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NARUMI-KATAYAMA AND MODIFIED NARUMI-KATAYAMA INDICES OF GRAPHS

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Abstract. Let G be a simple connected molecular graph in chemical graph theory, then its vertices correspond to the atoms and the edges to the bonds. Chemical graph theory is an important branch of graph theory, such that there exits many topological indices in it. Also, computing topological indices of molecular graphs is an important branch of chemical graph theory. Topological indices are numerical parameters of a molecular graph G which characterize its topology. In the present study we compute and report several results of the Narumi-Katayama and modified Narumi-Katayama indices for some widely used chemical molecular structures.

Key words : Zagreb indices, Narumi-Katayama index, multiple Zagreb index, chemical molecular structures, bridge Graph, triangular benzenoid.
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1. Introduction

A molecular graph $G = (V(G), E(G))$ with vertex set $V(G)$ and edge set $E(G)$ is a graph whose vertices denote atoms and edges denote bonds between the atoms of any underlying chemical structure. The degree of a vertex v, denoted by d_v, is the number of edges that are incident to it.

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The Zagreb indices were first introduced by Gutman in [25], they are important molecular descriptors and have been closely correlated with many chemical properties (see [28]) and defined as:

$$M_1(G) = \sum_{u\in V(G)} d_u^2 \quad \text{and}$$
$$M_2(G) = \sum_{uv\in E(G)} d_u d_v.$$

In 2012, Ghorbani and Azimi (see [24]) proposed the multiple versions of Zagreb indices of a graph G. These new indices are first multiplicative Zagreb index $PM_1(G)$, second multiplicative Zagreb index $PM_2(G)$ and defined as:

$$PM_1(G) = \prod_{uv\in E(G)} (d_u + d_v),$$

$$PM_2(G) = \prod_{uv\in E(G)} (d_u d_v).$$

In [26] authors studied some properties of Narumi-Katayama index which is defined as follows (see [27]):

$$NK(G) = \prod_{u\in V(G)} d_u.$$

The modified Narumi-Katayama index is defined by Ghorbani et al. as follows:

$$NK^*(G) = \prod_{u\in V(G)} d_u^{d_u}.$$

Clearly, second multiplicative Zagreb index and the modified Narumi-Katayama index are the same.

In order to calculate the number of edges of an arbitrary graph, the following lemma is significant for us.

Lemma 1. *Let G be a graph. Then*

$$\sum_{u\in V(G)} d_u = 2|E(G)|.$$

This is also known as handshaking Lemma. Several articles contributed to determining the topological indices of special molecular graphs (See Yan et al. [1] and [2], Gao and Shi [3] and [4], Gao and Wang [5], [6] and [7], Xi and Gao [8], Gao et al. [9], Gao et al., [10] and [11], Gao and Farahani [12], Farahani and Gao [13], and Farahani [14], [15], [16], [17], [18], [19], [20], [21], [22] and [23] for more details). In this paper, we compute the Narumi-Katayama and modified Narumi-Katayama indices for some widely used chemical molecular structures.

2. Narumi-Katayama and modified Narumi-Katayama indices of some graphs

Theorem 2. *Let G be a k-regular graph of n vertices, then*

(1) $NK(G) = k^n$;
(2) $NK^*(G) = (k)^{nk}$.

Proof. Since G is a k-regular graph, then each vertex of G has degree k and by Lemma 1 we have $\frac{kn}{2}$ edges. Consequently we get $NK(G) = k^n$ and $NK^*(G) = (k)^{nk}$. □

Let K_n denote the complete graph on n vertices and C_n denote the cycle on n vertices.

Theorem 3. *We have*

(1) $NK(K_n) = (n-1)^n$;
(2) $NK^*(K_n) = (n-1)^{n(n-1)}$;
(3) $NK(C_n) = 2^n$;
(4) $NK^*(C_n) = 2^{2n}$.

Proof. This proof can be obtained by using Theorem 2. □

Theorem 4. *Consider the wheel graph W_n and path P_n, then*

(1) $NK(W_n) = n3^n$;
(2) $NK^*(W_n) = n^n 3^{3n}$;
(3) $NK(P_n) = 2^{n-2}$;
(4) $NK^*(P_n) = 2^{2(n-2)}$.

