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On the Wiener Index of Pentachains

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Abstract

Topological index is the first effective choice in QSAR research and Wiener index is the most important topological index, since it can be obtained directly from molecular structures.In this paper we obtain wiener index for the graphs formed of concatenated 5-cycles in two rows of various lengths. Compounds represented by these chemical graphs include Octahedro-pentalene and Dodecahydro-Pentaleno [1,6-cd] pentalene.

Mathematics subject classification: 05C12

Keywords: Wiener index, Pentachain.

1 Introduction

The study of topological indices like wiener index,pi index…is helpful to build a correlation model between the chemical structures of various chemical compounds.The computation of general expressions for wiener indices of classes of polycyclic graphs gained importance with the explicit formula of Young and Yeh in 1995. Damir Vukicevic and Nenad Trinajstic[1] computed wiener indices of a class of pericondensed benzenoid graphs consisting of three rows of hexagons of various lengths.

Recently Ivan Gutman and co-authors[2] studied Schultz and modified Schultz of one row pentachains. In [3] we have obtained explicit formulas for wiener index of concatenated 5-cycles in one row.

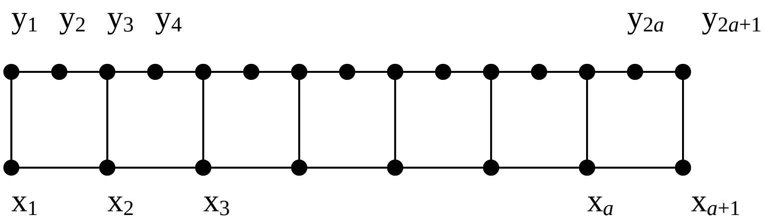
2 Preliminaries

The Wiener index of a graph is defined as $W(G)=\frac{1}{2}\sum_{u\in V}\sum_{v\in V} d_G(u,v)$ where $d_G(u,v)$ is the length of shortest path connecting u and v. A pentachain is a graph consisting of concatenated 5 cycles (Pentenes). We follow the following notation for convenience.

Throughout this paper N stands for the set of natural numbers and a,b,c are natural numbers.

5 cycles can be concatenated in two ways as explained below. We assume that the number of 5 cycles is a.

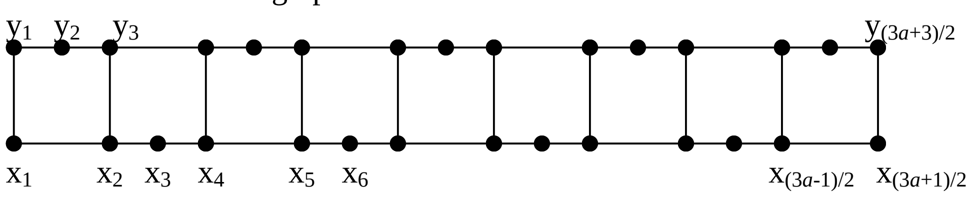
(i) Straight chaining: The graph when $a = 7$ is shown below.



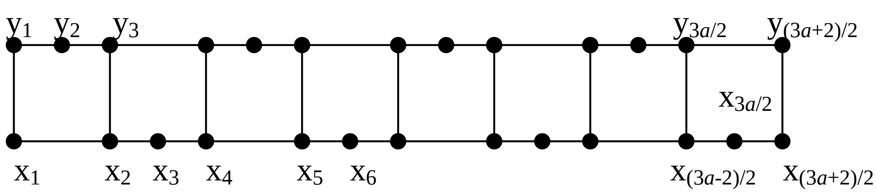
We denote the class of above graphs as G (a,S).

(ii) Alternate chaining:

(1) When a is odd: The graph when $a = 9$ is shown below.



(2) When a is even: The graph when $a = 8$ is shown below.



We denote the above class of alternate chaining graphs as G (a,A).

We state here the formulae[3] for the Wiener Index of above Pentagonal structures with out proof.

Result 2.1: $W(G(a,S)) = \frac{1}{2}\,(3a^3+21a^2-6a+14)$ if $2 \le a \in N$

Result 2.2: $W(G(a,A)) = \frac{1}{8}\,(18a^3+45a^2+58a-1)$ where $a \in N$ is odd

Result 2.3: $W(G(a,A)) = \frac{1}{8}\,(18a^3+45a^2+58a)$ where $a \in N$ is even

Note: In G(a,S) , $\sum_{u,v \in B} d(u,v) = 2 \sum_{i=1,3,5..}^{2a-1} \sum_{j=i+2,i+4,..}^{2a+1} ((j+1)/2-(i+1)/2+2) - 4(a-1)-3$

$$+\, 2 \sum_{i=2,4,6..}^{2a-2} \sum_{j=i+2,i+4,..}^{2a} (j/2-(i/2+1)+4) + a-(a-2)4 - 3\}$$

$$= \frac{1}{6}\,(4a^3+36a^2-46a+36)$$

where $B = \{y_1, y_2, ...y_{(2a+1)}\}$, $a>1$.

3 Main results

In this section we obtain formulae for Wiener Index of pentachains in two rows. The different cases are shown in the following figures.

