Bol. Soc. Paran. Mat. (3s.) **v. 36** 2 (2018): 9–15.
©SPM –ISSN-2175-1188 on line ISSN-00378712 in press
SPM: www.spm.uem.br/bspm doi:10.5269/bspm.v36i2.30613

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

V. Ahmadi and M. R. Darafsheh

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 defind, respectivly 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 defind by: $PM_1(G) = \prod_{u\in V} d(u)^2$ and $PM_2(G) = \prod_{u\in V} d(u)^{d(u)}$. The first and second Zagreb coindices of the graph are defind by: $\overline{M_1}(G) = \sum_{uv\notin E}(d(u) + d(v))$ and $\overline{M_2}(G) = \sum_{uv\notin E} d(u).d(v)$. $\overline{PM_1}(G) = \prod_{uv\notin E} d(u) + d(v)$ and $\overline{PM_2}(G) = \prod_{uv\notin E} d(u).d(v)$, named as multiplicative Zagreb coindices. In this article, we compute the first, second and the 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 Coind-ices, Multiplicative Zagreb Coindices.

Contents

1 Introduction 9

2 Preliminaries 10

3 Results and discussions 10

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 $\sum_{uv\in E}(d(u) + d(v))$.

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

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

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

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

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

2010 *Mathematics Subject Classification:* 05C10.
Submitted January 17, 2016. Published May 03, 2016

Recently,Ashrafi,Došlić and Hamzeh [1,2], define the first and second Zagreb coindices by:
$\overline{M_1}(G) = \sum_{uv \notin E}(d(u) + d(v)),\ \overline{M_2}(G) = \sum_{uv \notin E} d(u).d(v)$
In 2013 Xu, Das and Tang [7], defined multiplicative Zagreb coindices by:
$\overline{PM_1}(G) = \prod_{uv \notin E} d(u) + d(v),\ \overline{PM_2}(G) = \prod_{uv \notin E} d(u).d(v)$
They defined multiplicative sum Zagreb index and the total multiplicative sum Zagreb index by:
$PM_1{}^*(G) = \prod_{uv \in E} d(u) + d(v),\ PM^T(G) = \prod_{u,v \in V} d(u) + d(v)$

The goal of this article is to compute Zagreb indices, multiplicative Zagreb indices, Zagreb coindices, multiplicative Zagreb coindices, multiplicative sum Zagreb index and the total multiplicative sum Zagreb index of $NC_n(k)$ nanocones and $Ca_3(C_6)$, the third member of Capra- designed planar benzenoid series, graphs. The Harmonic index of $NC_n(k)$ are calculated in Ref. [8].

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 $\overline{x}_{ij}$ to be the number of paths connecting the vertex of degree i with a vertex of degree j, so that$\overline{x}_{ij}$ does not include the number of edges that connect vertices i, j . We define $\overline{x}_{ii}$ to be the number of paths connecting two vertices of degree i, so that $\overline{x}_{ii}$ does not include the number of edges which connect two vertices of degree i.

Lemma 2.1. The values of $\overline{x}_{ij}, \overline{x}_{ii}$ are equal to:

$$\overline{x}_{ij} = \begin{pmatrix} d_i \\ 1 \end{pmatrix}\begin{pmatrix} d_j \\ 1 \end{pmatrix} - x_{ij} = d_i d_j - x_{ij} \qquad \overline{x}_{ii} = \begin{pmatrix} d_i \\ 2 \end{pmatrix} - x_{ii} = \tfrac{d_i(d_i-1)}{2} - x_{ii}$$

Proof. Straight forward. □

We use the above formuli 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:

$$\begin{pmatrix} d_i \\ 2 \end{pmatrix} = \tfrac{d_i(d_i-1)}{2} \qquad\qquad \begin{pmatrix} d_i \\ 1 \end{pmatrix}\begin{pmatrix} d_j \\ 1 \end{pmatrix} = d_i d_j$$

Proof. straight forward. □

We use these formuli 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 $NC_n(k)$ nanocones (see Figures1-5) are computed as follows:

$M_1 = 9k^2n + 13kn + 4n, M_2 = \frac{27k^2n}{2} + \frac{33kn}{2} + 4n, M_3 = 2kn,$
$PM_1 = 2^{2kn+2n}.3^{2k^2n+2kn}, PM_2 = 2^{2kn+2n}.3^{3k^2n+3kn},$
$\overline{M_1} = 3n^2k^4 + 11n^2k^3 + (15n^2 - 12n)k^2 + (9n^2 - 18n)k + (2n^2 - 6n),$
$\overline{M_2} = \frac{9n^2}{2}k^4 + 15n^2k^3 + (\frac{37n^2}{2} - 18n)k^2 + (10n^2 - 23n)k + 2n^2 - 6n,$
$\overline{PM_1} = 2^{\frac{n^2k^4+2n^2k^3+(3n^2-4n)k^2+(4n^2-4n)k+2n^2-6n}{2}}.3^{\frac{n^2k^4+2n^2k^3+(n^2-4n)k^2-2nk}{2}}.$

$5^{n^2k^3+2n^2k^2+(n^2-2n)k}$,

$\overline{PM_2} = 2^{n^2k^3+3n^2k^2+(3n^2-3n)k+n^2-3n}.3^{n^2k^4+3n^2k^3+(3n^2-4n)k^2+(n^2-4n)k}$.

