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ON THE HYPER-WIENER INDEX OF TREES

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ABSTRACT

Let G be the connected graph. The Wiener index $W(G)$ is the sum of all distances between vertices of G, whereas the hyper-Wiener index $WW(G)$ is defined as $WW(G) = W(G) + \frac{1}{2}\sum_{\{u,v\}\subseteq V\{G\}} d(u,v)^2$. In this paper we prove some general results on the hyper-Wiener index of trees and some bounds on it.

Keywords: *acyclic graphs, molecular graphs and hyper-Wiener index.*

2000 mathematics subject classification: *05C12, 92E10.*

1. INTRODUCTION

In mathematical terms a graph is represented as $G = (V, E)$ where V is the set of vertices and E is the set of edges. Let G be an undirected connected graph without loops or multiple edges with n vertices, denoted by $1,2,\ldots,n$. The topological distance between the vertices u and v of $V(G)$ is denoted by $d(u,v)$ or d_{uv} and it is defined as the number of edges in a minimal path connecting the vertices u and v.

The Wiener index $W(G)$ of a connected graph G is defined as the sum the distances between all unordered pairs of vertices of G. It was put forward by Harold Wiener. The Wiener index is a graph invariant intensively studied both in mathematics and chemical literature, see for details$[1, 6, 7, 8, 10\ and\ 12-14]$.

The hyper-Wiener index was proposed by Randic [11] for a tree and extended by Klein *et al.* [2] to a connected graph. It is used to predict physicochemical properties of organic compounds. The hyper-Wiener index defined as,

$$WW(G) = \sum_{\{u,v\}\subseteq V(G)} \binom{d_{uv}+1}{2} = W(G) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d(u,v)^2$$

The hyper-Wiener index is studied both from a theoretical point of view and applications. We encourage the reader to consult $[4, 5, 10\ and\ 12-15]$ for further readings. The hyper-Wiener index of complete graph-K_n, path graph-P_n, star graph-$K_{1,(n-1)}$ and cycle graph C_n is given by the expressions

$$WW(K_n) = \frac{n(n-1)}{2}, WW(P_n) = \frac{n^4+2n^3-n^2-2n}{24},\ \ WW\left(K_{1,(n-1)}\right) = \frac{1}{2}(n-1)(3n-4)$$

And

$$WW(C_n) = \begin{cases} \frac{n^2(n+1)(n+2)}{48}, & if\ n\ is\ even \\ \frac{n(n^2-1)(n+3)}{48}, & if\ n\ is\ odd \end{cases}$$

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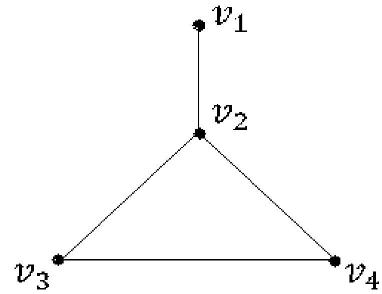
For example: Consider a graph G with vertices v_1, v_2, v_3 and v_4 as labeled in the figure below.



Here $d(v_1,v_2) = 1, d(v_1,v_3) = 2, d(v_1,v_4) = 2, d(v_2,v_3) = 1, d(v_2,v_4) = 1, d(v_3,v_4) = 1$.

Therefore $WW(G) = \sum_{\{u,v\}\subseteq V(G)} \binom{d_{uv}+1}{2}$
$$= \frac{2\times 1}{2} + \frac{3\times 2}{2} + \frac{3\times 2}{2} + \frac{2\times 1}{2} + \frac{2\times 1}{2} + \frac{2\times 1}{2}$$
$$= 1 + 3 + 3 + 1 + 1 + 1$$
$$= 10$$

2. MAIN RESULTS

Claim 1: If $\beta_1(T) = 2$, then $3 \leq diam(T) \leq 4$.

If $\beta_1(T) = 2$ then we have following two trees of diameter 3 and 4 and which we denote them by $A_n(k)$ and $B_n(k)$ respectively.

