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Leap Kepler Banhatti Indices of Some Chemical Drugs

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Abstract

In this paper, we introduce the leap Kepler Banhatti and modified leap Kepler Banhatti indices and their corresponding exponentials of a graph. Furthermore, we compute these newly defined leap Kepler Banhatti indices and their corresponding exponentials for certain important molecular structures such as chloroquine, hydroxychloroquine and remdesivir.

Keywords: leap Kepler Banhatti index; modified leap Kepler Banhatti index; molecular structure.
2020 Mathematics Subject Classification: 05C07, 05C09, 05C92.

1. Introduction

A graph index is a numerical parameter mathematically derived from the graph structure. In Chemical Graph Theory, concerning the definition of the graph index on the molecular graph and concerning chemical properties of drugs can be studied by the graph index calculation. Several graph indices have been considered in Theoretical Chemistry and many graph indices were defined by using vertex degree concept [1]. The Zagreb, Revan, Gourava, delta, Nirmala, Sombor indices are the most degree based graph indices in Chemical Graph Theory, see [2–40]. Graph indices have their applications in various disciplines in Science and Technology [41, 42]. Let G be a finite, simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex u is the number of edges incident to u. The number of edges in a shortest path connecting any two vertices u and v of G is the distance between these two vertices u and v, and denoted by $d(u,v)$. For a positive integer k and $v \in V(G)$, the open neighborhood of v in G is defined as $N_k(v/G) = \{u \in V(G) : d(u,v) = k\}$. The k-distance degree of v in G is the number of k neighbors of v in G and denoted by $d_k(v)$, see [43]. Any undefined terminologies and notations may be found in [44]. The Kepler Banhatti index [45] of a graph G is defined as

$$KB\,(G) = \sum_{uv \in E(G)} \left[(d_G(u) + d_G(v)) + \sqrt{d_G(u)^2 + d_G(v)^2} \right]$$

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Recently, some Kepler Banhatti indices were studied in [46-49]. The leap Kepler Banhatti index of a graph G is defined as

$$LKB(G) = \sum_{uv \in E(G)} \left((d_2(u) + d_2(v)) + \sqrt{d_2(u)^2 + d_2(v)^2} \right)$$

Considering the leap Kepler Banhatti index, we introduce the leap Kepler Banhatti exponential of a graph G and defined it as

$$LKB(G,x) = \sum_{uv \in E(G)} x^{(d_2(u)+d_2(v))+\sqrt{d_2(u)^2+d_2(v)^2}}$$

We define the modified leap Kepler Banhatti index of a graph G as

$${}^{m}LKB(G) = \sum_{uv \in E(G)} \frac{1}{(d_2(u) + d_2(v)) + \sqrt{d_2(u)^2 + d_2(v)^2}}$$

Considering the modified leap Kepler Banhatti index, we introduce the modified leap Kepler Banhatti exponential of a graph G and defined it as

$${}^{m}LKB(G,x) = \sum_{uv \in E(G)} x^{\frac{1}{(d_2(u)+d_2(v))+\sqrt{d_2(u)^2+d_2(v)^2}}}$$

Recently, some leap indices were studied in [50-54]. In this work, we determine the leap Kepler Banhatti and modified leap Kepler Banhatti indices and their exponentials for chloroquine, hydroxychloroquine and remdesivir.

2. Results for Chloroquine

Chloroquine is an antiviral compound (drug) which was discovered in 1934 by H. Andersag. This drug is medication primarily used to prevent and treat malaria. Let G_1 be the chemical structure of chloroquine. This structure has 21 atoms (vertices) and 23 bonds (edges), see Figure 1.

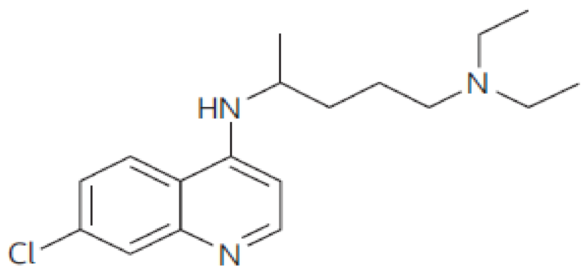

Figure 1: Chemical structure of chloroquine

From Figure 1, we obtain that $\{(d_2(u), d_2(v) \backslash uv \in E(G_1)\}$ has 9 edge set partitions.

$d_2(u), d_2(v)\backslash uv \in E(G_1)$	(1, 2)	(2, 2)	(2, 3)	(2, 4)	(3, 3)	(3, 4)	(3, 5)	(4, 4)	(4, 5)
Number of edges	2	2	8	1	2	3	1	2	2

Table 1: Edge set partitions of chloroquine

We determine the leap Kepler Banhatti index of chloroquine as follows.

