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Research Paper

MULTIVARIATE EXTENDED ADJACENCY DEGREE BASED GRAPHICAL INDEX : MATHEMATICAL AND CHEMICAL SIGNIFICANCES

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ABSRTACT

The Multivariate extended adjacency graphical index, which helps to analyze the molecular structures and predict properties of compounds, is that specific cases for randomly chosen values of the non zero real numbers a, b and c, which are coincide with the vast majority of pre-defined graphical indices being considered. In this paper, we obtained the index value for some specific families of graphs, bounds and characterization in terms of order, size, minimum and maximum degree. Also, we present the chemical applicability for some linear molecular graphs for the above said graphical index.

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1. INTRODUCTION

Let $G = (V, E)$ be a finite, undirected and simple graph with $n \geq 2$ vertices and $m \geq 1$ edges. The number of vertices are adjacent to vertex u is known as degree of u and is denoted by $d_G(u)$. The maximum (vertex) degree is denoted by $\Delta = \Delta(G)$ and the minimum degree by $\delta = \delta(G)$. Also, $d_G(e) = d_G(u) + d_G(v) - 2$ is the degree of an edge $e = uv$ in G. If vertices u and v are adjacent, we denote it as $i \sim j$. A graph G is r - regular if $\delta = \Delta = r$. For more graph terminologies and notations are not defined here we follow [14].

In 1994, Yi-Qiu Yang *et al.* [31] introduced the Extended Adjacency Index (EA index) of a graph G and defined as

$$EA(G) = \sum_{i\sim j} \tfrac{1}{2}\left(\tfrac{d_i}{d_j} + \tfrac{d_j}{d_i}\right).$$

The EA indices serves as an input features in QSAR models and is used to predict physiochemical properties like: Boiling point, melting point, solubility and Partition coefficient (log P). For more information about EA related indices, we refer to [3], [5], [12] and [30].

2. MULTIVARIATE EXTENDED ADJACENCY INDEX

Let $d_i = d_G(u)$ and $d_j = d_G(v)$ with $i \sim j$ (i.e., $e = uv \in E(G)$). Then the Multivariate extended adjacency index of a graph G is defined and denoted as

$$EA^{(a,b,c)}(G) = \sum_{i\sim j} \frac{1}{2}\left(\frac{d_i^a}{d_j^b} + \frac{d_j^b}{d_i^a}\right)^c = \frac{1}{2}\sum_{i\sim j}\left(\frac{d_i^{2a}+d_j^{2b}}{d_i^a d_j^b}\right)^c,$$

where $a, b, c \in \mathbb{R}$.

Chemical graph theory is a very active and widely used branch of Mathematical chemistry, which has the significance effect on the development of chemical sciences. Graphical indices are the numerical quantities which are derived from the structural features of a molecular graph which correlate to a molecule's physicochemical properties. It is also known as topological indices or molecular descriptors. It attracted much attention from scholars, and its mathematical properties and its chemical applicability were, and currently is, much investigated, see for instance [1], [2], [7] - [11], and [15].

2.1. The particular values of a, b and c in $EA^{(a,b,c)}(G)$.

For specific values of the $a, b, c \in \mathbb{R}$, majority of previously investigated degree-based graphical indices are special cases of the $EA^{(a,b,c)}(G)$ index of a graph G as given in the below table.

Multivariate Extended Adjacency Indices	Name of the Graphical Indices
$EA^{(\frac{1}{2},\frac{1}{2},1)}(G) = AG(G)$	Arithmetic Geometric Index, [20]
$EA^{(\frac{1}{2},\frac{1}{2},-1)}(G) = GA(G)$	Geometric-Arithmetic Index, [26]
$2EA^{(-1,-1,-1)}(G) = 2EA^{(1,1,1)}(G) = SDD(G)$	Symmetric Division Degree Index, [27]
$2EA^{(1,1,-1)}(G) = ISI(G)$	Inverse sum indegree index, [28]

3. MATHEMATICAL PROPERTIES

3.1. Special Class of Graphs.

Theorem 3.1. *Let G be regular graph with $n \geq 2$ and $d_G(v) = r$ such that for every $v \in V(G)$ and $\frac{nr}{2}$-edges. Then*

$$EA^{(a,b,c)}(G) = \frac{nr}{4}\left(r^{(a-b)} + r^{(b-a)}\right)^c. \tag{3.1}$$

Proof. Let G be regular graph with $n \geq 2$ and $d_G(v) = r$ such that for every $v \in V(G)$. Then

$$\begin{aligned} EA^{(a,b,c)}(G) &= \frac{1}{2}\sum_{i\sim j}\left(\frac{d_i^{2a}+d_j^{2b}}{d_i^a d_j^b}\right)^c \\ &= \frac{1}{2}\sum_{i\sim j}\left(\frac{r^{2a}+r^{2b}}{r^a r^b}\right)^c \\ &= \frac{1}{2}\left(\frac{r^{2a}+r^{2b}}{r^{(a+b)}}\right)^c \sum_{i\sim j}(1) \\ &= \frac{m}{2}\left(\frac{r^{2a}+r^{2b}}{r^{(a+b)}}\right)^c . \end{aligned}$$

Thus, the equation (3.1) follows. □

By using the above result, we have the following propositions of regular graphs.

Proposition 3.1.

(i) *For any Cycle C_n, which is 2-regular with $n \geq 3$ vertices,*

$$EA^{(a,b,c)}(C_n) = \frac{n}{2}\left(2^{(a-b)} + 2^{(b-a)}\right)^c . \tag{3.2}$$

(ii) *For any Complete graph K_n, which is $(n-1)$-regular with $n \geq 2$ vertices,*

$$EA^{(a,b,c)}(K_n) = \frac{n(n-1)}{2}\left[(n-1)^{a-b} + (n-1)^{b-a}\right]^c . \tag{3.3}$$

(iii) *For any k-hypercube graph Q_k, which is k-regular with 2^k - vertices and $k2^{k-1}$ - edges,*

$$EA^{(a,b,c)}(Q_k) = k2^{k-2}\left(k^{(a-b)} + k^{(b-a)}\right)^c . \tag{3.4}$$

where the hypercube Q_k is the simple graph whose vertices are the k-tuples with entries in $0, 1$ and whose edges are the pairs of k-tuples that differ in exactly one position.

