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On *K*-eccentric and *K*-hyper eccentric indices of Benzenoid *H_k* system

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Abstract

Let G be a connected graph with vertex set V(G) and edge set E(G). Bhanumathi and Easu Julia Rani introduced the first *K* -Eccentric index $B_1E(G)$ and the second *K* - Eccentric index $B_2E(G)$ of a graph *G* as $B_1E(G) = \sum_{ue} [e_G(u) + e_{L(G)}(e)]$, $B_2E(G) = \sum_{ue} [e_G(u)e_{L(G)}(e)]$ They also defined the first *K* -Hyper eccentric index $HB_1E(G)$ and the second *K* -Hyper eccentric index $HB_2E(G)$ of a graph *G* as $HB_1E(G) = \sum_{ue} [e_G(u) + e_{L(G)}(e)]^2$, $HB_2E(G) = \sum_{ue} [e_G(u)e_{L(G)}(e)]^2$ where in all the cases *ue* means that the vertex *u* and edge *e* are incident in *G* and $e_{L(G)}(e)$ is

the eccentricity of e in the line graph L(G) of G. They have defined the multiplicative version of these indices also. In this paper, we calculate the first and second K eccentric, the first and second K-hyper eccentric indices and their multiplicative versions of benzenoid H_k system.

Keywords

K-eccentric index, *K*-hyper eccentric index, Multiplicative *K*-eccentric index, Multiplicative *K*-hyper eccentric index, Circo.

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1. Introduction

A topological index is a real number associated with chemical constitution. It correlates the chemical structure with various physical and chemical properties and biological activity.

All graphs in this paper are simple, finite and undirected. A graph G is a finite nonempty set V(G) together with a prescribed set E(G) of unordered pair of distinct elements of V. The cardinality of V(G) and E(G) are represented by |V(G)| and |E(G)|, respectively. Let, $d_G(v)$ be the degree of a vertex v of G and $N_G(v)$ be the neighborhood of a vertex v of *G*. The distance between the vertices *u* and *v* of a connected graph *G* is represented by $d_G(u, v)$. It is defined as the number of edges in a shortest path connects the vertices *u* and *v*. The eccentricity $e_G(v)$ of a vertex *v* in *G* is the largest distance between *v* and any other vertices *u* of *G*.

To take an account on contributions of pairs of incident elements, Kulli [5] introduced the first and second *K* Banhatti indices. In [4], Bhanumathi and Easu Julia Rani introduced the first *K* -Eccentric index $B_1E(G)$ and the second *K* - Eccentric index $B_2E(G)$ of a graph *G* as

$$B_{1}E(G) = \sum_{ue} \left[e_{G}(u) + e_{L(G)}(e) \right], B_{2}E(G) = \sum_{ue} \left[e_{G}(u)e_{L(G)}(e) \right]$$

and also defined the first *K*-Hyper eccentric index $HB_1E(G)$ and the second *K*-Hyper eccentric index $HB_2E(G)$ of a graph *G* as $HB_1E(G) = \sum_{ue} [e_G(u) + e_{L(G)}(e)]^2$, $HB_2E(G) = \sum_{ue} [e_G(u)e_{L(G)}(e)]^2$ where in all the cases ue means that the vertex *u* and edge *e* are incident in *G* and $e_{L(G)}(e)$ is the eccentricity of *e* in the line graph L(G) of *G* [4].

