



The Computational Aspects of Topological Indices of the Chain Silicate and Ortho Chain Silicate Structures

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ABSTRACT

In recent years, the integration of topological indices into Quantitative Structure Property Relationship (QSPR) models has become increasingly prominent. These models leverage statistical techniques and machine learning algorithms to predict molecular properties based on topological descriptors, offering valuable insights for rational drug design, environmental risk assessment, and material properties optimization. In this article, we compute various topological indices of the chain silicate and ortho chain silicate structures. Also the computed indices are plotted in graphs and compared visually.

I. INTRODUCTION

Quantitative Structure-Property Relationship (QSPR) analysis represents a pivotal approach in computational chemistry and chemo-informatics, enabling the prediction of various molecular properties based on structural descriptors. Among the diverse methodologies employed in QSPR studies, topological indices have emerged as fundamental tools for characterizing molecular structure and properties. These indices encapsulate critical topological features of molecules, providing a quantitative framework for understanding and predicting their physicochemical behaviors.

The concept of topological indices dates back several decades, rooted in graph theory and mathematical chemistry. Initially devised to quantify molecular branching, symmetry, and connectivity without explicit consideration of atomic details, these indices have evolved into sophisticated descriptors that correlate with a wide range of molecular properties. The appeal of topological indices lies in their ability to condense complex molecular structures into numerical values, facilitating comparative analyses and predictive modeling across diverse chemical and biological systems.

In recent years, the integration of topological indices into QSPR methodologies has significantly advanced our ability to predict molecular properties such as solubility, toxicity, and biological activity. By leveraging computational

algorithms and statistical models, researchers can systematically explore the relationships between these indices and experimental data, thereby elucidating underlying structure-function relationships at a molecular level. Such insights are invaluable for drug discovery, environmental chemistry, and materials science, where predictive modeling plays a crucial role in guiding experimental design and decision-making processes.

Topological indices, also known as graph invariants, stand as fundamental tools in the realm of chemical graph theory and computational chemistry. These indices are numerical descriptors derived solely from the topology of molecular structures, capturing essential structural features without regard to specific atomic details. Originating from graph theory, which explores the mathematical properties of networks and inter connected structures, topological indices provide a quantitative framework for understanding and predicting various molecular properties and behaviors.

Graph theory and its applications in chemistry have provided significant insights into the understanding of molecular structures and properties. The foundational work of Gutman and Trinajstić [11] highlights the intersection of graph theory and molecular orbitals, establishing a theoretical framework that has been extensively utilized in the development of various molecular descriptors.

A critical advancement in this field is the concept of topological indices, which quantify the structure of

molecular graphs. Balaban [1] and Todeschini and Consonni [18] provide comprehensive overviews of these indices, discussing their derivation and applications in chemoinformatics. Balaban [1] specifically focuses on indices based on topological distances, which have proven useful in the study of molecular properties.

Ghorbani and Ashrafi [9] extended the Wiener index, a classical topological index, to provide more nuanced insights into molecular structures. Their work demonstrates the versatility of graph theoretical approaches in addressing complex chemical problems. Similarly, Klein and Jurcak [16] discuss various chemistry-relevant graph indices, highlighting their derivation and practical applications in understanding molecular behavior.

Recent advancements in computational methods have further enhanced the utility of topological indices. Zhang, Zhang, and Zou [14] review the application of these indices in the computational design of materials, showcasing how topological descriptors can predict material properties and guide the design process. Ivanciuc [15] also emphasizes the role of graph-theoretical models in nano-materials and drug design, underscoring the interdisciplinary nature of this research area.

In the realm of quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR), Gupta, Madan, and Singh [10] provide a detailed account of recent advances and future prospects. Their work highlights the integration of topological indices in predictive modeling, which is crucial for drug discovery and development.

The application of topological indices to specific chemical properties is explored by Mihai, Botezatu, and Al-Ahmad [17], who introduce novel descriptors for predicting the melting points of organic compounds. Their study illustrates the practical implications of topological indices in predicting physicochemical properties. Similarly, Barysz and Giziński [4] focus on modeling and predicting properties of chemical compounds, reinforcing the importance of topological indices in chemoinformatics.

Randić, Basak, and Trinajstić [13] delve into the properties of polycyclic aromatic hydrocarbons, using topological indices to elucidate their structure-property relationships. This work highlights the relevance of graph theoretical approaches in studying complex organic molecules.

