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Degree Ratio Dharwad Index of Certain Nanotubes

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Abstract. We put forward the degree ratio Dharwad and reciprocal degree ratio Dharwad indices of a graph. We determine the degree ratio Dharwad and the reciprocal degree ratio Dharwad indices for some chemical nanostructures, such as armchair polyhex nanotubes, zigzag polyhex nanotubes, and carbon nanocone networks.

Keywords: graph indices, degree ratio Dharwad index, reciprocal degree ratio Dharwad index, nanotube.

AMS Mathematics Subject Classification (2010): 05C07, 05C09, 05C92.

1. Introduction

Let $G = (V, E)$ be a finite, simple connected graph. Let $d(u)$ denote the degree of a vertex u [1, 2].

In the modeling of Mathematics, a molecular or chemical graph is a simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom of the molecule, and its edges represent the bonds between atoms. Topological indices are useful for finding correlations between the structure of a chemical compound and its physicochemical properties [3].

In [4], the degree ratio Nirmala index of a graph is defined as

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

Recently, some degree ratio indices were studied, for example, in [5, 6, 7, 8, 9, 10].

In [11], the Dharwad index of a graph G was introduced and it is defined as

$$D(G) = \sum_{uv \in E(G)} \sqrt{\left(d(u)^3 + d(v)^3\right)}.$$

Recently, some topological indices were studied, for example, in [12, 13, 14, 15].

We introduce the degree ratio Dharwad index of a graph G and it is defined as

$$DRD(G)=\sum_{uv\in E(G)}\sqrt{\frac{d(u)^3}{d(v)^3}+\frac{d(v)^3}{d(u)^3}}.$$

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

$$RDRD(G)=\sum_{uv\in E(G)}\sqrt{\frac{d(u)^3 d(v)^3}{d(u)^6+d(v)^6}}.$$

In this paper, we compute the degree ratio Dharwad and reciprocal degree ratio Dharwad indices of armchair polyhex nanotubes, zigzag polyhex nanotubes and carbon nanocone networks.

2. Armchair polyhex nanotubes

Carbon polyhex nanotubes exist in nature with remarkable stability and possess very interesting electrical, thermal and mechanical properties. The molecular graph of armchair polyhex nanotube $TUAC_6$ [*p*, *q*] is shown in the below graph.

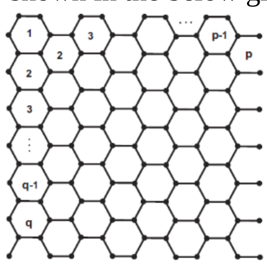

Figure 1:

The graphs of armchair polyhex nanotubes have 2*p*(*q*+1) vertices and 3*pq* + 2*p* edges are shown in the above graph. Let *A*= $TUAC_6$[*p*, *q*].

We obtain that {*d*(*u*), *d*(*v*): *uv* ∈ *E*(*A*)} has three edge set partitions.

d(*u*), *d*(*v*) \ *uv* ∈ *E*(*A*)	(2, 2)	(2, 3)	(3, 3)
Number of edges	*p*	2*p*	3*pq* – *p*

Theorem 1. The degree ratio Dharwad index of $TUAC_6$ [*p*, *q*] is given by

$$DRD(A)=3\sqrt{2}pq+2\sqrt{\frac{793}{216}}p.$$

Proof: Applying definition and edge partition of $TUAC_6$ [*p*, *q*], we conclude

$$DRD(A)=\sum_{uv\in E(A)}\sqrt{\frac{d(u)^3}{d(v)^3}+\frac{d(v)^3}{d(u)^3}}$$

$$= p\left(\sqrt{\frac{2^3}{2^3}+\frac{2^3}{2^3}}\right)+2p\left(\sqrt{\frac{2^3}{3^3}+\frac{3^3}{2^3}}\right)+(3pq-p)\left(\sqrt{\frac{3^3}{3^3}+\frac{3^3}{3^3}}\right)$$

By solving the above equation, we get the desired result.

Theorem 2. The reciprocal degree ratio Dharwad index of $TUAC_6\,[p, q]$ is

$$RDRD(A) == 3\sqrt{\frac{1}{2}}pq + 2\sqrt{\frac{216}{793}}p.$$

Proof: Applying definition and edge partition of $TUAC_6\,[p, q]$, we conclude

$$RDRD(A) = \sum_{uv\in E(A)} \sqrt{\frac{d(u)^3 d(v)^3}{d(u)^6 + d(v)^6}}$$

$$= p\left(\sqrt{\frac{2^3\times 2^3}{2^6+2^6}}\right)+2p\left(\sqrt{\frac{2^3\times 3^3}{2^6+3^6}}\right)+(3pq-p)\left(\sqrt{\frac{3^3\times 3^3}{3^6+3^6}}\right).$$

By solving the above equation, we get the desired result.

3. ZigZag polyhex nanotubes

The molecular graph of zigzag polyhex nanotube $TUZC_6\,[p, q]$ is depicted in below graph.

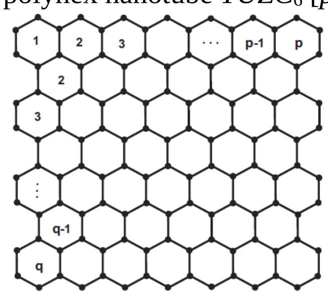

Figure 2:

The graphs of zigzag polyhex nanotubes have $2p(q+1)$ vertices and $3pq + 2p$ edges are shown in the above graph. Let $B = TUZC_6[p, q]$.