(vi) *For any generalized Petersen graph $GP(t,k)$ which is 3-regular with $2t$- vertices and $3t$-edges,*

$$EA^{(a,b,c)}(GP(t,k)) = \frac{3t}{2}\left(3^{(a-b)} + 3^{(b-a)}\right)^c . \tag{3.5}$$

where the generalized Petersen graph denoted by $GP(t,k)$ for $t \geq 3$ and $1 \leq k \leq \lfloor (t-1)/2 \rfloor$ is a connected cubic graph consisting of an inner star polygon $\{t,k\}$ (Circulant graph $C_t^i(k)$) and an outer regular polygon t (cycle graph C_t) with corresponding vertices in the inner and outer polygons connected with edges.

Proposition 3.2. *For any Complete bipartite graph $K_{p,q}$ with $1 \leq p \leq q$,*

$$EA^{(a,b,c)}(K_{p,q}) = \begin{cases} \frac{pq}{2}\left(q^a + q^{-a}\right)^c, & \text{if } p = 1 \quad \text{and} \quad q \geq 1; \\ \frac{p^2}{2}\left(p^{a-b} + p^{b-a}\right)^c, & \text{if } p = q \text{ and } p \geq 1; \\ \frac{pq}{2}\left(q^a p^{-b} + p^b q^{-a}\right)^c, & \text{if } p \neq q \text{ and } p, q \geq 1. \end{cases} \tag{3.6}$$

Proof. Let $K_{p,q}$ be a complete bipartite graph with $1 \leq p \leq q$ has $n = (p+q)$ - vertices and $m = pq$ - edges. For vertex $u \in V_1(K_{p,q})$ has q- degree and $v \in V_2(K_{p,q})$ has p-degree. Then, we have the following cases:

Case 1. If $p = 1$ and $q \geq 1$ in $K_{p,q}$, then $K_{1,q}$ has $n = (1+q)$-vertices and $m = q$-edges. For vertex $u \in V_1(K_{1,q})$ has q-degree and $v \in V_2(K_{1,q})$ has 1-degree. Therefore

$$\begin{aligned}
EA^{(a,b,c)}(K_{1,q}) &= \frac{1}{2}\sum_{i\sim j}\left(\frac{d_i^{2a}+d_j^{2b}}{d_i^a d_j^b}\right)^c \\
&= \frac{1}{2}\sum_{i\sim j}\left(\frac{q^{2a}+1^{2b}}{q^a 1^b}\right)^c \\
&= \frac{1}{2}\left(\frac{(q^{2a}+1}{q^a}\right)^c \sum_{i\sim j}(1) \\
&= \frac{pq}{2}\left[\left(\frac{q^{2a}+1}{q^a}\right)^c\right] \\
&= \frac{pq}{2}\left(q^a+q^{-a}\right)^c.
\end{aligned}$$

Case 2. If $p = q$ and $p \geq 1$ in $K_{p,q}$, then $K_{p,p}$ has $n = 2p$-vertices and $m = p^2$-edges. Also, each vertex of degree is p. By Theorem 3.1 with $r = p$, we have

$$EA^{(a,b,c)}(K_{p,p}) = \frac{p^2}{2}\left(p^{a-b}+p^{b-a}\right)^c$$

Case 3. If $p \neq q$ and $p, q \geq 1$ in $K_{p,q}$, then $K_{p,q}$ has $n = (p+q)$-vertices and $m = pq$-edges. For vertex $u \in V_1(K_{p,q})$ has q-degree and $v \in V_2(K_{p,q})$ has p-degree. Therefore

$$\begin{aligned}
EA^{(a,b,c)}(K_{p,q}) &= \frac{1}{2}\sum_{i\sim j}\left(\frac{d_i^{2a}+d_j^{2b}}{d_i^a d_j^b}\right)^c \\
&= \frac{1}{2}\sum_{i\sim j}\left(\frac{q^{2a}+p^{2b}}{q^a p^b}\right)^c \\
&= \frac{1}{2}\left(\frac{q^{2a}+p^{2b}}{q^a p^b}\right)^c \sum_{i\sim j}(1) \\
&= \frac{pq}{2}\left(\frac{q^{2a}+p^{2b}}{q^a p^b}\right)^c \\
&= \frac{pq}{2}\left(q^a p^{-b}+p^b q^{-a}\right)^c.
\end{aligned}$$

Hence, the proof. ☐

Proposition 3.3. *For any Path P_n with $n \geq 3$,*

$$EA^{(a,b,c)}(P_n) = \frac{1}{2}\left[(m-2)\left(2^{a-b}+2^{b-a}\right)^c + \left(2^{-b}+2^b\right)^c + \left(2^a+2^{-a}\right)^c\right]. \tag{3.7}$$

Proof. Let P_n be a path with $n \geq 3$ vertics and $m = n-1$ edges. Then every vertices other than the end vertices are of degree 2. In P_n, we have $k = (m-2)$ edges are of degree 2 and end vertices are pendent i.e., 2 edges are of (1, 2) and (2, 1) degrees ($d_G(u,v)$). On substituting all these in $EA^{(a,b,c)}(P_n)$, we get the desired result. ☐

To prove our next results, we make use of the following definition:

The Cartesian product of two graphs G_1 and G_2, denoted by $G_1 \Box G_2$, is a graph with vertex set $V(G_1 \Box G_2) = V(G_1) \times V(G_2)$, that is, the set $\{(u, v) : u \in G_1, v \in G_2\}$. The edge set of $G_1 \Box G_2$ consists of all pairs $[(u_1, v_1), (u_2, v_2)]$ of vertices with $[u_1, u_2] \in E(G_1)$ and $v_1 = v_2$, or $u_1 = u_2$ and $[v_1, v_2] \in E(G_2)$. For more details, we refer to [12],[16],[17] and [29].

Theorem 3.2. *Let $G = P_t \Box P_s$ be a $(t \times s)$-grid graph. Then*

$$EA^{(a,b,c)}(G) = \begin{cases} 2[2^{a-b} + 2^{b-a}]^c, & \textit{if } t = s = 2 \\ \frac{1}{2}\Big[2(2^{a-b} + 2^{b-a})^c \\ +4(2^a 3^{-b} + 3^b 2^{-a})^c \\ +(3s-8)(3^{a-b} + 3^{b-a})^c\Big] & \textit{if } t = 2, s \geq 3 \\ \frac{1}{2}\Big[8(2^a 3^{-b} + 3^b 2^{-a})^c \\ +2(t+s-6)(3^{a-b} + 3^{b-a})^c \\ +2(t+s-4)(3^a 4^{-b} + 4^b 3^{-a})^c \\ +(2ts - 5(t+s) + 12)(4^{a-b} + 4^{b-a})^c\Big] & \textit{if } t \geq 3, s \leq t \end{cases}$$

Proof. Let $(t \times s)$ grid graph G can be represented as a cartesian product of $P_t \Box P_s$ of a path of length $(t-1)$ and a path of length $(s-1)$ with (ts)-vertices and $(2ts - t - s)$-edges. By algebraic method, we have following vertex degree partitions and along with the number of edges of G. On substituting the degree values in the definition of $EA^{(a,b,c)}(G)$ and simplifying , we get the desired result of the theorem. $\Box$

$t \times s$ grid	Degree partitions (d_i, d_j)	Number of edges
2×2	$(2,2)$	4
$2 \times s,\ s \geq 3$	$(2,2)$	2
	$(2,3)$	4
	$(3,3)$	$3s-8$
$t \times s, t \leq s, t \geq 3$	$(2,3)$	8
	$(3,3)$	$2(t+s-6)$
	$(3,4)$	$2(t+s-4)$
	$(4,4)$	$2ts - 5(t+s) + 12$

TABLE 1. Edge degree partition of $G = P_t \Box P_s$.

