Research Article

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Computation of edge- and vertex-degree-based topological indices for tetrahedral sheets of clay minerals

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Abstract: In terms of soil conditions, clay minerals infrequently occur as homogenous mixtures of single constituents, gatherings, stages, or types of minerals. Rather, they contain intricate arrays of essential minerals and rippling intermediates of numerous basic and synergistic mixtures. There is also the possibility that a discrete mineral grain is composed of more than one clay type or has sections that are intermediate amongst two chosen minerals. Such minerals are alluded to as inter-stratified or mixed-layer minerals. The structures of clay minerals are the most researched compound in contemporary materials science. Tetrahedral sheets of clay minerals (TSCM) are one of the most well-known structures concentrated in materials science. QSPR/QSAR of the TSCM compounds requires articulations for the topological characteristic of these substances. Topological descriptors are indispensable gadgets for exploring chemical substances to understand the basic geography or physical properties of such chemical structures. In this article, we determine the edge-vertex-degree and vertex-edge-degree topological indices for TSCM.

Keywords: tetrahedral sheets of clay minerals, topological descriptors, complex chemical networks, edge-vertex-degree, vertex-edge-degree

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1 Introduction

Chemical graph theory aids the interpretation of a chemical graph's nuclear assistant properties. Chemical graph theory is expected to play an important role in showcasing and organizing any constructed framework or component organize out. A chemical compound or graph is a graphical portrayal that includes atoms called vertices and atom-to-atom bonds known as edges. The topological number is a quantitative assessment of molecular composition, whereas a topological index corresponds to specified chemical and physical properties of concealed chemical molecules that are not represented numerically.

Numerous complexes have almost the same molecular formula but have different structures; this is referred to as an isomer. Combinatorics and graph theory are much more appropriate scientific gadgets for contemplating the distinction between these isomers in mathematical branches that are firmly identified with one another. Such divisions are used to display the structures of chemical mixtures, investigating their chemical and physical properties. Throughout chemical graph theory, an atom is initiated as a vertex and the bonds between them are regarded as edges, and the developed illustration is referred to as a chemical graph. Chemical graph theory is an incredibly interesting branch of graph theory and has innumerable advancements in science, medicine architecture, and so on. The research work by Shao et al. (2017, 2018a) contains two examples of topological descriptors that have been studied in pharmaceutical research and theoretical science. In the concept of quantitative structure–property relationships (QSPR)/quantitative structure–activity relationships (QSAR), researchers are curious in comprehending a compound's network topology using certain numbers and boundaries derived given by the network's atomic structure.

Clay mineral structures are the most studied chemical substance in modern materials engineering. Probably, one of the best structures largely focused in materials science is the clay mineral sheet of tetrahedral. Clay minerals are versatile earth-rich ceramics with a variety of appealing properties and chemical stability under adverse conditions. Clay minerals are a collection of hydrous aluminosilicates that dominate the mud-measured (<2|xm) portion of soils. Such minerals are chemically and structurally similar to the essential minerals that originate in the Earth's crust; however, changes in the geometric arrangement of atoms and ions within their structures occur as a result of weathering. Indispensable minerals form at high temperatures and pressures and are typically formed from molten or trans-formative rocks (Barton, 2002).

All such minerals are relatively stable within the Earth, but alteration can occur when exposed to the bordering counties of the surface of the ground. While the safest chemical constituents (quartz, micas, and a few feldspars) can persist in soils, other less protected minerals (pyroxenes, amphiboles, and a large group of adornment minerals) are prone to disintegrate and erosional, resulting in the formation of ancillary minerals. The outcomes of entirely voluntary minerals are the culmination of either reconfiguration of the essential micronutrient framework (incongruent reaction) or neoformation via precipitation or recrystallization of fragmented individual components into a successively stable framework (congruent reaction). Such entirely voluntary minerals are frequently referred to as phyllosilicates even though, as the name implies (Greek: phyllon, leaf), leaf they have platy or flaky proclivity, and one of their primary core elements is an all-inclusive plate of SiO_4 tetrahedral (Barton, 2002).