We denote the graph consisting of 5-cycles in two rows with b cycles in row1 and a cycles in row2 as shown below by G(a,b,S_1)

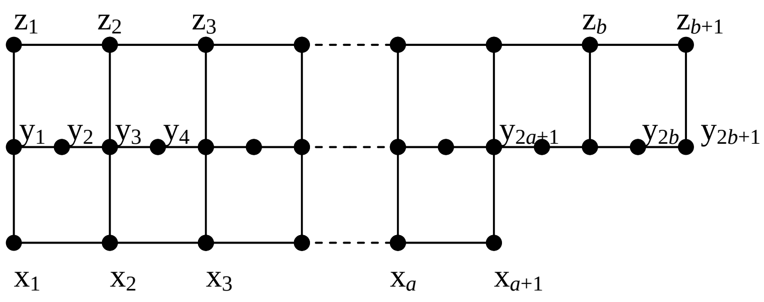


Fig.1

We denote the graph consisting of 5-cycles in two rows with b cycles in row1 and a cycles in row2 as shown below by G(a,b,S_2)

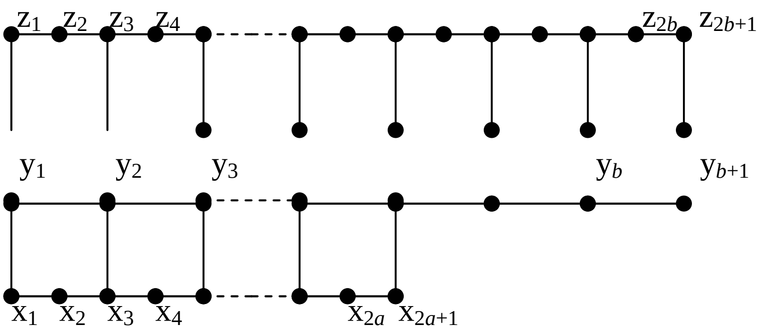


Fig.2

We denote the graph consisting of 5-cycles in two rows with *b* cycles in row1 and *a* cycles in row2 as shown below by G(*a*,*b*,A)

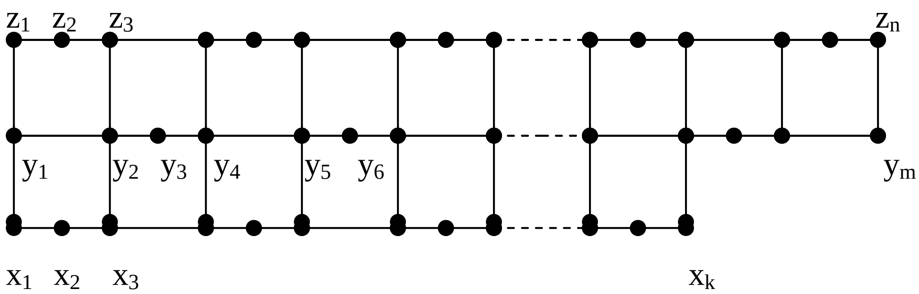


Fig.3

Where k = (3*a*+2)/2, m = n = (3*b*+2)/2 , if *a* = even and *b* = even
k = (3*a*+2)/2, m = (3*b*+1)/2, n = (3b+3)/2 ,if *a* = even and *b* = odd
k = (3*a*+3)/2, m = n = (3*b*+2)/2 , if *a* = odd and *b* = even
k = (3*a*+3)/2, m = (3*b*+1)/2, n = (3b+3)/2 ,if *a* = odd and *b* = odd

We explain the algorithm we adopted for the computation of Wiener Index,considering the case shown in Fig1,with *b*>*a*

1. Form the sets of vertices, A = $\{x_1, x_2, \ldots . x_{a+1}\}$, B = $\{y_1, y_2, \ldots . y_{(2a+1)}\}$, C = $\{y_{2a+2}, y_{2a+3}, \ldots y_{2b+1}\}$, D = $\{z_1, z_2, \ldots . z_{(b+1)}\}$ and take W=0.
2. Compute the Wiener Index (say $n_{1)}$ for the subgraph generated by B∪C∪D using the formula W(G(*b*,S)) and W=W+ n_1.
3. Compute the Wiener Index (say n_2) for the subgraph generated by A∪B using the formula W(G(*a*,S)), W=W+ $n_{2.}$
4. Compute $\sum_{u,v \in B} d(u,v)$, the sum of the shortest distances between vertices of B (say n_3), Now W=W- n_3,since these distances are repeated in steps 2 and 3.

5. Compute $\sum_{\substack{u\in A\\ v\in C}} d(u,v)$, the sum of the shortest distances between vertices of A and C (say n_4),W=W+ n_4.
6. Compute $\sum_{\substack{u\in A\\ v\in D}} d(u,v)$, the sum of the shortest distances between vertices of A and D (say n_5), W=W+ n_5.
7. W is the Wiener Index of the graph shown in Fig1.

By modifying the above algorithm suitably , Wiener Index for all other cases can be computed.

Theorem 3.1: $W(G(a,b,S_1)) = 36$,if $a=b=1$

$= \frac{1}{3}(8a^3+54a^2+19a+30)$, if $a=b\geq 2$

$= 95$, if $a=1, b=2$.

$= \frac{1}{3}(8a^3+72a^2+124a+81)$, if $b=a+1$, $a\geq 2$

$= \frac{1}{6}(7a^3-12a^2-25a) + \frac{1}{2}(3b^3+24b^2+13b+16ab -3a^2b+3ab^2) + 6$, if $a\geq 2$, $b>a+1$

$= \frac{1}{2}(3b^3+27b^2+26b+2)$, if $a=1$, $b>2$.

Proof: The proof is clear from the following lemmas.

Lemma 3.1: $W(G(a,a,S_1)) = \frac{1}{3}(8a^3+54a^2+19a+30)$, if $a\geq 2$.