The ongoing development of new topological indices, as discussed by Gutman and Zigert [12], continues to expand the toolkit available for chemists and materials scientists. Their review of the atom-bond connectivity index illustrates the continuous innovation in this field.

The theoretical foundations of chemical graph theory are thoroughly covered by Trinajstić [19] and Bonchev and Rouvray [3]. These works provide essential background knowledge and set the stage for the application of graph theory in modern chemical research.

Finally, Balakrishnan and Ranganathan [1] present advances in molecular descriptor research, offering insights into the development and application of new descriptors. This work underscores the dynamic nature of this research area and its importance in advancing chemical informatics.

Overall, the literature underscores the profound impact of graph theory and topological indices on chemical research, from theoretical foundations to practical applications in material design and drug discovery. The continuous development and refinement of these tools promise to drive further innovations in understanding and predicting molecular behavior.

II. TERMINOLOGIES

Given a graph $G = (V, E)$, by the term “degree” of a vertex x , we mean the number of edges incident with it and it is denoted as $\Gamma(x)$. The neighbourhood of a vertex x , denoted as $N(x)$ is a set containing the vertices incident with the edges incident with x and $N[x] = \{x\} \cup N(x)$. In this article, we compute the following topological indices for the proposed MOFs:

Definition 2.1. The following topological indices are used in this work:

$$(i) S_1(G) = \sum_{xy \in E(G)} \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right]$$

$$(ii) S_2(G) = \sum_{xy \in E(G)} \left[\frac{\Gamma(x) \times \Gamma(y)}{2} \right]$$

$$(iii) S_3(G) = \sum_{xy \in E(G)} \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right]^2$$

$$(iv) S_4(G) = \sum_{xy \in E(G)} \left[\frac{1}{\max\{\Gamma(x), \Gamma(y)\}} \right]$$

$$(v) S_5(G) = \sum_{xy \in E(G)} \left[\frac{\Gamma(x) \times \Gamma(y)}{\Gamma(x) + \Gamma(y)} \right]$$

$$(vi) S_6(G) = \sum_{xy \in E(G)} \left[\frac{1}{\sqrt{\Gamma(x) \times \Gamma(y)}} \right]$$

$$(vii) S_7(G) = \sum_{xy \in E(G)} \left[\frac{\Gamma(x) + \Gamma(y) - 2}{\Gamma(x) \times \Gamma(y)} \right]$$

$$(viii) S_8(G) = \sum_{xy \in E(G)} \sqrt{\Gamma(x)^2 \times \Gamma(y)^2}$$

III. RESULTS

In this section, we compute the topological indices of chain silicate and ortho chain silicate structures. Then we compare the computed values of these indices visually.

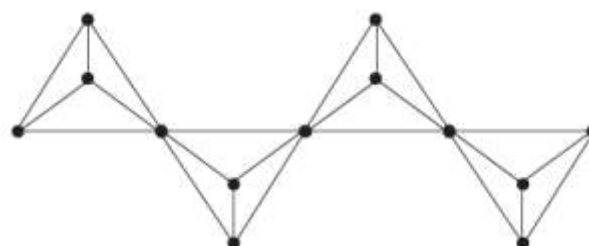


Figure 1: Chain silicate

We first consider the chain silicate structure which is shown in Fig.1. The edge partition for the chain silicates is as follows:

$$(i) E_1 = \{xy \in E(G) : \Gamma(x) = \Gamma(y) = 3\}$$

$$(ii) E_2 = \{xy \in E(G) : \Gamma(x) = 3, \Gamma(y) = 6\}$$

$$(iii) E_3 = \{xy \in E(G) : \Gamma(x) = \Gamma(y) = 6\}$$

Theorem 3.1 : For the chain silicate, the topological indices are:

$$(i) S_1(G) = 3(n + 4) + 9(2n - 1) + 6(n - 2)$$

$$(ii) S_2(G) = \frac{9}{2}(n + 4) + 18(2n - 1) + 18(n - 2)$$

$$(iii) S_3(G) = 9(n + 4) + \frac{81}{2}(2n - 1) + 36(n - 2)$$

$$(iv) S_4(G) = \frac{1}{3}(n + 4) + \frac{1}{12}(2n - 1) + \frac{1}{6}(n - 2)$$

$$(v) S_5(G) = \frac{3}{2}(n + 4) + 4(2n - 1) + 3(n - 2)$$

$$(vi) S_6(G) = \frac{1}{3}(n + 4) + \frac{1}{\sqrt{18}}(2n - 1) + \frac{1}{6}(n - 2)$$

