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Harmonic Eccentric Index of Hexagonal Chain

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ABSTRACT

Harmonic eccentric indices were proposed analogously to Harmonic indices already known and used for many years. We defined Harmonic eccentric index as $HEI\ (G) = \sum_{uv\epsilon E\ (G)} \frac{2}{e_u+e_v}$ .In his paper we have calculated Harmonic eccentric index for some particular chains.

Introduction

The harmonic index is one of the most important indices in chemical and mathematical field. It is a variant of the Randic index which is the most successful molecular descriptor in structure property and structure activity relationship studies and it is defined as $R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u \times d_v}}$ where d_u denotes the degree of the vertex u and the summation is taken over all pairs of adjacent vertices of the graph G.

The Harmonic index gives somewhat better correlations with physical and chemical properties comparing with the well known Randic index. The Harmonic index H(G) of a graph G is defined as $\sum_{uv\epsilon E\ (G)} \frac{2}{d_u+d_v}$, where d_u denotes the degree of the vertex u and the summation is taken over all pairs of adjacent vertices of the graph G.

Let G be a connected graph with vertex set V(G) and the edge set E(G).For a vertex $u \in V(G), e_G(u)\ or\ e_u$ denotes the eccentricity of u in G, where $e_u = max\{d(u,v): v \in V(G)\}$, where $d(u,v)$ denotes the distance between u and v in G.

The Harmonic eccentric indices are introduced in analogy with the Harmonic indices by replacing the vertex degrees with the vertex eccentricities.

We defined Harmonic eccentric index [9] as

$HEI\ (G) = \sum_{uv\epsilon E\ (G)} \frac{2}{e_u+e_v}$, where $e_G(u)\ or\ e_u$ denotes the eccentricity of u in G ..Note that degrees are " local properties", while eccentricities are " global properties" of the vertices.

Hexagonal chain:

A hexagonal system is a 2-connected plane graph whose every interior face is bounded by a regular hexagon of unit length 1. The hexagonal systems are of considerable importance in theoretical chemistry because they are the natural graph representation of Benzenoid hydrocarbons. A vertex of a hexagonal system belongs to, at most, three hexagons. A vertex shared by three hexagons is called an internal vertex of the respective hexagonal system. A hexagonal system H is said to be Catacondensed if it does not possess internal vertices, otherwise H is said to be Pericondensed. A hexagonal chain is a Catacondensed hexagonal system which has no hexagon adjacent to more than two hexagons. Some examples of hexagonal chains can be found in Fig. 1.

It is easy to see that any hexagonal chains H_{n+1} with $n+1$ hexagons can be obtained from a hexagonal chain Hn with n hexagons by attaching it to a new hexagon. Based on this fact, a hexagonal chain can be constructed inductively. There are three types of fusion for attaching a new hexagon h_{n+1} to a hexagonal chain H_n with n hexagons $h_1, h_2, h_3, \dots . h_n$:

(i) If h_{n+1} is on the line l, it is called $\propto -type$ fusing;

(ii) If h_{n+1} is on the left-hand side of l, it is called $\beta - type$ fusing;

(iii) If h_{n+1} is on the right-hand side of l, it is called $\gamma - type$ fusing

where l is the direct line from the center of h_{n-1} to the center of h_n . Any hexagonal chain $H_n (n \geq 2)$ can be obtained from H_2 by a stepwise fusion of new hexagons, and at each step a $\theta - type$ fusion is selected, where $\in \{\alpha, \beta, \gamma\}$.

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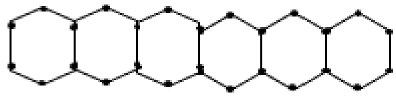
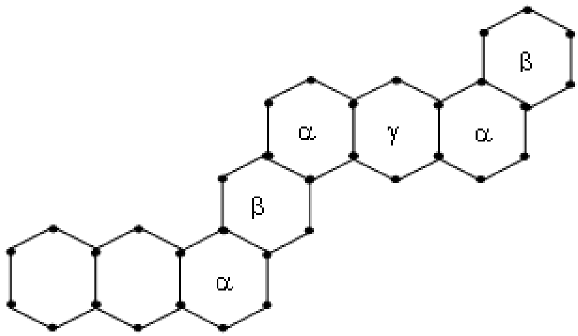
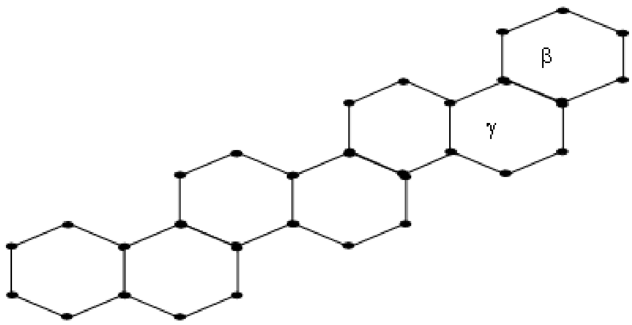


(i)A linear chain L_6



(ii) A hexagonal chain H_8



(iii)A zia-zag chain Z_7

Fig 1. Single hexagonal chains with different types of fusions.

Harmonic Eccentric index of Hexagonal system

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The eccentricities of $u, v \in V(G)$ are denoted by e_u, e_v. For $e = uv \in E(G)$, denote the eccentricities of the end vertices of e by (e_u, e_v).