Theorem 3.3. *Let $G = P_t \Box C_s$ be a cylinder graph. Then*

$$EA^{(a,b,c)}(G) = \begin{cases} \frac{3s}{s}[3^{a-b} + 3^{b-a}]^c, & \textit{if } t = 2,\ s \geq 2 \\ \frac{1}{2}\Big[2s(3^{a-b} + 3^{b-a})^c \\ +2s(3^a 4^{-b} + 4^b 3^{-a})^c \\ +(2ts - 5s)(4^{a-b} + 4^{b-a})^c\Big] & \textit{if } t \geq 3, s \leq t \end{cases}$$

Proof. Let cylinder graph G can be represented as a cartesian product of $P_t \square C_s$ of a path of length $(t-1)$ and a cycle of length s , $s \geq 3$, with (ts)-vertices and $3s$-edges. By algebraic method, we have following vertex degree partitions and along with the number of edges of that vertex partition for the graph G. On by substituting data provided in the TABLE 2. , in our definition, we follow the desired result. $\square$

$t \times s$	Degree partitions (d_i, d_j)	Number of edges
2×3	$(3,3)$	$3s$
$t \times s, t \leq s, t \geq 3$	$(2,3)$	8
	$(3,3)$	$2s$
	$(3,4)$	$2s$
	$(4,4)$	$2ts - 5s$

TABLE 2. Edge degree partition of $G = P_t \square C_s$

Theorem 3.4. *Let $G = P_2 \square P_s$ be a ladder graph. Then*

$$EA^{(a,b,c)}(G) = \begin{cases} 2[2^{a-b} + 2^{b-a}]^c, & if\, t = s = 2 \\ \frac{1}{2}\Big[2(2^{a-b} + 2^{b-a})^c \\ +4(2^a 3^{-b} + 3^b 2^{-a})^c \\ +(3^{a-b} + 3^{b-a})^c\Big] & if\, t = 2, s = 3 \\ \frac{1}{2}\Big[2(2^{a-b} + 2^{b-a})^c \\ +4(2^a 3^{-b} + 3^b 2^{-a})^c \\ +(3s-8)(3^{a-b} + 3^{b-a})^c\Big] & if\, t = 2, s \geq 4 \end{cases}$$

Proof. Let ladder graph G can be represented as a cartesian product of $P_2 \square P_s$ of a path of length 1 and a path of length $(s-1)$ with (ts)-vertices and $3s-2$-edges. By algebraic method, we have following vertex degree partitions and along with the number of edges of that vertex partition for the graph G. On by substituting data provided in the TABLE 3. , in our definition, we follow the desired result. $\square$

$t \times s$	Degree partitions (d_i, d_j)	Number of edge set partitions
2×2	$(2,2)$	4
2×3	$(2,2)$	2
	$(2,3)$	4
	$(3,3)$	1
$2 \times s, s \geq 4$	$(2,2)$	2
	$(2,3)$	4
	$(3,3)$	$3s-8$

TABLE 3. Edge degree partition of $G = P_2 \square P_s$

Theorem 3.5. *Let $G = P_2\Box C_s$ be a prism graph. Then*

$$EA^{(a,b,c)}(G) = \frac{3t}{2}(3^{a-b} + 3^{b-a})^c.$$

Proof. Let prism graph G be the graph which can be obtained by the cartesian product of $P_2\Box C_s$ of a path of length 1 and a cycle of length s which is like a cylidrical structure, where two C_s's joined pairwise, which consists of $(2s)$-vertices and $3s$-edges. In prism graph all the vertices are of degree 3 and we can say it is 3-regular graph. On substituting every edges along with their vertex degree in the definition of $EA^{(a,b,c)}(G)$, we get the desired result of the theorem. □

Theorem 3.6. *Let $G = C_t\Box C_s$ be a torus graph. Then*

$$EA^{(a,b,c)}(G) = ts(4^{a-b} + 4^{b-a})^c.$$

Proof. Let torus graph G be the cartesian product of $C_t\Box C_s$, forming a wrapped grid with no boundary. It consists two cycles, one cycle of length t and another cycle of length s, which has (ts)-vertices and $2ts$-edges. In torue graph all the vertices are of degree 4 and we can say it is 4-regular graph. On substituting every edges along with their vertex degree in the definition of $EA^{(a,b,c)}(G)$, we get the desired result of the theorem. □

3.2. **Bounds in terms of size, order, minimum, and maximum degree.**

Theorem 3.7. *Let G be a graph of order $n \geq 2$ and size $m \geq 1$. Then*

$$\frac{m}{2}\left[\frac{2^c}{(n-1)^{(a+b)c}}\right] \leq EA^{(a,b,c)}(G) \leq \frac{m}{2}\left[(n-1)^{2a} + (n-1)^{2b}\right]^c. \tag{3.8}$$

Proof. Let G be a graph of order $n \geq 2$ and size $m \geq 1$. Then we know that, $1 \leq d_i \leq (n-1)$. On rising the power to a in the above equation, we have

$$1^a \leq {d_i}^a \leq (n-1)^a$$
$$1^{2a} \leq {d_i}^{2a} \leq (n-1)^{2a}$$

$$1 \leq {d_i}^{2a} \leq (n-1)^{2a} \tag{3.9}$$

Similarly for d_j we have ,

$$1 \leq {d_j}^{2b} \leq (n-1)^{2b} \tag{3.10}$$

On adding equations (3.9) and (3.10), we have

$$2 \leq {d_i}^{2a} + {d_j}^{2b} \leq (n-1)^{2a} + (n-1)^{2b} \tag{3.11}$$

Now consider, $1^a 1^b \leq d_i d_j \leq (n-1)^a (n-1)^b$
$1 \leq d_i d_j \leq (n-1)^{a+b}$

$$\frac{1}{(n-1)^{a+b}} \leq \frac{1}{d_i d_j} \leq 1 \tag{3.12}$$

On multiplying equations (3.11) and (3.12), we get

$$\frac{2}{(n-1)^{a+b}} \leq \frac{{d_i}^{2a} + {d_j}^{2b}}{d_i d_j} \leq (n-1)^{2a} + (n-1)^{2b} \tag{3.13}$$

