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REVERSE NIRMALA INDEX

V. R. Kulli
Department of Mathematics Gulbarga University, Gulbarga, 585106, India

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ABSTRACT

In this paper, we propose the reverse Nirmala index, reverse Nirmala exponential of a graph. We determine the reverse Nirmala index and its corresponding exponential of chain silicate, silicate, oxide, honeycomb and hexagonal networks.

Keywords: reverse Nirmala index, reverse Nirmala exponential, silicate, oxide, honeycomb, hexagonal networks.

Mathematics Subject Classification: 05C05, 05C07, 05C12.

1. INTRODUCTION

A molecular 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 to the bonds between atoms. A topological index is a numerical parameter mathematically derived from the graph structure. These indices are useful for establishing correlation between the structure of a molecular compound and its physicochemical properties. Also these indices have been considered in Theoretical Chemistry and have found some applications, especially in QSPR/QSAR study, see [1].

Let G be a finite simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Let $d_G(u)$ denote the degree of a vertex u in G, which is the number of vertices adjacent to u. Let □(G) denote the largest of all degrees of G. The reverse vertex degree of a vertex u in G is defined as c_u = □(G) – $d_G(u)$ + 1. The reverse edge connecting the reverse vertices u and v will be denoted by uv. We refer to [2] for undefined term and notation.

In [3], Ediz introduced the first reverse Zagreb beta index and the second reverse Zagreb index of a graph G and they are defined as

$$CM_1(G) = \sum_{uv\in E(G)} (c_u + c_v), \qquad CM_2(G) = \sum_{uv\in E(G)} c_u c_v.$$

Recently, some reverse Zagreb indices were introduced and studied, see [4, 5, 6, 7, 8, 9].

The Nirmala index was introduced by Kulli in [10] and defined it as

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

Recently, some Nirmala indices were proposed and studied, for example, in [11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22].

Motivated by the definition of the Nirmala index and its applications, we introduce the reverse Nirmala index of a molecular graph as follows:

The reverse Nirmala index of a graph G is defined as

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$$CN(G) = \sum_{uv \in E(G)} \sqrt{c_u + c_v}. \qquad (1)$$

Considering the reverse Nirmala index, we propose the reverse Nirmala exponential of a graph G and defined it as

$$CN(G, x) = \sum_{uv \in E(G)} x^{\sqrt{c_u + c_v}}. \qquad (2)$$

In this paper, the reverse Nirmala index and its corresponding exponential of chain silicate, silicate, oxide, honeycomb and hexagonal networks are computed.

2. RESULTS FOR CHAIN SILICATE NETWORKS

Silicates are very important elements of Earth's crust. Sand and several minerals are constituted by silicates. A family of chain silicate network is symbolized by CS_n and is obtained by arranging $n \geq 2$ tetrahedral linearly, see Figure 1.

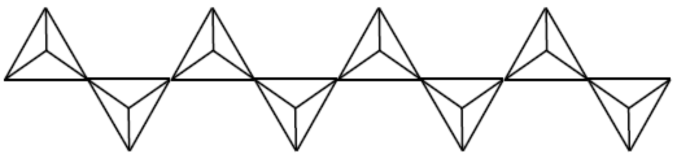

Figure 1. Chain silicate network

Let G be the graph of a chain silicate network CS_n with $3n+1$ vertices and $6n$ edges. From Figure 1, it is easy to see that $\Delta(G) = 6$. Thus $c_u = \Delta(G) - d_G(u) + 1 = 7 - d_G(u)$. In G, by algebraic method, there are three types of edges based on the degree of end vertices of each edge as follows:

$E_{33} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}$, $|E_{33}| = n + 4$.
$E_{36} = \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 6\}$, $|E_{36}| = 4n - 2$.
$E_{66} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 6\}$, $|E_{66}| = n - 2$.

Thus there are three types of reverse edges as given in Tabe 1.

