

On New Connectivity Topological Indices of Certain Chemical Graphs

Mohamad Nazri Husin¹, Muhammad Sharjeel², Ghulam Farid², Zainab Javid², Khurrem Shehzad², Murat Cancan³, Mehdi Alaeiyan⁴, Mohammad Reza Farahani⁴

¹Special Interest Group on Modelling & Data Analytics (SIGMDA),

Faculty of Ocean Engineering Technology & Informatics,

Universiti Malaysia Terengganu, 21030 Kuala Nerus, Terengganu, Malaysia.

nazri.husin@umt.edu.my

²Department of Mathematics and Statistics, University of Agriculture, Faisalabad, Pakistan.

mohammadsharjeel3550@gmail.com,

rgfarid76@gmail.com, khurremshehzad@gmail.com,

³Faculty of Education, Van Yuzuncu Yıl University, Zeve Campus, Tuşba, 65080, Van, Turkey.

m_cencen@yahoo.com, mcancan@yyu.edu.tr

⁴Department of Mathematics, Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran.

alaeiyan@iust.ac.ir, Mohammad_Farahani@mathdep.iust.ac.ir, Mrfarahani88@gmail.com

Correspondence should be addressed to Mohamad Nazri Husin; nazri.husin@umt.edu.my

(ORCID ID: 0000-0003-4196-4984, 0000-0002-0019-9131, 0000-0002-8606-2274, 0000-0003-2185-5967,

0000-0003-2969-4280)

Correspondence should be addressed to: nazri.husin@umt.edu.my

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Abstract

The goal of our research is to calculate degree-based connectivity Kulli-Basava indices of chemical graphs. These graphs include hammer-like-benzenoid and phenylene graphs. Several degree-based topological indices are calculated of hammer and phenylene graph.

Keywords: Degree-based Topological index, benzenoid graphs, sum connectivity index, product connectivity index, atom-bond connectivity index, geometric arithmetic connectivity index, reciprocal connectivity index.

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1. Introduction

Cheminformatics is a modern field that combines chemistry, computer science, mathematics. Mathematical chemistry is a subfield of chemistry in which we examine chemical structures by applying mathematical logic. The molecular graph is constructed by representing atoms as points or vertices and constraints as edges or lines, respectively. A graph is ‘joined’ if every two vertices have connectivity, a graph is ‘simple’ if there are no multiple edges and loops present between any two vertices. Molecular graphs are all connected and simple. The number of vertices connected to a vertex determines its degree. We recommend [4] for basic graph theory concepts. A topological index is a numerical value associated with a graph that describes the graph's topology and is invariant under graph auto-morphism. Distance-based

topological indices, degree-based topological indices, counting-related polynomials, graph indices are some of the most common types of topological indices. Degree-based topological indices are significantly vital in chemical graph theory, especially in chemistry. A topological index $Top(G')$ of a graph G' is a value having the characteristic that $Top(H') = Top(G')$ for any graph H' isomorphic to G' . Wiener developed the concept of the topological index while researching the boiling point of paraffin [1, 3, 9-11, 24, 31]. For more information about the topological indices, the reader can look at the articles [2, 7, 8, 17-23, 26-28, 30, 36-38, 40]

2. Definitions

For a graph G' , the Sum connectivity Kulli-Basava index, the Product connectivity Kulli-Basava index, the Atom bond connectivity Kulli-Basava index, the Geometric arithmetic connectivity Kulli-Basava index, the Reciprocal connectivity Kulli-Basava index are defined by

$$SKB(G') = \sum_{uv \in E(G)} \frac{1}{\sqrt{S_e(u) + S_e(v)}}, \quad (1)$$

$$PKB(G') = \sum_{uv \in E(G)} \frac{1}{\sqrt{S_e(u) S_e(v)}}, \quad (2)$$

$$ABC KB(G') = \sum_{uv \in E(G)} \sqrt{\frac{S_e(u) + S_e(v) - 2}{S_e(u) S_e(v)}}, \quad (3)$$

$$GAKB(G') = \sum_{uv \in E(G)} \frac{2\sqrt{S_e(u) S_e(v)}}{S_e(u) + S_e(v)}, \quad (4)$$

$$RKB(G') = \sum_{uv \in E(G)} \sqrt{S_e(u) S_e(v)}, \quad (5)$$

and

respectively (see [33]).

