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Computing Ga index of HAC_5C_7 [p, q] and $HAC_5C_6C_7$ [p, q] nanotubes

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Let $\sum$ be the class of finite graphs. A topological index is a function Top from $\sum$ in to real numbers with this property that Top(G) = Top(H), if G and H are isomorphic. Let G be a graph and e = uv be an edge of G. The GA index of G is defined as $GA(G)=\sum_{e\in E}\frac{2\sqrt{dudv}}{du+dv}$. In this paper we compute some results about this new topological index.

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1. Introduction

A nanostructure is an object of intermediate size between molecular and microscopic structures. It is product derived through engineering at molecular scale. The most important of these new materials are carbon nanotubes [1-3].

A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph also called vertices and edges of the graph, respectively. If e is an edge of G, connecting the vertices u and v, then we write e=uv and say "u and v are adjacent".

Let G be a graph and e = uv be an edge of G. The GA index of G was introduced by D. Vukicevic and co-authors as GA(G) = $\sum_{i=1}^{|E(G)|}\xi_i$ in which, for the edge $e_i = u_i v_i$ $\in$ E(G), $\xi_i=\frac{2\sqrt{du_i dv_i}}{du_i+dv_i}$ and du denoted to the degree of vertex u.[4-12].

For physico-chemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, and a centric factor. The predictive power of GA index is somewhat better than predictive power of the Randic connectivity index [13]. In [14-19], some topological indices are computed for some nanotubes and nanotori.

In this paper we compute some results about this new topological index.

2. Results and discussion

The aim of this section is to compute the GA index of HAC_5C_6 [p,q] and $HAC_5C_6C_7$[p,q] nanotubes.

Now we compute the GA index of HAC_5C_7 [p,q] nanotube.

A C_5C_7 net is a trivalent decoration made by alternating C_5 and C_7. It can cover either a cylinder or a torus. In Fig. 1 an HAC_5C_7 [4,2] lattic is shown.

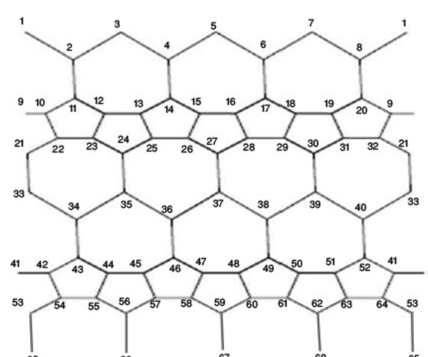

Fig. 1. 2-dimensional lattice of HAC_5C_7 [p,q] nanotube with p=4 , q=2.

We denote the number of heptagons in one row by P. In this nanotube, the three first rows of vertices and edges are repeated alternatively, and we denote the number of this repetition by q. In each period there are 8p vertices and p vertices which are joined to the end of the graph and hence the number of vertices in this nanotube is equal to 8pq + p.

$$V(HAC_5C_7[p,q]) = 8pq + p .$$

And in each period there are 12p edges and we have q repetition, hence the number of edges in this nanotube is equal to 12pq.

$$E(HAC_5C_7[p,q]) = 12pq .$$

We 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. We can see that $\xi_1 = \frac{2\sqrt{6}}{5}$, $\xi_2 = \frac{2\sqrt{3}}{4} = \frac{\sqrt{3}}{2}$ and $\xi_3 = 1$.

By the definition of GA index and Table 1 we can see that,

$$GA(HAC5C7[p,q]) = 2p(\frac{2\sqrt{6}}{5}) + p(\frac{\sqrt{3}}{2})$$
$$+12pq - 3p = \frac{4p\sqrt{6}}{5} + \frac{p\sqrt{3}}{2} + 12pq - 3p$$

Table 1. computing the ξ_i for the 2-dimensional lattice of HAC_5C_7 graph.

No.	ξ_i	Type of edges
2p	$\frac{2\sqrt{6}}{5}$	e_1
P	$\frac{2\sqrt{3}}{4} = \frac{\sqrt{3}}{2}$	e_2
12pq-2p-p	1	e_3

Now we compute GA index of $HAC_5C_6C_7$ [p,q] nanotube.

A $C_5C_6C_7$ net is a trivalent decoration made by alternating C_5, C_6, and C7. It can cover either cylinder or a torus. In this section we compute the GA index of $HAC_5C_6C_7$ [p,q] nanotube similar to the precious section. In Fig. 2 an HAC5C6C7[4,2] lattice is shown.

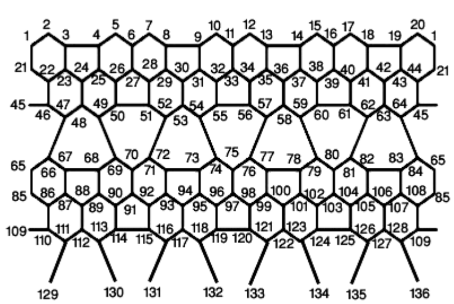

Fig. 2.2-dimensional lattice of $HAC_5C_6C_7$ [p,q] nanotube with p=4 , q=2.

We denote the number of pentagons in first row by P. In this nanotube, the three first rows of vertices and edges are repeated alternatively, and we denote the number of this repetition by q. In each period there are 16p vertices and 2p vertices which are joined to the end of the graph and hence the number of vertices in this nanotube is equal to 16pq + 2p.

$$V(HAC_5C_6C_7[p,q]) = 16pq + 2p.$$

And in each period there are 24p edges and we have q repetition, hence the number of edges in this nanotube is equal to 24pq.

$$E(HAC_5C_6C_7[p,q]) = 24pq.$$

We 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. We can see that $\xi_1 = \frac{2\sqrt{6}}{5}$, $\xi_2 = \frac{2\sqrt{3}}{4} = \frac{\sqrt{3}}{2}$ and $\xi_3 = 1$

By the definition of GA index and Table 2 we can see that,

$$GA(HAC_5C_6C_7[p,q]) = 4p(\frac{2\sqrt{6}}{5}) + 2p(\frac{\sqrt{3}}{2})$$
$$+24pq - 4p - 2p = \frac{8p\sqrt{6}}{5} + p\sqrt{3} + 24pq - 6p.$$

Table 2. Computing the ξ_i for the 2-dimensional lattice of $HAC_5C_6C_7$[p,q] graph.

No.	ξ_i	Type of edges
4p	$\frac{2\sqrt{6}}{5}$	e_1
2p	$\frac{2\sqrt{3}}{4} = \frac{\sqrt{3}}{2}$	e_2
24pq-4p-2p	1	e_3

3. Conclusion

In this paper, we obtained the GA index of nanotubes, HAC_5C_6 [p,q] nanotubes and $HAC_5C_6C_7$[p,q] nanotubes for the first time.

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