Table 1. Reverse edge partition of CS_n

$c_u, c_v \backslash uv \in E(G)$	(4, 4)	(4, 1)	(1, 1)
Number of edges	$n + 4$	$4n - 2$	$n - 2$

We now determine the reverse Nirmala index of a chain silicate network CS_n.

Theorem 1. The reverse Nirmala index of CS_n is

$$CN(CS_n) = \left(3\sqrt{2} + 4\sqrt{5}\right)n + 6\sqrt{2} - 2\sqrt{5}.$$

Proof: Let G be the graph of CS_n. By using equation (1) and Table 1, we deduce

$$CN(CS_n) = \sum_{uv \in E(G)} \sqrt{c_u + c_v}$$
$$= (n + 4)\sqrt{4 + 4} + (4n - 2)\sqrt{4 + 1} + (n - 2)\sqrt{1 + 1}$$
$$= \left(3\sqrt{2} + 4\sqrt{5}\right)n + 6\sqrt{2} - 2\sqrt{5}.$$

In the next theorem, we compute the reverse Nirmala exponential of a chain silicate network CS_n.

Theorem 2. The reverse Nirmala exponential of CS_n is

$$CN(CS_n, x) = (n + 4)x^{2\sqrt{2}} + (4n - 2)x^{\sqrt{5}} + (n - 2)x^{\sqrt{2}}.$$

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Proof: Let G be the graph of CS_n. From equation (2) and by using Table 1, we derive

$$CN(CS_n, x) = \sum_{uv \in E(G)} x^{\sqrt{c_u + c_v}}$$

$$= (n+4)x^{\sqrt{4+4}} + (4n-2)x^{\sqrt{4+1}} + (n-2)x^{\sqrt{1+1}}$$

$$= (n+4)x^{2\sqrt{2}} + (4n-2)x^{\sqrt{5}} + (n-2)x^{\sqrt{2}}.$$

3. RESULTS FOR SILICATE NETWORKS

Silicates are obtained by fusing metal oxide 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 2-dimensional silicate network is presented in Figure 2.

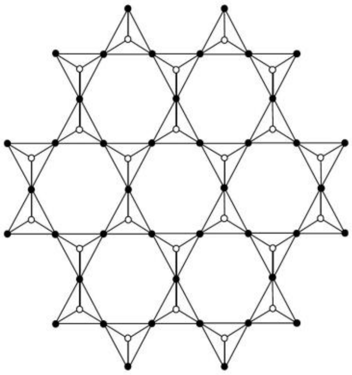

Figure 2. A 2-dimensional silicate network

Let G be the graph of a silicate network SL_n. From Figure 2, it is easy to see that $\Delta(G) = 6$. Clearly we have $c_u = \Delta(G) - d_G(u) + 1 = 7 - d_G(u)$. The graph G has $15n^2 + 3n$ vertices and $36n^2$ edges. In G, by algebraic method, there are three types of edges based on the degree of end vertices of each edge as follows:

$E_{33} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}$, $|E_{33}| = 6n$.
$E_{36} = \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 6\}$, $|E_{36}| = 18n^2 + 6n$.
$E_{66} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 6\}$, $|E_{66}| = 18n^2 - 12n$.

Thus there are three types of reverse edges as given in Tabe 2.

Table 2. Reverse edge partition of SL_n

$c_u, c_v \backslash uv \in E(G)$	(4, 4)	(4, 1)	(1, 1)
Number of edges	$6n$	$18n^2 + 6n$	$18n^2 - 12n$

In the following theorem, we compute the reverse Nirmala index of SL_n.

Theorem 3. The reverse Nirmala index of a silicate network SL_n is

$$CN(SL_n) = \left(18\sqrt{5}n^2 + 18\sqrt{2}\right)n^2 + 6\sqrt{5}n.$$

Proof: Let G be the graph of a silicate network SL_n. By using equation (1) and Table 2, we obtain

$$CN(SL_n) = \sum_{uv \in E(G)} \sqrt{c_u + c_v}$$

$$= 6n\sqrt{4+4} + \left(18n^2 + 6n\right)\sqrt{4+1} + \left(18n^2 - 12n\right)\sqrt{1+1}$$

$$= \left(18\sqrt{5}n^2 + 18\sqrt{2}\right)n^2 + 6\sqrt{5}n.$$

In Theorem 4, we calculate the reverse Nirmala exponential of SL_n.