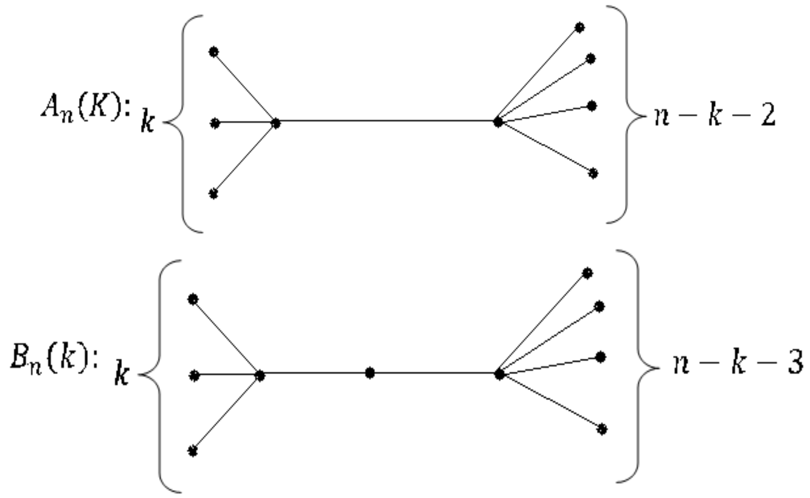


Figure-1

Lemma 2.1: Let $A_n(k)$ and $B_n(k)$ are the trees of order n, then its hyper wiener index given by

(i) $WW(A_n(K)) = \frac{1}{2}[k(6n-3k-11) + (n-k-2)(3n+3k-5) + 4n-6]$

(ii) $WW(B_n(k)) = \frac{1}{2}[k(10n-7k-23) + (n-k-3)(3n+7k-2) + 10n-20]$

Proof: To find hyper wiener index of: $A_n(k)$

$$WW(A_n(k)) = \sum_{\{u,v\}\subseteq V(G)} \binom{d_{uv}+1}{2}$$
$$= \frac{1}{2}\{\underbrace{(6n-3k-11)+\cdots+(6n-3k-11)}_{k\ times} + (3n-2k-5) + (n+2k-1)$$
$$+\underbrace{(3n+3k-5)+\cdots+(3n+3k-5)}_{(n-k-2)\ times}\}$$
$$WW(A_n(k)) = \frac{1}{2}[k(6n-3k-11) + (3n-2k-5) + (n+2k-1) + (n-k-2)(3n+3k-5)]$$
$$WW(A_n(k)) = \frac{1}{2}[k(6n-3k-11) + (n-k-2)(3n+3k-5) + 4n-6]$$

To find hyper wiener index of: $B_n(k)$

$$WW(B_n(k)) = \sum_{\{u,v\}\subseteq V(G)} \binom{d_{uv}+1}{2}$$

$$= \frac{1}{2}[(\underbrace{(10n-7k-23)+\cdots+(10n-7k-23)}_{k\ times})$$

$$+(6n-5k-14)+(3n-7)+(n+5k+1)$$

$$+(\underbrace{3n+7k-2)+\cdots+(3n+7k-2}_{(n-k-3)\ times})]$$

$$WW(B_n(k)) = \frac{1}{2}[k(10n-7k-23)+(6n-5k-14)+(3n-7)+(n+5k+1)+(n-k-3)(3n+7k-2)]$$

$$WW(B_n(k)) = \frac{1}{2}[k(10n-7k-23)+(n-k-3)(3n+7k-2)+10n-20]$$

Remark 1: Above result of the graph $A_n(k)$ used to find hyper-Wiener index of following chemical trees, Butane, 2-Methylbutane, 2, 2-Dimethylbutane, 2, 2, 3-Trimethylbutane, etc.

Theorem 2.2: Let $A_n(k)$ and $B_n(k)$ are the trees of orders n, as in figure 1. Then

(i) $WW(A_n(1)) < WW(A_n(2)) < WW(A_n(3)) \ldots < WW\left[A_n\left(\left\lfloor\frac{n-2}{2}\right\rfloor\right)\right]$

(ii) $WW(B_n(1)) < WW(B_n(2)) < WW(B_n(3)) \ldots < WW\left[B_n\left(\left\lfloor\frac{n-3}{2}\right\rfloor\right)\right]$

Proof: The integer valued function $f(n,k) = \frac{1}{2}[k(6n-3k-11)+(n-k-2)(3n+3k-5)+4n-6]$ has the maximum value if $k = \left\lfloor\frac{n-2}{2}\right\rfloor$ and also it is strictly increasing one and thus we have

$$WW(A_n(1)) < WW(A_n(2)) < WW(A_n(3)) \ldots < WW\left[A_n\left(\left\lfloor\frac{n-2}{2}\right\rfloor\right)\right]$$

Similarly, $\Phi(n,k) = \frac{1}{2}[k(10n-7k-23)+(n-k-3)(3n+7k-2)+10n-20]$ achieves maximum value, if $k = \left\lfloor\frac{n-3}{2}\right\rfloor$ and it is also increasing one. Hence we have,

$$WW(B_n(1)) < WW(B_n(2)) < WW(B_n(3)) \ldots < WW\left[B_n\left(\left\lfloor\frac{n-3}{2}\right\rfloor\right)\right]$$

Theorem 2.3: If $n > k+3$, then $WW(A_n(k)) < WW(B_n(k))$

Proof: Let $n > k+3$ and assume, to the contrary, that $WW(A_n(k)) \nless WW(B_n(k))$.