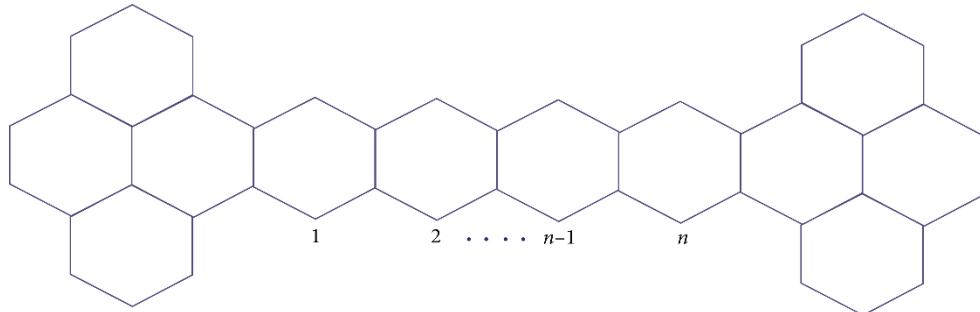


Figure 1: Hammer-like benzenoid graph $H_n(G')$.

The degree of an edge is determined by the formula $d_G(e) = d_G(u) + d_G(v) - 2$. The neighbourhood of vertices and sum of the degrees of all edges incident to a vertex are denoted by $N_G(v)$ and $S_e(v)$, respectively (see [5-6, 12-16, 25, 29, 32-35, 39]).

3. Main Results

3.1 Result for Hammer like-Benzoid Graph

The hammer-like benzenoid graph $H_n(G')$ has $2(2n+15)$ vertices and $(5n+37)$ edges. By simplification, the basis of the degree of vertices is divided into two portions $2(n+8)$ vertex of degree 2 and $2(n+7)$ vertex of degree 3. When two pyrene-fragments are joined at each

end of a linear polyacene chain of length n , the resulting structure is called a hammer-like structure $H_n(G')$.

Now, we construct a table by using section **Error! Reference source not found.** and calculate the partition of the edges to their sum of the degrees of all edges incident to vertices for the hammer-like benzenoid graph. So, for $e = uv \in E(G')$, we have:

Table 1: The number of edges partition of $(S_e(u), S_e(v))$ for Hammer like-Benzenoid Graph.

$(S_e(u), S_e(v))$	(4,5)	(5,5)	(5,10)	(5,11)	(6,10)	(6,11)
Number of edges	$n(n-2)$	2	$n(n-2)$	n	$n(n-1)$	n
$(S_e(u), S_e(v))$	(10,12)	(11,11)	(11,12)	(12,12)	(10,10)	
Number of edges	n	$n+2$	n	2	$n-1$	

Theorem 3.1.1. The Sum connectivity Kullibasava index $H_n(G')$ is defined by

$$\begin{aligned} SKB(G') &= \left(\frac{1}{3} + \frac{1}{\sqrt{15}} + \frac{1}{4} \right) n^2 + \left(\frac{1}{\sqrt{17}} + \frac{1}{\sqrt{20}} + \frac{2}{\sqrt{22}} + \frac{1}{\sqrt{23}} - \frac{2}{3} - \frac{2}{\sqrt{15}} \right) n \\ &\quad + \left(\frac{2}{\sqrt{10}} + \frac{2}{\sqrt{22}} + \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{20}} \right). \end{aligned}$$

Proof: By using sections **Error! Reference source not found.** and Table 1, we get

$$\begin{aligned} SKB(G') &= \sum_{uv \in E(G')} \frac{1}{\sqrt{S_e(u) + S_e(v)}} \\ &= n(n-2) \frac{1}{\sqrt{9}} + 2 \frac{1}{\sqrt{10}} + n(n-2) \frac{1}{\sqrt{15}} + n \frac{1}{\sqrt{16}} + n(n-1) \frac{1}{\sqrt{16}} + n \frac{1}{\sqrt{17}} + (n-1) \frac{1}{\sqrt{20}} \\ &\quad + n \frac{1}{\sqrt{22}} + (n+2) \frac{1}{\sqrt{22}} + n \frac{1}{\sqrt{23}} + 2 \frac{1}{\sqrt{24}} \\ &= n(n-2) \frac{1}{3} + 2 \frac{1}{\sqrt{10}} + n(n-2) \frac{1}{\sqrt{15}} + n \frac{1}{4} + n(n-1) \frac{1}{4} + n \frac{1}{\sqrt{17}} + (n-1) \frac{1}{\sqrt{20}} \\ &\quad + n \frac{1}{\sqrt{22}} + (n+2) \frac{1}{\sqrt{22}} + n \frac{1}{\sqrt{23}} + 2 \frac{1}{2\sqrt{6}} \\ &= \left(\frac{1}{3} + \frac{1}{\sqrt{15}} + \frac{1}{4} \right) n^2 + \left(\frac{1}{\sqrt{17}} + \frac{1}{\sqrt{20}} + \frac{2}{\sqrt{22}} + \frac{1}{\sqrt{23}} - \frac{2}{3} - \frac{2}{\sqrt{15}} \right) n \\ &\quad + \left(\frac{2}{\sqrt{10}} + \frac{1}{\sqrt{6}} + \frac{2}{\sqrt{22}} - \frac{1}{\sqrt{20}} \right). \end{aligned}$$

