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KG SOMBOR INDICES OF CERTAIN CHEMICAL DRUGS

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ABSTRACT
In this paper, we introduce the KG Sombor exponential, modified KG Sombor index, modified KG Sombor exponential, first and second Banhatti (a, b)-KA indices and their polynomials of a graph. We compute these KG Sombor indices for three chemical drugs such as chloroquine, hydrochloroquine and remdesivir.

Keywords: KG Sombor index, modified KG Sombor index, chemical drug.

Mathematics Subject Classification: 05C05, 05C12, 05C35..

1. INTRODUCTION
Let G be simple, connected graph with $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex u is the number of edges incident to u. If e= uv is an edge of G, then the vertex u and edge e are incident and it is denoted by ue. Let $d_G(e)$ denote the degree of an edge e in G, which is defined as $d_G(e) = d_G(u) + d_G(e) - 2$ with $e = uv$.

In 1972 [1], two degree based topological indices were introduced and studied. The first and second Banhatti indices of a graph G were introduced by Kulli in [2], and they are defined as

$$B_1(G) = \sum_{ue}\left[d_G(u) + d_G(e)\right], \qquad B_2(G) = \sum_{ue} d_G(u) d_G(e)$$

where ue means that the vertex u and edge e are incident in G.

Recently, some Banhatti indices were studied in [3, 4, 5, 6, 7, 8, 9, 10].

The KG Sombor index was introduced by Kulli et al. in [11], defined it as

$$KG(G) = \sum_{ue}\sqrt{d_G(u)^2 + d_G(e)^2}.$$

The true meaning of KG is Kulli and Gutman. So that we call this index as Kulli-Gutman Sombor index. Recently, some Sombor indices were studied in [12, 13, 14, 15, 16, 17, 18, 19, 20].

The KG Sombor exponential of a graph G is defined as

$$KG(G,x) = \sum_{ue} x^{\sqrt{d_G(u)^2 + d_G(e)^2}}.$$

We introduce the modified KG Sombor index of a graph G and it is defined as

$$^{m}KG(G) = \sum_{ue}\frac{1}{\sqrt{d_G(u)^2 + d_G(e)^2}}.$$

We define the modified KG Sombor exponential of a graph G as

$$^{m}KG(G,x) = \sum_{ue} x^{\frac{1}{\sqrt{d_G(u)^2 + d_G(e)^2}}}.$$

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We introduce the first and second Banhatti (*a*, *b*)-*KA* indices of a molecular graph *G* and they are defined as

$$BKA^1_{a,b}(G)=\sum_{ue}\left[d_G(u)^a+d_G(e)^a\right]^b, \qquad BKA^2_{a,b}(G)=\sum_{ue}\left[d_G(u)^a\cdot d_G(e)^a\right]^b.$$

Considering the first and second Banhatti (*a*, *b*)-*KA* indices, we define the first and second Banhatti (*a*, *b*)-*KA* polynomials of a graph *G* as

$$BKA^1_{a,b}(G,x)=\sum_{ue}x^{\left[d_G(u)^a+d_G(e)^a\right]^b}, \qquad BKA^2_{a,b}(G,x)=\sum_{ue}x^{\left[d_G(u)^a d_G(e)^a\right]^b}.$$

Recently, some (*a*,*b*)-*KA* indices were studied, for example, in [21, 22, 23, 24, 25, 26, 27]. In this paper, we determine the *KG* Sombor index, modified *KG* Sombor index, *KG* Sombor exponential, modified *KG* Sombor exponential, Banhatti (*a*,*b*)-*KA* indices and their corresponding polynomials of chloroquine, hydroxychloroquine and remdesivir.

2. CHLOROQUINE: RESULTS AND DISCUSSION

Let *G* be the graph of chloroquine. This graph has 21 vertices and 23 edges, see Figure 1.