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Theorem 4. The reverse exponential of a silicate network SL_n is

$$CN(SL_n, x) = 6nx^{2\sqrt{2}} + (18n^2 + 6n)x^{\sqrt{5}} + (18n^2 - 12n)x^{\sqrt{2}}.$$

Proof: Let G be the graph of a silicate network SL_n. From equation (2) and by using Table 2, we derive

$$CN(SL_n, x) = \sum_{uv \in E(G)} x^{\sqrt{c_u + c_v}}$$

$$= 6nx^{\sqrt{4+4}} + (18n^2 + 6n)x^{\sqrt{4+1}} + (18n^2 - 12n)x^{\sqrt{1+1}}$$

$$= 6nx^{2\sqrt{2}} + (18n^2 + 6n)x^{\sqrt{5}} + (18n^2 - 12n)x^{\sqrt{2}}.$$

4. 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.

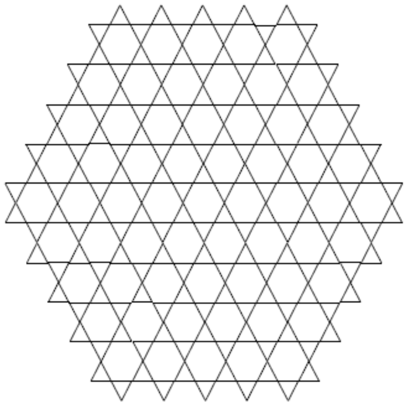

Figure 3. Oxide network of dimension 5

Let G be the graph of an oxide network OX_n. From Figure 3, it is easy to see that $\Delta(G)$=4. Thus $c_u = \Delta(G) - d_G(u) + 1 = 5 - d_G(u)$. By calculation, we obtain that G has $9n^2+3n$ vertices and $18n^2$ edges. In G, by algebraic method, there are two types of edges based on the degree of end vertices of each edge as follows:

$E_{24} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 4\}$, $|E_{24}| = 12n$.
$E_{44} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 4\}$, $|E_{44}| = 18n^2 - 12n$.

Thus there are two types of reverse edges as given in Table 3.

Table 3. Reverse edge partition of OX_n

$c_u, c_v \backslash uv \in E(G)$	(3, 1)	(1, 1)
Number of edges	$12n$	$18n^2 - 12n$

In the following theorem, we compute the reverse Nirmala index of OX_n.

Theorem 5. The reverse Nirmala index of an oxide network OX_n is

$$CN(OX_n) = 18\sqrt{2}n^2 + (24 - 12\sqrt{2})n.$$

Proof: Let G be the graph of OX_n. From equation (1) and by using Table 3, we have

$$CN(OX_n) = \sum_{uv \in E(G)} \sqrt{c_u + c_v}$$

$$= 12n\sqrt{3+1} + (18n^2 - 12n)\sqrt{1+1}$$

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$$= 18\sqrt{2}n^2 + \left(24 - 12\sqrt{2}\right)n.$$

In Theorem 6, we determine the reverse Nirmala exponential of OX_n.

Theorem 6. The reverse Nirmala exponential of an oxide network OX_n is

$$CN\left(OX_n, x\right) = 12nx^2 + \left(18n^2 - 12n\right)x^{\sqrt{2}}.$$

Proof: Let G be the graph of OX_n. By using equation (2) and Table 3, we deduce

$$CN\left(OX_n, x\right) = \sum_{uv \in E(G)} x^{\sqrt{c_u + c_v}}$$

$$= 12nx^{\sqrt{3+1}} + \left(18n^2 - 12n\right)x^{\sqrt{1+1}}$$

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

5. RESULTS FOR HONEYCOMB NETWORKS

Honeycomb networks are useful in Computer Graphics and Chemistry. 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.