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:

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

Elementary computation gives:

$M_1 = 9k^2n + 13kn + 4n$,

$PM_1 = 2^{2kn+2n}.3^{2k^2n+2kn}, PM_2 = 2^{2kn+2n}.3^{3k^2n+3kn}$.

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

Elementary computation gives: $M_2 = \frac{27k^2n}{2} + \frac{33kn}{2} + 4n, M_3 = 2kn$.

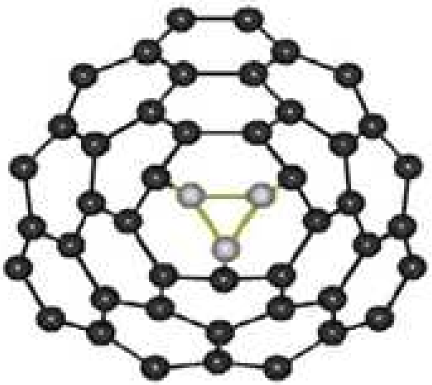

Figure 1. $NC_3(3)$ Nanocone

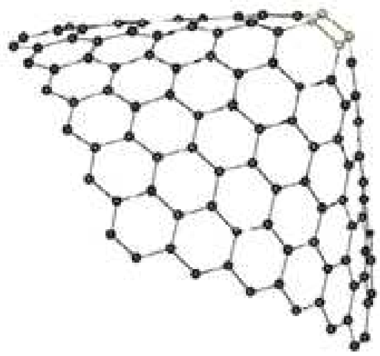

Figure 2. $NC_4(5)$ Nanocone

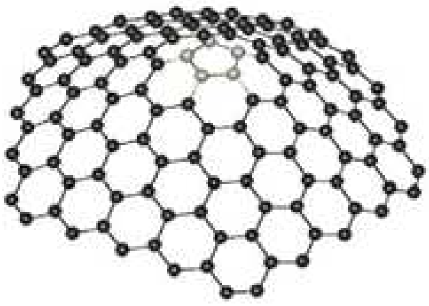

Figure 3. $NC_5(4)$ Nanocone

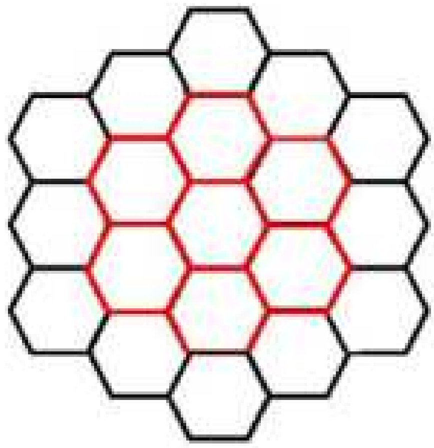

Figure 4. $NC_6(2)$ Nanocone

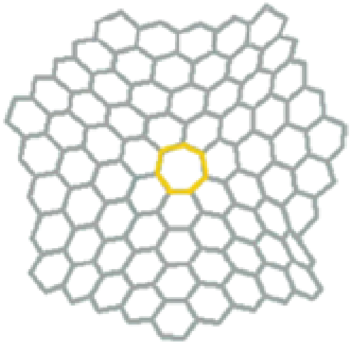

Figure 5. $NC_7(4)$ Nanocone

Similar calculation shows that:

$\overline{M_1} = 3n^2k^4 + 11n^2k^3 + (15n^2 - 12n)k^2 + (9n^2 - 18n)k + (2n^2 - 6n)$,

$\overline{M_2} = \frac{9n^2}{2}k^4 + 15n^2k^3 + (\frac{37n^2}{2} - 18n)k^2 + (10n^2 - 23n)k + 2n^2 - 6n$,

$\overline{PM_1} = 2^{\frac{n^2k^4+2n^2k^3+(3n^2-4n)k^2+(4n^2-4n)k+2n^2-6n}{2}}.3^{\frac{n^2k^4+2n^2k^3+(n^2-4n)k^2-2kn}{2}}.$
$5^{n^2k^3+2n^2k^2+(n^2-2n)k}$,

