ECCENTRIC AND WIENER INDICES OF NANO PENTACHAIN

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With the invention of Nano-technology, the study of topological indices gained much importance. In this paper we initiate the study of eccentric and Wiener indices of a pentagonal ring. We observe that the eccentric connectivity index is a second degree polynomial in both the structures (Straight chaining and Alternative chaining) where as Wiener index is a third degree polynomial.

KEYWORDS : Hyper wiener index, Wiener index, Narumi-Katayama index, pentachains.

INTRODUCTION

A nano pentachain is a closed chain of pentarings in one row. Ivan Gutman and [2] in 2007 presented the study of concatenated 5-cycles in one row and obtained explicit formulas for Schultz and modified Schultz indices of these graphs. Later Lakshmi prasanna [4] and the present author [5] obtained formulas for various topological indices. Recently in 2009, O. Halakoo [3] obtained bounds for Schultz index of pentachains.

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. In this paper, we obtained simple formulas for eccentric connectivity index and Wiener indices of nano pentachain.

Preliminaries

Iirst we state the definitions of W, WW, S, RW and eccentric indices.

Definition 2.1. [7] The Wiener index of a graph G = (V, E) is defined as

 $W(G) = \frac{1}{2} \sum_{v \in V} \sum_{u \in U} d_G(u, v) \text{ where } d_G(u, v) \text{ is the length of shortest path connecting } u \text{ and } v \text{ in } C$

 G_{\cdot}

Definition 2.2. [2] The Hyper wiener index of a graph G = (V, E) is defined as $WW(G) = \frac{1}{2} \sum_{i \le i} (d_{ij} + d_{ij}^2)$.

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Definition 2.3. [8] The Narumi-katayama index of a graph G is defined as $S = S(G) = \prod_{i=1}^{n} i$, where 'i' is the degree (= number of first neighbours) of the ith vertex and n is the number of the graph.

Definition 2.4. [1] The Reverse Wiener index of a graph G is defined as $RW(G) = \frac{1}{2}N(N-1)d - W$, where N is the number of vertices, d is the diameter and W is the Wiener index of the graph G.

Definition 2.5. [6] If G = (V, E) is a connected graph then the eccentric connectivity index of G is defined as $\xi(G) = \sum_{u \in V(G)} \deg(v) \in (v)$, where $\in (v) = \max \{d(u, v)/u \in V(G)\}$.

Notation

5-cycles can be concatenated in a chain as shown in figure 1, 2 (we call this case as Straight chaining) or as in figure 3 (we call this case as Alternative chaining).

In Straight chaining case the graph consisting of 5-cycles in a chain is denoted by G(a, S). The graph with a = 6 in a chain is as shown below.



The graph with a = 7 in a chain is as shown below.



Fig. 2.

In Alternative chaining case the graph consisting of 5-cycles in a chain is denoted by G(a, A). The graph with a = 6 in a chain is as shown below.





WIENER INDEX

Theorem 4.1. $W(G(a, S)) = \frac{1}{8}(9a^3 + 60a^2 - 101a)$, if a > 3 and a is odd.

Proof: Let the vertex set of G(a, S) be $A \cup B$, where $A = \{x_1, x_2, ..., x_a\}, B = \{y_1, y_2, ..., y_{2a}\}$.

Now
$$W(G(a,S)) = \sum_{u,v \in A} d(u,v) + \sum_{u,v \in B} d(u,v) + \sum_{u \in A, v \in B} d(u,v)$$

$$= \left\{ a \sum_{i=1}^{\frac{a-1}{2}} i \right\} + \left\{ 2a \sum_{i=1}^{4} i + 3a(5) + 4a \sum_{i=6}^{\frac{a+3}{2}} i + 2a \left(\frac{a+5}{2}\right) \right\} + \left\{ a(1) + 4a \sum_{i=2}^{\frac{a+1}{2}} i + a \left(\frac{a+3}{2}\right) \right\}$$

$$= \frac{1}{8} (a^3 - a) + \frac{1}{2} (a^3 + 10a^2 - 25a) + \frac{1}{2} (a^3 + 5a^2)$$

$$= \frac{1}{8} (9a^3 + 60a^2 - 101a).$$

Theorem 4.2. $W(G(a, S)) = \frac{1}{8}(9a^3 + 60a^2 - 100a)$, if a > 4 and a is even.