We obtain that $\{d(u), d(v): uv \in E(B)\}$ has three edge set partitions.

$d(u), d(v) \setminus uv \in E(B)$	(2, 3)	(3, 3)
Number of edges	$4p$	$3pq - 2p$

Theorem 3. The degree ratio Dharwad index of $TUZC_6\,[p, q]$ is given by

$$DRD(B) = 3\sqrt{2}pq + \left(4\sqrt{\frac{793}{216}} - 2\sqrt{2}\right)p.$$

Proof: Applying definition and edge partition of $TUZC_6\,[p, q]$, we conclude

$$DRD(B)=\sum_{uv\in E(B)}\sqrt{\frac{d(u)^3}{d(v)^3}+\frac{d(v)^3}{d(u)^3}}$$
$$=4p\left(\sqrt{\frac{2^3}{3^3}+\frac{3^3}{2^3}}\right)+(3pq-2p)\left(\sqrt{\frac{3^3}{3^3}+\frac{3^3}{3^3}}\right)$$

By solving the above equation, we get the desired result.

Theorem 4. The reciprocal degree ratio Dharwad index of $TUZC_6$ $[p, q]$ is

$$RDRD(B)=3\sqrt{\frac{1}{2}}pq+\left(4\sqrt{\frac{216}{793}}-2\sqrt{\frac{1}{2}}\right)p.$$

Proof: Applying definition and edge partition of $TUZC_6$ $[p, q]$, we conclude

$$RDRD(B)=\sum_{uv\in E(B)}\sqrt{\frac{d(u)^3 d(v)^3}{d(u)^6+d(v)^6}}$$
$$=4p\left(\sqrt{\frac{2^3\times 3^3}{2^6+3^6}}\right)+(3pq-2p)\left(\sqrt{\frac{3^3\times 3^3}{3^6+3^6}}\right).$$

By solving the above equation, we get the desired result.

4. Carbon nanocone networks

The molecular graph of pentagonal nanocone network $CNC_5\,[n]$ is depicted in below graph.

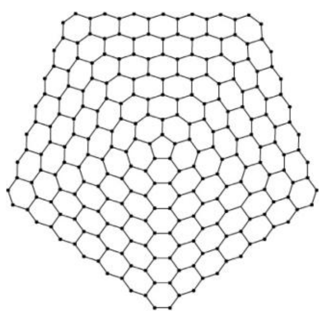

Figure 3:

The graphs of pentagonal nanocone networks have $5(n+1)^2$ vertices and $\frac{15}{2}n^2+\frac{25}{2}n+5$ edges. Let $C = CNC_5[n]$.

We obtain that $\{d(u), d(v): uv \in E(C)\}$ has three edge set partitions.

$d(u), d(v) \backslash uv\in E(C)$	(2, 2)	(2, 3)	(3, 3)
Number of edges	5	$10n$	$\frac{15}{2}n^2+\frac{5}{2}n$

Theorem 5. The degree ratio Dharwad index of $CNC_5[n]$ is given by

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Proof: Applying definition and edge partition of $CNC_5[n]$, we conclude

$$DRD(C)=\sum_{uv\in E(C)}\sqrt{\frac{d(u)^3}{d(v)^3}+\frac{d(v)^3}{d(u)^3}}$$

$$=5\sqrt{\frac{2^3}{2^3}+\frac{2^3}{2^3}}+10n\sqrt{\frac{2^3}{3^3}+\frac{3^3}{2^3}}+\left(\frac{15}{2}n^2+\frac{5}{2}n\right)\sqrt{\frac{3^3}{3^3}+\frac{3^3}{3^3}}.$$

By solving the above equation, we get the desired result.

Theorem 6. The reciprocal degree ratio Dharwad index of $CNC_5[n]$ is given by

$$RDRD(C)=\frac{15}{2}\sqrt{\frac{1}{2}}n^2+\left(10\sqrt{\frac{216}{793}}+\frac{5}{2}\sqrt{\frac{1}{2}}\right)n+\frac{5}{2}\sqrt{\frac{1}{2}}.$$

Proof: Applying definition and edge partition of $CNC_5[n]$, we conclude

$$RDRD(C)=\sum_{uv\in E(C)}\sqrt{\frac{d(u)^3 d(v)^3}{d(u)^6+d(v)^6}}$$

$$=5\left(\sqrt{\frac{2^3\times 2^3}{2^6+2^6}}\right)+10n\left(\sqrt{\frac{2^3\times 3^3}{2^6+3^6}}\right)+\left(\frac{15}{2}n^2+\frac{5}{2}n\right)\left(\sqrt{\frac{3^3\times 3^3}{3^6+3^6}}\right).$$

By solving the above equation, we get the desired result.

5. Conclusion

We have introduced the degree ratio Dharwad and reciprocal degree ratio Dharwad indices of a graph. Also, we have determined the newly defined degree ratios Dharwad indices of armchair polyhex nanotubes, zigzag polyhex nanotubes and carbon nanocone networks.

Conflicts of Interest: The author declares that there are no conflicts of interest regarding the research, authorship, or publication of this manuscript.

Author Contributions: The author independently conceived the study, carried out the research, prepared the manuscript, and approved the final version for publication.

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