Some topological polynomial indices of nanostructures

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Let G=(V,E) be a graph, where V is a non-empty set of vertices and E is a set of edges. Suppose that G be a graph, e=uv∈E(G), d(u) be degree of vertex u. In this paper we compute Zagreb, Randić and *ABC* indices Polynomial of TUC4C8(S), TUC4C8(R) nanotube and V-Phenylenic nanotorus.

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1. Introduction

All of the graphs in this paper are simple. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted [2].

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [3,4,5]. This theory had an important effect on the development of the chemical sciences.

A topological index is a numeric quantity from the structural graph of a molecule. 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 [6].

If $x,y \in V(G)$ then the distance $d_G(x,y)$ between x and y is defined as the length of any shortest path in G connecting x and y.

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajstić [3]. They are defined $ZG_1(G)=\sum_{e\in E(G)} d_u + d_v$, $ZG_2(G)=\sum_{e\in E(G)} d_v d_u$ and Zagreb Polynomial index is defined $ZG_1(G,x)=\sum_{e\in E(G)} x^{d_v+d_u}$, $ZG_2(G,x)=\sum_{e\in E(G)} x^{d_v d_u}$.

where d_u and d_v are the degrees of u and v. The connectivity index introduced in 1975 by Milan Randić [4, 5, 6], who has shown this index to reflect molecular branching. Randić index (Randić molecular connectivity index) was defined as follows $\chi(G)=\sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$.

Recently Furtula et al. [2] introduced atom-bond connectivity (*ABC*) index, which it has been applied up until now to study the stability of alkanes and the strain energy of cycloalkanes. This index is defined as follows $ABC(G)=\sum_{uv\in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u+d_v}}$. And Polynomial $\chi(G), ABC(G)$ indices is defined $\chi_P(G,x)=\sum_{uv\in E(G)} x^{\frac{1}{\sqrt{d_u d_v}}}$, $ABC_P(G,x)=\sum_{uv\in E(G)} x^{\sqrt{\frac{d_u+d_v-2}{d_u+d_v}}}$.

2. Main result and discusion

Diudea and his co-authors was the first scientist considered topological indices of nanostructures into account. In some research paper, he and his team computed the Wiener index of armchair, zig-zag and TUC_4C_8(R/S) nanotubes. One of us (ARA) continued this program to compute the Wiener index of a polyhex and TUC_4C_8(R/S) nanotori. In this sections, we compute this indices, for some well-known class of graphs, and in continue we calculate this indices for TUC_4C_8(S) nanotube and V-Phenylenic nanotorus.

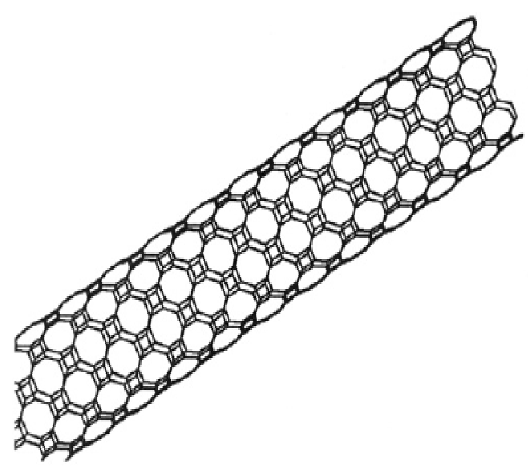

Fig. 1. A TUC_4C_8(S) nanotube.

Example 1. Let C_n be a cycle on n vertices. We know all of vertices are of degree 2 and so

$$ZG_1(C_n,x) = ZG_2(C_n,x) = nx^4 \,,\, \chi_P(C_n,x) = n\sqrt{x}$$

and $ABC_P(C_n,x) = n\sqrt[\sqrt{2}]{x}$

Example 2. Let K_n be a complete graph on n vertices. We know all of vertices of degree n-1 and so

$$ZG_1(K_n,x) = \sum_{uv\in E(K_n)} x^{2(n-1)} = nx^{2n-2}$$

$$ZG_2(K_n,x) = \sum_{uv\in E(K_n)} x^{(n-1)^2} = nx^{(n-1)^2} \,,$$

$$\chi(K_n,x) = \sum_{uv\in E(K_n)} x^{\frac{1}{\sqrt{(n+1)^2}}} = n\sqrt[(n+1)]{x} \quad \text{and}$$

$$ABC_P(K_n,x) = \sum_{uv\in E(K_n)} x^{\sqrt{\frac{(n-1)+(n-1)-2}{(n-1)+(n-1)}}} = nx^{\sqrt{\frac{2n-4}{2n-2}}}$$

