Intern. J. Fuzzy Mathematical Archive
Vol. 15, No. 1, 2018, 1-5
ISSN: 2320 –3242 (P), 2320 –3250 (online)
Published on 1 January 2018
www.researchmathsci.org
DOI: http://dx.doi.org/10.22457/ijfma.v15n1a1

International Journal of
Fuzzy Mathematical Archive

Atom Bond Connectivity Reverse and Product Connectivity Reverse Indices of Oxide and Honeycomb Networks

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Received 1 December 2017; accepted 16 December 2017

Abstract. The connectivity indices are applied to measure the chemical characteristics of compounds in Chemical Graph Theory. In this paper, we propose a new index known as the atom bond connectivity reverse index of a molecular graph. Furthermore, we determine the atom bond connectivity reverse index and product connectivity reverse index for oxide and honeycomb networks.

Keywords: atom bond connectivity reverse index, product connectivity reverse index, oxide network, honeycomb network.

AMS Mathematics Subject Classification (2010): 05*C*05, 05*C*12, 05*C*35

1. Introduction

Let $G = (V(G), E(G))$ be a simple, finite, connected graph. 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 a graph 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. Any undefined term in this paper may be found in Kulli [1].

We propose the atom bond connectivity reverse index of a graph G as

$$ABCC(G) = \sum_{uv \in E(G)} \sqrt{\frac{c_u + c_v - 2}{c_u c_v}}.$$

Recently some reverse indices were studied, for example, in [2, 3, 4, 5, 6].

The product connectivity reverse index was introduced by Kulli in [4]. The product connectivity reverse index of a graph G is defined as

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

Recently several topological indices were studied, for example, in [7, 8, 9, 10, 11, 12, 13, 14, 15, 16].

In this paper, the atom bond connectivity reverse index and product connectivity reverse index of oxide networks and honeycomb networks are determined. For networks see [17].

2. Results for Oxide networks

We consider oxide networks. These networks are 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 1.

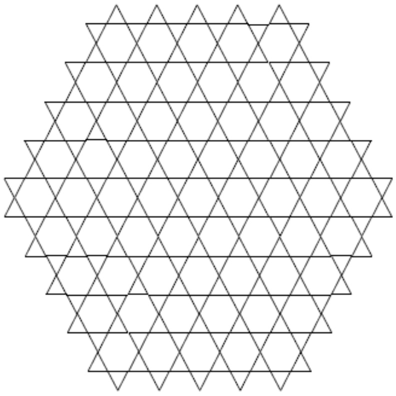

Figure 1: An oxide network of dimension five

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

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

Thus there are two types of reverse edges based on the degree of the reverse end vertices of each reverse edge as follows:

$CE_{31} = \{uv \in E(G) \mid c_u = 3, c_v = 1\}$, $\quad |CE_{31}| = 12n$.
$CE_{11} = \{uv \in E(G) \mid c_u = c_v = 1\}$, $\quad |CE_{11}| = 18n^2 – 12n$.

We compute the atom bond connectivity reverse index of oxide networks.

Theorem 1. The atom bond connectivity reverse index of an oxide network is given by

$$ABCC(OX_n) = 4\sqrt{6}n.$$

Proof: By definition, we have $ABCC(G) = \sum_{uv \in E(G)} \sqrt{\frac{c_u + c_v - 2}{c_u c_v}}$

$$ABCC(OX_n) = \sum_{CE_{31}} \sqrt{\frac{c_u + c_v - 2}{c_u c_v}} + \sum_{CE_{11}} \sqrt{\frac{c_u + c_v - 2}{c_u c_v}}$$

$$= \left(\sqrt{\frac{3+1-2}{3\times 1}} \right) 12n + \left(\sqrt{\frac{1+1-2}{1\times 1}} \right) \left(18n^2 - 12n\right)$$
$$= 4\sqrt{6}n.$$

In the following theorem, we compute the product connectivity reverse index of oxide networks.

