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SQUARE REVERSE INDEX AND ITS POLYNOMIAL OF CERTAIN NETWORKS

V. R. KULLI*

Department of Mathematics, Gulbarga University, Gulbarga, 585106, India.

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ABSTRACT

We propose the square reverse index of a molecular graph. Considering the square reverse index, we define the square reverse polynomial of a molecular graph. In this paper, we determine the square reverse index and its polynomial of certain networks of chemical importance like silicate, chain silicate, hexagonal, oxide and honeycomb networks.

Keywords: *square reverse index, square reverse polynomial, silicate, hexagonal, oxide, honeycomb networks.*

Mathematics Subject Classification: *05C05, 05C07, 05C12, 05C35.*

1. INTRODUCTION

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. In Chemistry, topological indices have found to be useful in chemical documentation, isomer discrimination, structure property relationships, structure activity relationships and pharmaceutical drug design. There has been considerable interest in the general problem of determining topological indices, see [1].

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

Recently, Kulli [3] proposed the square ve-degree index of a graph, defined as

$$Q_{ve}(G) = \sum_{uv \in E(G)} \left[d_{ve}(u) - d_{ve}(v) \right]^2.$$

Motivated by the definition of the square ve-degree index, we introduce the square reverse index as follows:

The square reverse index of a molecular graph G is defined as

$$QC(G) = \sum_{uv \in E(G)} \left(c_u - c_v \right)^2. \tag{1}$$

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

Considering the square reverse index, we introduce the square reverse polynomial of a graph G as

$$QC(G, x) = \sum_{uv \in E(G)} x^{\left(c_u - c_v \right)^2}. \tag{2}$$

Recently, some polynomials were studied, for example, in [12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22].

In this paper, the square reverse index and square reverse polynomial of silicate, chain silicate, hexagonal, oxide and honeycomb networks are determined. Silicates are very important elements of Earth's crust. Sand and several minerals are constituted by silicates. For more information about networks see [23].

Corresponding Author: V. R. Kulli*
Department of Mathematics, Gulbarga University, Gulbarga, 585106, India.

2. 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 1.

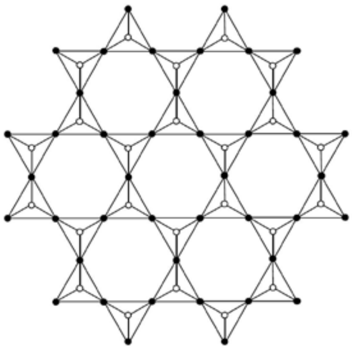

Figure-1: A 2-dimensional silicate network

Let G be the graph of a silicate network SL_n. From Figure 1, it is easy to see that the vertices of SL_n are either of degree 3 or 6. Therefore $\Delta(G) = 6$. 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 1.

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

Table-1: Reverse edge partition of SL_n

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

Theorem 1: The square reverse index of a silicate network SL_n is given by

$$QC(SL_n) = 162n^2 + 54n.$$

Proof: From equation (1) and Table 1, we see that

$$QC(SL_n) = \sum_{uv \in E(G)} [c_u - c_v]^2$$
$$= (4-4)^2 6n + (4-1)^2 (18n^2 + 6n) + (1-1)^2 (18n^2 - 12n)$$
$$= 162n^2 + 54n.$$

In the following theorem, we compute the square reverse polynomial of SL_n.

Theorem 2: The square reverse polynomial of a silicate network SL_n is given by

$$QC(SL_n, x) = (18n^2 + 6n)x^9 + (18n^2 - 6n)x^0.$$

Proof: From equation (2) and using Table 1, we see that

$$QC(SL_n, x) = \sum_{uv \in E(G)} x^{[c_u - c_v]^2}$$
$$= 6n\, x^{(4-4)^2} + (18n^2 + 6n)\, x^{(4-1)^2} + (18n^2 - 12n)\, x^{(1-1)^2}$$
$$= (18n^2 + 6n)x^9 + (18n^2 - 6n)x^0.$$

3. RESULTS FOR CHAIN SILICATE NETWORKS

We now consider a family of chain silicate networks. This network is symbolized by CS_n and is obtained by arranging $n \geq 2$ tetrahedral linearly, see Figure 2.