$\overline{PM_2} = 2^{n^2k^3+3n^2k^2+(3n^2-3n)k+n^2-3n}.3^{n^2k^4+3n^2k^3+(3n^2-4n)k^2+(n^2-4n)k}$,

also: $PM_1^* = 2^{\frac{3k^2n+kn+4n}{2}}.3^{\frac{3k^2n+kn}{2}}.5^{2kn}$,

$PM^T = 2^{\frac{n^2k^4+2n^2k^3+(3n^2-n)k^2+(4n^2-2n)k+2n^2-2n}{2}}.3^{\frac{n^2k^4+2n^2k^3+(n^2-n)k^2-nk}{2}}.$
$5^{n^2k^3+2n^2k^2+n^2k}$. □

Theorem 3.2. Zagreb, multiplicative Zagreb indices and Coindices of $Ca_3(C_6)$, the third member of Capra- designed planar benzenoid series (see Figure6) are computed as follows:

$M_1 = 4.3^n + 18.7^(n-1) - 6$,

$$M_2 = \begin{cases} 24 & n = 1 \\ 27.7^{n-1} + 10.3^{n-1} - 15 & n > 1 \end{cases},$$

$$M_3 = \begin{cases} 0 & n = 1 \\ 4.3^{n-1} & n > 1 \end{cases},$$

$PM_1 = 2^{2.3^n+6}.3^{4.7^{n-1}-4}$,

$PM_2 = 2^{2.3^n+6}.3^{6.7^{n-1}-6}$,

$$\overline{M_1} = \begin{cases} 36 & n = 1 \\ 12.7^{2n-2} + 2.3^{2n} + 10.3^n.7^{n-1} - 4.3^n - 18.7^{n-1} + 6 & n > 1 \end{cases},$$

$$\overline{M_2} = \begin{cases} 36 & n = 1 \\ 18.7^{2n-2} + 2.3^{2n} + 12.3^n.7^{n-1} - 16.3^{n-1} - 36.7^{n-1} + 18 & n > 1 \end{cases},$$

$$\overline{PM_1} = \begin{cases} 2^{18} & n = 1 \\ 2^{2.7^{2n-2}+3^{2n}+5.3^n-8.7^{n-1}+6}.3^{2.7^{2n-2}+2.3^{n-1}-8.7^{n-1}+6}. & n > 1 \\ 5^{2.3^n.7^{n-1}+6.7^{n-1}-10.3^{n-1}-6} & \end{cases},$$

$$\overline{PM_2} = \begin{cases} 2^{18} & n = 1 \\ 2^{2.3^n.7^{n-1}+3^{2n}+3^n+6.7^{n-1}-6}. & n > 1 \\ 3^{2.3^n7^{n-1}-2.3^n+4.7^{2n-2}-10.7^{n-1}+6} & \end{cases},$$

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:

$d_{2,n} = 6(\frac{d_{2,n-1}-2}{2}) = 3d_{2,n-1} - 6.$

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 sixtimes 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.

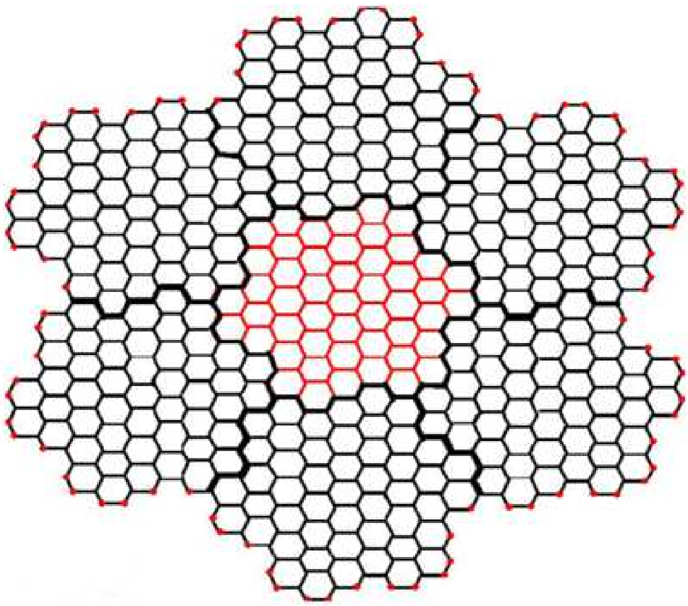

Figure 6. Graph $Ca_3(C_6)$ is the third member of Capra- designed planar benzenoid series $Ca_k(C_6)$

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

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

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:

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

So, the number of common vertices is equal to:

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

Therefore:

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

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:$d_3 = |V(G)| - d_2 = 2.7^{n-1} - 2.$
Elementary computation gives:

$M_1 = 4.3^n + 18.7^{n-1} - 6,$

$PM_1 = 2^{2.3^n+6}.3^{4.7^{n-1}-4}, PM_2 = 2^{2.3^n+6}.3^{6.7^{n-1}-6}.$

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

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

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.

