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Multiplicative Revan Indices of Rhombus Silicate Network and Rhombus Oxide Network

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Abstract: Early studies show that the chemical and pharmaceutical properties of compounds are closely related to their molecular structure. Theoretical chemistry provides a method to predict the characteristics of compounds through the topological index calculation. As the expansion of Zagreb index, the Zagreb connection indices were introduced to measure the stability of alkanes and strain energy of cycloalkanes, which can help the pharmaceutical, chemical and medical researchers test the chemical, biological features of new drugs, materials and compounds. In this paper, in light of molecular structure analysis and mathematical derivation, we study the multiplicative Revan indices of rhombus silicate network and rhombus oxide network which are widely applied in chemical and material engineering.
Keywords: Theoretical chemistry, molecular graph, multiplicative Revan index, rhombus silicate network, rhombus oxide network.

INTRODUCTION

Along with the improvement of experimental conditions and experimental methods, more and more high-performance materials, drugs were constructed from the laboratory. These synthetic materials and drugs have a large number of potential chemical properties that need to be tested, and can be put into the market after fully understanding their performance. Thus testing the physical, chemical, medical, medicinal properties of the new compound becomes a heavy boring workload. On the other hand, underdeveloped areas do not have enough equipment, reagents and manpower to do this job because of the shortage of funds.

From the early chemical experiments, scientists get an important rule: the properties of the compound are directly related to its molecular structure. This rule allows scholars to predict chemical properties from the theoretical point of view which is originally only determined by the experiment. As an important branch of theoretical chemistry, the chemical graph theory provides us with the following procedures: first we use the graph model to represent the molecular structure of the compound, and this kind of resulting graph is called the molecular graph; secondly, the topological index is defined on the molecular graph, and a topological indicator represents a kind of chemical, pharmaceutical or material property; finally, the performance of the compound is predicted by the calculation of the topological index on a particular molecular graph. This method is not subject to funding constraints, in the absence of instruments and reagent, it can also be carried out the prediction of the chemical properties, and therefore it's welcome by the researchers from developed countries and regions. In addition to the scholars in the field of chemistry, biology, materials and pharmaceutical, many mathematics experts also joined the study of chemical graph theory, and thus promoted the development of this discipline. For the contributions on the chemical graph theory and its engineering applications one can refer to Balaban [1], Munteanu *et al*. [2], Buscema *et al*. [3], Gao *et al*. [4] and [5], Bodlaj and Batagelj [6], Lokesha *et al*. [7], Khakpoor and Keshe [8], Ivanciuc [9] and Sardar *et al*. [10].

In chemical graph theory framework, the structure of chemical molecular is represented by a graph in which each atom is denoted as a vertex and each chemical bond is expressed as an edge. Let $G=(V(G),E(G))$ be a (molecular) graph, where $V(G)$ and $E(G)$ are vertex (atom) set and edge (chemical bond) set respectively. A topological index is defined on a graph as a function $f: G \rightarrow \mathbb{R}^{+}$ which maps each graph to a real number. In the past 40 years, inspired by chemistry applications, there were lots of degree-based, distance-based and spectral-based topological

indices being introduced, such as Zagreb index, atom-bond connectivity index, Wiener index, geometry arithmetic index, harmonic index, eccentric index, and PI index etc. There are several papers contributing to obtaining these topological indices of special molecular structures in material, biological, pharmaceutical and chemical engineering (See Gao and Siddiqui [11], Gao *et al*. [12-14], Gao and Wang [15] and [16], Ahmadi and Sadeghimehr [17], Guirao and de Bustos [18], Gutman and Das [19], and Dimitrov *et al*. [20] for more details).

As an important molecular structure, network structure (for example, dendrimer nanostars) is widely appeared in several of drugs, materials, and other chemical compounds, and it raised large interest from engineering scientists. Tada *et al*. [21] presented a fragment molecular orbital method which was applied to analyze how the orbitals of the dendrimer nanostars are localized in space as well as in energy. Mirzargar [22] calculated the PI, Szeged, edge Szeged indices and their polynomials of a class of nanostar dendrimers. Dorosti *et al*. [23] computed the the Cluj index of the first type of dendrimer nanostar. Palma *et al*. [24] presented a sequential molecular dynamics/quantum mechanics (MD/QM) study and steady-state spectroscopy measurements of the dendrimer nanostars to obtain the temperature dependence of the electronic absorption process. They considered the nanostar as separate units and performed MD simulations for each chromophore at 10 and 300 K to study the effects of the temperature on the structures. Khalifeh *et al.* [25] and Darafsheh and Khalifeh [26] determined several distance-based topological indices of dendrimer nanostars. Manuel *et al.* [27] studied the total-Szeged index of dendrimer nanostar NSC_5C_6. Alikhani and Iranmanesh [28] computed the Hosoya polynomial of an infinite family of dendrimer nanostar denoted by D_3 [72]. Alikhani *et al.* [29] manifested the Harary index of dendrimer nanostar NS_2 [*n*]. Quadras *et al*. [30] yielded the minimum wirelength of embedding circulant network into nanostar dendrimer, and the embedding of faulty circulant network into nanostar dendrimer were also studied. For more theoretical results and engineering applications on dendrimer nanostars, one can refer to Husin *et al.* [31], Sepulveda-Crespo *et al.* [32], Cevik *et al*. [33], and Rivero-Buceta *et al*. [34].

