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Augmented Euler Sombor Index of Certain Chemical Drugs

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Abstract: ***In this paper, we introduce the augmented Euler Sombor and the reciprocal augmented Euler Sombor indices of a graph. We compute these newly defined augmented Euler Sombor indices for certain chemical structures.***

Keywords: augmented Euler Sombor index, reciprocal augmented Euler Sombor 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.

The Euler Sombor index [1] or Nirmala alpha Gourava index [2] of a graph is defined as

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

Recently, some Sombor indices were studied in [3-10].

We introduce the augmented Euler Sombor index of a graph G as

$$AEU(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_G(u)^2+d_G(v)^2+d_G(u)d_G(v)}{d_G(u)+d_G(v)-2}}.$$

We define the reciprocal augmented Euler Sombor index of a graph G as

$$RAEU(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)^2+d_G(v)^2+d_G(u)d_G(v)}}.$$

In this research, we compute the augmented Euler Sombor and reciprocal augmented Euler Sombor indices for certain chemical structures.

Results and Discussion: Chloroquine

Let G be the molecular structure of chloroquine. Clearly G has 21 vertices and 23 edges, see Figure 1.

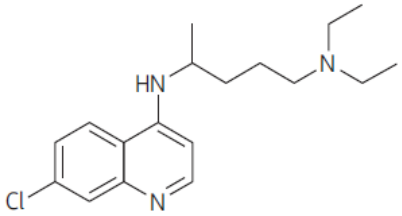

Figure 1

The edge set of G can be divided into five partitions based on the degree of end vertices of each edge as given in Table 1.

Table 1: Edge partition of G

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

We calculate the augmented Euler Sombor and reciprocal augmented Euler Sombor indices of chloroquine as follows.

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

$$AEU(G)=2\sqrt{7}+2\sqrt{\frac{13}{2}}+5\sqrt{6}+12\sqrt{\frac{19}{3}}+\sqrt{\frac{27}{4}}.$$

Proof: By using the definition and edge partition of G, we deduce

$$AEU(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_G(u)^2+d_G(v)^2+d_G(u)d_G(v)}{d_G(u)+d_G(v)-2}}$$

$$=2\sqrt{\frac{1^2+2^2+1\times 2}{1+2-2}}+2\sqrt{\frac{1^2+3^2+1\times 3}{1+3-2}}+5\sqrt{\frac{2^2+2^2+2\times 2}{2+2-2}}$$

$$+12\sqrt{\frac{2^2+3^2+2\times 3}{2+3-2}}+2\sqrt{\frac{3^2+3^2+3\times 3}{3+3-2}}$$

$$=2\sqrt{7}+2\sqrt{\frac{13}{2}}+5\sqrt{6}+12\sqrt{\frac{19}{3}}+\sqrt{\frac{27}{4}}.$$

Theorem 2. Let G be the chemical structure of chloroquine. Then

$$RAEU(G)=2\sqrt{\frac{1}{7}}+2\sqrt{\frac{2}{13}}+5\sqrt{\frac{1}{6}}+12\sqrt{\frac{3}{19}}+2\sqrt{\frac{4}{27}}.$$

Proof: By using the definition and edge partition of G, we deduce

$$RAEU(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)^2+d_G(v)^2+d_G(u)d_G(v)}}$$

$$=2\sqrt{\frac{1+2-2}{1^2+2^2+1\times 2}}+2\sqrt{\frac{1+3-2}{1^2+3^2+1\times 3}}+5\sqrt{\frac{2+2-2}{2^2+2^2+2\times 2}}$$

$$+12\sqrt{\frac{2+3-2}{2^2+3^2+2\times3}}+2\sqrt{\frac{3+3-2}{3^2+3^2+3\times3}}$$
$$=2\sqrt{\frac{1}{7}}+2\sqrt{\frac{2}{13}}+5\sqrt{\frac{1}{6}}+12\sqrt{\frac{3}{19}}+2\sqrt{\frac{4}{27}}.$$

Results and Discussion: Hydroxychloroquine

Let H be the molecular structure of hydroxychloroquine. Clearly H has 22 vertices and 24 edges, see Figure 2.