Thus $WW(A_n(k)) \geq WW(B_n(k))$. Since

$WW(A_n(k)) = \frac{1}{2}[k(6n-3k-11)+(n-k-2)(3n+3k-5)+4n-6]$ and

$$WW(B_n(k)) = \frac{1}{2}[k(10n-7k-23)+(n-k-3)(3n+7k-2)+10n-20]$$

Now consider n=5 and k=1, since $n > k+3$. We obtain $WW(A_n(k)) = 28$ and $WW(B_n(k)) = 35$, it contradicts the fact that $WW(A_n(k)) \geq WW(B_n(k))$. Therefore If $n > k+3$, then $WW(A_n(k)) < WW(B_n(k))$

Theorem 2.4: If $n > k+2$, then $WW(A_n(k+1)) < WW(B_n(k))$

Proof: Let $n > k+2$ and assume, to the contrary, that $WW(A_n(k+1)) \nless WW(B_n(k))$.

Thus $WW(A_n(k+1)) \geq WW(B_n(k))$. Since

$WW(A_n(k+1)) = \frac{1}{2}[(k+1)(6n-3\overline{k+1}-11)+(n-\overline{k+1}-2)(3n+3\overline{k+1}-5)+4n-6]$ and

$$WW(B_n(k)) = \frac{1}{2}[k(10n-7k-23)+(n-k-3)(3n+7k-2)+10n-20]$$

Now consider n=5 and k=1, since $n > k+2$. We obtain $WW(A_n(k+1)) = 28$ and $WW(B_n(k)) = 35$, it contradicts the fact that $WW(A_n(k+1)) \geq WW(B_n(k))$. Therefore If $n > k+2$, then $WW(A_n(k+1)) < WW(B_n(k))$

Claim 2: If $\beta_1(T) = 3$, then $4 \leq diam(T) \leq 6$.

If $\beta_1(T) = 3$ then we have following six trees of diameter 4, 5 and 6 and which we denote them by $C_n(l, m, k)$, $D_n(l, m, k)$, $E_n(k)$, $F_n(l, m, k)$ $G_n(k)$ and $H_n(l, m, k)$respectively.

