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DIFFERENT VERSIONS OF SOMBOR INDEX OF SOME CHEMICAL STRUCTURES

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ABSTRACT

Recently, a novel class of degree based topological indices was introduced, the so called Sombor indices. In this paper, we compute the Sombor index, second, third, fourth and neighborhood Sombor indices for some important chemical structures of drugs such as chloroquine, hydroxychloroquine and remdesivir.

Keywords: *Sombor index, second, third, fourth and neighborhood Sombor indices, chemical structure.*

Mathematics Subject Classification: *05C05, 05C07, 05C90*

1. INTRODUCTION

Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. Let $d(u)$ be the degree of a vertex u in a graph G. For undefined terms and notations, we refer [1].

Chemical Graph Theory is a branch of Mathematical Chemistry which has an important effect on the development of Chemical Sciences. A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. Topological indices are useful for establishing correlation between the structure of a molecular compound and its physicochemical properties. Numerous topological indices [2] have been considered in Theoretical Chemistry and have found some applications, especially in QSPR/QSAR research, see [3, 4].

In [5], Gutman introduced the Sombor index of a graph and defined it as

$$SO(G)=\sum_{uv\in E(G)}\sqrt{d(u)^2+d(v)^2}.$$

Motivated by the previous research on Sombor index and its applications, the second, third and fourth and neighborhood Sombor indices [6] of the molecular graph were defined as follows:

The second Sombor index of a molecular graph G is defined as

$$SO_2(G)=\sum_{uv\in E(G)}\sqrt{n(u)^2+n(v)^2}$$

where the number $n(u)$ of vertices of G lying closer to the vertex u than to the vertex v for the edge uv of a graph G.

The third Sombor index of a molecular graph G is defined as

$$SO_3(G)=\sum_{uv\in E(G)}\sqrt{m(u)^2+m(v)^2}$$

where the number $m(u)$ of edges of G lying closer to the vertex u than to the vertex v for the edge uv of a graph G.

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The fourth Sombor index of a molecular graph G is defined as

$$SO_4(G)=\sum_{uv\in E(G)}\sqrt{\varepsilon(u)^2+\varepsilon(v)^2}$$

where the number □(u) is the eccentricity of vertex u.

The neighborhood (or fifth) Sombor index of a molecular graph G is defined as

$$NSO(G)=\sum_{uv\in E(G)}\sqrt{s(u)^2+s(v)^2}$$

where $s(u)$ is the sum of the degrees of all vertices adjacent to vertex u.

Recently, some Sombor indices were studied, for example, in [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19] and some new versions of topological indices were studied [20, 21, 22, 23, 24, 25 26, 27].

In this study, we compute the Sombor index, second, third, fourth and neighborhood Sombor indices for certain chemical structures such as chloroquine, hydroxychloroquine and remdesivir. For chemical structures, see [28, 29].

2. 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_1 be the chemical structure of chloroquine. This structure has 21 atoms and 23 bonds, see Figure 1.

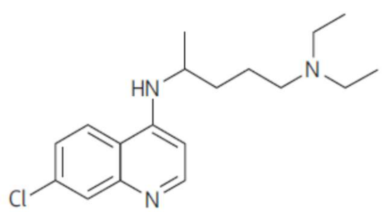

Figure 1. Chemical structure of chloroquine

From Figure 1, we obtain that
(i) $\{(d(u), d(v)) \setminus uv \in E(G_1)\}$ has 5 bond set partitions,
(ii) $\{(n(u), n(v)) \setminus uv \in E(G_1)\}$ has 10 bond set partitions,
(iii) $\{(m(u), m(v)) \setminus uv \in E(G_1)\}$ has 12 bond set partitions,
(iv) $\{(\varepsilon(u), \varepsilon(v)) \setminus uv \in E(G_1)\}$ has 7 bond set partitions,
(iv) $\{(s(u), s(v)) \setminus uv \in E(G_1)\}$ has 10 bond set partitions.