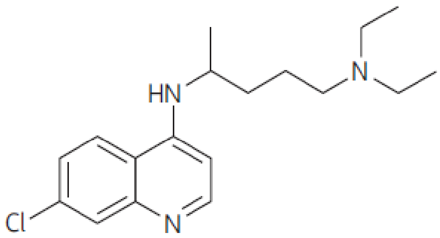

Figure 1. Structure of chloroquine

In *G*, the edge set of *G* can be divided into five partitions based on the degree of end vertices of each edge as follows:

$E_1=\{uv\in E(G) \mid d_G(u)=1, d_G(v)=2\}$, $|E_1|=2$,
$E_2=\{uv\in E(G) \mid d_G(u)=1, d_G(v)=3\}$, $|E_2|=2$,
$E_3=\{uv\in E(G) \mid d_G(u)=d_G(v)=2\}$, $|E_3|=5$,
$E_4=\{uv\in E(G) \mid d_G(u)=2, d_G(v)=3\}$, $|E_4|=12$,
$E_5=\{uv\in E(G) \mid d_G(u)=d_G(v)=3\}$, $|E_5|=2$.

Then the edge degree partition of *G* is given in Table 1:

Table 1. Edge degree partition of G

$d_G(u), d_G(v)\backslash uv\in E(G)$	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
$d_G(e)$	1	2	2	3	4
No. of edges	2	2	5	12	2

We compute the first Banhatti (*a*, *b*)-*KA* index of the molecular graph of chloroquine.

Theorem 1. The first Banhatti (*a*, *b*)-*KA* index of chloroquine is

$$BKA^1_{a,b}(G)=2(1^a+1^a)^b+2(2^a+1^a)^b+14(3^a+2^a)^b+10(2^a+2^a)^b+12(3^a+3^a)^b+4(3^a+4^a)^b.$$

Proof: By definition and cardinalities of the edge partitions of *G*, we have

$$BKA^1_{a,b}(G)=\sum_{ue}\left[d_G(u)^a+d_G(e)^a\right]^b$$

$$=2\left[(1^a+1^a)^b+(2^a+1^a)^b\right]+2\left[(1^a+2^a)^b+(3^a+2^a)^b\right]+5\left[(2^a+2^a)^b+(2^a+2^a)^b\right]$$

$$+12\left[\left(2^a+3^a\right)^b+\left(3^a+3^a\right)^b\right]+2\left[\left(3^a+4^a\right)^b+\left(3^a+4^a\right)^b\right].$$

After simplification, we get the desired result.

From Theorem 1, we establish the following results.
.
Corollary 1.1. The *KG* Sombor index of *G* is
$$KG(G)=BKA^1_{2,1/2}(G)=58\sqrt{2}+4\sqrt{5}+14\sqrt{13}+20.$$

Corollary 1.2. The modified *KG* Sombor index of *G* is
$${}^mKG(G)=BKA^1_{2,-1/2}(G)=\frac{11}{\sqrt{2}}+\frac{4}{\sqrt{5}}+\frac{14}{\sqrt{13}}+\frac{4}{5}.$$
In Theorem 2, we compute the second Banhatti (*a*, *b*)-*KA* index of the molecular graph of chloroquine.

Theorem 2. The second Banhatti (*a*, *b*)-*KA* index of *G* is
$$BKA^2_{a,b}(G)=2+\left(14\times 2^{ab}\right)+\left(14\times 6^{ab}\right)+\left(12\times 9^{ab}\right)+\left(4\times 12^{ab}\right).$$

Proof: From definition and by cardinalities of the edge partitions of *G*, we obtain
$$BKA^2_{a,b}(G)=\sum_{ue}\left[d_G(u)^a\cdot d_G(e)^a\right]^b$$
$$=2\left[\left(1^a\times 1^a\right)^b+\left(2^a\times 1^a\right)^b\right]+2\left[\left(1^a\times 2^a\right)^b+\left(3^a\times 2^a\right)^b\right]+5\left[\left(2^a\times 2^a\right)^b+\left(2^a\times 2^a\right)^b\right]$$
$$+12\left[\left(2^a\times 3^a\right)^b+\left(3^a\times 3^a\right)^b\right]+2\left[\left(3^a\times 4^a\right)^b+\left(3^a\times 4^a\right)^b\right]$$
gives the desired result after simplification.

In the following theorem, we compute the first Banhatti (*a*, *b*)-*KA* polynomial of the molecular graph of chloroquine.

