



Computation of Downhill Kepler Banhatti and Modified Downhill Kepler Banhatti Indices of Certain Chemical Structures

Kulli V R

Professor, Department of Mathematics, Gulbarga University, Kalaburgi, India

Abstract

In this paper, we introduce the downhill Kepler Banhatti and the modified downhill Kepler Banhatti indices of a graph. Furthermore, we compute these newly defined downhill Kepler Banhatti indices for some standard graphs, wheel graphs, gear graphs, helm graphs and certain chemical structures.

Keywords: downhill Kepler Banhatti index, modified downhill Kepler Banhatti index, structure.

1. Introduction

The simple graphs which are finite, undirected, connected graphs without loops and multiple edges are considered. Let G be such a graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u .

A u - v path P in G is a sequence of vertices in G , starting with u and ending at v , such that consecutive vertices in P are adjacent, and no vertex is repeated. A path $\pi = v_1, v_2, \dots, v_{k+1}$ in G is a downhill path if for every i , $1 \leq i \leq k$, $d_G(v_i) \geq d_G(v_{i+1})$.

A vertex v is downhill dominates a vertex u if there exists an downhill path originated from u to v . The downhill neighborhood of a vertex v is denoted by $N_{dn}(v)$ and defined as: $N_{dn}(v) = \{u: v$ downhill dominates $u\}$. The downhill degree $d_{dn}(v)$ of a vertex v is the number of downhill neighbors of v , see [1].

In [2], Kulli introduced the Kepler Banhatti index and this index is defined as

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

Recently, some Kepler Banhatti indices were studied in [3, 4, 5, 6, 7].

Motivated by the Kepler Banhatti index, the downhill Kepler Banhatti index of a graph G is defined as

$$DWKB(G) = \sum_{uv \in E(G)} \left(d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2} \right).$$

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

$${}^m DWKB(G) = \sum_{uv \in E(G)} \frac{1}{d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2}}.$$



Recently, some downhill indices were studied in [8-16].

In this paper, the downhill Kepler Banhatti and the modified downhill Kepler Banhatti indices for some chemical structures are determined.

2. Results for Some Standard Graphs

Proposition 1. Let G be r-regular with n vertices and $r \geq 2$. Then

$$DWKB(G) = \frac{(2 + \sqrt{2})n(n-1)r}{2}.$$

Proof: Let G be an r -regular graph with n vertices and $r \geq 2$ and $\frac{nr}{2}$ edges. Then $d_{dn}(v) = n-1$ for every v in G .

From definition,

$$\begin{aligned} DWKB(G) &= \sum_{uv \in E(G)} \left(d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2} \right) \\ &= \frac{nr}{2} \left((n-1) + (n-1) + \sqrt{(n-1)^2 + (n-1)^2} \right) \\ &= \frac{(2 + \sqrt{2})n(n-1)r}{2}. \end{aligned}$$

Corollary 1.1. Let C_n be a cycle with $n \geq 3$ vertices. Then

$$DWKB(C_n) = (2 + \sqrt{2})n(n-1).$$

Corollary 1.2. Let K_n be a complete graph with $n \geq 3$ vertices. Then

$$DWKB(K_n) = \frac{(2 + \sqrt{2})n(n-1)^2}{2}.$$

Proposition 2. Let G be r-regular with n vertices and $r \geq 2$. Then

$${}^m DWKB(G) = \frac{nr}{2(2 + \sqrt{2})(n-1)}.$$

Proof: Let G be an r -regular graph with n vertices and $r \geq 2$ and $\frac{nr}{2}$ edges. Then $d_{dn}(v) = n-1$ for every v in G .

$$\begin{aligned} {}^m DWKB(G) &= \sum_{uv \in E(G)} \frac{1}{d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2}} \\ &= \frac{nr}{2} \frac{1}{(n-1) + (n-1) + \sqrt{(n-1)^2 + (n-1)^2}} \\ &= \frac{nr}{2(2 + \sqrt{2})(n-1)}. \end{aligned}$$