Researchers defined the Harmonic index in the articles (Ediz, 2017; Zhong, 2012), and the majority of research is accomplished only using the conventional degree notion. Chellali et al. (2017) lately launched innovative degree notions, namely "vertex-edge-degree and edge-vertex-degree." The relationship between "classical degree-based" and "vertex-edge-degree and edge-vertex-degree" is shown by Horoldagva et al. (2019), Ediz (2018), Sahin and Ediz (2018), and Zhang et al. (2020), and it was discovered that the "vertex-edge-degree Zagreb index" has an instrumental growth than the "traditional Zagreb index."

2 Motivation and methodology

Topological descriptors play an important role in theoretical science. A topological descriptor, also known as a connectivity index throughout the areas of materials graph theory, is a type of molecular graph attribute that is determined by the chemical graph of a complex mixture. Generally, topological descriptors are distinguished by the use of vertex degree theory. Structural attributes have been used to comprehend and generate numerical attributes for real-world system models. Wiener (1947) presented the possibility of topological descriptors since attempting to reach the paraffin limit. As the first topological descriptor, he presented the Wiener descriptor. In scientific and chemical writing, the most commonly used topological descriptors are Zagreb, Randić, and Wiener descriptors (Ediz et al., 2017; Gutman and Trinajstic, 1972). Empowered by such considerations, we begin to investigate edge-vertex- and vertex-edge degree-based topological descriptors.

In this manuscript, we studied the structure of tetrahedral sheets of clay minerals (TSCM) and encountered the accurate value of vertex-edge and edge-vertex-degree-based topological properties for TSCM. Particularly, we determined the exact values of harmonic vertex-edge-degree index (H_{ve}), edge-vertex-degree Randić index, sum-connectivity vertex-edge-degree (X_{ve}) index, vertex-edge-degree Randić index, geometric-arithmetic vertex-edge-degree (GA_{ve}) index, atom-bond connectivity vertex-edge-degree (ABC_{ve}) index, first and second vertex-edge-degree Zagreb $\alpha(\beta)$ index, and Zagreb edge-vertex-degree index, for chemical structure of TSCM. For the basics of all these definitions in related literature, see studies by Ahmad (2018), Anjum and Safdar (2019), Gao et al. (2018), Shao et al. (2018a, 2018b), Siddiqui et al. (2016), Shao et al. (2019), and Raza et al. (2021).

The methodology of this article is as follows: first, we explain the topological indices, clay minerals, and their importance and applications. Second, we study the structure of TSCM. Third, we determine the vertex-edge- and edge-vertex degree-based topological descriptor and its numeric numbers. Then, we discuss the analogies of our computed theorems for TSCM, and finally, we give the closing remarks.

3 Definitions and results

"Let E and V be the edge set and vertex set of a connected graph $G = (V, E)$. The degree of a vertex x_1, denoted by $\xi(x_1)$, is the number of edges that are incident to x_1. The open neighborhood of a vertex x_1, denoted by $N(x_1)$, is the number of all vertices adjacent to x_1. The closed neighborhood of x_1, denoted by $N[x_1]$, is the union of x_1 and $N(x_1)$. The edge-vertex-degree, denoted by $\xi_{ev}(e)$, of any edge $e = x_1x_2 \in E$ is the total number of vertices of the closed neighborhoods union of x_1 and x_2. The vertex-edge-degree, denoted by $\xi_{ve}(x_1)$, of any vertex $x_1 \in V$ is

Table 1: The topological descriptors of vertex-edge-degree and edge-vertex-degree indices