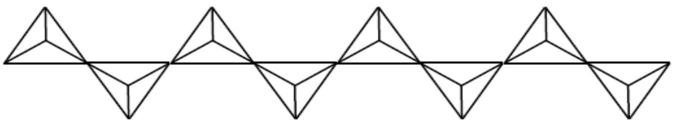

Figure-2: Chain silicate network

Let G be the graph of a chain silicate network CS_n with $3n+1$ vertices and $6n$ edges. From Figure 2, it is easy to see that the vertices of CS_n are either of degree 3 or 6. Therefore $\Delta(G) = 6$. 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:

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

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

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

Table-2: Reverse edge partition of CS_n

In the following theorem, we determine the square reverse index of CS_n.

Theorem 3: The square reverse index of a chain silicate network CS_n is given by

$$QC(CS_n) = 36n - 18.$$

Proof: From equation (1) and using Table 2, we see that

$$QC(CS_n) = \sum_{uv \in E(G)} \left[c_u - c_v\right]^2$$
$$= (4-4)^2(n+4) + (4-1)^2(4n-2) + (1-1)^2(n-2)$$
$$= 36n - 18.$$

In the following theorem, we compute the square reverse polynomial of CS_n.

Theorem 4: The square reverse polynomial of a chain silicate network CS_n is given by

$$QC(CS_n, x) = (4n-2)x^9 + (2n+2)x^0.$$

Proof: From equation (2) and Table 2, we see that

$$QC(CS_n, x) = \sum_{uv \in E(G)} x^{(c_u - c_v)^2}$$
$$= (n+4)x^{(4-4)^2} + (4n-2)x^{(4-1)^2} + (n-2)x^{(1-1)^2}$$
$$= (4n-2)x^9 + (2n+2)x^0.$$

4. 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 symbolized 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 3.

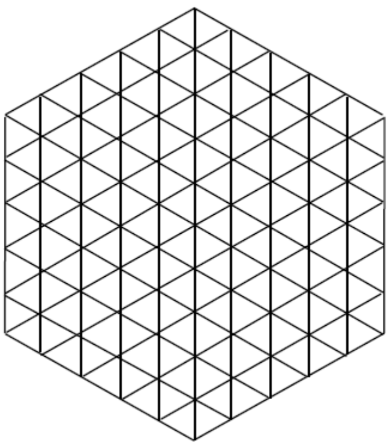

Figure-3: Hexagonal network of dimension six

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 3, it is easy to see that the vertices of HX_n are either of degree 3, 4 or 6. Therefore $\Delta(G)=6$ and $\delta(G)=3$. 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 Tabe 3.

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

Table-3: Reverse edge partition of HX_n

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

Theorem 5: The square reverse index of a hexagonal network HX_n is

$$QC(HX_n) = 48n – 30.$$

Proof: From equation (1) and Table 3, we deduce

$$QC(HX_n) = \sum_{uv \in E(G)} [c_u - c_v]^2$$
$$= (4–3)^2 12+(4–1)^2 6+(3–3)^2(6n–18) + (3–1)^2(12n – 24)+(1–1)^2(9n^2–33n + 30)$$
$$= 48n – 30.$$

In the following theorem, we calculate the square reverse polynomial of HX_n.

Theorem 6: The square reverse polynomial of a hexagonal network HX_n.

$$QC(HX_n, x) = 6x^9+(12n – 24)x^4 + 12x^1 + (9n^2 – 27n + 12)x^0.$$

Proof: From equation (2) and Table 3, we see that

$$QC(HX_n, x) = \sum_{uv \in E(G)} x^{[c_u - c_v]^2}$$
$$= 12x^{(4-3)^2} + 6x^{(4-1)^2} + (6n-18)x^{(3-3)^2} + (12n-24)x^{(3-1)^2} + (9n^2 - 33n + 30)x^{(1-1)^2}$$
$$= 6x^9 + (12n – 24)x^4 + 12x^1 + (9n^2 – 27n + 12)x^0.$$

5. 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-4.