Proof: Let the vertex set of G(a, S) be $A \cup B$, where $A = \{x_1, x_2, ..., x_a\}$, $B = \{y_1, y_2, ..., y_{2a}\}$.

Now
$$W(G(a,S)) = \sum_{u,v \in A} d(u,v) + \sum_{u,v \in B} d(u,v) + \sum_{u \in A, v \in B} d(u,v)$$

$$= \left\{ a \sum_{i=1}^{\frac{a-2}{2}} i + \left(\frac{a}{2}\right)^2 \right\} + \left\{ 2a \sum_{i=1}^{4} i + 3a(5) + 4a \sum_{i=6}^{\frac{a+2}{2}} i + \left(\frac{7a}{2}\right) \left(\frac{a+4}{2}\right) + \left(\frac{a}{2}\right) \left(\frac{a+6}{2}\right) \right\} + \left\{ a(1) + 4a \sum_{i=2}^{\frac{a}{2}} i + (3a) \left(\frac{a+2}{2}\right) \right\}$$

$$= \frac{1}{8} (a^3) + \frac{1}{2} (a^3 + 10a^2 - 25a) + \frac{1}{2} (a^3 + 5a^2)$$

$$= \frac{1}{8} (9a^3 + 60a^2 - 100a).$$

Theorem 4.3. $W(G(a, A)) = \frac{1}{16}(27a^3 + 18a^2 + 48a)$, if $\frac{a}{2}$ is odd.

Proof: Let the vertex set of G(a, A) be $A \cup B$, where $A = \{x_1, x_2, ..., x_{3a/2}\}, B = \{y_1, y_2, ..., y_{3a/2}\}.$

Now
$$W(G(a,S)) = \sum_{u,v\in A} d(u,v) + \sum_{u,v\in B} d(u,v) + \sum_{u\in A,v\in B} d(u,v)$$

$$= \left\{ \frac{3a}{2} \sum_{i=1}^{3a-2} i \right\} + \left\{ \frac{3a}{2} \sum_{i=1}^{3a-2} i \right\} + \left\{ a(1) + 4a(2) + 4a(3) + 3a \sum_{i=4}^{3a-2} i + \left(\frac{3a}{2}\right) \left(\frac{3a+2}{4}\right) \right\}$$

$$= \frac{1}{64}(27a^3 - 12a) + \frac{1}{64}(27a^3 - 12a) + \frac{1}{32}(27a^3 + 36a^2 + 108a)$$
$$= \frac{1}{16}(27a^3 + 18a^2 + 48a).$$

Theorem 4.4. $W(G(a, A)) = \frac{1}{16}(27a^3 + 18a^2 + 48a)$, if $\frac{a}{2}$ is even.

Proof: Let the vertex set of G(a, A) be $A \cup B$, where $A = \{x_1, x_2, ..., x_{3a/2}\}, B = \{y_1, y_2, ..., y_{3a/2}\}.$

Now
$$W(G(a,S)) = \sum_{u,v \in A} d(u,v) + \sum_{u,v \in B} d(u,v) + \sum_{u \in A,v \in B} d(u,v)$$

$$= \left\{ \frac{3a}{2} \sum_{i=1}^{3a-4} i + \left(\frac{3a}{4}\right)^2 \right\} + \left\{ \frac{3a}{2} \sum_{i=1}^{3a-4} i + \left(\frac{3a}{4}\right)^2 \right\} + \left\{ a(1) + 4a(2) + 4a(3) + 3a \sum_{i=4}^{3a} i \right\}$$

$$= \frac{1}{64} (27a^3) + \frac{1}{64} (27a^3) + \frac{1}{32} (27a^3 + 36a^2 + 96a)$$