Corollary 2.1. Let C_n be a cycle with $n \geq 3$ vertices. Then

$${}^m DWKB(C_n) = \frac{n}{(2 + \sqrt{2})(n-1)}.$$



Corollary 2.2. Let K_n be a complete graph with $n \geq 3$ vertices. Then

$${}^m DWKB(K_n) = \frac{n}{2(2 + \sqrt{2})}.$$

Proposition 3. Let P_n be a path with $n \geq 3$ vertices. Then

$$DWKB(P_n) = 2(n-1) + (2 + \sqrt{2})(n-3)(n-1).$$

Proof: Let P_n be a path with $n \geq 3$ vertices. Clearly, P_n has two types of edges based on the uphill degree of end vertices of each edge as follows:

$$E_1 = \{uv \in E(P_n) \mid d_{dn}(u)=0, d_{dn}(v)=n-1\}, |E_1| = 2.$$

$$E_2 = \{uv \in E(P_n) \mid d_{dn}(u)=d_{dn}(v)=n-1\}, |E_2| = n-3.$$

$$\begin{aligned} DWKB(P_n) &= \sum_{uv \in E(P_n)} \left(d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2} \right) \\ &= 2\left(0 + (n-1) + \sqrt{0^2 + (n-1)^2}\right) + (n-3)\left((n-1) + (n-1) + \sqrt{(n-1)^2 + (n-1)^2}\right) \\ &= 4(n-1) + (2 + \sqrt{2})(n-3)(n-1). \end{aligned}$$

Proposition 4. Let P_n be a path with $n \geq 3$ vertices. Then

$${}^m DWKB(P_n) = \frac{1}{(n-1)} + \frac{n-3}{(2 + \sqrt{2})(n-1)}.$$

Proof: We obtain

$$\begin{aligned} {}^m DWKB(P_n) &= \sum_{uv \in E(P_n)} \frac{1}{d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2}} \\ &= \frac{2}{0 + (n-1) + \sqrt{0^2 + (n-1)^2}} + \frac{(n-3)}{(n-1) + (n-1) + \sqrt{(n-1)^2 + (n-1)^2}} \\ &= \frac{1}{(n-1)} + \frac{n-3}{(2 + \sqrt{2})(n-1)}. \end{aligned}$$

3. Results for Wheel Graphs

Let W_n be a wheel with $n+1$ vertices and $2n$ edges, $n \geq 4$. Then there are two types of edges based on the uphill degree of end vertices of each edge as follows:

$$E_1 = \{uv \in E(W_n) \mid d_{dn}(u) = n, d_{dn}(v) = n-1\}, |E_1| = n.$$

$$E_2 = \{uv \in E(W_n) \mid d_{dn}(u) = d_{dn}(v) = n-1\}, |E_2| = n.$$

Theorem 1. Let W_n be a wheel with $n+1$ vertices and $2n$ edges, $n \geq 4$. Then

$$DWKB(W_n) = (4 + \sqrt{2})n^2.$$

Proof. We deduce

$$\begin{aligned}
DWKB(W_n) &= \sum_{uv \in E(W_n)} \left(d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2} \right) \\
&= n(n + (n-1) + \sqrt{n^2 + (n-1)^2}) + n((n-1) + (n-1) + \sqrt{(n-1)^2 + (n-1)^2}) \\
&= n(2n-1 + \sqrt{2n^2 - 2n+1}) + (2 + \sqrt{2})n(n-1).
\end{aligned}$$

Theorem 2. Let W_n be a wheel with $n+1$ vertices and $2n$ edges, $n \geq 4$. Then

$${}^m DWKB(W_n) = \frac{n}{2n-1+\sqrt{2n^2-2n+1}} + \frac{n}{(2+\sqrt{2})(n-1)}.$$