Proof. A wheel graph is a graph formed by connecting a single vertex to all vertices of a cycle. In wheel graph W_n, the total number of vertices are $n+1$, out of which n vertices of degree 3 and 1 vertex of degree n and by Lemma 1 we have $2n$ edges (see Fig. 1). Furthermore, we obtain $|E_6| = |E_9^*| = n$ and $|E_{3+n}| = |E_{3n}^*| = n$. Consequently we get $NK(W_n) = n3^n$ and $NK^*(W_n) = n^n 3^{3n}$. In path graph P_n, the total number of vertices are n, out of which $n-2$ vertices of degree 2 and 2 vertices of degree 1 and by Lemma 1 we have $n-1$ edges $|E_3| = |E_2^*| = 2$ and $|E_4| = |E_4^*| = n-3$. Consequently we get $NK(P_n) = 2^{n-2}$ and $NK^*(P_n) = 2^{2(n-2)}$. □

Theorem 5. *Let T_n be a graph of triangular benzenoid, then*

(1) $NK(T_n) = 2^{3n+3} 3^{n^2+n-2}$;
(2) $NK^*(T_n) = 2^{6n+6} 3^{3n^2+3n-6}$.

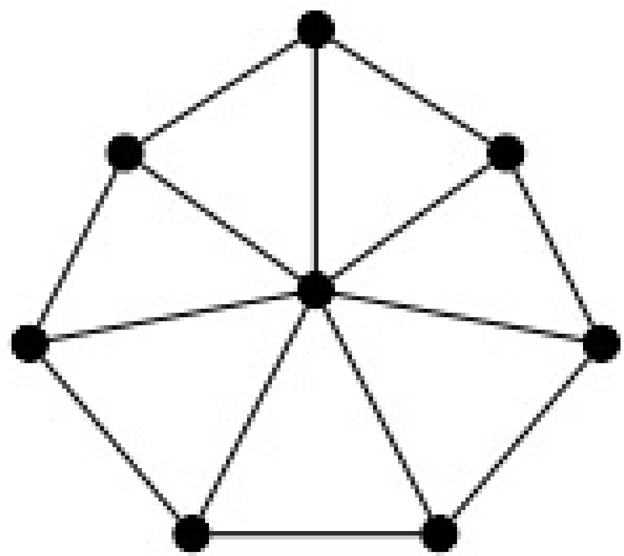

FIGURE 1. The wheel graph W_7

Proof. This graph has n^2+4n+1 vertices, out of which $3n+3$ vertices of degree 2 and n^2+n-2 vertices of degree 3 and by Lemma 1 we have $\frac{3(n^2+3n)}{2}$ edges (see Fig. 2). Furthermore, we obtain $|E_4| = |E_4^*| = 6$, $|E_6| = |E_9^*| = 6(n-1)$, and $|E_5| = |E_6^*| = \frac{3n(n-1)}{2}$. Consequently we get $NK(T_n) = 2^{3n+3}3^{n^2+n-2}$ and $NK^*(T_n) = 2^{6n+6}3^{3n^2+3n-6}$. □

3. Narumi-Katayama and modified Narumi-Katayama indices of bridge graph

Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint graphs with $v_i \in V(G_i)$. The bridge (molecular) graph $B(G_1, G_2, \cdots, G_d) = B(G_1, G_2, \cdots, G_d; v_1, v_2, \cdots, v_d)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ is yielded from the graphs $G_1, G_2, \cdots, G_d$ in which the vertices v_i and v_{i+1} are connected by an edge for $i = 1, 2, \cdots, d-1$. The main result of this section is determining the formulas of some degree based indices for the infinite family of nano structures of bridge graph with $G_1, G_2, \cdots, G_d$ (see Fig.3). We set $G_d(H, v) = B(H, H, \cdots, H; v, v, \cdots, v)$ for special situations of bridge graphs. In the following context of this section, we discuss the bridge graphs in which the main parts of graphs are path, cycle and complete graph, respectively.

Theorem 6. *Let $G_d(P_n, v)$ be a bridge graph, then*

(1) $NK(G_d(P_n, v)) = 2^{(n-2)d+2}3^{d-2}$;