Theorem 3. The first Banhatti (*a*, *b*)-*KA* polynomial of *G* is
$$BKA^1_{a,b}(G,x)=2x^{\left(1^a+1^a\right)^b+\left(2^a+1^a\right)^b}+2x^{\left(1^a+2^a\right)^b+\left(3^a+2^a\right)^b}+5x^{2\left(2^a+2^a\right)^b}+12x^{\left(2^a+3^a\right)^b+\left(3^a+3^a\right)^b}+2x^{2\left(3^a+4^a\right)^b}.$$
Proof: By definition and cardinalities of the edge partitions of *G*, we have
$$BKA^1_{a,b}(G)=\sum_{ue}x^{\left[d_G(u)^a+d_G(e)^a\right]^b}$$
$$=2x^{\left(1^a+1^a\right)^b+\left(2^a+1^a\right)^b}+2x^{\left(1^a+2^a\right)^b+\left(3^a+2^a\right)^b}+5x^{\left(2^a+2^a\right)^b+\left(2^a+2^a\right)^b}+12x^{\left(2^a+3^a\right)^b+\left(3^a+3^a\right)^b}+2x^{\left(3^a+4^a\right)^b+\left(3^a+4^a\right)^b}.$$

After simplification, we get the desired result.

From Theorem 3, we obtain the following results.

Corollary 3.1. The *KG* Sombor exponential of *G* is
$$KG(G,x)=2x^{\sqrt{2}+\sqrt{5}}+2x^{\sqrt{5}+\sqrt{13}}+5x^{4\sqrt{2}}+12x^{\sqrt{13}+3\sqrt{2}}+2x^{10}.$$

Corollary 3.2. The modified *KG* Sombor exponential of *G* is
$${}^mKG(G,x)=2x^{\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{5}}}+2x^{\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{13}}}+5x^{\frac{1}{\sqrt{2}}}+12x^{\frac{1}{\sqrt{13}}+\frac{1}{3\sqrt{2}}}+2x^{\frac{2}{5}}.$$

In the next theorem, we compute the second Banhatti (*a*, *b*)-*KA* polynomial of the molecular graph of chloroquine.

Theorem 4. The second Banhatti (*a*, *b*)-*KA* polynomial of *G* is

$$BKA^2_{a,b}(G,x) = 2x^{1^{ab}+2^{ab}} + 2x^{2^{ab}+6^{ab}} + 5x^{2\times 2^{ab}} + 12x^{6^{ab}+9^{ab}} + 2x^{2\times 12^{ab}}.$$

Proof: By definition and by using cardinalities of the edge partitions of *G*, we obtain

$$BKA^2_{a,b}(G,x) = \sum_{ue} x^{\left[d_G(u)^a d_G(e)^a\right]^b}$$

$$= 2x^{(1^a\times 1^a)^b+(2^a\times 1^a)^b} + 2x^{(1^a\times 2^a)^b+(3^a\times 2^a)^b} + 5x^{(2^a\times 2^a)^b+(2^a\times 2^a)^b} + 12x^{(2^a\times 3^a)^b+(3^a\times 3^a)^b} + 2x^{(3^a\times 4^a)^b+(3^a\times 4^a)^b}.$$

After simplification, we establish the desired result..

3. HYDROXYCHLOROQUINE: RESULTS AND DISCUSSION

Let *H* be the molecular graph of hydroxychloroquine and it has 22 vertices and 24 edges, see Figure 2.

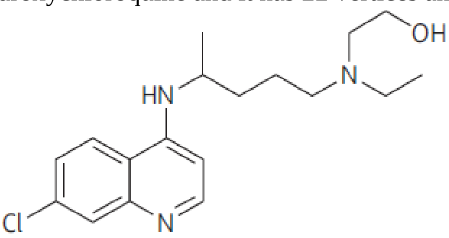

Figure 2. Structure of hydroxychloroquine

In *H*, the edge set of *E*(*H*) can be divided into five partitions based on the degree of end vertices of each edge as follows:

$E_1=\{uv \in E(H) \mid d_H(u)=1, d_H(v)=2\}$, $|E_1|=2$,
$E_2=\{uv \in E(H) \mid d_H(u)=1, d_H(v)=3\}$, $|E_2|=2$,
$E_3=\{uv \in E(H) \mid d_H(u)=2, d_H(v)=2\}$, $|E_3|=6$,
$E_4=\{uv\in E(H) \mid d_H(u)=2, d_H(v)=3\}$, $|E_4|=12$,
$E_5=\{uv \in E(H) \mid d_H(u) = d_H(v)=3\}$, $|E_5|=2$

Then the edge degree partition of *H* is given in Table 2:

Table 2. Edge degree partition of H

$d_H(u), d_H(v)\backslash$ uv□$E(H)$	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
$d_H(e)$	1	2	2	3	4
No. of edges	2	2	6	12	2

In the following theorem, we compute the first Banhatti (*a*, *b*)-*KA* index of the molecular graph of hydroxychloroquine.