Theorem 2.1:

Let $L_4, H_4,$ *and* Z_4 are the Linear chain with $\propto -type$ fusing, hexagonal chain with $\beta - type$ fusing, and Zig-zag chain with $\gamma - type$ fusing respectively , then

$$(i)\ HEI\ (L_4) = \begin{cases} 3.05452, \propto -type \text{ fusing} \\ 3.37228, \beta - type \text{ fusing} \\ 3.17850, \gamma - type \text{ fusing} \end{cases}$$

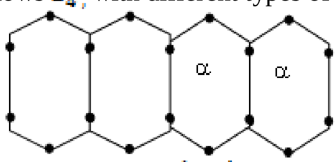
$$(ii)\ HEI\ (H_4) = \begin{cases} 3.3399858, \propto -type \text{ fusing} \\ 3.52168, \beta - type \text{ fusing} \\ 3.23609, \gamma - type \text{ fusing} \end{cases}$$

$$(iii)\ HEI\ (Z_4) = \begin{cases} 3.19713, \propto -type \text{ fusing} \\ 3.25427, \beta - type \text{ fusing} \\ 3.56208, \gamma - type \text{ fusing} \end{cases}$$

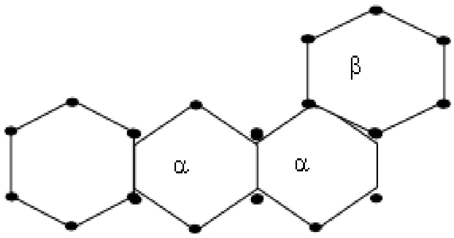
Proof

Consider the Linear chain L_4, in a line with $\propto -type, \beta - type$ and $\gamma - type$ fusing and which is denoted as

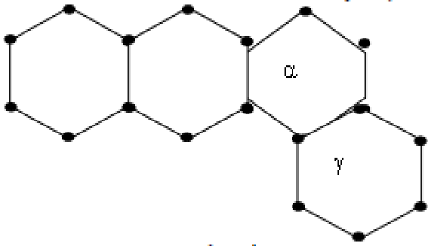
(i) $L_4(\alpha, \alpha), L_4(\alpha, \beta)$ *and* $L_4(\alpha, \gamma)$ .Fig 5. Shows L_4, with different types of fusing



$L_4(\alpha, \alpha)$



$L_4(\alpha,\beta)$



$L_4(\alpha,\gamma)$

Fig 2. Linear chain L_4 with α,β,γ type fusing.

Let V_1 be the vertex set and E_1 be the edge set in $L_4(\alpha,\alpha)$, then $|V_1| = 18$ and $|E_1| = 21$. Also the number of edges with eccentricities of end vertices are given as follows:

There are 1 edge with eccentricities of end vertices (5,5); 2 edges with eccentricities of end vertices (7,7); 2 edges with eccentricities of end vertices (9,9); 4 edges with eccentricities of end vertices (5,6); 4 edges with eccentricities of end vertices (6,7); 4 edges with eccentricities of end vertices (7,8); and 4 edges with eccentricity (8,9),

Hence $HEI\left(L_4(\alpha,\alpha)\right) = \sum_{uv\epsilon E(L_4(\alpha,\alpha))} \frac{2}{e_u+e_v}$

$= 1\left(\frac{2}{5+5}\right) + 2\left(\frac{2}{7+7}\right) + 2\left(\frac{2}{9+9}\right) + +4\left(\frac{2}{5+6}\right) + 4\left(\frac{2}{6+7}\right) + 4\left(\frac{2}{7+8}\right) + 4\left(\frac{2}{8+9}\right) = 3.05452.$

Also let V_2 be the vertex set and E_2 be the edge set in $L_4(\alpha,\beta)$, then $|V_2| = 18$ and $|E_2| = 21$. The number of edges with eccentricities of end vertices are given as follows:

There are 1 edge with eccentricities of end vertices (6,6);1 edge with eccentricities of end vertices (7,7); 1 edge with eccentricities of end vertices (9,7); 4 edges with eccentricities of end vertices (5,6); 3 edges with eccentricities of end vertices (5,5); 3 edges with eccentricities of end vertices (7,8); 3 edges with eccentricities of end vertices (8,9); and 5 edges with eccentricities of end vertices (7,6),

Hence $HEI\left(L_4(\alpha,\beta)\right) = \sum_{uv\epsilon E(L_4(\alpha,\beta))} \frac{2}{e_u+e_v}$

$= 1\left(\frac{2}{6+6}\right) + 1\left(\frac{2}{7+7}\right) + 1\left(\frac{2}{9+7}\right) + 3\left(\frac{2}{5+5}\right) + 3\left(\frac{2}{8+9}\right) + 3\left(\frac{2}{7+8}\right) + 4\left(\frac{2}{6+5}\right) + 5\left(\frac{2}{6+7}\right) = 3.37228$

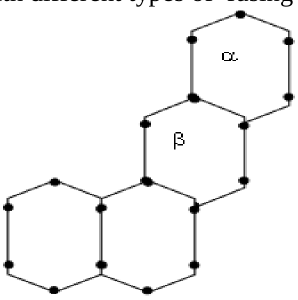
Similarly, let V_3 be the vertex set and E_3 be the edge set in $L_4(\alpha,\gamma)$, then $|V_3| = 18$ and $|E_3| = 21$. Also the number of edges with eccentricities of end vertices are given as follows:

There are1 edge with eccentricities of end vertices (6,6);1 edge with eccentricities of end vertices (7,7); 1 edge with eccentricities of end vertices (5,5); 2 edges with eccentricities of end vertices (9,8); 2 edges with eccentricities of end vertices (8,8); 4 edges with eccentricities of end vertices (7,8); 4 edges with eccentricities of end vertices (6,5); and 6 edges with eccentricities of end vertices (7,6),

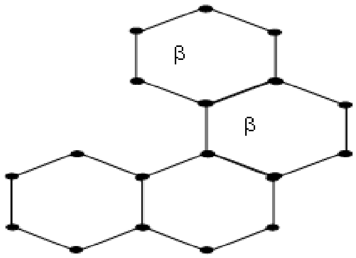
Hence $HEI\left(L_4(\alpha,\gamma)\right) = \sum_{uv\epsilon L_4(\alpha,\gamma))} \frac{2}{e_u+e_v}$

