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Original Article

Banhatti-Nirmala Index of certain Chemical Networks

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Abstract - *In Chemical Graph Theory, several degree based topological indices were introduced and studied since 1972. Recently, a novel invariant is concerned, which is the Nirmal index defined as the sum of the square root of the degrees of the pairs of adjacent vertices. In this paper, we introduce the Banhatti-Nirmala index and its exponential of a graph and compute exact formulas for certain chemical networks.*

Keywords - *Topological index, Banhatti-Nirmala index, Banhatti-Nirmala exponential, Network.*

Mathematics Subject Classification: *05C05, 05C12, 05C35.*

I. INTRODUCTION

Let G be a simple, finite, connected graph with the 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 additional definitions and notations, the reader may refer to [1].

A molecular graph is a graph in which the vertices correspond to the atoms and the edges to the bonds of a molecule. A topological index is a numeric quantity from structural graph of a molecule. Several topological indices have been considered in Theoretical Chemistry, and have found some applications, especially in *QSPR/QSAR* study, see [2, 3, 4].

In Chemical Science, numerous vertex degree based topological indices or graph indices have been introduced and extensively studied in [4, 5].

The first and second Banhatti indices of a graph G were introduced by Kulli in [6], and they are defined as

$$B_1(G)=\sum_{ue}\left[d_G(u)+d_G(e)\right], \qquad B_2(G)=\sum_{ue}d_G(u)d_G(e)$$

where ue means that the vertex u and edge e are incident in G.

Recently, some Banhatti indices were studied in [7, 8, 9, 10, 11, 12, 13, 14, 15].

In [16], Kulli introduced the Nirmala index of a graph G as follows:

The Nirmala index of a molecular graph G is defined as

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

Recently, some Nirmala indices were studied in [17, 18, 19, 20, 21, 22, 23, 24, 25].

Considering the Nirmala index, Kulli defined the Nirmala exponential of a graph G as

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

Motivated by the definitions of the Banhatti and Nirmala indices, we introduce the Banhatti-Nirmala index of a graph and defined it as,

$$BN(G)=\sum_{ue}\sqrt{d_G(u)+d_G(e)}.$$

Considering the Banhatti-Nirmala index, we define the Banhatti-Nirmala exponential of a graph G as

$$BN(G,x)=\sum_{ue}x^{\sqrt{d_G(u)+d_G(e)}}.$$

In this study, we compute the Banhatti-Nirmala index, Banhatti-Nirmala exponential of four families of networks. For networks, see [26].

II. RESULTS FOR SILICATE NETWORKS

Silicates are very important elements of Earth's crust. Sand and several minerals are constituted by silicates. Silicates are obtained by fusing metal oxides or metal carbonates with sand. A silicate network is symbolized by SL_n, where n is the number of hexagons between the center and boundary of SL_n. A silicate network of dimension two is shown in Figure 1.

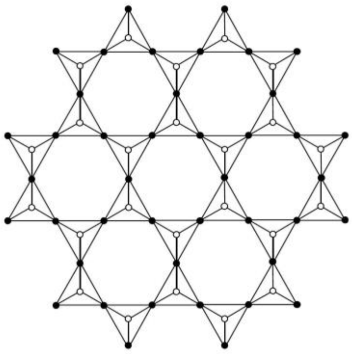

Fig. 1 Silicate network of dimension two

We compute the Banhatti-Nirmala index and Banhatti-Nirmala exponential for silicate networks.

Theorem 2.1. The Banhatti-Nirmala index and Banhatti-Nirmala exponential of SL_n silicate networks are given by

(i) $BN(SL_n)=12\times\sqrt{7}n+(18n^2+6n)(\sqrt{10}+\sqrt{13})+2(18n^2-12n)\sqrt{16}.$

(ii) $BN(SL_n,x)==6nx^{2\sqrt{7}}+(18n^2+6n)x^{\sqrt{10}+\sqrt{13}}+(18n^2-12n)x^{2\sqrt{16}}.$

Proof: Let $G = SL_n$ be the graph of silicate network with $|V(SL_n)| = 15n^2 + 3n$ and $|E(SL_n)| = 36n^2$. In SL_n, there are three types of edges based on the degree of the vertices of each edge. Further, by algebraic method, the edge degree partition of a silicate network SL_n is given in Table 1.