Theorem 3.1.2. The Product connectivity Kullibasava index $H_n(G')$ is given as

$$PKB(G') = \left(\frac{1}{\sqrt{20}} + \frac{1}{\sqrt{50}} + \frac{1}{\sqrt{60}} \right) n^2 + \left(\frac{1}{\sqrt{55}} + \frac{1}{\sqrt{66}} + \frac{1}{10} + \frac{1}{\sqrt{120}} + \frac{1}{11} + \frac{1}{\sqrt{132}} - \frac{2}{\sqrt{20}} - \frac{2}{\sqrt{50}} - \frac{1}{\sqrt{60}} \right) n + \left(\frac{2}{5} + \frac{2}{11} + \frac{1}{6} - \frac{1}{10} \right).$$

Proof: By using section **Error! Reference source not found.** and Table 1, we get

$$\begin{aligned} PKB(G') &= \sum_{uv \in E(G')} \frac{1}{\sqrt{S_e(u)S_e(v)}} \\ &= (n^2 - 2n) \frac{1}{\sqrt{20}} + 2 \frac{1}{\sqrt{25}} + (n^2 - 2n) \frac{1}{\sqrt{50}} + n \frac{1}{\sqrt{55}} + (n^2 - n) \frac{1}{\sqrt{60}} + n \frac{1}{\sqrt{66}} \\ &\quad + (n-1) \frac{1}{\sqrt{100}} + n \frac{1}{\sqrt{120}} + (n+2) \frac{1}{\sqrt{121}} + n \frac{1}{\sqrt{132}} + 2 \frac{1}{\sqrt{144}} \\ &= \left(\frac{1}{\sqrt{20}} + \frac{1}{\sqrt{50}} + \frac{1}{\sqrt{60}} \right) n^2 + \left(\frac{2}{5} + \frac{2}{11} + \frac{1}{6} - \frac{1}{10} \right) \\ &\quad + \left(\frac{1}{\sqrt{55}} + \frac{1}{\sqrt{66}} + \frac{1}{10} + \frac{1}{\sqrt{120}} + \frac{1}{11} + \frac{1}{\sqrt{132}} - \frac{2}{\sqrt{20}} - \frac{2}{\sqrt{50}} - \frac{1}{\sqrt{60}} \right) n. \end{aligned}$$

Theorem 3.1.3. The Atom bond connectivity Kullibasava index for $H_n(G')$ is given as

$$\begin{aligned} ABCK(G') &= \left(\sqrt{\frac{7}{20}} + \sqrt{\frac{13}{50}} + \sqrt{\frac{7}{30}} \right) n^2 + \left(\frac{2\sqrt{8}}{5} + \frac{\sqrt{22}}{6} + \frac{2\sqrt{20}}{11} - \frac{\sqrt{18}}{10} \right) \\ &\quad + \left(\sqrt{\frac{14}{55}} + \sqrt{\frac{15}{66}} + \frac{\sqrt{18}}{10} + \frac{1}{\sqrt{6}} + \frac{\sqrt{20}}{11} + \sqrt{\frac{21}{132}} - 2\sqrt{\frac{7}{20}} - \sqrt{\frac{7}{30}} - 2\sqrt{\frac{13}{50}} \right) n. \end{aligned}$$

Proof: It follows from section **Error! Reference source not found.** and Table 1 that

$$\begin{aligned} ABCKB(G') &= \sum_{uv \in E(G')} \sqrt{\frac{S_e(u) + S_e(v) - 2}{S_e(u)S_e(v)}} \\ &= n(n-2) \sqrt{\frac{7}{20}} + 2\sqrt{\frac{8}{25}} + n(n-2) \sqrt{\frac{13}{50}} + n\sqrt{\frac{14}{55}} + n(n-1) \sqrt{\frac{14}{60}} + n\sqrt{\frac{15}{66}} \\ &\quad + (n-1)\sqrt{\frac{18}{100}} + n\sqrt{\frac{20}{120}} + (n+2)\sqrt{\frac{20}{121}} + n\sqrt{\frac{21}{132}} + 2\sqrt{\frac{22}{144}} \\ &= (n^2 - 2n) \sqrt{\frac{7}{20}} + 2\frac{\sqrt{8}}{5} + (n^2 - 2n) \sqrt{\frac{13}{50}} + n\sqrt{\frac{14}{55}} + (n^2 - n) \sqrt{\frac{7}{30}} + n\sqrt{\frac{15}{66}} \\ &\quad + (n-1)\frac{\sqrt{18}}{10} + n\sqrt{\frac{1}{6}} + (n+2)\frac{\sqrt{20}}{11} + n\sqrt{\frac{21}{132}} + 2\frac{\sqrt{22}}{12} \\ &= \left(\sqrt{\frac{7}{20}} + \sqrt{\frac{13}{50}} + \sqrt{\frac{7}{30}} \right) n^2 + \left(\frac{2\sqrt{8}}{5} + \frac{\sqrt{22}}{6} + \frac{2\sqrt{20}}{11} - \frac{\sqrt{18}}{10} \right) \\ &\quad + \left(\sqrt{\frac{14}{55}} + \sqrt{\frac{15}{66}} + \frac{\sqrt{18}}{10} + \frac{1}{\sqrt{6}} + \frac{\sqrt{20}}{11} + \sqrt{\frac{21}{132}} - 2\sqrt{\frac{7}{20}} - \sqrt{\frac{7}{30}} - 2\sqrt{\frac{13}{50}} \right) n. \end{aligned}$$