Proof. We obtain

$$\begin{aligned}
{}^m DWKB(W_n) &= \sum_{uv \in E(W_n)} \frac{1}{d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2}} \\
&= \frac{n}{n + (n-1) + \sqrt{n^2 + (n-1)^2}} + \frac{n}{(n-1) + (n-1) + \sqrt{(n-1)^2 + (n-1)^2}} \\
&= \frac{n}{2n-1 + \sqrt{2n^2 - 2n+1}} + \frac{n}{(2+\sqrt{2})(n-1)}.
\end{aligned}$$

4. Results for Gear Graphs

A bipartite wheel graph is a graph obtained from W_n with $n+1$ vertices adding a vertex between each pair of adjacent rim vertices and this graph is denoted by G_n and also called as a gear graph. Clearly, $|V(G_n)| = 2n+1$ and $|E(G_n)| = 3n$. A gear graph G_n is depicted in Figure 1.

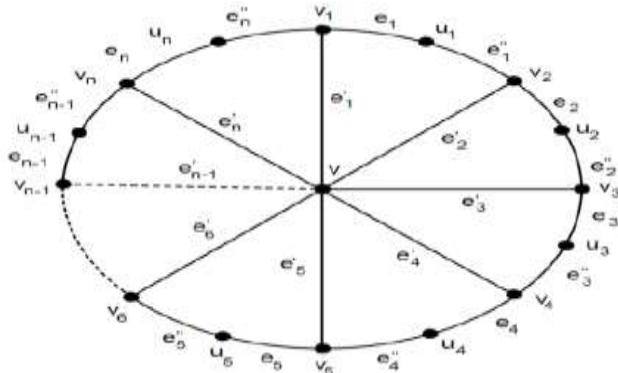


Figure 1. Gear graph G_n

Let G_n be a gear graph with $3n$ edges, $n \geq 4$. Then there are two types of edges based on the uphill degree of end vertices of each edge as follows:

$$\begin{aligned}
E_1 &= \{u \in E(G_n) \mid d_{dn}(u) = 2n, d_{dn}(v) = 2\}, & |E_1| &= n. \\
E_2 &= \{u \in E(G_n) \mid d_{dn}(u) = 2, d_{dn}(v) = 0\}, & |E_2| &= 2n.
\end{aligned}$$

Theorem 3. Let G_n be a gear graph with $2n+1$ vertices, $n \geq 3$. Then

$$DWKB(G_n) = 10n + 2n^2 + 2n\sqrt{n^2 + 1}.$$

Proof: We deduce

$$\begin{aligned}
DWKB(G_n) &= \sum_{uv \in E(G_n)} \left(d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2} \right) \\
&= n(2n + 2 + \sqrt{(2n)^2 + 2^2}) + 2n(2 + 0 + \sqrt{2^2 + 0^2}) \\
&= 10n + 2n^2 + 2n\sqrt{n^2 + 1}.
\end{aligned}$$

Theorem 4. Let G_n be a gear graph with $2n+1$ vertices, $n \geq 3$. Then

$${}^m DWKB(G_n) = \frac{n}{2n + 2 + 2\sqrt{n^2 + 1}} + \frac{n}{2}.$$

Proof: We deduce

$$\begin{aligned}
{}^m DWKB(G_n) &= \sum_{uv \in E(G_n)} \frac{1}{d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2}} \\
&= \frac{n}{2n + 2 + \sqrt{(2n)^2 + 2^2}} + \frac{2n}{2 + 0 + \sqrt{2^2 + 0^2}} \\
&= \frac{n}{2n + 2 + 2\sqrt{n^2 + 1}} + \frac{n}{2}.
\end{aligned}$$

5. Results for Helm Graphs

The helm graph H_n is a graph obtained from W_n (with $n+1$ vertices) by attaching an end edge to each rim vertex of W_n . Clearly, $|V(H_n)| = 2n+1$ and $|E(H_n)| = 3n$. A graph H_n is shown in Figure 2.

