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COMPUTING F-REVERSE INDEX AND F-REVERSE POLYNOMIAL OF CERTAIN NETWORKS

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ABSTRACT

In this paper, we introduce the F-reverse index of a molecular graph. Considering the F-reverse index, we define the F-reverse polynomial of a molecular graph. We compute the F-reverse index and F-reverse polynomial of silicate, chain silicate, hexagonal, oxide and honeycomb networks.

Keywords: *F-reverse index, F-reverse polynomial, silicate, hexagonal, oxide, honeycomb 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 physico-chemical properties. Also these indices have been considered in Theoretical Chemistry and have found some applications, especially in QSPR/QSAR study, see [1].

Throughout this paper, we consider finite simple connected graphs. Let G be a graph with a vertex set $V(G)$ and edge set $E(G)$. Let $d_G(v)$ denote the degree of a vertex v in G, which 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.

The first reverse Zagreb beta index and the second reverse Zagreb index of a graph G are defined as

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

These indices were introduced by Ediz in [3]. For more information and recent results about reverse Zagreb indices, see [4, 5, 6, 7, 8, 9].

The forgotten topological index or F-index of a graph G is defined as

$$F(G) = \sum_{uv\in E(G)} \left[d_G(u)^2 + d_G(v)^2 \right] = \sum_{u\in V(G)} d_G(u)^3.$$

The F-index was studied by Furtula and Gutman in [10] and also it was studied, for example, in [11, 12, 13, 14, 15, 16, 17, 18].

Motivated by the definition of the F-index and its applications, we introduce the F-reverse index and F_1-reverse index of a molecular graph as follows:

The F-reverse index of a molecular graph G is defined as

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

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The F_1-reverse index of a molecular graph G is defined as

$$F_1C(G) = \sum_{u \in V(G)} c_u^3.$$

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

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

Silicates are very important elements of Earth's crust. Sand and several minerals are constituted by silicates. The tetrahedron is a basic unit of silicates, in which the central vertex is silicon vertex and the corner vertices are oxygen vertices. For networks see [19]. In this paper, the F-reverse index and R-reverse polynomial of silicate, chain silicate, hexagonal, oxide and honeycomb networks are computed.

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.

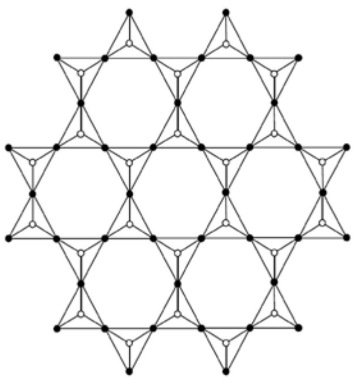

Figure-1: A 2-dimensional silicated network

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.

$c_u, c_v \backslash uv \in E(\underline{G})$	(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 F reverse index of SL_n.

Theorem 1: The F reverse index of a silicate network SL_n is
$FC(SL_n) = 342n^2 + 270n$.

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

$$FC(SL_n) = \sum_{uv \in E(G)} \left(c_u^2 + c_v^2\right)$$
$$= (4^2+4^2)6n + (4^2+1^2)(18n^2 + 6n) + (1^2+1^2)(18n^2 - 12n)$$
$$= 342n^2 + 270n.$$

In the following theorem, we calculate the F reverse polynomial of SL_n.

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Theorem 2: The F reverse polynomial of a silicate network SL_n is

$$FC(SL_n, x) = 6nx^{32} + (18n^2 + 6n)x^{17} + (18n^2 - 12n)x^2.$$

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

$$FC(SL_n, x) = \sum_{uv\in E(G)} x^{\left(c_u^2+c_v^2\right)}$$

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

$$= 6nx^{32} + (18n^2+6n)x^{17} + (18n^2 - 12n)x^2.$$

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.

