CERTAIN TOPOLOGICAL INDICES OF CHEMICAL INTERCONNECTION NETWORKS

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Article History: Received: 08.03.2023 **Revised:** 22.04.2023 **Accepted:** 06.06.2023

Abstract

Structure-based topological descriptors of chemical networks enable us the prediction of physicochemical properties and the bioactivities of compounds through QSAR/QSPR methods. Topological indices are the numerical values to represent a graph that characterize the graph. In this paper, we consider certain popular topological indices of chain oxide net- work COX_n, chain silicate network CS_n, ortho chain S_n, and para chain Q_n, for the first time. Moreover, analytically closed formulae for these structures are determined.

Keywords: Chain oxide network COX_n, Chain silicate network CS_n, Ortho chain S_n, Para chain Q_n.

2010 Math. Subject Classification: 05C12, 05C90, 05C76.

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DOI: 10.31838/ecb/2023.12.s3.471

1. INTRODUCTION AND PRELIMINARY RESULTS

All the graphs G in this paper are considered to be finite, undirected, and loopless. Graph G is the set made up of vertices (also called the nodes) that are connected with the edges (also called links). It consists on two sets V and E, where V is called the vertex set and E is called the edge set. In order to understand the properties and information contained in the connectivity pattern of graphs, there are many numbers of numerical quantities, known as structure invariants, topological indices, or topological descriptors, which have been derived and studied over the past few decades. Topological indices have vast number of applications in chemical graph theory which is a special branch of mathematical chemistry. Graph theory has a wide range of applications in engineering due to its diagrammatic nature. It is used in computer science to study the algorithms and flow of information. In engineering, it is used to model the graphics and designs of different networks by converting them in the form of graph. Topological indices are very much used for characterizing chemical graphs on the basis of their numerical values. [22] establish the relationship between the structure and properties of the molecule. Topological indices are widely used in QSAR and QSPR research studies [22].

For more new topological indices see [11, 23]. Many papers [1-24] are written on this simple graph invariant. A chemical graph is a simple graph in which atoms correspond to the vertices and edge denotes the bond between two atoms. [26] introduced the redefined versions of the some Zagreb indices, i.e. the redefined first, second and third Zagreb
indices for a graph G as:

$$ReZ_1(G) = \sum_{uv\in E(G)} \frac{d_u + d_v}{d_u d_v}.$$

$$ReZ_2(G) = \sum_{uv\in E(G)} \frac{d_u d_v}{d_u + d_v}.$$

$$ReZ_3(G) = \sum_{uv\in E(G)} d_u d_v (d_u + d_v).$$

2. MAIN RESULTS

The main goal of this article is to compute the redefined versions of the some Zagreb indices, i.e. the redefined first, second and third Zagreb indices of oxide chains, chain silicates, ortho chain, and para chain by using the technique of edge partition.

2.1 Results for the Chain Oxide Network COX_n

In this section, we discuss COX_n and compute the exact results for the redefined first, second and third Zagreb indices. If we remove the silicon atom from the silicate network, then the resulting network is an oxide network [25], which consists of three oxygen atoms. Oxide networkhas the triangular structure. If an oxide network shares its oxygen with other oxide network linearly, then the oxide chain is formed, as shown in Figure 1.

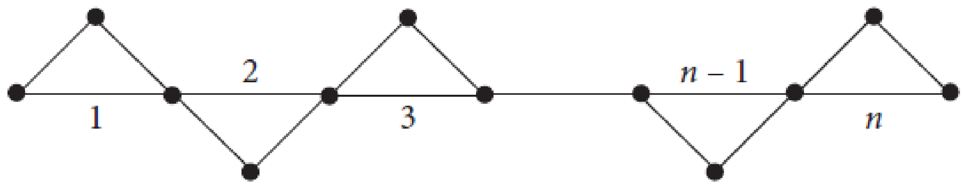

Figure 1: Oxide network.