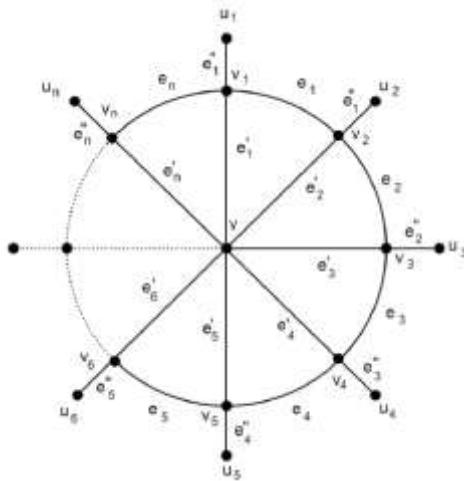


Figure 2. Helm graph H_n

Let H_n be a helm graph with $3n$ edges, $n \geq 3$. Then H_n has three types of the uphill degree of edges as follows:

$$\begin{aligned}
E_1 &= \{uv \in E(H_n) \mid d_{dn}(u) = 2n, d_{dn}(v) = 2n - 1\}. & |E_1| &= n. \\
E_2 &= \{uv \in E(H_n) \mid d_{dn}(u) = d_{dn}(v) = 2n - 1\}. & |E_2| &= n. \\
E_3 &= \{uv \in E(H_n) \mid d_{dn}(u) = 2n - 1, d_{dn}(v) = 0\}. & |E_3| &= n.
\end{aligned}$$

Theorem 5. Let H_n be a helm graph with $2n+1$ vertices, $n \geq 3$. Then

$$DWKB(H_n) = n(4n-1 + \sqrt{8n^2 - 4n+1}) + (4 + \sqrt{2})n(2n-1).$$

Proof: We obtain

$$\begin{aligned} DWKB(H_n) &= \sum_{uv \in E(H_n)} \left(d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2} \right) \\ &= n(2n+2n-1 + \sqrt{(2n)^2 + (2n-1)^2}) + n((2n-1) + (2n-1) + \sqrt{(2n-1)^2 + (2n-1)^2}) \\ &\quad + n((2n-1) + 0 + \sqrt{(2n-1)^2 + 0^2}) \\ &= n(4n-1 + \sqrt{8n^2 - 4n+1}) + (4 + \sqrt{2})n(2n-1). \end{aligned}$$

Theorem 6. Let H_n be a helm graph with $2n+1$ vertices, $n \geq 3$. Then

$${}^m DWKB(H_n) = \frac{n}{4n-1 + \sqrt{8n^2 - 4n+1}} + \frac{n}{(2 + \sqrt{2})(2n-1)} + \frac{n}{2(2n-1)}.$$

Proof: We deduce

$$\begin{aligned} {}^m DWKB(H_n) &= \sum_{uv \in E(H_n)} \frac{1}{d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2}} \\ &= \frac{n}{2n+2n-1 + \sqrt{(2n)^2 + (2n-1)^2}} + \frac{n}{(2n-1) + (2n-1) + \sqrt{(2n-1)^2 + (2n-1)^2}} \\ &\quad + \frac{n}{(2n-1) + 0 + \sqrt{(2n-1)^2 + 0^2}} \\ &= \frac{n}{4n-1 + \sqrt{8n^2 - 4n+1}} + \frac{n}{(2 + \sqrt{2})(2n-1)} + \frac{n}{2(2n-1)}. \end{aligned}$$

6. RESULTS AND DISCUSSION: 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 be the chemical structure of chloroquine. This structure has 21 vertices and 23 edges, see Figure 3.

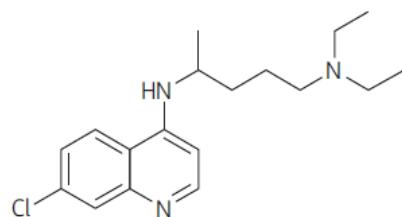


Figure 3. Chemical structure of chloroquine



From Figure 3, we obtain that

$\{(d_{dn}(u), d_{dn}(v)) \setminus uv \mid E(G)\}$ has 13 edge set partitions.