Theorem 3.1.4. The Geometric arithmetic connectivity Kullibasava index for $H_n(G')$ is defined by

$$\begin{aligned} GAKB(G') &= \left(\frac{2\sqrt{55}}{55} + \frac{\sqrt{66}}{33} + \frac{1}{5} + \frac{\sqrt{120}}{60} + \frac{2}{11} + \frac{\sqrt{132}}{66} - \frac{\sqrt{20}}{5} - \frac{2\sqrt{50}}{25} - \frac{\sqrt{60}}{30} \right) n \\ &\quad + \left(\frac{\sqrt{20}}{10} + \frac{\sqrt{50}}{25} + \frac{\sqrt{60}}{30} \right) n^2 + \left(\frac{4}{5} + \frac{4}{11} + \frac{1}{3} - \frac{1}{5} \right). \end{aligned}$$

Proof: By using section (2) and Table 1, we get

$$\begin{aligned} GAKB(G') &= \sum_{uv \in E(G')} \frac{2\sqrt{S_e(u)S_e(v)}}{S_e(u)+S_e(v)} \\ &= n(n-2) \frac{2\sqrt{20}}{20} + \frac{4\sqrt{25}}{25} + n(n-2) \frac{2\sqrt{50}}{50} + n \frac{2\sqrt{55}}{55} + n(n-1) \frac{2\sqrt{60}}{60} \\ &\quad + n \frac{2\sqrt{66}}{66} + (n-1) \frac{2\sqrt{100}}{100} + n \frac{2\sqrt{120}}{120} + (n+2) \frac{2\sqrt{121}}{121} + n \frac{2\sqrt{132}}{132} + \frac{4\sqrt{144}}{144} \\ &= n(n-2) \frac{\sqrt{20}}{10} + \frac{20}{25} + n(n-2) \frac{\sqrt{50}}{25} + n \frac{2\sqrt{55}}{55} + n(n-1) \frac{\sqrt{60}}{30} + n \frac{\sqrt{66}}{33} \\ &\quad + (n-1) \frac{1}{5} + n \frac{\sqrt{120}}{60} + (n+2) \frac{2}{11} + n \frac{\sqrt{132}}{66} + \frac{1}{3} \\ &= \left(\frac{2\sqrt{55}}{55} + \frac{\sqrt{66}}{33} + \frac{1}{5} + \frac{\sqrt{120}}{60} + \frac{2}{11} + \frac{\sqrt{132}}{66} - \frac{\sqrt{20}}{5} - \frac{2\sqrt{50}}{25} - \frac{\sqrt{60}}{30} \right) n \\ &\quad + \left(\frac{\sqrt{20}}{10} + \frac{\sqrt{50}}{25} + \frac{\sqrt{60}}{30} \right) n^2 + \left(\frac{4}{5} + \frac{4}{11} + \frac{1}{3} - \frac{1}{5} \right). \end{aligned}$$

Theorem 3.1.5. We define the Reciprocal connectivity Kullibasava index for $H_n(G')$ by

$$\begin{aligned} RKB(G') &= (7 + \sqrt{15})n^2 + (\sqrt{17} + \sqrt{20} + 2\sqrt{22} + \sqrt{23} - 6 - 2\sqrt{15})n \\ &\quad + (2\sqrt{10} + 2\sqrt{22} + 2\sqrt{24} - \sqrt{20}). \end{aligned}$$

