ECCENTRIC CONNECTIVITY INDEX OF V-PHENYLENIC NANOTUBES

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If G = (V, E) is a connected graph then the eccentric connectivity index of G is defined as $\xi(G) = \sum_{v \in V(G)} deg(v)\varepsilon(v)$. In this paper we obtain explicit formulas for eccentric connectivity index of phenylenic nanotubes.

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1. Introduction

Chemical compounds can be modeled by molecular graphs where the points represent atoms and the edges represents covalent bonds. This model has become an important tool in the prediction of physico-chemical, pharmacological and toxicological properties of a compound directly. The study of eccentric connectivity index gained more importance as the topological models involving this index show a high degree of predictability of pharmaceutical properties.

PI index of V-Phenylenic nanotube is computed by Amir Bahrani [1] in 2008. We compute eccentric connectivity index of nanotubes in this paper.

2. Main results

In this section, the eccentric connectivity index of the molecular graph of the V-Phenylenic nanotube VPHX [p, q] is computed, For simplicity, we denote this nanotube by V = V [p, q]. To compute eccentric connectivity index, we need $\varepsilon(v)$ which is maximum of $\{d(u,v)/u \in V(G)\}$. The edges in the longest path from $x_{1,1}$ in V[4,6] and V[3,7] are shown below with dark edges.

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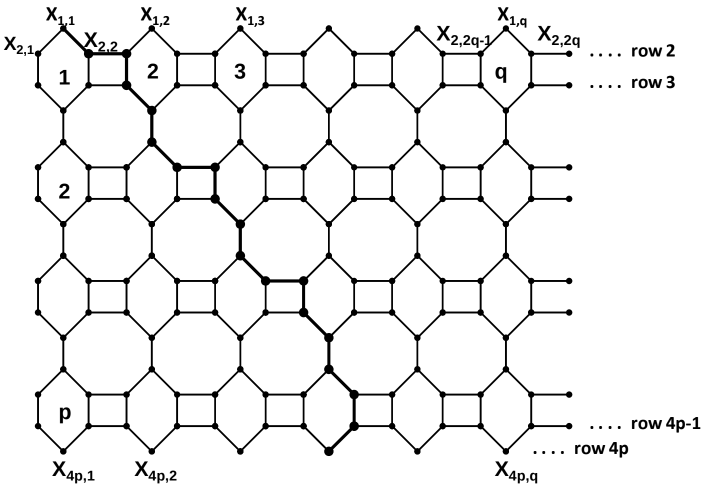
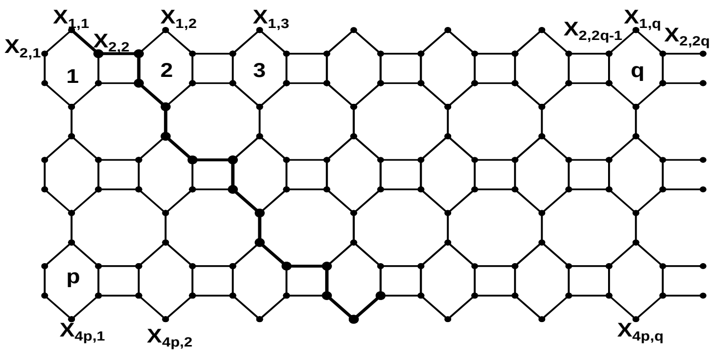


