Balaban index of $C_4C_8(S)$ nanotubes

Abbas Heydari

Department of Science, Arak University of Technology, Arak, Iran

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Abstract

Let G be a simple connected graph. the Balaban index of a G is defined as

$$J(G) = \frac{m}{1+\mu} \sum_{uv \in E(G)} [d(u)d(v)]^{-\frac{1}{2}},$$

which m is the number of edges, μ is the cyclomatic number of G, $d(u)$ is the sum of the distance between vertex u and all of the vertices of G and the summation goes over all edges from the edge set $E(G)$. In this paper we obtain a method to compute the Balaban index of the nanotubes which have square and octagon structure and denoted by $C_4C_8(S)$.

1 Introduction

Let G be an simple connected graph. The sets of vertices and edges of G are denoted by $V(G)$ and $E(G)$, respectively. For vertices u and v in $V(G)$, we denote by $d(u,v)$ the topological distance i.e., the number of edges on the shortest path, joining the two vertices of G. Since G is connected, $d(u,v)$ exists for all $u, v \in V(G)$. The distance sum of a vertex u of G is defined as $d(u) = \sum_{v \in V(G)} d(u,v)$. Let u and v be two adjacent vertices of the graph G and $e = uv$ be the edge between them. The Balaban index of a molecular graph G was introduced by Balaban [1] in 1982 as one of less degenerated topological indices. It calculate the average distance sum connectivity index according to the equation

$$J(G) = \frac{m}{1+\mu} \sum_{uv \in E(G)} [d(u)d(v)]^{-\frac{1}{2}}. \tag{1.1}$$

where m is number of edges of G and μ is the minimum number of edges that must be removed from G in order to transform it to an acyclic graph (called cyclomatic number of G). If G is a connected graphs and n denote the number of vertices of G then $\mu = m - n + 1$. The Balaban index appears to be a very useful molecular descriptor with attractive properties [2], [3]. It has also been extended to weighted graphs and used successfully in QSAR/QSPR modelling [4], [5]. Recently computing topological indices of nanostructures have been the object of many papers [6]-[11]. In this paper we obtain an exact formula for computation the Balaban index of nanotubes which have square and octagon structure and denoted by $C_4C_8(S)$ nanotubes.

2 Main results

In this section at first we compute $d(v)$ or sum distance for all of the vertices v of the graph. In order of this propose we must choose a coordinate labelling for vertices of graph $TUC_4C_8(S)$ nanotubes as shown in Figure (2). Let the graph contain q rows and $2p$ columns of vertices (q is an even positive integers). In this case we denote the graph by $T(p,q)$. If $q \leq p$ the graph of $T(p,q)$ is called short and if $q > p$, then the graph is called long.

* Corresponding Author's E-mail: heydari@arakut.ac.ir

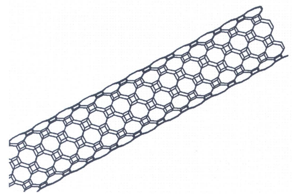

Figure 1: A $C_4C_8(S)$ nanotube.

To compute the value of Balaban index of $C_4C_8(S)$ nanotube by using equation (1.1), we most calculate $d(v)$ for all of the vertices of graph. So we compute the summation of distances between arbitrary vertex v of graph and all of the vertices of the graph in which are placed on k row bellow of the vertex v in the graph. Then by suitable summation on obtained results, we can derive summation of distances between vertex v and all of the vertices of the graph in which is equal to $d(v)$. For this propose we consider vertices x_{0p} and y_{0p} on the first row of the graph and calculate distance between vertices x_{0p} (or y_{0p}) and vertices where are placed on k-th row of the graph. The obtained results for these vertices can be used for vertices in which are placed on the other rows, by symmetry of the graph. Let x_{kt} and y_{kt} be vertices on k-th row and t-th column of the graph for $1 \leq k < q$ and $1 \leq t < p$. Put

$$d_x(k) = \sum_{t=0}^{p-1} \Big(d(x_{kt}, x_{0p}) + d(y_{kt}, x_{0p}) \Big).$$

$$d_y(k) = \sum_{t=0}^{p-1} \Big(d(x_{kt}, y_{0p}) + d(y_{kt}, y_{0p}) \Big).$$

In Lemma 3 of Ref. [7] we compute $d_x(k)$ and $d_y(k)$ as follows:

Let $0 \leq k < q$, then

$$d_x(k) = \begin{cases} p^2 + 2kp + 2(k^2 + k) & \text{if } 2k < p \\ \\ \frac{p^2}{2} + 4kp + p & \text{if } 2k \geq p \end{cases}$$

and

$$d_y(k) = \begin{cases} p^2 + 2kp + 2(k^2 - k) & \text{if } 2k < p \\ \\ \frac{p^2}{2} + 4kp - p & \text{if } 2k \geq p. \end{cases}$$

Now suppose for $0 \leq i < q$, x_{ip} and y_{ip} are vertices which are placed on the i-th row and p-th column of the graph. By using Lemma 1 we can compute distance sum of x_{ip} and y_{ip} in three cases as follow. By symmetry of the graph the obtained results can be used for vertices x_{it} and y_{it} where are placed on the t-th column of the graph. So the distance sum for all of the vertices can be calculated by symmetry of the graph.

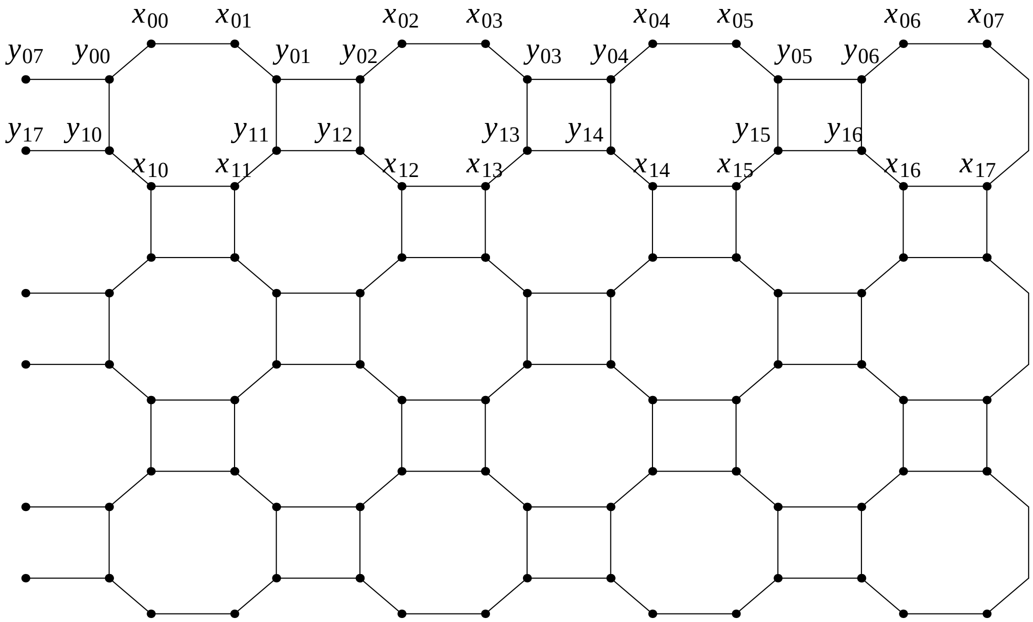

Figure 2: A $C_4C_8(S)$ Lattice with $p = 4$ and $q = 6$.

