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Calculation of Degree Ratio Harmonic Index of Certain Chemical Structures

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

Keywords: degree ratio harmonic index, reciprocal degree ratio harmonic 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.

In [1], the degree ratio Nirmala index of a graph is defined as

$$DRN(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_G(u)}{d_G(v)}+\frac{d_G(v)}{d_G(u)}}.$$

Recently, some degree ratio indices were studied in [2, 3, 4, 5, 6].

In view of the degree ratio Nirmala index, we propose the degree ratio Nirmala polynomial of a graph G and it is defined as

$$DRN(G,x)=\sum_{uv\in E(G)}x^{\sqrt{\frac{d_G(u)}{d_G(v)}+\frac{d_G(v)}{d_G(u)}}}.$$

The harmonic index [7] of a graph is defined as

$$H(G)=\sum_{uv\in E(G)}\frac{2}{d_G(u)+d_G(v)}.$$

Recently, some harmonic indices were studied in [8, 9].

We define the degree ratio harmonic index of a graph G as

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

In view of the degree ratio harmonic index, we propose the degree ratio harmonic polynomial of a graph G and it is defined as

$$DRH(G,x)=\sum_{uv\in E(G)}x^{\frac{2d_G(u)d_G(v)}{d_G(u)^2+d_G(v)^2}}.$$

We define the reciprocal degree ratio harmonic index of a graph G as

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

In view of the reciprocal degree ratio harmonic index, we propose the reciprocal degree ratio harmonic polynomial of a graph G and it is defined as

$$RDRH(G,x)=\sum_{uv\in E(G)}x^{\frac{d_G(u)^2+d_G(v)^2}{2d_G(u)d_G(v)}}.$$

In this research, we compute the degree ratio harmonic and reciprocal degree ratio harmonic indices for certain chemical structures.

2. Results and Discussion: Chloroquine

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

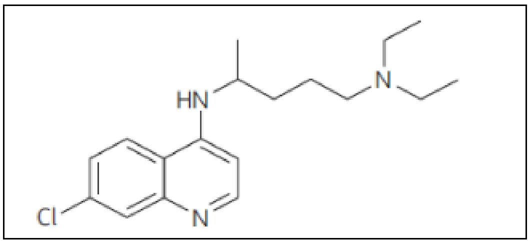

Figure 1

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

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

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

$$DRN(G)==2\sqrt{\frac{5}{2}}+2\sqrt{\frac{10}{3}}+7\sqrt{2}+12\sqrt{\frac{13}{6}}.$$

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

$$DRN(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_G(u)}{d_G(v)}+\frac{d_G(v)}{d_G(u)}}$$

$$=2\sqrt{\frac{1}{2}+\frac{2}{1}}+2\sqrt{\frac{1}{3}+\frac{3}{1}}+5\sqrt{\frac{2}{2}+\frac{2}{2}}$$
$$+12\sqrt{\frac{2}{3}+\frac{3}{2}}+2\sqrt{\frac{3}{3}+\frac{3}{3}}$$
$$=2\sqrt{\frac{5}{2}}+2\sqrt{\frac{10}{3}}+7\sqrt{2}+12\sqrt{\frac{13}{6}}.$$

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

$$DRN(G,x)=2x^{\sqrt{\frac{5}{2}}}+2x^{\sqrt{\frac{10}{3}}}+7x^{\sqrt{2}}+12x^{\sqrt{\frac{13}{6}}}.$$

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

$$DRN(G,x)=\sum_{uv\in E(G)} x^{\sqrt{\frac{d_G(u)}{d_G(v)}+\frac{d_G(v)}{d_G(u)}}}$$
$$=2x^{\sqrt{\frac{1}{2}+\frac{2}{1}}}+2x^{\sqrt{\frac{1}{3}+\frac{3}{1}}}+5x^{\sqrt{\frac{2}{2}+\frac{2}{2}}}$$
$$+12x^{\sqrt{\frac{2}{3}+\frac{3}{2}}}+2x^{\sqrt{\frac{3}{3}+\frac{3}{3}}}$$
$$=2x^{\sqrt{\frac{5}{2}}}+2x^{\sqrt{\frac{10}{3}}}+7x^{\sqrt{2}}+12x^{\sqrt{\frac{13}{6}}}.$$