Graph of V [p,q] with p=4, q=6



Graph of V[p,q] with p=3, q=7

Theorem 2.1. If G is a phenylenic nanotube (see above figures) then

$$\xi(G) = \begin{cases} 36, & \text{when } p = 1 \text{ and } q = 1; \\ 24q^2 + 16q, & \text{when } p = 1 \text{ and } q \text{ is even;} \\ 24q^2 + 8q, & \text{when } p = 1 \text{ and } q \text{ is odd;} \\ 54p^2q + 9pq^2 - 17pq - q^2 + 2q, & \text{when } q \le p,\ p \text{ and } q \text{ are even;} \\ 54p^2q + 9pq^2 - 26pq - q^2 + 3q, & \text{when } q \le p,\ p \text{ is even and } q \text{ is odd;} \\ 54p^2q + 9pq^2 - 17pq - q^2 - q, & \text{when } q \le p,\ p \text{ is odd and } q \text{ is even;} \\ 54p^2q + 9pq^2 - 26pq - q^2, & \text{when } q \le p,\ p \text{ and } q \text{ are odd;} \\ 9q^3 + 63p^2q - 9pq^2 - 17pq - q^2 + 2q, & \text{when } p+1 \le q \le 2p-1 \text{ and } q \text{ is even;} \\ 9q^3 + 63p^2q - 9pq^2 - 26pq - q^2, & \text{when } p+1 \le q \le 2p-1 \text{ and } q \text{ is odd;} \\ 27p^2q + 27pq^2 - 13pq - 3q^2 + 2q, & \text{when } 2p \le q \text{ and } q \text{ is even;} \\ 27p^2q + 27pq^2 - 22pq - 3q^2 + 3q, & \text{when } 2p \le q \text{ and } q \text{ is odd.} \end{cases}$$

Proof. From the lemmas given below the proof is clear.

Lemma. 2.2. $\xi(G) = \begin{cases} 36, & \text{when } p = 1 \text{ and } q = 1; \\ 24q^2 + 16q, & \text{when } p = 1 \text{ and } q \text{ is even}; \\ 24q^2 + 8q, & \text{when } p = 1 \text{ and } q \text{ is odd}. \end{cases}$

Proof. In this case the graph has only 4 rows. The degree of every vertex in first and 4th rows is 2 where as the degree of every vertex in 2nd and 3rd rows is 3. We have $\xi(G) = \sum_{v \in V(G)} deg(v)\varepsilon(v)$

Case (1). $p = 1 \text{ and } q = 1$

Then $\xi(G) = 2[(2)(3)+(2)(3)(2)] = 36$.

Case (2). $p = 1 \text{ and } q \text{ is even}$

In this case the eccentricity of every vertex in every row is $\frac{3q+2}{2}$.

Then $\xi(G) = 2\left[(2)(q)\left(\frac{3q+2}{2}\right) + (3)(2q)\left(\frac{3q+2}{2}\right)\right] = 24q^2 + 16q$.

Case (3). $p = 1 \text{ and } q \text{ is odd}$

In this case the eccentricity of every vertex in every row is $\frac{3q+1}{2}$.

Then $\xi(G) = 2\left[(2)(q)\left(\frac{3q+1}{2}\right) + (3)(2q)\left(\frac{3q+1}{2}\right)\right] = 24q^2 + 8q$.

Lemma 2.3. $\xi(G) = 54p^2q + 9pq^2 - 17pq - q^2 + 2q$ when $q \leq p$, p and q both are even.

Proof. In this case the graph has $4p$ rows and the eccentricity of a vertex in ith row is same as the eccentricity of a vertex in (4p+1-i)th row where $i = 1,2,\dots,2p$.

Here all the vertices in first and last rows are of degree 2 and the remaining vertices are of degree 3.

Let x_i be a vertex in ith row.

The eccentricity of x_i is $\varepsilon(x_i) = \left(\frac{8p+q}{2} - i\right)$ where $i = 1,2,\dots,2p$.

Hence $\xi(G) = \sum_{x_i \in V(G)} \deg(x_i)\, \varepsilon(x_i)$

$$= 2\Big[(2)(q)\left(\frac{8p+q}{2} - 1\right) + (3)(2q)\left(\frac{8p+q}{2} - 2\right) + (3)(2q)\left(\frac{8p+q}{2} - 3\right) + (3)(q)\left(\frac{8p+q}{2} - 4\right) + (3)(q)\left(\frac{8p+q}{2} - 5\right) + (3)(2q)\left(\frac{8p+q}{2} - 6\right) + (3)(2q)\left(\frac{8p+q}{2} - 7\right) + (3)(q)\left(\frac{8p+q}{2} - 8\right) + \dots + (3)(q)\left(\frac{8p+q}{2} - 2p\right)\Big]$$

$$= 54p^2q + 9pq^2 - 17pq - q^2 + 2q$$

Lemma 2.4. $\xi(G) = 54p^2q + 9pq^2 - 26pq - q^2 + 3q$ when $q \leq p$, p is even and q is odd.