Table 1. Bond set partitions of chloroquine

$d(u), d(v) \setminus uv \in E(G_1)$	(1, 2)	(1,3)	(2, 2)	(2, 3)	(3, 3)	
Number of bonds	2	2	5	12	2	
$n(u), n(v) \setminus uv \in E(G_1)$	(1,19)	(1,20)	(2,18)	(3,17)	(4,16)	
Number of bonds	2	4	2	4	1	
	(5,15)	(6,14)	(7,13)	(9,11)	(10,10)	
	4	1	3	1	1	
$m(u), m(v) \setminus uv \in E(G_1)$	(1,21)	(1,22)	(2,19)	(3,18)	(4,17)	(5,15)
Number of bonds	2	4	2	4	1	3
	(5,16)	(6,15)	(7,14)	(8,13)	(9,13)	(10,12)
	1	1	2	1	1	1

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$\varepsilon(u), \varepsilon(v) \setminus uv \in E(G_1)$	(7,7)	(8,7)	(8,9)	(9,10)	(10,11)
Number of bonds	1	3	3	4	5
	(11,12)	(12,13)			
	4	3			
$s(u), s(v) \setminus uv \in E(G_1)$					
Number of bonds	(2,4)	(3,5)	(4,5)	(4,6)	(5,5)
	2	2	4	2	3
	(5,6)	(5,7)	(5,8)	(6,7)	(7,8)
	3	2	1	2	2

In the following theorem, we compute the different versions Sombor indices of chloroquine.

Theorem 1. Let G_1 be the chemical structure of chloroquine. Then

(i) $SO(G_1) = 76.6907235789.$

(ii) $SO_2(G_1) = 400.246770763.$

(iii) $SO_3(G_1) = 417.159690973.$

(iv) $SO_4(G_1) = 324.250256459.$

(v) $NSO(G_1) = 171.622842421.$

Proof: By using the definitions and cardinalities of the bond partition of G_1, we deduce

(i) $$SO(G_1) = \sum_{uv \in E(G_1)} \sqrt{d(u)^2 + d(v)^2}$$

$$= (1^2+2^2)^{\frac{1}{2}} 2 + (1^2+3^2)^{\frac{1}{2}} 2 + (2^2+2^2)^{\frac{1}{2}} 5 + (2^2+3^2)^{\frac{1}{2}} 12 + (3^2+3^2)^{\frac{1}{2}} 2.$$

After simplification, we get the desired result.

(ii) $$SO_2(G_1) = \sum_{uv \in E(G_1)} \sqrt{n(u)^2 + n(v)^2}$$

$$= (1^2+19^2)^{\frac{1}{2}} 2 + (1^2+20^2)^{\frac{1}{2}} 4 + (2^2+18^2)^{\frac{1}{2}} 2 + (3^2+17^2)^{\frac{1}{2}} 4 + (4^2+16^2)^{\frac{1}{2}}$$
$$+ (5^2+15^2)^{\frac{1}{2}} 4 + (6^2+14^2)^{\frac{1}{2}} + (7^2+13^2)^{\frac{1}{2}} 3 + (9^2+11^2)^{\frac{1}{2}} + (10^2+10^2)^{\frac{1}{2}}.$$

After simplification, we get the desired result.

(iii) $$SO_3(G_1) = \sum_{uv \in E(G_1)} \sqrt{m(u)^2 + m(v)^2}$$

$$= (1^2+21^2)^{\frac{1}{2}} 2 + (1^2+22^2)^{\frac{1}{2}} 4 + (2^2+19^2)^{\frac{1}{2}} 2 + (3^2+18^2)^{\frac{1}{2}} 4 + (4^2+17^2)^{\frac{1}{2}} + (5^2+15^2)^{\frac{1}{2}} 3$$
$$+ (5^2+16^2)^{\frac{1}{2}} + (6^2+15^2)^{\frac{1}{2}} + (7^2+14^2)^{\frac{1}{2}} 2 + (8^2+13^2)^{\frac{1}{2}} + (9^2+13^2)^{\frac{1}{2}} + (10^2+112^2)^{\frac{1}{2}}.$$

After simplification, we get the desired result.

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(iv) $$SO_4(G_1) = \sum_{uv \in E(G_1)} \sqrt{\varepsilon(u)^2 + \varepsilon(v)^2}$$

$$= (7^2+7^2)^{\frac{1}{2}} + (8^2+7^2)^{\frac{1}{2}}3 + (8^2+9^2)^{\frac{1}{2}}3 + (9^2+10^2)^{\frac{1}{2}}4 + (10^2+11^2)^{\frac{1}{2}}5$$

$$+ (11^2+12^2)^{\frac{1}{2}}4 + (12^2+13^2)^{\frac{1}{2}}3.$$

After simplification, we get the desired result.