Proof: By using section **Error! Reference source not found.** and Table 1, we get

$$\begin{aligned} RKB(G') &= \sum_{uv \in E(G')} \sqrt{S_e(u)S_e(v)} \\ &= n(n-2)\sqrt{4+5} + 2\sqrt{5+5} + n(n-2)\sqrt{5+10} + n\sqrt{5+11} + n(n-1)\sqrt{6+10} \\ &\quad + n\sqrt{6+11} + (n-1)\sqrt{10+10} + n\sqrt{10+12} + (n+2)\sqrt{11+11} + n\sqrt{11+12} + 2\sqrt{12+12} \\ &= (n^2 - 2n)3 + 2\sqrt{10} + (n^2 - 2n)\sqrt{15} + 4n + (n^2 - n)4 + n\sqrt{17} + (n-1)\sqrt{20} \\ &\quad + n\sqrt{22} + n\sqrt{23} + 2\sqrt{24} + (n+2)\sqrt{22} \\ &= (3 + 4 + \sqrt{15})n^2 + (-6 - 2\sqrt{15} + 4 - 4 + \sqrt{17} + \sqrt{20} + \sqrt{22} + \sqrt{23} + \sqrt{22})n \\ &\quad + (2\sqrt{10} + 2\sqrt{22} + 2\sqrt{24} - \sqrt{20}) \\ &= (7 + \sqrt{15})n^2 + (\sqrt{17} + \sqrt{20} + 2\sqrt{22} + \sqrt{23} - 6 - 2\sqrt{15})n + (2\sqrt{10} + 2\sqrt{22} + 2\sqrt{24} - \sqrt{20}). \end{aligned}$$

3.2 Results for Linear Benzenoid Phenylenes

The descriptor phenylene is generally reserved for chemical graphs formed by inserting a square between all pairs of neighbouring hexagons in catacondensed benzenoid systems. There are two types of vertices one vertex is of degree Two and the other vertex is of degree Three. The number of vertices is equal to $V(G') = h'^2 + q'^2 + n'^2 + h'q' + q'n' - 5$ and the total number of edges in the graph $E(G') = h'^2 + q'^2 + n'^2 + 5(h' + q' + n') - 4$, where h' is the number of hexagons in each hexagon segment q' is the number of squares joining the hexagon and n' is the total number of hexagons segments. Therefore, linear benzenoid phenylenes can be a suitable term for these graphs.

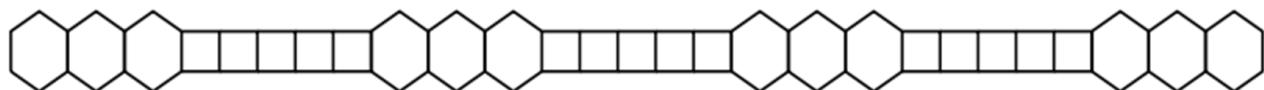


Figure 2: Linear Benzenoid Phenylene where $h' = 3$, $q' = 5$ and $n' = 4$.

Now, we construct the table using section 2 and we calculate the partitions of the edges to their sum of the degrees of all edge's incident to vertices of fluoranthene type benzenoid linear generalized phenylene graph for $e = uv \in E(G')$ in Table 2.

Table 2: The number of edges partition of $(S_e(u), S_e(v))$ for Linear Benzenoid Phenylene.

$(S_e(u), S_e(v))$	(4,4)	(4,5)	(5,10)	(6,6)	(6,10)
Number of edges	2	n'	n'	$q'+1$	q'^2
$(S_e(u), S_e(v))$	(6,11)	(10,10)	(11,11)	(11,12)	(12,12)
Number of edges	$h'+q'+n'$	q'	$q'+1$	$h'+q'+n'$	$h'^2+n'^2+5$

Theorem 3.2.1. The Sum connectivity Kulli basava index for linear generalized phenylene is defined by

$$\begin{aligned} SKB(G') &= \left(\frac{1}{\sqrt{24}} \right) h'^2 + \left(\frac{1}{\sqrt{17}} + \frac{1}{\sqrt{23}} \right) h' + \left(\frac{1}{\sqrt{12}} + \frac{1}{\sqrt{17}} + \frac{1}{\sqrt{20}} + \frac{1}{\sqrt{22}} + \frac{1}{\sqrt{23}} \right) q' \\ &\quad + \left(\frac{1}{4} \right) q'^2 + \left(\frac{1}{\sqrt{24}} \right) n'^2 + \left(\frac{1}{3} + \frac{1}{\sqrt{15}} + \frac{1}{\sqrt{17}} + \frac{1}{\sqrt{23}} \right) n' + \left(\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{12}} + \frac{1}{\sqrt{22}} + \frac{5}{\sqrt{24}} \right). \end{aligned}$$