Table 1							
	Edge set	No. of edges	Eccentricity of end vertices	Eccentricity of <i>e</i> in			
		e = uv	(e(u), e(v))	$L(G)e_{L(G)}(e)$			
	E_1	6	(2k+1, 2k+1)	2k + 1			
	E_2	6	(2k+1, 2k+2)	2k + 1			
	E_3	12	(2k+2, 2k+3)	2k + 2			
	E_4	6	(2k+3, 2k+3)	2k + 3			
	E_5	12	(2k+3, 2k+4)	2k + 3			
	E_6	24	(2k+4, 2k+5)	2k + 4			
	E_7	6	(2k+5, 2k+5)	2k + 5			
	E_8	18	(2k+5, 2k+6)	2k + 5			
	E_9	36	(2k+6, 2k+7)	2k + 6			
	•	•	: :	÷			
	$E_{3(k-2)-2}$	6	(2k+2(k-2)-1, 2k+2(k-2)-1)	2k+2(k-2)-1			
	$E_{3(k-2)-1}$	6(k-2)	(2k+2(k-2)-1, 2k+2(k-2))	2k+2(k-2)-1			
	$E_{3(k-2)}$	12(k-2)	(2k+2(k-2), 2k+2(k-1)-1)	2k + 2(k - 2)			
	$E_{3(k-1)-2}$	6	(2k+2(k-1)-1, 2k+2(k-1)-1)	2k+2(k-1)-1			
	$E_{3(k-1)-1}$	6(k-1)	(2k+2(k-1)-1, 2k+2(k-1))	2k+2(k-1)-1			
	$E_{3(k-1)}$	12(k-1)	(2k+2(k-1), 2k+2(k-1)+1)	2k + 2(k - 1)			
	$E_{3(k-1)+1}$	6	(2k+2(k-1)+1, 2k+2(k-1)+1)	2k + 2(k - 1) + 1			

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2. First and second *K*-Eccentric indices, First and Second *K*-Hyper Eccentric indices of Benzenoid *H_k* system:

The circumcoronene homologous series of benzenoid also belongs to the family of molecular graphs that has several copy of benzene C_6 on its circumference. The terms of this series are represented as, H_1 -benzene, H_2 -coronene, H_3 circumcoronene and H_4 circumcircumcoronene etc. A benzeniod system is a connected geometric figure. It is obtained by arranging congruent regular hexagons in a plane. Consequently two hexagons are either disjoint or have a common edge.

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) respectively and for $e = uv \in E(G)$, denote the eccentricities of the end vertices of the edge e by (e(u), e(v)).

Let *V* be the vertex set of H_k and *E* be the edge set in H_k , then $|V| = 6k^2$ and $|E| = 9k^2 - 3k$ for the structure of H_k . First, we shall determine the number of edges e = uv with the eccentricity of the end vertices e(u), e(v) and eccentricity of the edge e in L(G). We give these values in the following Table 1.

Theorem 2.1. For any positive integer number k, let H_k be the general form of circumcoronene series of benzenoid system, then

(i)
$$B_1 E(H_k) = 6 \sum_{i=1}^{k} [8k + 4(2i - 1)] + 6 \sum_{i=1}^{k-1} [8k + 4(2i - 1)] + 1] + 12 \sum_{i=1}^{k-1} i[8k + 4(2i) + 1]$$

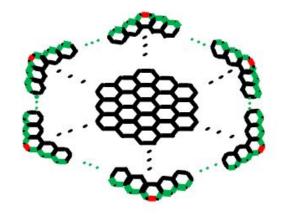


Figure 1. The Circumcoronene homologous Series of Benzenoid $H_k (k \ge 1)$ with edges

$$\begin{array}{ll} (ii) \quad B_{2}E\left(H_{k}\right)=6\sum_{i=1}^{k}\left[\left(2(2k+2i-1)\right)^{2}\right]\\ &+6\sum_{i=1}^{k-1}i\left[\left(2k+2i-1\right)^{2}+(2k+2i)(2k+2i-1)\right]\\ &+12\sum_{i=1}^{k-1}i\left[\left(2k+2i\right)^{2}+(2k+2i)(2k+2i-1)\right]\\ (iii) \quad HB_{1}E\left(H_{k}\right)=6\sum_{i=1}^{k}\left[\left(2(2k+2i-1)\right)^{2}+\left(2(2k+2i-1)\right)^{2}\right] \end{array}$$

$$+6\sum_{i=1}^{k-1} i \left[(2(2k+2i-1))^2 + ((2k+2i) + (2k+2i-1))^2 \right] \\ +12\sum_{i=1}^{k-1} i \left[(2(2k+2i))^2 + ((2k+2i+1) + (2k+2i))^2 \right]$$

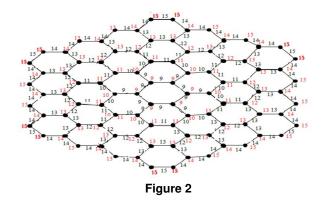


(iv)
$$HB_{2}E(H_{k}) = 6\sum_{i=1}^{k} \left[\left((2k+2i-1)^{2} \right)^{2} + \left((2k+2i-1)^{2} \right)^{2} \right] \\ + 6\sum_{i=1}^{k-1} i \left[\left((2k+2i-1)^{2} \right)^{2} + \left((2k+2i)(2k+2i-1))^{2} \right] \\ + 12\sum_{i=1}^{k-1} i \left[\left((2k+2i)^{2} \right)^{2} + \left((2k+2i+1)(2k+2i))^{2} \right] \right]$$