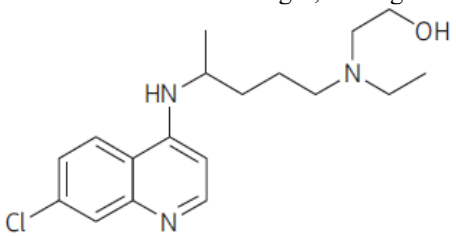

Figure 2

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 given in Table 2:

Table 2: Edge partition of H

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

We calculate the augmented Euler Sombor and reciprocal augmented Euler Sombor indices of hydroxychloroquine as follows.

Theorem 3. Let H be the chemical structure of hydroxychloroquine. Then

$$AEU(H)=2\sqrt{7}+2\sqrt{\frac{13}{2}}+6\sqrt{6}+12\sqrt{\frac{19}{3}}+\sqrt{\frac{27}{4}}.$$

Proof: By using the definition and edge partition of H, we deduce

$$AEU(H)=\sum_{uv\in E(H)}\sqrt{\frac{d_H(u)^2+d_H(v)^2+d_H(u)d_H(v)}{d_H(u)+d_H(v)-2}}$$

$$=2\sqrt{\frac{1^2+2^2+1\times2}{1+2-2}}+2\sqrt{\frac{1^2+3^2+1\times3}{1+3-2}}+6\sqrt{\frac{2^2+2^2+2\times2}{2+2-2}}$$
$$+12\sqrt{\frac{2^2+3^2+2\times3}{2+3-2}}+2\sqrt{\frac{3^2+3^2+3\times3}{3+3-2}}$$
$$=2\sqrt{7}+2\sqrt{\frac{13}{2}}+6\sqrt{6}+12\sqrt{\frac{19}{3}}+\sqrt{\frac{27}{4}}.$$

Theorem 4. Let H be the chemical structure of chloroquine. Then

$$RAEU(H)=2\sqrt{\frac{1}{7}}+2\sqrt{\frac{2}{13}}+6\sqrt{\frac{1}{6}}+12\sqrt{\frac{3}{19}}+2\sqrt{\frac{4}{27}}.$$

Proof: By using the definition and edge partition of H, we deduce

$$RAEU(H)=\sum_{uv\in E(H)}\sqrt{\frac{d_H(u)+d_H(v)-2}{d_H(u)^2+d_H(v)^2+d_H(u)d_H(v)}}$$

$$=2\sqrt{\frac{1+2-2}{1^2+2^2+1\times2}}+2\sqrt{\frac{1+3-2}{1^2+3^2+1\times3}}+6\sqrt{\frac{2+2-2}{2^2+2^2+2\times2}}$$
$$+12\sqrt{\frac{2+3-2}{2^2+3^2+2\times3}}+2\sqrt{\frac{3+3-2}{3^2+3^2+3\times3}}$$
$$=2\sqrt{\frac{1}{7}}+2\sqrt{\frac{2}{13}}+6\sqrt{\frac{1}{6}}+12\sqrt{\frac{3}{19}}+2\sqrt{\frac{4}{27}}.$$

Results and Discussion: Remdesvir

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

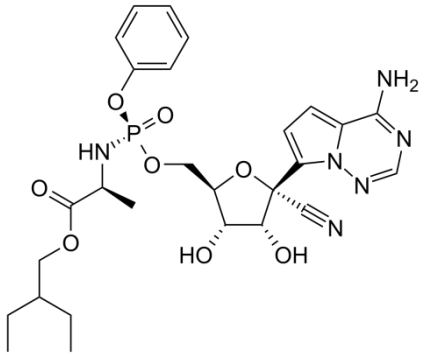

Figure 3

In R, the edge set $E(R)$ can be divided into eight partitions based on the degree of end vertices of each edge as given in Table 3:

Table 3: Edge partition of R

$d_G(u)$, $d_G(v)$\ $uv\in E(R)$	(1, 2)	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(2, 4)	(3,3)	(3,4)
No. of edges	2	5	2	9	14	4	6	2

We calculate the augmented Euler Sombor and reciprocal augmented Euler Sombor indices of remdesivir as follows.