Table 1. Edge degree partition of $G = SL_n$

$d_G(u), d_G(v)\backslash e = uv \in E(G)$	(3,3)	(3, 6)	(6, 6)
$d_G(e)$	4	7	10
Number of edges	$6n$	$18n^2 + 6n$	$18n^2 - 12n$

(i) To compute $BN(SL_n)$, we see that

$$BN(SL_n)=\sum_{ue}\sqrt{d_G(u)+d_G(e)}$$

$$=6n\left[\sqrt{3+4}+\sqrt{3+4}\right]+(18n^2+6n)\left[\sqrt{3+7}+\sqrt{6+7}\right]+(18n^2-12n)\left[\sqrt{6+10}+\sqrt{6+10}\right]$$

$$=12\times\sqrt{7}n+(18n^2+6n)(\sqrt{10}+\sqrt{13})+2(18n^2-12n)\sqrt{16}.$$

(ii) To compute $BN(SL_n, x)$, we see that

$$BN(SL_n, x) = \sum_{uv \in E(G)} x^{\sqrt{d_G(u)+d_G(e)}}$$

$$= 6nx^{2\sqrt{7}} + (18n^2 + 6n)x^{\sqrt{10}+\sqrt{13}} + (18n^2 - 12n)x^{2\sqrt{16}}.$$

III. RESULTS FOR CHAIN SILICATE NETWORKS

In this section, we consider a family of chain silicate networks. This network is symbolized by CS_n and is obtained by arranging n tetrahedra linearly, see Fig. 2

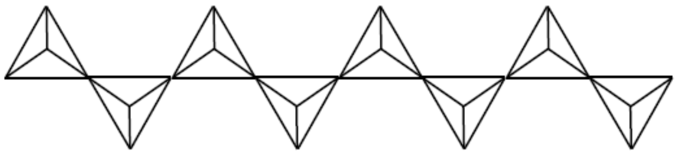

Fig. 2 Chain silicate network

We determine the Banhatti-Nirmala index and Banhatti-Nirmala exponential for chain silicate networks.

Theorem 3.1. The Banhatti-Nirmala index and Banhatti-Nirmala exponential of CS_n *chain* silicate networks are given by

(i) $BN(CS_n) == (2\times\sqrt{7} + 4\times\sqrt{10} + 4\times\sqrt{13} + 2\times\sqrt{16})n + (8\times\sqrt{7} - 2\times\sqrt{10} - 2\times\sqrt{13} - 4\times\sqrt{16}).$

(ii) $BN(CS_n, x) = (n+4)x^{2\sqrt{7}} + (4n-2)x^{2\sqrt{10}} + (n-2)x^{2\sqrt{16}}.$

Proof: Let $G = CS_n$ be the graph of chain silicate network, $n\geq 2$. By algebraic method, we obtain $|V(CS_n)|=3n+1$ and $|E(CS_n)| = 6n$. Also in CS_n, there are three types of edges based on the degree of the vertices of each edge. Further, by algebraic method, the edge degree partition of a chain silicate network CS_n, $n\geq 2$ is given in Table 2.

Table 2. Edge degree partition of CS_n, $n\geq 2$

$d_G(u), d_G(v)\backslash e = uv \in E(G)$	(3,3)	(3, 6)	(6, 6)
$d_G(e)$	4	7	10
Number of edges	$n + 4$	$4n - 2$	$n - 2$

(i) To compute $B_1^a(CS_n)$, we see that

$$BN(CS_n) = \sum_{ue} \sqrt{d_G(u) + d_G(e)}$$

$$= (n+4)\left[\sqrt{3+4} + \sqrt{3+4}\right] + (4n-2)\left[\sqrt{3+7} + \sqrt{3+7}\right] + (n-2)\left[\sqrt{6+10} + \sqrt{6+10}\right]$$

$$= (2\times\sqrt{7} + 4\times\sqrt{10} + 4\times\sqrt{13} + 2\times\sqrt{16})n + (8\times\sqrt{7} - 2\times\sqrt{10} - 2\times\sqrt{13} - 4\times\sqrt{16}).$$

(ii) To compute $BN(CS_n, x)$, we see that

$$BN(CS_n, x) = \sum_{uv \in E(G)} x^{\sqrt{d_G(u)+d_G(e)}}$$

$$= (n+4)x^{2\sqrt{7}} + (4n-2)x^{2\sqrt{10}} + (n-2)x^{2\sqrt{16}}.$$

IV. RESULTS FOR OXIDE NETWORKS

The oxide networks are of vital importance in the study of silicate networks. An oxide network of dimension n is denoted by OX_n. A 5 -dimensional oxide network is shown in Figure-3.

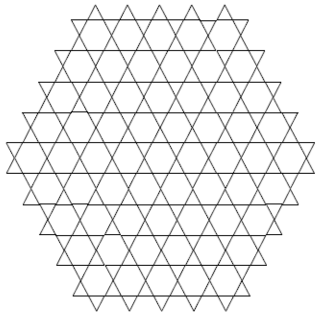

Fig. 3 Oxide network of dimension 5

We compute the values of $BN(OX_n)$ and $B(OX_n, x)$ for oxide networks.

