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Research Article

Calculating Some Topological Indices of SiO_2 Layer Structure

Fatima Farrukh[1], Sabeel-e-Hafi[1], Rashid Farooq[1] and Mohammad R. Farahani[2,*]

[1] *School of Natural Sciences, National University of Sciences and Technology, H-12, Islamabad, Pakistan*
[2] *Department of Applied Mathematics, Iran University of Science and Technology, Narmak, Tehran, Iran*
***Corresponding author:** mr_farahani@mathdep.iust.ac.ir, mrfarahani88@gmail.com

Abstract. Topological indices are closely related to the toxicological, physicochemical, pharmacological etc. properties of a chemical compound. This paper focuses on calculating topological indices namely Randić index, sum-connectivity index, reciprocal Randić index, reduced second Zagreb index and reduced reciprocal Randić index of SiO_2 layer structure for all values of p and q.

Keywords. Degree based indices; Topological indices; SiO_2 layer structure

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1. Introduction

For a molecular graph G, with the vertex set $V(G)$ and the edge set $E(G)$, a topological index is defined as a numeric quantity that can be calculated from G. Topological indices are numerical invariants that are associated with the topological characterization of a compound. By topological characterization, we mean that these indices relate to certain properties of the compound including the toxicological, physicochemical, pharmacological etc. properties. From chemistry's point of view, compounds' properties give a measure of how a certain compound will behave and react but the process is both time and energy consuming. Chemical graph theory provides an easy alternative to that. Mathematically a topological index is a function from a set of finite graphs ξ to real numbers i.e., $\text{Top}: \zeta \to \mathbb{R}$. Calculating topological indices is not only useful for verifying the existing properties of chemical compound but also for calculating new applications of naturally occurring molecules and more interestingly these can be used to design new compounds with specifically required properties [11].

In this paper, we focus on calculating the topological indices of the SiO_2 layer structure. We know that the silicates (SiO_2) consist of one silicon ion and four oxygen ions, as shown in Figure 1.

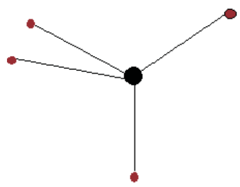

Figure 1. SiO_2 ion

Silicates form different networks, based on their polymerization but the networks are usually motivated by the original silicate network. The SiO_2 layer structure, on the other hand is the original silicate structure. Silicate, in its naturally occurring form, forms an octagon of sorts, as shown in Figure 2.

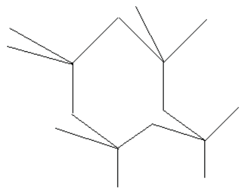

Figure 2. SiO_2 octagon

And finally, these octagons join together to form the SiO_2 layer structure. We define the rows as the number of lines of vertical octagons and columns as the number of lines of horizontal octagons. We denote the number of rows with p and the number of columns with q. For better understanding, Figure 3 gives the SiO_2 layer structure with $p = 4$ and $q = 5$. The concept can be extended to any number of rows and columns.

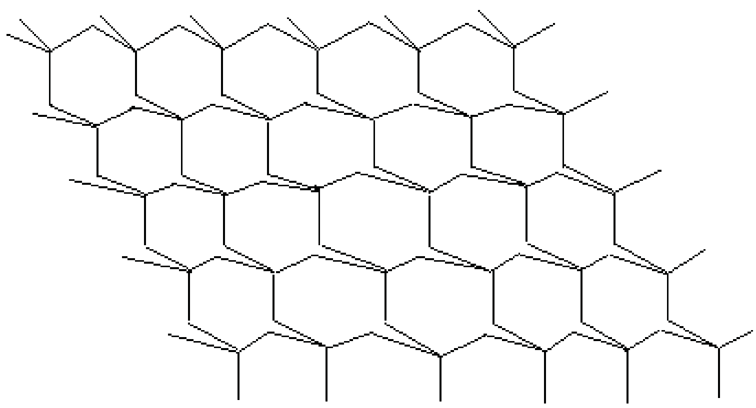

Figure 3. $SiO_2(4,5)$

This study calculates the Randić, sum-connectivity, reciprocal Randić, reduced second Zagreb and reduced reciprocal Randić indices of the SiO_2 layer structure. To start off we will define and explain the indices in the next section.

2. Preliminaries

In this section, the topological indices being calculated are introduced, defined and explained. As explained in the above section, topological indices relate to specific properties of molecular structures. The topological indices chosen here are extremely useful in this regard. Before starting we define the following:

(1) If two vertices x and y are adjacent in G, then xy is an edge in G.