On multiplying $\frac{1}{2}$ in equation (3.13), rising the power to c, and taking summation for each $i \sim j$, we have

$$\frac{1}{2}\sum_{i\sim j}\left[\frac{2}{(n-1)^{a+b}}\right]^c \leq \frac{1}{2}\sum_{i\sim j}\left[\frac{{d_i}^{2a}+{d_j}^{2b}}{d_i d_j}\right]^c \leq \frac{1}{2}\sum_{i\sim j}\left[(n-1)^{2a}+(n-1)^{2b}\right]^c.$$

Thus, the desired result of equation (3.8) follows. □

Theorem 3.8. *Let G be graph with $n \geq 2$ vertices. Then*

$$\frac{m}{2}\left[\frac{(\delta^{2a}+\delta^{2b})^c}{\Delta^{(a+b)^c}}\right] \leq EA^{(a,b,c)}(G) \leq \frac{m}{2}\left[\frac{(\Delta^{2a}+\Delta^{2b})^c}{\delta^{(a+b)^c}}\right]. \tag{3.14}$$

Proof. Let G be graph with $n \geq 2$ vertices. Then, we know that $\delta \leq d_i \leq \Delta$.

$$\delta^a \leq d_i^a \leq \Delta^a$$

$$\delta^{2a} \leq d_i^{2a} \leq \Delta^{2a} \tag{3.15}$$

Similarly for d_j, we have

$$\delta^{2b} \leq d_j^{2b} \leq \Delta^{2b} \tag{3.16}$$

On adding equations (3.15) and (3.16)), we have

$$\delta^{2a}+\delta^{2b} \leq d_i^{2a}+d_j^{2b} \leq \Delta^{2a}+\Delta^{2b}. \tag{3.17}$$

On multiplying d_i^a and d_j^b, we get $\delta^a\delta^b \leq d_i^a d_j^b \leq \Delta^a\Delta^b$

$$\delta^{a+b} \leq d_i^a d_j^b \leq \Delta^{a+b}$$

$$\frac{1}{\Delta^{a+b}} \leq \frac{1}{d_i^a d_j^b} \leq \frac{1}{\delta^{a+b}} \tag{3.18}$$

On multiplying equations (3.17) and (3.18), we have

$$\frac{\delta^{2a}+\delta^{2b}}{\Delta^{a+b}} \leq \frac{d_i^{2a}+d_j^{2b}}{d_i^a d_j^b} \leq \frac{\Delta^{2a}+\Delta^{2b}}{\delta^{a+b}}.$$

On multiplying $\frac{1}{2}$ in the above equation, rising the power to c, and taking summation for each $i \sim j$, we have

$$\frac{1}{2}\sum_{i\sim j}\left[\frac{\delta^{2a}+\delta^{2b}}{\Delta^{a+b}}\right]^c \leq \frac{1}{2}\sum_{i\sim j}\left[\frac{d_i^{2a}+d_j^{2b}}{d_i^a d_j^b}\right]^c \leq \frac{1}{2}\sum_{i\sim j}\left[\frac{\Delta^{2a}+\Delta^{2b}}{\delta^{a+b}}\right]^c$$

$$\frac{m}{2}\left[\frac{\delta^{2a}+\delta^{2b}}{\Delta^{a+b}}\right]^c \leq EA^{(a,b,c)}(G) \leq \frac{m}{2}\left[\frac{\Delta^{2a}+\Delta^{2b}}{\delta^{a+b}}\right]^c.$$

Thus, the desired equation (3.14) follows. □

4. CHEMICAL APPLICABILITY

4.1. **Linear[k] - Benzenoid structures.** The term "benzenoid aromatic compounds" refers to molecules containing one or more fused benzene rings. The concept of benzenoid compound is not attributed to a single inventor, but it was evolved through the work of the several scientists over time. In 1825, Michael Faraday isolated benzene from the oily residue of compressed illuminating gas, initially it was called as "bicarburet of hydrogen". In 1834, Eilhard Mitscherlich determined its emperical formula and named it as benzene in

1836. Later, in 1865, August Kekule proposed its cyclic structure, with alternating single and double bonds. The Linear $[k]$-Benzenoid graph is symbolized by $B[k]$. Where k is the number of Benzene structures. It is also denoted by $C_6, C_6, \dots, C_6$, as shown in Figure 1. For more information, we refer to [6] ,[24].

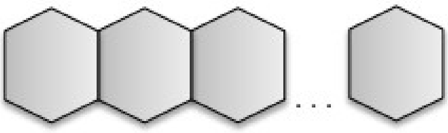

Figure 1. Linear $[k]$-Benzenoid

Theorem 4.1. *Let $B[k]$ be a molecular graph of Linear[k]-Benzenoid. Then*

$$EA^{(a,b,c)}(B[k]) = \frac{1}{2}\Big[6\left(2^{a-b}+2^{b-a}\right)^c + 4(k-1)\left(2^a3^{-b}+3^b2^{-a}\right)^c$$
$$+(k-1)\left(3^{a-b}+3^{b-a}\right)^c\Big].$$

Proof. Let $B[k]$ be a molecular graph of linear$[k]$-Benzenoid with $4k+2$ vertices and $5k+1$ edges for $k \in \mathbb{N}$ is the number rings of a benzenoid. Further, linear$[k]$-Benzenoid consists of 6 edges are of degree 2, $4(k-1)$ edges are of degree $(2,3)$ and $(k-1)$ edges are of degree 3. On substituting this in our definition we get,

$$EA^{(a,b,c)}(B[k]) = \frac{1}{2}\Big[6\left(2^{a-b}+2^{b-a}\right)^c + 4(k-1)\left(2^a3^{-b}+3^b2^{-a}\right)^c$$
$$+(k-1)\left(3^{a-b}+3^{b-a}\right)^c\Big].$$

□

4.2. **Linear[k]-Cyclohexane.** In 1874, Adolf von Baeyer was synthesized Cyclohexane using a ketonic decarboxylation of pimelic acid followed by multiple reductions. During this year only, E. Haworth and W. H. Perkin Jr. also synthesized it using a Wurtz reaction of 1,6-dibromohexane. in 1890, Germann Sachse proposed the chair and boat conformations of cyclohexane. The Linear $[k]$-Cyclohexane is symbolized by $C[k]$ and is denoted by $C_6, C_4, C_6, C_4, \dots, C_4, C_6$ as shown in Figure 2.

