

Computing Ga index for some nanotubes

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Let Σ be the class of finite graphs. A topological index is a function Top from Σ in to real numbers with this property that $\text{Top}(G) = \text{Top}(H)$, 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 $GA(G) = \sum_{e \in E} \frac{2\sqrt{du dv}}{du + dv}$. In this paper we compute some results about this new topological index.

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1. Introduction

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_i denoted to the degree

of vertex u.

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 [1]. In [2-15], 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 for some nanotubes.

Now we compute the GA index of TUAC₆ [p,q] nanotube.

A C₆ net is a trivalent decoration made by C₆. It can cover either a cylinder or a torus. In Fig. 1 an lattic TUAC₆ [4,8] is shown.

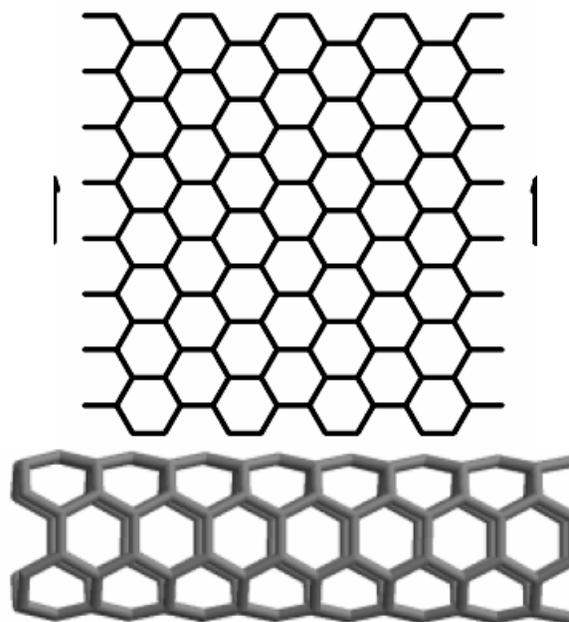


Fig. 1. 2-dimensional lattice of nanotube TUAC₆ [4,8].

We denote the number of hexagonal in the first row by P. In this nanotube, 8 rows of vertices and edges are repeated alternatively, and we denote the number of this repetition by q. In each period there are 4p vertices and we have q repetition.. Hence the number of vertices in this nanotube is equal to 4pq. That is

$$V(\text{TUAC}_6 [p,q]) = 4pq .$$

In each period there are 6p edges and we have q repetition, hence the number of edges in this nanotube is equal to 6pq, but there are 2p edges that are repeated in the end of graph hence the number of edges in this

nanotube is equal to $6pq-2p$. That is $E(TUAC_6[p,q]) = 6pq-2p$.

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

$$\xi_1 = \frac{2\sqrt{6}}{5}, \xi_2 = \frac{2\sqrt{4}}{4} = 1, \text{ and } \xi_3 = 1.$$

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

$$GA(TUAC_6[p,q]) = 8p \frac{\sqrt{6}}{5} + 6pq - 8p + 2p = 8p \frac{\sqrt{6}}{5} + 4pq - 6p.$$

Now we compute GA index of $TUZC_6[p,q]$ nanotube.

A C_6 net is a trivalent decoration made by C_6 . It can cover either a cylinder or a torus. In Fig. 2, an lattic $TUZC_6 [8,4]$ is shown.

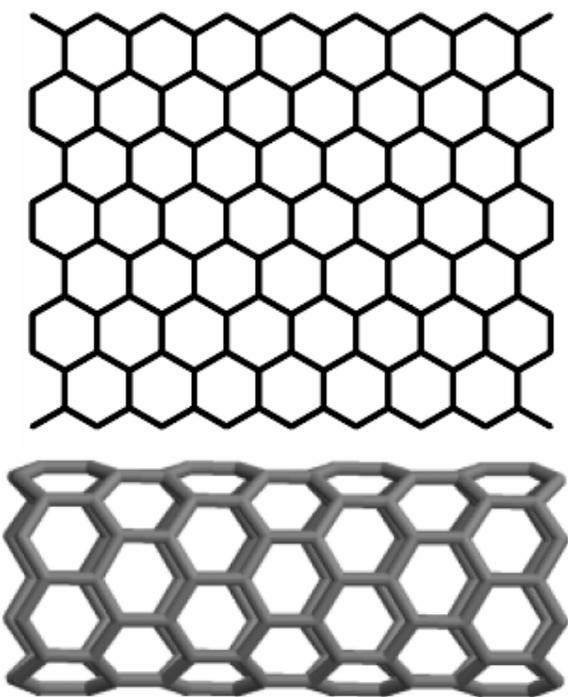


Fig. 2. 2-dimensional lattice of nanotube $TUZC_6 [8,4]$.