Theorem 2.1. *Let G be the oxide network of order n. Then*

$$R_eZ_1(G) = 2 + \frac{3n}{2} + \frac{n-2}{2}.$$

$$R_eZ_2(G) = 2 + \frac{8n}{3} + 2(n-2).$$

$$R_eZ_3(G) = 32 + 96n + 128(n-2).$$

Proof. Let $G \cong OX_n$, where $n \geqslant 2$; also, n is an integer. One can partition the set edge of OX_n as follow:

$$E_1 = \{uv : uv \in E(OX_n) \ and \ du = 2, d_v = 2\}$$

$$E_2 = \{uv : uv \in E(OX_n) \ and \ du = 2, d_v = 4\}$$

$$E_3 = \{uv : uv \in E(OX_n) \ and \ du = 4, d_v = 4\}$$

and $|E_1| = 2$, $|E_2| = 2n$, $|E_3| = n - 2$. Hence

$$\begin{aligned} ReZ_1(OX_n) &= \sum_{uv \in E(OX_n)} \frac{d_u + d_v}{d_u d_v} = \sum_{uv \in E_1} \frac{d_u + d_v}{d_u d_v} + \sum_{uv \in E_2} \frac{d_u + d_v}{d_u d_v} + \sum_{uv \in E_3} \frac{d_u + d_v}{d_u d_v} \\ &= \sum_{uv \in E_1} \frac{2+2}{2 \times 2} + \sum_{uv \in E_2} \frac{2+4}{2 \times 4} + \sum_{uv \in E_3} \frac{4+4}{4 \times 4} \\ &= |E_1| + \frac{3}{4}|E_2| + \frac{1}{2}|E_3| \\ &= 2 + \frac{3n}{2} + \frac{n-2}{2}. \end{aligned}$$

And,

$$\begin{aligned} ReZ_2(OX_n) &= \sum_{uv \in E(OX_n)} \frac{d_u d_v}{d_u + d_v} = \sum_{uv \in E_1} \frac{d_u d_v}{d_u + d_v} + \sum_{uv \in E_2} \frac{d_u d_v}{d_u + d_v} + \sum_{uv \in E_3} \frac{d_u d_v}{d_u + d_v} \\ &= \sum_{uv \in E_1} \frac{2 \times 2}{2+2} + \sum_{uv \in E_2} \frac{2 \times 4}{2+4} + \sum_{uv \in E_3} \frac{4 \times 4}{4+4} \\ &= |E_1| + \frac{4}{3}|E_2| + 2|E_3| \\ &= 2 + \frac{8n}{3} + 2(n-2). \end{aligned}$$

$$\begin{aligned} R_eZ_3(G) &= \sum_{uv \in E(G)} d_u d_v(d_u + d_v) = \sum_{uv \in E_1} d_u d_v(d_u + d_v) + \sum_{uv \in E_2} d_u d_v(d_u + d_v) \\ &+ \sum_{uv \in E_3} d_u d_v(d_u + d_v) \\ &= \sum_{uv \in E_1} 4(2+2) + \sum_{uv \in E_2} 8(2+4) + \sum_{uv \in E_3} 16(4+4) \\ &= 16|E_1| + 48|E_2| + 128|E_3| \\ &= 32 + 96n + 128(n-2). \end{aligned}$$

