International Journal of Engineering Sciences & Research Technology

(A Peer Reviewed Online Journal)
Impact Factor: 5.164

IJESRT

RESEARCHERID
THOMSON REUTERS

[Nandargi *et al.*, 11(2): February, 2022]
IC™ Value: 3.00

ISSN: 2277-9655
Impact Factor: 5.164
CODEN: IJESS7

IJESRT

INTERNATIONAL JOURNAL OF ENGINEERING SCIENCES & RESEARCH TECHNOLOGY

THE (*a*, *b*)-NIRMALA INDEX

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DOI: 10.29121/ijesrt.v11.i2.2022.5

ABSTRACT

Graphical indices are applied to measure to chemical characteristics of chemical compounds. In this paper, we introduce the (a,b)-Nirmala index of a graph. Furthermore we compute this index for benzenoid systems and polycyclic aromatic hydrocarbons. We also establish some other well known graphical indices directly as special case of this index for some special values of *a* and *b*, in particular Nirmala index and mean Sombor index.

KEYWORDS: (a,b)-Nirmala index, benzenoid system, polycyclic aromatic hydrocarbon.

AMS Mathematics Subject Classification): 05*C*05, 05*C*07, 05*C*09, 05.

1. INTRODUCTION

Let *G* be a finite, simple, connected 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*. We refer [1], for other undefined notations and terminologies.

A molecular graph is a graph such that its vertices correspond to the atoms and edges to the bonds. Chemical Graph Theory is a branch of mathematical chemistry, which has an important effect on the development of Chemical Sciences. Several graphical indices have been considered in Theoretical Chemistry and have found some applications.

The Nirmala index [2] of a graph *G* is defined as

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

This index was studied, for example, in [3].

Motivated by the definition of Nirmala index of a graph *G*, we define the (a,b)-Nirmala index as

$$N_{a,b}(G)=\sum_{uv\in E(G)}\left(\frac{d_G(u)^a+d_G(v)^a}{2}\right)^b,$$

where *a* and *b* are real numbers.

The first Zagreb index [4] of a graph *G* is defined as

$$M_1(G)=\sum_{uv\in E(G)}\left[d_G(u)+d_G(v)\right].$$

The Sombor index was introduced by Gutman in [5] and defined it as

ISSN: 2277-9655
Impact Factor: 5.164
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$$SO(G)=\sum_{uv\in E(G)}\sqrt{d_G(u)^2+d_G(v)^2}.$$

The harmonic index proposed in [6], as

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

The K_1index [7] was defined as

$$K_1(G)=\sum_{uv\in E(G)}\frac{\sqrt{2}}{\sqrt{\left(d_G(u)^2+d_G(v)^2\right)}}.$$

The sum-connectivity index [8] is defined as

$$S(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_G(u)+d_G(v)}}.$$

The misbalance prodeg index of a graph G was defined by Kulli et al. [9] as

$$MPI(G)=\sum_{uv\in E(G)}\left[\sqrt{d_G(u)}+\sqrt{d_G(v)}\right].$$

The inverse sum indeg index was defined by Vukicevic et al. [10] as

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

The mean Sombor index was defined by Mendez-Bermudez et al. in [11] as

$$mSO_a(G)=\sum_{uv\in E(G)}\left(\frac{d_G(u)^a+d_G(v)^a}{2}\right)^{1/a},$$

We easily see that

(1) $N_{1,1}(G)=\frac{1}{2}M_1(G).$

(2) $N_{1,-1}(G)=H(G).$

(3) $N_{1,\frac{1}{2}}(G)=\frac{1}{\sqrt{2}}N(G).$

(4) $N_{1,-\frac{1}{2}}(G)=\sqrt{2}S(G).$

(5) $N_{-1,-1}(G)=2ISI(G).$

(6) $N_{2,\frac{1}{2}}(G)=\frac{1}{\sqrt{2}}SO(G).$

(7) $N_{2,-\frac{1}{2}}(G)=K_1(G).$

(8) $N_{\frac{1}{2},1}(G)=\frac{1}{2}MPI(G).$

(9) $N_{a,\frac{1}{a}}(G)=mSO_a(G).$

ISSN: 2277-9655
Impact Factor: 5.164
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We compute the newly defined novel graph index for benzenoid systems and polycyclic aromatic hydrocarbons. For benzenoid systems, etc. see [12].

