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ON NEW CONNECTIVITY TOPOLOGICAL INDICES OF CERTAIN MOLECULAR GRAPHS

Muhammad Sharjeel[1], Muhammad Mohsin Abbas[2], Mohammad Reza Farahani[3,*], Mehdi Alaeiyan[4], Murat Cancan[5]

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Abstract

Topological index is a graphic invariant of digital quantity, which can be used by researchers to analyze various physical and chemical aspects of molecules. In this paper, the molecular graph of the benzenoid hydrocarbon structure of benzenoid triangular and benzenoid rhombus are explored. Furthermore, degree-based topological indices including product connectivity Kulli-Basava index, sum connectivity Kulli-Basava index, atom-bond connectivity Kulli-Basava index, geometric arithmetic connectivity Kulli-Basava index, and the reciprocal connectivity Kulli-Basava index are determined.

Mathematics Subject Classification: 05C90, 05C35, 05C12.

Keywords: Degree-based Topological index, benzenoid networks, Sum connectivity index, Product connectivity index, Atom-bond connectivity index, Geometric arithmetic connectivity index, Reciprocal connectivity index.

[1]Department of Mathematics and Statistics, University of Agriculture, Faisalabad, Pakistan. E-mail:mohammadsharjeel3550@gmail.com

[2]Department of Mathematics, Air University Multan Campus, Multan, Pakistan. E-mail:mohsinabas.05@gmail.com

[3] Department of Mathematics, Iran University of Science and Technology, Tehran 16844, Iran. E-mail: mrfarahani88@gmail.com

[4]Department of Mathematics, Iran University of Science and Technology, Tehran 16844, Iran. E-mail: alaeiyan@iust.ac.ir

[5]Faculty of Education, Van Yuzuncu Yıl University, Zeve Campus, Tuşba, 65080, Van, Turkey
E-mail: m_cencen@yahoo.com

* **Corresponding author: Mohammad Reza Farahani,** Department of Mathematics, Iran University of Science and Technology, Tehran 16844, Iran. E-mail: mrfarahani88@gmail.com

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1 Introduction

Graph theory is a field of mathematics that enables demonstration of any structure. It has recently attracted a lot of attention because of its wide variety of applications in computer science, electrical networks, interconnected networks, biological networks, chemistry, and other fields. Chemical graph theory is a field of research that is growing quickly. It facilitates the explanation of a molecular graph's structural characteristics. Several chemical compounds with a wide range of uses in commercial, industrial, medical, and everyday life as well as in the laboratory are applied. Chemical compounds and molecular structures have a correlation. Molecular descriptors enable the modelling and analysis of chemical structure for information. Chemical graph theory is a subfield of mathematical chemistry in which graph theory techniques are used to mathematically represent chemical occurrences. It, therefore, has something to do with graph theory's non-trivial applications in molecular phenomena. This concept has a significant impact on disciplines related to chemical sciences(see [1-3]).

Chem-informatics is a new field that brings together chemistry, mathematics, and information science. It investigates the quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR), both of which are used to evaluate the bioactivity and physicochemical qualities of chemical compounds. Chemical graph theory has obtained a lot of interest and attention of researchers (see [4, 13-15]).

A lot of topological indices based on degree have been proposed and studied, and rich research results have been produced. Jia-Bao Liu studied the degree based topological index of generalized Sierpiński networks and Euler graphs from the pure theory. [17,18]Xiujun Zhang studied the degree based and distance based topological index of interconnection networks.[14]Topological indices of polymers such as bridge molecular diagram are researched in [19,20].Topological indices of Nanosheet, Nanotube are researched in [23,24].Topologcial indices of Benzenoids are researched in [27].Weidong Zhao recently researched Triangular Benzenoids and Starphene Nanotubes Topological Co-Indices.[29] For some recent work on topological indices, interested readers can refer to [22,25,26-37].In this paper, we will focus on the molecular graph of the benzenoid hydrocarbon structure of benzenoid triangular and benzenoid rhombus.