Let $0 \leq i < q$, then

$$d(x_{ip}) = \begin{cases} 2(p+q)i^2 - 2(pq+q^2-p)i + \frac{2}{3}(q^3-q) + pq(q+p-1), & \text{if } 2i < p \\ \frac{2i^3}{3} + 3pi^2 + (\frac{p^2}{2} - 4pq + 2p - \frac{2}{3})i + \frac{p}{12}(p^2-4) + \frac{pq}{2}(p+4q-2), & \text{if } p \leq 2i \leq 2p \\ 4pi^2 + 2p(1-2q)i + \frac{p}{6}(p^2-4) + pq(\frac{p}{2} + 2q - 1), & \text{if } i > p \end{cases}$$

and

$$d(y_{ip}) = \begin{cases} 2(p+q)i^2 - 2(pq+q^2-p+2q)i + \frac{2q}{3}(q^2-3q+2) \\ \quad +pq(q+p-1), & \text{if } 2i < p \\ \frac{2i^3}{3} + (3p+2)i^2 + (\frac{p^2}{2} - 4pq + 4p - \frac{4}{3})i \\ \quad + \frac{p}{12}(p^2+6p+8) + \frac{pq}{2}(p+4q-6), & \text{if } p \leq 2i \leq 2p \\ 4pi^2 + 2p(3-2q)i + \frac{p}{6}(p^2+8) + pq(\frac{p}{2} + 2q - 3), & \text{if } i > p \end{cases}$$

Proof. Let $0 \leq i < q$. By using Lemma 1 the summation of distances between vertex x_{ip} (or y_{ip}) and vertices on the j-th row of the graph (where are placed up of i-th row) can be computed as $d_x(i-j)$ (or $d_y(i-j)$). But the summation of distances between vertex x_{ip} (or y_{ip}) and vertices on the j-th row of the graph (where are placed below of the i-th row) can be computed as $d_y(j-i)$ (or $d_x(j-i)$). Suppose $2i < p$ and $d_1(x_{ip})$ (or $d_1(y_{ip})$) denotes the sum distance of vertex x_{ip} (or y_{ip}). Thus

$$\begin{aligned} d_1(x_{ip}) &= \sum_{k=0}^{i} d_y(i) + \sum_{k=1}^{q-i-1} d_x(i) \\ &= \sum_{k=0}^{i}(p^2+2kp+2(k^2-k)) + \sum_{k=1}^{q-i-1}(p^2+2kp+2(k^2+k)) \\ &= 2(p+q)i^2 - 2(pq+q^2-p)i + \frac{2}{3}(q^3-q) + pq(q+p-1). \end{aligned}$$

and

$$\begin{aligned} d_1(y_{ip}) &= \sum_{k=0}^{i} d_x(i) + \sum_{k=1}^{q-i-1} d_y(i) \\ &= \sum_{k=0}^{i}(p^2+2kp+2(k^2+k)) + \sum_{k=1}^{q-i-1}(p^2+2kp+2(k^2-k)) \\ &= 2(p+q)i^2 - 2(pq+q^2-p+2q)i + \frac{2q}{3}(q^2-3q+2) \\ &\quad +pq(q+p-1). \end{aligned}$$

Now suppose $p \leq i < p$. By Lemma 1, for j-th row of the graph where are placed below of the i-th row we most consider two cases such that $j-i < \frac{p}{2}$ or $j-i \geq \frac{p}{2}$.

$$\begin{aligned} d_2(x_{ip}) &= \sum_{k=0}^{i} d_y(i) + \sum_{k=1}^{q-i-1} d_x(i) \\ &= \sum_{k=0}^{i}(p^2+2kp+2(k^2-k)) + \sum_{k=1}^{\frac{p}{2}-1}(p^2+2kp+2(k^2+k)) \\ &\quad + \sum_{k=\frac{p}{2}}^{q-i-1}(\frac{p^2}{2}+4kp+p) \\ &= \frac{2i^3}{3} + 3pi^2 + (\frac{p^2}{2} - 4pq + 2p - \frac{2}{3})i + \frac{p}{12}(p^2-4) + \frac{pq}{2}(p+4q-2). \end{aligned}$$