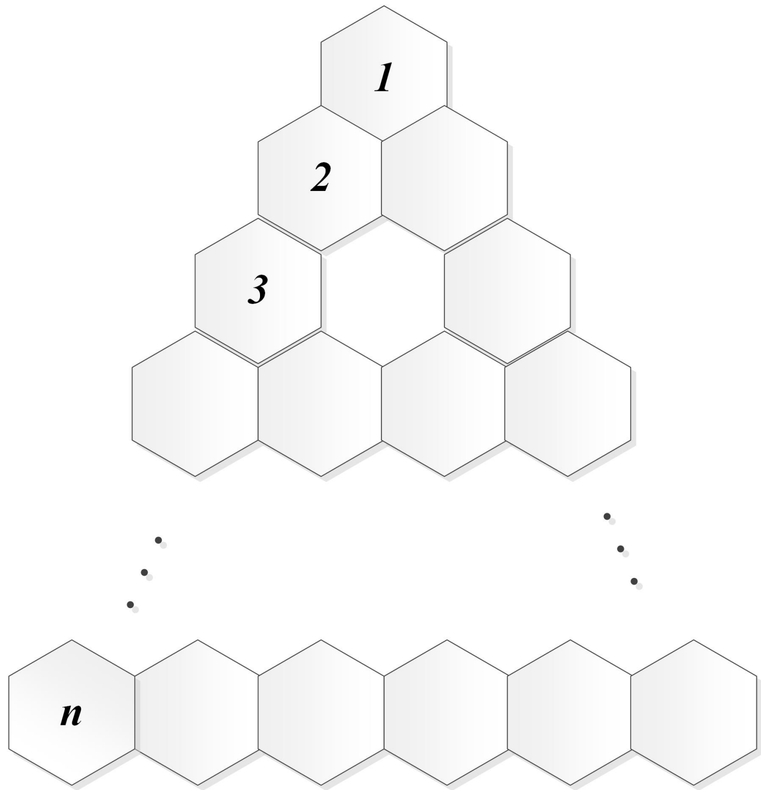

FIGURE 2. The triangular benzenoid T_n.

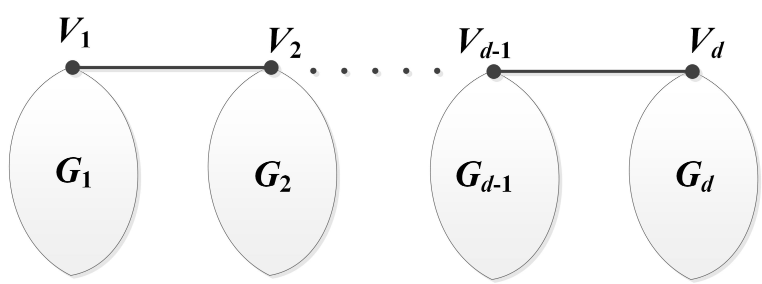

FIGURE 3. The bridge graph T_n.

(2) $NK^*(G_d(P_n, v)) = 2^{2((n-2)d+2)}3^{3(d-2)}$.

Proof. This graph has nd vertices, out of which d vertices of degree 1, $(n-2)d+2$ vertices of degree 2 and $d-2$ vertices of degree 3 and by Lemma 1 we have $nd-1$ edges (see Fig. 4). Furthermore, we obtain $|E_5| = |E_6^*| =$

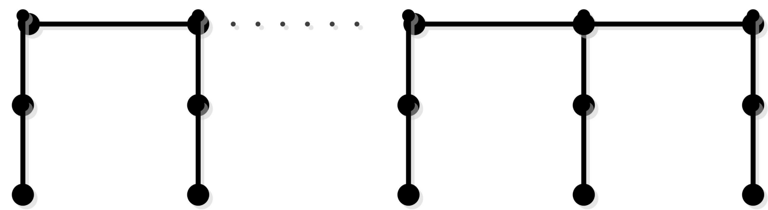

FIGURE 4. The nano structures bridge graph $G_d(P_n; v1)$.

d, $|E_6| = |E_9^*| = d-3$, $|E_4| = |E_4^*| = d(n-3)+2$, $|E_3| = |E_2^*| = d$. Consequently we get $NK(G_d(P_n,v)) = 2^{(n-2)d+2}3^{d-2}$ and $NK^*(G_d(P_n,v)) = 2^{2((n-2)d+2)}3^{3(d-2)}$. □

Theorem 7. *Let $G_d(C_n,v)$ be a bridge graph, then*

(1) $NK(G_d(C_n,v)) = 2^{(n-1)d}4^{d-2}9$;
(2) $NK^*(G_d(C_n,v)) = 3^{2(3)}2^{2(n-1)d}4^{4(d-2)}$.