$$(vii) S_7(G) = \frac{2}{3}(n + 4) + \sqrt{\frac{7}{18}}(2n - 1) + \frac{1}{\sqrt{3}}(n - 2)$$

$$(viii) S_8(G) = \sqrt{18}(n + 4) + \sqrt{45}(2n - 1) + \sqrt{72}(n - 2)$$

Proof:

$$\begin{aligned} (i) S_1 &= \sum_{xy \in E(G)} \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right] \\ &= \sum_{xy \in E_1} \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right] + \sum_{xy \in E_2} \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right] \\ &\quad + \sum_{xy \in E_3} \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right] \\ &= (n + 4) \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right] + 2(2n - 1) \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right] \\ &\quad + (n - 2) \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right] \end{aligned}$$

$$= 3(n + 4) + 9(2n - 1) + 6(n - 2).$$

$$\begin{aligned} (ii) S_2 &= \sum_{xy \in E(G)} \left[\frac{\Gamma(x) \times \Gamma(y)}{2} \right] \\ &= \sum_{xy \in E_1} \left[\frac{\Gamma(x) \times \Gamma(y)}{2} \right] + \sum_{xy \in E_2} \left[\frac{\Gamma(x) \times \Gamma(y)}{2} \right] \\ &\quad + \sum_{xy \in E_3} \left[\frac{\Gamma(x) \times \Gamma(y)}{2} \right] \\ &= (n + 4) \left[\frac{\Gamma(x) \times \Gamma(y)}{2} \right] + 2(2n - 1) \left[\frac{\Gamma(x) \times \Gamma(y)}{2} \right] \\ &\quad + (n - 2) \left[\frac{\Gamma(x) \times \Gamma(y)}{2} \right] \end{aligned}$$

$$= \frac{9}{2}(n + 4) + 18(2n - 1) + 18(n - 2).$$

$$\begin{aligned} (iii) S_3 &= \sum_{xy \in E(G)} \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right]^2 \\ &= \sum_{xy \in E_1} \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right]^2 + \sum_{xy \in E_2} \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right]^2 \\ &\quad + \sum_{xy \in E_3} \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right]^2 \\ &= (n + 4) \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right]^2 \\ &\quad + 2(2n - 1) \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right]^2 \\ &\quad + (n - 2) \left[\frac{\Gamma(x) + \Gamma(y)}{2} \right]^2 \\ &= 9(n + 4) + \frac{81}{2}(2n - 1) + 36(n - 2). \end{aligned}$$

$$\begin{aligned} (iv) S_4 &= \sum_{xy \in E(G)} \left[\frac{1}{\lfloor \max\{\Gamma(x), \Gamma(y)\} \rfloor} \right] \\ &= \sum_{xy \in E_1} \left[\frac{1}{\lfloor \max\{\Gamma(x), \Gamma(y)\} \rfloor} \right] \\ &\quad + \sum_{xy \in E_2} \left[\frac{1}{\lfloor \max\{\Gamma(x), \Gamma(y)\} \rfloor} \right] \\ &\quad + \sum_{xy \in E_3} \left[\frac{1}{\lfloor \max\{\Gamma(x), \Gamma(y)\} \rfloor} \right] \\ &= (n + 4) \left[\frac{1}{\lfloor \max\{\Gamma(x), \Gamma(y)\} \rfloor} \right] \\ &\quad + 2(2n - 1) \left[\frac{1}{\lfloor \max\{\Gamma(x), \Gamma(y)\} \rfloor} \right] \\ &\quad + (n - 2) \left[\frac{1}{\lfloor \max\{\Gamma(x), \Gamma(y)\} \rfloor} \right] \\ &= \frac{1}{3}(n + 4) + \frac{1}{12}(2n - 1) + \frac{1}{6}(n - 2). \end{aligned}$$