Example 3. Let S_n be a star on *n + 1* vertices. One can see there are *n* vertices of degree *1* and a vertex of degree *n*. So,

$$ZG_1(S_n,x) = xZG_2(S_n,x) = \sum_{uv\in E(S_n)} x^{n+1} = nx^{n+1}$$

$$\chi_P(S_n,x) = \sum_{uv\in E(S_n)} x^{\frac{1}{\sqrt{n\times 1}}} = n\cdot\sqrt[\sqrt{n}]{x} \quad \text{and}$$

$$ABC_P(S_n,x) = \sum_{uv\in E(S_n)} x^{\sqrt{\frac{n+1-2}{n+1}}} = nx^{\sqrt{\frac{n-1}{n+1}}} \,.$$

Example 4. Let Wn be a graph of wheel on *n + 1* vertices. One can see there are *n* vertices of degree *3* and a vertex of degree *n*. So $|E(W_n)|=2n$, we have e_1 and e_2 cases of edges in E(Wn) is different and $|E(e_1)|=n$, $|E(e_2)|=n$. Then

$$ZG_1(W_n,x) = \sum_{uv\in E(W_n)} x^{d_v+d_v} =$$

$$\sum_{uv\in E(e_1)} x^6 + \sum_{uv\in E(e_2)} x^{n+3} = nx^3(x^{n-1}+x^3+1)$$

$$ZG_2(W_n,x) = \sum_{uv\in E(W_n)} x^{d_v d_v} =$$

$$\sum_{uv\in E(e_1)} x^9 + \sum_{uv\in E(e_2)} x^{3n} = nx^n(x^{2n}+1)$$

$$\chi_P(W_n,x) = \sum_{uv\in E(W_n)} x^{\frac{1}{\sqrt{d_v d_u}}} =$$

$$\sum_{uv\in E(e_1)} \sqrt[3]{x} + \sum_{uv\in E(e_2)} \sqrt[3n]{x} = n(\sqrt[3n]{x}+\sqrt[3]{x})$$

$$ABC_P(W_n,x) = \sum_{uv\in E(W_n)} x^{\sqrt{\frac{d_v+d_u-2}{d_v+d_u}}} =$$

$$\sum_{uv\in E(e_1)} x^{\sqrt{\frac{2}{3}}} + \sum_{uv\in E(e_2)} x^{\sqrt{\frac{n+1}{n+3}}} =$$

$$n(\sqrt[\sqrt{3}]{x^{\sqrt{2}}} + \sqrt[\sqrt{n+3}]{x^{\sqrt{n+1}}})$$

Now we compute Zagreb, Randić and *ABC* indices of a $TUC_4C_8(S)$ nanotube as described above. The Randić, Zagreb and *ABC* indices of the 2-dimensional lattice of $TUC_4C_8(S)$ graph K= KTUC[p,q] (Fig 2) is also computed. Following Diudea [8,9], we denote a TUC4C8(R) nanotorus by H = HTUC[p,q] (Fig 3).
It is easy to see that |V(K)| = |V(H)| =8pq, |E(K)| = 12pq - 2p-2q and |E(H)| = 12pq. We also denote an V-Phenylenic nanotorus by Y = VPHY[4p,2q] where |E(Y)|=36pq see Fig 4.

One can see that $ZG_1(G,x) = \sum_{i=1}^{|E(G)|} x^{\beta_i}$,

$$ZG_2(G,x) = \sum_{i=1}^{|E(G)|} x^{\alpha_i} \,,\, \chi_P(G,x) = \sum_{i=1}^{|E(G)|} x^{\frac{1}{\sqrt{\alpha_i}}} \,.$$

And $ABC_P(G,x) = \sum_{i=1}^{|E(G)|} x^{\sqrt{\frac{\beta_i-2}{\beta_i}}}$ where $\alpha_i = d_{v_i} d_{u_i}$ and $\beta_i = d_{v_i} + d_{u_i}$. So whit respect the molecular graph of K (Fig. 2), one can see that there are three separate cases and the number of edges is different. Suppose e_1, e_2 and e_3 are representative edges for these cases. Then $\alpha_1 = \alpha_3 = \beta_1 = \beta_3 = 4$, $\alpha_2 = 6$ and $\beta_2 = 5$.