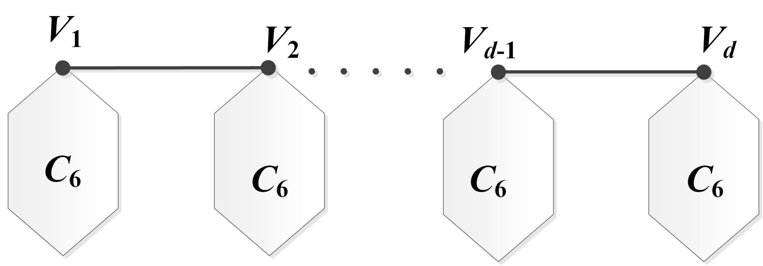

FIGURE 5. The nano structures bridge graph $G_d(C_6; v)$.

Proof. This graph has dn vertices, out of which $(n-1)d$ vertices of degree 2, 2 vertices of degree 3 and $d-2$ vertices of degree 4 and by Lemma 1 we have $dn+d-1$ edges (see Fig. 5). Furthermore, we obtain $|E_5| = |E_6^*| = 4$, $|E_6| = |E_8^*| = 2d-4$, $|E_4| = |E_4^*| = d(n-2)$, $|E_8| = |E_{16}^*| = d-3$ and $|E_7| = |E_{12}^*| = 2$. Consequently we get $NK(G_d(C_n,v)) = 2^{(n-1)d}4^{d-2}9$ and $NK^*(G_d(C_n,v)) = 3^{2(3)}2^{2(n-1)d}4^{4(d-2)}$. □

Theorem 8. *Let $G_d(K_n,v)$ be a bridge graph, then*

(1) $NK(G_d(K_n,v)) = n^2.(n+1)^{d-2}(n-1)^{(n-1)d}$;
(2) $NK^*(G_d(K_n,v)) = n^{2n}.(n+1)^{(d-2)(n+1)}(n-1)^{(n-1)^2d}$.

Proof. This graph has dn vertices, out of which 2 vertices of degree n, $d-2$ vertices of degree $n+1$ and $(n-1)d$ vertices of degree $n-1$ and by Lemma

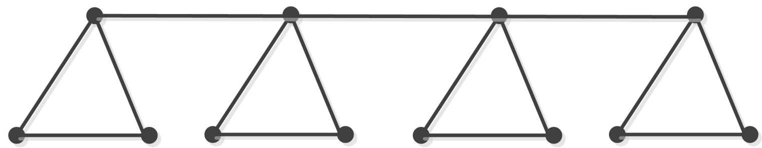

FIGURE 6. The nano structures bridge graph $G_d(K_3; v)$.

1 we have $\frac{dn(n-1)}{2} + d - 1$ edges (see Fig. 6). Furthermore, we obtain $|E_{2n+1}| = |E^*_{n^2+n}| = 2$, $|E_{2(n+1)}| = |E^*_{(n+1)^2}| = d - 3$, $|E_{2n}| = |E^*_{n^2-1}| = (d-2)(n-1)$, $|E_{2n-1}| = |E^*_{n^2-n}| = 2n - 2$ and $|E_{2(n-1)}| = |E^*_{(n-1)^2}| = [\frac{(n-1)(n-2)}{2}]d$. Consequently we get $NK(G_d(K_n, v)) = n^2.(n+1)^{d-2}(n-1)^{(n-1)d}$ and $NK^*(G_d(K_n, v)) = n^{2n}.(n+1)^{(d-2)(n+1)}(n-1)^{(n-1)^2 d}$. □

REFERENCES

[1] L. Yan, J. S. Li, W. Gao: *Vertex PI index and Szeged index of certain special molecular graphs*, The Open Biotechnology Journal, 8(2014), 19-22.

[2] L. Yan, W. Gao, J. S. Li: *General harmonic index and general sum connectivity index of polyomino chains and nanotubes*, Journal of Computational and Theoretical Nanoscience, In press.

[3] W. Gao, L. Shi: *Szeged related indices of unilateral polyomino chain and unilateral hexagonal chain*, IAENG International Journal of Applied Mathematics, 45(2)(2015), 138-150.

[4] W. Gao, L. Shi: *Wiener index of gear fan graph and gear wheel graph*, Asian Journal of Chemistry, 26(11)(2014), 3397-3400.

[5] W. Gao, W. F. Wang: *The vertex version of weighted wiener number for bicyclic molecular structures*, Computational and Mathematical Methods in Medicine, Volume 2015, Article ID 418106, 10 pages, http://dx.doi.org/10.1155/2015/418106.

[6] W. Gao, W. F. Wang: *Second atom-bond connectivity index of special chemical molecular structures*, Journal of Chemistry, Volume 2014, Article ID 906254, 8 pages, http://dx.doi.org/10.1155/2014/906254.