Theorem 5. The first Banhatti (*a*, *b*)-*KA* index of hydroxychloroquine is

$$BKA^1_{a,b}(G) = 2(1^a+1^a)^b + 2(2^a+1^a)^b + 14(3^a+2^a)^b + 12(2^a+2^a)^b + 12(3^a+3^a)^b + 4(3^a+4^a)^b.$$

Proof: By definition and cardinalities of the edge partitions of *H*, we have

$$BKA^1_{a,b}(H) = \sum_{ue}\left[d_H(u)^a + d_H(e)^a\right]^b$$

$$= 2\left[(1^a+1^a)^b + (2^a+1^a)^b\right] + 2\left[(1^a+2^a)^b + (3^a+2^a)^b\right] + 6\left[(2^a+2^a)^b + (2^a+2^a)^b\right]$$
$$+12\left[(2^a+3^a)^b + (3^a+3^a)^b\right] + 2\left[(3^a+4^a)^b + (3^a+4^a)^b\right]$$

gives the desired result.

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The following results are obtained from Theorem 5.

Corollary 5.1. The *KG* Sombor index of *H* is

$$KG(H) = BKA^1_{2,1/2}(H) = 62\sqrt{2} + 4\sqrt{5} + 14\sqrt{13} + 20.$$

Corollary 5.2. The modified *KG* Sombor index of *H* is

$$^mKG(H) = BKA^1_{2,-1/2}(H) = \frac{12}{\sqrt{2}} + \frac{4}{\sqrt{5}} + \frac{14}{\sqrt{13}} + \frac{4}{5}.$$

In the following theorem, we compute the second Banhatti (*a*, *b*)-*KA* index of the molecular graph of hydroxychloroquine.

Theorem 6. The second Banhatti (*a*, *b*)-*KA* index of *H* is

$$BKA^2_{a,b}(H) = 2 + (16 \times 2^{ab}) + (14 \times 6^{ab}) + (12 \times 9^{ab}) + (4 \times 12^{ab}).$$

Proof: From definition and by using cardinalities of the partitions of *H*, we get

$$BKA^2_{a,b}(H) = \sum_{ue}\left[d_H(u)^a \cdot d_H(e)^a\right]^b$$
$$= 2\left[(1^a \times 1^a)^b + (2^a \times 1^a)^b\right] + 2\left[(1^a \times 2^a)^b + (3^a \times 2^a)^b\right] + 6\left[(2^a \times 2^a)^b + (2^a \times 2^a)^b\right]$$
$$+12\left[(2^a \times 3^a)^b + (3^a \times 3^a)^b\right] + 2\left[(3^a \times 4^a)^b + (3^a \times 4^a)^b\right].$$

After simplification, we get the desired result.

In the next theorem, we compute the first Banhatti (*a*, *b*)-*KA* polynomial of the molecular graph of hydroxychloroquine.

Theorem 7. The first Banhatti (*a*, *b*)-*KA* polynomial of *H* is

$$BKA^1_{a,b}(H,x) = 2x^{(1^a+1^a)^b+(2^a+1^a)^b} + 2x^{(1^a+2^a)^b+(3^a+2^a)^b} + 6x^{2(2^a+2^a)^b} + 12x^{(2^a+3^a)^b+(3^a+3^a)^b} + 2x^{2(3^a+4^a)^b}.$$

Proof: By definition and using cardinalities of the edge partitions of *H*, we have

$$BKA^1_{a,b}(H) = \sum_{ue} x^{\left[d_H(u)^a + d_H(e)^a\right]^b}$$
$$= 2x^{(1^a+1^a)^b+(2^a+1^a)^b} + 2x^{(1^a+2^a)^b+(3^a+2^a)^b} + 6x^{(2^a+2^a)^b+(2^a+2^a)^b} + 12x^{(2^a+3^a)^b+(3^a+3^a)^b} + 2x^{(3^a+4^a)^b+(3^a+4^a)^b}.$$

After simplification, We get the desired result after simplification.