Proof. Consider the General form of H_k -Circumcoronene graph.

$$\begin{array}{ll} (i) \quad B_{1}E\left(H_{k}\right)=\sum_{ue}\left[e_{H_{k}}(u)+e_{L(H_{k})}(e)\right] \\ &=\sum_{e=uv\in E(G)}\left[e_{H_{k}}(u)+e_{L(H_{k})}(e)+e_{H_{k}}(v)+e_{L(H_{k})}(e)\right] \\ &=\sum_{uv\in E_{1}(G)}\left[e_{G}(u)+e_{L(G)}(e)+e_{G}(v)+e_{L(G)}(e)\right]+\ldots \\ &+\sum_{uv\in E_{3(k-1)+1}(G)}\left[e_{G}(u)+e_{L(G)}(e)+e_{G}(v)+e_{L(G)}(e)\right] \\ &=6\sum_{i=1}^{k}\left[8k+4(2i-1)\right]+6\sum_{i=1}^{k-1}\left[8k+4(2i-1)+1\right] \\ &+12\sum_{i=1}^{k-1}i\left[8k+4(2i)+1\right] \\ (ii) \quad B_{2}E\left(H_{k}\right)=\sum_{ue}\left[e_{H_{k}}(u)\times e_{L(H_{k})}(e)\right] \\ &=\sum_{uv\in E_{1}(G)}\left[e_{G}(u)e_{L(G)}(e)+e_{G}(v)e_{L(G)}(e)\right]+\ldots \\ &+\sum_{uv\in E_{3(k-1)+1}}\left[e_{G}(u)e_{L(G)}(e)+e_{G}(v)e_{L(G)}(e)\right] \\ &=6\sum_{i=1}^{k}\left[\left(2(2k+2i-1)\right)^{2}\right] \\ &+6\sum_{i=1}^{k-1}i\left[(2k+2i-1)^{2}+(2k+2i)(2k+2i-1)\right] \\ (iii) \quad HB_{1}E\left(H_{k}\right)=\sum_{ue}\left[e_{H_{k}}(u)+e_{L(H_{k})}(e)\right]^{2} \\ &=\sum_{uv\in E_{1}(G)}\left[\left[e_{G}(u)+e_{L(G)}(e)\right]^{2}+\left[e_{G}(v)+(e)\right]\right]^{2}+\ldots \\ &+\sum_{uv\in E_{3(k-1)+1}(G)}\left[\left[e_{G}(u)+e_{L(G)}(e)\right]^{2}+\left[e_{G}(v)+e_{L(G)}(e)\right]\right]^{2} \\ &=6\sum_{i=1}^{k}\left[\left(2(2k+2i-1)^{2}\right)+\left(2(2k+2i-1)\right)^{2}\right] \\ &=6\sum_{i=1}^{k}\left[\left(2(2k+2i-1)^{2}\right)+\left(2(2k+2i-1)\right)^{2}\right] \\ &+6\sum_{i=1}^{k-1}i\left[\left(2(2k+2i-1)^{2}\right)+\left((2k+2i-1)^{2}\right)^{2}\right] \\ &+12\sum_{i=1}^{k-1}i\left[\left(2(2k+2i-1)^{2}\right)^{2}+\left((2k+2i-1)^{2}\right)^{2}\right] \\ &=6\sum_{i=1}^{k}\left[\left(2(2k+2i-1)^{2}\right)^{2}+\left((2k+2i-1)^{2}\right)^{2}\right] \\ &+12\sum_{i=1}^{k-1}i\left[\left(2(2k+2i-1)^{2}\right)^{2}+\left((2k+2i-1)^{2}\right)^{2}\right] \\ &+12\sum_{i=1}^{k-1}i\left[\left(2(2k+2i)^{2}\right)^{2}+\left(2(2k+2i-1)^{2}\right)^{2}\right] \\ &+12\sum_{i=1}^{k-1}i\left[\left(2(2k+2i)^{2}\right)^{2}+\left(2(2k+2i-1)^{2}\right)^{2}\right] \\ &+12\sum_{i=1}^{k-1}i\left[\left(2(2k+2i)^{2}\right)^{2}+\left(2(2k+2i-1)^{2}\right)^{2}\right] \\ &+12\sum_{i=1}^{k-1}i\left[\left(2(2k+2i)^{2}\right)^{2}+\left(2(2k+2i-1)^{2}\right)$$

For example, let us evaluate the indices for H_4 . Consider the H_4 -Circumcircumcoronene graph.