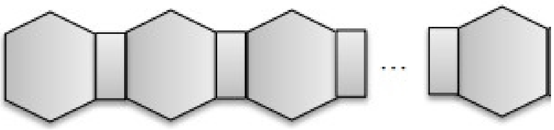

Figure 2. Linear $[k]$-Cyclohexane

Theorem 4.2. *Let $C[k]$ be a molecular graph of Linear[k]-Cyclohexane. Then*

$$EA^{(a,b,c)}(C[k]) = \Big[6\left(2^{a-b}+2^{b-a}\right)^c + 4(k-1)\left(2^a3^{-b}+3^b2^{-a}\right)^c$$

$$+4(k-1)\left(3^{a-b}+3^{b-a}\right)^{c}\Bigg].$$

Proof. Let $C[k]$ be a molecular graph of linear$[k]$-Cyclohexane with $6k$ vertices and $8k-2$ edges for $k \in \mathbb{N}$ is the number rings of a Cyclohexane. Further, linear$[k]$-Cyclohexane consists of 6 edges are of degree 2, $4(k-1)$ edges are of degree $(2,3)$ and $4(k-1)$ edges are of degree 3. On substituting this in our definition we get,

$$EA^{(a,b,c)}(C[k]) = \Bigg[6\left(2^{a-b}+2^{b-a}\right)^{c} + 4(k-1)\left(2^{a}3^{-b}+3^{b}2^{-a}\right)^{c}$$
$$+4(k-1)\left(3^{a-b}+3^{b-a}\right)^{c}\Bigg].$$

□

4.3. **Linear[k]-Naphthalene.** Naphthalene was first identified in 1819 by Alexnder Garden, a Scottish chemist. Further, its name was proposed in 1821 by John Kidd. In 1826, Michael Faraday determined its chemical formula and in 1866, Emil Erlenmeyer proposed the structure of two fused benzene rings and three year later it was confirmed by Carl Grabe.The Linear $[k]$-Naphthalene is symbolized by $N[k]$ and is denoted by $C_6, C_6, C_4, C_6, C_6, C_4, \ldots, C_4, C_6, C_6$ as shown in Figure 3. For more information, we refer to [25].

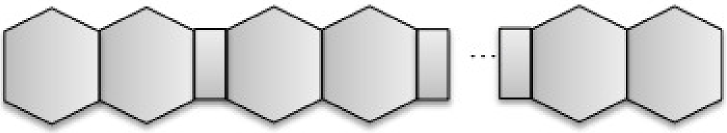

FIGURE 3. Linear $[k]$-Naphthalene

Theorem 4.3. *Let $N[k]$ be a molecular graph of Linear[k]-Naphthalene. Then*

$$EA^{(a,b,c)}(N[k]) = \Bigg[6\left(2^{a-b}+2^{b-a}\right)^{c} + +(8k-4)\left(2^{a}3^{-b}+3^{b}2^{-a}\right)^{c}$$
$$+(5k-4)\left(3^{a-b}+3^{b-a}\right)^{c}\Bigg].$$

Proof. Let $N[k]$ be a molecular graph of linear$[k]$-Naphthalene with $10k$ vertices and $13k-2$ edges for $k \in \mathbb{N}$ is the number rings of a Naphthalene. Further, linear$[k]$-Naphthalene consists of 6 edges are of degree 2, $8k-4$ edges are of degree $(2,3)$ and $5k-4$ edges are of degree 3. On substituting this in our definition we get,

$$EA^{(a,b,c)}(N[k]) = \Bigg[6\left(2^{a-b}+2^{b-a}\right)^{c} + (8k-4)\left(2^{a}3^{-b}+3^{b}2^{-a}\right)^{c}$$
$$+(5k-4)\left(3^{a-b}+3^{b-a}\right)^{c}\Bigg].$$

□

4.4. **Linear $[k]$-Anthracene.** In 1832, Dumas and Auguste Laurent discovered Anthracene in coal tar. The Linear $[k]$-Anthracene is symbolized by $A[k]$ and is denoted by $C_6, C_6, C_6, C_4, C_6, C_6, C_6, C_4, \ldots, C_4, C_6, C_6, C_6$ as shown in Figure 4. For more information, we refer to [4].

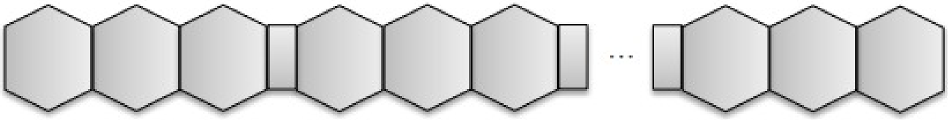

Figure 4. Linear $[k]$-Anthracene

Theorem 4.4. *Let $A[k]$ be a molecular graph of Linear[k]-Anthracene. Then*

$$EA^{(a,b,c)}(A[k]) = \Big[6\left(2^{a-b}+2^{b-a}\right)^c + (12k-4)\left(2^a3^{-b}+3^b2^{-a}\right)^c + (6k-4)\left(3^{a-b}+3^{b-a}\right)^c\Big].$$

Proof. Let $A[k]$ be a molecular graph of linear$[k]$-Anthracene with $14k$ vertices and $18k-2$ edges for $k \in \mathbb{N}$ is the number rings of a Anthracene. Further, linear$[k]$-Anthracene consists of 6 edges are of degree 2, $12k-4$ edges are of degree $(2,3)$ and $6k-4$ edges are of degree 3. On substituting this in our definition we get,

$$EA^{(a,b,c)}(A[k]) = \Big[6\left(2^{a-b}+2^{b-a}\right)^c + (12k-4)\left(2^a3^{-b}+3^b2^{-a}\right)^c + (6k-4)\left(3^{a-b}+3^{b-a}\right)^c\Big].$$

. □

4.5. **Linear $[k]$-Tetracene.** During his time at Bell Labs, Jan Hendrik Schon claimed to have developed an electrically pumped laser based on Tetracene. Tetracene is also known as Naphthacene. The Linear $[k]$-Tetracene is symbolized by $T[k]$ and is denoted by $C_6, C_6, C_6, C_6, C_4, C_6, C_6, C_6, C_6, C_4, \ldots, C_4, C_6, C_6, C_6, C_6$ as shown in Figure 5. For more information, we refer to [21].