$X_{ve}(G) = \sum_{x_1x_2 \in E}(\xi_{ve}(x_1) + \xi_{ve}(x_2))^{-\frac{1}{2}}$	Sum-connectivity vertex-edge-degree index
$H_{ve}(G) = \sum_{x_1x_2 \in E}\frac{2}{\xi_{ve}(x_1) + \xi_{ve}(x_2)}$	Harmonic index of vertex-edge-degree
$GA_{ve}(G) = \sum_{x_1x_2 \in E}\frac{2(\xi_{ve}(x_1) \times \xi_{ve}(x_2))^{\frac{1}{2}}}{\xi_{ve}(x_1) + \xi_{ve}(x_2)}$	Geometric–arithmetic vertex-edge-degree index
$ABC_{ve}(G) = \sum_{x_1x_2 \in E}\left(\frac{\xi_{ve}(x_1) + \xi_{ve}(x_2) - 2}{\xi_{ve}(x_1) \times \xi_{ve}(x_2)}\right)^{\frac{1}{2}}$	Atom–bond connectivity vertex-edge-degree index
$R_{ev}(G) = \sum_{e_1 \in E}(\xi_{ve}e_1)^{-\frac{1}{2}}$	Randić edge-vertex-degree index
$R_{ve}(G) = \sum_{x_1x_2 \in E}(\xi_{ve}(x_1) \times \xi_{ve}(x_2))^{-\frac{1}{2}}$	Randić vertex-edge-degree index
$M_{ve}^{2}(G) = \sum_{x_1x_2 \in E}(\xi_{ve}(x_1) \times \xi_{ve}(x_2))$	Second Zagreb vertex-edge-degree index
$M_{\beta ve}^{1}(G) = \sum_{x_1x_2 \in E}(\xi_{ve}(x_1) + \xi_{ve}(x_2))$	First Zagreb β vertex-edge-degree index
$M_{\alpha ve}^{1}(G) = \sum_{x_1 \in V}(\xi_{ve}x_1)^2$	First Zagreb α vertex-edge-degree index
$M_{ev}(G) = \sum_{e_1 \in E}(\xi_{ev}e_1)^2$	ZAGREB edge-vertex-degree index

the number of different edges that are incident to any vertex from the closed neighborhood of x_1." Chellali et al. (2017), Ediz (2018), Horoldagva et al. (2019), and Sahin and Ediz (2018) studied some vertex- and edge-degree-based topological descriptors which are available in the main body of our draft, particularly shown in Table 1. Furthermore, the basic definitions are also available in these basic research articles.

4 Structure of TSCM

The properties that decide the formation of a mineral are derived from its chemical foundation, geometric arrangement of atoms and ions, and the electrical powers that dilemma them together. Silicon will quite often be found in geochemical arrangements since silicate minerals are so universal. Underneath the pH of 9 or 10, most solvent silicon is found as silicic acid, $Si(OH)_4$ (Figure 1).

In whatsoever scenario, the phyllosilicate structure's predominance of silicon and oxygen is logical. All silicate structures are found on the SiC > 4 tetrahedron. It has four O_2 particles at the apexes of a conventional tetrahedron facilitated by one Si^{4+} particle in the middle (Figure 1). A hexagonal system called the tetrahedral sheet is formed by an interlocking array of these tetrahedral associated at three corners in a similar plane by shared oxygen anions. Figure 2 depicts the clay mineral sheet of tetrahedral $TSCM_{p,q}$ for $p = 2$ and $q = 2$.

The graph $TSCM_{p,q}$ contains $10pq + 7p + q$ vertices and $24pq + 12p$ edges. The vertex partitions of $TSCM_{p,q}$ are $V_3 = \{x_1 \in V(TSCM_{p,q}) : \xi(x_1) = 3\}$ and $V_6 = \{x_1 \in V(TSCM_{p,q}) : \xi(x_1) = 6\}$ with $|V_3| = 4pq + 6p + 2q$ and $|V_6| = 6pq + p - q$. The edge partitions based on the degree of vertices are $E_{3,3} = \{x_1x_2 \in E(TSCM_{p,q}) : \xi(x_1) = 3, \xi(x_2) = 3\}$, $E_{3,6} = \{x_1x_2 \in E(TSCM_{p,q}) : \xi(x_1) = 3, \xi(x_2) = 6\}$, and $E_{6,6} = \{x_1x_2 \in E(TSCM_{p,q}) : \xi(x_1) = 6, \xi(x_2) = 6\}$ with $|E_{3,3}| = 4p + 2q$, $|E_{3,6}| = 12pq + 10p + 2q$ and $|E_{6,6}| = 12pq - 2p - 4q$. The topological number is calculated for $TSCM_{p,q}$, which are defined above.