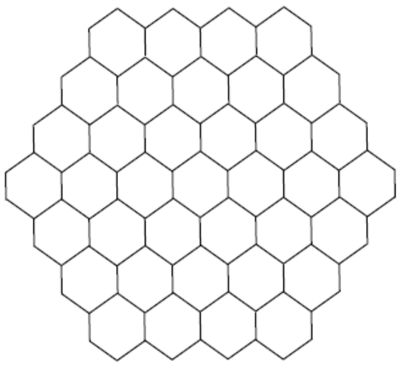

Figure 4. A 4-dimensional honeycomb network

Let G be the graph of a honeycomb network HC_n. From Figure 4, it is easy to see that $\Delta(G) = 3$. Therefore $c_u = \Delta(G) - d_G(u) + 1 = 4 - d_G(u)$. By calculation, we obtain that G has $6n^2$ vertices and $9n^2 – 3n$ edges. In G, by algebraic method, there are three types of edges based on the degree of end vertices of each edge as follows:

$E_{22} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_{22}| = 6$.
$E_{23} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_{23}| = 12n – 12$.
$E_{33} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}$, $|E_{33}| = 9n^2 – 15n + 6$.

Thus there are three types of reverse edges as given in Table 4.

Table 4. Reverse edge partition of HC_n

$c_u, c_v \backslash uv \in E(G)$	(2, 2)	(2, 1)	(1, 1)
Number of edges	6	$12n – 12$	$9n^2 – 15n + 6$

In the following theorem, we compute the reverse Nirmala index of HC_n.

Theorem 7. The reverse Nirmala index of a honeycomb network HC_n is

$$CN\left(HC_n\right) = 9\sqrt{2}n^2 + \left(12\sqrt{3} - 15\sqrt{2}\right)n + 12 - 12\sqrt{3} - 6\sqrt{2}.$$

Proof: Let G be the graph of a honeycomb network HC_n. By using equation (1) and Table 4, we derive

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$$CN(HC_n) = \sum_{uv\in E(G)} \sqrt{c_u + c_v}$$
$$= 6\sqrt{2+2} + (12n-12)\sqrt{2+1} + (9n^2 - 15n+6)\sqrt{1+1}$$
$$= 9\sqrt{2}n^2 + \left(12\sqrt{3} - 15\sqrt{2}\right)n + 12 - 12\sqrt{3} - 6\sqrt{2}.$$

In the next theorem, we calculate the reverse Nirmala exponential of HC_n.

Theorem 8. The reverse Nirmala exponential of a honeycomb network HC_n is
$$CN(HC_n, x) = (12n-6)x^2 + (9n^2 - 15n + 6)x^{\sqrt{2}}.$$

Proof: Let G be the graph of a honeycomb network HC_n. By using equation (2) and Table 4, we deduce
$$CN(HC_n, x) = \sum_{uv\in E(G)} x^{\sqrt{c_u+c_v}}$$
$$= 6x^{\sqrt{2+2}} + (12n-12)x^{\sqrt{3+1}} + (9n^2 - 15n + 6)x^{\sqrt{1+1}}$$
$$= (12n-6)x^2 + (9n^2 - 15n + 6)x^{\sqrt{2}}.$$

6. RESULTS FOR HEXAGONAL NETWORKS

It is known that there exist three regular plane tilings with composition of some kind of regular polygons such as triangular, hexagonal and square. Triangular tiling is used in the construction of hexagonal networks. This network is denoted by HX_n, where n is the number of vertices in each side of hexagon. A hexagonal network of dimension six is shown in Figure 5.