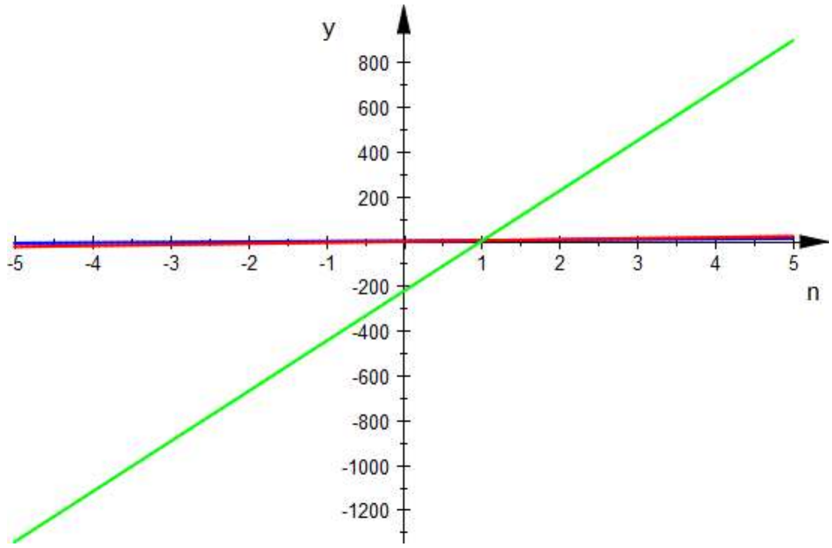

Figure 2: Graphical representation of the redefined first, second, and third Zagreb indices of the oxide network

2.2 Results for the Chain Silicate Network CS_n.

In this section, we discuss CS_n and compute the exact results for $R_eZ_1(CS_n)$, $R_eZ_2(CS_n)$ and $R_eZ_3(CS_n)$. Silicates are the compounds which consist of silicon and oxygen, having a tetra- hadron structure with a bond angle of 109.5°. SiO_4 is found in almost all of the silicates. A singletetrahedron has a shape like a pyramid with triangular base. It has four oxygen atoms at its corners, and the silicon atom is bounded equally with oxygen atoms with a bond length of 162 pm. A single tetrahedron is shown in Figure 3(*a*). If a single tetrahedron shares its oxygen with othertetrahedrons; then, a linear silicate chain [8] is formed, as shown in Figure 3(b).

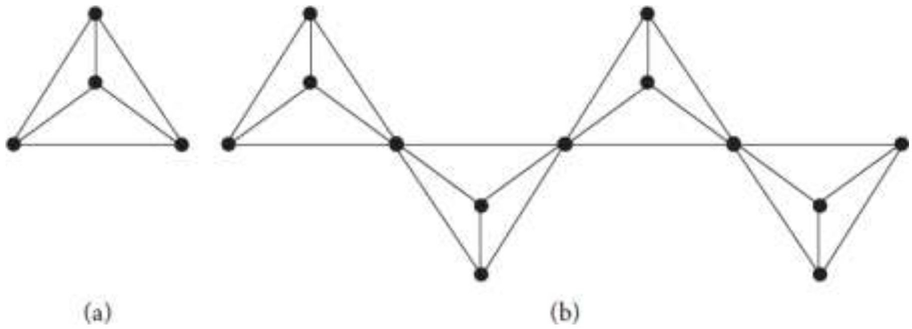

Figure 3: (a) Single silicate and (b) chain silicate

Theorem 2.2. *Let G_2 be the chain silicate network of n order; then,*

$$R_eZ_1(G_2) = \frac{3(n+4)}{2} + \frac{2(2n-1)}{9} + \frac{n-2}{3}.$$

$$R_eZ_2(G_2) = \frac{2(n+4)}{3} + 18(2n-1) + 3(n-2).$$

$$R_eZ_3(G_2) = 54(n+4) + 324(2n-1) + 432(n-2).$$

Proof. Let G_2 be the chain silicate network of *n* order, then the the partition of chain silicatenetwork is