Table 1. Edge set partitions of chloroquine

| | | | | | |
|---|-------|-------|-------|-------|-------|
| $d_{dn}(u), d_{dn}(v) \setminus uv \sqsubset$ | (9,9) | (2,9) | (1,9) | (2,7) | (1,7) |
| $E(G)$ | 2 | 2 | 1 | 1 | 2 |
| Number of edges | (2,5) | (1,4) | (2,2) | (1,1) | (0,9) |
| | 1 | 1 | 4 | 1 | 2 |
| | (0,5) | (0,4) | (0,1) | | |
| | 2 | 2 | 2 | | |

In the following theorem, we compute the different versions of multiplicative arithmetic-geometric indices of chloroquine.

Theorem 7. Let G be the chemical structure of chloroquine. Then

$$DWKB(G) = 199 + 27\sqrt{2} + 2\sqrt{85} + \sqrt{82} + \sqrt{53} + 2\sqrt{50} + \sqrt{29} + \sqrt{17}.$$

Proof: We obtain

$$\begin{aligned} DWKB(G) &= \sum_{uv \in E(G)} \left(d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2} \right) \\ &= 2(9 + 9 + \sqrt{9^2 + 9^2}) + 2(2 + 9 + \sqrt{2^2 + 9^2}) + 1(1 + 9 + \sqrt{1^2 + 9^2}) + 1(2 + 7 + \sqrt{2^2 + 7^2}) + 2(1 + 7 + \sqrt{1^2 + 7^2}) \\ &\quad + 1(2 + 5 + \sqrt{2^2 + 5^2}) + 1(1 + 4 + \sqrt{1^2 + 4^2}) + 4(2 + 2 + \sqrt{2^2 + 2^2}) + 1(1 + 1 + \sqrt{1^2 + 1^2}) + 2(0 + 9 + \sqrt{0^2 + 9^2}) \\ &\quad + 2(0 + 5 + \sqrt{0^2 + 5^2}) + 2(0 + 4 + \sqrt{0^2 + 4^2}) + 2(0 + 1 + \sqrt{0^2 + 1^2}) \end{aligned}$$

After simplification, we obtain the desired result.

Theorem 8. Let G be the chemical structure of chloroquine. Then

$$\begin{aligned} {}^m DWKB(G) &= \frac{2}{18 + 9\sqrt{2}} + \frac{2}{11 + \sqrt{85}} + \frac{1}{10 + \sqrt{82}} + \frac{1}{9 + \sqrt{53}} + \frac{2}{8 + \sqrt{50}} + \frac{1}{7 + \sqrt{29}} + \frac{1}{5 + \sqrt{17}} \\ &\quad + \frac{3}{2 + \sqrt{2}} + \frac{281}{180}. \end{aligned}$$

Proof: We deduce

$$\begin{aligned} {}^m DWKB(G) &= \sum_{uv \in E(G)} \frac{1}{d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2}} \\ &= \frac{2}{9 + 9 + \sqrt{9^2 + 9^2}} + \frac{2}{2 + 9 + \sqrt{2^2 + 9^2}} + \frac{1}{1 + 9 + \sqrt{1^2 + 9^2}} + \frac{1}{2 + 7 + \sqrt{2^2 + 7^2}} + \frac{2}{1 + 7 + \sqrt{1^2 + 7^2}} \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2+5+\sqrt{2^2+5^2}} + \frac{1}{1+4+\sqrt{1^2+4^2}} + \frac{4}{2+2+\sqrt{2^2+2^2}} + \frac{1}{1+1+\sqrt{1^2+1^2}} + \frac{2}{0+9+\sqrt{0^2+9^2}} \\
& + \frac{2}{0+5+\sqrt{0^2+5^2}} + \frac{2}{0+4+\sqrt{0^2+4^2}} + \frac{2}{0+1+\sqrt{0^2+1^2}}.
\end{aligned}$$

After simplifying, we get the desired result.

