International Journal of Mathematics And its Applications
Volume 5, Issue 4–B (2017), 175–179.
ISSN: 2347-1557
Available Online: http://ijmaa.in/

International Journal of Mathematics And its Applications

On the Product Connectivity Reverse Index of Silicate and Hexagonal Networks

Research Article

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Abstract: In this paper, we introduce the product connectivity reverse index of a molecular graph. In Chemical Graph Theory, the connectivity indices are applied to measure the chemical characteristics of compounds. We determine the product connectivity reverse index for silicate networks and hexagonal networks.

MSC: 05C05, 05C12, 05C35.

Keywords: Product connectivity reverse index, silicate network, hexagonal network.

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1. Introduction

Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. Let $\Delta(G)$ denote the maximum degree among the vertices of G. The reverse vertex degree of a vertex v in G is defined as $c_v = \Delta(G) + 1 - d_G(v)$. The reverse edge connecting the reverse vertices u and v will be denoted by uv. We refer [1] for undefined term and notation. Chemical graph theory is a branch of Mathematical Chemistry which has an important effect on the development of the chemical sciences. Several topological indices have been considered in Theoretical Chemistry, see [2]. In [3], Ediz defined the first reverse Zagreb beta index and the second reverse Zagreb index of a graph G. These indices are defined respectively as

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

In [4], Kulli introduced the sum connectivity reverse index of a graph G and defined it as

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

We now introduce the product connectivity reverse index of a graph G as follows:

$$PC(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{c_u c_v}}. \tag{1}$$

Recently several topological indices were studied, for example, in [5–13]. In this paper, we compute the first and second reverse Zagreb indices and the product connectivity reverse index of some important chemical structures like silicate networks and hexagonal networks. For networks see [14] and references cited therein.

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2. Silicate Networks

A silicate network is symbolized by SL_n where n is the number of hexagons between the center and boundary of SL_n. Silicates are obtained by fusing metal oxide or metal carbonates with sand. A silicate network of dimension two is shown in Figure 1.

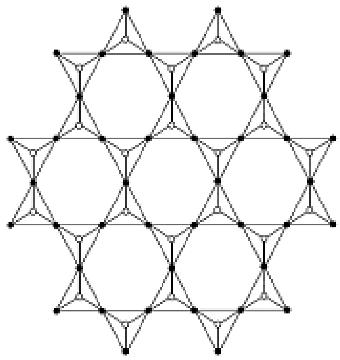

Figure 1. A 2-dimensional silicate network

In the following theorem, we determine the value of $CM_1(SL_n)$, $CM_2(SL_n)$ for silicate networks.

Theorem 2.1. *Let SL_n be the silicate networks. Then*

(1). $CM_1(SL_n) = 126n^2 + 54n$.

(2). $CM_2(SL_n) = 90n^2 + 108n$.

Proof. Let G be the graph of silicate network SL_n. The graph G has 15 $n^2 + 3n$ vertices and $36n^2$ edges. From Figure 1, we see that the vertices of SL_n are either of degree 3 or 6. In G, by algebraic method, there are three types of edges as follows:

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

We have $c_u = \Delta(G) - d_G(u) + 1 = 7 - d_G(u)$. Thus there are three types of reverse edges of follows:

$$CE_{44} = \{uv \in E(G) | c_u = c_v = 4\}, \quad |CE_{44}| = 6n.$$
$$CE_{41} = \{uv \in E(G) | c_u = 4, c_v = 1\}, \quad |CE_{41}| = 18n^2 + 6n.$$
$$CE_{11} = \{uv \in E(G) | c_u = c_v = 1\}, \quad |CE_{11}| = 18n^2 - 12n.$$

(1). To determine $CM_1(SL_n)$, we see that

$$\begin{aligned} CM_1(SL_n) &= \sum_{uv \in E(G)} (c_u + c_v) \\ &= \sum_{CE_{44}} (c_u + c_v) + \sum_{CE_{41}} (c_u + c_v) + \sum_{CE_{11}} (c_u + c_v) \\ &= (4+4)6n + (4+1)(18n^2 + 6n) + (1+1)(18n^2 - 12n) \\ &= 126n^2 + 54n. \end{aligned}$$

(2). To determine $CM_2(SL_n)$, we see that

$$\begin{aligned} CM_2(SL_n) &= \sum_{uv\in E(G)} c_u c_v \\ &= \sum_{CE_{44}} c_u c_v + \sum_{CE_{41}} c_u c_v + \sum_{CE_{11}} c_u c_v \\ &= (4\times 4)6n + (4\times 1)(18n^2+6n) + (1\times 1)(18n^2-12n) \\ &= 90n^2 + 108n. \end{aligned}$$

□

In the next theorem, we determine the product connectivity reverse index of SL_n.