By using Theorem 7, we get the following results.

Corollary 7.1. The *KG* Sombor exponential of *H* is

$$KG(H,x) = 2x^{\sqrt{2}+\sqrt{5}} + 2x^{\sqrt{5}+\sqrt{13}} + 6x^{4\sqrt{2}} + 12x^{\sqrt{13}+3\sqrt{2}} + 2x^{10}.$$

Corollary 7.2. The modified *KG* Sombor exponential of *H* is

$$^mKG(H,x) = 2x^{\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{5}}} + 2x^{\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{13}}} + 6x^{\frac{1}{\sqrt{2}}} + 12x^{\frac{1}{\sqrt{13}}+\frac{1}{3\sqrt{2}}} + 2x^{\frac{2}{5}}.$$

In Theorem 8, we compute the second Banhatti (*a*, *b*)-*KA* polynomial of the molecular graph of hydroxychloroquine.

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Theorem 8. The second Banhatti (*a*, *b*)-*KA* polynomial of *H* is

$$BKA_{a,b}^{2}(H,x) = 2x^{1^{ab}+2^{ab}} + 2x^{2^{ab}+6^{ab}} + 6x^{2\times 2^{ab}} + 12x^{6^{ab}+9^{ab}} + 2x^{2\times 12^{ab}}.$$

Proof: By definition and using cardinalities of the edge partitions of *H*, we obtain

$$BKA_{a,b}^{2}(H,x) = \sum_{ue} x^{\left[d_H(u)^a d_H(e)^a\right]^b}$$

$$= 2x^{(1^a\times 1^a)^b+(2^a\times 1^a)^b} + 2x^{(1^a\times 2^a)^b+(3^a\times 2^a)^b} + 6x^{(2^a\times 2^a)^b+(2^a\times 2^a)^b} + 12x^{(2^a\times 3^a)^b+(3^a\times 3^a)^b} + 2x^{(3^a\times 4^a)^b+(3^a\times 4^a)^b}.$$

After simplification, we get the desired result.

4. RESULTS AND DISCUSSION: REMDESVIR

Let *R* be the molecular structure of remdesivir. Clearly *R* has 41 vertices and 44 edges, see Figure 3.

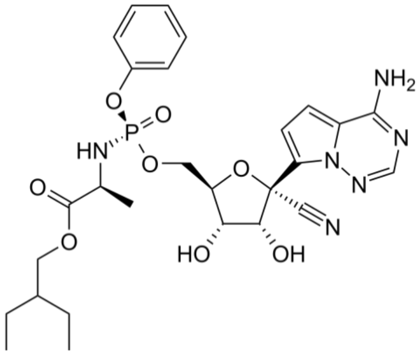

Figure 3. Structure of remdesivir

In *R*, the edge set *E*(*R*) can be divided into eight partitions based on the degree of end vertices of each edge as follows:

$E_1=\{uv \in E(R) \mid d_R(u)=1, d_R(v)=2\}$, $|E_1|=2$,
$E_2=\{uv \in E(R) \mid d_R(u)=1, d_R(v)=3\}$, $|E_2|=5$,
$E_3=\{uv \in E(R) \mid d_R(u)=1, d_R(v)=4\}$, $|E_3|=2$,
$E_4=\{uv \in E(R) \mid d_R(u)=2, d_R(v)=2\}$, $|E_4|=9$,
$E_5=\{uv \in E(R) \mid d_R(u)=2, d_R(v)=3\}$, $|E_5|=14$.
$E_6=\{uv \in E(R) \mid d_R(u)=2, d_R(v)=4\}$, $|E_6|=4$,
$E_7=\{uv \in E(R) \mid d_R(u)=3, d_R(v)=3\}$, $|E_7|=6$,
$E_8=\{uv \in E(R) \mid d_R(u)=3, d_R(v)=4\}$, $|E_8|=2$.

Then the edge degree partition of *R* is given in Table 3.