And,

$$E_1 = \{uv : uv \in E(CS_n) \ \ and \ \ du = 3, d_v = 3\}$$

$$E_2 = \{uv : uv \in E(CS_n) \ \ and \ \ du = 3, d_v = 6\}$$

$$E_3 = \{uv : uv \in E(CS_n) \ \ and \ \ du = 6, d_v = 6\}$$

and $|E_1| = n + 4$, $|E_2| = 2(2n - 1)$, $|E_3| = n - 2$. Hence

$$\begin{aligned} R_eZ_1(G_2) &= \sum_{uv\in E(G_2)} \frac{d_u + d_v}{d_u d_v} = \sum_{uv\in E_1} \frac{d_u + d_v}{d_u d_v} + \sum_{uv\in E_2} \frac{d_u + d_v}{d_u d_v} + \sum_{uv\in E_3} \frac{d_u + d_v}{d_u d_v} \\ &= \sum_{uv\in E_1} \frac{3+3}{3\times 3} + \sum_{uv\in E_2} \frac{3+6}{3\times 6} + \sum_{uv\in E_3} \frac{6+6}{6\times 6} \\ &= \frac{3}{2}|E_1| + \frac{1}{9}|E_2| + \frac{1}{3}|E_3| \\ &= \frac{3(n+4)}{2} + \frac{2(2n-1)}{9} + \frac{n-2}{3}. \end{aligned}$$

$$\begin{aligned} ReZ_2(G_2) &= \sum_{uv\in E(G_2)} \frac{d_u d_v}{d_u + d_v} = \sum_{uv\in E_1} \frac{d_u d_v}{d_u + d_v} + \sum_{uv\in E_2} \frac{d_u d_v}{d_u + d_v} + \sum_{uv\in E_3} \frac{d_u d_v}{d_u + d_v} \\ &= \sum_{uv\in E_1} \frac{3\times 3}{3+3} + \sum_{uv\in E_2} \frac{3\times 6}{3+6} + \sum_{uv\in E_3} \frac{6\times 6}{6+6} \\ &= \frac{2}{3}|E_1| + 9|E_2| + 3|E_3| \\ &= \frac{2(n+4)}{3} + 18(2n-1) + 3(n-2). \end{aligned}$$

$$\begin{aligned} R_eZ_3(G_2) &= \sum_{uv\in E(G_2)} d_u d_v(d_u + d_v) = \sum_{uv\in E_1} d_u d_v(d_u + d_v) + \sum_{uv\in E_2} d_u d_v(d_u + d_v) \\ &+ \sum_{uv\in E_3} d_u d_v(d_u + d_v) \\ &= \sum_{uv\in E_1} 9(3+3) + \sum_{uv\in E_2} 18(3+6) + \sum_{uv\in E_3} 36(6+6) \\ &= 54|E_1| + 162|E_2| + 432|E_3| \\ &= 54(n+4) + 324(2n-1) + 432(n-2). \end{aligned}$$

□

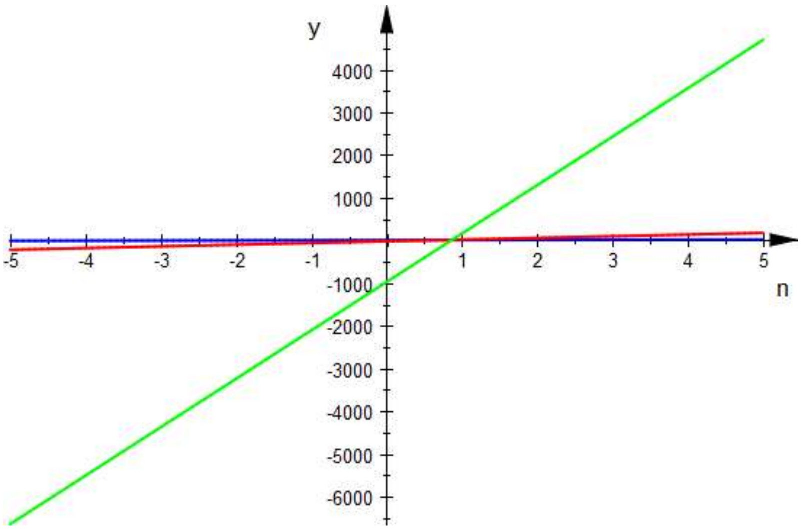

Figure 4: Graphical representation of the redefined first, second and third Zagreb indices of thechain silicate network

2.3 Results for the Ortho Chain S_n

In this section, we discuss S_n and compute the exact results for $R_eZ_1(S_n)$, $R_eZ_2(S_n)$ and $R_eZ_3(S_n)$. The single molecule of para and ortho chain has the same structure. Basically, it is a cycle graph having 4 sides denoted as C_4 and represented as a four-sided regular polygon. The ortho chain has a zig-zag structure where each corner of C_4 is attached linearly, as shownin Figure 5.