We define $N(e)=|\{e' \in E(G) \text{ s.t } e||e'\}|$, in graph G, so we have $N(e_1)$= 2p+2q+4 , $N(e_2)$= 4(p + q - 2) and $N(e_3)$= 12pq – 8 p -8 q + 4.

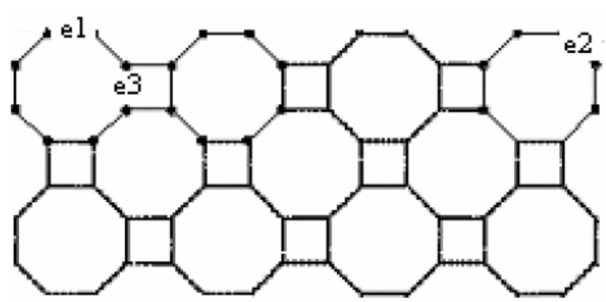

Fig. 2. 2-Dimensional Lattice of TUC4C8(S) Nanotorus with p = 4 and q = 2.

$$ZG_1(TUC_4C_8(S),x) = \sum_{i=1}^{|E(G)|} x^{\beta_i}$$

$$= N(e_1)x^{\beta_1} + N(e_2)x^{\beta_2} + N(e_3)x^{\beta_3}$$

$=6(2pq-p-q+1)x^4+4(p+q-2)x^5$

$$ZG_2(TUC_4C_8(S),x) = \sum_{i=1}^{|E(G)|} x^{\alpha_i}$$

$$= N(e_1)x^{\alpha_1} + N(e_2)x^{\alpha_2} + N(e_3)x^{\alpha_3}$$

$=6(2pq-p-q+1)x^4+4(p+q-2)x^6$

$$ABC_P(TUC_4C_8(S),x) = \sum_{i=1}^{|E(G)|} x^{\sqrt{\frac{\beta_i-2}{\beta_i}}}$$

$$= N(e_1)x^{\sqrt{\frac{\beta_1-2}{\beta_1}}} + N(e_2)x^{\sqrt{\frac{\beta_2-2}{\beta_2}}}$$

$$+ N(e_3)x^{\sqrt{\frac{\beta_3-2}{\beta_3}}}$$

$=6(2pq-p-q+1)\, x^{\frac{\sqrt{2}}{2}} +4(p+q-2)\, x^{\sqrt{\frac{3}{5}}}$

$$\chi_P(TUC_4C_8(S),x) = \sum_{i=1}^{|E(G)|} x^{\frac{1}{\sqrt{\alpha_i}}} =$$

$$N(e_1)x^{\frac{1}{\sqrt{\alpha_1}}} + N(e_2)x^{\frac{1}{\sqrt{\alpha_2}}} + N(e_3)x^{\frac{1}{\sqrt{\alpha_3}}}$$

$=6(2pq-p-q+1)\sqrt{x} +4(p+q-2)\sqrt[\sqrt{6}]{x}$

We now consider the molecular graph H=HTUC[p,q], Fig. 3, and Y=V-Phenylenic nanotorus Fig. 7.

Theorem 1. For an arbitrary graph G,

(a) $ZG_1(G,x) = |E(G)| \cdot x^{2k}$ if and only if G be a k-regular graph.

(b) $ZG_2(G,x) = |E(G)| \cdot x^{k^2}$ if and only if G be a k-regular graph.

(c) $\chi_P(G,x) = |E(G)| \cdot \sqrt[k]{x}$ if and only if G be a k-regular graph.

(d) $ABC_P(G,x) = |E(G)| \cdot x^{\sqrt{\frac{k-1}{k}}}$ if and only if G be a k-regular graph.

Proof: If G be k-regular then it is easy to see that for every $e \in V(G)$, $\alpha_i = k^2$ and $\beta_i = \sqrt{\frac{k-1}{k}}$, then $ZG_1(G)$, $ZG_2(G)$, $\chi(G)$ and $ABC(G)$ implies that this indices Polynomial.