Theorem 3. Let G be the chemical structure of chloroquine. Then

$$DRH(G)=\frac{1357}{65}.$$

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

$$DRH(G)=\sum_{uv\in E(G)}\frac{2d_G(u)d_G(v)}{d_G(u)^2+d_G(v)^2}$$
$$=2\frac{2\times1\times2}{1^2+2^2}+2\frac{2\times1\times3}{1^2+3^2}+5\frac{2\times2\times2}{2^2+2^2}$$
$$+12\frac{2\times2\times3}{2^2+3^2}+2\frac{2\times3\times3}{3^2+3^2}$$
$$=\frac{1357}{65}.$$

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

$$DRH(G,x)==2x^{\frac{4}{5}}+2x^{\frac{3}{5}}+7x^{1}+12x^{\frac{12}{13}}.$$

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

$$DRH(G,x)=\sum_{uv\in E(G)} x^{\frac{2d_G(u)d_G(v)}{d_G(u)^2+d_G(v)^2}}$$
$$=2x^{\frac{2\times1\times2}{1^2+2^2}}+2x^{\frac{2\times1\times3}{1^2+3^2}}+5x^{\frac{2\times2\times2}{2^2+2^2}}$$
$$+12x^{\frac{2\times2\times3}{2^2+3^2}}+2x^{\frac{2\times3\times3}{3^2+3^2}}$$
$$=2x^{\frac{4}{5}}+2x^{\frac{3}{5}}+7x^{1}+12x^{\frac{12}{13}}.$$

Theorem 5. Let G be the chemical structure of chloroquine. Then

$$RDRH(G)=\frac{155}{6}.$$

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

$$RDRH(G)=\sum_{uv\in E(G)}\frac{d_G(u)^2+d_G(v)^2}{2d_G(u)d_G(v)}$$
$$=2\frac{1^2+2^2}{2\times1\times2}+2\frac{1^2+3^2}{2\times1\times3}+5\frac{2^2+2^2}{2\times2\times2}$$
$$+12\frac{2^2+3^2}{2\times2\times3}+2\frac{3^2+3^2}{2\times3\times3}$$
$$=\frac{155}{6}.$$

Theorem 6. Let G be the chemical structure of chloroquine. Then

$$RDRH(G,x)=2x^{\frac{5}{4}}+2x^{\frac{5}{3}}+2x^{1}+12x^{\frac{13}{12}}.$$

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

$$RDRH(G,x)=\sum_{uv\in E(G)} x^{\frac{d_G(u)^2+d_G(v)^2}{2d_G(u)d_G(v)}}$$
$$=2x^{\frac{1^2+2^2}{2\times1\times2}}+2x^{\frac{1^2+3^2}{2\times1\times3}}+5x^{\frac{2^2+2^2}{2\times2\times2}}$$
$$+12x^{\frac{2^2+3^2}{2\times2\times3}}+2x^{\frac{3^2+3^2}{2\times3\times3}}$$
$$=2x^{\frac{5}{4}}+2x^{\frac{5}{3}}+2x^{1}+12x^{\frac{13}{12}}.$$

3. Results and Discussion: Hydroxychloroquine

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

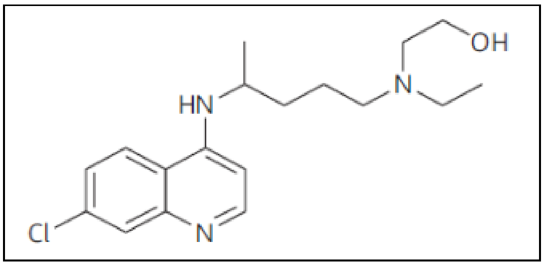

Figure 2

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

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

Theorem 7. Let H be the chemical structure of hydroxychloroquine. Then

$$DRN(H) == 2\sqrt{\frac{5}{2}} + 2\sqrt{\frac{10}{3}} + 8\sqrt{2} + 12\sqrt{\frac{13}{6}}.$$

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

$$DRN(H) = \sum_{uv\in E(G)} \sqrt{\frac{d_H(u)}{d_H(v)} + \frac{d_H(v)}{d_H(u)}}$$
$$= 2\sqrt{\frac{1}{2}+\frac{2}{1}} + 2\sqrt{\frac{1}{3}+\frac{3}{1}} + 6\sqrt{\frac{2}{2}+\frac{2}{2}}$$
$$+12\sqrt{\frac{2}{3}+\frac{3}{2}} + 2\sqrt{\frac{3}{3}+\frac{3}{3}}$$
$$= 2\sqrt{\frac{5}{2}} + 2\sqrt{\frac{10}{3}} + 8\sqrt{2} + 12\sqrt{\frac{13}{6}}.$$