$$= \frac{1}{16} (27a^3 + 18a^2 + 48a).$$

Hyper wiener index

$$+ \left\{ a(1)^{2} + 4a \sum_{i=2}^{\frac{a+1}{2}} i^{2} + a \left(\frac{a+3}{2}\right)^{2} \right\} \right]$$
$$= \frac{1}{2} \left[\frac{1}{8} (a^{3} - a) + \frac{1}{2} (a^{3} + 10a^{2} - 25a) + \frac{1}{2} (a^{3} + 5a^{2}) + \frac{1}{24} (a^{4} - a^{2}) + \frac{1}{6} (a^{4} + 15a^{3} + 77a^{2} - 375a) + \frac{1}{12} (2a^{4} + 15a^{3} + 40a^{2} + 3a) \right]$$
$$= \frac{1}{16} (3a^{4} + 39a^{3} + 189a^{2} - 599a).$$

Theorem 5.2. $WW(G(a,S)) = \frac{1}{16}(3a^4 + 39a^3 + 190a^2 - 600a)$, where a > 4 and a is even.

Proof: Let the vertex set of
$$G(a, S)$$
 be $A \cup B$, where $A = \{x_1, x_2, ..., x_a\}$, $B = \{y_1, y_2, ..., y_{2a}\}$.

Now
$$WW(G(a,S)) = \frac{1}{2} \left(\sum_{u,v \in A} d(u,v) + \sum_{u,v \in B} d(u,v) + \sum_{u \in A,v \in B} d(u,v) + \sum_{u,v \in A} d^2(u,v) + \sum_{u \in A,v \in B} d^2(u,v) \right)$$

$$= \frac{1}{2} \left[\left\{ a \sum_{i=1}^{\frac{a-2}{2}} i + \left(\frac{a}{2}\right)^2 \right\} + \left\{ 2a \sum_{i=1}^{4} i + 3a(5) + 4a \sum_{i=6}^{\frac{a+2}{2}} i + \left(\frac{7a}{2}\right) \left(\frac{a+4}{2}\right) + \left(\frac{a}{2}\right) \left(\frac{a+6}{2}\right) \right\} \right]$$

$$+ \left\{ a(1) + 4a \sum_{i=2}^{\frac{a}{2}} i + (3a) \left(\frac{a+2}{2}\right) \right\} + \left\{ a \sum_{i=1}^{\frac{a-2}{2}} i^2 + \left(\frac{a}{2}\right) \left(\frac{a}{2}\right)^2 \right\}$$

$$+ \left\{ 2a \sum_{i=1}^{4} i^2 + 3a(5)^2 + 4a \sum_{i=6}^{\frac{a+2}{2}} i^2 + \left(\frac{7a}{2}\right) \left(\frac{a+4}{2}\right)^2 + \left(\frac{a}{2}\right) \left(\frac{a+6}{2}\right)^2 \right\}$$

$$+ \left\{ a(1)^2 + 4a \sum_{i=2}^{\frac{a}{2}} i^2 + (3a) \left(\frac{a+2}{2}\right)^2 \right\}$$

$$= \frac{1}{2} \left[\frac{1}{8} (a^3) + \frac{1}{2} (a^3 + 10a^2 - 25a) + \frac{1}{2} (a^3 + 5a^2) + \frac{1}{24} (a^4 + 2a^2) \right]$$

$$+ \frac{1}{6} (a^4 + 15a^3 + 77a^2 - 375a) + \frac{1}{12} (2a^4 + 15a^3 + 40a^2) \right]$$

Theorem 5.3.
$$WW(G(a, A)) = \frac{1}{64}(27a^4 + 81a^3 + 60a^2 + 460a)$$
, where $\frac{a}{2}$ is odd

Proof: Let the vertex set of G(a, A) be $A \cup B$, where $A = \{x_1, x_2, ..., x_{3a/2}\}, B = \{y_1, y_2, ..., y_{3a/2}\}.$