Proof. In this case the graph has $4p$ rows and the eccentricity of a vertex in ith row is same as the eccentricity of a vertex in (4p+1-i)th row where $i = 1,2,\dots,2p$.

Here all the vertices in first and last rows are of degree 2 and the remaining vertices are of degree 3.

Let x_i be a vertex in ith row.

The eccentricity of x_i is $\varepsilon(x_i) = \left(\frac{8p+q-1}{2} - i\right)$ where $i = 1,2,\ldots,2p$.

Hence $\xi(G) = \sum_{x_i \in V(G)} \deg(x_i)\, \varepsilon(x_i)$

$$= 2\left[(2)(q)\left(\frac{8p+q-1}{2} - 1\right) + (3)(2q)\left(\frac{8p+q-1}{2} - 2\right) + (3)(2q)\left(\frac{8p+q-1}{2} - 3\right) + (3)(q)\left(\frac{8p+q-1}{2} - 4\right) + (3)(q)\left(\frac{8p+q-1}{2} - 5\right) + (3)(2q)\left(\frac{8p+q-1}{2} - 6\right) + (3)(2q)\left(\frac{8p+q-1}{2} - 7\right) + (3)(q)\left(\frac{8p+q-1}{2} - 8\right) + \cdots + (3)(q)\left(\frac{8p+q-1}{2} - 2p\right)\right]$$

$$= 54p^2q + 9pq^2 - 26pq - q^2 + 3q$$

Lemma 2.5. $\xi(G) = 54p^2q + 9pq^2 - 17pq - q^2 - q$ *when* $q \le p$, p *is odd and* q *is even.*

Proof. In this case the graph has $4p$ rows and the eccentricity of a vertex in i^{th} row is same as the eccentricity of a vertex in $(4p+1-i)^{th}$ row where $i = 1,2,\ldots,2p$.
Here all the vertices in first and last rows are of degree 2 and the remaining vertices are of degree 3.
Let x_i be a vertex in i^{th} row.
The eccentricity of x_i is $\varepsilon(x_i) = \left(\frac{8p+q}{2} - i\right)$ where $i = 1,2,\ldots,2p$.
Hence $\xi(G) = \sum_{x_i \in V(G)} \deg(x_i)\, \varepsilon(x_i)$

$$= 2\left[(2)(q)\left(\frac{8p+q}{2} - 1\right) + (3)(2q)\left(\frac{8p+q}{2} - 2\right) + (3)(2q)\left(\frac{8p+q}{2} - 3\right) + (3)(q)\left(\frac{8p+q}{2} - 4\right) + (3)(q)\left(\frac{8p+q}{2} - 5\right) + (3)(2q)\left(\frac{8p+q}{2} - 6\right) + (3)(2q)\left(\frac{8p+q}{2} - 7\right) + (3)(q)\left(\frac{8p+q}{2} - 8\right) + \cdots + (3)(2q)\left(\frac{8p+q}{2} - 2p\right)\right]$$

$$= 54p^2q + 9pq^2 - 17pq - q^2 - q.$$

Lemma 2.6. $\xi(G) = 54p^2q + 9pq^2 - 26pq - q^2$ *when* $q \le p$, p *and* q *both are odd.*

Proof. In this case the graph has $4p$ rows and the eccentricity of a vertex in i^{th} row is same as the eccentricity of a vertex in $(4p+1-i)^{th}$ row where $i = 1,2,\ldots,2p$.
Here all the vertices in first and last rows are of degree 2 and the remaining vertices are of degree 3.
Let x_i be a vertex in i^{th} row.
The eccentricity of x_i is $\varepsilon(x_i) = \left(\frac{8p+q-1}{2} - i\right)$ where $i = 1,2,\ldots,2p$.