Theorem 2.1. *Let G_1 be the chemical structure of chloroquine. Then*

$$LKB\,(G_1) = 150 + 18\sqrt{2} + 4\sqrt{5} + 8\sqrt{13} + \sqrt{34} + 2\sqrt{41}.$$

Proof. By using the definition and edge partition of G_1, we deduce

$$\begin{aligned} LKB\,(G_1) &= \sum_{uv\in E(G_1)} \left((d_2\,(u) + d_2\,(v)) + \sqrt{d_2\,(u)^2 + d_2\,(v)^2} \right) \\ &= \left((1+2) + \sqrt{1^2+2^2}\right)2 + \left((2+2) + \sqrt{2^2+2^2}\right)2 + \left((2+3) + \sqrt{2^2+3^2}\right)8 \\ &+ \left((2+4) + \sqrt{2^2+4^2}\right)1 + \left((3+3) + \sqrt{3^2+3^2}\right)2 + \left((3+4) + \sqrt{3^2+4^2}\right)3 \\ &+ \left((3+5) + \sqrt{3^2+5^2}\right)1 + \left((4+4) + \sqrt{4^2+4^2}\right)2 + \left((4+5) + \sqrt{4^2+5^2}\right)2 \end{aligned}$$

By simplifying the above equation, we get the desired result. □

We calculate the leap Kepler Banhatti exponential of chloroquine as follows.

Theorem 2.2. *Let G_1 be the chemical structure of chloroquine. Then*

$$LBK\,(G_1, x) = 2x^{3+\sqrt{5}} + 2x^{4+2\sqrt{2}} + 8x^{5+\sqrt{13}} + 1x^{6+2\sqrt{5}} + 2x^{6+3\sqrt{2}} + 3x^{7+5} + 1x^{8+\sqrt{34}} + 2x^{8+4\sqrt{2}} + 2x^{9+\sqrt{41}}$$

Proof. By using the definition and edge partition of G_1, we deduce

$$\begin{aligned} LKB\,(G_1, x) &= \sum_{uv\in E(G_1)} x^{(d_2(u)+d_2(v))+\sqrt{d_2(u)^2+d_2(v)^2}} \\ &= 2x^{(1+2)+\sqrt{1^2+2^2}} + 2x^{(2+2)+\sqrt{2^2+2^2}} + 8x^{(2+3)+\sqrt{2^2+3^2}} + 1x^{(2+4)+\sqrt{2^2+4^2}} + 2x^{(3+3)+\sqrt{3^2+3^2}} \\ &+ 3x^{(3+4)+\sqrt{3^2+4^2}} + 1x^{(3+5)+\sqrt{3^2+5^2}} + 2x^{(4+4)+\sqrt{4^2+4^2}} + 2x^{(4+5)+\sqrt{4^2+5^2}}. \end{aligned}$$

By simplifying the above equation, we obtain the desired result. □

We find the modified leap Kepler Banhatti index of chloroquine as follows.

Theorem 2.3. *Let G_1 be the chemical structure of chloroquine. Then*

$${}^{m}LKB\,(G_1) = \frac{2}{3+\sqrt{5}} + \frac{1}{2+\sqrt{2}} + \frac{8}{5+\sqrt{13}} + \frac{1}{6+2\sqrt{5}} + \frac{2}{6+3\sqrt{2}} + \frac{1}{4} + \frac{1}{8+\sqrt{34}} + \frac{1}{4+2\sqrt{2}} + \frac{2}{9+\sqrt{41}}$$

Proof. By using the definition and edge partition of G_1, we deduce

$$\begin{aligned}
{}^{m}LKB\left(G_1\right) &= \sum_{uv\in E(G_1)} \frac{1}{\left(d_2\left(u\right)+d_2\left(v\right)\right)+\sqrt{d_2\left(u\right)^2+d_2\left(v\right)^2}} \\
&= \frac{2}{(1+2)+\sqrt{1^2+2^2}}+\frac{2}{(2+2)+\sqrt{2^2+2^2}}+\frac{8}{(2+3)+\sqrt{2^2+3^2}}+\frac{1}{(2+4)+\sqrt{2^2+4^2}} \\
&+\frac{2}{(3+3)+\sqrt{3^2+3^2}}+\frac{3}{(3+4)+\sqrt{3^2+4^2}}+\frac{1}{(3+5)+\sqrt{3^2+5^2}}+\frac{2}{(4+4)+\sqrt{4^2+4^2}} \\
&+\frac{2}{(4+5)+\sqrt{4^2+5^2}}
\end{aligned}$$

By simplifying the above equation, we get the desired result. □

We compute the modified leap Kepler Banhatti exponential of chloroquine as follows.

Theorem 2.4. *Let G_1 be the chemical structure of chloroquine. Then*

$${}^{m}LBK\left(G_1,x\right)=2x^{3+\sqrt{5}}+2x^{4+2\sqrt{2}}+8x^{5+\sqrt{13}}+1x^{6+2\sqrt{5}}+2x^{6+3\sqrt{2}}+3x^{12}+1x^{8+\sqrt{34}}+2x^{8+4\sqrt{2}}+2x^{9+\sqrt{41}}$$