Now
$$WW(G(a, S)) = \frac{1}{2} \left(\sum_{u,v \in A} d(u,v) + \sum_{u,v \in B} d(u,v) + \sum_{u \in A,v \in B} d(u,v) + \sum_{u,v \in A} d^2(u,v) + \sum_{u,v \in A} d^2(u,v) \right)$$

$$= \frac{1}{2} \left[\left\{ \frac{3a}{2} \sum_{i=1}^{\frac{3a-2}{4}} i \right\} + \left\{ \frac{3a}{2} \sum_{i=1}^{\frac{3a-2}{4}} i \right\} + \left\{ a(1) + 4a(2) + 4a(3) + 3a \sum_{i=4}^{\frac{3a-2}{4}} i + \left(\frac{3a}{2} \right) \left(\frac{3a+2}{4} \right) \right\} \right]$$

$$+ \left\{ \frac{3a}{2} \sum_{i=1}^{\frac{3a-2}{4}} i^2 \right\} + \left\{ \frac{3a}{2} \sum_{i=1}^{\frac{3a-2}{4}} i^2 \right\} + \left\{ a(1)^2 + 4a(2)^2 + 4a(3)^2 + 3a \sum_{i=4}^{\frac{3a-2}{4}} i^2 + \left(\frac{3a}{2} \right) \left(\frac{3a+2}{4} \right)^2 \right\} \right]$$

$$= \frac{1}{2} \left[\frac{1}{64} (27a^3 - 12a) + \frac{1}{64} (27a^3 - 12a) + \frac{1}{32} (27a^3 + 36a^2 + 108a) + \frac{1}{128} (27a^4 - 12a^2) + \frac{1}{128} (27a^4 - 12a^2) + \frac{1}{64} (27a^4 + 54a^3 + 60a^2 + 728a) \right]$$

$$= \frac{1}{64} (27a^4 + 81a^3 + 60a^2 + 460a).$$

Theorem 5.4. $WW(G(a, A)) = \frac{1}{64}(27a^4 + 81a^3 + 60a^2 + 448a)$, where $\frac{a}{2}$ is even.

Proof: Let the vertex set of G(a, A) be $A \cup B$, where $A = \{x_1, x_2, ..., x_{3a/2}\}, B = \{y_1, y_2, ..., y_{3a/2}\}.$

Now
$$WW(G(a,S)) = \frac{1}{2} \left(\sum_{u,v \in A} d(u,v) + \sum_{u,v \in B} d(u,v) + \sum_{u \in A,v \in B} d(u,v) + \sum_{u,v \in A} d^2(u,v) + \sum_{u,v \in A} d^2(u,v) \right)$$

$$= \frac{1}{2} \left[\left\{ \frac{3a}{2} \sum_{i=1}^{3a-2} i \right\} + \left\{ \frac{3a}{2} \sum_{i=1}^{3a-2} i \right\} + \left\{ a(1) + 4a(2) + 4a(3) + 3a \sum_{i=4}^{3a-2} i + \left(\frac{3a}{2} \right) \left(\frac{3a+2}{4} \right) \right\} \right]$$

$$+ \left\{ \frac{3a}{2} \sum_{i=1}^{3a-2} i^{2} \right\} + \left\{ \frac{3a}{2} \sum_{i=1}^{3a-2} i^{2} \right\} + \left\{ a(1)^{2} + 4a(2)^{2} + 4a(3)^{2} + 3a \sum_{i=4}^{3a-2} i^{2} + \left\{ \frac{3a}{2} \sum_{i=1}^{4} i^{2} + \left(\frac{3a}{2} \right) \left(\frac{3a+2}{4} \right)^{2} \right\} \right]$$
$$= \frac{1}{2} \left[\frac{1}{64} (27a^{3}) + \frac{1}{64} (27a^{3}) + \frac{1}{32} (27a^{3} + 36a^{2} + 96a) + \frac{1}{128} (27a^{4} + 24a^{2}) + \frac{1}{128} (27a^{4} + 24a^{2}) + \frac{1}{64} (27a^{4} + 54a^{3} + 24a^{2} + 704a) \right]$$
$$= \frac{1}{64} (27a^{4} + 81a^{3} + 60a^{2} + 448a).$$

S INDEX

Theorem 6.1. $S(G(a, S)) = 12a^2$, if $a \ge 2$.