Theorem 2.2. *Let SL_n be the silicate networks. Then*

$$PC(SL_n) = 27n^2 - \frac{15}{2}n.$$

Proof. Let $G = SL_n$. From equation (1) and by cardinalities of the reverse edge partition of SL_n, we have

$$\begin{aligned} PC(SL_n) &= \sum_{uv\in E(G)} \frac{1}{\sqrt{c_u c_v}} \\ &= \sum_{CE_{44}} \frac{1}{\sqrt{c_u c_v}} + \sum_{CE_{41}} \frac{1}{\sqrt{c_u c_v}} + \sum_{CE_{11}} \frac{1}{\sqrt{c_u c_v}} \\ &= \frac{1}{\sqrt{4\times 4}}(6n) + \frac{1}{\sqrt{4\times 1}}\left(18n^2+6n\right) + \frac{1}{\sqrt{1\times 1}}\left(18n^2-12n\right) \\ &= 27n^2 - \frac{15}{2}n. \end{aligned}$$

□

3. 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 6-dimensional hexagonal network is shown in Figure 2.

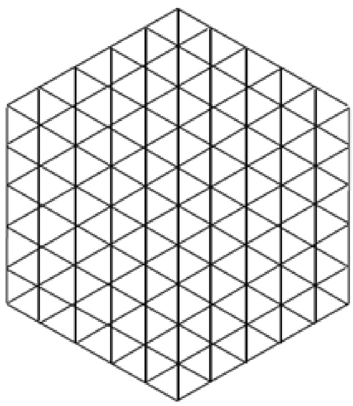

Figure 2. **Hexagonal network of dimension six**

In the following theorem, we determine the exact formulas of $CM_1(HX_n)$, $CM_2(HX_n)$ for hexagonal networks.

Theorem 3.1. *Let HX_n be the hexagonal networks. Then*

(1). $CM_1(HX_n) = 18n^2 + 18n - 30$.

(2). $CM_2(HX_n) = 9n^2 + 57n - 36$.

Proof. Let H be the graph of hexagonal networks. The graph H has $3n^2 - 3n + 1$ vertices and $9n^2 - 15n + 6$ edges. From Figure 2, it is easy to see that the vertices of HX_n are either of degree 3, 4 or 6. Thus $\Delta(H) = 6$. In H, by algebraic method, there are five types of edges as follows:

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

We have $c_u = \Delta(H) - d_H(u) + 1 = 7 - d_H(u)$. Thus there are five types of reverse edges as follows:

$$CE_{43} = \{uv \in E(H) | c_u = 4, c_v = 3\}, \quad |CE_{43}| = 12.$$
$$CE_{41} = \{uv \in E(H) | c_u = 4, c_v = 1\}, \quad |CE_{41}| = 6.$$
$$CE_{33} = \{uv \in E(H) | c_u = c_v = 3\}, \quad |CE_{33}| = 6n - 18.$$
$$CE_{31} = \{uv \in E(H) | c_u = 3, c_v = 1\}, \quad |CE_{31}| = 12n - 24.$$
$$CE_{11} = \{uv \in E(H) | c_u = c_v = 1\}, \quad |CE_{11}| = 9n^2 - 33n + 30.$$

(1). To determine $CM_1(XL_n)$, we see that

$$\begin{aligned} CM_1(HX_n) &= \sum_{uv \in E(H)} (c_u + c_v) \\ &= \sum_{CE_{43}} (c_u + c_v) + \sum_{CE_{41}} (c_u + c_v) + \sum_{CE_{33}} (c_u + c_v) + \sum_{CE_{31}} (c_u + c_v) + \sum_{CE_{11}} (c_u + c_v) \\ &= (4+3)12 + (4+1)6 + (3+3)(6n-18) + (3+1)(12n-24) + (1+1)(9n^2 - 33n + 30) \\ &= 18n^2 + 18n - 30. \end{aligned}$$

(2). To determine $CM_2(HX_n)$, we see that

$$\begin{aligned} CM_2(HX_n) &= \sum_{uv \in E(H)} c_u c_v \\ &= \sum_{CE_{43}} c_u c_v + \sum_{CE_{41}} c_u c_v + \sum_{CE_{33}} c_u c_v + \sum_{CE_{31}} c_u c_v + \sum_{CE_{11}} c_u c_v \\ &= (4 \times 3)12 + (4 \times 1)6 + (3 \times 3)(6n-18) + (3 \times 1)(12n-24) + (1 \times 1)(9n^2 - 33n + 30) \\ &= 9n^2 + 57n - 36. \end{aligned}$$

□

In the next theorem, we determine the product connectivity reverse index of HX_n.

Theorem 3.2. *Let HX_n be the hexagonal networks. Then*

$$PC\left(HX_n\right) = 9n^2 - \left(4\sqrt{3} - 31\right)n + \left(27 - 6\sqrt{3}\right)$$

Proof. Let $H = HX_n$. From equation (1) and by cardinalities of the reverse edge partition of HX_n, we have

$$\begin{aligned} PC\left(HX_n\right) &= \sum_{uv \in E(H)} \frac{1}{\sqrt{c_u c_v}} \\ &= \left(\frac{1}{\sqrt{4 \times 3}}\right) 12 + \left(\frac{1}{\sqrt{4 \times 1}}\right) 6 + \left(\frac{1}{\sqrt{3 \times 3}}\right)(6n - 18) + \left(\frac{1}{\sqrt{3 \times 1}}\right)(12n - 24) + \left(\frac{1}{\sqrt{1 \times 1}}\right)\left(9n^2 - 33n + 30\right) \\ &= 9n^2 - \left(4\sqrt{3} - 31\right)n + \left(27 - 6\sqrt{3}\right). \end{aligned}$$

□

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