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Some New Temperature Indices of Oxide and Honeycomb Networks

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Abstract. A graph index is a numerical parameter mathematically derived from the graph structure. In this paper, we introduce the first temperature index, modified first temperature index, temperature inverse degree, total temperature index, temperature zeroth order index, *F*-temperature index and general vertex temperature index of a graph. We compute these newly defined temperature indices for oxide networks and honeycomb networks.

Keywords: Temperature, first temperature index, *F*-temperature index, general vertex temperature index, oxide network, honeycomb network.

AMS Mathematics Subject Classification (2010): 05*C*05, 05*C*07, 05*C*12

1. Introduction

A molecular graph or a chemical graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. Chemical Graph Theory is a branch of Mathematical Chemistry. This branch of Mathematics has an important effect on the development of Science and Technology. Several graph indices have found many applications, especially, in QSPR/QSAR research, see [1, 2]. Let G be a finite, simple, connected graph. Let $V(G)$ and $E(G)$ denote the vertex set and edge set of G respectively. The degree $d_G(v)$ of a vertex v in G is the number of vertices adjacent to v. For undefined term and notation, we refer the book [3].

The temperature of a vertex u of a graph G is defined by Fajtlowicz [5] as

$$T(u) = \frac{d_G(u)}{n - d_G(u)},$$

where n is the number of vertices of G.

We introduce the following temperature indices.

The first temperature index of a graph G is defined as

$$T_1(G) = \sum_{u \in V(G)} T(u)^2.$$

The modified first temperature index of a graph G is defined as

$$ {}^{m}T_1(G) = \sum_{u \in V(G)} \frac{1}{T(u)^2}. $$

The temperature inverse degree of a graph G is defined as

$$ TID(G) = \sum_{u \in V(G)} \frac{1}{T(u)}. $$

The total temperature index of a graph G is defined as

$$ TT(G) = \sum_{u \in V(G)} T(u). $$

The temperature zeroth order index of a graph G is defined as

$$ TZ(G) = \sum_{u \in V(G)} \frac{1}{\sqrt{T(u)}}. $$

The F-temperature index of a graph G is defined as

$$ FT(G) = \sum_{u \in V(G)} T(u)^3. $$

The general vertex temperature index of a graph G is defined as

$$ T_1^a(G) = \sum_{u \in V(G)} T(u)^a, $$

where a is a real number.

Recently, some temperature indices were introduced and studied, for example, in [5,6,7,8,9]. Recently, some graph indices were studied in [10,11, 12,13, 14]. In this paper, the first temperature index, modified first temperature index, temperature zeroth order index, F-temperature index, general vertex temperature index for oxide and honeycomb networks are computed.

2. Results for Oxide networks

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 1.

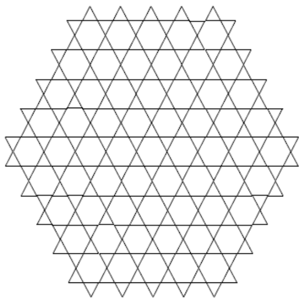

Figure 1: A 5-dimensional oxide network

Theorem 1. The general vertex temperature index of an oxide network OX_n is given by

$$ T_1^a(OX_n) = 6n\left(\frac{2}{9n^2+3n-2}\right)^a + \left(9n^2-3n\right)\left(\frac{4}{9n^2+3n-4}\right)^a. \qquad \text{(i)} $$

Proof: Let G be the graph of oxide network OX_n. Clearly the vertices of OX_n are either of degree 2 or 4, see Figure 1. By calculation, we obtain that G has $9n^2 + 3n$ vertices and $18n^2$ edges. We partition $V(G)$ into two sets, vertices of degree 2 and 4 respectively.

$V_1 = \{u \in V(G) \mid d_G(u) = 2\}$, $\qquad |V_1| = 6n$.

$V_2 = \{u \in V(G) \mid d_G(u) = 4\}$, $\qquad |V_2| = 9n^2 - 3n$.

Therefore we obtain the vertex partition based on the temperature of the vertices as given in Table 1.

$T(u) \setminus u \in V(G)$	$\dfrac{2}{9n^2+3n-2}$	$\dfrac{4}{9n^2+3n-4}$
Number of edges	$6n$	$9n^2 - 3n$

Table 1: Vertex partition of OX_n

By definition, we have $T_1^a(G) = \sum_{u \in V(G)} T(u)^a$. Thus by using Table 1, we deduce

$$T_1^a(OX_n) = 6n\left(\frac{2}{9n^2+3n-2}\right)^a + \left(\frac{4}{9n^2+3n-4}\right)^a.$$

From Theorem 1, we obtain the following results.