$$\begin{aligned} (v) S_5 &= \sum_{xy \in E(G)} \left[\frac{\Gamma(x) \times \Gamma(y)}{\Gamma(x) + \Gamma(y)} \right] \\ &= \sum_{xy \in E_1} \left[\frac{\Gamma(x) \times \Gamma(y)}{\Gamma(x) + \Gamma(y)} \right] + \sum_{xy \in E_2} \left[\frac{\Gamma(x) \times \Gamma(y)}{\Gamma(x) + \Gamma(y)} \right] \\ &\quad + \sum_{xy \in E_3} \left[\frac{\Gamma(x) \times \Gamma(y)}{\Gamma(x) + \Gamma(y)} \right] \\ &= (n + 4) \left[\frac{\Gamma(x) \times \Gamma(y)}{\Gamma(x) + \Gamma(y)} \right] \\ &\quad + 2(2n - 1) \left[\frac{\Gamma(x) \times \Gamma(y)}{\Gamma(x) + \Gamma(y)} \right] \\ &\quad + (n - 2) \left[\frac{\Gamma(x) \times \Gamma(y)}{\Gamma(x) + \Gamma(y)} \right] \end{aligned}$$

$$\begin{aligned}
 &= \frac{3}{2}(n+4) + 4(2n-1) + 3(n-2), \\
 (vi) S_6 &= \sum_{xy \in E(G)} \left[\frac{1}{\sqrt{\Gamma(x) \times \Gamma(y)}} \right] \\
 &= \sum_{xy \in E_1} \left[\frac{1}{\sqrt{\Gamma(x) \times \Gamma(y)}} \right] \\
 &+ \sum_{xy \in E_2} \left[\frac{1}{\sqrt{\Gamma(x) \times \Gamma(y)}} \right] \\
 &+ \sum_{xy \in E_3} \left[\frac{1}{\sqrt{\Gamma(x) \times \Gamma(y)}} \right] \\
 &= (n+4) \left[\frac{1}{\sqrt{\Gamma(x) \times \Gamma(y)}} \right] \\
 &+ 2(2n-1) \left[\frac{1}{\sqrt{\Gamma(x) \times \Gamma(y)}} \right] \\
 &+ (n-2) \left[\frac{1}{\sqrt{\Gamma(x) \times \Gamma(y)}} \right] \\
 &= \frac{1}{3}(n+4) + \frac{1}{\sqrt{18}}(2n-1) + \frac{1}{6}(n-2). \\
 (vii) S_7 &= \sum_{xy \in E(G)} \left[\frac{\Gamma(x) + \Gamma(y) - 2}{\Gamma(x) \times \Gamma(y)} \right] \\
 &= \sum_{xy \in E_1} \left[\frac{\Gamma(x) + \Gamma(y) - 2}{\Gamma(x) \times \Gamma(y)} \right] \\
 &+ \sum_{xy \in E_2} \left[\frac{\Gamma(x) + \Gamma(y) - 2}{\Gamma(x) \times \Gamma(y)} \right] \\
 &+ \sum_{xy \in E_3} \left[\frac{\Gamma(x) + \Gamma(y) - 2}{\Gamma(x) \times \Gamma(y)} \right] \\
 &= (n+4) \left[\frac{\Gamma(x) + \Gamma(y) - 2}{\Gamma(x) \times \Gamma(y)} \right] \\
 &+ 2(2n-1) \left[\frac{\Gamma(x) + \Gamma(y) - 2}{\Gamma(x) \times \Gamma(y)} \right] \\
 &+ (n-2) \left[\frac{\Gamma(x) + \Gamma(y) - 2}{\Gamma(x) \times \Gamma(y)} \right] \\
 &= \frac{2}{3}(n+4) + \sqrt{\frac{7}{18}}(2n-1) + \frac{1}{\sqrt{3}}(n-2). \\
 (viii) S_8 &= \sum_{xy \in E(G)} \sqrt{\Gamma(x)^2 + \Gamma(y)^2} \\
 &= \sum_{xy \in E_1} \sqrt{\Gamma(x)^2 + \Gamma(y)^2} \\
 &+ \sum_{xy \in E_2} \sqrt{\Gamma(x)^2 + \Gamma(y)^2} \\
 &+ \sum_{xy \in E_3} \sqrt{\Gamma(x)^2 + \Gamma(y)^2} \\
 &= (n+4)\sqrt{\Gamma(x)^2 + \Gamma(y)^2}
 \end{aligned}$$

$$\begin{aligned}
 &+ 2(2n-1)\sqrt{\Gamma(x)^2 + \Gamma(y)^2} \\
 &+ (n-2)\sqrt{\Gamma(x)^2 + \Gamma(y)^2} \\
 &= \sqrt{18}(n+4) + \sqrt{45}(2n-1) + \sqrt{72}(n-2).
 \end{aligned}$$

Next, we compute the topological indices of the ortho chain, shown in Fig. 2.