and

$$\begin{aligned} d_2(y_{ip}) &= \sum_{k=0}^{i} d_x(i) + \sum_{k=1}^{q-i-1} d_y(i) \\ &= \sum_{k=0}^{i}(p^2+2kp+2(k^2+k)) + \sum_{k=1}^{\frac{p}{2}-1}(p^2+2kp+2(k^2-k)) \\ &\quad + \sum_{k=\frac{p}{2}}^{q-i-1}(\frac{p^2}{2}+4kp-p) \\ &= \frac{2i^3}{3}+(3p+2)i^2+(\frac{p^2}{2}-4pq+4p-\frac{4}{3})i+\frac{p}{12}(p^2+6p+8) \\ &\quad +\frac{pq}{2}(p+4q-6). \end{aligned}$$

If $i \geq p$, by Lemma 1, for the j-th row of the graph where are placed below (or up) of the i-th row we most consider two cases such that $|j-i| < \frac{p}{2}$ or $|j-i| \geq \frac{p}{2}$. So

$$\begin{aligned} d_3(x_{ip}) &= \sum_{k=0}^{i} d_y(i) + \sum_{k=1}^{q-i-1} d_x(i) \\ &= \sum_{k=0}^{\frac{p}{2}-1}(p^2+2kp+2(k^2-k)) + \sum_{k=\frac{p}{2}}^{i}(\frac{p^2}{2}+4kp-p) \\ &\quad + \sum_{k=1}^{\frac{p}{2}-1}(p^2+2kp+2(k^2+k)) + \sum_{k=\frac{p}{2}}^{q-i-1}(\frac{p^2}{2}+4kp+p) \\ &= 4pi^2+2p(1-2q)i+\frac{p}{6}(p^2-4)+pq(\frac{p}{2}+2q-1). \end{aligned}$$

and

$$\begin{aligned} d_3(y_{ip}) &= \sum_{k=0}^{i} d_x(i) + \sum_{k=1}^{q-i-1} d_y(i) \\ &= \sum_{k=0}^{\frac{p}{2}-1}(p^2+2kp+2(k^2+k)) + \sum_{k=\frac{p}{2}}^{i}(\frac{p^2}{2}+4kp+p) \\ &\quad + \sum_{k=1}^{\frac{p}{2}-1}(p^2+2kp+2(k^2-k)) + \sum_{k=\frac{p}{2}}^{q-i-1}(\frac{p^2}{2}+4kp-p) \\ &= 4pi^2+2p(1-2q)i+\frac{p}{6}(p^2-4)+pq(\frac{p}{2}+2q-1). \end{aligned}$$

Therefore the Lemma is proved. □

Now the Balaban index of the graph can be computed by using the previous results of distance sum for all of the vertices of the graph. Since the number of the vertices and edges of the graph are equal to $n = 4pq$ and $m = 6pq - 2p$, so $\mu = m - n + 1 = 2p(q-1) + 1$. Thus

$$J(G) = \frac{m}{1+\mu} \sum_{uv \in E(G)} [d(u)d(v)]^{\frac{-1}{2}} = \frac{p(3q-1)}{p(q-1)+1} \sum_{uv \in E(G)} [d(u)d(v)]^{\frac{-1}{2}}.$$

Suppose $0 \leq i < q$, by using symmetry of the graph, $d(x_{it}) = d(x_{ip})$ and $d(y_{it}) = d(y_{ip})$ for $t = 0, 1, 2, \ldots, 2p-1$. Therefore if $2q < p$. we have