Let *V* be the vertex set and *E* be the edge set in H_4 = Circumcircumcoronene, then |V| = 96 and |E| = 132. Also, the number of edges with eccentricities of end vertices $e = uv \in E(G)$ and $e \in L(G)$ are given as follows:

Table 2					
Edge	No. of	Eccentricity	Eccentricity		
set	edges	of end vertices	of <i>e</i> in		
		(e(u), e(v))	$L(G)e_{L(G)}(e)$		
E_1	6	(9,9)	9		
E_2	6	(9,10)	9		
E_3	12	(10,11)	10		
E_4	6	(11,11)	11		
E_5	12	(11,12)	11		
E_6	24	(12,13)	12		
E_7	6	(13,13)	13		
E_8	18	(13,14)	13		
E_9	36	(14,15)	14		
E_{10}	6	(15,15)	15		



(i)
$$B_1E(H_4) = \sum_{ue} \left[e_{H_4}(u) + e_{L(H_4)}(e) \right]$$

$$= \sum_{uv \in E_1(G)} \left[e_G(u) + e_{L(G)}(e) + e_G(v) + e_{L(G)}(e) \right] + \dots$$

$$+ \sum_{uv \in E_{10}(G)} \left[e_G(u) + e_{L(G)}(e) + e_G(v) + e_{L(G)}(e) \right]$$

$$= 6588$$
(ii) $B_2E(H_4) = \sum \left[e_{H_4}(u) \times e_{L(H_4)}(e) \right]$

$$= \sum_{e=uv \in E_1(G)} \left[e_G(u) e_{L(G)}(e) + e_G(v) e_{L(G)}(e) \right] + \dots + \sum_{e=uv \in E_{10}(G)} \left[e_G(u) e_{L(G)}(e) + e_G(v) e_{L(G)}(e) \right] = 41868$$

(iii)
$$HB_1E(H_4) = \sum_{ue} \left[e_{H_4}(u) + e_{L(H_4)}(e) \right]^2$$

$$= \sum_{e=uv \in E_1(G)} \left[\left[e_G(u) + e_{L(G)}(e) \right]^2 + \left[e_G(v) + e_{L(G)}(e) \right] \right]^2 + \dots + \sum_{e=uv \in E_{10}(G)} \left[\left[e_G(u) + e_{L(G)}(e) \right]^2 + \left[e_G(v) + e_{L(G)}(e) \right] \right]^2$$

$$= 167580$$

(iv)
$$HB_2E(H_4) = \sum_{ue} \left[e_{H_4}(u) \times e_{L(H_4)}(e) \right]^2$$

 $= \sum_{e=uv \in E_1(G)} \left[\left[e_G(u) \times e_{L(G)}(e) \right]^2 + \left[e_G(v) \times e_{L(G)}(e) \right] \right]^2 + \dots$
 $+ \sum_{e=uv \in E_{10}(G)} \left[\left[e_G(u) \times e_{L(G)}(e) \right]^2 + \left[e_G(v) \times e_{L(G)}(e) \right] \right]^2$
 $= 7105236$

Thus we have $B_1E(H_4) = 6588$, $B_2E(H_4) = 41868$, $HB_1E(H_4) = 167580$ and $HB_2E(H_4) = 7105236$.