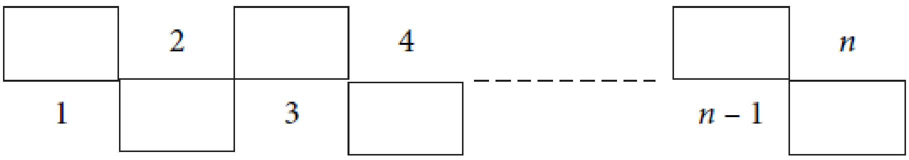

Figure 5: Ortho chain of n vertices.

Theorem 2.3. *Let G_3 be the ortho chain of n order; then,*

$$R_eZ_1(G_3) = n + 2 + \frac{4n-2}{2}.$$

$$R_eZ_2(G_3) = 3n - 2 + \frac{8n}{3}.$$

$$R_eZ_3(G_3) = 240n - 224.$$

Proof. Let $G_3 \cong S_n$, where $n \geq 2$; also, n is an integer. The edge partition of ortho chain of norder is $E_1 = \{uv : uv \in E(S_n)$ *and* $du = 2, d_v = 2\}$ $E_2 = \{uv : uv \in E(S_n)$ *and* $du = 2, d_v = 4\}$ $E_3 = \{uv : uv \in E(S_n)$ *and* $du = 4, d_v = 4\}$

$$E_1 = \{uv : uv \in E(S_n) \ \ and \ \ du = 2, d_v = 2\}$$

$$E_2 = \{uv : uv \in E(S_n) \ \ and \ \ du = 2, d_v = 4\}$$

$$E_3 = \{uv : uv \in E(S_n) \ \ and \ \ du = 4, d_v = 4\}$$

and $|E_1| = n+2$, $|E_2| = 2n$, $|E_3| = n-2$. Hence

$$\begin{aligned} R_eZ_1(G_3) &= \sum_{uv\in E(G_3)} \frac{d_u+d_v}{d_ud_v} = \sum_{uv\in E_1} \frac{d_u+d_v}{d_ud_v} + \sum_{uv\in E_2} \frac{d_u+d_v}{d_ud_v} + \sum_{uv\in E_3} \frac{d_u+d_v}{d_ud_v} \\ &= \sum_{uv\in E_1} \frac{2+2}{2\times 2} + \sum_{uv\in E_2} \frac{2+4}{2\times 4} + \sum_{uv\in E_3} \frac{4+4}{4\times 4} \\ &= |E_1| + \frac{3}{4}|E_2| + \frac{1}{2}|E_3| \\ &= n+2+\frac{3n}{2}+\frac{n-2}{2} \\ &= n+2+\frac{4n-2}{2} \end{aligned}$$

And,

$$\begin{aligned} R_eZ_2(G_3) &= \sum_{uv\in E(G_3)} \frac{d_ud_v}{d_u+d_v} = \sum_{uv\in E_1} \frac{d_ud_v}{d_u+d_v} + \sum_{uv\in E_2} \frac{d_ud_v}{d_u+d_v} + \sum_{uv\in E_3} \frac{d_ud_v}{d_u+d_v} \\ &= \sum_{uv\in E_1} \frac{4}{2+2} + \sum_{uv\in E_2} \frac{8}{2+4} + \sum_{uv\in E_3} \frac{16}{4+4} \\ &= |E_1| + \frac{4}{3}|E_2| + 2|E_3| \\ &= n+2+\frac{8n}{3}+2(n-2) \\ &= 3n-2+\frac{8n}{3}. \end{aligned}$$

$$\begin{aligned} R_eZ_3(G_3) = \sum_{uv\in E(G_3)} d_ud_v(d_u+d_v) &= \sum_{uv\in E_1} d_ud_v(d_u+d_v) + \sum_{uv\in E_2} d_ud_v(d_u+d_v) \\ &+ \sum_{uv\in E_3} d_ud_v(d_u+d_v) \\ &= \sum_{uv\in E_1} 4(2+2) + \sum_{uv\in E_2} 8(2+4) + \sum_{uv\in E_3} 16(4+4) \\ &= 16|E_1| + 48|E_2| + 128|E_3| \\ &= 16n+32+96n+128n-256 \\ &= 240n-224. \end{aligned}$$