2 Definitions

For a graph G', the Sum connectivity Kulli-Basava index [5], the Product connectivity Kulli-Basava index [6], the Atom bond connectivity Kulli-Basava index [7], the Geometric arithmetic connectivity Kulli-Basava index [9], and the Reciprocal connectivity Kulli-Basava index [11, 12] are defined by

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

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

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

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

and

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

Respectively (see [10]).

The degree of an edge is determined by the formula $d_G(e) = d_G(u) + d_G(v) - 2.$ The neighborhood 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 [10]).

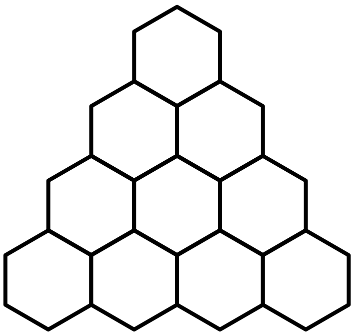

Figure 1. Benzenoid Triangular T_4.

3 Main Results

3.1 Results for Triangular benzenoid

In this section, the graph of a triangular benzenoid is discussed. This graph is denoted by T_q where q is the number of hexagons in the base graph(for example see Figure 1). Hence the total number of hexagons T_q is found by $\frac{1}{2}q(q+1)$. we obtain the result by using the arithmetical method is denoted by the number of vertices and the number of edges is given below:

$$\left|V\left(T_q\left(G'\right)\right)\right| = \mathrm{q}^2+4q+1$$

and

$$\left|E\left(T_q\left(G'\right)\right)\right| = \frac{3}{2}q\left(q+3\right).$$

We calculate the partitions of the edges for their sum of the degrees of all edges incident to vertices of the triangular benzenoid graph (see Table 1). We construct Table 1 by using mathematical procedures.

$S_e\left(u\right)$, $S_e\left(v\right)$ where $e=uv\in \mathrm{E}\left(T_q\left(G'\right)\right)$	Number of edges $(q \geq 2)$
(4,5)	6
(5,10)	$6(q-1)$
(10,12)	$3\left(q-1\right)$
(12,12)	$\frac{3}{2}q^2+\frac{9}{2}q+3$

Table 1. The sum of the degrees of all edges incident to vertices of the triangular benzenoid graph.

Theorem 1. We define the sum connectivity Kulli-Basava index for $T_q\left(G'\right)$ by

$$SKB\left(G'\right)=\sqrt{\frac{3}{32}}q^2+(\sqrt{\frac{12}{5}}+\sqrt{\frac{27}{32}}+\frac{3}{\sqrt{22}})q-\frac{3}{\sqrt{22}}+\sqrt{\frac{3}{8}}-\sqrt{\frac{12}{5}}+2, q\geq 2.$$

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

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

$$=6\left(\frac{1}{\sqrt{4+5}}\right)+6(q-1)\left(\frac{1}{\sqrt{5+10}}\right)+3(q-1)\left(\frac{1}{\sqrt{10+12}}\right)+\left(\frac{3}{2}q^2+\frac{9}{2}q+3\right)\left(\frac{1}{\sqrt{12+12}}\right)$$

$$=\sqrt{\frac{3}{32}}q^2+(\sqrt{\frac{12}{5}}+\sqrt{\frac{27}{32}}+\frac{3}{\sqrt{22}})q-\frac{3}{\sqrt{22}}+\sqrt{\frac{3}{8}}-\sqrt{\frac{12}{5}}+2$$

Theorem 2. The Product connectivity Kulli-Basava index for $T_q\left(G'\right)$ is defined by

$$PKB\left(G'\right)=\frac{1}{8}q^2+(\frac{3}{8}+\sqrt{\frac{3}{40}}+\frac{3\sqrt{2}}{5})q+\frac{3}{\sqrt{5}}-\frac{3\sqrt{2}}{5}-\sqrt{\frac{3}{40}}+\frac{1}{4}, q\geq 2.$$

