

Reduced Second Hyper-Zagreb Index and its Polynomial of Certain Silicate Networks

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Abstract. We introduce the reduced second hyper-Zagreb index of a graph. Considering this index, we define the reduced second hyper-Zagreb polynomial of a graph. Also we define the reduced second Zagreb polynomial of a graph. In this paper, we compute the reduced second hyper-Zagreb index and its polynomial of certain families of networks such as silicate and chain silicate networks. Also we determine the reduced second Zagreb polynomial of certain silicate networks.

Keywords: reduced second hyper-Zagreb index, silicate 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 . We refer [1], for other undefined notations and terminologies.

A molecular graph is a graph such that its vertices correspond to the atoms and edges to the bonds. Chemical Graph Theory is a branch of mathematical chemistry, which has an important effect on the development of Chemical Sciences. Several topological indices have been considered in Theoretical Chemistry and have found some applications.

Recently Furtula et al. proposed the reduced second Zagreb index, defined as [2]

$$RM_2(G) = \sum_{uv \in E(G)} (d_G(u)-1)(d_G(v)-1). \quad (1)$$

Recently, some new reduced indices were studied, for example, in [3, 4, 5, 6, 7].

Considering the reduced second Zagreb index, we introduce the reduced second Zagreb polynomial of a graph G as

$$RM_2(G, x) = \sum_{uv \in E(G)} x^{(d_G(u)-1)(d_G(v)-1)}. \quad (2)$$

We now introduce the reduced second hyper-Zagreb index of a graph G , defined as,

V.R.Kulli

$$RHM_2(G) = \sum_{uv \in E(G)} [(d_G(u)-1)(d_G(v)-1)]^2. \quad (3)$$

Considering the reduced second hyper-Zagreb index, we introduce the reduced second hyper-Zagreb polynomial of a graph G as

$$RHM_2(G, x) = \sum_{uv \in E(G)} x^{[(d_G(u)-1)(d_G(v)-1)]^2}. \quad (4)$$

Recently, some new topological indices were studied, for example, in [8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23]. Also some new polynomials were studied, for example, in [24, 25, 26, 27, 28, 29, 30, 31].

In this paper, the reduced second Zagreb polynomial, reduced second hyper-Zagreb index and its polynomial of silicate and chain silicate networks are computed. For more information about silicate networks see [32].

2. Results for silicate networks

Silicate networks 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 silicate network of dimension two is shown in Figure 1.

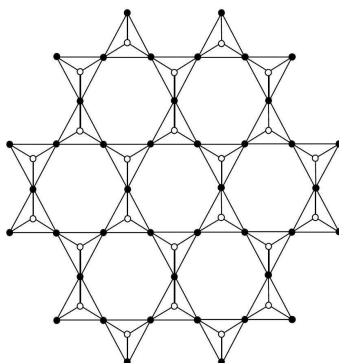


Figure 1: Silicate network of dimension two

Let G be the graph of a silicate network SL_n with $|V(SL_n)|=15n^2+3n$ and $|E(SL_n)|=36n^2$. By algebraic method, there are three types of edges in G based on the degree of end vertices of each edge as in Table 1.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(3, 3)	(3, 6)	(6, 6)
Number of edges	$6n$	$18n^2 + 6n$	$18n^2 - 12n$

Table 1: Edge partition of SL_n

Theorem 1. The reduced second Zagreb index and its polynomial of a silicate network SL_n are

- (i) $RM_2(SL_n) = 630n^2 + 216n$.
- (ii) $RM_2(SL_n, x) = 6nx^4 + (18n^2+6n)x^{10} + (18n^2 - 12n)x^{25}$.

Proof: Let $G = SL_n$ be the graph of a silicate network.

Reduced Second Hyper-Zagreb Index and its Polynomial of Certain Silicate Networks

(i) By using equation (1) and Table 1, we obtain

$$\begin{aligned} RM_2(SL_n) &= \sum_{uv \in E(G)} (d_G(u)-1)(d_G(v)-1) \\ &= (3-1)(3-1)6n + (3-1)(6-1)(18n^2+6n) + (6-1)(6-1)(18n^2-12n) \\ &= 630n^2 - 216n. \end{aligned}$$

(ii) By using equation (2) and Table 1, we obtain

$$\begin{aligned} RM_2(SL_n, x) &= \sum_{uv \in E(G)} x^{(d_G(u)-1)(d_G(v)-1)} \\ &= 6nx^{(3-1)(3-1)} + (18n^2+6n)x^{(3-1)(6-1)} + (18n^2-12n)x^{(6-1)(6-1)} \\ &= 6nx^4 + (18n^2+6n)x^{10} + (18n^2-12n)x^{25}. \end{aligned}$$

Theorem 2. The reduced second hyper-Zagreb index and its polynomial of a silicate network SL_n are

- (i) $RHM_2(SL_n) = 13050n^2 - 6804n$.
(ii) $RHM_2(SL_n, x) = 6nx^{16} + (18n^2+6n)x^{100} + (18n^2-12n)x^{625}$.