Conversely, for (b) suppose $ZG_2(G,x) = |E(G)| \cdot x^{k^2}$

So $x^{\alpha_1} + x^{\alpha_2} + \cdots + x^{\alpha_{|E(G)|}} = |E(G)|\, x^{k^2}$ this implies $\alpha_i = d_{v_i} d_{u_i} = k^2$ and $d_{v_i} = d_{u_i} = k$ then G, k-regular. And for (d) suppose $ABC_P(G,x) = |E(G)| \cdot x^{\sqrt{\frac{k-1}{k}}}$ then $x^{\beta_1} + x^{\beta_2} + \cdots + x^{\beta_{|E(G)|}} = x^{\sqrt{\frac{k-1}{k}}}\, |E(G)|$, so $x^{\beta_i}\, |E(G)| = x^{\sqrt{\frac{k-1}{k}}}\, |E(G)| \Rightarrow \beta_i = \sqrt{\frac{k-1}{k}}$ for $1 \le i \le |E(G)|$ and this proof (d) is completed. Proof (a) and (c) are similarly.

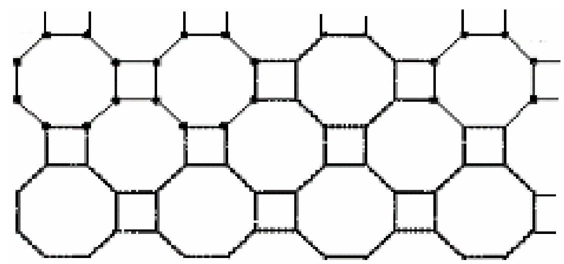

Fig. 3. The 2-Dimensional Lattice of TUC4C8(R) Nanotorus.

By using Theorem 1, consider the Fig. 3. One can see that $TUC_4C_8(S)$ graph is 3-regular, so

$$ZG_1(TUC_4C_8(R),x) = |E(TUC_4C_8(R))| x^{2k}$$

$$= 12pqx^6$$

$$ZG_2(TUC_4C_8(R),x) = |E(TUC_4C_8(R))| x^{k^2}$$

$$=12pqx^9$$

$$\chi_P(TUC_4C_8(R),x) = |E(TUC_4C_8(R))|\, \sqrt[k]{x}$$

$$= 12pq\sqrt[3]{x}$$

and

$$ABC_P(TUC_4C_8(R),x) = |E(TUC_4C_8(R))|\, x^{\sqrt{\frac{k-1}{k}}} =$$

$$12pq\sqrt[\sqrt{3}]{x^{\sqrt{2}}}$$

Naw by using Theorem 1, consider the Y=V-Phenylenic nanotorus, Fig. 4.

$$ZG_1(Y,x) = |E(Y)| x^{2k} = 36pqx^6,$$

$$ZG_2(Y,x) = |E(Y)| x^{k^2} = 36pqx^9,$$

$$\chi_P(Y,x) = |E(Y)|\, \sqrt[k]{x} = 36pq\sqrt[3]{x}.$$

And $ABC_P(Y,x) = |E(Y)|\, x^{\sqrt{\frac{k-1}{k}}} = 36pqx^{\sqrt{\frac{2}{3}}}$

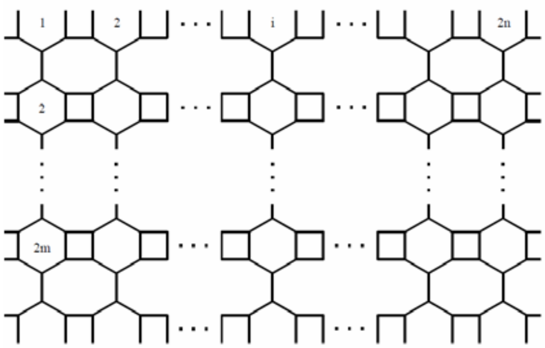

Fig. 4. A V-Phenylenic nanotorus.

3. Conclusions

In this paper a method for computing Polynomial of Zagreb Index, Randić Index, *ABC* Index over a new class of nanostructures is presented. This method is useful for working by all nanostructures. We applied our method on an infinite class of nanostructures.

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