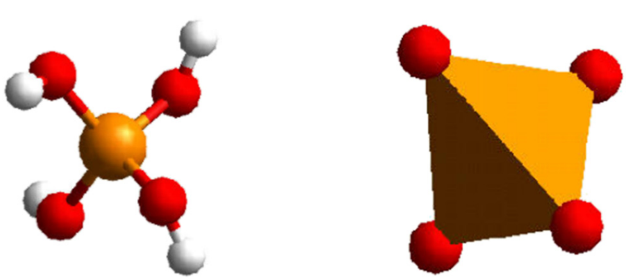

Figure 1: Tetrahedron.

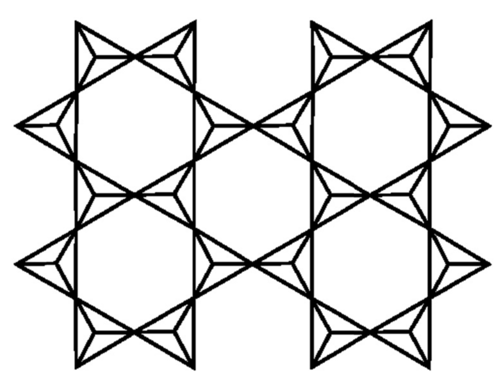

Figure 2: A clay mineral's sheet of tetrahedral for $p = q = 2$.

Table 2: Edge-vertex-degree of $TSCM_{p,q}$

$(\xi(x_1), \xi(x_2))$	Edge-vertex-degree	Frequency
(3, 3)	6	$4p + 2q$
(3, 6)	9	$12pq + 10p + 2q$
(6, 6)	12	$12pq - 2p - 4q$

5 Main results

This section contains the main results we determined. Particularly, harmonic vertex-edge-degree index (H_{ve}), sum-connectivity vertex-edge-degree (X_{ve}) index, Randić vertex-edge-degree and edge-vertex-degree index, geometric–arithmetic vertex-edge-degree (GA_{ve}) index, atom–bond connectivity vertex-edge-degree (ABC_{ve}) index, second Zagreb vertex-edge-degree β index, first Zagreb vertex-edge-degree $\alpha(\beta)$ index, and the Zagreb edge-vertex-degree index for $\mathrm{TSCM}_{p,q}$.

5.1 The edge-vertex-degree Zagreb index

Using Table 2 in $M_{ev}(\mathrm{TSCM}_{p,q}) = \sum_{e_1 \in E}(\xi_{ev}(e_1)^2$, we obtain the Zagreb edge-vertex-degree index:

$$M_{ev}(\mathrm{TSCM}_{p,q}) = 2700pq + 666p - 342q$$

5.2 The first vertex-edge-degree Zagreb α index

We compute the first vertex-edge-degree Zagreb α index using the values from Table 3 in the equation $M^1_{\alpha\mathrm{ve}}(\mathrm{TSCM}_{p,q}) = \sum_{x_1 \in V}(\xi_{ve}(x_1)^2$. After simplification, we obtain:

$$M^1_{\alpha ve}(\mathrm{TSCM}_{p,q}) = 6696pq + 720p - 1332q + 72$$

5.3 The first vertex-edge-degree Zagreb β index

Using the values from Table 4 in the equation $M^1_{\beta\mathrm{ve}}(\mathrm{TSCM}_{p,q}) = \sum_{x_1x_2 \in E}(\xi_{\mathrm{ve}}(x_1) + \xi_{\mathrm{ve}}(x_2))$, after simple calculation, we obtain the first vertex-edge-degree Zagreb β index as follows:

$$M^1_{\beta ve}(\mathrm{TSCM}_{p,q}) = 1296pq + 288p - 180q$$

Table 3: Edge-vertex-degree of $TSCM_{p,q}$

$\xi(x_1)$	Vertex-edge-degree	Frequency
3	15	$8p + 4q$
3	18	$4pq - 2p - 2q$
6	24	$2p + 4$
6	27	$4q - 8 + 4p$
6	30	$4 - 5q - 5p + 6pq$