Table 3. Edge partition of R

$d_G(u), d_G(v)\backslash uv$ □ $E(G)$	(1, 2)	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(2, 4)	(3, 3)	(3, 4)
$d_G(e)$	1	2	3	2	3	4	4	5
No. of edges	2	5	2	9	14	4	6	2

In the following theorem, we compute the first Banhatti (*a*, *b*)-*KA* index of the molecular graph of remdesivir.

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Theorem 9. The first Banhatti (*a*, *b*)-*KA* index of remdesivir is

$$BKA^1_{a,b}(R)=2(1^a+1^a)^b+2(2^a+1^a)^b+14(3^a+2^a)^b+12(2^a+2^a)^b+12(3^a+3^a)^b+4(3^a+4^a)^b.$$

Proof: By definition and cardinalities of the edge partitions of *R*, we get

$$BKA^1_{a,b}(R)=\sum_{ue}\left[d_R(u)^a+d_R(e)^a\right]^b$$

$$=2\left[(1^a+1^a)^b+(2^a+1^a)^b\right]+5\left[(1^a+2^a)^b+(3^a+2^a)^b\right]+2\left[(1^a+3^a)^b+(4^a+3^a)^b\right]$$
$$+9\left[(2^a+2^a)^b+(2^a+2^a)^b\right]+14\left[(2^a+3^a)^b+(3^a+3^a)^b\right]+4\left[(2^a+4^a)^b+(4^a+4^a)^b\right]$$
$$+6\left[(3^a+4^a)^b+(3^a+4^a)^b\right]+2\left[(3^a+5^a)^b+(4^a+5^a)^b\right].$$

After simplification, we get the desired result.

We obtain the following results from Theorem 9.

Corollary 9.1. The *KG* Sombor index of *R* is

$$KG(R)=BKA^1_{2,1/2}(R)=96\sqrt{2}+15\sqrt{5}+2\sqrt{10}+19\sqrt{13}+2\sqrt{34}+2\sqrt{41}+70.$$

Corollary 9.2. The modified *KG* Sombor index of *R* is

$$^{m}KG(R)=BKA^1_{2,-1/2}(R)=\frac{50}{3\sqrt{2}}+\frac{9}{\sqrt{5}}+\frac{2}{\sqrt{10}}+\frac{19}{\sqrt{13}}+\frac{2}{\sqrt{34}}+\frac{2}{\sqrt{41}}+\frac{14}{5}.$$

In the following theorem, we compute the second Banhatti (*a*, *b*)-*KA* index of the molecular graph of remdesivir

Theorem 10. The second Banhatti (*a*, *b*)-*KA* index of *R* is

$$BKA^2_{a,b}(R)=2+(7\times 2^{ab})+(2\times 3^{ab})+(18\times 4^{ab})+(19\times 6^{ab})+(4\times 8^{ab})+(14\times 9^{ab})+(14\times 12^{ab})$$
$$+(4\times 16^{ab})+(2\times 15^{ab})+(2\times 20^{ab}).$$

Proof: By definition and cardinalities of the edge partitions of *R*, we have

$$BKA^2_{a,b}(R)=\sum_{ue}\left[d_R(u)^a\times d_R(e)^a\right]^b$$

$$=2\left[(1^a\times 1^a)^b+(2^a\times 1^a)^b\right]+5\left[(1^a\times 2^a)^b+(3^a\times 2^a)^b\right]+2\left[(1^a\times 3^a)^b+(4^a\times 3^a)^b\right]$$
$$+9\left[(2^a\times 2^a)^b+(2^a\times 2^a)^b\right]+14\left[(2^a\times 3^a)^b+(3^a\times 3^a)^b\right]+4\left[(2^a\times 4^a)^b+(4^a\times 4^a)^b\right]$$
$$+6\left[(3^a\times 4^a)^b+(3^a\times 4^a)^b\right]+2\left[(3^a\times 5^a)^b+(4^a\times 5^a)^b\right].$$

After simplification, we obtain the desired result.

In Theorem 11, we compute the first Banhatti (*a*, *b*)-*KA* polynomial of the molecular graph of remdesivir.