We denote the number of hexagonal in the first row by P . In this nanotube, 4 rows of vertices and edges are repeated alternatively, and we denote the number of this repetition by q . In each period there are $4p$ vertices and we have q repetition. Hence the number of vertices in this nanotube is equal to $4pq$.

$$V(TUZC_6 [p,q]) = 4pq .$$

In each period there are $6p$ edges and we have q repetition, hence the number of edges in this nanotube is equal to $6pq$, but there are p edges that are repeated in

the end of graph hence the number of edges in this nanotube is equal to $6pq-p$.

$$E(TUZC_6 [p,q]) = 6pq-p .$$

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

$$\xi_1 = \frac{2\sqrt{6}}{5} \text{ and } \xi_2 = 1$$

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

$$GA(TUZC_6 [p,q]) = 8p \frac{\sqrt{6}}{5} + 6pq - p - 4p = 8p \frac{\sqrt{6}}{5} + 4pq - 5p.$$

Table 1. Computing the ξ_i for the 2-dimensional lattice of $TUZC_6 [p,q]$ graph.

No.	ξ_i	Type of edges
$4p$	$\frac{2\sqrt{6}}{5}$	e_1
$6pq-5p$	$2 \frac{\sqrt{9}}{6} = 1$	e_2

Now we compute GA index of $HC_5C_7[p,q]$ 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. 3 a $HC_5C_7 [8, 4]$ lattic is shown.

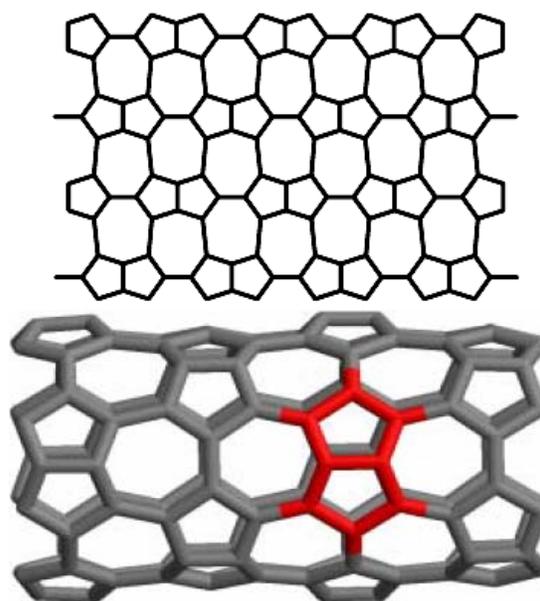


Fig. 3. 2-dimensional lattice of nanotube $HC_5C_7 [8,4]$.

We denote the number of heptagones in the first row by P . In this nanotube, 4 rows of pentagones are repeated alternatively, and we denote the number of this repetition by q . In each period there are $4p$ vertices and we have q repetition. Hence the number of vertices in this nanotube is equal to $4pq$. That is $V(HC_5C_7 [p,q]) = 4pq$.

In each period there are $6p$ edges and we have q repetition, hence the number of edges in this nanotube is equal to $6pq$, but there are p edges that are repeated in the end of graph hence the number of edges in this nanotube is equal to $6pq$. That is $E(HC_5C_7 [p,q]) = 6pq - p$. 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

$\xi_1 = \frac{2\sqrt{6}}{5}$, and $\xi_2 = 1$. By the definition of GA index and Table 2, we can see that, $GA(HC_5C_7 [p,q]) = 8p \frac{\sqrt{6}}{5} + 6pq - p - 4p = 8p \frac{\sqrt{6}}{5} + 4pq - 5p$.

Table 2. Computing the ξ_i for the 2-dimensional lattice of $HC_5C_7 [p,q]$ graph.

No.	ξ_i	Type of edges
$4p$	$\frac{2\sqrt{6}}{5}$	e_1
$6pq - 5p$	$2 \frac{\sqrt{9}}{6} = 1$	e_2

Now we compute GA index of $SC_5C_7 [p,q]$ 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. 4, a $SC_5C_7 [8, 4]$ lattice is shown.

