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DHARWAD INDICES

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ABSTRACT

Recently, Gutman considered a class of novel graph invariants of which the Sombor index was defined. In this paper, we introduce the Dharwad index, reduced Dharwad index, δ-Dharwad index and their exponentials of a graph and compute exact formulas for polycyclic aromatic hydrocarbons and benzenoid systems.

Keywords: *Dharwad index, Dharwad exponential, reduced Dharwad index, reduced Dharwad exponential, nanostructure.*
Mathematics Subject Classification: *05C05, 05C07, 05C90..*

1. INTRODUCTION

Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex u is denoted by $d_G(u)$. The edge connecting the vertices u and v will be denoted by uv. We refer [1] for undefined notations and terminologies.

The Sombor index of a graph G was introduced by Gutman in [2] and defined it as

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

Recently, some Sombor indices were studied, for example, in [3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13].

Motivated by the definition of Sombor index and its applications, we now introduce the Dharwad index as follows:

The Dharwad index of a graph G is defined as

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

Considering the Dharwad index, we introduce the Dharwad exponential of a graph G and defined it as

$$D(G,x)=\sum_{uv\in E(G)}x^{\sqrt{d_G(u)^3+d_G(v)^3}}.$$

We also define the reduced Dharwad index of a graph G as

$$RD(G)=\sum_{uv\in E(G)}\sqrt{(d_G(u)-1)^3+(d_G(v)-1)^3}.$$

Considering the reduced Dharwad index, we propose the reduced Dharwad exponential of a graph G and it is defined as

$$RD(G,x)=\sum_{uv\in E(G)}x^{\sqrt{(d_G(u)-1)^3+(d_G(v)-1)^3}}.$$

We introduce the δ-Dharwad index of a graph G and it is defined as

$$\delta D(G)=\sum_{uv\in E(G)}\sqrt{(d_G(u)-\delta(G)+1)^3+(d_G(v)-\delta(G)+1)^3}.$$

Considering the δ-Dharwad index, we introduce the δ-Dharwad exponential of a graph G, defined as

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$$\delta D(G,x) = \sum_{uv \in E(G)} x^{\sqrt{(d_G(u)-(\delta(G)+1))^3+(d_G(v)-\delta(G)+1)^3}}.$$

In Chemical Graph Theory, many graph indices were introduced and studied, see [14, 15]. The reduced first [16] and second [17] Zagreb indices were introduced and studied.

In this paper, we establish some results on the Dharwad indices and their corresponding exponentials for certain nanostructures. For nanostructures, see [18].

2. OBSERVATIONS

(1) If $\delta(G) = 1$, then $\delta D(G)$ is the Dharwad index $D(G)$.

(2) If $\delta(G) = 1$, then $\delta D(G,x)$ is the Dharwad exponential $D(G,x)$.

(3) If $\delta(G) = 2$, then $\delta D(G)$ is the reduced Dharwad index $RD(G)$.

(4) If $\delta(G) = 2$, then $\delta D(G,x)$ is the reduced Dharwad exponential $RD(G,x)$.

3. RESULTS FOR POLYCYCLIC AROMATIC HYDROCARBONS

We focus on the chemical graph structure of the family polycyclic aromatic hydrocarbons, denoted by PAH_n. The first three members of the family PAH_n are presented in Figure 1.

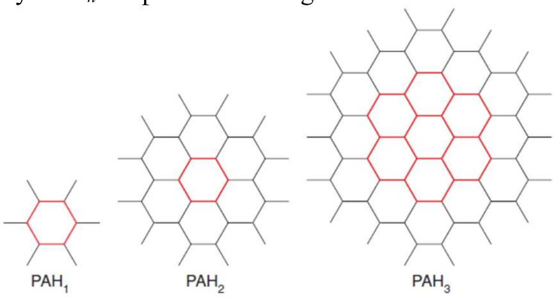

Figure 1

Let $G = PAH_n$. Clearly, the vertices of G are either of degree 1 or 3, see Figure 1. By calculation, we see that G has $6n^2+6n$ vertices and $9n^2+3n$ edges. In G, there are two types of edges based on the degree of end vertices of each edge as given in Table 1.