Proof: Let the vertex set of $G(a,a,S_1) = A\cup B\cup C$, where $A=\{x_1, x_2, ...x_{a+1}\}$, $B=\{y_1, y_2, ...y_{(2a+1)}\}$, $C=\{z_1, z_2, ...z_{(a+1)}\}$. Now

$$W(G(a,a,S_1)) = 2W(a) - \sum_{u,v\in B} d(u,v) + \sum_{\substack{u\in A\\ v\in C}} d(u,v)$$

$$= (3a^3+21a^2-6a+14) - \frac{1}{6}(4a^3+36a^2-46a+36) + \sum_{i=1}^{a+1}\sum_{j=1}^{a+1}(|i-j|+2)$$

$$= \frac{1}{3}(8a^3+54a^2+19a+30).$$

Lemma 3.2: $W(G(a,a+1,S_1)) = \frac{1}{3}(8a^3+72a^2+124a+81)$, if $a\geq 2$.

Proof: Let the vertex set of $G(a,a+1,S_1) = A\cup B\cup C\cup D$, where $A=\{x_1, x_2, ...x_{a+1}\}$, $B=\{y_1, y_2, ...y_{(2a+1)}\}$, $C=\{y_{2a+2}, y_{2a+3}\}$, $D=\{z_1, z_2, ...z_{(a+2)}\}$.
Now

$$W(G(a,a+1,S_1)) = W(a) + W(a+1) - \sum_{u,v\in B} d(u,v) + \sum_{\substack{u\in A\\ v\in C}} d(u,v) + \sum_{\substack{u\in A\\ v\in D}} d(u,v)$$

$$= \frac{1}{2}(3a^3+21a^2-6a+14) + \frac{1}{2}(3a^3+30a^2+45a+32)$$

$$- \frac{1}{6}(4a^3+36a^2-46a+36) + \{\sum_{i=2}^{a+2} i + \sum_{i=3}^{a+3} i\} + \sum_{i=1}^{a+1}\sum_{j=1}^{a+2}(|i-j|+2)$$

$$= \frac{1}{3}(8a^3+72a^2+124a+81).$$

Lemma 3.3: $W(G(a,b,S_1)) = \frac{1}{6}(7a^3-12a^2-25a) + \frac{1}{2}(3b^3+24b^2+13b+16ab$
$-3a^2b+3ab^2) + 6$, if $a\geq 2$, $b>a+1$.

Proof: Let the vertex set of $G(a,b,S_1) = A\cup B\cup C\cup D$, where
$A = \{x_1, x_2, ...x_{a+1}\}$, $B = \{y_1, y_2, ...y_{(2a+1)}\}$, $C = \{y_{2a+2}, y_{2a+3}, ...y_{2b+1}\}$,
$D = \{z_1, z_2, ...z_{(b+1)}\}$. Now

$$W(G(a,b,S_1)) = W(a) + W(b) - \sum_{u,v\in B} d(u,v) + \sum_{\substack{u\in A\\ v\in C}} d(u,v) + \sum_{\substack{u\in A\\ v\in D}} d(u,v)$$

$$= \frac{1}{2}(3a^3+21a^2-6a+14) + \frac{1}{2}(3b^3+21b^2-6b+14)$$

$$- \frac{1}{6}(4a^3+36a^2-46a+36) + \{ |C| \sum_{u\in A} d(u, y_{2a+1})$$

$$+ |A| \sum_{u\in C} d(u, y_{2a+1}) \} + \sum_{i=1}^{a+1}\sum_{j=1}^{b+1}(|i-j|+2)$$

$$= \frac{1}{2}(3a^3+21a^2-6a+14) + \frac{1}{2}(3b^3+21b^2-6b+14)$$

$$- \frac{1}{6}(4a^3+36a^2-46a+36) + \{2(b-a)\sum_{i=1}^{a+1}(a+1-i+1)$$

$$+ (a+1)\,[2\sum_{i=2a+3,2a+5,...}^{2b+1}((i+1)/2-(a+1)+2)-4\,]\}$$

$$+ \sum_{i=1}^{a+1}\sum_{j=1}^{b+1}(|i-j|+2)$$

$$= \frac{1}{6}(7a^3-12a^2-25a) + \frac{1}{2}(3b^3+24b^2+13b+16ab-3a^2b+3ab^2) + 6.$$

Lemma 3.4: $W(G(1,b,S_1)) = \frac{1}{2}(3b^3+27b^2+26b+2)$, $b>2$.

Proof: Let the vertex set of $G(1,b,S_1) = A\cup B\cup C\cup D$, where $A = \{x_1, x_2\}$,
$B = \{y_1, y_2, y_3\}$, $C = \{y_4, y_5, ...y_{2b+1}\}$, $D = \{z_1, z_2, ...z_{(b+1)}\}$. Now

$$W(G(1,b,S_1)) = d(x_1,x_2) + W(b) + \sum_{\substack{u\in A\\ v\in D}} d(u,v) + \sum_{\substack{u\in A\\ v\in B}} d(u,v) + \sum_{\substack{u\in A\\ v\in C}} d(u,v)$$

$$= 1 + \frac{1}{2}(3b^3+21b^2-6b+14) + \{ \sum_{i=2}^{b+2} i + (\sum_{i=2}^{b+1} i + 3) \} + \{5+5\}$$

$$+ \{|C|\sum_{u\in A} d(u,y_3) + |A|\sum_{u\in C} d(u,y_3)\}$$

$$= 1 + \frac{1}{2}(3b^3+21b^2-6b+14) + \{ \sum_{i=2}^{b+2} i + (\sum_{i=2}^{b+1} i + 3) \} + \{5+5\}$$