(2) The number of vertices adjacent to a particular vertex x is known as the degree of the vertex, denoted by d_x.

Starting off with the Randić index, it was initially proposed by a chemist named Milan Randić in 1975 [10]. Also known as the product-connectivity index, it was limited to measure the extent of molecular branching relevant to carbon-atom skeleton of saturated hydrocarbons. But on the positive side, it showed a good co-relation with several physicochemical properties of alkanes that include enthalpies of formation, boiling points, parameters in the Antoine equation for vapor pressure, Kovats constants, chromatographic retention times, surface areas, etc. [7,8]. Verbally Randić index is defined as the sum of square root of the product of all the degrees of adjacent vertices. Mathematically, for a graph G, the Randić index $R(G)$ is given by:

$$R(G) = \sum_{xy\in E(G)} \frac{1}{\sqrt{d_x d_y}}. \tag{2.1}$$

In order to reach the full extent of the index, Bollobas and Erdös [1] generalized the index in 1998 by replacing the square root with an α root, where α is any real number. They called it the general Randić index and it is defined as follows:

$$R_g(G) = \sum_{xy\in E(G)} \frac{1}{\sqrt{d_x d_y}}. \tag{2.2}$$

Further examination of the Randić index yielded another index, known as the reciprocal Randić index. The index was first encountered by Favaron, Maheo and Sacle as a part of their study [6]. Verbally, it is defined as the sum of the square root of the product of degrees of the vertices of a molecular graph. For a graph G, the index is defined as follows:

$$RR(G) = \sum_{xy\in E(G)} \sqrt{d_x d_y}. \tag{2.3}$$

Another invariant related to the Randić index is the reduced reciprocal Randić index [9]. It is a slight variation of the reciprocal Randić index defined as follows:

$$RRR(G) = \sum_{xy\in E(G)} \sqrt{(d_x - 1)(d_y - 1)}. \tag{2.4}$$

Next, we have the sum-connectivity index, which was introduced by Zhou and Trinajstić in 2008 [10]. It is a relatively new index closely related to the Randić (product-connectivity) index. This index also shows a good co-relation with physicochemical properties which are explained in detail by Todeschini and Consonni in '*Handbook of Molecular Descriptors*' [12] and research articles [3–5]. Verbally, it is defined as the sum of square root of the sum of all the degrees of adjacent vertices. Mathematically, for a graph G, the sum-connectivity index $R^+(G)$ is given by:

$$R^+(G) = \sum_{xy \in E(G)} \frac{1}{\sqrt{d_x + d_y}} . \tag{2.5}$$

Like product-connectivity index, sum-connectivity index can be also be generalized to an α root instead of a square root, where α is any real number. The general sum-connectivity index $R_g^+(G)$ for a graph G is defined as follows:

$$R_g^+(G) = \sum_{xy \in E(G)} \frac{1}{\sqrt[\alpha]{d_x + d_y}} . \tag{2.6}$$

In the next section, we calculate these indices for the SiO_2 layer structure.

3. Results

Based on the degree of each vertex, there are two types of edges in the SiO_2 layer structure. Table 1 gives the different types of edges and the formulae to calculate the number of edges of each type.

Table 1. Types of edges and formulae to calculate the number of edges of each type in the SiO_2 network

Types of edges	Number of edges
$(1,4)$	$2p+2q+4$
$(2,4)$	$2p+2q+4pq$

Using Table 1, we have the following theorems.

Theorem 3.1. *The Randić index of* $SiO_2(p,q)$ *layer structure is given by:*

$$R(SiO_4) = \left(1+\frac{\sqrt{2}}{2}\right)p + \left(1+\frac{\sqrt{2}}{2}\right)q + \sqrt{2}pq + 2 .$$

Proof. Replacing the values from Table 1 in (2.1), we get

$$\begin{aligned} R(SiO_4) &= \sum_{xy \in (1,4)} \frac{1}{\sqrt{(1)(4)}} + \sum_{xy \in (2,4)} \frac{1}{\sqrt{(2)(4)}} \\ &= (2p+2q+4)\frac{1}{2} + (2p+2q+4pq)\frac{\sqrt{2}}{4} \\ &= p+q+2+\frac{\sqrt{2}}{2}p + \frac{\sqrt{2}}{2}q + \sqrt{2}pq \\ &= \left(1+\frac{\sqrt{2}}{2}\right)p + \left(1+\frac{\sqrt{2}}{2}\right)q + \sqrt{2}pq + 2. \end{aligned}$$

