
3^{n-1} + 3 & n > 1
\end{cases}, \
x_{23} = \begin{cases} 
0 & n = 1 \\
4.3^{n-1} & n > 1
\end{cases}, \
x_{33} = \begin{cases} 
0 & n = 1 \\
3.7n^{-1} - 2.3n^{-1} - 3 & n > 1
\end{cases}
\]

Elementary computation gives:

\[
M_2 = \begin{cases} 
24 & n = 1 \\
27.7^{n-1} + 10.3^{n-1} - 15 & n > 1
\end{cases}, \
M_3 = \begin{cases} 
0 & n = 1 \\
4.3^{n-1} & n > 1
\end{cases}
\]

Similar calculation shows that:

\[
M_1 = \begin{cases} 
36 & n = 1 \\
12.7n^{-2} + 2.3n + 10.3^n - 7n^{-1} - 4.3^n - 18.7^n - 6 & n > 1
\end{cases}, \
M_2 = \begin{cases} 
18.7n^{-2} + 2.3n + 12.3^n - 6n^{-1} - 16.3^n - 18 & n > 1
\end{cases}, \
P M_1 = \begin{cases} 
2^{13} & n = 1 \\
2^{7n^{-2} + 5n + 2} + 8.7^{-1} + 6n - 12.7^{n-2} + 2.3^n + 10.3^n - 7n^{-1} & n > 1
\end{cases}, \
P M_2 = \begin{cases} 
2^{13} & n = 1 \\
2^{3n - 1} + 3n + 6.7^{n-1} - 2.3^n + 4.7^{n-2} - 10.7^{n-1} & n > 1
\end{cases}
\]

also: \( PM_1^* = \begin{cases} 
2^{12} & n = 1 \\
2^{3n - 1} + 5.3^{n-1} - 3.543^{n-1} & n > 1
\end{cases}, \
PM_2^T = 2^{2.7n^{-2} + 5n + 2} + 5.3^{n-1} + 6.7^{n-1} + 9.3^{2.7n^{-2} - 5.7^{n-1} + 3n} \]

\( 5.2^{3n - 1} + 6.7^{n-1} - 2.3^n - 6. \)

\( \square \)

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