7. RESULTS AND DISCUSSION: HYDROXYCHLOROQUINE

Hydroxychloroquine is another antiviral compound (drug) which has antiviral activity very similar to that of chloroquine. These compounds have been repurposed for the treatment of a number of other conditions including HIV, systemic lupus erythematosus and rheumatoid arthritis.

Let H be the chemical structure of hydroxychloroquine. This structure has 22 vertices and 24 edges, see Figure 4.

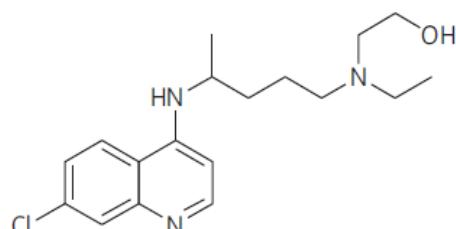


Figure 4. Chemical structure of hydroxychloroquine

From Figure 4, we obtain that

$\{(d_{dn}(u), d_{dn}(v)) \setminus uv \mid uv \in E(H)\}$ has 14 edge set partition

Table 2. Edge set partitions of hydroxychloroquine

| | | | | | |
|---|-------|-------|-------|-------|-------|
| $d_{dn}(u), d_{dn}(v) \setminus uv \sqsubset$ | (9,9) | (2,9) | (1,9) | (2,8) | (1,8) |
| $E(H)$ | 2 | 2 | 1 | 2 | 1 |
| Number of edges | (2,5) | (1,4) | (2,2) | (1,1) | (0,9) |
| | 1 | 1 | 5 | 1 | 2 |
| | (0,5) | (0,4) | (0,2) | (0,1) | |
| | 2 | 2 | 1 | 1 | |

Theorem 9. Let H be the chemical structure of hydroxychloroquine. Then

$$DWKB(H) = 209 + 29\sqrt{2} + 2\sqrt{85} + \sqrt{82} + 5\sqrt{17} + \sqrt{65} + \sqrt{29}.$$

Proof: We obtain

$$DWKB(H) = \sum_{uv \in E(H)} \left(d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2} \right)$$

$$\begin{aligned}
&= 2(9 + 9 + \sqrt{9^2 + 9^2}) + 2(2 + 9 + \sqrt{2^2 + 9^2}) + 1(1 + 9 + \sqrt{1^2 + 9^2}) + 2(2 + 8 + \sqrt{2^2 + 8^2}) + 1(1 + 8 + \sqrt{1^2 + 8^2}) \\
&+ 1(2 + 5 + \sqrt{2^2 + 5^2}) + 1(1 + 4 + \sqrt{1^2 + 4^2}) + 5(2 + 2 + \sqrt{2^2 + 2^2}) + 1(1 + 1 + \sqrt{1^2 + 1^2}) + 2(0 + 9 + \sqrt{0^2 + 9^2}) \\
&+ 2(0 + 5 + \sqrt{0^2 + 5^2}) + 2(0 + 4 + \sqrt{0^2 + 4^2}) + 1(0 + 2 + \sqrt{0^2 + 2^2}) + 1(0 + 1 + \sqrt{0^2 + 1^2})
\end{aligned}$$

Simplification gives the desired result.

Theorem 10. Let H be the chemical structure of hydroxychloroquine. Then

$$\begin{aligned}
{}^m DWKB(H) &= \frac{2}{18 + 9\sqrt{2}} + \frac{2}{11 + \sqrt{85}} + \frac{1}{10 + \sqrt{82}} + \frac{2}{5 + \sqrt{17}} + \frac{1}{9 + \sqrt{65}} + \frac{1}{7 + \sqrt{29}} \\
&+ \frac{5}{4 + 2\sqrt{2}} + \frac{1}{2 + \sqrt{2}} + \frac{59}{45}.
\end{aligned}$$