□

Theorem 3.2. *The general Randić index of* $\mathrm{SiO_2}(p,q)$ *layer structure is given by:*

$$R_g(\mathrm{SiO_4})=\left(\frac{2}{(4)^{\frac{1}{a}}}+\frac{2}{(8)^{\frac{1}{a}}}\right)p+\left(\frac{2}{(4)^{\frac{1}{a}}}+\frac{2}{(8)^{\frac{1}{a}}}\right)q+\frac{4}{(8)^{\frac{1}{a}}}pq+\frac{4}{(4)^{\frac{1}{a}}}\,.$$

Proof. Replacing the values from Table 1 in (2.2), we get

$$\begin{aligned}R_g(\mathrm{SiO_4})&=\sum_{xy\in(1,4)}\frac{1}{\sqrt[a]{(1)(4)}}+\sum_{xy\in(2,4)}\frac{1}{\sqrt[a]{(2)(4)}}\\&=(2p+2q+4)\frac{1}{(4)^{\frac{1}{a}}}+(2p+2q+4pq)\frac{1}{(8)^{\frac{1}{a}}}\\&=\left(\frac{2}{(4)^{\frac{1}{a}}}+\frac{2}{(8)^{\frac{1}{a}}}\right)p+\left(\frac{2}{(4)^{\frac{1}{a}}}+\frac{2}{(8)^{\frac{1}{a}}}\right)q+\frac{4}{(8)^{\frac{1}{a}}}pq+\frac{4}{(4)^{\frac{1}{a}}}\,.\end{aligned}$$ □

Theorem 3.3. *The reciprocal Randić index of* $\mathrm{SiO_2}(p,q)$ *layer structure is given by:*

$$RR(\mathrm{SiO_4})=(4+4\sqrt{2})p+(4+4\sqrt{2})q+8\sqrt{2}pq+8\,.$$

Proof. Replacing the values from Table 1 in (2.3), we get

$$\begin{aligned}RR(\mathrm{SiO_4})&=\sum_{xy\in(1,4)}\sqrt{(1)(4)}+\sum_{xy\in(2,4)}\sqrt{(2)(4)}\\&=(2p+2q+4)2+(2p+2q+4pq)\sqrt{8}\\&=4p+4q+8+2\sqrt{8}p+2\sqrt{8}q+4\sqrt{8}\\&=(4+4\sqrt{2})p+(4+4\sqrt{2})q+8\sqrt{2}pq+8\,.\end{aligned}$$ □

Theorem 3.4. *The reverse reciprocal Randić index of* $\mathrm{SiO_2}(p,q)$ *layer structure is given by:*

$$RRR(\mathrm{SiO_4})=2\sqrt{3}p+2\sqrt{3}q+4\sqrt{3}pq\,.$$

Proof. Replacing the values from Table 1 in (2.4), we get

$$\begin{aligned}RRR(\mathrm{SiO_4})&=\sum_{xy\in(1,4)}\sqrt{(1-1)(4-1)}+\sum_{xy\in(2,4)}\sqrt{(2-1)(4-1)}\\&=0+(2p+2q+4pq)\sqrt{3}\\&=2\sqrt{3}p+2\sqrt{3}q+4\sqrt{3}pq\,.\end{aligned}$$ □

Theorem 3.5. *The sum-connectivity index of* $\mathrm{SiO_2}(p,q)$ *layer structure is given by:*

$$R^+(\mathrm{SiO_4})=\left(\frac{2}{\sqrt{5}}+\frac{2}{\sqrt{6}}\right)p+\left(\frac{2}{\sqrt{5}}+\frac{2}{\sqrt{6}}\right)q+\frac{4}{\sqrt{6}}pq+\frac{4}{\sqrt{5}}\,.$$