$$+\{2(b-1)(2+1) + 2[2\sum_{i=5,7,9...}^{2b+1}((i+1)/2-2+2)-4]\}$$

$$= \frac{1}{2}(3b^3+27b^2+26b+2).$$

Theorem 3.2: $W(G(a,b,S_2)) = 55$, if $a=b=1$

$$= \frac{1}{6}(25a^3+195a^2+26a+96), \text{ if } a=b\geq 2$$

$$= \frac{1}{6}(16a^3+45a^2+5a+9b^3+72b^2+21b) + 13ab$$

$$-3a^2b+3ab^2+16, \text{ if } b > a \geq 2$$

$$= \frac{1}{2}(3b^3+30b^2+27b+52), \text{ if } a=1, b>1.$$

Proof: The proof is clear from the following lemmas.

Lemma 3.5: $W(G(a,a,S_2)) = \frac{1}{6}(25a^3+195a^2+26a+96)$, $a\geq 2$.

Proof: Let the vertex set of $G(a,a,S_2) = A\cup B\cup C$, where $A = \{x_1, x_2, ...x_{2a+1}\}$, $B = \{y_1, y_2, ...y_{a+1}\}$, $C = \{z_1, z_2, ...z_{2a+1}\}$. Now

$$W(G(a,a,S_2)) = 2W(a) - \sum_{u,v\in B} d(u,v) + \sum_{\substack{u\in A\\ v\in C}} d(u,v)$$

$$= (3a^3+21a^2-6a+14) - \sum_{i=1}^{a}\sum_{j=i+1}^{a+1}(j-i)$$

$$+ \{2[\sum_{i=1,3,5,...}^{2a+1}\sum_{j=1,3,5,...}^{i-2}((i+1)/2-(j+1)/2+2)$$

$$+ \sum_{i=1,3,5,...}^{2a+1}\sum_{j=i+2,i+4,..}^{2a+1}((j+1)/2-(i+1)/2+2)] + 2(a+1)$$

$$+ [2\sum_{i=2,4,6,...}^{2a}\sum_{j=1,3,5,...}^{i-1}(i/2-(j+1)/2+3) - 3a]$$

$$+ [2\sum_{i=2,4,6,...}^{2a}\sum_{j=i+1,i+3...}^{2a+1}((j+1)/2-(i/2+1)+3) - 3a] + 4a\}$$

$$= \frac{1}{6}(25a^3+195a^2+26a+96).$$

Lemma 3.6: $W(G(a,b,S_2) = \frac{1}{6}(16a^3+45a^2+5a+9b^3+72b^2+21b) + 13ab$
$-3a^2b+3ab^2+16,\ b> a\geq 2.$

Proof: Let the vertex set of $G(a,b,S_2) = A\cup B\cup C\cup D$, where $A = \{x_1, x_2, ...x_{2a+1}\}$, $B = \{y_1, y_2, ...y_{a+1}\}$, $C = \{y_{a+2}, y_{a+3}, ...y_{b+1}\}$, $D = \{z_1, z_2, ...z_{2b+1}\}$. Now

$$W(G(a,b,S_2)) = W(a) + W(b) - \sum_{u,v\in B} d(u,v) + \sum_{\substack{u\in A\\ v\in D}} d(u,v) + \sum_{\substack{u\in A\\ v\in C}} d(u,v)$$

$$= \frac{1}{2}(3a^3+21a^2-6a+14) + \frac{1}{2}(3b^3+21b^2-6b+14) - \sum_{i=1}^{a}\sum_{j=i+1}^{a+1}(j-i)$$

$$+ \{ 2[\sum_{i=1,3,5,...}^{2a+1}\sum_{j=1,3,5,...}^{i-2}((i+1)/2-(j+1)/2+2)$$

$$+ \sum_{i=1,3,5,...}^{2a+1}\sum_{j=i+2,i+4,..}^{2b+1}((j+1)/2-(i+1)/2+2)\,] + 2(a+1)$$

$$+ [2\sum_{i=2,4,6,...}^{2a}\sum_{j=1,3,5,...}^{i-1}(i/2-(j+1)/2+3) - 3a]$$

$$+ [2\sum_{i=2,4,6,...}^{2a}\sum_{j=i+1,i+3...}^{2b+1}((j+1)/2-(i/2+1)+3) - 3a] + 4a\}$$

$$+\{2\sum_{i=a+2}^{b+1}\sum_{j=1,3,5...}^{2a-1}(i-(j+1)/2+1) + \sum_{i=2}^{b-a+1} i\,\}$$

$$= \frac{1}{6}(16a^3+45a^2+5a+9b^3+72b^2+21b) + 13ab - 3a^2b + 3ab^2 + 16.$$

Lemma 3.7: $W(G(1,b,S_2) = \frac{1}{2}(3b^3+30b^2+27b+52),\ b>1.$

Proof: Let the vertex set of $G(1,b,S_2) = A\cup B\cup C$, where $A = \{x_1, x_2, x_3\}$, $B = \{y_1, y_2, ...y_{b+1}\}$, $C = \{z_1, z_2, ...z_{2b+1}\}$.Now

$$W(G(1,b,S_2)) = \sum_{u,v\in A} d(u,v) + W(b) + \sum_{\substack{u\in A\\ v\in B}} d(u,v) + \sum_{\substack{u\in A\\ v\in C}} d(u,v)$$

$$= 4 + \frac{1}{2}(3b^3+21b^2-6b+14) + \{ \sum_{i=1}^{b+1} i + (\sum_{i=2}^{b+1} i+2) + (\sum_{i=1}^{b} i+2)\}$$

$$+\{ 2\sum_{i=1,3,5...}^{2b+1}((i+1)/2-1+2) - 2 + 2\sum_{i=4,6,...}^{2b}(i/2-2+4) + 10$$

$$+2\sum_{i=3,5,7,..}^{2b+1}((i+1)/2-2+2)-2+6\}$$

$$= \frac{1}{2}(3b^3+30b^2+27b+52).$$

Theorem 3.3: $W(G(a,b,A)) = \frac{1}{16}(81a^3+261a^2+487a+51)$, if $a=b$ is odd.