$= 1\left(\frac{2}{6+6}\right) + 1\left(\frac{2}{7+7}\right) + 1\left(\frac{2}{5+5}\right) + 2\left(\frac{2}{8+8}\right) + 2\left(\frac{2}{8+8}\right) + 4\left(\frac{2}{8+7}\right) + 6\left(\frac{2}{7+6}\right) + 4\left(\frac{2}{6+5}\right) = 3.17850.$

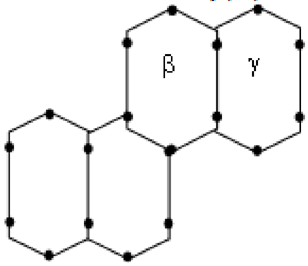
(ii) Consider the Hexogonal chain $H_{4,}$ in a line with $\propto -type, \beta - type$ and $\gamma - type$ fusing and which is denoted as $H_4(\beta,\alpha), H_4(\beta,\beta)$ and $H_4(\beta,\gamma)$ .Fig 6. Shows H_4 with different types of fusing



$H_4(\beta,\alpha)$



$H_4(\beta,\beta)$



$H_4(\beta,\gamma)$

Fig 3. Hexogonal chain H_4, with α,β,γ type fusing.

Let V_4 be the vertex set and E_4 be the edge set in $H_4(\beta,\alpha)$, then $|V_4| = 18$ and $|E_4| = 21$. Also the number of edges with eccentricities of end vertices are given as follows:

There are 1 edge with eccentricities of end vertices (7,7); 2 edges with eccentricities of end vertices (5,5); 4 edges with eccentricities of end vertices (9,8); 4 edges with eccentricities of end vertices (8,7); 4 edges with eccentricities of end vertices (6,5); and 6 edges with eccentricities of end vertices (7,6),

Hence $HEI\left(H_4(\beta,\alpha)\right) = \sum_{uv\epsilon E(H_4(\beta,\alpha))}\frac{2}{e_u+e_v}$

$= 1\left(\frac{2}{7+7}\right) + 2\left(\frac{2}{5+5}\right) + +4\left(\frac{2}{9+8}\right) + 4\left(\frac{2}{8+7}\right) + 4\left(\frac{2}{5+6}\right) + 6\left(\frac{2}{7+6}\right) = 3.3399858$.

Also let V_5 be the vertex set and E_5 be the edge set in $H_4(\beta,\beta)$, then $|V_5| = 18$ and $|E_5| = 21$. The number of edges with eccentricities of end vertices are given as follows:

3 edge with eccentricities of end vertices (5,4); 4 edge with eccentricities of end vertices (8,7); 6 edge with eccentricities of end vertices (6,5); and 8 edges with eccentricities of end vertices (7,6),

Hence $HEI\left(H_4(\beta,\beta)\right) = \sum_{uv\epsilon E(H_4(\beta,\beta))}\frac{2}{e_u+e_v}$

$= 3\left(\frac{2}{5+4}\right) + 4\left(\frac{2}{8+7}\right) + 6\left(\frac{2}{6+5}\right) + 8\left(\frac{2}{7+6}\right) = 3.52168$

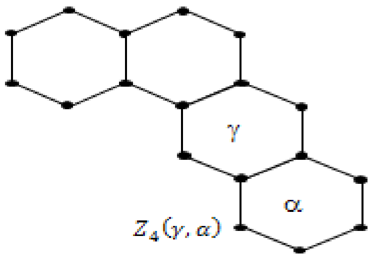
Similarly, let V_6 be the vertex set and E_6 be the edge set in $H_4(\beta,\gamma)$, then $|V_6| = 18$ and $|E_6| = 21$. Also the number of edges with eccentricities of end vertices are given as follows:

There are 2 edges with eccentricities of end vertices (5,5); 4 edges with eccentricities of end vertices (9,8); 4 edges with eccentricities of end vertices (8,7); 5 edges with eccentricities of end vertices (6,5); and 6 edges with eccentricities of end vertices (7,6),

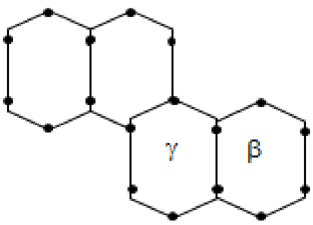
Hence $HEI\left(H_4(\beta,\gamma)\right) = \sum_{uv\epsilon H_4(\beta,\gamma))}\frac{2}{e_u+e_v}$

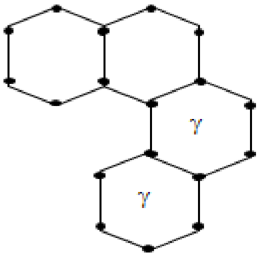
$= 2\left(\frac{2}{5+5}\right) + 4\left(\frac{2}{9+8}\right) + 4\left(\frac{2}{8+7}\right) + 5\left(\frac{2}{6+5}\right) + 6\left(\frac{2}{7+6}\right) = 3.23609$

(iii) Consider the Zig-zag chain Z_4, in a line with $\propto -type, \beta - type$ and $\gamma - type$ fusing and which is denoted as $Z_4(\gamma,\alpha)$, $Z_4(\gamma,\beta)$ and $Z_4(\gamma,\gamma)$. Fig 7 Shows Z_4 with different types of fusing.



$Z_4(\gamma,\alpha)$





(γ,γ)

Fig 4. Zig-zag chain Z_4 , with α,β,γ type fusing.