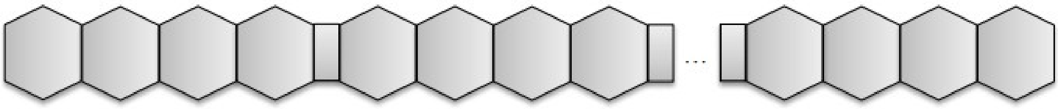

Figure 5. Linear $[k]$-Tetracene

Theorem 4.5. *Let $T[k]$ be a molecular graph of Linear[k]-Tetracene. Then*

$$EA^{(a,b,c)}(T[k]) = \Big[6\left(2^{a-b}+2^{b-a}\right)^c + (16k-4)\left(2^a3^{-b}+3^b2^{-a}\right)^c + (7k-4)\left(3^{a-b}+3^{b-a}\right)^c\Big].$$

Proof. Let $T[k]$ be a molecular graph of linear$[k]$-Tetracene with $18k$ vertices and $23k-2$ edges for $k \in \mathbb{N}$ is the number rings of a Tetracene. Further, linear$[k]$-Tetracene consists of

6 edges are of degree 2, $16k-4$ edges are of degree $(2,3)$ and $7k-4$ edges are of degree 3. On substituting this in our definition we get,

$$EA^{(a,b,c)}(T[k]) = \Big[6\left(2^{a-b}+2^{b-a}\right)^c + (16k-4)\left(2^a3^{-b}+3^b2^{-a}\right)^c + (7k-4)\left(3^{a-b}+3^{b-a}\right)^c\Big].$$

□

4.6. **Linear $[k]$-Pentacene.**

In 1912, Mills and Mills of the Northern Polytechnic Institute in London first synthesized Pentacene and some of its derivatives. The Linear $[k]$-Pentacene is symbolized by $P[k]$ and is denoted by $C_6, C_6, C_6, C_6,$ $C_6, C_4, C_6, C_6, C_6, C_6, C_6, C_4, \ldots, C_4, C_6, C_6, C_6, C_6, C_6$ as shown in Figure 6. For more information, we refer to[18].

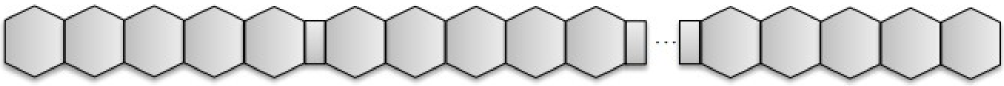

Figure 6. Linear $[k]$-Pentacene

Theorem 4.6. *Let $P[k]$ be a molecular graph of Linear[k]-Pentacene. Then*

$$EA^{(a,b,c)}(P[k]) = \Big[6\left(2^{a-b}+2^{b-a}\right)^c + (20k-4)\left(2^a3^{-b}+3^b2^{-a}\right)^c + (8k-4)\left(3^{a-b}+3^{b-a}\right)^c\Big].$$

Proof. Let $P[k]$ be a molecular graph of linear$[k]$-Pentacene with $22k$ vertices and $28k-2$ edges for $k \in \mathbb{N}$ is the number rings of a Pentacene. Further, linear$[k]$-Pentacene consists of 6 edges are of degree 2, $20k-4$ edges are of degree $(2,3)$ and $8k-4$ edges are of degree 3. On substituting this in our definition we get,

$$EA^{(a,b,c)}(P[k]) = \Big[6\left(2^{a-b}+2^{b-a}\right)^c + (20k-4)\left(2^a3^{-b}+3^b2^{-a}\right)^c + (8k-4)\left(3^{a-b}+3^{b-a}\right)^c\Big].$$

□

4.7. **Sensitive Analysis.**

The family of expressions $EA^{(a,b,c)}(X[k])$, where $X[k] \in \{C[k], N[k], A[k], T[k], P[k], B[k]\}$, exhibits a structured and interpretable behavior governed by the parameters a, b, c, and k. These expressions are composed of symmetric exponential terms designed to emphasize the interaction between variables a and b, modulated by the exponent c, which controls the degree of nonlinearity.

As c increases, the expressions become increasingly sensitive to differences between a and b, with sharp peaks emerging when $a \neq b$, and a flattening trend when $a = b$. The parameter

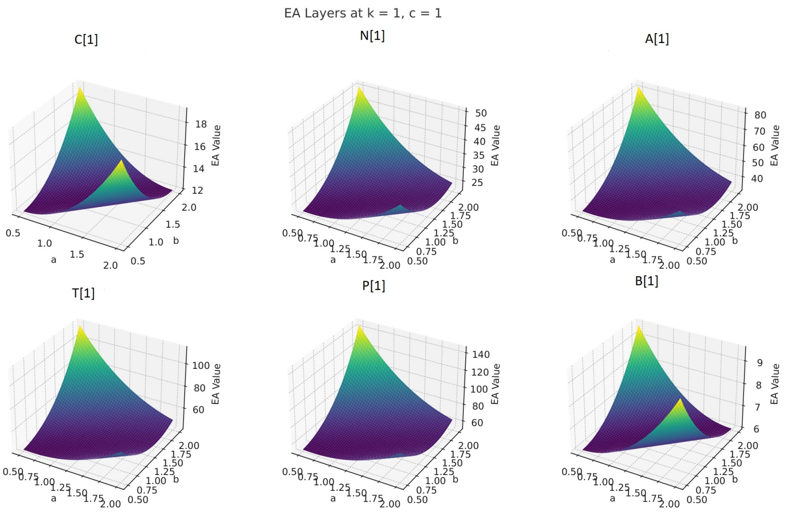

FIGURE 7. $EA^{(a,b,c)}(X[1])$ at $c = 1$

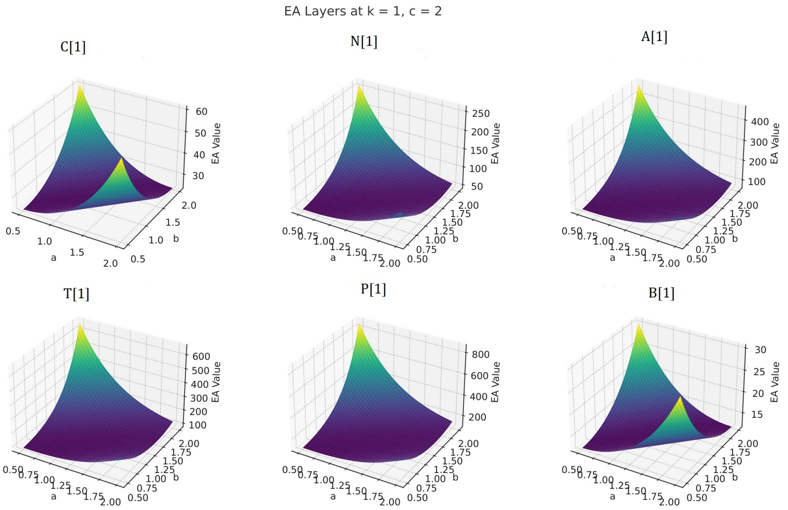

FIGURE 8. $EA^{(a,b,c)}(X[1])$ at $c = 2$

k acts as a scaling factor that progressively amplifies the influence of the second and third terms across layers, resulting in significant variation in growth behavior.