Theorem 8. Let H be the chemical structure of hydroxychloroquine. Then

$$DRN(H,x) = 2x^{\sqrt{\frac{5}{2}}} + 2x^{\sqrt{\frac{10}{3}}} + 8x^{\sqrt{2}} + 12x^{\sqrt{\frac{13}{6}}}.$$

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

$$DRN(H,x) = \sum_{uv\in E(H)} x^{\sqrt{\frac{d_H(u)}{d_H(v)}+\frac{d_H(v)}{d_H(u)}}}$$
$$= 2x^{\sqrt{\frac{1}{2}+\frac{2}{1}}} + 2x^{\sqrt{\frac{1}{3}+\frac{3}{1}}} + 6x^{\sqrt{\frac{2}{2}+\frac{2}{2}}}$$
$$+12x^{\sqrt{\frac{2}{3}+\frac{3}{2}}} + 2x^{\sqrt{\frac{3}{3}+\frac{3}{3}}}$$
$$= 2x^{\sqrt{\frac{5}{2}}} + 2x^{\sqrt{\frac{10}{3}}} + 8x^{\sqrt{2}} + 12x^{\sqrt{\frac{13}{6}}}.$$

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

$$DRH(H) = \frac{1422}{65}.$$

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

$$DRH(H) = \sum_{uv\in E(G)} \frac{2d_H(u)d_H(v)}{d_H(u)^2 + d_H(v)^2}$$
$$= 2\frac{2\times1\times2}{1^2+2^2} + 2\frac{2\times1\times3}{1^2+3^2} + 6\frac{2\times2\times2}{2^2+2^2}$$
$$+12\frac{2\times2\times3}{2^2+3^2} + 2\frac{2\times3\times3}{3^2+3^2}$$
$$= \frac{1422}{65}.$$

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

$$DRH(H,x) == 2x^{\frac{4}{5}} + 2x^{\frac{3}{5}} + 8x^{1} + 12x^{\frac{12}{13}}.$$

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

$$DRH(H,x) = \sum_{uv\in E(H)} x^{\frac{2d_H(u)d_H(v)}{d_H(u)^2+d_H(v)^2}}$$
$$= 2x^{\frac{2\times1\times2}{1^2+2^2}} + 2x^{\frac{2\times1\times3}{1^2+3^2}} + 6x^{\frac{2\times2\times2}{2^2+2^2}}$$
$$+12x^{\frac{2\times2\times3}{2^2+3^2}} + 2x^{\frac{2\times3\times3}{3^2+3^2}}$$
$$= 2x^{\frac{4}{5}} + 2x^{\frac{3}{5}} + 8x^{1} + 12x^{\frac{12}{13}}.$$

Theorem 11. Let H be the chemical structure of hydroxychloroquine. Then

$$RDRH(H) = \frac{161}{6}.$$

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

$$RDRH(H) = \sum_{uv\in E(H)} \frac{d_H(u)^2 + d_H(v)^2}{2d_H(u)d_H(v)}$$
$$= 2\frac{1^2+2^2}{2\times1\times2} + 2\frac{1^2+3^2}{2\times1\times3} + 6\frac{2^2+2^2}{2\times2\times2}$$
$$+12\frac{2^2+3^2}{2\times2\times3} + 2\frac{3^2+3^2}{2\times3\times3}$$
$$= \frac{161}{6}.$$

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

$$RDRH(H,x) = 2x^{\frac{5}{4}} + 2x^{\frac{5}{3}} + 8x^{1} + 12x^{\frac{13}{12}}.$$

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

$$RDRH(H,x) = \sum_{uv\in E(H)} x^{\frac{d_H(u)^2+d_H(v)^2}{2d_H(u)d_H(v)}}$$
$$= 2x^{\frac{1^2+2^2}{2\times1\times2}} + 2x^{\frac{1^2+3^2}{2\times1\times3}} + 6x^{\frac{2^2+2^2}{2\times2\times2}}$$
$$+12x^{\frac{2^2+3^2}{2\times2\times3}} + 2x^{\frac{3^2+3^2}{2\times3\times3}}$$
$$= 2x^{\frac{5}{4}} + 2x^{\frac{5}{3}} + 8x^{1} + 12x^{\frac{13}{12}}.$$