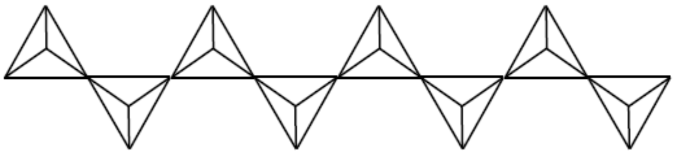

Figure-2: Chain silicate network

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:

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

Thus there are three types of reverse edges as given in Tabe 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 F reverse index of CS_n.

Theorem 3: The F reverse index of a chain silicate network CS_n is

$$FC(CS_n) = 102n + 90.$$

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

$$FC(CS_n) = \sum_{uv\in E(G)} \left(c_u^2 + c_v^2\right)$$

$$= (4^2+4^2)(n + 4) + (4^2+1^2)\,(4n - 2) + (1^2+1^2)\,(n - 2)$$

$$= 102n + 90.$$

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

Theorem 4: The F reverse polynomial of a chain silicate network CS_n is

$$FC(CS_n, x) = (n + 4)x^{32} + (4n - 2)x^{17} + (n - 2)x^2.$$

Proof: Let G be the graph of a chain silicate network CS_n. By using equation (2) and Table 2, we derive

$$FC(CS_n, x) = \sum_{uv\in E(G)} x^{\left(c_u^2+c_v^2\right)}$$

$$= (n+4)\,x^{\left(4^2+4^2\right)} + (4n-2)\,x^{\left(4^2+1^2\right)} + (n-2)\,x^{\left(1^2+1^2\right)}$$

$$= (n+4)x^{32} + (4n - 2)x^{17} + (n - 2)x^2.$$

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4. RESULTS FOR HEXAGONAL NETWORKS

It is known that there exist three regular plane tilings with composition of same 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.

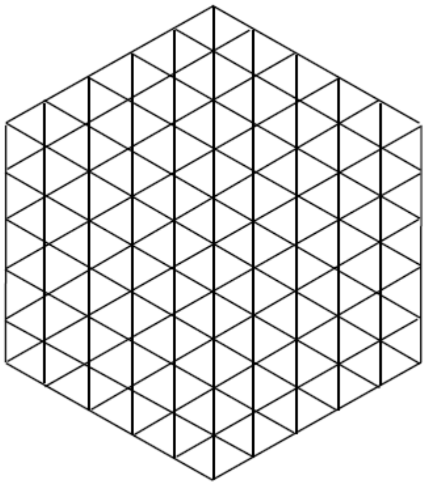

Figure-3: Hexagonal network of dimension six

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 compute the F reverse index of HX_n.

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

$$FC(HX_n) = 18n^2 + 162n - 102.$$

Proof: Let G be the graph of a hexagonal network HX_n. By using equation (1) and Table 3, we deduce

$$FC(HX_n) = \sum_{uv\in E(G)} \left(c_u^2 + c_v^2\right)$$
$$= (4^2+3^2)12 + (4^2+1^2)6 + (3^2+3^2)(6n - 18) + (3^2+1^2)(12n - 24) + (1^2+1^2)(9n^2 - 33n + 30)$$
$$= 18n^2 + 162n - 102.$$

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

Theorem 6: The F reverse polynomial of a hexagonal network HX_n is

$$FC(HX_n, x) = 12x^{25} + 6x^{17} + (6x - 18)x^{18} + (12x - 24)x^{10} + (9n^2 - 33n + 30)x^2.$$

Proof: Let G be the graph of a hexagonal network HX_n. By using equation (2) and Table 3, we derive

$$FC(HX_n, x) = \sum_{uv\in E(G)} x^{\left(c_u^2+c_v^2\right)}$$
$$= 12x^{\left(4^2+3^2\right)} + 6x^{\left(4^2+1^2\right)} + (6n-18)x^{\left(3^2+3^2\right)} + (12n-24)x^{\left(3^2+1^2\right)} + \left(9n^2-33n+30\right)x^{\left(1^2+1^2\right)}$$
$$= 12x^{25} + 6x^{17} + (6x - 18)x^{18} + (12x - 24)x^{10} + (9n^2 - 33n + 30)x^2.$$

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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.