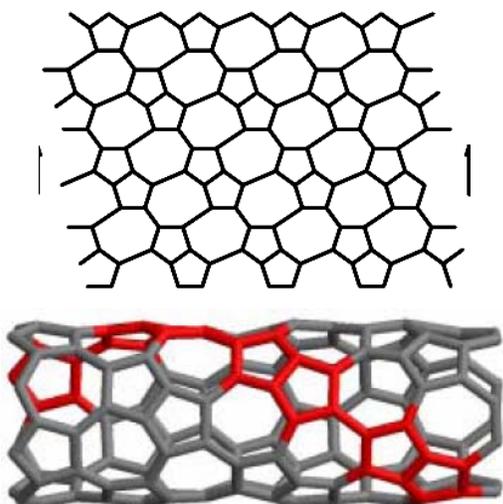


Fig. 4. 2-dimensional lattice of nanotube $SC_5C_7 [8,4]$.

We denote the number of heptagones in the first row by P . In this nanotube p is 8. In this nanotube, 4 rows of vertices and edges are repeated alternatively, and we denote the number of this repetition by q . In each period there are $4p$ vertices and we have q repetition. Hence the number of vertices in this nanotube is equal to $4pq$. That is $V(SC_5C_7 [p,q]) = 4pq$.

In each period there are $6p$ edges and we have q repetition, hence the number of edges in this nanotube is equal to $6pq$, but there are p edges that are repeated in the end of graph hence the number of edges in this nanotube is equal to $6pq - p$. That is $E(SC_5C_7 [p,q]) = 6pq - p$. 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

$\xi_1 = \frac{2\sqrt{6}}{5}$, $\xi_2 = \frac{2\sqrt{4}}{4} = 1$, and $\xi_3 = 1$.

By the definition of GA index and table 3 we can see that,

$GA(SC_5C_7 [p,q]) = 12q \frac{\sqrt{6}}{5} + q + 6pq - p - q - 6q = 12q \frac{\sqrt{6}}{5} + 6pq - p - 6q$.

Table 3. Computing the ξ_i for the 2-dimensional lattice of $SC_5C_7 [p,q]$ graph.

No.	ξ_i	Type of edges
$6q$	$\frac{2\sqrt{6}}{5}$	e_1
Q	$2 \frac{\sqrt{4}}{4} = 1$	e_2
$6pq - p - 7q$	$2 \frac{\sqrt{9}}{6} = 1$	e_3

3. Conclusion

In this paper, we obtained the GA index of $TUZC_6 [p,q]$ nanotubes, $TUAC_6 [p,q]$ nanotubes, $HC_5C_7 [p,q]$ nanotubes and $SC_5C_7 [p,q]$ nanotubes for the first time.

References

- [1] Yan Yuan, Bo Zhou, Nenad Trinajstić, J. Math. Chem 47 (2010).
- [2] A. Sousarai, A. Mahmiani, O. Khormali, Iranian Journal of Mathematical Sciences and Informatics, 3(1) 49 (2008).
- [3] A. Iranmanesh, B. Soliemani, MATCH Communications in Mathematical and in Computer Chemistry, 57, 251 (2007).
- [4] A. Iranmanesh, B. Soliemani, A. Ahmadi, Journal of

- Computational and Theoretical Nanoscience, **4**, 147 (2007).
- [5] A. Iranmanesh, A. R. Ashrafi, Journal of Computational and Theoretical Nanoscience, **4**, 514 (2007).
- [6] A. Iranmanesh, Y. Pakraves, Ars Combinatorics, **84**, 247 (2007).
- [7] A. Iranmanesh, Y. Pakraves, Utilitas Mathematica, **75**, 89 (2008).
- [8] Anehgaldi Mahmiani, Omid Khormali, A. Iranmanesh, Optoelectron. Adv. Mater. - Rapid Commun. **2**, 252 (2010).
- [10] Anehgaldi Mahmiani, Omid Khormali, A. Iranmanesh, Ali Ahmadi, Optoelectron. Adv. Mater. - Rapid Commun. **2**, 256 (2010).
- [11] A. Iranmanesh, Y. Pakraves, Optoelectron. Adv. Mater. - Rapid Commun., **2**, 264 (2010).
- [12] A. Iranmanesh, O. Khormali, J. Comput. Theor. Nanosci., **5**(1), 131 (2008).
- [13] A. R. Ashrafi, M. Jalali, M. Ghorbani, Optoelectron. Adv. Mater-Rapid Comm. **3**(8), 823 (2009).
- [14] A. R. Ashrafi, M. Ghorbani, Optoelectron. Adv. Mater-Rapid Comm. **3**(6), 596 (2009).
- [15] A. Iranmanesh, A. Soltani, O. Khormali, Optoelectron. Adv. Mater. - Rapid Commun., **4**(2), 242 (2010).

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