Let V_7 be the vertex set and E_7 be the edge set in $Z_4(\gamma,\alpha)$, then $|V_7| = 18$ and $|E_7| = 21$. Also the number of edges with eccentricities of end vertices are given as follows:

There are1 edge with eccentricities of end vertices (7,7); 2 edges with eccentricities of end vertices (5,5); 4 edges with eccentricities of end vertices (6,5); 4 edges with eccentricities of end vertices (8,7); 4 edges with eccentricities of end vertices (8,9); and 6 edges with eccentricities of end vertices (7,6),

Hence $HEI\ (\ Z_4(\gamma,\alpha)) = \sum_{uv\in E(Z_4(\gamma,\alpha))} \frac{2}{e_u+e_v}$

$= 1\left(\frac{2}{7+7}\right) + 2\left(\frac{2}{5+5}\right) + +4\left(\frac{2}{6+5}\right) + 4\left(\frac{2}{8+7}\right) + 4\left(\frac{2}{8+9}\right) + 6\left(\frac{2}{7+6}\right) \quad = 3.19173$

Also let V_8 be the vertex set and E_8 be the edge set in $Z_4(\gamma,\beta)$, then $|V_8| = 18$ and $|E_8| = 21$. The number of edges with eccentricities of end vertices are given as follows:

There are 3 edges with eccentricities of end vertices (5,5); 4 edges with eccentricities of end vertices (8,7); 4 edges with eccentricities of end vertices (8,9); 4 edges with eccentricities of end vertices (6,5); and 6 edges with eccentricities of end vertices (7,6),

Hence $HEI\ (Z_4(\gamma,\beta)) = \sum_{uv\in E(Z_4(\gamma,\beta))} \frac{2}{e_u+e_v}$

$= 3\left(\frac{2}{5+5}\right) + 4\left(\frac{2}{8+7}\right) + 4\left(\frac{2}{8+9}\right) + \ 4\left(\frac{2}{6+5}\right) + 6\left(\frac{2}{7+6}\right) \quad = 3.25427$.

Similarly, let V_9 be the vertex set and E_9 be the edge set in $Z_4(\gamma,\gamma)$, then $|V_9| = 18$ and $|E_9| = 21$. Also the number of edges with eccentricities of end vertices are given as follows:

4 edges with eccentricities of end vertices (5, 4); 4 edges with eccentricities of end vertices (7,8); 5 edges with eccentricities of end vertices (6,5); and 8 edges with eccentricities of end vertices (6,7)

Hence $HEI\ (Z_4(\gamma,\gamma)) = \sum_{uv\in E(Z_4(\gamma,\gamma))} \frac{2}{e_u+e_v}$

$= 4\left(\frac{2}{5+4}\right) + 4\left(\frac{2}{7+8}\right) + 5\left(\frac{2}{6+5}\right) + 8\left(\frac{2}{7+6}\right) = 3.23609$.

Theorem 2.2:

Let $L_5, H_5,$ and Z_5 are the Linear chain with $\propto -type$ fusing, hexagonal chain with $\beta - type$ fusing, and Zig-zag chain with $\gamma - type$ fusing respectively , then

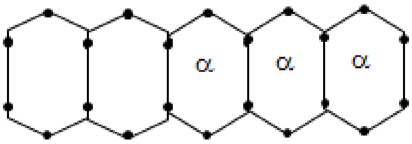
$$(i)\ HEI\ (L_5) = \begin{cases} 2.38124, \propto -type \text{ fusing} \\ 3.327934, \beta - type \text{ fusing} \\ 3.343620, \gamma - type \text{ fusing} \end{cases}$$

$$(ii)\ HEI\ (H_5) = \begin{cases} 3.290804, \propto -type \text{ fusing} \\ 2.670662\ \ , \beta - type \text{ fusing} \\ 3.273821\ \ , \gamma - type \text{ fusing} \end{cases}$$

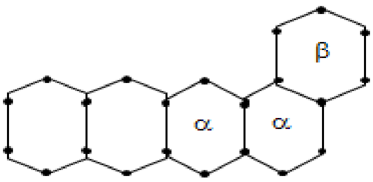
$$(iii)\ HEI\ (Z_5) = \begin{cases} 3.391749\ \ , \propto -type \text{ fusing} \\ 3.133432\ \ , \beta - type \text{ fusing} \\ 3.677155, \gamma - type \text{ fusing} \end{cases}$$

Proof:

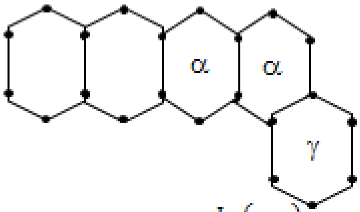
Consider the Linear chain L_4, in a line with $\propto -type, \beta - type$ and $\gamma - type$ fusing and which is denoted as $L_5(\alpha,\alpha)$, $L_5(\alpha,\beta)$ and $L_5(\alpha,\gamma)$



$L_5(\alpha,\alpha)$



$L_5(\alpha,\beta)$



$L_5(\alpha,\gamma)$

Fig 5. Linear chain L_5 with α,β,γ type fusing.

Let V_1 be the vertex set and E_1 be the edge set in $L_5(\alpha,\alpha)$, then $|V_1| = 22$ and $|E_1| = 26$. Also the number of edges with eccentricities of end vertices are given as follows:

There are 2 edges with eccentricities of end vertices (11,11); 4 edges with eccentricities of end vertices (10,11); 4 edges with eccentricities of end vertices (9,10); 2 edges with eccentricities of end vertices (9,9); 2 edges with eccentricities of end vertices (7,7); 4 edges with eccentricities of end vertices (9,8); 4 edges with eccentricity (8,7); and 4 edges with eccentricity (6,7)

Hence $HEI\left(L_5(\alpha,\alpha)\right) = \sum_{uv\in E(L_5(\alpha,\alpha))} \frac{2}{e_u+e_v}$

$= 2\left(\frac{2}{11+11}\right) + 2\left(\frac{2}{7+7}\right) + 2\left(\frac{2}{9+9}\right) + +4\left(\frac{2}{10+11}\right) + 4\left(\frac{2}{9+10}\right) + 4\left(\frac{2}{7+8}\right) + 4\left(\frac{2}{8+9}\right) + 4\left(\frac{2}{7+6}\right) = 2.38124\cdot$

Also let V_2 be the vertex set and E_2 be the edge set in $L_5(\alpha,\beta)$, then $|V_2| = 22$ and $|E_2| = 26$. The number of edges with eccentricities of end vertices are given as follows:

There are 1 edge with eccentricities of end vertices (10,7);2 edges with eccentricities of end vertices (6,5); 4 edges with eccentricities of end vertices (11,10); 4 edges with eccentricities of end vertices (9,10); 4 edges with eccentricities of end vertices (8,7); 5 edges with eccentricities of end vertices (9,8); 6 edges with eccentricities of end vertices (7,6)

Hence $HEI\left(L_5(\alpha,\beta)\right) = \sum_{uv\in E(L_5(\alpha,\beta))} \frac{2}{e_u+e_v}$

$= 1\left(\frac{2}{10+7}\right) + 2\left(\frac{2}{6+5}\right) + 4\left(\frac{2}{10+11}\right) + 4\left(\frac{2}{10+9}\right) + 4\left(\frac{2}{8+7}\right) + 5\left(\frac{2}{9+8}\right) + 6\left(\frac{2}{6+7}\right) = 3.327934$

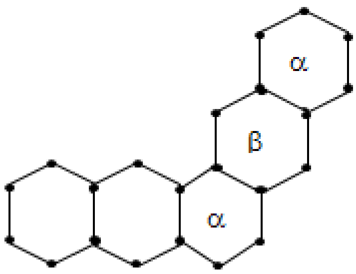
Similarly, let V_3 be the vertex set and E_3 be the edge set in $L_5(\alpha,\gamma)$, then $|V_3| = 22$ and $|E_3| = 26$. Also the number of edges with eccentricities of end vertices are given as follows:

There are 2 edges with eccentricities of end vertices (6,5); 4 edges with eccentricities of end vertices (10,11); 4 edges with eccentricities of end vertices (10,9); 5 edges with eccentricities of end vertices (8,7); 5 edges with eccentricities of end vertices (8,9); 6 edges with eccentricities of end vertices (7,6)

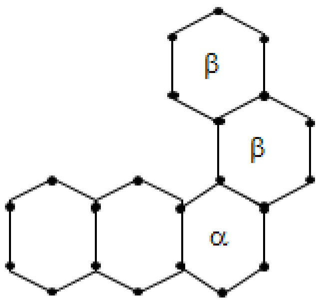
Hence $HEI\left(L_5(\alpha,\gamma)\right) = \sum_{uv\in L_5(\alpha,\gamma))} \frac{2}{e_u+e_v}$

$= 2\left(\frac{2}{6+5}\right) + 4\left(\frac{2}{10+11}\right) + 4\left(\frac{2}{10+9}\right) + 5\left(\frac{2}{8+7}\right) + 5\left(\frac{2}{9+8}\right) + 6\left(\frac{2}{6+7}\right) = 3.343620\cdot$

(ii) Consider the Hexogonal chain H_5, in a line with $\propto -type, \beta - type$ and $\gamma - type$ fusing and which is denoted as $H_5(\beta,\alpha), H_5(\beta,\beta)$ and $H_5(\beta,\gamma)$ .Fig 6. Shows H_5 with different types of fusing.



$H_5(\beta,\alpha)$



$H_5(\beta,\beta)$

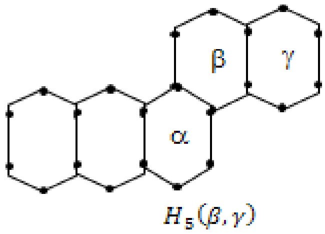


Fig 6. Hexogonal chain H_5 with α, β, γ type fusing.

Let V_4 be the vertex set and E_4 be the edge set in $H_5(\beta,\alpha)$, then $|V_4| = 22$ *and* $|E_4| = 26$. Also the number of edges with eccentricities of end vertices are given as follows:

There are 1 edge with eccentricities of end vertices (7,5); 1 edge with eccentricities of end vertices (6,5); 2 edges with eccentricities of end vertices (7,7); 4 edges with eccentricities of end vertices (9,10); 4 edges with eccentricities of end vertices (8,7); 4 edges with eccentricities of end vertices (10,11); 4 edges with eccentricities of end vertices (7,6); and 6 edges with eccentricities of end vertices (9,8)

Hence $HEI\left(H_5(\beta,\alpha)\right) = \sum_{uv\epsilon E(H_5(\beta,\alpha))} \frac{2}{e_u+e_v}$

$= 1\left(\frac{2}{7+5}\right) + 1\left(\frac{2}{6+5}\right) + 2\left(\frac{2}{7+7}\right) + 4\left(\frac{2}{8+7}\right) + 4\left(\frac{2}{9+10}\right) + 4\left(\frac{2}{11+10}\right) + 4\left(\frac{2}{6+7}\right) + 6\left(\frac{2}{9+8}\right) = 3.290804$.

Also let V_5 be the vertex set and E_5 be the edge set in $H_5(\beta,\beta)$, then $|V_5| = 22$ *and* $|E_5| = 26$. The number of edges with eccentricities of end vertices are given as follows:

4 edges with eccentricities of end vertices (10,9); 4 edges with eccentricities of end vertices (8,9); 4 edges with eccentricities of end vertices (7,6); 6 edges with eccentricities of end vertices (8,7);and 8 edges with eccentricities of end vertices (5,6)

Hence $HEI\left(H_5(\beta,\beta)\right) = \sum_{uv\epsilon E(H_5(\beta,\beta))} \frac{2}{e_u+e_v}$

$= 4\left(\frac{2}{10+9}\right) + 4\left(\frac{2}{8+9}\right) + 4\left(\frac{2}{7+6}\right) + 6\left(\frac{2}{8+7}\right) + 8\left(\frac{2}{5+6}\right) = 2.670662$

Similarly, let V_6 be the vertex set and E_6 be the edge set in $H_5(\beta,\gamma)$, then $|V_6| = 22$ *and* $|E_6| = 26$. Also the number of edges with eccentricities of end vertices are given as follows:

There are 1 edge with eccentricities of end vertices (5,5); 1 edge with eccentricities of end vertices (6,6); 4 edges with eccentricities of end vertices (9,10); 4 edges with eccentricities of end vertices (11,10); 4 edges with eccentricities of end vertices (8,7); 6 edges with eccentricities of end vertices (6,7); and 6 edges with eccentricities of end vertices (8,9),

Hence $HEI\left(H_5(\beta,\gamma)\right) = \sum_{uv\epsilon H_5(\beta,\gamma))} \frac{2}{e_u+e_v}$

$= 1\left(\frac{2}{7+7}\right) + 1\left(\frac{2}{6+6}\right) + 4\left(\frac{2}{9+10}\right) + 4\left(\frac{2}{11+10}\right) + 4\left(\frac{2}{8+7}\right) + 6\left(\frac{2}{6+7}\right) + 6\left(\frac{2}{8+9}\right) = 3.273821$

(iii) Consider the Zig-zag chain Z_5 in a line with $\propto -type, \beta - type$ and $\gamma - type$ fusing and which is denoted as $Z_5(\gamma,\alpha)$, $Z_5(\gamma,\beta)$ *and* $Z_5(\gamma,\gamma)$. Fig 7 Shows Z_5 with different types of Fusing

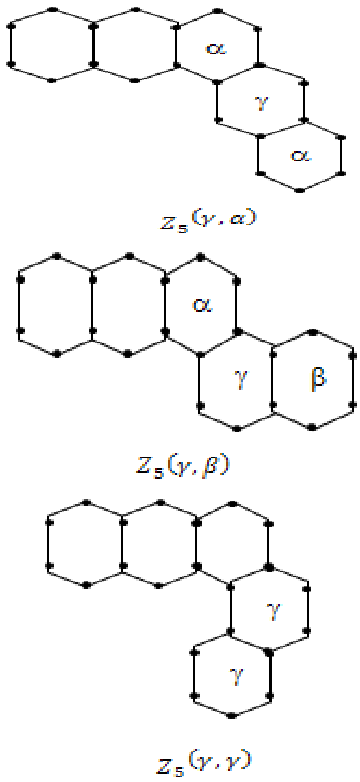


Fig 7. Zig-zag chain Z_5 with α, β, γ type fusing.

Let V_7 be the vertex set and E_7 be the edge set in $Z_5(\gamma,\alpha)$, then $|V_7| = 22$ and $|E_7| = 26$. Also the number of edges with eccentricities of end vertices are given as follows:

There are 2 edges with eccentricities of end vertices (6,6); 4 edges with eccentricities of end vertices (10,11); 4 edges with eccentricities of end vertices (8,7); 4 edges with eccentricities of end vertices (10,9); 6 edges with eccentricities of end vertices (7,6) ; and 6 edges with eccentricities of end vertices (7,8),

Hence $HEI\left(Z_5(\gamma,\alpha)\right) = \sum_{uv\in E(Z_5(\gamma,\alpha))} \frac{2}{e_u+e_v}$

$= 2\left(\frac{2}{6+6}\right) + 4\left(\frac{2}{10+11}\right) + +4\left(\frac{2}{10+9}\right) + 4\left(\frac{2}{8+7}\right) + 6\left(\frac{2}{8+7}\right) + 6\left(\frac{2}{7+6}\right) = 3.391749$

Also let V_8 be the vertex set and E_8 be the edge set in $Z_5(\gamma,\beta)$, then $|V_8| = 22$ and $|E_8| = 26$. The number of edges with eccentricities of end vertices are given as follows:

There are 1 edge with eccentricities of end vertices (6, 6); 3 edge with eccentricities of end vertices (6, 5); 4 edges with eccentricities of end vertices (8,7); 4 edges with eccentricities of end vertices (10,9); 4 edges with eccentricities of end vertices (6,7); 4 edges with eccentricities of end vertices (10,11); and 6 edges with eccentricities of end vertices (8,9),

Hence $HEI\left(Z_5(\gamma,\beta)\right) = \sum_{uv\in E(Z_5(\gamma,\beta))} \frac{2}{e_u+e_v}$

$= 1\left(\frac{2}{6+6}\right) + 3\left(\frac{2}{6+5}\right) + 4\left(\frac{2}{8+7}\right) + 4\left(\frac{2}{10+9}\right) + 4\left(\frac{2}{10+11}\right) + 4\left(\frac{2}{7+6}\right) + 4\left(\frac{2}{8+9}\right) = 3.133432$.

Similarly, let V_9 be the vertex set and E_9 be the edge set in $Z_5(\gamma,\gamma)$, then $|V_9| = 22$ and $|E_9| = 26$. Also the number of edges with eccentricities of end vertices are given as follows:

There are 1 edge with eccentricities of end vertices (7, 7); 4 edges with eccentricities of end vertices (6, 7); 3 edges with eccentricities of end vertices (6, 6); 4 edges with eccentricities of end vertices (6, 5); 4 edges with eccentricities of end vertices (8, 9); 4 edges with eccentricities of end vertices (9,10); and 6 edges with eccentricities of end vertices (8,7)

Hence $HEI\left(Z_5(\gamma,\gamma)\right) = \sum_{uv\in E(Z_5(\gamma,\gamma))} \frac{2}{e_u+e_v}$

$= 1\left(\frac{2}{7+7}\right) + 3\left(\frac{2}{6+6}\right) + 4\left(\frac{2}{6+5}\right) + 4\left(\frac{2}{6+7}\right) + 4\left(\frac{2}{8+9}\right) + 4\left(\frac{2}{9+10}\right) + 6\left(\frac{2}{7+8}\right) = 3.677155$. .