Proof: By using section 2 and Table 1, we obtain

$$PKB\left(G'\right)=\sum_{uv\in E(G')}\frac{1}{\sqrt{S_e\left(u\right)\mathrm{S}_e\left(v\right)}}$$

$$=6\left(\frac{1}{\sqrt{4\times 5}}\right)+6(q-1)\left(\frac{1}{\sqrt{5\times 10}}\right)+3(q-1)\left(\frac{1}{\sqrt{10\times 12}}\right)+(\frac{3}{2}q^2+\frac{9}{2}q+3)\left(\frac{1}{\sqrt{12\times 12}}\right)$$

$$=\frac{1}{8}q^2+(\frac{3}{8}+\sqrt{\frac{3}{40}}+\frac{3\sqrt{2}}{5})q+\frac{3}{\sqrt{5}}-\frac{3\sqrt{2}}{5}-\sqrt{\frac{3}{40}}+\frac{1}{4}$$

Theorem 3. The Atom bond connectivity Kulli-Basava index for $T_q\left(G'\right)$ is written as

$$ABCKB\left(G'\right)=\sqrt{\frac{11}{32}}q^2+(\sqrt{\frac{3}{2}}+\sqrt{\frac{99}{32}}+\frac{3\sqrt{26}}{5})q-\frac{3\sqrt{26}}{5}+\sqrt{\frac{11}{8}}-\sqrt{\frac{3}{2}}+3\sqrt{\frac{7}{5}}, q\geq 2.$$

Proof: By using section 2 and Table 1, it follows that

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

$$=6\left(\sqrt{\frac{4+5-2}{4\times 5}}\right)+6(q-1)\left(\sqrt{\frac{5+10-2}{5\times 10}}\right)+3(q-1)\left(\sqrt{\frac{10+12-2}{10\times 12}}\right)+\left(\frac{3}{2}q^2+\frac{9}{2}q+3\right)\left(\sqrt{\frac{12+12-2}{12\times 12}}\right)$$

$$=\sqrt{\frac{11}{32}}q^2+(\sqrt{\frac{3}{2}}+\sqrt{\frac{99}{32}}+\frac{3\sqrt{26}}{5})q-\frac{3\sqrt{26}}{5}+\sqrt{\frac{11}{8}}-\sqrt{\frac{3}{2}}+3\sqrt{\frac{7}{5}}$$

Theorem 4. The Geometric arithmetic connectivity Kulli-Basava index for $T_q(G')$ is defined as

$$GAKB(G') = \frac{3}{2}q^2+(\frac{9}{2}+4\sqrt{2}+\frac{6\sqrt{30}}{11})q-\frac{6\sqrt{30}}{11}+\frac{8\sqrt{5}}{3}-4\sqrt{2}+3, q\geq 2.$$

Proof: By using section 2 and Table 1, it follows that

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

$$=6\left(\frac{2\sqrt{4\times5}}{4+5}\right)+6(q-1)\left(\frac{2\sqrt{5\times10}}{5+10}\right)+3(q-1)\left(\frac{2\sqrt{10\times12}}{10+12}\right)+\left(\frac{3}{2}q^2+\frac{9}{2}q+3\right)\left(\frac{2\sqrt{12\times12}}{12+12}\right)$$

$$=\frac{3}{2}q^2+(\frac{9}{2}+4\sqrt{2}+\frac{6\sqrt{30}}{11})q-\frac{6\sqrt{30}}{11}+\frac{8\sqrt{5}}{3}-4\sqrt{2}+3$$

Theorem 5. The Reciprocal connectivity Kulli-Basava index for $T_q(G')$ is given by

$$RKB(G')=18q^2+(54+30\sqrt{2}+6\sqrt{30})q-6\sqrt{30}+12\sqrt{5}-30\sqrt{2}+36, q\geq 2.$$

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

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

$$=6\left(\sqrt{4\times5}\right)+6(q-1)\left(\sqrt{5\times10}\right)+3(q-1)\left(\sqrt{10\times12}\right)+\left(\frac{3}{2}q^2+\frac{9}{2}q+3\right)\left(\sqrt{12\times12}\right)$$

$$=18q^2+(54+30\sqrt{2}+6\sqrt{30})q-6\sqrt{30}+12\sqrt{5}-30\sqrt{2}+36$$

3.2 Results for Rhombus Benzenoid

In this section, the graph of the Rhombus benzenoid $R_{q'}$ is discussed. By calculation, we find that graph of $R_{q'}$ has $3q'(q'^2-2q'-4)$ vertices and $2q'^2+8q'-1$ edges (for example see Figure 1). In this graph, there are three types of edges based on the degree of the end vertices of each edge. Calculate the partitions of the edges to their sum of the degrees of all edges incident to vertices of Rhombus benzenoid graph in Table 2. Construct the Table 2 by using Mathematical procedure.