Theorem 4.1. The Banhatti-Nirmala index and Banhatti-Nirmala exponential of OX_n oxide networks are given by

(i) $BN(OX_n) == 36\sqrt{10}n^2 + \left(\sqrt{6}+\sqrt{8}-2\times\sqrt{10}\right)12n.$

(ii) $BN(OX_n, x) = 12nx^{\sqrt{6}+\sqrt{8}} + \left(18n^2 - 12n\right)x^{2\sqrt{10}}.$

Proof: Let G be the graph of oxide network OX_n, see Figure 3. By algebraic method, G has $9n^2 + 3n$ vertices and $18n^2$ edges. In OX_n, there are two types of edges based on the degree of the vertices of each edge. Further by algebraic method, the edge degree partition of an oxide network OX_n is given in Table 3.

Table 3. Edge degree partition of OX_n

$d_G(u), d_G(v)\backslash e = uv \in E(G)$	(2,4)	(4,4)
$d_G(e)$	4	6
Number of edges	$12n$	$18n^2 - 12n$

(i) To compute $BN(OX_n)$, we see that

$$BN(OX_n) = \sum_{ue} \sqrt{d_G(u) + d_G(e)}$$

$$= 12n\left[\sqrt{2+4} + \sqrt{4+4}\right] + \left(18n^2 - 12n\right)\left[\sqrt{4+6} + \sqrt{4+6}\right]$$

$$= 36\sqrt{10}n^2 + \left(\sqrt{6}+\sqrt{8}-2\times\sqrt{10}\right)12n.$$

(ii) To compute $BN(OX_n, x)$, we see that

$$BN(OX_n, x) = \sum_{uv\in E(G)} x^{\sqrt{d_G(u)+d_G(e)}}$$

$$= 12nx^{\sqrt{6}+\sqrt{8}} + \left(18n^2 - 12n\right)x^{2\sqrt{10}}.$$

V. RESULTS FOR HONEYCOMB NETWORKS

If we recursively use hexagonal tiling in a particular pattern, honeycomb networks are formed. These networks are useful in chemistry and also in computer graphics. A honeycomb network of dimension n is denoted by HC_n, where n is the number of hexagons between central and boundary hexagon. A 4-dimensional honeycomb network is shown in Figure 4.

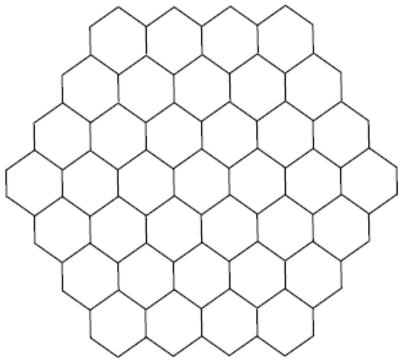

Fig. 4 Honeycomb network of dimension four

Now we compute the values of $BN(HC_n)$ and $BN(HC_n, x)$ for honeycomb networks.

Theorem 5.1. The Banhatti-Nirmala index and Banhatti-Nirmala exponential of HC_n oxide networks are given by

(i) $BN(HC_n) = 24 + (12n - 12)(\sqrt{5} + \sqrt{6}) + 2(9n^2 - 15n + 6)\sqrt{7}.$

(ii) $BN(HC_n, x) = 6x^4 + (12n - 12)x^{\sqrt{5}+\sqrt{6}} + (9n^2 - 15n + 6)x^{2\sqrt{7}}.$

Proof: Let G be the graph of honeycomb network HC_n with $6n^2$ vertices and $9n^2 - 3n$ edges. In HC_n, there are three types of edges based on the degree of the vertices of each edge. Further, by algebraic method, the edge degree partition of a honeycomb network HC_n is given in Table 4.

Table 4. Edge degree partition of HC_n

$d_G(u), d_G(v)\backslash e = uv \in E(G)$	(2, 2)	(2, 3)	(3, 3)
$d_G(e)$	2	3	4
Number of edges	6	$12n - 12$	$9n^2 - 15n + 6$

(i) To compute $BN(HC_n)$, we see that

$$BN(HC_n) = \sum_{ue} \sqrt{d_G(u) + d_G(e)}$$

$$= 6\left[\sqrt{2+2} + \sqrt{2+2}\right] + (12n - 12)\left[\sqrt{2+3} + \sqrt{3+3}\right] + (9n^2 - 15n + 6)\left[\sqrt{3+4} + \sqrt{3+4}\right]$$

$$= 24 + (12n - 12)(\sqrt{5} + \sqrt{6}) + 2(9n^2 - 15n + 6)\sqrt{7}.$$

(ii) To compute $BN(HC_n)$, we see that

$$BN(HC_n, x) = \sum_{uv \in E(G)} x^{\sqrt{d_G(u) + d_G(e)}}$$

$$= 6x^4 + (12n - 12)x^{\sqrt{5}+\sqrt{6}} + (9n^2 - 15n + 6)x^{2\sqrt{7}}.$$

VI. CONCLUSION

In this study, a novel invariant is considered which is the Banhatti-Nirmala index. Also we have defined the Banhatti-Nirmala exponential of a molecular graph. Furthermore, the Banhatti-Nirmala index and its corresponding exponential for certain networks are determined.

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