Proof. Replacing the values from Table 1 in (2.5), we get

$$R(\mathrm{SiO_4})=\sum_{xy\in(1,4)}\frac{1}{\sqrt{(1)+(4)}}+\sum_{xy\in(2,4)}\frac{1}{\sqrt{(2)+(4)}}$$

$$
\begin{aligned}
&= (2p+2q+4)\frac{1}{\sqrt{5}} + (2p+2q+4pq)\frac{1}{\sqrt{6}} \\
&= \frac{2}{\sqrt{5}}p + \frac{2}{\sqrt{5}}q + \frac{4}{\sqrt{5}} + \frac{2}{\sqrt{6}}p + \frac{2}{\sqrt{5}}q\frac{4}{\sqrt{6}}pq \\
&= \left(\frac{2}{\sqrt{5}} + \frac{2}{\sqrt{6}}\right)p + \left(\frac{2}{\sqrt{5}} + \frac{2}{\sqrt{6}}\right)q + \frac{4}{\sqrt{6}}pq + \frac{4}{\sqrt{5}}\,. \qquad \square
\end{aligned}
$$

Theorem 3.6. *The sum-connectivity index of* $\mathrm{SiO}_2(p,q)$ *layer structure is given by:*

$$R_g^+(\mathrm{SiO}_4) = \left(\frac{2}{(5)^{\frac{1}{a}}} + \frac{2}{(6)^{\frac{1}{a}}}\right)p + \left(\frac{2}{(5)^{\frac{1}{a}}} + \frac{2}{(6)^{\frac{1}{a}}}\right)q + \frac{4}{(6)^{\frac{1}{a}}}pq + \frac{4}{(5)^{\frac{1}{a}}}\,.$$

Proof. Replacing the values from Table 1 in (2.6), we get

$$
\begin{aligned}
R_g^+(\mathrm{SiO}_4) &= \sum_{xy\in(1,4)} \frac{1}{\sqrt[a]{(1)+(4)}} + \sum_{xy\in(2,4)} \frac{1}{\sqrt[a]{(2)+(4)}} \\
&= (2p+2q+4)\frac{1}{(5)^{\frac{1}{a}}} + (2p+2q+4pq)\frac{1}{(6)^{\frac{1}{a}}} \\
&= \left(\frac{2}{(5)^{\frac{1}{a}}} + \frac{2}{(6)^{\frac{1}{a}}}\right)p + \left(\frac{2}{(5)^{\frac{1}{a}}} + \frac{2}{(6)^{\frac{1}{a}}}\right)q + \frac{4}{(6)^{\frac{1}{a}}}pq + \frac{4}{(5)^{\frac{1}{a}}}\,. \qquad \square
\end{aligned}
$$

4. Conclusion

In this study we have calculated the Randić, general Randić, sum-connectivity, general sum-connectivity, reciprocal Randić and reduced reciprocal Randić indices of the SiO$_2$ layer structure for all values of p and q.

References

[1] B. Bollobás and P. Erdös, Graphs of extremal weights, *Ars. Combin.*, **50** (1998), 225–233.

[2] S. Fajtlowicz, On conjectures of Graffitti-II, *Congr. Numer.*, **60** (1987), 187–197.

[3] M.R. Farahani, On the Randić and sum-connectivity index of some graphs, *Algebras, Groups and Geometries* (Hadronic Journal), **29** (4) (2012), 415–422.

[4] M.R. Farahani, On the Randić and sum-connectivity index of nanotubes, *Annals of West University of Timisoara-Mathematics and Computer Science*, **51** (2) (2013), 39–46.

[5] M.R. Farahani, On the higher Randić indices of nanotubes, *Journal of Computational Methods in Molecular Design*, **5** (3) (2015), 10–15.

[6] O. Favaron, M. Mahéo and J.F. Saclé, Some eigenvalues properties in graphs (conjectures of Graffitti-II), *Dicrete Math.*, **111** (1993), 197–220.

[7] X. Li and Y. Shi, A survey on the Randić index, *MATCH Commun. Math. Comput. Chem.*, **59** (2008), 127–156.

[8] H. Liu, M. Lu and F. Tian, On the Randić index, *J. Math. Chem.*, **38** (2005), 345–354.

[9] W. Luo and B. Zhou, On the irregularity of trees and unicyclic graphs with given matching number, *Util. Math.*, **83** (2010), 141–148.

[10] M. Randić, On characterization of molecular branching, *J. Mol. Graphics Modell.*, **97** (1975), 6609–6615.

[11] M. Rosary, C.J. Deeni and D.A. Xavier, Computing some topological indices of triangular silicate network, *Proceedings of the International Conference on Applied Mathematics and Theoretical Computer Sciences* (2013), 124–128.

[12] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim (2000).

[13] B. Zhou and N. Trinajstić, On a novel connectivity index, *J. Math. Chem.*, **46** (2009), 1252–1270.