Proof: Let $G = SL_n$ be the graph of a silicate network.

(i) By using equation (3) and Table 1, we obtain

$$\begin{aligned} RHM_2(SL_n) &= \sum_{uv \in E(G)} [(d_G(u)-1)(d_G(v)-1)]^2 \\ &= [(3-1)(3-1)]^2 6n + [(3-1)(6-1)]^2 (18n^2+6n) + [(6-1)(6-1)]^2 (18n^2-12n) \\ &= 13050n^2 - 6804n. \end{aligned}$$

(ii) By using equation (4) and Table 1, we obtain

$$\begin{aligned} RHM_2(SL_n, x) &= \sum_{uv \in E(G)} x^{[(d_G(u)-1)(d_G(v)-1)]^2} \\ &= 6nx^{[(3-1)(3-1)]^2} + (18n^2+6n)x^{[(3-1)(6-1)]^2} + (18n^2-12n)x^{[(6-1)(6-1)]^2} \\ &= 6nx^{16} + (18n^2+6n)x^{100} + (18n^2-12n)x^{625}. \end{aligned}$$

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 tetrahedral linearly, see Figure 2.

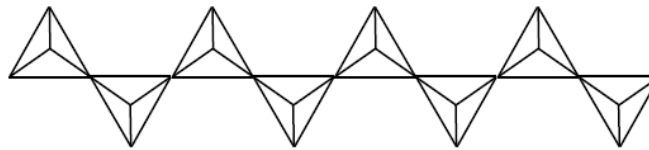


Figure 2: Chain silicate network

Let G be the graph of chain silicate network CS_n with $|V(CS_n)|=3n+1$ and $|E(CS_n)|=6n$. By algebraic method, CS_n , $n \geq 2$, there are three types of edges based on the degree of end vertices of each edge as in Table 2.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(3, 3)	(3, 6)	(6, 6)
Number of edges	$n + 4$	$4n - 2$	$n - 2$

Table 2: Edge partition of CS_n

V.R.Kulli

Theorem 3. The reduced second Zagreb index and its polynomial of a chain silicate network CS_n are

- (i) $RM_2(CS_n) = 69n - 54$.
(ii) $RM_2(CS_n, x) = (n+4)x^4 + (4n-2)x^{10} + (n-2)x^{25}$.

Proof: Let $G = CS_n$ be the graph of chain silicate network.

- (i) By using equation (1) and Table 2, we deduce

$$\begin{aligned} RM_2(CS_n) &= \sum_{uv \in E(G)} (d_G(u)-1)(d_G(v)-1) \\ &= (3-1)(3-1)(n+4) + (3-1)(6-1)(4n-2) + (6-1)(6-1)(n-2) \\ &= 69n - 54. \end{aligned}$$

- (ii) By using equation (2) and Table 2, we deduce

$$\begin{aligned} RM_2(CS_n, x) &= \sum_{uv \in E(G)} x^{(d_G(u)-1)(d_G(v)-1)} \\ &= (n+4)x^{(3-1)(3-1)} + (4n-2)x^{(3-1)(6-1)} + (n-2)x^{(6-1)(6-1)} \\ &= (n+4)x^4 + (4n-2)x^{10} + (n-2)x^{25}. \end{aligned}$$

Theorem 4. The reduced second hyper-Zagreb index and its polynomial of a chain silicate network CS_n are

- (i) $RHM_2(CS_n) = 1041n - 1386$.
(ii) $RHM_2(CS_n, x) = (n+4)x^{16} + (4n-2)x^{100} + (n-2)x^{625}$.

Proof: Let $G = CS_n$ be the graph of chain silicate network.

- (i) By using equation (3) and Table 2, we deduce

$$\begin{aligned} RHM_2(CS_n) &= \sum_{uv \in E(G)} [(d_G(u)-1)(d_G(v)-1)]^2 \\ &= [(3-1)(3-1)]^2(n+4) + [(3-1)(6-1)]^2(4n-2) + [(6-1)(6-1)]^2(n-2) \\ &= 1041n - 1386 \end{aligned}$$

- (ii) By using equation (4) and Table 2, we deduce

$$\begin{aligned} RHM_2(CS_n, x) &= \sum_{uv \in E(G)} x^{[(d_G(u)-1)(d_G(v)-1)]^2} \\ &= (n+4)x^{[(3-1)(3-1)]^2} + (4n-2)x^{[(3-1)(6-1)]^2} + (n-2)x^{[(6-1)(6-1)]^2} \\ &= (n+4)x^{16} + (4n-2)x^{100} + (n-2)x^{625}. \end{aligned}$$

4. Conclusion

In this paper, the explicit formulas for the reduced hyper-Zagreb index and its polynomial of silicate and chain silicate networks are computed. These expressions can correlate the molecular structure of silicate and chain silicate networks to information about their physical structures.

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Reduced Second Hyper-Zagreb Index and its Polynomial of Certain Silicate Networks

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V.R.Kulli

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