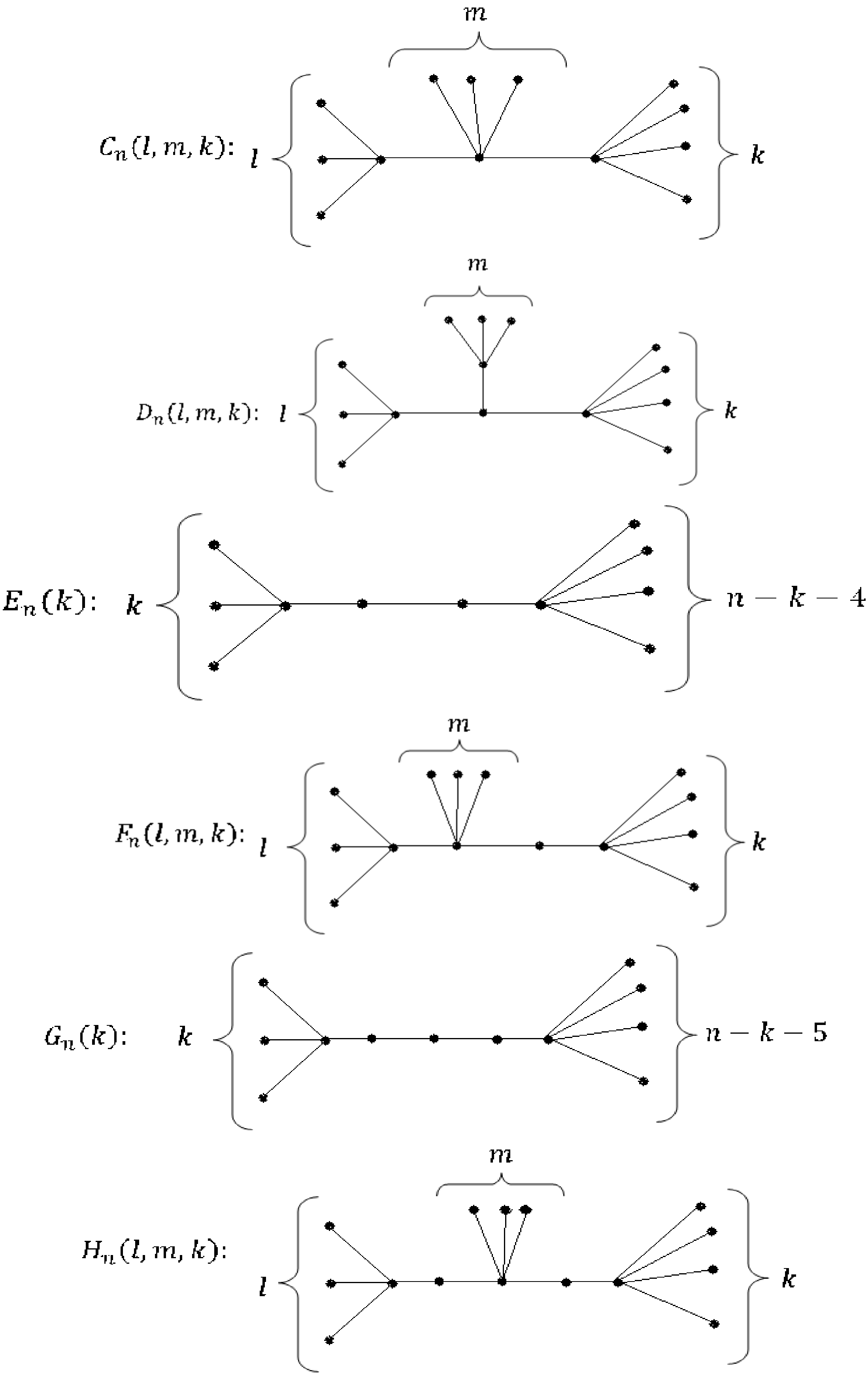


Figure-2

Lemma 2.5: Let $C_n(l,m,k)$, $D_n(l,m,k)$, $E_n(k), F_n(l,m,k)$ $G_n(k)$ and $H_n(l,m,k)$ are the trees of orders n, then its hyper wiener index given by

(i) $WW\big(C_n(l,m,k)\big) = \frac{1}{2}[l(3l+6m+10k+7)+m(6l+3m+6k+4) + k(10l+6m+3k+7)+10l+7m+10k+10]$, Where $l+m+k+3=n$

(ii) $WW\big(D_n(l,m,k)\big) = \frac{1}{2}[l(3l+10m+10k+13)+m(10l+3m+10k+13) +k(10l+10m+3k+13)+16l+16m+16k+24]$, Where $l+m+k+4=n$

(iii) $WW\big(E_n(k)\big) = \frac{1}{2}[k(15n-12k-43)+(n-k-4)(3n+12k+5)+20n-50]$

(iv) $WW\big(F_n(l,m,k)\big) = \frac{1}{2}[l(3l+6m+15k+17)+m(6l+3m+10k+10) +k(15l+10m+3k+17)+20l+13m+20k+30]$, Where $l+m+k+4=n$

(v) $WW\big(G_n(k)\big) = \frac{1}{2}[k(21n-18k-73)+(n-k-5)(3n+18k+17)+35n-105]$

(vi) $WW\big(H_n(l,m,k)\big) = \frac{1}{2}[l(3l+10m+21k+32)+m(10l+3m+10k+16) +k(21l+10m+3k+32)+35l+19m+35k+70]$, Where $l+m+k+5=n$