Proof. By using the definition and edge partition of G_1, we deduce

$$\begin{aligned}
{}^{m}LKB\left(G_1,x\right) &= \sum_{uv\in E(G_1)} x^{\frac{1}{\left(d_2(u)+d_2(v)\right)+\sqrt{d_2(u)^2+d_2(v)^2}}} \\
&= 2x^{\frac{1}{(1+2)+\sqrt{1^2+2^2}}}+2x^{\frac{1}{(2+2)+\sqrt{2^2+2^2}}}+8x^{\frac{1}{(2+3)+\sqrt{2^2+3^2}}}+1x^{\frac{1}{(2+4)+\sqrt{2^2+4^2}}}+2x^{\frac{1}{(3+3)+\sqrt{3^2+3^2}}} \\
&+3x^{\frac{1}{(3+4)+\sqrt{3^2+4^2}}}+1x^{\frac{1}{(3+5)+\sqrt{3^2+5^2}}}+2x^{\frac{1}{(4+4)+\sqrt{4^2+4^2}}}+2x^{\frac{1}{(4+5)+\sqrt{4^2+5^2}}}.
\end{aligned}$$

By simplifying the above equation, we obtain the desired result. □

3. Results for Hydrochloroquine

Let G_2 be the chemical structure of hydroxychloroquine. This structure has 22 atoms (vertices) and 24 bonds (edges), see Figure 2.

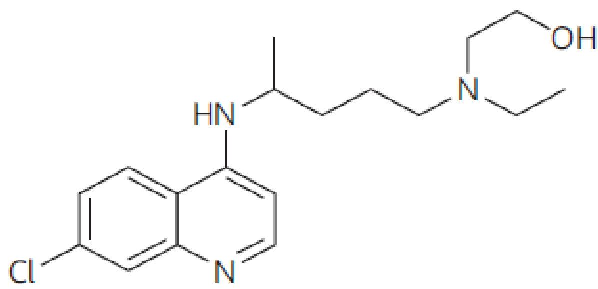

Figure 2: Chemical structure of hydroxychloroquine

From Figure 2, we obtain that $\{(d_2(u), d_2(v)\backslash uv \in E(G_2)\}$ has 11 edge set partitions.

$d_2(u), d_2(v) \backslash uv \in E(G_2)$	(1, 1)	(1, 2)	(1, 3)	(2, 2)	(2, 3)	(2, 4)
Number of edges	1	1	1	2	8	1
$d_2(u), d_2(v) \backslash uv \in E(G_2)$	(3, 3)	(3, 4)	(3, 5)	(4, 4)	(4, 5)	
Number of edges	2	3	1	2	2	

Table 2: Edge set partitions of hydroxychloroquine

We calculate the leap Kepler Banhatti index of hydroxychloroquine as follows.

Theorem 3.1. *Let G_2 be the chemical structure of hydroxychloroquine. Then*

$$LKB\,(G_2) = 153 + 19\sqrt{2} + 3\sqrt{5} + \sqrt{10} + 8\sqrt{13} + \sqrt{34} + 2\sqrt{41}$$

Proof. By using the definition and edge partition of G_2, we deduce

$$\begin{aligned} LKB\,(G_2) &= \sum_{uv \in E(G_2)} \left((d_2\,(u) + d_2\,(v)) + \sqrt{d_2\,(u)^2 + d_2\,(v)^2} \right) \\ &= \left((1+1) + \sqrt{1^2+1^2} \right) 1 + \left((1+2) + \sqrt{1^2+2^2} \right) 1 + \left((1+3) + \sqrt{1^2+3^2} \right) 1 \\ &+ \left((2+2) + \sqrt{2^2+2^2} \right) 2 + \left((2+3) + \sqrt{2^2+3^2} \right) 8 + \left((2+4) + \sqrt{2^2+4^2} \right) 1 \\ &+ \left((3+3) + \sqrt{3^2+3^2} \right) 2 + \left((3+4) + \sqrt{3^2+4^2} \right) 3 + \left((3+5) + \sqrt{3^2+5^2} \right) 1 \\ &+ \left((4+4) + \sqrt{4^2+4^2} \right) 2 + \left((4+5) + \sqrt{4^2+5^2} \right) 2 \end{aligned}$$

By simplifying the above equation, we get the desired result. □

We find the leap Kepler Banhatti exponential of hydroxychloroquine as follows.

Theorem 3.2. *Let G_2 be the chemical structure of hydroxychloroquine. Then*

$$\begin{aligned} LBK\,(G_2, x) &= 1x^{2+\sqrt{2}} + 1x^{3+\sqrt{5}} + 1x^{4+\sqrt{10}} + 2x^{4+2\sqrt{2}} + 8x^{5+\sqrt{13}} + 1x^{6+2\sqrt{5}} \\ &+ 2x^{6+3\sqrt{2}} + 3x^{7+5} + 1x^{8+\sqrt{34}} + 2x^{8+4\sqrt{2}} + 2x^{9+\sqrt{41}} \end{aligned}$$

Proof. By using the definition and edge partition of G_1, we deduce

$$\begin{aligned} LKB\,(G_2, x) &= \sum_{uv \in E(G_2)} x^{(d_2(u)+d_2(v))+\sqrt{d_2(u)^2+d_2(v)^2}} \\ &= 1x^{(1+1)+\sqrt{1^2+1^2}} + 1x^{(1+2)+\sqrt{1^2+2^2}} + 1x^{(1+3)+\sqrt{1^2+3^2}} + 2x^{(2+2)+\sqrt{2^2+2^2}} + 8x^{(2+3)+\sqrt{2^2+3^2}} \\ &+ 1x^{(2+4)+\sqrt{2^2+4^2}} + 2x^{(3+3)+\sqrt{3^2+3^2}} + 3x^{(3+4)+\sqrt{3^2+4^2}} + 1x^{(3+5)+\sqrt{3^2+5^2}} + 2x^{(4+4)+\sqrt{4^2+4^2}} \\ &+ 2x^{(4+5)+\sqrt{4^2+5^2}} \end{aligned}$$

By simplifying the above equation, we obtain the desired result. □

We compute the modified leap Kepler Banhatti index of hydroxychloroquine as follows.