(v) $$NSO(G_1) = \sum_{uv \in E(G_1)} \sqrt{s(u)^2 + s(v)^2}$$

$$= (2^2+4^2)^{\frac{1}{2}}2 + (3^2+5^2)^{\frac{1}{2}}2 + (4^2+5^2)^{\frac{1}{2}}4 + (4^2+6^2)^{\frac{1}{2}}2 + (5^2+5^2)^{\frac{1}{2}}3$$

$$+ (5^2+6^2)^{\frac{1}{2}}3 + (5^2+7^2)^{\frac{1}{2}}2 + (5^2+8^2)^{\frac{1}{2}} + (6^2+7^2)^{\frac{1}{2}}2 + (7^2+8^2)^{\frac{1}{2}}2.$$

After simplification, we get the desired result.

3. 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 erythmatosus and rheumatoid arthritis .

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

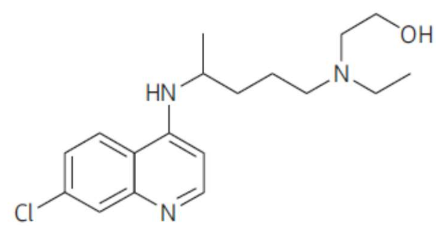

Figure 2. Chemical structure of hydroxychloroquine

From Figure 2, we obtain that

(i) $\{(d(u), d(v)) \setminus uv \in E(G_2)\}$ has 5 bond set partitions,
(ii) $\{(n(u), n(v)) \setminus uv \in E(G_2)\}$ has 9 bond set partitions,
(iii) $\{(m(u), m(v)) \setminus uv \in E(G_2)\}$ has 12 bond set partitions,
(iv) $\{(\varepsilon(u), \varepsilon(v)) \setminus uv \in E(G_2)\}$ has 7 bond set partitions,
(iv) $\{(s(u), s(v)) \setminus uv \in E(G_2)\}$ has 11 bond set partitions.

Table 2. Bond set partitions of hydroxychloroquine

$d(u), d(v) \setminus uv \in E(G_2)$	(1, 2)	(1,3)	(2, 2)	(2, 3)	(3, 3)	
Number of bonds	2	2	6	12	2	
$n(u), n(v) \setminus uv \in E(G_2)$	(1,20)	(1,21)	(2,19)	(3,18)	(5,16)	
Number of bonds	2	4	3	4	4	
	(6,15)	(7,14)	(10,11)	(8,13)		
	3	2	1	1		
$m(u), m(v) \setminus uv \in E(G_2)$	(1,22)	(1,23)	(2,20)	(2,21)	(3,19)	(5,16)
Number of bonds	2	4	2	1	4	3
	(5,17)	(6,16)	(7,15)	(8,14)	(10,13)	(11,12)
	1	1	1	3	1	1
$\varepsilon(u), \varepsilon(v) \setminus uv \in E(G_2)$	(7,8)	(8,9)	(9,10)	(10,11)	(11,12)	
Number of bonds	3	2	3	4	6	
	(12,13)	(13,14)				
	4	2				
$s(u), s(v) \setminus uv \in E(G_2)$						
Number of bonds	(2,3)	(2,4)	(3,5)	(4,5)	(4,6)	(5,5)
	1	1	3	4	1	3
	(5,6)	(5,7)	(5,8)	(6,7)	(7,8)	
	4	2	1	2	2	

In the following theorem, we compute the different versions of Sombor indices of hydroxychloroquine.

Theorem 2. Let G_2 be the chemical structure of hydroxychloroquine. Then
(i) $SO(G_2) = 79.5191507036.$
(ii) $SO_2(G_2) = 431.407282519.$
(iii) $SO_3(G_2) = 457.072156788.$
(iv) $SO_4(G_2) = 362.448867704.$
(v) $NSO(G_2) = 177.186356761.$

Proof: By using the definitions and cardinalities of the bond partition of G_1, we deduce

(i) $$SO(G_2) = \sum_{uv \in E(G_2)} \sqrt{d(u)^2 + d(v)^2}$$

$$= (1^2+2^2)^{\frac{1}{2}} 2 + (1^2+3^2)^{\frac{1}{2}} 2 + (2^2+2^2)^{\frac{1}{2}} 6 + (2^2+3^2)^{\frac{1}{2}} 12 + (3^2+3^2)^{\frac{1}{2}} 2.$$

After simplification, we get the desired result.