Proof: By using definition (2) and **Error! Reference source not found.**, we get

$$\begin{aligned} SKB(G') &= \sum_{uv \in E(G')} \frac{1}{\sqrt{S_e(u) + S_e(v)}} \\ &= 2 \frac{1}{\sqrt{8}} + n' \frac{1}{\sqrt{9}} + n' \frac{1}{\sqrt{15}} + (q'+1) \frac{1}{\sqrt{12}} + q'^2 \frac{1}{\sqrt{16}} + (h'+q'+n') \frac{1}{\sqrt{17}} + q' \frac{1}{\sqrt{20}} + \\ &\quad (q'+1) \frac{1}{\sqrt{22}} + (h'+q'+n') \frac{1}{\sqrt{23}} + (h'^2 + n'^2 + 5) \frac{1}{\sqrt{24}} \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{\sqrt{2}} + \frac{n'}{3} + \frac{n'}{\sqrt{15}} + q' \frac{1}{\sqrt{12}} + \frac{1}{\sqrt{12}} + q'^2 \frac{1}{4} + h' \frac{1}{\sqrt{17}} + q' \frac{1}{\sqrt{17}} + \frac{n'}{\sqrt{17}} + q' \frac{1}{\sqrt{20}} \\
&\quad + q' \frac{1}{\sqrt{22}} + \frac{1}{\sqrt{22}} + h' \frac{1}{\sqrt{23}} + q' \frac{1}{\sqrt{23}} + \frac{n'}{\sqrt{23}} + h'^2 \frac{1}{\sqrt{24}} + n'^2 \frac{1}{\sqrt{24}} + 5 \frac{1}{\sqrt{24}} \\
&= \left(\frac{1}{\sqrt{24}} \right) h'^2 + \left(\frac{1}{4} \right) q'^2 + \left(\frac{1}{\sqrt{24}} \right) n'^2 + \left(\frac{1}{\sqrt{12}} + \frac{1}{\sqrt{17}} + \frac{1}{\sqrt{20}} + \frac{1}{\sqrt{22}} + \frac{1}{\sqrt{23}} \right) q' \\
&\quad + \left(\frac{1}{\sqrt{17}} + \frac{1}{\sqrt{23}} \right) h' + \left(\frac{1}{3} + \frac{1}{\sqrt{15}} + \frac{1}{\sqrt{17}} + \frac{1}{\sqrt{23}} \right) n' + \left(\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{12}} + \frac{1}{\sqrt{22}} + \frac{5}{\sqrt{24}} \right).
\end{aligned}$$

Theorem 3.2.2. The Product connectivity Kulli basava index for linear generalized phenylene is given by

$$\begin{aligned}
PKB(G') &= \left(\frac{1}{12} \right) h'^2 + \left(\frac{1}{\sqrt{60}} \right) q'^2 + \left(\frac{1}{12} \right) n'^2 + \left(\frac{1}{6} + \frac{1}{\sqrt{66}} + \frac{1}{10} + \frac{1}{11} + \frac{1}{\sqrt{132}} \right) q' \\
&\quad + \left(\frac{1}{\sqrt{66}} + \frac{1}{\sqrt{132}} \right) h' + \left(\frac{1}{\sqrt{20}} + \frac{1}{\sqrt{50}} + \frac{1}{\sqrt{66}} + \frac{1}{\sqrt{132}} \right) n' + \left(\frac{1}{2} + \frac{1}{6} + \frac{1}{11} + \frac{5}{12} \right)
\end{aligned}$$

Proof: By using definition (2) and **Error! Reference source not found.**, it follows that

$$\begin{aligned}
PKB(G') &= \sum_{uv \in E(G')} \frac{1}{\sqrt{S_e(u)S_e(v)}} \\
&= 2 \frac{1}{\sqrt{16}} + n' \frac{1}{\sqrt{20}} + n' \frac{1}{\sqrt{50}} + q' \frac{1}{\sqrt{36}} + \frac{1}{\sqrt{36}} + q'^2 \frac{1}{\sqrt{60}} + h' \frac{1}{\sqrt{66}} + q' \frac{1}{\sqrt{66}} \\
&\quad + n' \frac{1}{\sqrt{66}} + q' \frac{1}{\sqrt{100}} + q' \frac{1}{\sqrt{121}} + \frac{1}{\sqrt{121}} + h' \frac{1}{\sqrt{132}} + q' \frac{1}{\sqrt{132}} + n' \frac{1}{\sqrt{132}} \\
&\quad + h'^2 \frac{1}{\sqrt{144}} + n'^2 \frac{1}{\sqrt{144}} + 5 \frac{1}{\sqrt{144}} \\
&= \frac{1}{2} + n' \frac{1}{\sqrt{120}} + n' \frac{1}{\sqrt{50}} + q' \frac{1}{6} + \frac{1}{6} + q'^2 \frac{1}{\sqrt{60}} + h' \frac{1}{\sqrt{66}} + q' \frac{1}{\sqrt{66}} + n' \frac{1}{\sqrt{66}} \\
&\quad + q' \frac{1}{10} + q' \frac{1}{11} + \frac{1}{11} + h' \frac{1}{\sqrt{132}} + q' \frac{1}{\sqrt{132}} + n' \frac{1}{\sqrt{132}} + h'^2 \frac{1}{12} + n' \frac{1}{12} + 5 \frac{1}{12} \\
&= \left(\frac{1}{12} \right) h'^2 + \left(\frac{1}{\sqrt{60}} \right) q'^2 + \left(\frac{1}{12} \right) n'^2 + \left(\frac{1}{6} + \frac{1}{\sqrt{66}} + \frac{1}{10} + \frac{1}{11} + \frac{1}{\sqrt{132}} \right) q' \\
&\quad + \left(\frac{1}{\sqrt{66}} + \frac{1}{\sqrt{132}} \right) h' + \left(\frac{1}{\sqrt{120}} + \frac{1}{\sqrt{50}} + \frac{1}{\sqrt{66}} + \frac{1}{\sqrt{132}} \right) n' + \left(\frac{1}{2} + \frac{1}{6} + \frac{1}{11} + \frac{5}{12} \right).
\end{aligned}$$