Theorem 1. The sum connectivity Kulli-Basava index for $R_{q'}(G')$ is given by

$$SKB(G')=\sqrt{\frac{3}{8}}q'^2+(\sqrt{\frac{8}{11}}-\sqrt{\frac{8}{3}}+\frac{8}{\sqrt{15}})q'-\frac{8}{\sqrt{15}}+\frac{5}{2\sqrt{6}}+\sqrt{\frac{2}{5}}-2\sqrt{\frac{2}{11}}+\frac{4}{3}, q'\geq 2.$$

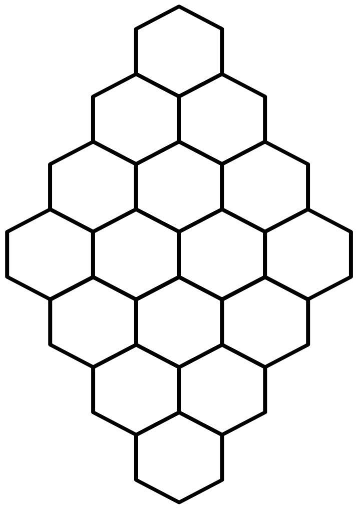

Figure 2. The Rhombus benzenoid R$_4$.

$S_e(u)$, $S_e(v)$ where $e=uv\in E(R_{q'}(G'))$	Number of edges $(q'\geq 2)$
(4,5)	4
(5,5)	2
(5,10)	$8(q'-1)$
(10,12)	$4(q'-1)$
(12,12)	$3q'^2-8q'+5$

Table 2. The sum of the degrees of all edges incident to vertices of Rhombus benzenoid graph.

Proof: By using section 2 and Table 2, we get

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

$$=4\frac{1}{\sqrt{4+5}}+2\frac{1}{\sqrt{5+5}}+8(q'-1)\frac{1}{\sqrt{5+10}}+4(q'-1)\frac{1}{\sqrt{10+12}}+(3q'^2-8q'+5)\frac{1}{\sqrt{12+12}}$$

$$=\sqrt{\frac{3}{8}}q'^2+(\sqrt{\frac{8}{11}}-\sqrt{\frac{8}{3}}+\frac{8}{\sqrt{15}})q'-\frac{8}{\sqrt{15}}+\frac{5}{2\sqrt{6}}+\sqrt{\frac{2}{5}}-2\sqrt{\frac{2}{11}}+\frac{4}{3}$$

Theorem 2. We define the Product connectivity Kulli-Basava index for $E\left(R_{q'}\left(G'\right)\right)$ by

$$PKB(G') = \frac{1}{4}q'^2 + (\frac{4\sqrt{2}}{5} + \sqrt{\frac{2}{15}} - \frac{2}{3})q' + \frac{2}{\sqrt{5}} - \frac{4\sqrt{2}}{5} - \sqrt{\frac{2}{15}} + \frac{49}{60}, q' \geq 2.$$

Proof: By using section 2 and Table 2, it follows that

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

$$= 4\frac{1}{\sqrt{4\times5}} + 2\frac{1}{\sqrt{5\times5}} + 8(q'-1)\frac{1}{\sqrt{5\times10}} + 4(q'-1)\frac{1}{\sqrt{10\times12}} + (3q'^2 - 8q' + 5)\frac{1}{\sqrt{12\times12}}$$

$$= \frac{1}{4}q'^2 + (\frac{4\sqrt{2}}{5} + \sqrt{\frac{2}{15}} - \frac{2}{3})q' + \frac{2}{\sqrt{5}} - \frac{4\sqrt{2}}{5} - \sqrt{\frac{2}{15}} + \frac{49}{60}$$