Corollary 2.2. H_1 be the first terms of this Circumcoronene series of Benzene H_k . Then

- (*i*) $B_1E(H_1) = 72$
- (*ii*) $B_2E(H_1) = 108$
- (*iii*) $HB_1E(H_1) = 432$
- (*iv*) $HB_2E(H_1) = 972.$

Corollary 2.3. H_2 be the second terms of this Circumcoronene series of Benzene H_k . Then

- (*i*) $B_1E(H_2) = 714$
- (*ii*) $B_2E(H_2) = 2154$
- (*iii*) $HB_1E(H_2) = 8634$
- (*iv*) $HB_2E(H_2) = 82182$

Corollary 2.4. H_3 be the third terms of this Circumcoronene series of Benzene H_k . Then

(i)
$$B_1E(H_3) = 2646$$

(ii) $B_2E(H_3) = 12366$
(iii) $HB_1E(H_3) = 49770$
(iv) $HB_2E(H_3) = 1134150$

3. Multiplicative First and Second *K*-Eccentric indices, Multiplicative First and Second *K* Hyper Eccentric indices of Benzenoid *H_k* system:

Theorem 3.1. For any positive integer number k, let H_k be the general form of circumcoronene series of benzenoid system, then

$$\begin{array}{ll} (i) & B\Pi_{1}E\left(H_{k}\right)=6\prod_{i=1}^{k}\left[4(2k+2i-1)^{2}\right] \\ & \times 6\prod_{i=1}^{k-1}i[2(2k+2i-1)(4k+4i-1)] \\ & \times 12\prod_{i=1}^{k-1}i[2(2k+2i)(4k+4i+1)] \\ (ii) & B\Pi_{2}E\left(H_{k}\right)=6\prod_{i=1}^{k}\left[(2k+2i-1)^{4}\right] \\ & \times 6\prod_{i=1}^{k-1}i\left[(2k+2i-1)^{3}(2k+2i)\right] \\ & \times 12\prod_{i=1}^{k-1}i\left[(2k+2i)^{3}(2k+2i+1)\right] \\ (iii) & HB\Pi_{1}\left(H_{k}\right)=6\prod_{i=1}^{k}\left[16(2k+2i-1)^{4}\right] \\ & \times 6\prod_{i=1}^{k-1}i\left[(4(2k+2i-1))^{2}\right] \\ & \times \left[\left((2k+2i)+(2k+2i-1)\right)^{2}\right] \\ & \times \left[\left((2k+2i)+(2k+2i-1)\right)^{2}\right] \\ & \times 12\prod_{i=1}^{k-1}i\left[4(2k+2i)^{2}\right]+\left[\left((2k+2i+1)+(2k+2i)\right)^{2}\right] \\ (iv) & HB\Pi_{2}\left(H_{k}\right)=6\prod_{i=1}^{k}\left[(2k+2i-1)^{8}\right] \\ & \times 6\prod_{i=1}^{k-1}i\left[(2k+2i-1)^{6}\right] \times \left[(2k+2i)\right] \\ & \times 12\prod_{i=1}^{k-1}i\left[(2k+2i)^{6}\right]\left[(2k+2i+1)\right] \end{array}$$

Proof. Consider the General form of Hk - Circumcoronene



graph, Using Table 1, we obtain the following:

$$\begin{array}{ll} (i) & B\Pi_{1}E\left(H_{k}\right)=\prod_{uv}\left[e_{H_{k}}\left(u\right)+e_{L(H_{k})}\left(e\right)\right] \\ &=\prod_{uv\in E_{i}(G)}\left[\left[e_{G}(u)+e_{L(G)}(e)\right]\left[e_{G}(v)+e_{L(G)}(e)\right]\right]\right]\times\ldots \\ &\times\prod_{uv\in E_{i}(d-1)+1}\left(G\right)\left[\left[e_{G}(u)+e_{L(G)}(e)\right]\left[e_{G}(v)+e_{L(G)}(e)\right]\right] \\ &=6\prod_{i=1}^{k}\left[4(2k+2i-1)^{2}\right] \\ &\times 6\prod_{i=1}^{k-1}i[2(2k+2i)(4k+4i-1)] \\ &\times 12\prod_{i=1}^{k-1}i[2(2k+2i)(4k+4i+1)] \\ (ii) & B\prod_{2}(H_{k})=\prod_{uv}\left[e_{H_{k}}(u)\times e_{L(H_{k})}(e)\right] \\ &=\prod_{e=uv\in E_{1}(G)}\left[\left[e_{G}(u)\times e_{L(G)}(e)\right]\left[e_{G}(v)\times e_{L(G)}(e)\right]\right]\times\ldots \\ &\times \prod_{e=uv\in E_{2}(k-1)+1}\left(G\right]\left[e_{G}(u)\times e_{L(G)}(e)\right]\left[e_{G}(v)+e_{L(G)}(e)\right]\right] \\ &=1i\left[(2k+2i-1)^{4}\times 6\prod_{i=1}^{k-1}i\left[(2k+2i-1)^{3}(2k+2i)\right] \\ &\times 12\prod_{i=1}^{k-1}i\left[(2k+2i)^{3}(2k+2i+1)\right] \\ (iii) & HB\Pi_{1}(H_{k})=\Pi_{ue}\left[e_{H_{k}}(u)+e_{L(H_{k})}(e)\right]^{2} \\ &=\prod_{e=uv\in E_{1}(G)}\left[\left[e_{G}(u)+e_{L(G)}(e)\right]^{2}\left[e_{G}(v)+e_{L(G)}(e)\right]^{2}\right]\times\ldots \\ &\times \prod_{e=uv\in E_{1}(G)}\left[\left[e_{G}(u)+e_{L(G)}(e)\right]^{2}\left[e_{G}(v)+e_{L(G)}(e)\right]^{2}\right] \\ &+\left[\left((2k+2i)+(2k+2i-1)^{4}\right]\times 6\prod_{i=1}^{k-1}i\left[\left(4(2k+2i-1)\right)^{2}\right] \\ &+\left[\left((2k+2i)+(2k+2i-1)\right)^{2}\right]\times 12\prod_{i=1}^{k-1}i\left[4(2k+2i)^{2}\right] \\ &+\left[\left((2k+2i+1)+(2k+2i)^{2}\right]\right] \\ (iv) & HB\Pi_{1}(H_{k})=\prod_{ue}\left[e_{H_{k}}(u)\times e_{L(H_{k})}(e)\right]^{2} \\ &=\prod_{e=uv\in E_{1}(G)}\left[\left[e_{G}(u)\times e_{L(G)}(e)\right]^{2}\left[e_{G}(v)\times e_{L(G)}(e)\right]^{2}\right]\times \\ &\times \prod_{e=uv\in E_{1}(G)}\left[e_{E}(u)\times e_{E}(e)\right]^{2}\left[e_{E}(v)\times e_{E}(e)\right]^{2}\left[e_{E}(v)\times e_{E}(e)\right]^{2}$$

Using MATLAB programme, we have calculated these indices for H_1, H_2 and H_3 . Those values are given below corollaries.

Corollary 3.2. H_1 be the first terms of this Circumcoronene series of Benzene H_k . Then

- (*i*) $B\Pi_1 E(H_1) = 2176782336$
- (*ii*) $B\Pi_2 E(H_1) = 2.824295365 \times 10^{11}$
- (*iii*) $HB\Pi_1 E(H_1) = 4.738381338 \times 10^{18}$
- (*iv*) $HB\Pi_2 E(H_1) = 7.976644308 \times 10^{22}$

Corollary 3.3. H_2 be the second terms of this Circumcoronene series of Benzene H_k . Then

- (*i*) $B\Pi_1 E(H_2) = 2.086352657 \times 10^{64}$
- (*ii*) $B\Pi_2 E(H_2) = 2.901497086 \times 10^{92}$
- (*iii*) $HB\Pi_1E(H_2) = 3.1023e + 040$
- (*iv*) $HB\Pi_2 E(H_2) = 8.4187e + 184$

Corollary 3.4. H_3 be the third terms of this Circumcoronene series of Benzene H_k . Then

- (*i*) $B\Pi_1 E(H_3) = 1.3789e^{+093}$
- (*ii*) $B\Pi_2 E(H_3) = 7.3558e^{+128} \times 1.0328e^{+234}$
- (*iii*) $HB\Pi_1E(H_3) = 1.9013e^{+186}$
- (*iv*) $HB\prod_2 E(H_3) = 5.4107e^{+257} \times 5.7517e^{+151} \times 6.7910e^{+251} \times 2.7308e^{+064}$

4. Conclusion

In chemical graph theory a topological index of a molecular graph characterizes its topology. Here, we have computed the first, second *K*-eccentric indices, *K*-hyper eccentric indices and multiplicative first, second *K*-eccentric and *K*-hyper eccentric indices of benzenoid H_k system.

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