In this paper, we focus on the multiplicative Revan indices of special kind of networks.

Setting and network graph description

For $v \in V(G)$, set $d(v)$ as the degree of *v*. Let $\delta(G) = \min\{d(v) : v \in V(G)\}$ and $\Delta(G) = \max\{d(v) : v \in V(G)\}$ be the minimum and maximum degree of molecular graph *G*. The Revan vertex degree of a vertex *v* in *G* is defined as $r(v) = \Delta(G) + \delta(G) - d(v)$. The first and second Revan indices of a graph *G* are defined as (see Kulli [35]):

$$r_1(G) = \sum_{uv \in E(G)} (r(u) + r(v));$$

$$r_2(G) = \sum_{uv \in E(G)} r(u)r(v).$$

In this paper, we first introduce the first and second multiplicative Revan indices of a graph *G*, which are described as follows:

$$r_1\Pi(G) = \prod_{uv \in E(G)} (r(u) + r(v));$$

$$r_2\Pi(G) = \prod_{uv \in E(G)} r(u)r(v).$$

We consider a family of rhombus silicate networks. A rhombus silicate network is symbolized by $RHSL_n$. A 3-dimensional rhombus silicate network is depicted in Figure 1.

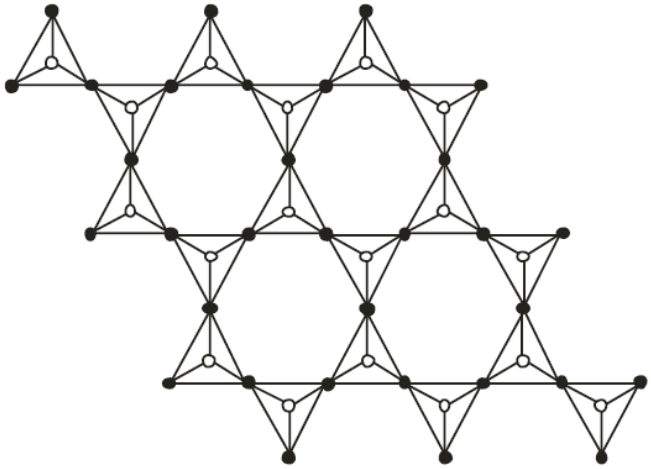

Fig-1: A 3-dimensional rhombus silicate network

Next, we consider a family of rhombus oxide networks. A rhombus oxide network of dimension *n* is denoted by $RHOX_n$. A rhombus oxide network of dimension 3 is depicted in Figure 2.

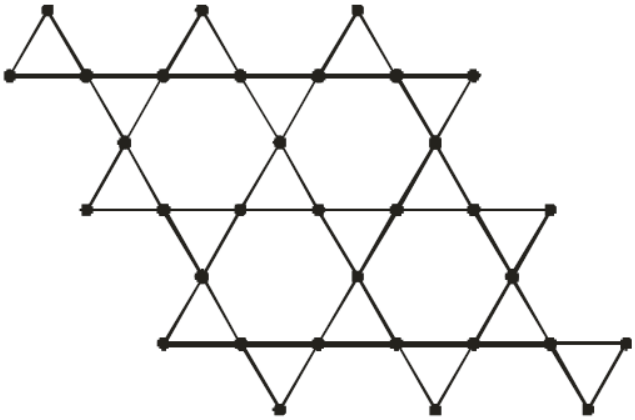

Fig-2: Rhombus oxide network of dimension 3.

Main results and proofs

In this section, we present the main conclusions.

Theorem 1. The first and second multiplicative Revan indices of $RHSL_n$ are:

$$r_1\Pi(RHSL_n) = 12^{4n+2}9^{6n^2+4n-4}6^{6n^2-8n+2};$$

$$r_2\Pi(RHSL_n) = 36^{4n+2}18^{6n^2+4n-4}9^{6n^2-8n+2}.$$

Proof. It is easy to check that $RHSL_n$ has $5n^2+2n$ vertices and $12n^2$ edges. According to the value of $d(u)$ and $d(v)$ for each edge *uv*, the whole edge set can be divided into three subsets:

- $E_{33}=\{uv \in E(G): d(u)=d(v)=3\}$, $|E_{33}|=4n+2$;
- $E_{36}=\{uv \in E(G): d(u)=3; d(v)=6\}$, $|E_{36}|=6n^2+4n-4$;
- $E_{66}=\{uv \in E(G): d(u)=d(v)=6\}$, $|E_{66}|=6n^2-8n+2$.