Theorem 2.3:

If L_6 is a Linear chain with $\propto -type$ fusing , H_6 is the Hexagonal chain with $\beta - type$ fusing, and Z_6 is a Zig-zag chain with $\gamma - type$ fusing then,

$(i)\, HEI\,(L_6) = 3.1745$

$(ii)\, HEI\,(H_6) = 3.37713$

$(iii)\, HEI\,(Z_6) = 3.29196$

Proof:

(i) Consider the Linear chain L_6 as in the diagram

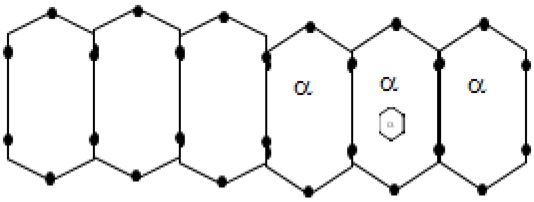


Fig 8. Linear chain L_6 .

Let V_1 be the vertex set and E_1 be the edge set in L_6, then $|V_1| = 26$ and $|E_1| = 31$. Also the number of edges with eccentricities of end vertices are given as follows:

There are 2 edges with eccentricities of end vertices (13,13); 2 edges with eccentricities of end vertices (11,11); 2 edges with eccentricities of end vertices (9,9); 1 edge with eccentricities of end vertices (7,7); 4 edges with eccentricities of end vertices (13,12); 4 edges with eccentricities of end vertices (11,12); 4 edges with eccentricities of end vertices (10,11); 4 edges with eccentricities of end vertices (10,9); 4 edges with eccentricities of end vertices (9,8); and 4 edges with eccentricities of end vertices (8,7),

Hence $HEI\,(L_6) = \sum_{uv\in E\,(L_6)} \frac{2}{e_u+e_v}$

$= 1\left(\frac{2}{7+7}\right) + 2\left(\frac{2}{13+13}\right) + 2\left(\frac{2}{11+11}\right) + 2\left(\frac{2}{9+9}\right) + 4\left(\frac{2}{13+12}\right) + 4\left(\frac{2}{11+12}\right) + 4\left(\frac{2}{11+10}\right) + 4\left(\frac{2}{10+9}\right) + 4\left(\frac{2}{9+8}\right) + 4 = 3.1745$.

(ii)Consider the Hexagonal chain H_6 as in the diagram

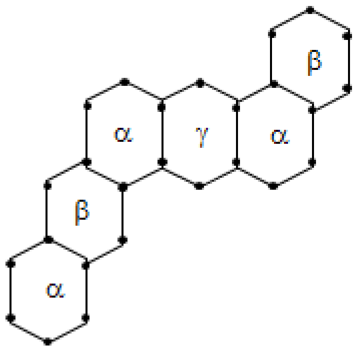


Fig 9. A Hexagonal chain H_6.

Let V_2 be the vertex set and E_2 be the edge set in L_6, then $|V_2| = 26$ and $|E_2| = 31$. Also the number of edges with eccentricities of end vertices are given as follows:
There are 2 edges with eccentricities of end vertices (12,12); 2 edges with eccentricities of end vertices (11,11); 3 edges with eccentricities of end vertices (7,7); 4 edges with eccentricity (11,12); 6 edges with eccentricities of end vertices (10,11); 3 edges with eccentricities of end vertices (10,9); 4 edges with eccentricities of end vertices (9,8); 4 edges with eccentricities of end vertices eccentricity (8,7); 2 edges with eccentricities of end vertices (8,8); and 1 edge with eccentricities of end vertices (10,8)

Hence $HEI\ (H_6) = \sum_{uv\in E\ (H_6)} \frac{2}{e_u+e_v}$

$$= 1\left(\frac{2}{10+8}\right) + 2\left(\frac{2}{12+12}\right) + 2\left(\frac{2}{11+11}\right) + 2\left(\frac{2}{8+8}\right) + 3\left(\frac{2}{10+9}\right) + 3\left(\frac{2}{7+7}\right) + 4\left(\frac{2}{11+12}\right) + 4\left(\frac{2}{8+7}\right) + 4\left(\frac{2}{9+8}\right) + 6\left(\frac{2}{11+10}\right) = 3.37713.$$

Consider the Zig-zag chain Z_6 as in the diagram

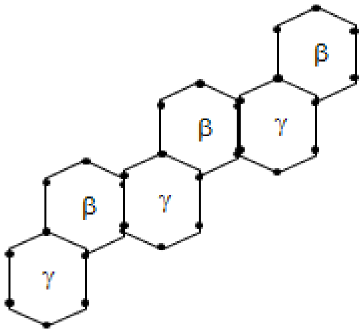


Fig 10. A Zig-zag chain Z_6

Let V_3 be the vertex set and E_3 be the edge set in Z_6, then $|V_3| = 26$ and $|E_3| = 31$. Also the number of edges with eccentricities of end vertices are given as follows:
There are 2 edges with eccentricities of end vertices (13,13); 2 edges with eccentricities of end vertices (12,11); 2 edges with eccentricities of end vertices (13,11); 1 edge with eccentricities of end vertices (6,6); 2 edges with eccentricities of end vertices (13,12); 2 edge with eccentricities of end vertices (8,6); 2 edge with eccentricities of end vertices (8,7); 2 edge with eccentricities of end vertices (7,6); 4 edges with eccentricities of end vertices (10,9); 6 edges with eccentricities of end vertices (10,11); and 6 edges with eccentricities of end vertices (9,8),

Hence $HEI\ (L_6) = \sum_{uv\in E\ (Z_6)} \frac{2}{e_u+e_v}$

$$= 1\left(\frac{2}{6+6}\right) + 2\left(\frac{2}{13+13}\right) + 2\left(\frac{2}{12+11}\right) + 2\left(\frac{2}{13+11}\right) + 2\left(\frac{2}{13+12}\right) + 2\left(\frac{2}{8+6}\right) + 4\left(\frac{2}{7+6}\right) + 4\left(\frac{2}{10+9}\right) + 6\left(\frac{2}{10+11}\right) + 6\left(\frac{2}{9+8}\right) = 3.296196$$