$= \frac{1}{16}(81a^3+234a^2+424a-32)$, if $a=b$ is even.

$= \frac{1}{16}(45a^3+81a^2+179a+36b^3+144b^2+302b+36ab-54a^2b+54ab^2+47)$, if a is odd and b is even , $b>a$

$= \frac{1}{16}(45a^3+36a^2+236a+36b^3+126b^2+188b+72ab-54a^2b+54ab^2+16)$, if a is even and b is even , $b>a$

$= \frac{1}{16}(45a^3+36a^2+242a+36b^3+126b^2+188b+72ab-54a^2b+54ab^2+18)$, if a is even and b is odd , $b>a$

$= \frac{1}{16}(45a^3+81a^2+185a+36b^3+144b^2+302b+36ab-54a^2b+54ab^2+51)$, if a is odd and b is odd , $b>a$.

Proof: The proof is clear from the following lemmas**.**

Lemma 3.8: $W(G(a,a,A)) = \frac{1}{16}(81a^3+261a^2+487a+51)$, where a is odd.

Proof: Let the vertex set of $G(a,a,A) = A\cup B\cup C\cup D\cup E$, where

$A=\{x_1,x_4,....x_{(3a-1)/2}\}$, $B=\{x_3,x_6,....x_{(3a+3)/2}\}$, $C=\{x_2,x_5,....x_{(3a+1)/2}\}$,

$D=\{y_1,y_2,....y_{(3a+1)/2}\}$,E= $\{z_1,z_2,....z_{(3a+3)/2}\}$, Now

$$W(G(a,a,A)) = \sum_{u,v\in A\cup B\cup C\cup D} d(u,v) + \sum_{u,v\in D\cup E} d(u,v) - \sum_{u,v\in D} d(u,v) + \sum_{\substack{u\in A\cup B\cup C\\ v\in E}} d(u,v)$$

$$= \frac{2}{8}(18a^3+45a^2+58a-1) - \sum_{i=1}^{(3a-1)/2}\sum_{j=i+1}^{(3a+1)/2}(j-i)$$

$$+ \{[\sum_{i=4,7,10..}^{(3a-1)/2}\sum_{j=1}^{i-3}((i-3)-j+4) + \sum_{i=1,4,7,...}^{(3a-1)/2}\sum_{j=i+2}^{(3a+3)/2}(j-(i+2)+3)$$

$$+ (\frac{a-1}{2}\text{x}12)+5] + [\sum_{i=3,6,9...}^{(3a+3)/2}\sum_{j=1}^{i-2}((i-2)-j+3)$$

$$+ \sum_{i=3,6,9..}^{(3a-3)/2} \sum_{j=i+3}^{(3a+3)/2} (j-(i+3)+4) \ + (\frac{a-1}{2} \text{ x } 12\ ) + 5\ ]$$

$$+ \ [\sum_{i=5,8,..}^{(3a+1)/2} \sum_{j=1}^{i-4} ((i-4)-j+5) \ + \sum_{i=2,5,8...}^{(3a-5)/2} \sum_{j=i+4}^{(3a+3)/2} (j-(i+4)+5)$$

$$+ (\frac{a-3}{2} \text{ x } 28) + 19 + 19]\ \}$$

$$= \frac{1}{16}(81a^3+261a^2+487a+51).$$

Lemma 3.9: $W(G(a,a,A)) = \frac{1}{16}(81a^3+234a^2+424a-32)$, where a is even.

Proof: Let the vertex set of $G(a,a,A) = A \cup B \cup C \cup D$, where $A = \{x_1, x_2, ...x_{3a/2}\}$, $B = \{y_1, y_2, ...y_{(3a-2)/2}\}$, $C = \{z_1, z_2, ...z_{3a/2}\}$, $D = \{x_{(3a+2)/2}, y_{3a/2}, y_{(3a+2)/2}, z_{(3a+2)/2}\}$

Now

$$W(G((a,a,A)) = W(G(a\text{-}1,a\text{-}1,A)) + \sum_{\substack{u \in A \cup B \cup C \\ v \in D}} d(u,v) \ + \sum_{u,v \in D} d(u,v)$$

$$= \frac{1}{16}\ (81(a\text{-}1)^3+261(a\text{-}1)^2+ 487(a\text{-}1)+51) + \sum_{u \in A} d(u, x_{(3a+2)/2})$$

$$+ \sum_{u \in B} d(u, x_{(3a+2)/2}) + \sum_{u \in C} d(u, x_{(3a+2)/2}) + \sum_{u \in A} d(u, z_{(3a+2)/2})$$

$$+ \sum_{u \in B} d(u, z_{(3a+2)/2}) + \sum_{u \in C} d(u, z_{(3a+2)/2}) + \sum_{u \in A} d(u, y_{3a/2})$$