Theorem 3.3. *Let G_2 be the chemical structure of hydroxychloroquine. Then*

$$
\begin{aligned}
{}^{m}LKB\left(G_2\right) = {} & \frac{1}{2+\sqrt{2}} + \frac{1}{3+\sqrt{5}} + \frac{1}{4+\sqrt{10}} + \frac{1}{2+\sqrt{2}} + \frac{8}{5+\sqrt{13}} + \frac{1}{6+2\sqrt{5}} + \frac{2}{6+3\sqrt{2}} \\
& + \frac{1}{4} + \frac{1}{8+\sqrt{34}} + \frac{1}{4+2\sqrt{2}} + \frac{2}{9+\sqrt{41}}
\end{aligned}
$$

Proof. By using the definition and edge partition of G_2, we deduce

$$
\begin{aligned}
{}^{m}LKB\left(G_2\right) &= \sum_{uv\in E(G_2)} \frac{1}{\left(d_2\left(u\right)+d_2\left(v\right)\right)+\sqrt{d_2\left(u\right)^2+d_2\left(v\right)^2}} \\
&= \frac{1}{(1+1)+\sqrt{1^2+1^2}} + \frac{1}{(1+2)+\sqrt{1^2+2^2}} + \frac{1}{(1+3)+\sqrt{1^2+3^2}} + \frac{2}{(2+2)+\sqrt{2^2+2^2}} \\
&+ \frac{8}{(2+3)+\sqrt{2^2+3^2}} + \frac{1}{(2+4)+\sqrt{2^2+4^2}} + \frac{2}{(3+3)+\sqrt{3^2+3^2}} + \frac{3}{(3+4)+\sqrt{3^2+4^2}} \\
&+ \frac{1}{(3+5)+\sqrt{3^2+5^2}} + \frac{2}{(4+4)+\sqrt{4^2+4^2}} + \frac{2}{(4+5)+\sqrt{4^2+5^2}}
\end{aligned}
$$

By simplifying the above equation, we get the desired result. □

We determine the modified leap Kepler Banhatti exponential of hydroxychloroquine as follows.

Theorem 3.4. *Let G_2 be the chemical structure of hydroxychloroquine. Then*

$$
\begin{aligned}
{}^{m}LBK\left(G_2,x\right) = {} & 1x^{2+\sqrt{2}} + 1x^{3+\sqrt{5}} + 1x^{4+\sqrt{10}} + 2x^{4+2\sqrt{2}} + 8x^{5+\sqrt{13}} + 1x^{6+2\sqrt{5}} \\
& + 2x^{6+3\sqrt{2}} + 3x^{12} + 1x^{8+\sqrt{34}} + 2x^{8+4\sqrt{2}} + 2x^{9+\sqrt{41}}.
\end{aligned}
$$

Proof. By using the definition and edge partition of G_1, we deduce

$$
\begin{aligned}
{}^{m}LKB\left(G_2,x\right) &= \sum_{uv\in E(G_2)} x^{\frac{1}{\left(d_2(u)+d_2(v)\right)+\sqrt{d_2(u)^2+d_2(v)^2}}} \\
&= 1x^{\frac{1}{(1+1)+\sqrt{1^2+1^2}}} + 1x^{\frac{1}{(1+2)+\sqrt{1^2+2^2}}} + 1x^{\frac{1}{(1+3)+\sqrt{1^2+3^2}}} + 2x^{\frac{1}{(2+2)+\sqrt{2^2+2^2}}} + 8x^{\frac{1}{(2+3)+\sqrt{2^2+3^2}}} + 1x^{\frac{1}{(2+4)+\sqrt{2^2+4^2}}} \\
&+ 2x^{\frac{1}{(3+3)+\sqrt{3^2+3^2}}} + 3x^{\frac{1}{(3+4)+\sqrt{3^2+4^2}}} + 1x^{\frac{1}{(3+5)+\sqrt{3^2+5^2}}} + 2x^{\frac{1}{(4+4)+\sqrt{4^2+4^2}}} + 2x^{\frac{1}{(4+5)+\sqrt{4^2+5^2}}}.
\end{aligned}
$$

By simplifying the above equation, we obtain the desired result. □

4. Results for Remdesivir

Let G_3 be the molecular structure of remdesivir. This graph has 41 atoms (vertices) and 44 bonds (edges).

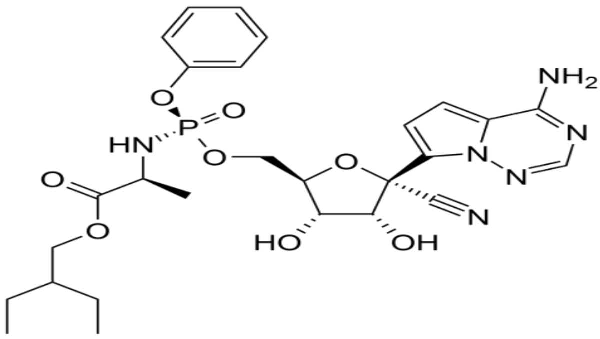

Figure 3: Chemical structure of remdesivir

From Figure 3, we obtain that $\{(d_2(u), d_2(v)\backslash uv \in E(G_3)\}$ has 13 edge set partitions.