Specifically, layers such as $A[k]$, $T[k]$, and $P[k]$ demonstrate accelerated EA value increases with higher k, while $C[k]$ and its scaled counterpart $B[k]$ maintain a smoother, more uniform structure. The symmetry of the EA surfaces about the line $a = b$ confirms the balanced design of the exponential terms.

Both surface and contour visualizations support these observations and highlight the layers' suitability for modeling systems with varying degrees of response sensitivity — from linear or stable interactions to nonlinear, threshold-driven dynamics.

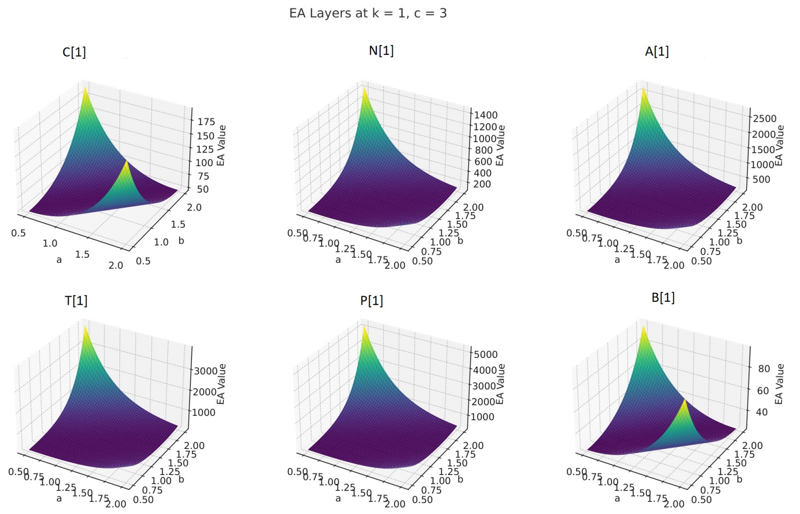

FIGURE 9. $EA^{(a,b,c)}(X[1])$ at $c = 3$

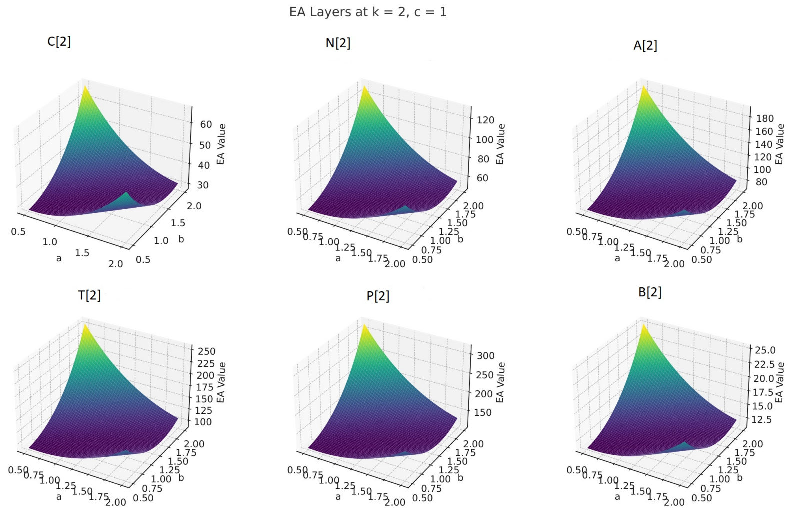

FIGURE 10. $EA^{(a,b,c)}(X[2])$ at $c = 1$

5. COMPARISON OF $EA^{(a,b,c)}(G)$ WITH SOME CLASSICAL INDICES

In this section we provided comparison of $EA^{(a,b,c)}(G)$ index value with some selected indices index value like: $ISI(G)$, $SDD(G)$, $AG(G)$, and $GA(G)$ for Linear[1]- molecular graphs like: Benzene ($B[1]$), Cyclohexane ($C[1]$), Naphthalene ($N[1]$), Anthracene ($A[1]$), Tetracene ($T[1]$), and Pentacene ($P[1]$). Here for the instance we fixed the values for our variables a, b, c as 1.

Based on both the table values and the plotted graph, the Extended Adjacency index EA(G) shows the clearest and most consistent growth pattern among all the classical indices considered. While indices such as $ISI(G)$, $SDD(G)$, $AG(G)$, and $GA(G)$ also increase from B[1]/C[1] to P[1], their rate of change is not as uniform as that of $EA(G)$. $EA(G)$ begins with the lowest value of 6.00 for $B[1]/C[1]$, indicating minimal adjacency contribution, and then increases steadily through $N[1]$ and $A[1]$. The gradual rise reflects $EA(G)$'s sensitivity