Theorem 3.2.3. We define the Atom bond connectivity Kullibasava index for linear generalized phenylene

$$\begin{aligned} ABCK(G') &= \left(\frac{\sqrt{22}}{12} \right) h'^2 + \left(\sqrt{\frac{7}{30}} \right) q'^2 + \left(\frac{\sqrt{10}}{6} + \sqrt{\frac{15}{66}} + \sqrt{\frac{18}{10}} + \sqrt{\frac{20}{11}} + \sqrt{\frac{21}{132}} \right) q' \\ &\quad + \left(\frac{\sqrt{22}}{12} \right) n'^2 + \left(\sqrt{\frac{15}{66}} + \sqrt{\frac{21}{132}} \right) h' + \left(\sqrt{\frac{7}{20}} + \sqrt{\frac{13}{50}} + \sqrt{\frac{15}{66}} + \sqrt{\frac{21}{132}} \right) n' \\ &\quad + \left(\frac{\sqrt{6}}{2} + \frac{\sqrt{10}}{6} + \frac{\sqrt{20}}{11} + \frac{5\sqrt{22}}{12} \right). \end{aligned}$$

Proof: By using definition (2) and **Error! Reference source not found.**, we get

$$\begin{aligned} ABCKB(G') &= \sum_{uv \in E(G')} \sqrt{\frac{S_e(u) + S_e(v) - 2}{S_e(u)S_e(v)}} \\ &= 2\sqrt{\frac{6}{16}} + n'\sqrt{\frac{7}{20}} + n'\sqrt{\frac{13}{50}} + (q'+1)\sqrt{\frac{10}{36}} + q'^2\sqrt{\frac{14}{60}} + (h'+q'+n')\sqrt{\frac{15}{66}} \\ &\quad + q'\sqrt{\frac{18}{100}} + (q'+1)\sqrt{\frac{20}{121}} + (h'+q'+n')\sqrt{\frac{21}{132}} + (h'^2 + n'^2 + 5)\sqrt{\frac{22}{144}} \\ &= \frac{\sqrt{6}}{2} + n'\sqrt{\frac{7}{20}} + n'\sqrt{\frac{13}{50}} + q'\frac{\sqrt{10}}{6} + \frac{\sqrt{10}}{6} + q'^2\sqrt{\frac{7}{30}} + h'\sqrt{\frac{15}{66}} + q'\sqrt{\frac{15}{66}} \\ &\quad + n'\sqrt{\frac{15}{66}} + q'\frac{\sqrt{18}}{10} + q'\frac{\sqrt{20}}{11} + \frac{\sqrt{20}}{11} + h'\sqrt{\frac{21}{132}} + q'\sqrt{\frac{21}{132}} + n'\sqrt{\frac{21}{132}} \\ &\quad + h'^2\frac{\sqrt{22}}{12} + n'^2\frac{\sqrt{22}}{12} + \frac{5\sqrt{22}}{12} \\ &= \left(\frac{\sqrt{22}}{12} \right) h'^2 + \left(\sqrt{\frac{7}{30}} \right) q'^2 + \left(\frac{\sqrt{10}}{6} + \sqrt{\frac{15}{66}} + \sqrt{\frac{18}{10}} + \sqrt{\frac{20}{11}} + \sqrt{\frac{21}{132}} \right) q' \\ &\quad + \left(\frac{\sqrt{22}}{12} \right) n'^2 + \left(\sqrt{\frac{15}{66}} + \sqrt{\frac{21}{132}} \right) h' + \left(\sqrt{\frac{7}{20}} + \sqrt{\frac{13}{50}} + \sqrt{\frac{15}{66}} + \sqrt{\frac{21}{132}} \right) n' \\ &\quad + \left(\frac{\sqrt{6}}{2} + \frac{\sqrt{10}}{6} + \frac{\sqrt{20}}{11} + \frac{5\sqrt{22}}{12} \right). \end{aligned}$$