Table 4: The $\mathrm{TSCM}_{p,q}$ structure edge's end vertices vertex-edge-degrees

$(\xi(x_1), \xi(x_2))$	Vertex-edge-degree	Frequency
(3, 3)	(15, 15)	$4p + 2q$
(3, 6)	(15, 24)	$8p + 16$
(3, 6)	(15, 27)	$8p + 8q - 16$
(3, 6)	(18, 27)	$4p + 4q - 8$
(3, 6)	(18, 30)	$12pq - 10p - 10q + 8$
(6, 6)	(24, 24)	4
(6, 6)	(24, 27)	$4p$
(6, 6)	(27, 27)	$4q - 6$
(6, 6)	(27, 30)	$8p + 4q - 12$
(6, 6)	(30, 30)	$12pq - 14p - 12q + 14$

5.4 The second vertex-edge-degree Zagreb index

We obtain the second vertex-edge-degree Zagreb index using the values from Table 4 in the equation $M^2_{\mathrm{ve}}(\mathrm{TSCM}_{p,q}) = \sum_{x_1x_2 \in E}(\xi_{\mathrm{ve}}(x_1) \times \xi_{\mathrm{ve}}(x_2))$. After simplification, it is as follows:

$$M^2_{ve}(\mathrm{TSCM}_{p,q}) = 17280pq + 36p - 4410q + 522$$

5.5 The vertex-edge-degree Randić index

We acquire the vertex-edge-degree Randić index by using the values from Table 4 in the formula $R_{\mathrm{ve}}(\mathrm{TSCM}_{p,q}) = \sum_{x_1x_2 \in E}(\xi_{\mathrm{ve}}(x_1) \times \xi_{\mathrm{ve}}(x_2))^{-\frac{1}{2}}$. After simplification, it is as follows:

$$\begin{aligned} R_{\mathrm{ve}}(\mathrm{TSCM}_{p,q}) = {} & \left(\frac{2\sqrt{15} + 6}{15}\right)pq \\ & + \left(\frac{24\sqrt{5} - 15\sqrt{15} + 10\sqrt{6} + 6\sqrt{10} - 16}{135}\right)q \\ & + \left(\frac{30\sqrt{10} + 24\sqrt{5} + 10\sqrt{6} - 9\sqrt{15} + 15\sqrt{2} - 27}{135}\right)p \end{aligned}$$

Table 5: Numerical results for the Sections 5.1 to 5.5.

(p, q)	M_{ev}	$M^1_{\alpha ve}$	$M^1_{\beta ve}$	M^2_{ve}	R_{ve}
(2, 2)	11448	25632	5400	60894	5.9682
(3, 3)	25272	58500	11988	142920	11.701
(4, 4)	44496	104760	21168	259506	19.267
(5, 5)	69120	164412	32940	410652	28.666
(6, 6)	99144	237456	47304	596358	39.898
(7, 7)	134568	323892	64260	816624	52.962
(8, 8)	175392	423720	83808	1071450	67.859
(9, 9)	221616	536940	105948	1360836	84.590
(10, 10)	273240	663552	130680	1684782	103.15

Table 6: Numerical results for the Sections 5.6 to 5.10.