Proof: We obtain

$$\begin{aligned}
{}^m DWKB(H) &= \sum_{uv \in E(H)} \frac{1}{d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2}} \\
&= \frac{2}{9 + 9 + \sqrt{9^2 + 9^2}} + \frac{2}{2 + 9 + \sqrt{2^2 + 9^2}} + \frac{1}{1 + 9 + \sqrt{1^2 + 9^2}} + \frac{2}{2 + 8 + \sqrt{2^2 + 8^2}} + \frac{1}{1 + 8 + \sqrt{1^2 + 8^2}} \\
&+ \frac{1}{2 + 5 + \sqrt{2^2 + 5^2}} + \frac{1}{1 + 4 + \sqrt{1^2 + 4^2}} + \frac{5}{2 + 2 + \sqrt{2^2 + 2^2}} + \frac{1}{1 + 1 + \sqrt{1^2 + 1^2}} + \frac{2}{0 + 9 + \sqrt{0^2 + 9^2}} \\
&+ \frac{2}{0 + 5 + \sqrt{0^2 + 5^2}} + \frac{2}{0 + 4 + \sqrt{0^2 + 4^2}} + \frac{1}{0 + 2 + \sqrt{0^2 + 2^2}} + \frac{1}{0 + 1 + \sqrt{0^2 + 1^2}}.
\end{aligned}$$

After simplification, we get the required result.

8. RESULTS AND DISCUSSION: REMDESIVIR

Remdesivir is an antiviral drug which was developed by the biopharmaceutical company Gilead Sciences. Let R be the molecular graph of remdesivir. This graph has 41 vertices and 44 edges.

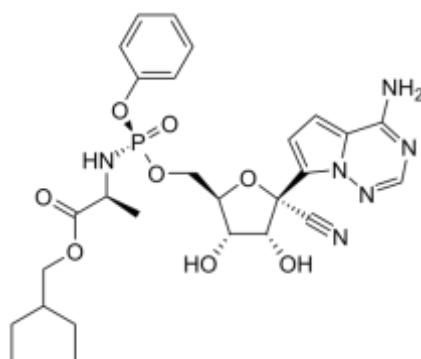


Figure 5. Chemical structure of remdesivir

From Figure 5, we obtain that



$\{(d_{dn}(u), d_{dn}(v)) \setminus uv \mid uv \in E(R)\}$ has 20 edge set partitions.

Table 3. Edge set partitions of remdesivir

| | | | | | | | | |
|-------------------------|--------|--------|-------|-------|-------|-------|--------|-------|
| $d_{dn}(u), d_{dn}(v)$ | (9,19) | (7,19) | (9,9) | (2,9) | (1,9) | (7,7) | (1,7) | (6,6) |
| $\setminus uv \in E(R)$ | 1 | 1 | 3 | 2 | 2 | 2 | 1 | 1 |
| Number of edges | (4,6) | (1,6) | (1,5) | (4,4) | (2,2) | (1,1) | (0,19) | (0,9) |
| | 2 | 4 | 1 | 4 | 2 | 3 | 2 | 1 |
| | (0,7) | (0,6) | (0,5) | (0,1) | | | | |
| | 3 | 4 | 3 | 2 | | | | |

Theorem 11. Let R be the chemical structure of remdesivir. Then

$$DWKB(R) = 516 + 70\sqrt{2} + \sqrt{442} + \sqrt{410} + 2\sqrt{85} + 2\sqrt{82} + \sqrt{50} + 4\sqrt{13} + 4\sqrt{57} + \sqrt{26}.$$