Now $\xi(G) = \sum_{x_i \in V(G)} \deg(x_i)\, \varepsilon(x_i)$

$$= 2\left[(2)(q)\left(\frac{8p+q-1}{2} - 1\right) + (3)(2q)\left(\frac{8p+q-1}{2} - 2\right) + (3)(2q)\left(\frac{8p+q-1}{2} - 3\right) + (3)(q)\left(\frac{8p+q-1}{2} - 4\right) + (3)(q)\left(\frac{8p+q-1}{2} - 5\right) + (3)(2q)\left(\frac{8p+q-1}{2} - 6\right) + \right.$$

$$(3)(2q)\left(\frac{8p+q-1}{2}-7\right)+(3)(q)\left(\frac{8p+q-1}{2}-8\right)+\cdots+(3)(2q)\left(\frac{8p+q-1}{2}-2p\right)\Big]$$

$$= 54p^2q + 9pq^2 - 26pq - q^2.$$

Lemma 2.7. ξ(G) = $9q^3 + 63p^2q - 9pq^2 - 17pq - q^2 + 2q$ *when* $p+1 \le q \le 2p-1$ *and* q *is even.*

Proof. In this case the graph has $4p$ rows and the eccentricity of a vertex in i^{th} row is same as the eccentricity of a vertex in $(4p+1-i)^{th}$ row where $i = 1,2,\ldots,2p$.

Here all the vertices in first and last rows are of degree 2 and the remaining vertices are of degree 3.

Let x_i be a vertex in i^{th} row.

The eccentricity of x_i is $\varepsilon(x_i) = \left(\frac{8p+q}{2} - i\right)$ where $i = 1,2,\ldots,(4p-2q)$.

Let x_i be a vertex in $(4p-2q+2i-1)^{th}$ or $(4p-2q+2i)^{th}$ row.

The eccentricity of x_i is $\varepsilon(x_i) = \left(\frac{8p+q}{2} - (4p-2q+i)\right)$ where $i = 1,2,\ldots,(q-p)$.

Hence ξ(G) = $\sum_{x_i \in V(G)} \deg(x_i)\, \varepsilon(x_i)$

$$= 2\Big[(2)(q)\left(\frac{8p+q}{2}-1\right)+(3)(2q)\left(\frac{8p+q}{2}-2\right)+(3)(2q)\left(\frac{8p+q}{2}-3\right)+$$
$$(3)(q)\left(\frac{8p+q}{2}-4\right)+(3)(q)\left(\frac{8p+q}{2}-5\right)+(3)(2q)\left(\frac{8p+q}{2}-6\right)+$$
$$(3)(2q)\left(\frac{8p+q}{2}-7\right)+(3)(q)\left(\frac{8p+q}{2}-8\right)+\cdots+(3)(q)\left(\frac{8p+q}{2}-(4p-2q)\right)\Big]+$$
$$2\Big[(3)(3q)\left(\frac{8p+q}{2}-(4p-2q+1)\right)+(3)(3q)\left(\frac{8p+q}{2}-(4p-2q+2)\right)+\ldots+$$
$$(3)(q)\left(\frac{8p+q}{2}-(3p-q)\right)\Big]$$
$$= 9q^3 + 63p^2q - 9pq^2 - 17pq - q^2 + 2q$$

Lemma 2.8. ξ(G) = $9q^3 + 63p^2q - 9pq^2 - 26pq - q^2$ *when* $p+1 \le q \le 2p-1$ *and* q *is odd*.

Proof. In this case the graph has $4p$ rows and the eccentricity of a vertex in i^{th} row is same as the eccentricity of a vertex in $(4p+1-i)^{th}$ row where $i = 1,2,\ldots,2p$.

Here all the vertices in first and last rows are of degree 2 and the remaining vertices are of degree 3.

Let x_i be a vertex in i^{th} row.

The eccentricity of x_i is $\varepsilon(x_i) = \left(\frac{8p+q-1}{2} - i\right)$ where $i = 1,2,\ldots,(4p-2q)$.

Let x_i be a vertex in $(4p-2q+2i-1)^{th}$ or $(4p-2q+2i)^{th}$ row.

The eccentricity of x_i is $\varepsilon(x_i) = \left(\frac{8p+q-1}{2} - (4p-2q+i)\right)$ where $i = 1,2,\ldots,(q-p)$.