$d_2(u), d_2(v)\backslash uv \in E(G_3)$	(1, 2)	(2, 2)	(2, 3)	(2, 4)	(2, 5)	(3, 3)	(3, 4)
Number of edges	2	3	10	1	1	7	3
$d_2(u), d_2(v)\backslash uv \in E(G_3)$	(3, 5)	(3, 6)	(4, 4)	(4, 5)	(5, 5)	(5, 6)	
Number of edges	8	1	1	2	3	2	

Table 3: Edge set partitions of remdesivir

We compute the leap Kepler Banhatti index of remdesivir as follows.

Theorem 4.1. *Let G_2 be the chemical structure of remdesivir. Then*

$$LKB\left(G_3\right) = 394 + 46\sqrt{2} + 7\sqrt{5} + 10\sqrt{13} + \sqrt{29} + 8\sqrt{34} + 2\sqrt{41} + 2\sqrt{61}.$$

Proof. By using the definition and edge partition of G_2, we deduce

$$\begin{aligned}
LKB\left(G_3\right) &= \sum_{uv\in E(G_3)} \left(\left(d_2\left(u\right) + d_2\left(v\right)\right) + \sqrt{d_2\left(u\right)^2 + d_2\left(v\right)^2} \right) \\
&= \left((1+2) + \sqrt{1^2+2^2}\right) 2 + \left((2+2) + \sqrt{2^2+2^2}\right) 3 + \left((2+3) + \sqrt{2^2+3^2}\right) 10 \\
&+ \left((2+4) + \sqrt{2^2+4^2}\right) 1 + \left((2+5) + \sqrt{2^2+5^2}\right) 1 + \left((3+3) + \sqrt{3^2+3^2}\right) 7 \\
&+ \left((3+4) + \sqrt{3^2+4^2}\right) 3 + \left((3+5) + \sqrt{3^2+5^2}\right) 8 + \left((3+6) + \sqrt{3^2+6^2}\right) 1 \\
&+ \left((4+4) + \sqrt{4^2+4^2}\right) 1 + \left((4+5) + \sqrt{4^2+5^2}\right) 2 + \left((5+5) + \sqrt{5^2+5^2}\right) 3 \\
&+ \left((5+6) + \sqrt{5^2+6^2}\right) 2
\end{aligned}$$

By simplifying the above equation, we get the desired result. □

We determine the leap Kepler Banhatti exponential of remdesivir as follows.

Theorem 4.2. *Let G_3 be the chemical structure of remdesivir. Then*

$$\begin{aligned}
LBK\left(G_3, x\right) = 2x^{3+\sqrt{5}} + 3x^{4+2\sqrt{2}} + 10x^{5+\sqrt{13}} + 1x^{6+2\sqrt{5}} + 1x^{7+\sqrt{29}} + 7x^{6+3\sqrt{2}} + 3x^{12} \\
+ 8x^{8+\sqrt{34}} + 1x^{9+3\sqrt{5}} + 1x^{8+4\sqrt{2}} + 2x^{9+\sqrt{41}} + 3x^{10+5\sqrt{2}} + 2x^{11+\sqrt{61}}
\end{aligned}$$

Proof. By using the definition and edge partition of G_3, we deduce

$$\begin{aligned}
LKB\left(G_3, x\right) &= \sum_{uv \in E(G_3)} x^{(d_2(u)+d_2(v))+\sqrt{d_2(u)^2+d_2(v)^2}} \\
&= 2x^{(1+2)+\sqrt{1^2+2^2}} + 3x^{(2+2)+\sqrt{2^2+2^2}} + 10x^{(2+3)+\sqrt{2^2+3^2}} + 1x^{(2+4)+\sqrt{2^2+4^2}} + 1x^{(2+5)+\sqrt{2^2+5^2}} \\
&+ 7x^{(3+3)+\sqrt{3^2+3^2}} + 3x^{(3+4)+\sqrt{3^2+4^2}} + 8x^{(3+5)+\sqrt{3^2+5^2}} + 1x^{(3+6)+\sqrt{3^2+6^2}} + 1x^{(4+4)+\sqrt{4^2+4^2}} \\
&+ 2x^{(4+5)+\sqrt{4^2+5^2}} + 3x^{(5+5)+\sqrt{5^2+5^2}} + 2x^{(5+6)+\sqrt{5^2+6^2}}
\end{aligned}$$

By simplifying the above equation, we obtain the desired result. □

We calculate the modified leap Kepler Banhatti index of remdesivir as follows.