Proof: We obtain

$$\begin{aligned} DWKB(R) &= \sum_{uv \in E(R)} \left(d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2} \right) \\ &= 1(9+19+\sqrt{9^2+19^2}) + 1(7+19+\sqrt{7^2+19^2}) + 3(9+9+\sqrt{9^2+9^2}) + 2(2+9+\sqrt{2^2+9^2}) + 2(1+9+\sqrt{1^2+9^2}) \\ &\quad + 2(7+7+\sqrt{7^2+7^2}) + 1(1+7+\sqrt{1^2+7^2}) + 1(6+6+\sqrt{6^2+6^2}) + 2(4+6+\sqrt{4^2+6^2}) + 4(1+6+\sqrt{1^2+6^2}) \\ &\quad + 1(1+5+\sqrt{1^2+5^2}) + 4(4+4+\sqrt{4^2+4^2}) + 2(2+2+\sqrt{2^2+2^2}) + 3(1+1+\sqrt{1^2+1^2}) + 2(0+19+\sqrt{0^2+19^2}) \\ &\quad + 1(0+9+\sqrt{0^2+9^2}) + 3(0+7+\sqrt{0^2+7^2}) + 4(0+6+\sqrt{0^2+6^2}) + 3(0+5+\sqrt{0^2+5^2}) + 2(0+1+\sqrt{0^2+1^2}). \end{aligned}$$

After simplifying the above equation, we get the desired result.

Theorem 12. Let R be the chemical structure of hydroxychloroquine. Then

$$\begin{aligned} {}^m DWKB(R) &= \frac{1}{28+\sqrt{442}} + \frac{1}{26+\sqrt{410}} + \frac{1}{6+3\sqrt{2}} + \frac{2}{11+\sqrt{85}} + \frac{2}{10+\sqrt{82}} \\ &\quad + \frac{2}{14+7\sqrt{2}} + \frac{1}{8+\sqrt{50}} + \frac{1}{12+6\sqrt{2}} + \frac{1}{5+\sqrt{13}} + \frac{4}{7+\sqrt{37}} \\ &\quad + \frac{1}{6+\sqrt{26}} + \frac{5}{2+\sqrt{2}} + \frac{1}{19} + \frac{1}{18} + \frac{3}{14} + \frac{1}{3} + \frac{3}{10} + 1. \end{aligned}$$

Proof: We obtain

$${}^m DWKB(R) = \sum_{uv \in E(R)} \frac{1}{d_{dn}(u) + d_{dn}(v) + \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2}}$$



$$\begin{aligned} &= \frac{1}{9+19+\sqrt{9^2+19^2}} + \frac{1}{7+19+\sqrt{7^2+19^2}} + \frac{3}{9+9+\sqrt{9^2+9^2}} + \frac{2}{2+9+\sqrt{2^2+9^2}} + \frac{2}{1+9+\sqrt{1^2+9^2}} \\ &+ \frac{2}{7+7+\sqrt{7^2+7^2}} + \frac{1}{1+7+\sqrt{1^2+7^2}} + \frac{1}{6+6+\sqrt{6^2+6^2}} + \frac{2}{4+6+\sqrt{4^2+6^2}} + \frac{4}{1+6+\sqrt{1^2+6^2}} \\ &+ \frac{1}{1+5+\sqrt{1^2+5^2}} + \frac{4}{4+4+\sqrt{4^2+4^2}} + \frac{2}{2+2+\sqrt{2^2+2^2}} + \frac{3}{1+1+\sqrt{1^2+1^2}} + \frac{2}{0+19+\sqrt{0^2+19^2}} \\ &+ \frac{1}{0+9+\sqrt{0^2+9^2}} + \frac{3}{0+7+\sqrt{0^2+7^2}} + \frac{4}{0+6+\sqrt{0^2+6^2}} + \frac{3}{0+5+\sqrt{0^2+5^2}} + \frac{2}{0+1+\sqrt{0^2+1^2}}. \end{aligned}$$

By simplifying, the result is obtained.

9. Conclusion

In this paper, the downhill Kepler Banhatti and modified downhill Kepler Banhatti indices of a graph are defined. Also these newly defined the downhill Kepler Banhatti indices of some standard graphs, wheel graphs, gear graphs, helm graphs and some chemical structures are determined.

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