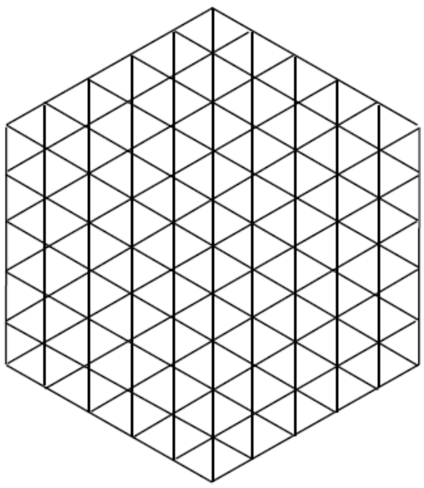

Figure 5. Hexagonal network of dimension six

Let G be the graph of a hexagonal network HX_n. The graph G has $3n^2–3n+1$ vertices and $9n^2–15n+6$ edges. From Figure 5, it is easy to see that $\Delta(G)=6$. Thus $c_u = \Delta(G) – d_G(u) + 1 = 7 – d_G(u)$. In G, by algebraic method, there are five types of edges based on the degree of end vertices of each edge as follows:

$E_{34} = \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 4\}$, $|E_{34}| = 12$.
$E_{36} = \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 6\}$, $|E_{36}| = 6$.
$E_{44} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 4\}$, $|E_{44}| = 6n – 18$.
$E_{46} = \{uv \in E(G) \mid d_G(u) = 4, d_G(v) = 6\}$, $|E_{46}| = 12n – 24$.
$E_{66} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 6\}$, $|E_{66}| = 9n^2 – 33n + 30$.

Thus there are five types of reverse edges as given in Table 5.

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Table 5. Reverse edge partition of HX_n

$c_u, c_v \backslash uv \in E(G)$	(4, 3)	(4, 1)	(3, 3)	(3, 1)	(1, 1)
Number of edges	12	6	$6n – 18$	$12n – 24$	$9n^2 – 33n + 30$

In the following theorem, we determine the reverse Nirmala index of HX_n.

Theorem 9. The reverse Nirmala index of a hexagonal network HX_n is

$$CN(HX_n) = 9\sqrt{2}n^2 + \left(6\sqrt{6} + 24 - 33\sqrt{2}\right)n + 12\sqrt{7} + 6\sqrt{5} - 18\sqrt{6} - 48 + 30\sqrt{2}.$$

Proof: Let G be the graph of a hexagonal network HX_n. By using equation (1) and Table 5, we deduce

$$CN(HX_n) = \sum_{uv\in E(G)} \sqrt{c_u + c_v}$$

$$= 12\sqrt{4+3} + 6\sqrt{4+1} + (6n-18)\sqrt{3+3} + (12n-24)\sqrt{3+1} + \left(9n^2 - 33n + 30\right)\sqrt{1+1}$$

$$= 9\sqrt{2}n^2 + \left(6\sqrt{6} + 24 - 33\sqrt{2}\right)n + 12\sqrt{7} + 6\sqrt{5} - 18\sqrt{6} - 48 + 30\sqrt{2}.$$

We now calculate the reverse Nirmala exponential of HX_n.

Theorem 10. The reverse Nirmala exponential of a hexagonal network HX_n is

$$CN(HX_n, x) = 12x^{\sqrt{7}} + 6x^{\sqrt{5}} + (6n-18)x^{\sqrt{6}} + (12n-24)x^2 + \left(9n^2 - 33n + 30\right)x^{\sqrt{2}}.$$

Proof: Let G be the graph of HX_n. By using equation (2) and using Table 5, we derive

$$CN(HX_n, x) = \sum_{uv\in E(G)} x^{\sqrt{c_u + c_v}}$$

$$= 12x^{\sqrt{4+3}} + 6x^{\sqrt{4+1}} + (6n-18)x^{\sqrt{3+3}} + (12n-24)x^{\sqrt{3+1}} + (9n^2 - 33n + 30)x^{\sqrt{1+1}}$$

$$= 12x^{\sqrt{7}} + 6x^{\sqrt{5}} + (6n-18)x^{\sqrt{6}} + (12n-24)x^2 + (9n^2 - 33n + 30)x^{\sqrt{2}}.$$

7. CONCUSION

In this study, we have proposed the reverse Nirmala index and its corresponding exponential of a graph. Furthermore, we have calculated exact values of this novel topological index and its corresponding exponential for certain networks.

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