Theorem 4.3. *Let G_3 be the chemical structure of remdesivir. Then*

$$\begin{aligned}
{}^{m}LKB\left(G_3\right) = \frac{2}{3+\sqrt{5}} + \frac{3}{4+2\sqrt{2}} + \frac{10}{5+\sqrt{13}} + \frac{1}{6+2\sqrt{5}} + \frac{1}{7+\sqrt{29}} + \frac{7}{6+3\sqrt{2}} \\
+ \frac{1}{4} + \frac{8}{8+\sqrt{34}} + \frac{1}{9+3\sqrt{5}} + \frac{1}{8+4\sqrt{2}} + \frac{2}{9+\sqrt{41}} + \frac{3}{10+5\sqrt{2}} + \frac{2}{11+\sqrt{61}}.
\end{aligned}$$

Proof. By using the definition and edge partition of G_3, we deduce

$$\begin{aligned}
{}^{m}LKB\left(G_3\right) &= \sum_{uv \in E(G_3)} \frac{1}{\left(d_2\left(u\right)+d_2\left(v\right)\right)+\sqrt{d_2\left(u\right)^2+d_2\left(v\right)^2}} \\
&= \frac{2}{(1+2)+\sqrt{1^2+2^2}} + \frac{3}{(2+2)+\sqrt{2^2+2^2}} + \frac{10}{(2+3)+\sqrt{2^2+3^2}} + \frac{1}{(2+4)+\sqrt{2^2+4^2}} \\
&+ \frac{1}{(2+5)+\sqrt{2^2+5^2}} + \frac{7}{(3+3)+\sqrt{3^2+3^2}} + \frac{3}{(3+4)+\sqrt{3^2+4^2}} + \frac{8}{(3+5)+\sqrt{3^2+5^2}} \\
&+ \frac{1}{(3+6)+\sqrt{3^2+6^2}} + \frac{1}{(4+4)+\sqrt{4^2+4^2}} + \frac{2}{(4+5)+\sqrt{4^2+5^2}} + \frac{3}{(5+5)+\sqrt{5^2+5^2}} \\
&+ \frac{2}{(5+6)+\sqrt{5^2+6^2}}
\end{aligned}$$

By simplifying the above equation, we get the desired result. □

We obtain the modified leap Kepler Banhatti exponential of remdesivir as follows.

Theorem 4.4. *Let G_3 be the chemical structure of remdesivir. Then*

$$\begin{aligned}
{}^{m}LBK\left(G_3, x\right) = 2x^{\frac{1}{3+\sqrt{5}}} + 3x^{\frac{1}{4+2\sqrt{2}}} + 10x^{\frac{1}{5+\sqrt{13}}} + 1x^{\frac{1}{6+2\sqrt{5}}} + 1x^{\frac{1}{7+\sqrt{29}}} + 7x^{\frac{1}{6+3\sqrt{2}}} + 3x^{12} \\
+ 8x^{\frac{1}{8+\sqrt{34}}} + 1x^{\frac{1}{9+3\sqrt{5}}} + 1x^{\frac{1}{8+4\sqrt{2}}} + 2x^{\frac{1}{9+\sqrt{41}}} + 3x^{\frac{1}{10+5\sqrt{2}}} + 2x^{\frac{1}{11+\sqrt{61}}}.
\end{aligned}$$

Proof. By using the definition and edge partition of G_3, we deduce

$$ {}^{m}LKB\left(G_3, x\right) = \sum_{uv \in E(G_3)} x^{\frac{1}{(d_2(u)+d_2(v))+\sqrt{d_2(u)^2+d_2(v)^2}}} $$

$$= 2x^{\frac{1}{(1+2)+\sqrt{1^2+2^2}}} + 3x^{\frac{1}{(2+2)+\sqrt{2^2+2^2}}} + 10x^{\frac{1}{(2+3)+\sqrt{2^2+3^2}}} + 1x^{\frac{1}{(2+4)+\sqrt{2^2+4^2}}} + 1x^{\frac{1}{(2+5)+\sqrt{2^2+5^2}}}$$
$$+ 7x^{\frac{1}{(3+3)+\sqrt{3^2+3^2}}} + 3x^{\frac{1}{(3+4)+\sqrt{3^2+4^2}}} + 8x^{\frac{1}{(3+5)+\sqrt{3^2+5^2}}} + 1x^{\frac{1}{(3+6)+\sqrt{3^2+6^2}}} + 1x^{\frac{1}{(4+4)+\sqrt{4^2+4^2}}}$$
$$+ 2x^{\frac{1}{(4+5)+\sqrt{4^2+5^2}}} + 3x^{\frac{1}{(5+5)+\sqrt{5^2+5^2}}} + 2x^{\frac{1}{(5+6)+\sqrt{5^2+6^2}}}.$$

By simplifying the above equation, we obtain the desired result. □

5. Conclusion

In this study, we have introduced the leap Kepler Banhatti and modified leap Kepler Banhatti indices and their exponentials of a graph. We have computed these newly defined leap Kepler Banhatti indices and their exponentials for chloroquine, hydroxychloroquine and remdesivir.

References

[1] V. R. Kulli, *Graph indices*, Hand Book of Research on Advanced Applications of Application Graph Theory in Modern Society, M. Pal. S. Samanta and A. Pal, (eds) IGI Global, USA, (2019), 66-91.

[2] I. Gutman and N. Trinajstic, *Graph Theory and Molecular Orbitals. Total phi-electron energy of alternant hydrocarbons*, Chemical Physics Letters, 17(4)(1972), 535-538.