Proof: The total number of vertices in this graph is 3*a*.

The number of vertices of degree 2 is a where as the number of vertices of degree 3 is 2a.

Hence
$$S(G(a, S)) = \prod_{i=1}^{n} i = (a)(2)(2a)(3) = 12a^2$$

Theorem 6.1. $S(G(a, A)) = 12a^2$, if $a \ge 2$.

Proof: The total number of vertices in this graph is 3*a*.

The number of vertices of degree 2 is a where as the number of vertices of degree 3 is 2a.

Hence
$$S(G(a, A)) = \prod_{i=1}^{n} i = (a)(2)(2a)(3) = 12a^2$$

Reverse wiener index

heorem 7.1.
$$RW(G(a,S)) = \frac{1}{8}(9a^3 + 24a^2 + 71a)$$
, where $a > 3$ and a is odd.

Proof: The total number of vertices in this graph *N* is 3*a*.

The diameter in this graph *d* is $\frac{a+5}{2}$.

And the Wiener index of this graph is $W(G(a, S)) = \frac{1}{8}(9a^3 + 60a^2 - 101a).$

Now
$$RW(G(a, S)) = \frac{1}{2}N(N-1)d - W.$$

= $\frac{1}{2}(3a)(3a-1)(\frac{a+5}{2}) - \frac{1}{8}(9a^3 + 60a^2 - 101a)$
= $\frac{1}{8}(9a^3 + 24a^2 + 71a).$

Theorem 7.2. $RW(G(a, S)) = \frac{1}{8}(9a^3 + 42a^2 + 64a)$, where a > 4 and a is even. **Proof:** The total number of vertices in this graph *N* is 3*a*.

The diameter in this graph d is $\frac{a+6}{2}$.

And the Wiener index of this graph is $W(G(a, S)) = \frac{1}{8}(9a^3 + 60a^2 - 100a)$.

Now
$$RW(G(a, S)) = \frac{1}{2}N(N-1)d - W.$$

= $\frac{1}{2}(3a)(3a-1)(\frac{a+6}{2}) - \frac{1}{8}(9a^3 + 60a^2 - 100a)$
= $\frac{1}{8}(9a^3 + 42a^2 + 64a).$

Theorem 7.3. $RW(G(a, A)) = \frac{1}{16}(27a^3 - 60a)$, where $\frac{a}{2}$ is odd. **Proof:** The total number of vertices in this graph N is 3a.

The diameter in this graph d is $\frac{3a+2}{4}$.

And the Wiener index of this graph is $W(G(a, A)) = \frac{1}{16}(27a^3 + 18a^2 + 48a)$.

Now
$$RW(G(a, A)) = \frac{1}{2}N(N-1)d - W.$$

= $\frac{1}{2}(3a)(3a-1)\left(\frac{3a+2}{2}\right) - \frac{1}{16}(27a^3 + 18a^2 + 48a)$
= $\frac{1}{16}(27a^3 - 60a).$

Theorem 7.4. $RW(G(a, A)) = \frac{1}{16}(27a^3 - 36a^2 - 48a)$, where $\frac{a}{2}$ is even. **Proof:** The total number of vertices in this graph *N* is 3*a*. Acta Ciencia Indica, Vol. XLIII M, No. 2 (2017)

The diameter in this graph d is $\frac{3a}{4}$.

And the Wiener index of this graph is $W(G(a, A)) = \frac{1}{16}(27a^3 + 18a^2 + 48a)$.