2.4 Results for the Para Chain Q_n

In this section, we discuss Q_n and compute the exact results for $R_eZ_1(Q_n)$, $R_eZ_2(Q_n)$ and $R_eZ_3(Q_n)$. The para chain has a structure in which each C_4 is attached at corner to corner with

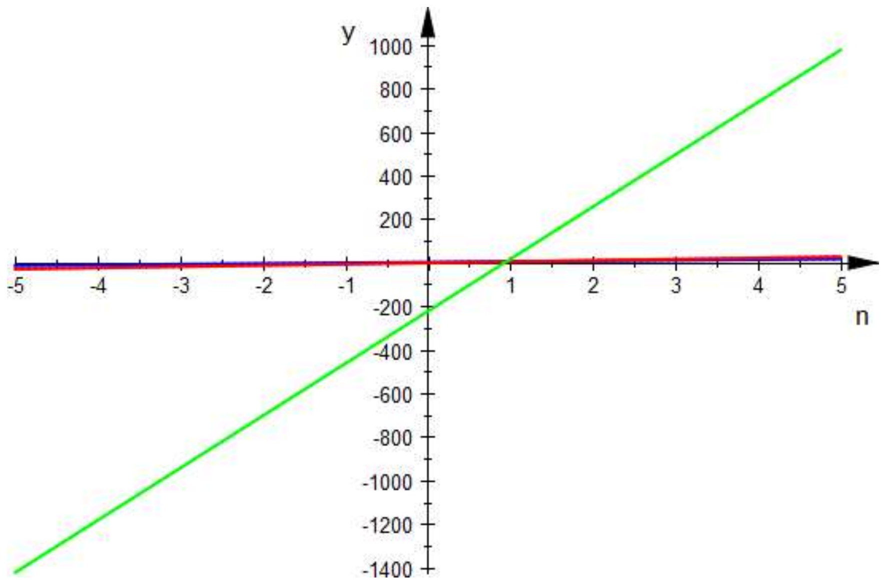

Figure 6: Graphical representation of the redefined first, second and third Zagreb indices of theortho chain

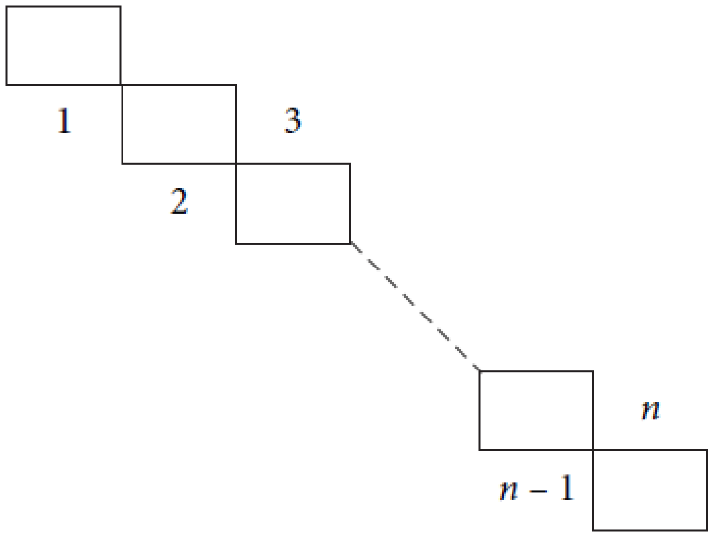

Figure 7: Para chain of n order.

other C_4 but not linearly, as shown in Figure 7.