Proof: To find hyper wiener index of: $\boldsymbol{C_n(l,m,k)}$

$$WW\big(C_n(l,m,k)\big) = \sum_{\{u,v\}\subseteq V(G)} \binom{d_{uv}+1}{2}$$

$$= \frac{1}{2}[\underbrace{(3l+6m+10k+7)+\cdots+(3l+6m+10k+7)}_{l\ times}+(l+3m+6k+4)$$

$$+(3l+m+3k+2)+\underbrace{(6l+3m+6k+4)+\cdots+(6l+3m+6k+4)}_{m\ times}$$

$$+(6l+3m+k+4)+\underbrace{(10l+6m+3k+7)+\cdots+(10l+6m+3k+7)}_{k\ times}$$

$$WW\big(C_n(l,m,k)\big) = \frac{1}{2}[l(3l+6m+10k+7)+(l+3m+6k+4)+(3l+m+3k+2) +m(6l+3m+6k+4)+(6l+3m+k+4)+k(10l+6m+3k+7)]$$

$$WW\big(C_n(l,m,k)\big) = \frac{1}{2}[l(3l+6m+10k+7)\ +m(6l+3m+6k+4)+ k(10l+6m+3k+7)+10l+7m+10k+10]$$

To find hyper wiener index of: $\boldsymbol{D_n(l,m,k)}$

$$WW\big(D_n(l,m,k)\big) = \sum_{\{u,v\}\subseteq V(G)} \binom{d_{uv}+1}{2}$$

$$= \frac{1}{2}[\underbrace{(3l+10m+10k+13)+\cdots+(3l+10m+10k+13)}_{l\ times}$$

$$+(l+6m+6k+7)+(3l+3m+3k+3)+(6l+m+6k+7)$$

$$+\underbrace{(10l+3m+10k+13)+\cdots+(10l+3m+10k+13)}_{m\ times}$$

$$+(6l+6m+k+7)$$

$$+\underbrace{(10l+10m+3k+13)+\cdots+(10l+10m+3k+13)}_{k\ times}$$

$$WW\big(D_n(l,m,k)\big) = \frac{1}{2}[l(3l+10m+10k+13)+(l+6m+6k+7)+(3l+3m+3k+3) +(6l+m+6k+7)+m(10l+3m+10k+13)+(6l+6m+k+7) +k(10l+10m+3k+13)]$$

$$WW\big(D_n(l,m,k)\big) = \frac{1}{2}[l(3l+10m+10k+13)+m(10l+3m+10k+13) +k(10l+10m+3k+13)+16l+16m+16k+24]$$

To find hyper wiener index of: $E_n(k)$

$$WW(E_n(k)) = \sum_{\{u,v\}\subseteq V(G)} \binom{d_{uv}+1}{2}$$

$$= \frac{1}{2}[\underbrace{(15n-12k-43)+\cdots+(15n-12k-43)}_{k\ times}+(k+10n-10k-30)$$
$$+(3k+6n-6k-19)+(6k+3n-3k-7)+(n+9k+6)$$
$$+\underbrace{(3n+12k+5)+\cdots+(3n+12k+5)}_{(n-k-4)\ times}]$$

$$WW(E_n(k)) = \frac{1}{2}[k(15n-12k-43)+(n-k-4)(3n+12k+5)+(10n-9k-30)$$
$$+(6n-3k-19)+(3n+3k-7)+(n+9k+6)]$$

$$WW(E_n(k)) = \frac{1}{2}[k(15n-12k-43)+(n-k-4)(3n+12k+5)+20n-50]$$

To find hyper wiener index of: $F_n(l,m,k)$

$$WW(F_n(l,m,k)) = \sum_{\{u,v\}\subseteq V(G)} \binom{d_{uv}+1}{2}$$

$$WW(F_n(l,m,k)) = \frac{1}{2}[\underbrace{(3l+6m+15k+17)+\cdots+(3l+6m+15k+17)}_{l\ times}$$
$$+(l+3m+10k+10)+(3l+m+6k+5)$$
$$+\underbrace{(6l+3m+10k+10)+\cdots+(6l+3m+10k+10)}_{m\ times}$$
$$+(6l+3m+3k+5)+(10l+6m+k+10)$$
$$+\underbrace{(15l+10m+3k+17)+\cdots+(15l+10m+3k+17)}_{k\ times}]$$

$$WW(F_n(l,m,k)) = \frac{1}{2}[l(3l+6m+15k+17)+(l+3m+10k+10)+(3l+m+6k+5)$$
$$+m(6l+3m+10k+10)+(6l+3m+3k+5)+(10l+6m+k+10)$$
$$+k(15l+10m+3k+17)]$$

$$WW(F_n(l,m,k)) = \frac{1}{2}[l(3l+6m+15k+17)+m(6l+3m+10k+10)$$
$$+k(15l+10m+3k+17)+20l+13m+20k+30]$$