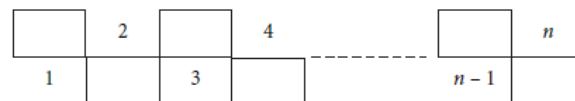


Figure 2: Ortho silicate

The edge partition for the ortho chain silicate structure is as follows:

- (i) $E_1 = \{xy \in E(G) : \Gamma(x) = \Gamma(y) = 2\}$
- (ii) $E_2 = \{xy \in E(G) : \Gamma(x) = 2, \Gamma(y) = 4\}$
- (iii) $E_3 = \{xy \in E(G) : \Gamma(x) = \Gamma(y) = 4\}$

Theorem 3.2: For the ortho chain silicate, the topological indices are:

- (i) $S_1(G) = 2(n+2) + 6n + 4(n-2)$
- (ii) $S_2(G) = 2(n+2) + 8n + 8(n-2)$
- (iii) $S_3(G) = 4(n+2) + 36n + 16(n-2)$
- (iv) $S_4(G) = \frac{1}{2}(n+2) + \frac{1}{2}n + \frac{1}{4}(n-2)$
- (v) $S_5(G) = (n+2) + \frac{8}{3}n + 2(n-2)$
- (vi) $S_6(G) = \frac{1}{2}(n+2) + \frac{2}{\sqrt{6}}n + 2(n-2)$
- (vii) $S_7(G) = \frac{1}{\sqrt{2}}(n+2) + \sqrt{2}n + \sqrt{\frac{3}{8}}(n-2)$
- (viii) $S_8(G) = \sqrt{8}(n+2) + \sqrt{20}n + \sqrt{32}(n-2)$

The proof of the Theorem 3.2 follows the same procedure of the proof of Theorem 3.1. The computed topological indices are plotted in the following graphs.

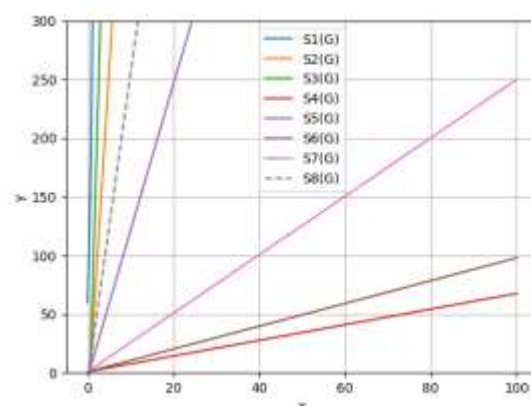


Figure 3: Topological Indices of Chain silicate

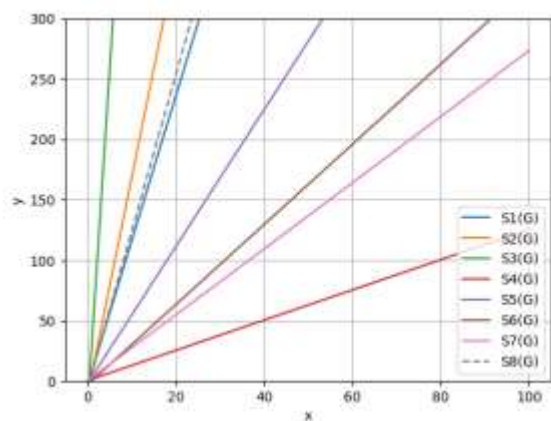


Figure 4: Topological Indices of Ortho silicate

4. CONCLUDING REMARKS

In this work, we computed various topological indices of chain silicate and ortho chain silicate structures. The computed indices are graphically visualized and are plotted. The computed topological indices have interconnections with various properties of the silicate structures. These numerical values may be used to investigate the physiochemical properties of the silicate structures.

Conflicts of Interest: The authors declare that they have no conflicts of interest regarding the publication of this article.

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