4. Results and Discussion: Remdesivir

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

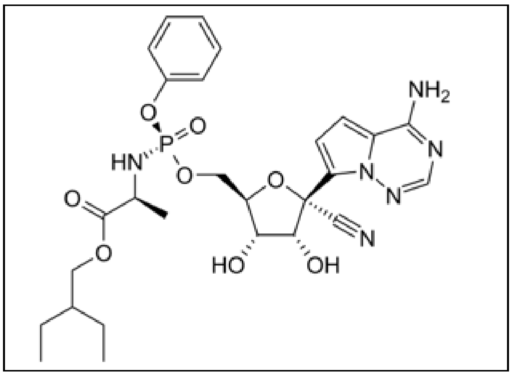

Figure 3

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

$d_G(u), d_G(v)\backslash uv\in E(R)$	(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

Theorem 13. Let R be the chemical structure of remdesivir. Then

$$DRN(R)=6\sqrt{\frac{5}{2}}+5\sqrt{\frac{10}{3}}+\sqrt{17}+15\sqrt{2}+14\sqrt{\frac{13}{6}}+5\sqrt{\frac{1}{3}}.$$

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

$$DRN(R)=\sum_{uv\in E(R)}\sqrt{\frac{d_R(u)}{d_R(v)}+\frac{d_R(v)}{d_R(u)}}$$

$$=2\sqrt{\frac{1}{2}+\frac{2}{1}}+5\sqrt{\frac{1}{3}+\frac{3}{1}}+2\sqrt{\frac{1}{4}+\frac{4}{1}}+9\sqrt{\frac{2}{2}+\frac{2}{2}}$$

$$+14\sqrt{\frac{2}{3}+\frac{3}{2}}+4\sqrt{\frac{2}{4}+\frac{4}{2}}+6\sqrt{\frac{3}{3}+\frac{3}{3}}+2\sqrt{\frac{3}{4}+\frac{4}{3}}$$

$$=6\sqrt{\frac{5}{2}}+5\sqrt{\frac{10}{3}}+\sqrt{17}+15\sqrt{2}+14\sqrt{\frac{13}{6}}+5\sqrt{\frac{1}{3}}.$$

Theorem 14. Let R be the chemical structure of remdesivir. Then

$$DRN(R,x)=6x^{\sqrt{\frac{5}{2}}}+5x^{\sqrt{\frac{10}{3}}}+2x^{\sqrt{\frac{17}{4}}}+15x^{\sqrt{2}}+14x^{\sqrt{\frac{13}{6}}}+2x^{\sqrt{\frac{25}{12}}}$$

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

$$DRN(R,x)=\sum_{uv\in E(R)}x^{\sqrt{\frac{d_R(u)}{d_R(v)}+\frac{d_R(v)}{d_R(u)}}}$$

$$=2x^{\sqrt{\frac{1}{2}+\frac{2}{1}}}+5x^{\sqrt{\frac{1}{3}+\frac{3}{1}}}+2x^{\sqrt{\frac{1}{4}+\frac{4}{1}}}+9x^{\sqrt{\frac{2}{2}+\frac{2}{2}}}$$

$$+14x^{\sqrt{\frac{2}{3}+\frac{3}{2}}}+4x^{\sqrt{\frac{2}{4}+\frac{4}{2}}}+6x^{\sqrt{\frac{3}{3}+\frac{3}{3}}}+2x^{\sqrt{\frac{3}{4}+\frac{4}{3}}}$$

$$=6x^{\sqrt{\frac{5}{2}}}+5x^{\sqrt{\frac{10}{3}}}+2x^{\sqrt{\frac{17}{4}}}+15x^{\sqrt{2}}$$

$$+14x^{\sqrt{\frac{13}{6}}}+2x^{\sqrt{\frac{25}{12}}}.$$

Theorem 15. Let R be the chemical structure of remdesivir. Then

$$DRH(R)=\frac{24}{5}+\frac{16}{17}+\frac{168}{13}+\frac{48}{25}+18.$$

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

$$DRH(R)=\sum_{uv\in E(R)}\frac{2d_R(u)d_R(v)}{d_R(u)^2+d_R(v)^2}$$

$$=2\frac{2\times1\times2}{1^2+2^2}+5\frac{2\times1\times3}{1^2+3^2}+2\frac{2\times1\times4}{1^2+4^2}+9\frac{2\times2\times2}{2^2+2^2}$$