(ii) $$SO_2(G_2) = \sum_{uv \in E(G_2)} \sqrt{n(u)^2 + n(v)^2}$$

$$= (1^2+20^2)^{\frac{1}{2}} 2 + (1^2+21^2)^{\frac{1}{2}} 4 + (2^2+19^2)^{\frac{1}{2}} 3 + (3^2+18^2)^{\frac{1}{2}} 4 + (5^2+16^2)^{\frac{1}{2}} 4$$
$$+ (6^2+15^2)^{\frac{1}{2}} 3 + (7^2+14^2)^{\frac{1}{2}} 2 + (10^2+11^2)^{\frac{1}{2}} + (8^2+13^2)^{\frac{1}{2}}.$$

After simplification, we get the desired result.

(iii) $$SO_3(G_2) = \sum_{uv \in E(G_2)} \sqrt{m(u)^2 + m(v)^2}$$

$$= (1^2 + 22^2)^{\frac{1}{2}} 2 + (1^2 + 23^2)^{\frac{1}{2}} 4 + (2^2 + 20^2)^{\frac{1}{2}} 2 + (2^2 + 21^2)^{\frac{1}{2}} + (3^2 + 19^2)^{\frac{1}{2}} 4 + (5^2 + 16^2)^{\frac{1}{2}} 3$$
$$+ (5^2 + 17^2)^{\frac{1}{2}} + (6^2 + 16^2)^{\frac{1}{2}} + (7^2 + 15^2)^{\frac{1}{2}} + (8^2 + 14^2)^{\frac{1}{2}} 3 + (10^2 + 13^2)^{\frac{1}{2}} + (11^2 + 12^2)^{\frac{1}{2}}.$$

After simplification, we get the desired result.

(iv) $$SO_4(G_2) = \sum_{uv \in E(G_2)} \sqrt{\varepsilon(u)^2 + \varepsilon(v)^2}$$

$$= (7^2 + 8^2)^{\frac{1}{2}} 3 + (8^2 + 9^2)^{\frac{1}{2}} 2 + (9^2 + 10^2)^{\frac{1}{2}} 3 + (10^2 + 11^2)^{\frac{1}{2}} 4 + (11^2 + 12^2)^{\frac{1}{2}} 6$$
$$+ (12^2 + 13^2)^{\frac{1}{2}} 4 + (13^2 + 14^2)^{\frac{1}{2}} 2.$$

After simplification, we get the desired result.

(v) $$NSO(G_2) = \sum_{uv \in E(G_2)} \sqrt{s(u)^2 + s(v)^2}$$

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

After simplification, we get the desired result.

4. RESULTS AND DISCUSSION: REMDESIVIR

Let G_3 be the molecular graph of remdesivir. This graph has 41 atoms and 44 bonds.

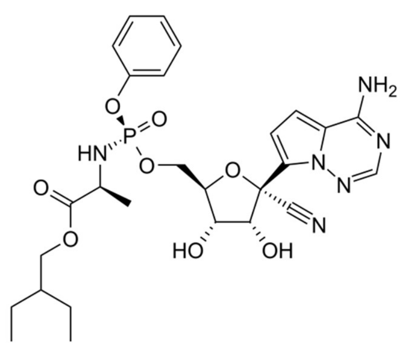

Figure 3. Chemical structure of remdesivir

From Figure 2, we obtain that

(i) $\{(d(u), d(v)) \setminus uv \in E(G_3)\}$ has 8 bond set partitions,
(ii) $\{(n(u), n(v)) \setminus uv \in E(G_3)\}$ has 25 bond set partitions,
(iii) $\{(m(u), m(v)) \setminus uv \in E(G_3)\}$ has 23 bond set partitions,
(iv) $\{(\varepsilon(u), \varepsilon(v)) \setminus uv \in E(G_3)\}$ has 11 bond set partitions,
(iv) $\{(s(u), s(v)) \setminus uv \in E(G_3)\}$ has 23 bond set partitions.