$$+ \sum_{u \in B} d(u, y_{3a/2}) + \sum_{u \in C} d(u, y_{3a/2}) + \sum_{u \in A} d(u, y_{(3a+2)/2})$$

$$+ \sum_{u \in B} d(u, y_{(3a+2)/2}) + \sum_{u \in C} d(u, y_{(3a+2)/2}) + \sum_{u,v \in D} d(u,v)$$

$$= \frac{1}{16}(81a^3+18a^2+208a\text{-}256) + \{\ 2[\sum_{i=1}^{3a/2} i + (\sum_{i=1}^{3a/2} i \text{ -}1) + (\sum_{i=1}^{(3a+2)/2} i \ \text{-}6\text{+}7)]\}$$

$$+\{\sum_{i=1}^{(3a-2)/2} i \ + (\sum_{i=1}^{3a/2} i \text{ -}3\text{+}5) +(\sum_{i=1}^{3a/2} i \text{ -}3\text{+}5)\}+ \{(\sum_{i=1}^{3a/2} i \text{ -}1) + 2(\sum_{i=1}^{(3a+2)/2} i \ \text{-}1)\}+9$$

$$= \frac{1}{16}(81a^3+234a^2+ 424a\text{-}32).$$

Lemma 3.10: $W(G(a,b,A)) = \frac{1}{16}(45a^3+81a^2+179a+36b^3+144b^2+302b+36ab$ $-54a^2b+54ab^2+47)$, if a is odd and b is even , $b>a$.

Proof: Let the vertex set of $G(a,b,A) = A \cup B \cup C \cup D$, where
$A = \{x_1, x_2, ...x_{(3a+3)/2}\}$, $B = \{y_1, y_2, ...y_{(3a+1)/2}\}$,

$C = \{y_{(3a+3)/2}, y_{(3a+5)/2}, \ldots. y_{(3b+2)/2}\}$, $D = \{z_1, z_2, \ldots. z_{(3b+2)/2}\}$ Now

$$W(G(a,b,A)) = W(a) + W(b) - \sum_{u,v\in B} d(u,v) + \sum_{\substack{u\in A\\ v\in C}} d(u,v) + \sum_{\substack{u\in A\\ v\in D}} d(u,v)$$

$$= \frac{1}{8}(18a^3+45a^2+58a-1) + \frac{1}{8}(18b^3+45b^2+58b) - \sum_{i=1}^{(3a-1)/2} \sum_{j=i+1}^{(3a+1)/2} (j-i)$$

$$+ \{ |A| \sum_{u\in C} d(u, y_{(3a+1)/2}) + |C| \sum_{u\in A} d(u, y_{(3a+1)/2}) \}$$

$$+ \sum_{\substack{u\in A\\ v\in D}} d(u,v)$$

$$= \frac{1}{8}(18a^3+45a^2+58a-1) + \frac{1}{8}(18b^3+45b^2+58b)$$

$$- \sum_{i=1}^{(3a-1)/2} \sum_{j=i+1}^{(3a+1)/2} (j-i) + \{(3a+3)/2 \sum_{i=1}^{(3b-3a+1)/2} i$$

$$+ (3b-3a+1)/2 \; [\sum_{i=1,4,7\ldots}^{(3a-1)/2} ((3a+1)/2-(i+1)+2)$$

$$+ \sum_{i=2,5,8\ldots}^{(3a+1)/2} ((3a+1)/2-(i+2)+3) + 1$$

$$+ \sum_{i=3,6,9\ldots}^{(3a+3)/2} ((3a+1)/2-(i+1)+2) + 1]\}$$

$$+ \{[\sum_{i=4,7,10..}^{(3a-1)/2} \sum_{j=1}^{i-3} ((i-3)-j+4) + \sum_{i=1,4,7,\ldots}^{(3a-1)/2} \sum_{j=i+2}^{(3b+2)/2} (j-(i+2)+3)$$

$$+ (\frac{a-1}{2} \text{x}12) + 5] + [\sum_{i=3,6,9\ldots}^{(3a+3)/2} \sum_{j=1}^{i-2} ((i-2)-j+3)$$

$$+ \sum_{i=3,6,9..}^{(3a-3)/2} \sum_{j=i+3}^{(3b+2)/2} (j-(i+3)+4) + (\frac{a-1}{2} \text{ x } 12) + 3$$

$$+ \sum_{i=(3a+3)/2}^{(3b+2)/2} (i-(3a+3)/2+2)] + [\sum_{i=5,8,..}^{(3a+1)/2} \sum_{j=1}^{i-4} ((i-4)-j+5)$$

$$+ \sum_{i=2,5,8\ldots}^{(3a-5)/2} \sum_{j=i+4}^{(3b+2)/2} (j-(i+4)+5) + (\frac{a-3}{2} \text{ x } 28) + 19 + 16$$

$$+ \sum_{i=(3a+3)/2}^{(3b+2)/2} (i-(3a+3)/2+3)]\}$$

$$= \frac{1}{16}(45a^3+81a^2+179a+36b^3+144b^2+302b+36ab-54a^2b+54ab^2+47).$$

Lemma 3.11: W(G(a,b,A))= $\frac{1}{16}$(45a^3+36a^2+236a+36b^3+126b^2+188b+72ab -54a^2b+54ab^2+16), if a is even and b is even , $b>a$.