[3] I. Gutman, V. R. Kulli, B. Chaluvaraju and H. S. Boregowda, *On Banhatti and Zagreb indices*, Journal of the International Mathematical Virtual Institute, 7(2017), 53-67.

[4] A. Q. Baig, M. Naeem and W. Gao, *Revan and Hyper-Revan indices of octahedral and icosahedral networks*, Applied Mathematics and Nonlinear Sciences, 3(1)(2018), 33-40.

[5] R. Aguilar-Sanchez, I. F. Herrera-Gonzalez, J. A. Mendez-Bermudez and J. M. Sigaareta, *Revan degree indices on random graphs*, arXiv: 2210.04749v1 [math. CO] 10 Oct, (2022).

[6] M. Kamran, N. Salamat, R. H. Khan, M. A. Ullah, M. S. Hameed and M. K. Pandit, *Computation of Revan topological indices for phenol-formaldehyde resin*, Journal of Mathematics, 2022(2022), 10 pages.

[7] V. R. Kulli, *Elliptic Revan Sombor index and its exponential of certain networks*, International Journal of Mathematics and Computer Research, 12(2)(2024), 4055-4061.

[8] V. R. Kulli, *Modified elliptic Revan index of two families of nanotubes*, Annals of Pure and Applied Mathematics, 29(2)(2024), 103-107.

[9] V. R. Kulli, *Revan Kepler Banhatti and modified Revan Kepler Banhatti indices of certain nanotubes*, Annals of Pure and Applied Mathematics, 30(2)(2024), 129-136.

[10] B. K. Majhi, V. R. Kulli and I. N. Cangul, *Revan indices and their polynomials of square snake graphs*, Montes Taurus J. Pure Appl. Math., 6(1)(2024), 12-17.

[11] D. Narasmhan, R. Vignesh and K. Desikan, *Results on Revan and hyper Revan indices of some HEX derived networks*, Fuzzy Mathematical Analysis and Advances in Computational Mathematics, 2022(2022), 209-220.

[12] G. N. Adithya, N. D. Soner and M. Kirankumar, *Gourava indices for Jahangir graph and phase transfer catalyst*, Journal of Emerging Technologies and Innovative Research, 10(6)(2023), f394-f399.

[13] M. Aruvi, J. M. Joseph and E. Ramganesh, *The second Gourava index of some graph products*, Advances in Mathematics: Scientific Journal, 9(12)(2020), 10241-10249.

[14] V. R. Kulli, *Gourava domination indices of graphs*, International Journal of Mathematics and Computer Research, 11(8)(2023), 3680-3684.

[15] V. R. Kulli, *On hyper Gourava domination indices*, International Journal of Engineering Sciences & Research Technology, 12(10)(2023), 12-20.

[16] I. Gutman and V. R. Kulli, *Estimating the Gourava Sombor index*, Ser. A: Appl. Math. Inform. And Mech., 16(1)(2024), 47-52.

[17] V. R. Kulli, *On alpha and gamma Gourava indices*, International Journal of Mathematics and Computer Research, 12(4)(2024), 4139-4144.

[18] V. R. Kulli, *Nirmala alpha Gourava and modified Nirmala alpha Gourava indices of certain dendrimers*, International Journal of Mathematics and Computer Research, 12(5)(2024), 4256-4263.

[19] V. R. Kulli, *On delta Nirmala and multiplicative delta Nirmala indices of certain nanotubes*, Annals of Pure and Applied Mathematics, 28(2)(2023), 49-53.

[20] V. R. Kulli, *Delta atom bond connectivity indices of certain networks*, International Journal of Mathematics and its Applications, 11(4)(2023), 89-98.

[21] V. R. Kulli, *On delta harmonic and multiplicative delta harmonic indices of some nanostructures*, International Journal of Mathematics and Statistics Invention, 11(5)(2023), 38-45.

[22] B. K. Majhi, V. R. Kulli and I. N. Cangul, *Sum connectivity delta Banhatti and product connectivity delta Banhatti indices of certain nanotubes*, Montes Taurus J.Pure Appl. Math., 5(2)(2023), 89-97.

[23] V. R. Kulli, *Delta geometric-arithmetic and delta arithmetic-geometric indices of certain nanotubes*, International Journal of Mathematics and its Applications, 12(1)(2024), 43-51.

[24] S. B. B. Altindag, I. Milovannovic, E. Milovanocic, M. Matejic and S. Stankov, *Remark on delta and reverse degree indices*, Sci. Pub. State Univ. Novi Pazar, Ser. A: Appl. Math. Inform. Mech., 15(1)(2022), 37-47.

[25] S. B. B. Altindag, M. Matejic, S. Stankov, E. Milovannovic and I. Milovanocic, *Some new bounds on the delta and reverse Zagreb indices*, Sci. Pub. State Univ. Novi Pazar, Ser. A: Appl. Math. Inform. Mech., 14(2)(2022), 53-63.

[26] E. Milovannovic, I. Milovanocic, M. Matejic, S. Stankov and S. B. B. Altindag, *Bounds for the reverse (delta) first Zagreb indices*, Sci. Pub. State Univ. Novi Pazar, Ser. A: Appl. Math. Inform. Mech., 15(1)(2023), 49-59.