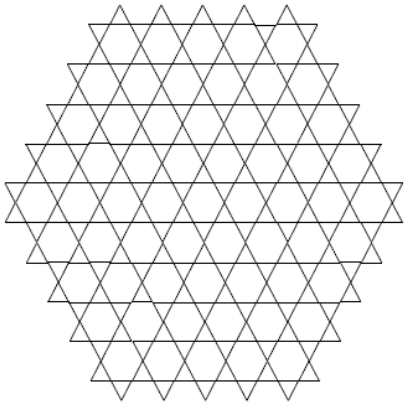

Figure-4: Oxide network of dimension 5

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 Tabe 4.

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

Table-4: Reverse edge partition of OX_n

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

Theorem 7: The F reverse index of an oxide network OX_n is
$FC(OX_n) = 36n^2 + 96n$.

Proof: Let G be the graph of an oxide network OX_n. By using equation (1) and Table 4, we obtain

$$FC(OX_n) = \sum_{uv \in E(G)} \left(c_u^2 + c_v^2\right)$$
$$= (3^2+1^2)12n + (1^2+1^2)(18n^2 - 12n)$$
$$= 36n^2 + 96n.$$

In the following theorem, we determine the F reverse polynomial of OX_n.

Theorem 8: The F reverse polynomial of an oxide network OX_n is
$FC(OX_n, x) = 12nx^{10} + (18n^2 - 12n)x^2$.

Proof: Let G be the graph of an oxide network OX_n. By using equation (2) and Table 4, we deduce

$$FC(OX_n, x) = \sum_{uv \in E(G)} x^{\left(c_u^2 + c_v^2\right)}$$
$$= 12nx^{\left(3^2+1^2\right)} + \left(18n^2 - 12n\right)x^{\left(1^2+1^2\right)}$$
$$= 12nx^{10} + (18n^2 - 12n)x^2.$$

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.

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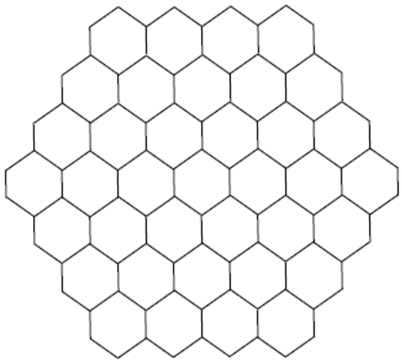

Figure-5: A 4-dimensional honeycomb network

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 compute the F reverse index of HC_n.

Theorem 9: The F reverse index of a honeycomb network HC_n is
$FC(HC_n) = 18n^2 + 30n$.

Proof: Let G be the graph of a honeycomb network HC_n. By using equation (1) and Table 5, we derive

$$FC(HC_n) = \sum_{uv \in E(G)} \left(c_u^2 + c_v^2\right)$$
$$= (2^2+2^2)6 + (2^2+1^2)(12n - 12) + (1^2+1^2)(9n^2 - 12n + 6)$$
$$= 18n^2 + 30n.$$

In the following theorem, we calculate the F reverse polynomial of HC_n.

Theorem 10: The F reverse polynomial of a honeycomb network HC_n is
$FC(HC_n, x) = 6x^8 + (12n - 12)x^5 + (9n^2 - 15n + 6)x^2$.

Proof: Let G be the graph of a honeycomb network HC_n. By using equation (2) and Table 5, we deduce

$$FC(HC_n, x) = \sum_{uv \in E(G)} x^{\left(c_u^2 + c_v^2\right)}$$
$$= 6x^{\left(2^2+2^2\right)} + (12n - 12)x^{\left(2^2+1^2\right)} + \left(9n^2 - 15n + 6\right)x^{\left(1^2+1^2\right)}$$
$$= 6x^8 + (18n^2 - 12n)x^5 + (9n^2 - 15n + 6)x^2.$$

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