Proof: Let the vertex set of G(a,b,A) = A∪B∪C∪D, where

A = $\{x_1, x_2, ...x_{(3a+2)/2}\}$, B = $\{y_1, y_2, ...y_{(3a+2)/2}\}$,

C = $\{y_{(3a+4)/2}, y_{(3a+6)/2}, ...y_{(3b+2)/2}\}$,D = $\{z_1, z_2, ...z_{(3b+2)/2}\}$ Now

$$W(G(a,b,A)) = W(a) + W(b) - \sum_{u,v\in B} d(u,v) + \sum_{\substack{u\in A\\ v\in C}} d(u,v) + \sum_{\substack{u\in A\\ v\in D}} d(u,v)$$

$$= \frac{1}{8}(18a^3+45a^2+58a) + \frac{1}{8}(18b^3+45b^2+58b) - \sum_{i=1}^{(3a-1)/2}\sum_{j=i+1}^{(3a+1)/2}(j-i)$$

$$+ \{|A| \sum_{u\in C} d(u, y_{(3a+2)/2}) + |C| \sum_{u\in A} d(u, y_{(3a+2)/2})\}$$

$$+ \sum_{\substack{u\in A\\ v\in D}} d(u,v)$$

$$= \frac{1}{8}(18a^3+45a^2+58a) + \frac{1}{8}(18b^3+ 45b^2+58b) - \sum_{i=1}^{(3a-1)/2}\sum_{j=i+1}^{(3a+1)/2}(j-i)$$

$$+ \{(3a+2)/2 \sum_{i=1}^{(3b-3a)/2} i + (3b-3a)/2 [\sum_{i=1,4,7...}^{(3a+2)/2}((3a+2)/2-(i+1)+2)$$

$$+ \sum_{i=2,5,8...}^{(3a-2)/2}((3a+2)/2-(i+2)+3) + \sum_{i=3,6,9...}^{3a/2}((3a+2)/2-(i+1)+2)]\}$$

$$+ \{[\sum_{i=4,7,10..}^{(3a+2)/2}\sum_{j=1}^{i-3}((i-3)-j+4) + \sum_{i=1,4,7,...}^{(3a+2)/2}\sum_{j=i+2}^{(3b+2)/2}(j-(i+2)+3)$$

$$+ (\frac{a}{2}\text{x}12) +5] + [\sum_{i=3,6,9...}^{3a/2}\sum_{j=1}^{i-2}((i-2)-j+3)$$

$$+ \sum_{i=3,6,9..}^{3a/2}\sum_{j=i+3}^{(3b+2)/2}(j-(i+3)+4) + (\frac{a}{2}\text{x } 12)]$$

$$+ [\sum_{i=5,8,..}^{(3a-2)/2}\sum_{j=1}^{i-4}((i-4)-j+5) + \sum_{i=2,5,8...}^{(3a-2)/2}\sum_{j=i+4}^{(3b+2)/2}(j-(i+4)+5)$$

$$+ (\frac{a-2}{2}\text{x } 28)+19]\}$$

$$= \frac{1}{16}(45a^3+36a^2+236a+36b^3+126b^2+188b+72ab-54a^2b+54ab^2+16).$$

Lemma 3.12: W(G(a,b,A)) = $\frac{1}{16}$(45a^3+36a^2+242a+36b^3+126b^2+188b+72ab

$-54a^2b+54ab^2+18)$, if a is even and b is odd , $b>a$.

Proof: Let the vertex set of G(a,b,A) = A∪B∪C∪D, where
A = $\{x_1, x_2, ...x_{(3a+2)/2}\}$, B = $\{y_1, y_2, ...y_{(3a+2)/2}\}$,
C = $\{y_{(3a+4)/2}, y_{(3a+6)/2}, ...y_{(3b+1)/2}\}$, D = $\{z_1, z_2, ...z_{(3b+3)/2}\}$ Now

$$W(G(a,b,A)) = W(a) + W(b) - \sum_{u,v\in B} d(u,v) + \sum_{\substack{u\in A\\ v\in C}} d(u,v) + \sum_{\substack{u\in A\\ v\in D}} d(u,v)$$

$$= \frac{1}{8}(18a^3+45a^2+58a) + \frac{1}{8}(18b^3+45b^2+58b-1) - \sum_{i=1}^{(3a-1)/2}\sum_{j=i+1}^{(3a+1)/2}(j-i)$$
$$+ \{ |A| \sum_{u\in C} d(u, y_{(3a+2)/2}) + |C| \sum_{u\in A} d(u, y_{(3a+2)/2})\}$$
$$+ \sum_{\substack{u\in A\\ v\in D}} d(u,v)$$

$$= \frac{1}{8}(18a^3+45a^2+58a) + \frac{1}{8}(18b^3+45b^2+58b-1) - \sum_{i=1}^{(3a-1)/2}\sum_{j=i+1}^{(3a+1)/2}(j-i)$$
$$+\{(3a+2)/2 \sum_{i=1}^{(3b-3a-1)/2} i + (3b-3a-1)/2\ [\sum_{i=1,4,7...}^{(3a+2)/2}((3a+2)/2-(i+1)+2)$$
$$+ \sum_{i=2,5,8...}^{(3a-2)/2}((3a+2)/2-(i+2)+3) + \sum_{i=3,6,9...}^{3a/2}((3a+2)/2-(i+1)+2)\ ]\}$$
$$+\{[\sum_{i=4,7,10..}^{(3a+2)/2}\sum_{j=1}^{i-3}((i-3)-j+4) + \sum_{i=1,4,7,...}^{(3a+2)/2}\sum_{j=i+2}^{(3b+3)/2}(j-(i+2)+3)$$
$$+ (\frac{a}{2}\text{x}12) + 5] + [\sum_{i=3,6,9...}^{3a/2}\sum_{j=1}^{i-2}((i-2)-j+3)$$
$$+ \sum_{i=3,6,9..}^{3a/2}\sum_{j=i+3}^{(3b+3)/2}(j-(i+3)+4) + (\frac{a}{2}\text{x }12)]$$
$$+ [\sum_{i=5,8,..}^{(3a-2)/2}\sum_{j=1}^{i-4}((i-4)-j+5) + \sum_{i=2,5,8...}^{(3a-2)/2}\sum_{j=i+4}^{(3b+3)/2}(j-(i+4)+5)$$
$$+ (\frac{a-2}{2}\text{x }28) +19]\}$$
$$= \frac{1}{16}(45a^3+36a^2+242a+36b^3+126b^2+188b+72ab-54a^2b+54ab^2+18).$$