Theorem 3.2.4. The Geometric arithmetic connectivity Kulli basava index for linear generalized phenylene is given by

$$\begin{aligned} GAKB(G') &= h'^2 + \left(\frac{\sqrt{60}}{8} \right) q'^2 + n'^2 + \left(\frac{2\sqrt{66}}{17} + \frac{2\sqrt{132}}{23} \right) h' + \left(3 + \frac{2\sqrt{66}}{17} + \frac{2\sqrt{132}}{23} \right) q' \\ &\quad + \left(\frac{2\sqrt{20}}{9} + \frac{2\sqrt{50}}{15} + \frac{2\sqrt{66}}{17} + \frac{2\sqrt{132}}{23} \right) n' + 9 \end{aligned}$$

Proof: By using definition (2) and **Error! Reference source not found.**, we get

$$GAKB(G') = \sum_{uv \in E(G')} \frac{2\sqrt{S_e(u)S_e(v)}}{S_e(u) + S_e(v)}$$

$$\begin{aligned}
&= 4 \frac{\sqrt{16}}{8} + n' \frac{2\sqrt{20}}{9} + n' \frac{2\sqrt{50}}{15} + (q'+1) \frac{2\sqrt{36}}{12} + q'^2 \frac{2\sqrt{60}}{16} + (h'+q'+n') \frac{2\sqrt{66}}{17} \\
&\quad + q' \frac{2\sqrt{100}}{20} + (q'+1) \frac{2\sqrt{121}}{22} + (h'+q'+n') \frac{2\sqrt{132}}{23} + (h'^2 + n'^2 + 5) \frac{2\sqrt{144}}{24} \\
&= 2 + n' \frac{2\sqrt{20}}{9} + n' \frac{2\sqrt{50}}{15} + q'+1+q'^2 \frac{\sqrt{60}}{8} + h' \frac{2\sqrt{66}}{17} + q' \frac{2\sqrt{66}}{17} + n' \frac{2\sqrt{66}}{17} \\
&\quad + q'+q'+1+h' \frac{2\sqrt{132}}{23} + q' \frac{2\sqrt{132}}{23} + n' \frac{2\sqrt{132}}{23} + h'^2 + n'^2 + 5 \\
&= h'^2 + \left(\frac{\sqrt{60}}{8} \right) q'^2 + n'^2 + \left(\frac{2\sqrt{66}}{17} + \frac{2\sqrt{132}}{23} \right) h' + \left(3 + \frac{2\sqrt{66}}{17} + \frac{2\sqrt{132}}{23} \right) q' \\
&\quad + \left(\frac{2\sqrt{20}}{9} + \frac{2\sqrt{50}}{15} + \frac{2\sqrt{66}}{17} + \frac{2\sqrt{132}}{23} \right) n' + 9.
\end{aligned}$$

Theorem 3.2.5. The Reciprocal connectivity Kulli basava index for linear generalized phenylene is given by

$$\begin{aligned}
RKB(G') &= (12)h'^2 + (\sqrt{60})q'^2 + (12)n'^2 + (\sqrt{66} + \sqrt{132})h' + (27 + \sqrt{66} + \sqrt{132})q' \\
&\quad + (\sqrt{20} + \sqrt{50} + \sqrt{66} + \sqrt{132})n' + 85.
\end{aligned}$$

Proof: By using section **Error! Reference source not found.** and **Error! Reference source not found.**, we get

$$\begin{aligned}
RKB(G') &= \sum_{uv \in E(G')} \sqrt{S_e(u)S_e(v)} \\
&= 2\sqrt{16} + n'\sqrt{20} + n'\sqrt{50} + (q'+1)\sqrt{36} + q'^2\sqrt{60} + (h'+q'+n')\sqrt{66} + q'\sqrt{100} \\
&\quad + (q'+1)\sqrt{121} + (h'+q'+n')\sqrt{132} + (h'^2 + n'^2 + 5)\sqrt{144} \\
&= 2.4 + n'\sqrt{20} + n'\sqrt{50} + (q'+1)(6) + q'^2\sqrt{60} + (h'+q'+n')\sqrt{66} + q'(10) \\
&\quad + (q'+1)(11) + (h'+q'+n')\sqrt{132} + (h'^2 + n'^2 + 5)(12) \\
&= (12)h'^2 + (\sqrt{60})q'^2 + (12)n'^2 + (\sqrt{66} + \sqrt{132})h' + (27 + \sqrt{66} + \sqrt{132})q' \\
&\quad + (\sqrt{20} + \sqrt{50} + \sqrt{66} + \sqrt{132})n' + 85.
\end{aligned}$$

Conclusion

Graph theory has given researchers several helpful tools, such as topological indices. It investigates quantitative structure-activity (QSAR) and structure-property (QSPR) correlations, which are used to determine chemical compound biological activities and characteristics. In this paper, the Kulli-Basava indices of chemical graphs have been computed. Our results may play a vital role in estimating the melting and boiling points.

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