$$\begin{aligned} J(G) &= \frac{p(3q-1)}{p(q-1)+1}\Bigg(p\sum_{i=0}^{q-1}[d_1(x_{ip})d_1(y_{ip})]^{\frac{-1}{2}} \\ &\quad + \frac{p}{2}\sum_{i=0}^{q-1}\bigg([d_1(x_{ip})d_1(x_{i,p+1})]^{\frac{-1}{2}} + [d_1(y_{ip})d_1(y_{i,p+1}]^{\frac{-1}{2}})\bigg) \\ &\quad + p\sum_{i=0}^{q-1}[d_1(x_{i+1,p})d_1(y_{i,p}]^{\frac{-1}{2}}\Bigg) \\ &= \frac{p^2(3q-1)}{p(q-1)+1}\Bigg(2\sum_{i=0}^{q/2-1}[d_1(x_{ip})d_1(y_{ip})]^{\frac{-1}{2}} \\ &\quad + \sum_{i=0}^{q/2-1}\bigg([d_1(x_{ip})]^{-1} + [d_1(y_{ip}]^{-1})\bigg) \\ &\quad + \bigg(\sum_{i=0}^{q/2-2}[d_1(x_{i+1,p})d_1(y_{i,p}]^{\frac{-1}{2}}) + \sum_{q/2-1}^{q/2-1}[d_1(x_{i+1,p})d_1(y_{i,p})]^{\frac{-1}{2}}\Bigg). \end{aligned} \tag{2.1}$$

If $p \leq 2q < 2p$. Then the Balaban index of $C_4C_8(S)$ computed as follows:

$$\begin{aligned} J(G) &= \frac{p^2(3q-1)}{p(q-1)+1}\Bigg(2\sum_{i=0}^{q/2-1}[d_2(x_{ip})d_2(y_{ip})]^{\frac{-1}{2}} + \\ &\quad \sum_{i=0}^{q/2-1}\bigg([d_2(x_{ip})]^{-1} + [d_2(y_{ip})]^{-1}\bigg) + \sum_{i=0}^{q/2-2}[d_1(x_{i+1,p})d_1(y_{i,p})]^{\frac{-1}{2}} \\ &\quad + \sum_{q/2-1}^{q/2-1}[d_1(x_{i+1,p})d_1(y_{i,p})]^{\frac{-1}{2}}\Bigg). \end{aligned} \tag{2.2}$$

p	q	$J(G)$	p	q	$J(G)$
2	2	1.9264	6	6	.5688
2	4	1.2522	6	10	.4442
2	8	.7397	8	2	.6900
2	10	.6129	8	4	.5276
4	2	1.2211	8	8	.4195
4	4	.8819	10	2	.5658
4	6	.7202	10	10	.3323
4	10	.5222	12	10	.2931
6	2	.8830	12	12	.2751
6	4	.6626	20	20	.1629

Table 1: Balaban index of $TUC_4C_8(S)$ Nanotubes.

Now suppose $q > p$. Similar to previous cases we have

$$\begin{aligned} J(G) \quad &= \quad \frac{p^2(3q-1)}{p(q-1)+1}\Bigg(2\sum_{i=0}^{p/2-1}[d_2(x_{ip})d_2(y_{ip})]^{\frac{-1}{2}} + 2\sum_{i=p/2}^{q/2-1}[d_3(x_{ip})d_3(y_{ip})]^{\frac{-1}{2}} \\ &+ \sum_{i=0}^{p/2-1}\Big([d_2(x_{ip})]^{-1} + [d_2(y_{ip})]^{-1}\Big) + \sum_{i=p/2}^{q/2-1}\Big([d_3(x_{ip})]^{-1} + [d_3(y_{ip})]^{-1}\Big) \\ &+ \sum_{i=0}^{p/2-1}[d_2(x_{i+1,p})d_2(y_{i,p})]^{\frac{-1}{2}} + \sum_{i=p/2}^{q/2-2}[d_3(x_{i+1,p})d_3(y_{i,p}]^{\frac{-1}{2}} \\ &+ \sum_{q/2-1}^{q/2-1}[d_1(x_{i+1,p})d_1(y_{i,p})]^{\frac{-1}{2}}\Bigg). \end{aligned} \tag{2.3}$$

Therefore the Balaban index of $C_4C_8(S)$ nanotubes can be computed by using formulas (2.1), (2.2) and (2.3) in three cases. To consideration the variation of the Balaban index of the graph in the following table the Balaban index of $C_4C_8(S)$ nanotubes is computed for various integer numbers.

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