Theorem 3. The Atom bond connectivity Kulli-Basava index for $E\left(R_{q'}\left(G'\right)\right)$ is given as

$$ABCKB(G') = \sqrt{\frac{11}{8}}q'^2 + \left(\sqrt{\frac{8}{3}} - \frac{2}{3}\sqrt{22} + \frac{4}{5}\sqrt{26}\right)q' + \left(\frac{5}{6}\sqrt{\frac{11}{2}} - \frac{4}{5}\sqrt{26} + \frac{4}{5}\sqrt{2} + \sqrt{\frac{28}{5}} - \sqrt{\frac{8}{3}}\right), q' \geq 2.$$

Proof: By using section 2 and Table 2, we get

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

$$= 4\sqrt{\frac{4+5-2}{4\times5}} + 2\sqrt{\frac{5+5-2}{5\times5}} + 8(q'-1)\sqrt{\frac{5+10-2}{5\times10}} + 4(q'-1)\sqrt{\frac{10+12-2}{10\times12}} + (3q'^2 - 8q' + 5)\sqrt{\frac{12+12-2}{12\times12}}$$

$$= \sqrt{\frac{11}{8}}q'^2 + \left(\sqrt{\frac{8}{3}} - \frac{2}{3}\sqrt{22} + \frac{4}{5}\sqrt{26}\right)q' + \left(\frac{5}{6}\sqrt{\frac{11}{2}} - \frac{4}{5}\sqrt{26} + \frac{4}{5}\sqrt{2} + \sqrt{\frac{28}{5}} - \sqrt{\frac{8}{3}}\right).$$

Theorem 4. We define The Geometric arithmetic connectivity Kulli-Basava index for $E\left(R_{q'}\left(G'\right)\right)$ by

$$GAKB(G') = 3q'^2 + (\frac{16}{3}\sqrt{2} + \frac{8}{11}\sqrt{30} - 8)q' + \frac{16}{9}\sqrt{5} - \frac{8}{11}\sqrt{30} - \frac{16}{3}\sqrt{2} + 7, q' \geq 2.$$

Proof: By using section 2 and Table 2, we get

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

$$= 4\frac{2\sqrt{4\times5}}{4+5} + 2\frac{2\sqrt{5\times5}}{5+5} + 8(q'-1)\frac{2\sqrt{5\times10}}{5+10} + 4(q'-1)\frac{2\sqrt{10\times12}}{10+12} + (3q'^2 - 8q' + 5)\frac{2\sqrt{12\times12}}{12+12}$$

$$= 3q'^2 + (\frac{16}{3}\sqrt{2} + \frac{8}{11}\sqrt{30} - 8)q' + \frac{16}{9}\sqrt{5} - \frac{8}{11}\sqrt{30} - \frac{16}{3}\sqrt{2} + 7$$

Theorem 5. The Reciprocal connectivity Kulli-Basava index for $E\left(R_{q'}\left(G'\right)\right)$ is defined as

$$RKB(G') = 36q'^2 + (40\sqrt{2} + 8\sqrt{30} - 96)q' + 8\sqrt{5} - 8\sqrt{30} - 40\sqrt{2} + 70, q' \geq 2.$$

Proof: By using section 2 and Table 2, we get

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

$$= 4\sqrt{4\times5} + 2\sqrt{5\times5} + 8(q'-1)\sqrt{5\times10} + 4(q'-1)\sqrt{10\times12} + (3q'^2 - 8q' + 5)\sqrt{12\times12}$$

$$= 36q'^2 + (40\sqrt{2} + 8\sqrt{30} - 96)q' + 8\sqrt{5} - 8\sqrt{30} - 40\sqrt{2} + 70$$

Conclusion

Chemical graph theory is useful in modeling and developing chemical structures. In this work, Kulli-Basava indices of molecular graphs have been analyzed and the topological index has been computed for two types of benzenoid graphs. One may try to correlate these results with chemical compounds which have some structures such as triangular benzenoid graph and rhombus benzenoid graph to obtain useful results after conducting the experiments.

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