Table 1. Edge partition of PAH_n

$d_G(u), d_G(v) \backslash uv \in E(G)$	(1, 3)	(3, 3)
Number of edges	$6n$	$9n^2 - 3n$

In the following theorem, we compute the Dharwad index and its corresponding exponential of PAH_n.

Theorem 1. Let G be the graph of PAH_n. Then

(i) $D(PAH_n) = 27\sqrt{6}n^2 + (6\sqrt{28} - 9\sqrt{6})n.$

(ii) $D(PAH_n, x) = 6nx^{\sqrt{28}} + (9n^2 - 3n)x^{3\sqrt{6}}.$

Proof: From definitions and by using Table 1, we deduce

(i) $D(PAH_n) = (1^3+3^3)^{\frac{1}{2}} 6n + (3^3+3^3)^{\frac{1}{2}} (9n^2 - 3n)$

$= 27\sqrt{6}n^2 + (6\sqrt{28} - 9\sqrt{6})n.$

(ii) $D(PAH_n, x) = 6nx^{(1^3+3^3)^{\frac{1}{2}}} + (9n^2 - 3n)^{(3^3+3^3)^{\frac{1}{2}}}$

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$$= 6nx^{\sqrt{28}} + (9n^2 - 3n)x^{3\sqrt{6}}.$$

In the following theorem, we compute the reduced Dharwad index and its corresponding exponential of PAH_n.

Theorem 2. Let G be the graph of PAH_n. Then

(i) $RD(PAH_n) = 36n^2 + (12\sqrt{2} - 12)n.$

(ii) $RD(PAH_n, x) = 6nx^{2\sqrt{2}} + (9n^2 - 3n)x^4.$

Proof: From definitions and by using Table 1, we deduce

(i) $$RD(PAH_n) = \left[(1-1)^3 + (3-1)^3\right]^{\frac{1}{2}} 6n + \left[(3-1)^3 + (3-1)^3\right]^{\frac{1}{2}} (9n^2 - 3n)$$
$$= 36n^2 + (12\sqrt{2} - 12)n.$$

(ii) $$RD(PAH_n, x) = 6nx^{\left[(1-1)^3 + (3-1)^3\right]^{\frac{1}{2}}} + (9n^2 - 3n)^{\left[(3-1)^3 + (3-1)^3\right]^{\frac{1}{2}}}$$
$$= 6nx^{2\sqrt{2}} + (9n^2 - 3n)x^4.$$

In the following theorem, we compute the δ-Dharwad index and its corresponding exponential of PAH_n.

Theorem 3. Let G be the graph of PAH_n and $\delta(G) = 1$.Then

(i) $\delta D(PAH_n) = 27\sqrt{6}n^2 + (6\sqrt{28} - 9\sqrt{6})n.$

(ii) $\delta D(PAH_n, x) = 6nx^{\sqrt{28}} + (9n^2 - 3n)x^{3\sqrt{6}}.$

Proof: By observations (1), (2) and Theorem 1, the results follow.

4. RESULTS FOR BENZENOID SYSTEMS

We focus on the chemical graph structure of a jagged rectangle benzenoid system, denoted by $B_{m,n}$ for all m, n, in N. Three chemical graphs of a jagged rectangle benzenoid system are depicted in Figure 2.

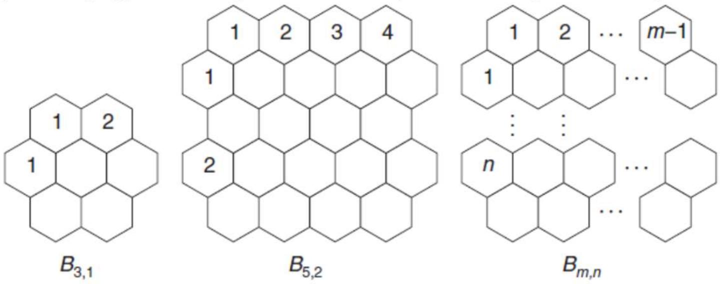

Figure 2

Let $H = B_{m,n}$. Clearly the vertices of H are either of degree 2 or 3, see Figure 2. By calculation, we obtain that H has $4mn + 4m + m - 2$ vertices and $6mn + 5m + n - 4$ edges. In H, there are three types of edges based on the degree of end vertices of each edge as given in Table 2.