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Table 3. Bond set partitions of remdesivir

$d(u), d(v) \backslash uv\in E(G_3)$	(1,2)	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(2, 4)	(3, 3)	(3, 4)
Number of bonds	2	5	2	9	14	4	6	2
$n(u), n(v) \backslash uv\in E(G_3)$	(1,6)	(1,34)	(1,38)	(1,39)	(2,37)	(3,12)	(3,23)	(3,36)
Number of bonds	1	1	2	9	8	1	1	2
	(4,32)	(4,33)	(4,34)	(4,35)	(5,34)	(6,32)	(6,33)	(8,31)
	1	1	1	1	2	1	2	1
	(9,30)	(10,29)	(11,28)	(12,24)	(13,24)	(13,25)	(17,22)	(18,21)
	1	1	1	1	1	1	1	1
	(19,20)							
	1							
$m(u),m(v)\backslash uv\in E(G_3)$	(1,42)	(1,43)	(2,8)	(2,32)	(2,40)	(2,41)	(3,39)	(4,15)
Number of bonds	2	9	1	1	2	6	2	1
	(4,39)	(4,26)	(5,37)	(5,38)	(6,35)	(6,37)	(7,36)	(8,35)
	1	1	2	1	1	2	1	2
	(10,33)	(11,32)	(15,27)	(16,26)	(16,27)	(20,23)	(21,22)	
	1	2	1	1	1	1	2	
$\varepsilon(u),\varepsilon(v)\backslash uv\in E(G_3)$	(9,10)	(10,11)	(11,12)	(12,13)	(13,13)	(13,14)	(14,15)	(15,16)
Number of bonds	2	4	4	7	1	7	5	4
	(16,16)	(16,17)	(17,18)					
	1	4	5					
$s(u),s(v)\backslash uv\in E(G_3)$	(2,4)	(3,6)	(3,7)	(3,8)	(4,4)	(4,5)	(4,6)	(4,7)
Number of bonds	2	3	1	1	2	4	2	1
	(4,9)	(5,5)	(5,6)	(5,7)	(5,8)	(5,9)	(6,6)	(6,7)
	1	2	6	1	2	1	1	3
	(6,8)	(7,7)	(7,8)	(7,9)	(8,8)	(8,9)	(9,9)	
	1	4	1	1	1	2	1	

In the following theorem, we compute the different versions of Sombor indices of remdesivir.

Theorem 3. Let G_3 be the chemical structure of remdesivir. Then

(i) $SO(G_3) = 157.807685429.$

(ii) $SO_2(G_3) = 1464.25762961.$

(iii) $SO_3(G_3) = 1613.39486006.$

(iv) $SO_4(G_3) = 857.569848801.$

(v) $NSO(G_3) = 369.156352285.$

Proof: By using the definitions and cardinalities of the bond partition of G_3, we deduce

(i) $$SO(G_3) = \sum_{uv\in E(G_3)} \sqrt{d(u)^2 + d(v)^2}$$

$$= (1^2+2^2)^{\frac{1}{2}}2 + (1^2+3^2)^{\frac{1}{2}}5 + (1^2+4^2)^{\frac{1}{2}}2 + (2^2+2^2)^{\frac{1}{2}}9 + (2^2+3^2)^{\frac{1}{2}}14$$

$$+(2^2+4^2)^{\frac{1}{2}}4 + (3^2+3^2)^{\frac{1}{2}}6 + (3^2+4^2)^{\frac{1}{2}}2.$$

After simplification, we get the desired result.

(ii) $$SO_2(G_3) = \sum_{uv\in E(G_3)} \sqrt{n(u)^2 + n(v)^2}$$

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$$=(1^2+6^2)^{\frac{1}{2}}+(1^2+34^2)^{\frac{1}{2}}+(1^2+38^2)^{\frac{1}{2}}2+(1^2+39^2)^{\frac{1}{2}}9+(2^2+37^2)^{\frac{1}{2}}8+(3^2+12^2)^{\frac{1}{2}}$$
$$+(3^2+23^2)^{\frac{1}{2}}+(3^2+36^2)^{\frac{1}{2}}2+(4^2+32^2)^{\frac{1}{2}}+(4^2+33^2)^{\frac{1}{2}}+(4^2+34^2)^{\frac{1}{2}}+(4^2+35^2)^{\frac{1}{2}}$$
$$+(5^2+34^2)^{\frac{1}{2}}2+(6^2+32^2)^{\frac{1}{2}}+(6^2+33^2)^{\frac{1}{2}}2+(8^2+31^2)^{\frac{1}{2}}+(9^2+30^2)^{\frac{1}{2}}+(10^2+29^2)^{\frac{1}{2}}$$
$$+(11^2+28^2)^{\frac{1}{2}}+(12^2+24^2)^{\frac{1}{2}}+(13^2+24^2)^{\frac{1}{2}}+(13^2+25^2)^{\frac{1}{2}}+(17^2+22^2)^{\frac{1}{2}}$$
$$+(18^2+21^2)^{\frac{1}{2}}+(19^2+20^2)^{\frac{1}{2}}.$$

After simplification, we get the desired result.