Lemma 3.13: W(G(a,b,A))= $\frac{1}{16}$ $(45a^3+81a^2+185a+36b^3+144b^2+302b+36ab$
$-54a^2b+54ab^2+51)$, if a is odd and b is odd , $b>a$.

Proof: Let the vertex set of G(a,b,A) = A∪B∪C∪D, where
A = $\{x_1, x_2, ...x_{(3a+3)/2}\}$, B = $\{y_1, y_2, ...y_{(3a+1)/2}\}$,
C = $\{y_{(3a+3)/2}, y_{(3a+5)/2}, ...y_{(3b+1)/2}\}$, D = $\{z_1, z_2, ...z_{(3b+3)/2}\}$ Now

$$W(G(a,b,A)) = W(a) + W(b) - \sum_{u,v\in B} d(u,v) + \sum_{\substack{u\in A\\ v\in C}} d(u,v) + \sum_{\substack{u\in A\\ v\in D}} d(u,v)$$

$$= \frac{1}{8}(18a^3 + 45a^2 + 58a - 1) + \frac{1}{8}(18b^3 + 45b^2 + 58b - 1)$$
$$- \sum_{i=1}^{(3a-1)/2} \sum_{j=i+1}^{(3a+1)/2} (j-i) + \{|A| \sum_{u\in C} d(u, y_{(3a+1)/2})$$
$$+ |C| \sum_{u\in A} d(u, y_{(3a+1)/2})\} + \sum_{\substack{u\in A\\ v\in D}} d(u,v)$$

$$= \frac{1}{8}(18a^3 + 45a^2 + 58a - 1) + \frac{1}{8}(18b^3 + 45b^2 + 58b - 1) - \sum_{i=1}^{(3a-1)/2} \sum_{j=i+1}^{(3a+1)/2} (j-i)$$
$$+ \{(3a+3)/2 \sum_{i=1}^{(3b-3a)/2} i + (3b-3a)/2\, [\sum_{i=1,4,7...}^{(3a-1)/2} ((3a+1)/2 - (i+1) + 2)$$

$$+ \sum_{i=2,5,8...}^{(3a+1)/2} ((3a+1)/2 - (i+2) + 3) + 1 + \sum_{i=3,6,9...}^{(3a+3)/2} ((3a+1)/2 - (i+1) + 2)$$
$$+ 1]\} + \{[\sum_{i=4,7,10..}^{(3a-1)/2} \sum_{j=1}^{i-3} ((i-3) - j + 4) + \sum_{i=1,4,7,...}^{(3a-1)/2} \sum_{j=i+2}^{(3b+3)/2} (j - (i+2) + 3)$$

$$+ (\frac{a-1}{2} \text{ x} 12) + 5] + [\sum_{i=3,6,9...}^{(3a+3)/2} \sum_{j=1}^{i-2} ((i-2) - j + 3)$$

$$+ \sum_{i=3,6,9..}^{(3a-3)/2} \sum_{j=i+3}^{(3b+3)/2} (j - (i+3) + 4) + (\frac{a-1}{2} \text{ x } 12) + 3$$

$$+ \sum_{i=(3a+3)/2}^{(3b+3)/2} (i - (3a+3)/2 + 2)] + [\sum_{i=5,8,..}^{(3a+1)/2} \sum_{j=1}^{i-4} ((i-4) - j + 5)$$

$$+ \sum_{i=2,5,8...}^{(3a-5)/2} \sum_{j=i+4}^{(3b+3)/2} (j - (i+4) + 5) + (\frac{a-3}{2} \text{ x } 28) + 19 + 16$$

$$+ \sum_{i=(3a+3)/2}^{(3b+3)/2} (i - (3a+3)/2 + 3)]\}$$

$$= \frac{1}{16}(45a^3 + 81a^2 + 185a + 36b^3 + 144b^2 + 302b + 36ab - 54a^2b + 54ab^2 + 51).$$

4. Conclusion:

All the formulas presented in this paper are verified with a computer program using Floyd Warshall algorithm.The work related to three rows of fused 5-cycles is in progress and will be communicated in future papers.

References:

[1] Damir Verkicevic, Nenod Trinajstic, Wiener index of Benzenoid graphs, Bulletin of chemists and Technologists of Macedonia, 2004, Vol 23, No 2, page113-129.

[2] Ivan Gutman, Weigen Yan, Bo-Yin Yang, Yenong-Nan Yeh, Generalized Wiener indices of zigzagging pentachians, Journal of Mathematical Chemistry, Vol 42, No 2, Aug 2007, Springer.

[3] Prabhakara Rao N, Laxmi Prasanna A, Wiener Indices of Pentachains, presented at National Conference on Discrete Mathematics and its applications, NCDMA 2007, Madurai, India.

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