Now
$$RW(G(a, A)) = \frac{1}{2}N(N-1)d - W.$$

= $\frac{1}{2}(3a)(3a-1)\left(\frac{3a}{4}\right) - \frac{1}{16}(27a^3 + 18a^2 + 48a)$
= $\frac{1}{16}(27a^3 - 36a^2 - 48a).$

Eccentric connectivity index

Theorem 8.1. $\xi(G(a, S)) = 4a^2 + 17a$, where a > 3 and a is odd.

Proof: The total number of vertices in this graph is 3*a*.

In the first row the number of vertices of degree 2 is a, the number of vertices of degree 3 is 0.

In the second row the number of vertices of degree 2 is 0, the number of vertices of degree 3 is a.

In the third row the number of vertices of degree 2 is 0, the number of vertices of degree 3 is a.

In this graph the eccentricity of every vertex in the first row is $\frac{a+5}{2}$.

The eccentricity of every vertex in the second row is $\frac{a+5}{2}$.

And the eccentricity of every vertex in the second row is $\frac{a+3}{2}$.

Then
$$\xi(G(a,S)) = 2a\left(\frac{a+5}{2}\right) + 3a\left(\frac{a+5}{2}\right) + 3a\left(\frac{a+3}{2}\right) = 4a^2 + 17a.$$

Theorem 8.2. $\xi(G(a, S)) = 4a^2 + 15a$, where a > 4 and *a* is even.

Proof: The total number of vertices in this graph is 3*a*.

In the first row the number of vertices of degree 2 is a, the number of vertices of degree 3 is 0.

In the second row the number of vertices of degree 2 is 0, the number of vertices of degree 3 is a.

In the third row the number of vertices of degree 2 is 0, the number of vertices of degree 3 is a.

In this graph the eccentricity of every vertex in the first row is $\frac{a+6}{2}$.

The eccentricity of every vertex in the second row is $\frac{a+4}{2}$.

And the eccentricity of every vertex in the second row is $\frac{a+2}{2}$.

Then
$$\xi(G(a,S)) = 2a\left(\frac{a+6}{2}\right) + 3a\left(\frac{a+4}{2}\right) + 3a\left(\frac{a+2}{2}\right) = 4a^2 + 15a$$
.

Theorem 8.3. $\xi(G(a, A)) = 6a^2 + 4a$, where $\frac{a}{2}$ is odd.

Proof: The total number of vertices in this graph is 3*a*.

In the first row the number of vertices of degree 2 is a, the number of vertices of degree 3 is 0.

In the second row the number of vertices of degree 2 is 0, the number of vertices of degree 3 is a.

In the third row the number of vertices of degree 2 is 0, the number of vertices of degree 3 is a.

In this graph the eccentricity of every vertex in the first row is $\frac{3a+2}{4}$.

The eccentricity of every vertex in the second row is $\frac{3a+2}{4}$.

And the eccentricity of every vertex in the second row is $\frac{3a+2}{4}$.

Then
$$\xi(G(a, A)) = 2a\left(\frac{3a+2}{4}\right) + 3a\left(\frac{3a+2}{4}\right) + 3a\left(\frac{3a+2}{4}\right) = 6a^2 + 4a$$
.

Theorem 8.4. $\xi(G(a, A)) = 6a^2$, where $\frac{a}{2}$ is even.

Proof: The total number of vertices in this graph is 3*a*.

In the first row the number of vertices of degree 2 is a, the number of vertices of degree 3 is 0.

In the second row the number of vertices of degree 2 is 0, the number of vertices of degree 3 is a.

In the third row the number of vertices of degree 2 is 0, the number of vertices of degree 3 is a.

In this graph the eccentricity of every vertex in the first row is $\frac{3a}{4}$.

The eccentricity of every vertex in the second row is $\frac{3a}{4}$.

And the eccentricity of every vertex in the second row is $\frac{3a}{4}$.

Then
$$\xi(G(a, A)) = 2a\left(\frac{3a}{4}\right) + 3a\left(\frac{3a}{4}\right) + 3a\left(\frac{3a}{4}\right) = 6a^2$$
.

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