$$+14\frac{2\times2\times3}{2^2+3^2}+4\frac{2\times2\times4}{2^2+4^2}+6\frac{2\times3\times3}{3^2+3^2}+2\frac{2\times3\times4}{3^2+4^2}$$

$$=\frac{24}{5}+\frac{16}{17}+\frac{168}{13}+\frac{48}{25}+18.$$

Theorem 16. Let R be the chemical structure of remdesivir. Then

$$DRH(R,x)=6x^{\frac{4}{5}}+5x^{\frac{3}{5}}+2x^{\frac{8}{17}}+15x^{1}+14x^{\frac{12}{13}}+2x^{\frac{24}{25}}.$$

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

$$DRH(R,x)=\sum_{uv\in E(G)}x^{\frac{2d_R(u)d_R(v)}{d_R(u)^2+d_R(v)^2}}$$

$$=2x^{\frac{2\times1\times2}{1^2+2^2}}+5x^{\frac{2\times1\times3}{1^2+3^2}}+2x^{\frac{2\times1\times4}{1^2+4^2}}+9x^{\frac{2\times2\times2}{2^2+2^2}}$$

$$+14x^{\frac{2\times2\times3}{2^2+3^2}}+4x^{\frac{2\times2\times4}{2^2+4^2}}+6x^{\frac{2\times3\times3}{3^2+3^2}}+2x^{\frac{2\times3\times4}{3^2+4^2}}$$

$$=6x^{\frac{4}{5}}+5x^{\frac{3}{5}}+2x^{\frac{8}{17}}+15x^{1}$$

$$+14x^{\frac{12}{13}}+2x^{\frac{24}{25}}.$$

Theorem 17. Let R be the chemical structure of remdesivir. Then

$$RDRH(R)=\frac{97}{3}+20.$$

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

$$RDRH(R)=\sum_{uv\in E(R)}\frac{d_R(u)^2+d_R(v)^2}{2d_R(u)d_R(v)}$$

$$=2\frac{1^2+2^2}{2\times1\times2}+5\frac{1^2+3^2}{2\times1\times3}+2\frac{1^2+4^2}{2\times1\times4}+9\frac{2^2+2^2}{2\times2\times2}$$

$$+14\frac{2^2+3^2}{2\times2\times3}+4\frac{2^2+4^2}{2\times2\times4}+6\frac{3^2+3^2}{2\times3\times3}+2\frac{3^2+4^2}{2\times3\times4}$$

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$$=\frac{97}{3}+20.$$

Theorem 18. Let R be the chemical structure of remdesivir. Then

$$RDRH(R,x)=6x^{\frac{5}{4}}+5x^{\frac{5}{3}}+2x^{\frac{17}{8}}+15x^{1}+14x^{\frac{13}{12}}+2x^{\frac{25}{24}}$$

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

$$RDRH(R,x)=\sum_{uv\in E(G)} x^{\frac{d_R(u)^2+d_R(v)^2}{2d_R(u)d_R(v)}}$$

$$=2x^{\frac{1^2+2^2}{2\times1\times2}}+5x^{\frac{1^2+3^2}{2\times1\times3}}+2x^{\frac{1^2+4^2}{2\times1\times4}}+9x^{\frac{2^2+2^2}{2\times2\times2}}$$

$$+14x^{\frac{2^2+3^2}{2\times2\times3}}+4x^{\frac{2^2+4^2}{2\times2\times4}}+6x^{\frac{3^2+3^2}{2\times3\times3}}+2x^{\frac{3^2+4^2}{2\times3\times4}}$$

$$=6x^{\frac{5}{4}}+5x^{\frac{5}{3}}+2x^{\frac{17}{8}}+15x^{1}$$

$$+14x^{\frac{13}{12}}+2x^{\frac{25}{24}}.$$

5. Conclusion

In this research, the degree ratio Nirmala, degree ratio harmonic and reciprocal degree ratio harmonic indices and their polynomials for certain chemical structures are determined.

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