Theorem 2. The product connectivity reverse index of oxide networks is given by

$$PC(OX_n) = 18n^2 + \left(4\sqrt{3} - 12\right)n.$$

Proof: By definition, we have $PC(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{c_u c_v}}.$

Thus $$PC(OX_n) = \sum_{CE_{31}} \frac{1}{\sqrt{c_u c_v}} + \sum_{CE_{11}} \frac{1}{\sqrt{c_u c_v}}$$
$$= \left(\frac{1}{\sqrt{3\times 1}} \right) 12n + \left(\frac{1}{\sqrt{1\times 1}} \right) \left(18n^2 - 12n\right)$$
$$= 18n^2 + \left(4\sqrt{3} - 12\right)n.$$

3. Results for Honeycomb networks

Honeycomb networks are very 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 2.

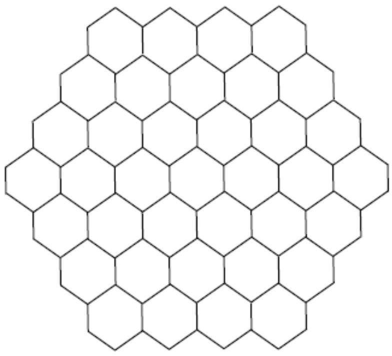

Figure 2: A honeycomb network of dimension four

Let H be the graph of honeycomb network HC_n. From Figure 2, we see that the vertices of HC_n are either of degree 2 or 3. By algebraic method, we obtain that $|V(HC_n)| = 6n^2$ and $|E(HC_n)| = 9n^2 - 3n$. Clearly we have $c_u = \Delta(H) - d_H(u) + 1 = 4 - d_H(u)$. By algebraic method, in HC_n, there are three types of edges based on the degree of the end vertices of each edge as follows:

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

Thus there are three types of reverse edges based on the degree of the reverse end vertices of each reverse edge as follows:

$CE_{22} = \{uv \in E(H) \mid c_u = c_v = 2\}$, $|CE_{22}| = 6$.
$CE_{21} = \{uv \in E(H) \mid c_u = 2, c_u = 1\}$, $|CE_{21}| = 12n - 12$.
$CE_{11} = \{uv \in E(H) \mid c_u = c_u = 1\}$, $|CE_{11}| = 9n^2 - 15n + 6$.

In the following theorem, we compute the atom bond connectivity reverse index of honeycomb networks.

Theorem 3. The atom bond connectivity reverse index of honeycomb networks is given by

$$ABCC(HC_n) = 6\sqrt{2}n - 3\sqrt{2}.$$

Proof: By definition, we have $ABCC(H) = \sum_{uv \in E(H)} \sqrt{\frac{c_u + c_v - 2}{c_u c_v}}$

Thus, $ABCC(HC_n) = \sum_{CE_{22}} \sqrt{\frac{c_u + c_v - 2}{c_u c_v}} + \sum_{CE_{21}} \sqrt{\frac{c_u + c_v - 2}{c_u c_v}} + \sum_{CE_{11}} \sqrt{\frac{c_u + c_v - 2}{c_u c_v}}$

$$= \left(\sqrt{\frac{2+2-2}{2\times 2}}\right)6 + \left(\sqrt{\frac{2+1-2}{2\times 1}}\right)(12n-12) + \left(\sqrt{\frac{1+1-2}{1\times 1}}\right)\left(9n^2 - 15n + 6\right)$$

$$= 6\sqrt{2}n - 3\sqrt{2}.$$

In the following theorem, we compute the product connectivity reverse index of honeycomb networks.

Theorem 4. The product connectivity reverse index of honeycomb networks is given by

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

Proof: By definition, we have $PC(H) = \sum_{uv \in E(H)} \frac{1}{\sqrt{c_u c_v}}$.

Thus $PC(HC_n) = \sum_{CE_{22}} \frac{1}{\sqrt{c_u c_v}} + \sum_{CE_{21}} \frac{1}{\sqrt{c_u c_v}} + \sum_{CE_{11}} \frac{1}{\sqrt{c_u c_v}}$

$$= \left(\frac{1}{\sqrt{2\times 2}}\right)6 + \left(\frac{1}{\sqrt{2\times 1}}\right)(12n-12) + \left(\frac{1}{\sqrt{1\times 1}}\right)\left(9n^2 - 15n + 6\right)$$

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

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