.In the following theorem we find Harmonic eccentric index of $L_n(\alpha,\alpha,\alpha,\ldots..\alpha)$

Theorem 2.4

If L_n is a linear chain with n hexagons, then

$$(i) HEI\ (L_n) = 4\left[\frac{2}{(n+1)+(n+2)}\right] + 2\left[\frac{2}{(n+2)+(n+2)}\right] + \cdots + 4\left[\frac{2}{(n+2)+(n+3)}\right] + 2\left[\frac{2}{(n+4)+(n+4)}\right] + \cdots + 4\left[\frac{2}{(2n)+(2n+1)}\right].$$

$$HEI\ (L_n) = 1\left[\frac{2}{(n+1)+(n+1)}\right] + 4\left[\frac{2}{(n+1)+(n+2)}\right] + 4\left[\frac{2}{(n+2)+(n+3)}\right] + 2\left[\frac{2}{(n+2)+(n+2)}\right] + \cdots + 4\left[\frac{2}{(2n)+(2n+1)}\right] + 2\left[\frac{2}{(2n+1)+(2n+1)}\right].$$

Proof: (i) Suppose n is odd , Let V_n be the vertex set in L_n, and E_n be the edge set in L_n, then $|V_n| = 8n-2$ and $|E_n| = 10n-4$. Let x ,y denote the central vertices with eccentricity $e_x = n+1$ and $e_y = n+1$.

Here there are 4 edges with eccentricities of end vertices $(n+1, n+2)$; 2 edges with eccentricities of end vertices $(n+2, n+2)$; 4 edges with eccentricities of end vertices $(n+2, n+3)$; 2 edges with eccentricities of end vertices $(n+4, n+4)$; 4 edges with eccentricities of end vertices $(n+1, n+2)$………; 4 edges with eccentricities of end vertices $(2n, 2n+1)$.

$$(i) HEI\ (L_n) = 4\left[\frac{2}{(n+1)+(n+2)}\right] + 2\left[\frac{2}{(n+2)+(n+2)}\right] + \cdots + 4\left[\frac{2}{(n+2)+(n+3)}\right] + 2\left[\frac{2}{(n+4)+(n+4)}\right] + \cdots + 4\left[\frac{2}{(2n)+(2n+1)}\right].$$

$$HEI\ (L_n) = 1\left[\frac{2}{(n+1)+(n+1)}\right] + 4\left[\frac{2}{(n+1)+(n+2)}\right] + 4\left[\frac{2}{(n+2)+(n+3)}\right] + 2\left[\frac{2}{(n+2)+(n+2)}\right] + \cdots + 4\left[\frac{2}{(2n)+(2n+1)}\right] + 2\left[\frac{2}{(2n+1)+(2n+1)}\right].$$

Proof: (i) Suppose n is odd , Let V_n be the vertex set in L_n, and E_n be the edge set in L_n, then $|V_n| = 8n-2$ and $|E_n| = 10n-4$. Let x ,y denote the central vertices with eccentricity $e_x = n+1$ and $e_y = n+1$.

Here there are 4 edges with eccentricities of end vertices $(n+1, n+2)$; 2 edges with eccentricities of end vertices $(n+2, n+2)$; 4 edges with eccentricities of end vertices $(n+2, n+3)$; 2 edges with eccentricities of end vertices $(n+4, n+4)$; 4 edges with eccentricities of end vertices $(n+1, n+2)$………; 4 edges with eccentricities of end vertices $(2n, 2n+1)$.

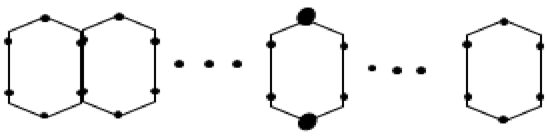


Fig 11. Linear chain L_n ,n is odd.

The above diagram shows the Linear chain L_n, when n is odd. Hence

$$HEI\,(L_n) = 4\left[\frac{2}{(n+1)+(n+2)}\right] + 2\left[\frac{2}{(n+2)+(n+2)}\right] + \cdots + 4\left[\frac{2}{(n+2)+(n+3)}\right] + 2\left[\frac{2}{(n+4)+(n+4)}\right] + \cdots + 4\left[\frac{2}{(2n)+(2n+1)}\right].$$

(ii) Suppose n is even ,

Let V_n be the vertex set in L_n, and E_n be the edge set in L_n, then $|V_n| = 8n - 2$ and $|E_n| = 10n - 4$. Let x,y denote the central vertices with eccentricity $e_x = n + 1$ and $e_y = n + 1$.

Here there are 1 edge with eccentricities of end vertices $(n+1, n+1)$; 4 edges with eccentricities of end vertices $(n+1, n+2)$; 4 edges with eccentricities of end vertices $(n+2, n+3)$; 2 edges with eccentricities of end vertices $(n+2, n+2)$………; 4 edges with eccentricities of end vertices $(2n, 2n+1)$; 2 edges with eccentricities of end vertices $(2n+1, 2n+1)$.

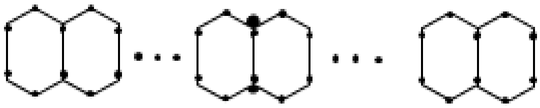


Fig 12. Linear chain L_n ,n is even.

The above diagram shows the Linear chain L_n, when n is even. Hence

$$HEI\,(L_n) = 1\left[\frac{2}{(n+1)+(n+1)}\right] + 4\left[\frac{2}{(n+1)+(n+2)}\right] + 4\left[\frac{2}{(n+2)+(n+3)}\right] + 2\left[\frac{2}{(n+2)+(n+2)}\right] + \cdots + 4\left[\frac{2}{(2n)+(2n+1)}\right] + 2\left[\frac{2}{(2n+1)+(2n+1)}\right].$$

Conclusion

In this paper we have calculated Harmonic eccentric index of Hexagonal chain. In future we will compare the various eccentric index of hexagonal chain.

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