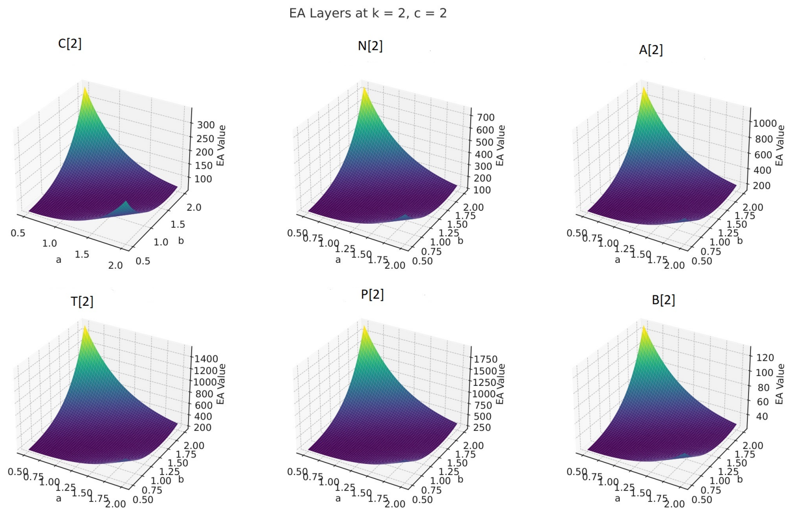

FIGURE 11. $EA^{(a,b,c)}(X[2])$ at $c = 2$

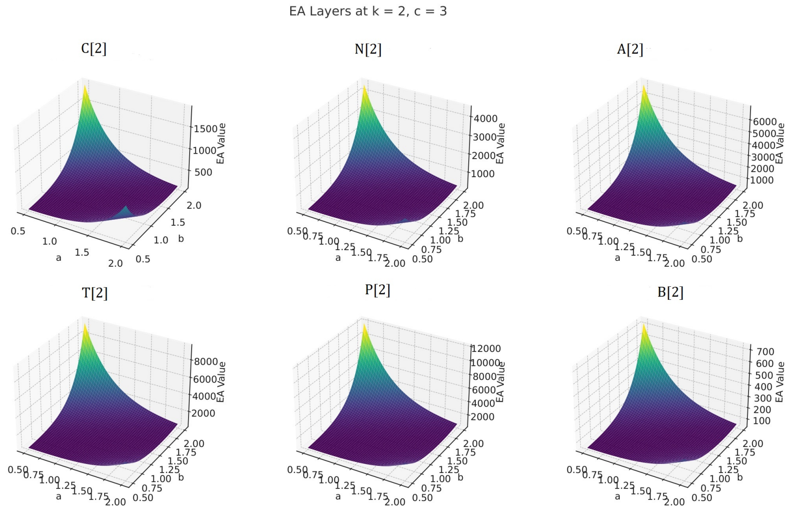

FIGURE 12. $EA^{(a,b,c)}(X[2])$ at $c = 3$

Graph	**ISI(G)**	**SDD(G)**	**AG(G)**	**GA(G)**	**EA(G)**
B[1]/C[1]	6.000000	6.000000	6.000000	6.000000	6.000000
N[1]	9.800000	14.833333	11.262742	10.357723	11.333333
A[1]	13.600000	21.666667	16.525484	14.715446	16.666667
T[1]	17.400000	28.500000	21.788226	19.073169	22.000000
P[1]	21.200000	35.333333	27.050968	23.430892	27.33333

TABLE 4. Comparison of $EA^{(1,1,1)}(G)$ with selected graphical indices

to changes in degree distribution, even in graphs with moderate structural complexity. For $T[1]$, $EA(G)$ increases further, capturing the enhanced connectivity of the graph. The index reaches its maximum value of 27.33 for $P[1]$, highlighting $P[1]$ as the graph with the richest

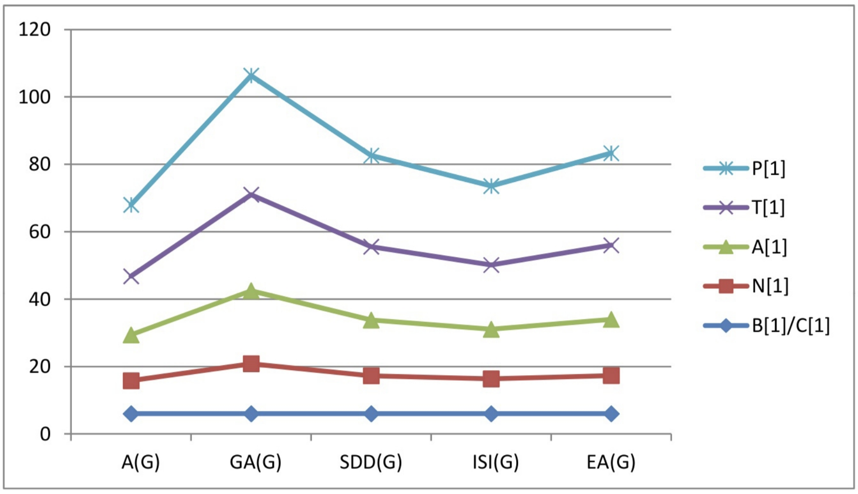

Figure 13. Graph showing comparison of $EA^{(1,1,1)}(G)$ with some selected indices index value.

adjacencies and highest structural contribution.

As observed from both the tabulated values and the plotted graph, all indices exhibit strictly increasing behaviour from single-ring to five-ring systems, following the order: $P[1] > T[1] > A[1] > N[1] > B[1]/C[1]$. Among the indices, $SDD(G)$ records the highest magnitude and the most rapid escalation, reflecting its strong dependence on vertex–vertex distances, which expand considerably in elongated polyacenes. Conversely, $ISI(G)$ maintains the smallest values and exhibits minimal variation, indicating its weaker discriminatory ability for larger graph structures. The indices $AG(G)$ and $GA(G)$ show closely parallel trends, whereas the our index $EA(G)$ aligns well with these degree-based measures while offering slightly enhanced separation between larger polyacenes, highlighting its ability to blend degree and structural contributions effectively. The smallest and most uniform values are consistently associated with $B[1]$ / $C[1]$ owing to their high symmetry and minimal internal distances. Overall, the analysis confirms that $EA(G)$ behaves coherently with established indices and accurately captures the structural progression within this chemical graph family.

The plotted graph visually confirms this behavior: the $EA(G)$ curve follows a stable upward trend and remains close to the order imposed by the structural complexity of the graphs. Compared with the other indices—some of which show sharper fluctuations (like $SDD(G)$) or slower growth (like $ISI(G)$). $EA(G)$ offers the most balanced, reliable, and discriminative measure. Its smooth progression across the graphs demonstrates its effectiveness in capturing structural variations and makes it particularly useful for distinguishing between graph families with increasing adjacency interactions.

6. Conclusion and Future Scope

In this work, we have conducted a comprehensive analysis of the Multivariate extended adjacency graphical index $EA^{(a,b,c)}(G)$, across diverse graph families, including many degree based graphical indices, where a, b and c are set of non zero real numbers. Here, we have established fundamental mathematical properties including order, size, minimum and maximum degrees for these. Our investigation has yielded precise bounds and characterizations for the $EA^{(a,b,c)}(G)$, positioning it within the broader framework of Chemical graph theory. Furthermore, we have demonstrated its practical significance through a comparative and sensitive analysis of $EA^{(a,b,c)}(G)$ for some certain class of chemical graphs. For the comparative advantages, practical applications, and mathematical point of view, many open problems are suggested by this research, among them are the following.

1. Find the extremal values and extremal graphs of this novel Multivariate extended adjacency graphical index.
2. Find the values of the Multivariate extended adjacency graphical index and coindex of certain classes of chemical graphs and explore some results towards QSPR / QSAR / QSTR Model.
3. Obtain the relationship between Multivariate extended adjacency graphical index in terms of other degree/distance/spectral based graphical indices.

7. Declaration

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Conflicts of Interest: The authors declare that there is no conflict of interest regarding the publication of this article.

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