(iii) $$SO_3(G_3)=\sum_{uv\in E(G_3)}\sqrt{m(u)^2+m(v)^2}$$
$$=(1^2+42^2)^{\frac{1}{2}}2+(1^2+43^2)^{\frac{1}{2}}9+(2^2+8^2)^{\frac{1}{2}}+(2^2+32^2)^{\frac{1}{2}}+(2^2+40^2)^{\frac{1}{2}}2+(2^2+41^2)^{\frac{1}{2}}6$$
$$+(3^2+39^2)^{\frac{1}{2}}2+(4^2+15^2)^{\frac{1}{2}}+(4^2+39^2)^{\frac{1}{2}}+(4^2+26^2)^{\frac{1}{2}}+(5^2+37^2)^{\frac{1}{2}}2+(5^2+38^2)^{\frac{1}{2}}$$
$$+(6^2+35^2)^{\frac{1}{2}}+(6^2+37^2)^{\frac{1}{2}}2+(7^2+36^2)^{\frac{1}{2}}+(8^2+35^2)^{\frac{1}{2}}2+(10^2+33^2)^{\frac{1}{2}}+(11^2+32^2)^{\frac{1}{2}}2$$
$$+(15^2+27^2)^{\frac{1}{2}}+(16^2+26^2)^{\frac{1}{2}}+(16^2+27^2)^{\frac{1}{2}}+(20^2+23^2)^{\frac{1}{2}}+(21^2+22^2)^{\frac{1}{2}}2.$$

After simplification, we get the desired result.

(iv) $$SO_4(G_3)=\sum_{uv\in E(G_3)}\sqrt{\varepsilon(u)^2+\varepsilon(v)^2}$$

$$=(9^2+10^2)^{\frac{1}{2}}2+(10^2+11^2)^{\frac{1}{2}}4+(11^2+12^2)^{\frac{1}{2}}4+(12^2+13^2)^{\frac{1}{2}}7+(13^2+13^2)^{\frac{1}{2}}+(13^2+14^2)^{\frac{1}{2}}7$$
$$+(14^2+15^2)^{\frac{1}{2}}5+(15^2+16^2)^{\frac{1}{2}}4+(16^2+16^2)^{\frac{1}{2}}+(16^2+17^2)^{\frac{1}{2}}4+(17^2+18^2)^{\frac{1}{2}}5.$$

After simplification, we get the desired result.

(v) $$NSO(G_3)=\sum_{uv\in E(G_3)}\sqrt{s(u)^2+s(v)^2}$$
$$=(2^2+4^2)^{\frac{1}{2}}2+(3^2+6^2)^{\frac{1}{2}}3+(3^2+7^2)^{\frac{1}{2}}+(3^2+8^2)^{\frac{1}{2}}+(4^2+4^2)^{\frac{1}{2}}2+(4^2+5^2)^{\frac{1}{2}}4$$
$$+(4^2+6^2)^{\frac{1}{2}}2+(4^2+7^2)^{\frac{1}{2}}+(4^2+9^2)^{\frac{1}{2}}+(5^2+5^2)^{\frac{1}{2}}2+(5^2+6^2)^{\frac{1}{2}}6+(5^2+7^2)^{\frac{1}{2}}$$
$$+(5^2+8^2)^{\frac{1}{2}}2+(5^2+9^2)^{\frac{1}{2}}+(6^2+6^2)^{\frac{1}{2}}+(6^2+7^2)^{\frac{1}{2}}3+(6^2+8^2)^{\frac{1}{2}}+(7^2+7^2)^{\frac{1}{2}}4$$
$$+(7^2+8^2)^{\frac{1}{2}}+(7^2+9^2)^{\frac{1}{2}}+(8^2+8^2)^{\frac{1}{2}}+(8^2+9^2)^{\frac{1}{2}}2+(9^2+9^2)^{\frac{1}{2}}.$$

After simplification, we get the desired result.

5. CONCLUSION

In this study, we have found computational values of molecular structures such as chloroquine, hydroxychloroquine and remdesivir. These values can be useful in planning the effective use of these drugs in Medical Science.

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