Theorem 2.4. *Let G_4 be the para chain of n order; then*

$$R_eZ_1(G_4) = n - 3.$$

$$R_eZ_2(G_4) = 4 + \frac{16n - 16}{3}.$$

$$R_eZ_3(G_4) = 192n - 128.$$

Proof. Let $G_4 \cong Q_n$, where $n \geq 2$; also, n is an integer. Then the edge partition of para chainof n order is

$$E_1 = \{uv : uv \in E(S_n) \;\; and \;\; du = 2, d_v = 2\}$$

$$E_2 = \{uv : uv \in E(S_n) \;\; and \;\; du = 2, d_v = 4\}$$

and $|E_1| = 4$, $|E_2| = 4n - 4$. Hence

$$\begin{aligned} R_eZ_1(G_4) &= \sum_{uv\in E(G_4)} \frac{d_u+d_v}{d_ud_v} = \sum_{uv\in E_1} \frac{d_u+d_v}{d_ud_v} + \sum_{uv\in E_2} \frac{d_u+d_v}{d_ud_v} \\ &= \sum_{uv\in E_1} \frac{2+2}{2\times 2} + \sum_{uv\in E_2} \frac{2+4}{2\times 4} \\ &= |E_1| + \frac{3}{4}|E_2| \\ &= 4 + (n-1) \\ &= n-3. \end{aligned}$$

And,

$$\begin{aligned} R_eZ_2(G_4) &= \sum_{uv\in E(G_4)} \frac{d_ud_v}{d_u+d_v} = \sum_{uv\in E_1} \frac{d_ud_v}{d_u+d_v} + \sum_{uv\in E_2} \frac{d_ud_v}{d_u+d_v} \\ &= \sum_{uv\in E_1} \frac{4}{2+2} + \sum_{uv\in E_2} \frac{8}{2+4} \\ &= |E_1| + \frac{4}{3}|E_2| \\ &= 4 + \frac{16n-16}{3}. \end{aligned}$$

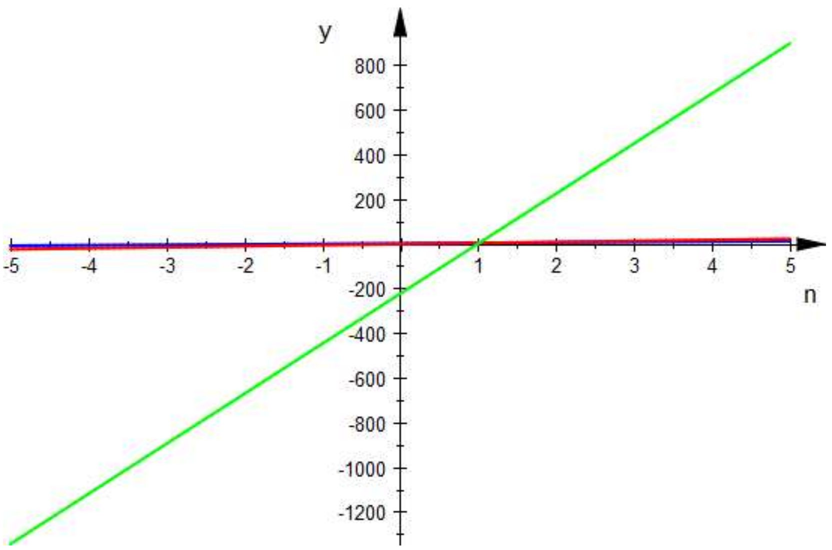

Figure 8: Graphical representation of the redefined first, second and third Zagreb indices of thepara chain

3. CONCLUSION

In this article, we have figured out several degree-based topological indices such as $R_eZ_1(G)$, $R_eZ_2(G)$ and $R_eZ_3(G)$ of a graph G. We calculated the closed formulae for abovementionedtopological indices of chain silicate, oxide network, para, and ortho chain. The above outcomes contribute in the field of natural sciences and pharmaceutical science.

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