Hence, we have $\delta(RHSL_n)=3$ and $\Delta(RHSL_n)=6$. By means of definition of Revan vertex degree, the divided subset of $E(G)$ can be re-written as follows:

- $RE_{66}=\{uv\in E(G):r(u)=r(v)=6\}$, $|RE_{66}|=4n+2$;
- $RE_{63}=\{uv\in E(G):r(u)=6;r(v)=3\}$, $|RE_{63}|=6n^2+4n-4$;
- $RE_{33}=\{uv\in E(G):r(u)=r(v)=3\}$, $|RE_{33}|=6n^2-8n+2$.

Using the definition of the first and second multiplicative Revan index, we have

$$r_1\Pi(RHSL_n)=\prod_{uv\in E(RHSL_n)}(r(u)+r(v))$$

$$=\prod_{uv\in RE_{66}}(r(u)+r(v))\prod_{uv\in RE_{63}}(r(u)+r(v))\prod_{uv\in RE_{33}}(r(u)+r(v))$$

$$=12^{4n+2}9^{6n^2+4n-4}6^{6n^2-8n+2}$$

Using the definition of the second multiplicative Revan index, we get

$$r_2\Pi(RHSL_n)=\prod_{uv\in E(RHSL_n)}r(u)r(v).$$

$$=\prod_{uv\in RE_{66}}(r(u)r(v))\prod_{uv\in RE_{63}}(r(u)r(v))\prod_{uv\in RE_{33}}(r(u)r(v))$$

$$=36^{4n+2}18^{6n^2+4n-4}9^{6n^2-8n+2}.$$

Thus, we finish the proof of Theorem 1.

Theorem 2. The first and second multiplicative Revan indices of $RHOX_n$ are:

$$r_1\Pi(RHOX_n)=64\cdot 6^{8n-4}4^{6n^2-8n+2};$$

$$r_2\Pi(RHOX_n)=256\cdot 8^{8n-4}4^{6n^2-8n+2}.$$

Proof. It is easy to check that $RHOX_n$ has $3n^2+2n$ vertices and $6n^2$ edges. According to the value of $d(u)$ and $d(v)$ for each edge *uv*, the whole edge set can be divided into three subsets:

- $E_{22}=\{uv\in E(G):d(u)=d(v)=2\}$, $|E_{22}|=2$;
- $E_{24}=\{uv\in E(G):d(u)=2;d(v)=4\}$, $|E_{24}|=8n-4$;
- $E_{44}=\{uv\in E(G):d(u)=d(v)=4\}$, $|E_{44}|=6n^2-8n+2$.

Hence, we have $\delta(RHOX_n)=2$ and $\Delta(RHOX_n)=4$. By means of definition of Revan vertex degree, the divided subset of $E(G)$ can be re-written as follows:

- $RE_{44}=\{uv\in E(G):r(u)=r(v)=4\}$, $|RE_{44}|=2$;
- $RE_{42}=\{uv\in E(G):r(u)=4;r(v)=2\}$, $|RE_{42}|=8n-4$;
- $RE_{22}=\{uv\in E(G):r(u)=r(v)=2\}$, $|RE_{22}|=6n^2-8n+2$.

Using the definition of the first and second multiplicative Revan index, we have

$$r_1\Pi(RHOX_n)=\prod_{uv\in E(RHOX_n)}(r(u)+r(v))$$

$$=\prod_{uv\in RE_{44}}(r(u)+r(v))\prod_{uv\in RE_{42}}(r(u)+r(v))\prod_{uv\in RE_{22}}(r(u)+r(v))$$

$$=64\cdot 6^{8n-4}4^{6n^2-8n+2}$$

Using the definition of the second multiplicative Revan index, we get

$$r_2\Pi(RHOX_n) = \prod_{uv\in E(RHOX_n)} r(u)r(v).$$

$$= \prod_{uv\in RE_{44}} (r(u)r(v)) \prod_{uv\in RE_{42}} (r(u)r(v)) \prod_{uv\in RE_{22}} (r(u)r(v))$$

$$= 256\cdot 8^{8n-4}4^{6n^2-8n+2}.$$

Thus, we finish the proof of Theorem 2.

CONCLUSION

By means of the graph structure analysis and mathematical tricks, we finally infer the multiplicative Revan indices of rhombus silicate network and rhombus oxide network. The conclusions deduced in this work also demonstrate the promising and wide application prospects in chemical, biological, pharmaceutical and nanoscience engineering.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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