[27] V. R. Kulli, *Reverse Nirmala index*, International Journal of Engineering Sciences & Research Technology, 11(8)(2022), 12-19.

[28] V. R. Kulli, *Multiplicative Nirmala and Banhatti-Nirmala indices of certain nanostar dendrimers*, International Journal of Mathematical Archive, 13(10)(2022), 8-15.

[29] B. K. Majhi, V. R. Kulli and I. N. Cangul, *Nirmala leap indices of some chemical drugs against COVID-19*, Journal of Discrete Mathematics and its Applications, 10(1)(2023), 13-21.

[30] V. R. Kulli, *Irregularity domination Nirmala and domination Sombor indices of certain drugs*, International Journal of Mathematical Archive, 14(8)(2023), 1-7.

[31] S. Raghu, V. R. Kulli, K. M. Niranjan and V. M. Goudar, *Nirmala indices of certain antiviral drugs*, International Journal of Mathematics and Computer Research, 11(11)(2023), 3862-3866.

[32] V. R. Kulli, I. Gutman, B. Furtula and I. Redzepovic, *Sombor, Nirmala Dharwad and F-Sombor indices: A Comparative Study*, SSRG International Journal of Applied Chemistry, 10(2)(2023), 7-10.

[33] I. Gutman, V. R. Kulli and I. Redzepovic, *Irregularity Sombor, index*, Bull. Acad. Serbe. Sci. Arts (Cl. Sci. Math. Natur.), 156(2023), 31-37.

[34] V. R. Kulli, *Modified elliptic Sombor index and its exponential of a graph*, International Journal of Mathematics and Computer Research, 12(1)(2024), 3949-3954.

[35] V. R. Kulli, *Reverse elliptic Sombor and modified reverse elliptic Sombor indices*, International Journal of Mathematical Archive, 15(1)(2024), 1-7.

[36] V. R. Kulli, *Multiplicative elliptic Sombor and multiplicative modified elliptic Sombor indices*, Annals of Pure and Applied Mathematics, 29(1)(2024), 19-23.

[37] V. R. Kulli, *Euler Sombor Banhatti indices*, International Journal of Engineering Sciences & Research Technology, 13(5)(2024), 12-45.

[38] V. R. Kulli, *Status elliptic Sombor and modified status elliptic Sombor indices of graphs*, Journal of Mathematics and Informatics, 27(2024), 49-54.

[39] V. R. Kulli, *Temperature elliptic Sombor and modified temperature elliptic Sombor indices*, International Journal of Mathematics and Computer Research, 13(3)(2025), 4906-4910.

[40] I. Gutman, B. Furtula and M. S. Oz, *Geometric approach to vertex degree based topological indices-Elliptic Sombor index, theory and application*, Int. J. Quantum Chem., 124(2)(2024), e27346.

[41] S. Wagner and H. Wang, *Introduction Chemical Graph Theory*, Boca Raton, CRC Press, (2018).

[42] M. V. Diudea, *QSPR/QSAR Studies by Molecular Descriptors*, NOVA New York, (2001).

[43] A. M. Naji, N. D. Soner and I. Gutman, *On leap Zagreb indices of graphs*, Communications in Combinatorics and Optimization, 2(2)(2017), 99-117.

[44] V. R. Kulli, *College Graph Theory*, Vishwa International Publications, Gulbarga, India, (2012).

[45] V. R. Kulli, *Kepler Banhatti and modified Kepler Banhatti indices*, International Journal of Mathematics and Computer Research, 12(6)(2024), 4310-4314.

[46] V. R. Kulli, *Reverse Kepler Banhatti and modified reverse Kepler Banhatti indices*, International Journal of Mathematical Archive, 15(7)(2024), 1-8.

[47] V. R. Kulli, *Revan Kepler Banhatti and modified Revan Kepler Banhatti indices of certain nanotubes*, Annals of Pure and Applied Mathematics, 30(2)(2024), 129-136.

[48] V. R. Kulli, *Domination Kepler Banhatti and modified domination Kepler Banhatti indices of graphs*, Annals of Pure and Applied Mathematics, 31(1)(2025), 23-29.

[49] V. R. Kulli, *Delta Kepler Banhatti indices of certain nanostructures*, International Journal of Mathematical Archive, 16(2025), to be appear.

[50] B. Basavagoud and E. Chitra, *On leap hyper Zagreb indices of some nanostructures*, International Journal Mathematics Trends and Technology, 64(1)(2018), 30-36.

[51] F. Dayan, M. Javaid and M. A. Rehman, *On leap Gourava indices of some wheel related graphs*, Scientific Inquiry and Review, 2(4)(2018), 14-24.

[52] I. Gutman, Z. Shao, Z. Li, S. Wang and P. Wu, *Leap Zagreb indices of trees and unicyclic graphs*, Communications in Combinatorics and Optimization, 3(2)(2018), 179-194.

[53] V. R. Kulli, *Leap indices of graphs*, International Journal of Current Research in Life Sciences, 8(1)(2019), 2998-3006.

[54] V. R. Kulli, *Computation of leap Adriatic indices and their polynomials of polycyclic aromatic hydrocarbons*, International Journal of Mathematics Trends and Technology, 67(4)(2021), 20-25.