$x_{22} = 6(\frac{x_{22,n-1}-2}{2}) = 3x_{22,n-1} - 6 = 3^{n-1} + 3,$

$x_{23} = 6(\frac{x_{23,n-1}}{2}) = 3x_{23,n-1} = 4.3^{n-1}$

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:

$$x_{22} = \begin{cases} 6 & n = 1 \\ 3^{n-1} + 3 & n > 1 \end{cases}, x_{23} = \begin{cases} 0 & n = 1 \\ 4.3^{n-1} & n > 1 \end{cases},$$

$$x_{33} = \begin{cases} 0 & n = 1 \\ 3.7^{n-1} - 2.3^{n-1} - 3 & n > 1 \end{cases},$$

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:

$$\overline{M_1} = \begin{cases} 36 & n = 1 \\ 12.7^{2n-2} + 2.3^{2n} + 10.3^n.7^{n-1} - 4.3^n - 18.7^{n-1} + 6 & n > 1 \end{cases},$$

$$\overline{M_2} = \begin{cases} 36 & n = 1 \\ 18.7^{2n-2} + 2.3^{2n} + 12.3^n.7^{n-1} - 16.3^{n-1} - 36.7^{n-1} + 18 & n > 1 \end{cases},$$

$$\overline{PM_1} = \begin{cases} 2^{18} & n = 1 \\ 2^{2.7^{2n-2}+3^{2n}+5.3^n-8.7^{n-1}+6}.3^{2.7^{2n-2}+2.3^{n-1}-8.7^{n-1}+6}. & n > 1 \\ 5^{2.3^n.7^{n-1}+6.7^{n-1}-10.3^{n-1}-6} & \end{cases},$$

$$\overline{PM_2} = \begin{cases} 2^{18} & n = 1 \\ 2^{2.3^n.7^{n-1}+3^{2n}+3^n+6.7^{n-1}-6}. & n > 1 \\ 3^{2.3^n 7^{n-1}-2.3^n+4.7^{2n-2}-10.7^{n-1}+6} & \end{cases},$$

also: $PM_1^* = \begin{cases} 2^{12} & n = 1 \\ 2^{3.7^{n-1}+3}.3^{3.7^{n-1}-2.3^{n-1}-3}.5^{4.3^{n-1}} & n > 1 \end{cases},$

$PM^T = 2^{2.7^{2n-2}+3^{2n}+5.3^n-5.7^{n-1}+9}.3^{2.7^{2n-2}-5.7^{n-1}+3}.$
$5^{2.3^n.7^{n-1}+6.7^{n-1}-2.3^n-6}.$ □

Acknowledgments

The authors are thankful to the anonymous referee for his expert and valuable comments to improve this article.

References

1. A. R. Ashrafi, T. Došlić, A. Hamzeh, The Zagreb Coindices of graph operations, Discrete Appl. Math. 158, (2010), 1571-1578.
2. A. R. Ashrafi, T. Došlić, A. Hamzeh, Extremal graphs with respect to the Zagreb coindices, MATCH Commun. Math. Comput. Chem., 65, (2011), 85-92.
3. G. H. Fath-Tabar, Old and new Zagreb indices of graphs, Communications in Mathematical and in Computer Chemistry, 65, (2011), 79-84.
4. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. III. Total $\pi_{-}electron$ energy of alternant hydrocarbons, Chem. Phys. Lett. 17, (1972), 535-538.
5. R. Todeschini, D. Ballabio and V. Consonni, Novel molecular descriptors based on functions of new vertex degrees. in: I. Gutman and B. Furtula (Eds.), Novel Molecular Structure Descriptors-Theory and Applications I, Univ. Kragujevac, Kragujevac, (2010), 73-100.
6. R. Todeschini and V. Consonni, New local vertex invariants and molecular descriptors based on functions of the vertex degrees, MATCH Commun. Math. Comput. Chem. 64, (2010), 359-372.
7. K. Xu, K. Ch. Das, K. Tang, On the multiplicative Zagreb coindex of graphs, Opuscula Math. 33, (2013), 191-204.
8. L. Yang, H. Hua, The Harmonic index of general graphs, nanoc-ones and triangular benzenoid graphs, Optoelectronics and Advanced Materials-Rapid Communications, 6, (2012), 660-663.

Vida Ahmadi
Department of Mathematics, Chamran University, Ahvaz, Iran.
E-mail address: `vidaahmadi_math@yahoo.com`

and

Mohammad Reza Darafsheh
Department of Mathematics, Tehran University, Tehran, Iran
E-mail address: `mrdaraf@yahoo.com`