Hence ξ(G) = $\sum_{x_i \in V(G)} \deg(x_i)\, \varepsilon(x_i)$

$$= 2\Big[(2)(q)\left(\frac{8p+q-1}{2}-1\right)+(3)(2q)\left(\frac{8p+q-1}{2}-2\right)+(3)(2q)\left(\frac{8p+q-1}{2}-3\right)+$$
$$(3)(q)\left(\frac{8p+q-1}{2}-4\right)+(3)(q)\left(\frac{8p+q-1}{2}-5\right)+(3)(2q)\left(\frac{8p+q-1}{2}-6\right)+$$
$$(3)(2q)\left(\frac{8p+q-1}{2}-7\right)+(3)(q)\left(\frac{8p+q-1}{2}-8\right)+\cdots+$$

$$(3)(2q)\left(\frac{8p+q}{2}-(4p-2q)\right)\Big]+2\Big[(3)(3q)\left(\frac{8p+q}{2}-(4p-2q+1)\right)+(3)(3q)\left(\frac{8p+q}{2}-(4p-2q+2)\right)+\cdots+(3)(3q)\left(\frac{8p+q}{2}-(3p-q)\right)\Big]$$

$$= 9q^3+63p^2q-9pq^2-26pq-q^2.$$

Lemma 2.9. ξ (G) = $27p^2q+27pq^2-13pq-3q^2+2q$ *when* $2p \le q$ *and* q *is even.*

Proof. In this case the graph has $4p$ rows and the eccentricity of a vertex in i$^{\text{th}}$ row is same as the eccentricity of a vertex in (4p+1-i)$^{\text{th}}$ row where $i = 1,2,\dots,2p$.

Here all the vertices in first and last rows are of degree 2 and the remaining vertices are of degree 3.

Let x_i be a vertex in $(2i-1)^{\text{th}}$ or $(2i)^{\text{th}}$ row.

The eccentricity of x_i is $\varepsilon(x_i) = \left(\frac{4p+3q}{2}-i\right)$ where $i = 1,2,\dots,p$.

Now $\xi(G) = \sum_{x_i \in V(G)} \deg(x_i)\,\varepsilon(x_i)$

$$= 2\Big[(2)(q)\left(\frac{4p+3q}{2}-1\right)+(3)(2q)\left(\frac{4p+3q}{2}-1\right)+(3)(3q)\left(\frac{4p+3q}{2}-2\right)+(3)(3q)\left(\frac{4p+3q}{2}-3\right)+(3)(3q)\left(\frac{4p+3q}{2}-4\right)+(3)(3q)\left(\frac{4p+3q}{2}-5\right)+(3)(3q)\left(\frac{4p+3q}{2}-6\right)+(3)(3q)\left(\frac{4p+3q}{2}-7\right)+\cdots+(3)(3q)\left(\frac{4p+3q}{2}-p\right)\Big]$$

$$= 27p^2q+27pq^2-13pq-3q^2+2q.$$

Lemma 2.10. ξ (G) = $27p^2q+27pq^2-22pq-3q^2+3q$ *when* $2p \le q$ *and* q *is odd.*

Proof. In this case the graph has $4p$ rows and the eccentricity of a vertex in i$^{\text{th}}$ row is same as the eccentricity of a vertex in (4p+1-i)$^{\text{th}}$ row where $i = 1,2,\dots,2p$.

Here all the vertices in first and last rows are of degree 2 and the remaining vertices are of degree 3.

Let x_i be a vertex in $(2i-1)^{\text{th}}$ or $(2i)^{\text{th}}$ row.

The eccentricity of x_i is $\varepsilon(x_i) = \left(\frac{4p+3q-1}{2}-i\right)$ where $i = 1,2,\dots,p$.

Hence $\xi(G) = \sum_{x_i \in V(G)} \deg(x_i)\,\varepsilon(x_i)$

$$= 2\Big[(2)(q)\left(\frac{4p+3q-1}{2}-1\right)+(3)(2q)\left(\frac{4p+3q-1}{2}-1\right)+(3)(3q)\left(\frac{4p+3q-1}{2}-2\right)+(3)(3q)\left(\frac{4p+3q-1}{2}-3\right)+(3)(3q)\left(\frac{4p+3q-1}{2}-4\right)+(3)(3q)\left(\frac{4p+3q-1}{2}-5\right)+(3)(3q)\left(\frac{4p+3q-1}{2}-6\right)+(3)(3q)\left(\frac{4p+3q-1}{2}-7\right)+\cdots+(3)(3q)\left(\frac{4p+3q-1}{2}-p\right)\Big]$$

$$= 27p^2q+27pq^2-22pq-3q^2+3q.$$

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