2. 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 1.

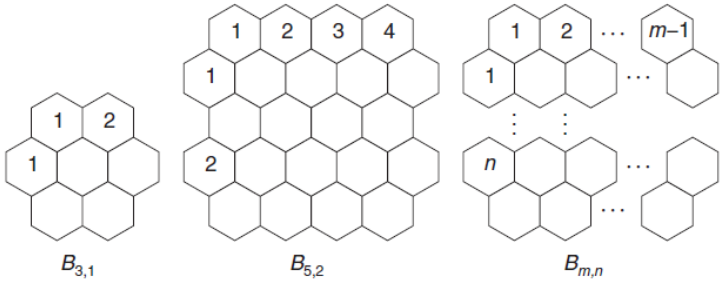

Figure 1

Let $G = B_{m,n}$. Clearly the vertices of G are either of degree 2 or 3, see Figure 1. By calculation, we obtain that H has $4mn + 4m + m - 2$ vertices and $6mn + 5m + n - 4$ edges. In G, there are three types of edges based on the degree of end vertices of each edge as given in Table 1.

Table 1. Edge partition of $B_{m,n}$

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

In the following theorem, we determine the (a,b)-Nirmala index of $B_{m,n}$.

Theorem 1. Let $G = B_{m,n}$ be the family of a jagged rectangle benzenoid system. Then

$$N_{a,b}(G) = (2n+4)2^{ab} + (4m+4n-4)\left(\frac{2^a+3^a}{2}\right)^b + (6mn+m-5n-4)3^{ab}.$$

Proof: Let $G = B_{m,n}$. By using equation and Table 1, we deduce

$$N_{a,b}(G) = \sum_{uv\in E(G)} \left(\frac{d_G(u)^a + d_G(v)^a}{2}\right)^b$$

$$= (2n+4)\left(\frac{2^a+2^a}{2}\right)^b + (4m+4n-4)\left(\frac{2^a+3^a}{2}\right)^b + (6mn+m-5n-4)\left(\frac{3^a+3^a}{2}\right)^b$$

After simplification, we obtain the desired result.

We establish the following results by using Theorem 1.

Corollary 1.1. Let $G = B_{m,n}$ be the family of a jagged rectangle benzenoid system. Then

(1) $N_{1,1}(G) = \frac{1}{2}M_1(G) = 18mn + 13m - n - 14.$

(2) $N_{1,-1}(G) = H(G) = 3mn + \frac{29}{15}m + \frac{14}{15}n - \frac{14}{15}.$

(3) $N_{1,\frac{1}{2}}(G) = \frac{1}{\sqrt{2}}N(G) = 6\sqrt{3}mn + \left(2\sqrt{10}+\sqrt{3}\right)m + \left(2\sqrt{2}+2\sqrt{10}-5\sqrt{3}\right)n + 4\sqrt{2} - 2\sqrt{10} - 4\sqrt{3}$

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(4) $N_{1,-\frac{1}{2}}(G)=\sqrt{2}S(G)=\frac{6}{\sqrt{3}}mn+\left(\frac{4\sqrt{2}}{\sqrt{5}}+\frac{1}{\sqrt{3}}\right)m+\left(\frac{2}{\sqrt{2}}+\frac{4\sqrt{2}}{\sqrt{5}}-\frac{5}{\sqrt{3}}\right)n+\left(\frac{4}{\sqrt{2}}-\frac{4\sqrt{2}}{\sqrt{5}}-\frac{4}{\sqrt{3}}\right).$

(5) $N_{-1,-1}(G)=2ISI(G)=18mn+\frac{63}{5}m-\frac{7}{5}n-\frac{68}{5}.$

(6) $N_{2,\frac{1}{2}}(G)=\frac{1}{\sqrt{2}}SO(G)=18mn+\left(2\sqrt{26}+3\right)m+\left(2\sqrt{26}-11\right)n-\left(2\sqrt{26}+4\right).$