Table 2. Edge partition of $B_{m,n}$

$d_H(u)\, d_H(v) \backslash uv \in E(H)$	(2,2)	(2,3))	(3, 3)
Number of edges	$2n+4$	$4m+4n-4$	$6mn + m - 5n - 4$

In the following theorem, we compute the Dharwad index and its corresponding exponential of $B_{m,n}$.

Theorem 4. Let G be the graph of $B_{m,n}$. Then

(i) $D(B_{m,n}) = 18\sqrt{6}mn + (4\sqrt{35} + 3\sqrt{6})m + (8 + 4\sqrt{35} - 15\sqrt{6})n + 16 - 4\sqrt{35} - 12\sqrt{6}.$

(ii) $D(B_{m,n}, x) = (2n+4)x^4 + (4m + 4n - 4)x^{\sqrt{35}} + (6mn + m - 5n - 4)x^{3\sqrt{6}}.$

Proof: From definitions and by using Table 2, we deduce

(i) $$D(B_{m,n}) = (2^3 + 2^3)^{\frac{1}{2}}(2n+4) + (2^3 + 3^3)^{\frac{1}{2}} 4m + 4n - 4) + (3^3 + 3^3)^{\frac{1}{2}}(6mn + m - 5n - 4)$$
$$= 18\sqrt{6}mn + (4\sqrt{35} + 3\sqrt{6})m + (8 + 4\sqrt{35} - 15\sqrt{6})n + 16 - 4\sqrt{35} - 12\sqrt{6}.$$

(ii) $$D(B_{m,n}, x) = (2n+4)x^{(2^3+2^3)^{\frac{1}{2}}} + (4m + 4n - 4)x^{(2^3+3^3)^{\frac{1}{2}}} + (6mn + m - 5n - 4)^{(3^3+3^3)^{\frac{1}{2}}}$$
$$= (2n+4)x^4 + (4m + 4n - 4)x^{\sqrt{35}} + (6mn + m - 5n - 4)x^{3\sqrt{6}}.$$

In the following theorem, we compute the reduced Dharwad index and its corresponding exponential of $B_{m,n}$.

Theorem 5. Let G be the graph of $B_{m,n}$. Then

(i) $RD(B_{m,n}) = 24mn + 16m + (2\sqrt{2} - 8)n + 4\sqrt{2} - 28.$

(ii) $RD(B_{m,n}, x) = (2n+4)x^{\sqrt{2}} + (4m + 4n - 4)x^3 + (6mn + m - 5n - 4)x^4.$

Proof: From definitions and by using Table 2, we deduce

(i) $$RD(B_{m,n}) = (1^3 + 1^3)^{\frac{1}{2}}(2n+4) + (1^3 + 2^3)^{\frac{1}{2}} 4m + 4n - 4) + (2^3 + 2^3)^{\frac{1}{2}}(6mn + m - 5n - 4)$$
$$= 24mn + 16m + (2\sqrt{2} - 8)n + 4\sqrt{2} - 28.$$

(ii) $$RD(B_{m,n}, x) = (2n+4)x^{(1^3+1^3)^{\frac{1}{2}}} + (4m + 4n - 4)x^{(1^3+2^3)^{\frac{1}{2}}} + (6mn + m - 5n - 4)^{(2^3+2^3)^{\frac{1}{2}}}$$
$$= (2n+4)x^{\sqrt{2}} + (4m + 4n - 4)x^3 + (6mn + m - 5n - 4)x^4.$$

In the following theorem, we compute the δ-Dharwad index and its corresponding exponential of $B_{m,n}$.

Theorem 6. Let G be the graph of $B_{m,n}$ and $\delta(G) = 2$. Then

(i) $\delta D(B_{m,n}) = 24mn + 16m + (2\sqrt{2} - 8)n + 4\sqrt{2} - 28.$

(ii) $\delta D(B_{m,n}, x) = (2n+4)x^{\sqrt{2}} + (4m + 4n - 4)x^3 + (6mn + m - 5n - 4)x^4.$

Proof: By observations (3), (4) and Theorem 5, we obtain the desired results.

5. CONCLUSION

In this paper, we have introduced the Dharwad index, reduced Dharwad index, δ-Dharwad index and their corresponding exponentials of a graph. Also we have computed exact formulas for polycyclic aromatic hydrocarbons and benzenoid systems.

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