Theorem 11. The first Banhatti (*a*, *b*)-*KA* polynomial of *R* is

$$BKA^1_{a,b}(R,x)=2x^{(1^a+1^a)^b+(2^a+1^a)^b}+5x^{(1^a+2^a)^b+(3^a+2^a)^b}+2x^{(1^a+3^a)^b+(4^a+3^a)^b}+9x^{2(2^a+2^a)^b}+14x^{(2^a+3^a)^b+(3^a+3^a)^b}$$
$$+4x^{(2^a+4^a)^b+(4^a+4^a)^b}+6x^{2(3^a+4^a)^b}+2x^{(3^a+5^a)^b+(4^a+5^a)^b}.$$

Proof: From definition and by cardinalities of the edge partitions of *R*, we obtain

$$BKA^1_{a,b}(R)=\sum_{ue}x^{\left[d_R(u)^a+d_R(e)^a\right]^b}$$

$$=2x^{(1^a+1^a)^b+(2^a+1^a)^b}+5x^{(1^a+2^a)^b+(3^a+2^a)^b}+2x^{(1^a+3^a)^b+(4^a+3^a)^b}+9x^{(2^a+2^a)^b+(2^a+2^a)^b}$$
$$+14x^{(2^a+3^a)^b+(3^a+3^a)^b}+4x^{(2^a+4^a)^b+(4^a+4^a)^b}+6x^{(3^a+4^a)^b+(3^a+4^a)^b}+2x^{(3^a+5^a)^b+(4^a+5^a)^b}.$$

After simplification, we get the desired result.

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From Theorem 11, we obtain the following results.

Corollary 11.1. The *KG* Sombor exponential of *R* is

$$KG(R,x) = 2x^{\sqrt{2}+\sqrt{5}} + 5x^{\sqrt{5}+\sqrt{13}} + 2x^{\sqrt{10}+5} + 9x^{4\sqrt{2}} + 14x^{\sqrt{13}+3\sqrt{2}} + 4x^{2\sqrt{5}+4\sqrt{2}} + 6x^{10} + 2x^{\sqrt{34}+\sqrt{41}}.$$

Corollary 11.2. The modified *KG* Sombor exponential of *R* is

$${}^{m}KG(R,x) = 2x^{\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{5}}} + 5x^{\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{13}}} + 2x^{\frac{1}{\sqrt{10}}+\frac{1}{5}} + 9x^{\frac{1}{\sqrt{2}}} + 14x^{\frac{1}{\sqrt{13}}+\frac{1}{3\sqrt{2}}} + 4x^{\frac{1}{2\sqrt{5}}+\frac{1}{4\sqrt{2}}} + 6x^{\frac{2}{5}} + 2x^{\frac{1}{\sqrt{34}}+\frac{1}{\sqrt{41}}}.$$

We now compute the second Banhatti (*a*, *b*)-*KA* polynomial of the molecular graph of remdesivir.

Theorem 12. The second Banhatti (*a*, *b*)-*KA* polynomial of *R* is

$$BKA_{a,b}^{2}(R,x) = 2x^{(1^a+1^a)^b \times (2^a+1^a)^b} + 2x^{(1^a+2^a)^b \times (3^a+2^a)^b} + 5x^{(2^a+2^a)^{2b}} + 12x^{(2^a+3^a)^b \times (3^a+3^a)^b} + 2x^{(3^a+4^a)^{2b}}.$$

Proof: By definition and cardinalities of the edge partitions of *R*, we have

$$BKA_{a,b}^{2}(G) = \sum_{ue} x^{\left[d_G(u)^a \times d_G(e)^a\right]^b}$$

$$= 2x^{(1^a\times 1^a)^b+(2^a\times 1^a)^b} + 5x^{(1^a\times 2^a)^b+(3^a\times 2^a)^b} + 2x^{(1^a\times 3^a)^b+(4^a\times 3^a)^b} + 9x^{(2^a\times 2^a)^b+(2^a\times 2^a)^b}$$

$$+14x^{(2^a\times 3^a)^b+(3^a\times 3^a)^b} + 4x^{(2^a\times 4^a)^b+(4^a\times 4^a)^b} + 6x^{(3^a\times 4^a)^b+(3^a\times 4^a)^b} + 2x^{(3^a\times 5^a)^b+(4^a\times 5^a)^b}$$

gives the desired result after simplification.

5. CONCLUSION

In this paper, the expressions of some *KG* indices and their corresponding exponentials of chloroquine, hydroxychloroquine, remdesivir have been computed.

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