To find hyper wiener index of: $G_n(k)$

$$WW(G_n(k)) = \sum_{\{u,v\}\subseteq V(G)} \binom{d_{uv}+1}{2}$$

$$WW(G_n(k)) = \frac{1}{2}[\underbrace{(21n-18k-73)+\cdots+(21n-18k-73)}_{k\ times}+(15n-14k-55)$$
$$+(10n-7k-39)+(6n-22)+(3n+7k-4)+(n+14k+15)$$
$$+\underbrace{(3n+18k+17)+\cdots+(3n+18k+17)}_{(n-k-5)times}]$$

$$WW(G_n(k)) = \frac{1}{2}[k(21n-18k-73)+(15n-14k-55)+(10n-7k-39)+(6n-22)$$
$$+(3n+7k-4)+(n+14k+15)+(n-k-5)(3n+18k+17)]$$

$$WW(G_n(k)) = \frac{1}{2}[k(21n-18k-73)+(n-k-5)(3n+18k+17)+35n-105]$$

To find hyper wiener index of: $H_n(l,m,k)$

$$WW(H_n(l,m,k)) = \sum_{\{u,v\}\subseteq V(G)} \binom{d_{uv}+1}{2}$$

$$WW(H_n(l,m,k)) = \frac{1}{2}[\underbrace{(3l+10m+21k+32)+\cdots+(3l+10m+21k+32)}_{l\ times}$$
$$+(l+6m+15k+20)+(3l+3m+10k+11)+(6l+m+6k+8)$$
$$+\underbrace{(10l+3m+10k+16)+\cdots+(10l+3m+10k+16)}_{m\ times}$$
$$+(10l+3m+3k+11)+(15l+6m+k+20)$$
$$+\underbrace{(21l+10m+3k+32)+\cdots+(21l+10m+3k+32)}_{k\ times}]$$

$$WW(H_n(l,m,k)) = \frac{1}{2}[l(3l+10m+21k+32)+(l+6m+15k+20)$$
$$+(3l+3m+10k+11)+(6l+m+6k+8)$$
$$+m(10l+3m+10k+16)+(10l+3m+3k+11)$$
$$+(15l+6m+k+20)+k(21l+10m+3k+32)]$$

$$WW(H_n(l,m,k)) = \frac{1}{2}[l(3l+10m+21k+32)+m(10l+3m+10k+16)$$
$$+k(21l+10m+3k+32)+35l+19m+35k+70]$$

Remark 2: Above results of the graphs $B_n(k)$ and $C_n(l,m,k)$ used to find hyper-Wiener index of Pentane, 2, 4-Dimethylpentane, 2,2-Dimethylpentane, etc.

Remark 3: Similar way the results of the graphs $D_n(l,m,k)$, $E_n(k), F_n(l,m,k)$ $G_n(k)$ and $H_n(l,m,k)$ used to find hyper-Wiener index of 3,3-Dimethylpentane, 2,3-Dimethylpentane, etc.

Theorem 2.6: For trees of the classes $C_n(l,m,k)$, $D_n(l,m,k)$, $E_n(k), F_n(l,m,k)$ $G_n(k)$ and $H_n(l,m,k)$ following relations holds good

(i) $WW(C_n(1,n-5,1)) \le WW(C_n(l,m,k))$ for all $l,m,k \ge 1$ where $l+m+k+3=n$.
(ii) $WW(D_n(1,n-6,1)) \le WW(D_n(l,m,k))$ for all $l,m,k \ge 1$ where $l+m+k+4=n$.
(iii) $WW(F_n(1,n-6,1)) \le WW(F_n(l,m,k))$ for all $l,m,k \ge 1$ where $l+m+k+4=n$.
(iv) $WW(H_n(1,n-7,1)) \le WW(H_n(l,m,k))$ for all $l,m,k \ge 1$ where $l+m+k+5=n$.

Proof is similar to that of **theorem 2.4**

Theorem 2.7: Let $WW(E_n(k))$ and $WW(G_n(k))$ are trees as in the figure 2, then,

(iii) $WW(E_n(1)) < WW(E_n(2)) < WW(E_n(3)) \ldots < WW\left[E_n\left(\left\lfloor\frac{n-4}{2}\right\rfloor\right)\right]$
(iv) $WW(G_n(1)) < WW(G_n(2)) < WW(G_n(3)) \ldots < WW\left[G_n\left(\left\lfloor\frac{n-5}{2}\right\rfloor\right)\right]$

Proof is similar to that of **theorem 2.2**

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