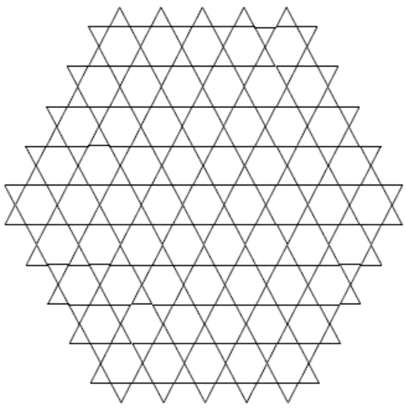

Figure-4: Oxide network of dimension 5

Let G be the graph of an oxide network OX_n. From Figure 4, it is easy to see that the vertices of OX_n are either of degree 2 or 4. Therefore $\Delta(G)=4$. 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 4.

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

Table-4: Reverse edge partition of OX_n

In the following theorem, we calculate the square reverse index of OX_n.

Theorem 7: The square reverse index of an oxide network OX_n is given by

$$QC(OX_n) = 48n.$$

Proof: From equation (1) and using Table 4, we see that

$$QC(OX_n) = \sum_{uv \in E(G)} [c_u - c_v]^2$$
$$= (3-1)^2 12n + (1-1)^2 (18n^2 - 12n)$$
$$= 48n.$$

In the following theorem, we calculate the square reverse polynomial of OX_n.

Theorem 8: The square reverse polynomial of an oxide network OX_n is given by

$$QC(OX_n, x) = 12nx^4 + (18n^2 - 12n)x^0.$$

Proof: From equation (2) and using Table 4, we see that

$$QC(OX_n, x) = \sum_{uv \in E(G)} x^{[c_u - c_v]^2}$$
$$= 12nx^{(3-1)^2} + (18n^2 - 12n)x^{(1-1)^2}$$
$$= 12nx^4 + (18n^2 - 12n)x^0.$$

6. 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 5.

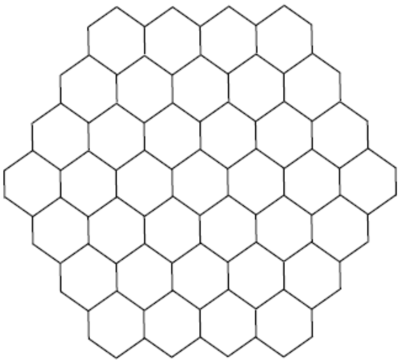

Figure-5: A 4-dimensional honeycomb network

Let G be the graph of a honeycomb network HC_n. From Figure 5, it is easy to see that the vertices of HC_n are either of degree 2 or 3. Thus $\Delta(G) = 3$. 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 Tabe 5.

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

Table-5: Reverse edge partition of HC_n

In the following theorem, we derive the square reverse index of HC_n.

Theorem 9: The square reverse index of a honeycomb network HC_n is

$$QC(HC_n) = 12n – 12.$$

Proof: From equation (1) and Table 5, we see that

$$QC(HC_n) = \sum_{uv \in E(G)} [c_u - c_v]^2$$
$$= (2 – 2)^2 6 + (2 – 1)^2 (12n – 12) + (1 – 1)^2 (9n^2 – 12n + 6)$$
$$= 12n – 12.$$

In the following theorem, we derive the square reverse polynomial of HC_n.

Theorem 10: The square reverse polynomial of a honeycomb network HC_n is given by

$$QC(HC_n, x) = (12n – 12)x^1 + (9n^2 – 15n + 12)x^0.$$

Proof: From equation (2) and Table 5, we see that

$$QC(HC_n, x) = \sum_{uv \in E(G)} x^{[c_u - c_v]^2}$$
$$= 6x^{(2-2)^2} + (12n - 12)x^{(2-1)^2} + (9n^2 - 15n + 6)x^{(1-1)^2}$$
$$= (12n^2 – 12)x^1 + (9n^2 – 15n + 12)x^0.$$

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