[7] W. Gao, W. F. Wang: *Revised szeged index and revised edge-szeged index of special chemical molecular structures*, Journal of Interdisciplinary Mathematics, In press.

[8] W. F. Xi, W. Gao: *Geometric-arithmetic index and Zagreb indices of certain special molecular graphs*, Journal of Advances in Chemistry, 10(2)(2014), 2254-2261.

[9] Y. Gao, W. Gao, L. Liang: *Revised Szeged index and revised edge Szeged index of certain special molecular graphs*, International Journal of Applied Physics and Mathematics, 4(6)(2014), 417-425.

[10] W. Gao, L. Liang, Y. Gao: *Some results on Wiener related index and Shultz index of molecular graphs*, Energy Education Science and Technology: Part A, 32(6)(2014), 8961-8970.

[11] W. Gao, L. Liang, Y. Gao: *Total eccentricity, adjacent eccentric distance sum and Gutman index of certain special molecular graphs*, The BioTechnology: An Indian Journal, 10(9)(2014), 3837-3845.

[12] W. Gao, M. R. Farahani: *The theta polynomial $\Theta(G,x)$ and the theta index $\Theta(G)$ of molecular graph polycyclic aromatic hydrocarbons PAHk*, Journal of Advances in Chemistry, 12(1)(2015), 3934-3939.

[13] M. R. Farahani, W. Gao: *The multiply version of Zagreb indices of a family of molecular graph "polycyclic aromatic hydrocarbons (PAHS)"*, Journal of Chemical and Pharmaceutical Research, 7(10)(2015), 535-539.

[14] M. R. Farahani: *The theta $\Theta(G,x)$ polynomial of an infinite family of the linear parallelogram $P(n,m)$*, Journal of Applied Physical Science International, 4(4)(2015), 206-209.

[15] M. R. Farahani: *The Wiener index and hosoya polynomial of a class of Jahangir graphs $J_{3,m}$*, Fundamental Journal of Mathematics and Mathematical Science, 3(1)(2015), 91-96.

[16] M. R. Farahani: *Hosoya, Schultz, modified Schultz polynomials and their topological indices of benzene molecules: first members of polycyclic aromatic hydrocarbons (PAHs)*, International Journal of Theoretical Chemistry, 1(2)(2013), 9-16.

[17] M. R. Farahani: *On the Schultz polynomial, modified Schultz polynomial, Hosoya polynomial and Wiener index of circumcoronene series of benzenoid*, Journal of Applied Mathematics and Informatics, 31(5-6)(2013), 595-608.

[18] M. R. Farahani: *Computing eccentricity connectivity polynomial of circumcoronene series of benzenoid H_k by ring-cut method*, Annals of West University of Timisoara-Mathematics and Computer Science, 51(2)(2013), 29-37.

[19] M. R. Farahani: *Third-connectivity and third-sum-connectivity indices of circumcoronene series of benzenoid H_k*, Acta Chimica Slovenica, 60(2013), 198-202.

[20] M. R. Farahani: *A new version of Zagreb index of circumcoronene series of benzenoid*, Chemical Physics Research Journal, 6(1)(2013), 27-33.

[21] M. R. Farahani: *On multiple Zagreb indices of dendrimer nanostars*, International Letters of Chemistry, Physics and Astronomy, 52(2015), 147-151.

[22] M. R. Farahani: *Hosoya polynomial of jahangir graphs $J_{4,m}$*, Global Journal of Mathematics, 3(1)(2015), 232-236.

[23] M. R. Farahani: *Using the cut method to computing GA_3 of circumcoronene series of benzenoid H_k*, International Journal of Chemical Model, 6(1)(2014), 9-16.

[24] M. Ghorbani, N. Azimi: *Note on multiple Zagreb indices*, Iran. J. Math. Chem., 3(2)(2012), 137-143.

[25] I. Gutman, N. Trinajstić: *Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons*, Chem. Phys. Assumet., 17(1972), 535–538.

[26] I. Gutman, M. Ghorbani.: *Some properties of Narumi-Katayama index*, Appl. Math. Lett., 25(10)(2012), 1435-1438.

[27] H. Narumi, M. Katayama.: *Simple topological index, A newly devised index characterizing the topological nature of structural isomers of saturated hydrocarbons*, Mem. Fac. Engin. Hokkaido Univ., 16(1984), 209-214.

[28] R. Todeschini, V. Consonni.: Handbook of molecular descriptors, Wiley-VCH, Weinheim, (2000).