Corollary 1.1. Let OX_n be an oxide network of dimension n. Then

(1) $$T_1(OX_n) = 6n\left(\frac{2}{9n^2+3n-2}\right)^2 + \left(9n^2-3n\right)\left(\frac{4}{9n^2+3n-4}\right)^2.$$

(2) $$^mT_1(OX_n) = \frac{1}{16}\left[24n\left(9n^2+3n-2\right)^2 + \left(9n^2-3n\right)\left(9n^2+3n-4\right)^2\right].$$

(3) $$TID(OX_n) = \frac{1}{4}\left[12n\left(9n^2+3n-2\right) + \left(9n^2-3n\right)\left(9n^2+3n-4\right)\right].$$

(4) $$TT(OX_n) = \frac{12n}{9n^2+3n-2} + \frac{4\left(9n^2-3n\right)}{9n^2+3n-4}.$$

(5) $$TZ(OX_n) = 6n\left(\frac{2}{9n^2+3n-2}\right)^{\frac{1}{2}} + \left(9n^2-3n\right)\left(\frac{4}{9n^2+3n-4}\right)^{\frac{1}{2}}.$$

(6) $$FT(OX_n) = 6n\left(\frac{2}{9n^2+3n-2}\right)^3 + \left(9n^2-3n\right)\left(\frac{4}{9n^2+3n-4}\right)^3.$$

Proof: Put a = 2, –2, 1, –1, –½, 3 in equation (i), we obtain the desired results.

3. Results for Honeycomb networks

Honeycomb networks are very useful in chemistry and also in computer graphics. 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 presented in Figure 2.

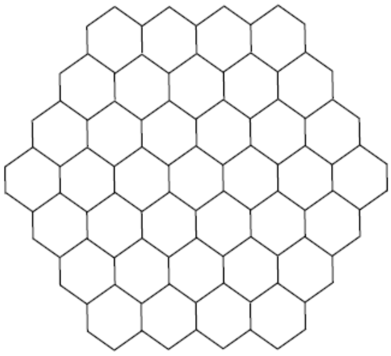

Figure 2: A 4-dimensional honeycomb network

Theorem 2. The general vertex temperature index of a honeycomb network HC_n is

$$T_1^a(HC_n) = 6n\left(\frac{1}{3n^2-1}\right)^a + \left(6n^2-6n\right)\left(\frac{1}{2n^2-1}\right)^a. \qquad \text{(ii)}$$

Proof: Let H be the graph of honeycomb network HC_n. The vertices of HC_n are either of degree 2 or 3, see Figure 2. By calculation, we obtain that H has $6n^2$ vertices and $9n^2 - 3n$ edges. We partition the vertex set of H into two sets, vertices of degree 2 and 3 respectively.

$V_1 = \{u \in V(H) \mid d_H(u) = 2\}$, $\quad |V_1| = 6n$.

$V_2 = \{u \in V(H) \mid d_H(u) = 3\}$, $\quad |V_2| = 6n^2 - 6n$.

Therefore we find the vertex partition based on the temperature of the vertices as follows:

$$TV_1 = \left\{u \in V(H) \mid T(u) = \frac{2}{6n^2-2}\right\}, \qquad |TV_1| = 6n.$$

$$TV_2 = \left\{u \in V(H) \mid T(u) = \frac{3}{6n^2-3}\right\}, \qquad |TV_2| = 6n^2 - 6n.$$

By definition, we have $T_1^a(H) = \sum_{u \in V(H)} T(u)^a$. Thus

$$T_1^a(HC_n) = |TV_1|\left(\frac{2}{6n^2-2}\right)^a + |TV_2|\left(\frac{3}{6n^2-3}\right)^a$$

$$= 6n\left(\frac{1}{3n^2-1}\right)^a + \left(6n^2-6n\right)\left(\frac{1}{2n^2-1}\right)^a$$

Corollary 2.1. Let HC_n be a honeycomb network of dimension n. Then

(1) $T_1(HC_n) = \dfrac{6n}{\left(3n^2-1\right)^2} + \dfrac{6n^2-6n}{\left(2n^2-1\right)^2}$.

(2) ${}^mT_1(HC_n) = 6n\left(3n^2-1\right)^2 + \left(6n^2-6n\right)\left(2n^2-1\right)^2$.

(3) $TID(HC_n) = 6n\left(3n^2-1\right) + \left(6n^2-6n\right)\left(2n^2-1\right)$.

(4) $$TT(HC_n) = \frac{6n}{3n^2-1} + \frac{6n^2-6n}{2n^2-1}.$$

(5) $$TZ(HC_n) = 6n\left(\frac{1}{3n^2-1}\right)^{\frac{1}{2}} + \left(6n^2-6n\right)\left(\frac{1}{3n^2-1}\right)^{\frac{1}{2}}.$$

(6) $$FT(HC_n) = 6n\left(\frac{1}{3n^2-1}\right)^{3} + \left(6n^2-6n\right)\left(\frac{1}{2n^2-1}\right)^{3}.$$

Proof: Put a = 2, –2, 1, –1, –½, 3 in equation (ii), we get the desired results.

4. Conclusion

In this paper, the first temperature index, modified first temperature index, temperature zeroth order index, F-temperature index, general first temperature index for oxide and honeycomb networks are computed.

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