(7) $N_{2,-\frac{1}{2}}(G)=K_1(G)=2mn+\left(\frac{4\sqrt{2}}{\sqrt{13}}+\frac{1}{\sqrt{3}}\right)m+\left(\frac{4\sqrt{2}}{\sqrt{13}}-\frac{2}{3}\right)n+\frac{2}{3}-\frac{4\sqrt{2}}{\sqrt{13}}.$

(8) $N_{\frac{1}{2},1}(G)=\frac{1}{2}MPI(G)=2\sqrt{3}mn+\left(2\sqrt{2}+\frac{7}{\sqrt{3}}\right)m+\left(3\sqrt{2}+\frac{1}{\sqrt{3}}\right)n-\frac{10}{\sqrt{3}}.$

(9) $N_{a,\frac{1}{a}}(G)=mSO_a(G)=(2n+4)2+(4m+4n-4)\left(\frac{2^a+3^a}{2}\right)^{\frac{1}{a}}+(6mn+m-5n-4)3$

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.

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 2.

Table 2. Edge partition of PAH_n

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

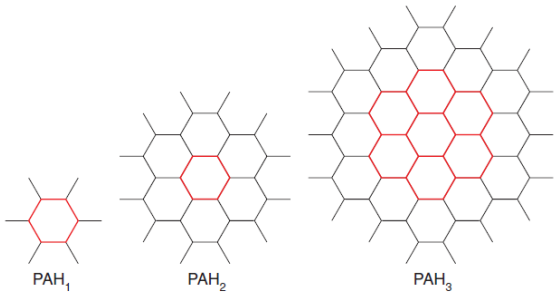

Figure 2

In the following theorem, we determine the (a,b)-Nirmala index of PAH_n.

Theorem 2. Let $G=PAH_n$ be the family of a polycyclic aromatic hydrocarbon. Then

$$N_{a,b}(G)==6n\left(\frac{1^a+3^a}{2}\right)^b+(9n^2-3n)3^{ab}.$$

ISSN: 2277-9655
Impact Factor: 5.164
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Proof: Let $G = PAH_n$. By using equation and Table 2, we deduce

$$N_{a,b}(G) = \sum_{uv \in E(G)} \left(\frac{d_G(u)^a + d_G(v)^a}{2} \right)^b = 6n \left(\frac{1^a + 3^a}{2} \right)^b + (9n^2 - 3n) \left(\frac{3^a + 3^a}{2} \right)^b .$$

After simplification, we obtain the desired result.

We establish the following results by using Theorem 2.

Corollary 2.1. Let $G = PAH_n$ be the family of a polycyclic aromatic hydrocarbon. Then

(1) $N_{1,1}(G) = \frac{1}{2} M_1(G) = 27n^2 + 3n$

(2) $N_{1,-1}(G) = H(G) = 3n^2 + 2n.$

(3) $N_{1,\frac{1}{2}}(G) = \frac{1}{\sqrt{2}} N(G) = 9\sqrt{3}n^2 + (6\sqrt{2} - 3\sqrt{3})n.$

(4) $N_{1,-\frac{1}{2}}(G) = \sqrt{2} S(G) = 3\sqrt{3}n^2 + (3\sqrt{2} - \sqrt{3})n.$

(5) $N_{-1,-1}(G) = 2ISI(G) = 27n^2.$

(6) $N_{2,\frac{1}{2}}(G) = \frac{1}{\sqrt{2}} SO(G) = 27n^2 + (6\sqrt{5} - 9)n.$

(7) $N_{2,-\frac{1}{2}}(G) = K_1(G) = \frac{9}{\sqrt{3}} n^2 + \left(\frac{6}{\sqrt{5}} - \frac{3}{\sqrt{3}} \right) n.$

(8) $N_{\frac{1}{2},1}(G) = \frac{1}{2} MPI(G) = 9\sqrt{3}n^2 + 3n.$

(9) $N_{a,\frac{1}{a}}(G) = mSO_a(G) = 27n^2 - 9n + \left(\frac{1 + 3^a}{2} \right) 6n.$

4. CONCLUSION

In this paper, we have introduced the (a,b)-Nirmala index of a graph. Also we have determined exact values of this novel graph index for benzenoid systems and polycyclic aromatic hydrocarbons.

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