Theorem 5. Let R be the chemical structure of remdesivir. Then

$$AEU(R)=8\sqrt{7}+5\sqrt{\frac{13}{2}}+9\sqrt{6}+14\sqrt{\frac{19}{3}}+6\sqrt{\frac{27}{4}}+2\sqrt{\frac{37}{5}}.$$

Proof: By using the definitions and edge partition of R, we deduce

$$AEU(R)=\sum_{uv\in E(R)}\sqrt{\frac{d_R(u)^2+d_R(v)^2+d_R(u)d_R(v)}{d_R(u)+d_R(v)-2}}$$
$$=2\sqrt{\frac{1^2+2^2+1\times2}{1+2-2}}+5\sqrt{\frac{1^2+3^2+1\times3}{1+3-2}}+2\sqrt{\frac{1^2+4^2+1\times4}{1+4-2}}$$
$$+9\sqrt{\frac{2^2+2^2+2\times2}{2+2-2}}+14\sqrt{\frac{2^2+3^2+2\times3}{2+3-2}}+4\sqrt{\frac{2^2+4^2+2\times4}{2+4-2}}$$
$$+6\sqrt{\frac{3^2+3^2+3\times3}{3+3-2}}+2\sqrt{\frac{3^2+4^2+3\times4}{3+4-2}}$$

$$=8\sqrt{7}+5\sqrt{\frac{13}{2}}+9\sqrt{6}+14\sqrt{\frac{19}{3}}+6\sqrt{\frac{27}{4}}+2\sqrt{\frac{37}{5}}.$$

Theorem 6. Let R be the chemical structure of remdesivir. Then

$$RAEU(R)=8\sqrt{\frac{1}{7}}+5\sqrt{\frac{2}{13}}+9\sqrt{\frac{1}{6}}+14\sqrt{\frac{3}{19}}+6\sqrt{\frac{4}{27}}+2\sqrt{\frac{5}{37}}.$$

Proof: By using the definitions and edge partition of R, we deduce

$$RAEU(R)=\sum_{uv\in E(G)}\sqrt{\frac{d_R(u)+d_R(v)-2}{d_R(u)^2+d_R(v)^2+d_R(u)d_R(v)}}$$

$$=2\sqrt{\frac{1+2-2}{1^2+2^2+1\times 2}}+5\sqrt{\frac{1+3-2}{1^2+3^2+1\times 3}}+2\sqrt{\frac{1+4-2}{1^2+4^2+1\times 4}}$$

$$+9\sqrt{\frac{2+2-2}{2^2+2^2+2\times 2}}+14\sqrt{\frac{2+3-2}{2^2+3^2+2\times 3}}+4\sqrt{\frac{2+4-2}{2^2+4^2+2\times 4}}$$

$$+6\sqrt{\frac{3+3-2}{3^2+3^2+3\times 3}}+2\sqrt{\frac{3+4-2}{3^2+4^2+3\times 4}}$$

$$=8\sqrt{\frac{1}{7}}+5\sqrt{\frac{2}{13}}+9\sqrt{\frac{1}{6}}+14\sqrt{\frac{3}{19}}+6\sqrt{\frac{4}{27}}+2\sqrt{\frac{5}{37}}.$$

2. Conclusion

In this research, the augmented Euler Sombor and reciprocal augmented Euler Sombor indices of a graph are defined. Furthermore, the augmented Euler Sombor and reciprocal augmented Euler Sombor indices for certain chemical structures are determined.

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