(p, q)	R_{ev}	ABC_{ve}	GA_{ve}	H_{ve}	χ_{ve}
(2, 2)	39.292	36.100	117.77	5.5340	18.135
(3, 3)	81.330	73.788	247.44	10.988	37.030
(4, 4)	138.30	124.58	424.34	18.242	62.489
(5, 5)	210.19	188.47	648.47	27.295	94.508
(6, 6)	297.02	265.46	919.85	38.149	133.09
(7, 7)	398.77	355.52	1238.5	50.803	178.23
(8, 8)	515.45	458.69	1604.31	65.257	229.95
(9, 9)	647.06	574.97	2017.4	81.510	288.20
(10, 10)	793.60	704.35	2477.7	99.564	353.04

5.6 The edge-vertex-degree Randić index

Using Table 2 in the equation $R_{ev}((\text{TSCM}_{p,q})) = \sum_{e_1\in E}(\xi_{ve}(e_1))^{-\frac{1}{2}}$, we compute the edge-vertex-degree Randić index as follows:

$$R_{ev}(\text{TSCM}_{p,q}) = (4 + 2\sqrt{3})pq + \left(\frac{2\sqrt{6} - \sqrt{3} + 10}{3}\right)p + \left(\frac{\sqrt{6} - 2\sqrt{3} + 2}{3}\right)q$$

5.7 The vertex-edge-degree atom–bond connectivity index

Using values from Table 4 in the equation $ABC_{\text{ve}}(\text{TSCM}_{p,q}) = \sum_{x_1x_2\in E}\left(\frac{\xi_{\text{ve}}(x_1)+\xi_{\text{ve}}(x_2)-2}{\xi_{\text{ve}}(x_1)\times\xi_{\text{ve}}(x_2)}\right)^{\frac{1}{2}}$, after simple calculation, we compute the vertex-edge-degree atom–bond connectivity index as follows:

$$\begin{aligned}ABC_{\text{ve}}(\text{TSCM}_{p,q}) &= \left(\frac{2\sqrt{690}}{15} + \frac{2\sqrt{58}}{5}\right)pq \\ &+ \left(\frac{23}{9}\sqrt{2} + \frac{2\sqrt{370}}{15} - \frac{\sqrt{690}}{9} + \frac{2}{27}\sqrt{258} + \frac{8}{15}\sqrt{7} + \frac{4\sqrt{22}}{9} - \frac{7}{15}\sqrt{58}\right)p \\ &+ \left(\frac{-2\sqrt{58}}{5} + \frac{16}{9}\sqrt{2} + \frac{4}{15}\sqrt{7} + \frac{2}{27}\sqrt{258} + \frac{8}{27}\sqrt{13} - \frac{\sqrt{690}}{9}\right)q \\ &+ \frac{7}{15}\sqrt{58} - \frac{4\sqrt{13}}{9} - \frac{32}{9}\sqrt{2} + \frac{4}{15}\sqrt{370} - \frac{4}{27}\sqrt{258} + \frac{4}{45}\sqrt{690}\end{aligned}$$

5.8 The geometric–arithmetic vertex-edge-degree index

We obtain the vertex-edge-degree geometric–arithmetic index using values from Table 4 in the equation $GA_{\text{ve}}(\text{TSCM}_{p,q}) = \sum_{x_1x_2\in E}\frac{2(\xi_{\text{ve}}(x_1)\times\xi_{\text{ve}}(x_2))^{\frac{1}{2}}}{\xi_{\text{ve}}(x_1)+\xi_{\text{ve}}(x_2)}$. It is as follows:

$$\begin{aligned}GA_{ve}(\text{TSCM}_{p,q}) &= (3\sqrt{15} + 12)pq \\ &+ \left(\frac{24}{7}\sqrt{5} - 5/2\sqrt{15} + 8/5\sqrt{6} + \frac{24}{19}\sqrt{10} - 6\right)q \\ &+ \left(\frac{1232}{247}\sqrt{10} + \frac{24}{7}\sqrt{5} + 8/5\sqrt{6} - 5/2\sqrt{15} + \frac{48}{17}\sqrt{2} - 10\right) \\ &p - \frac{48}{7}\sqrt{5} - \frac{16}{5}\sqrt{6} + \frac{280}{247}\sqrt{10} + 2\sqrt{15} + 12\end{aligned}$$

5.9 The vertex-edge-degree harmonic index

We obtain the vertex-edge-degree harmonic index using values from Table 4 in the equation $H_{\text{ve}}(\text{TSCM}_{p,q}) = \sum_{x_1x_2\in E}\frac{2}{\xi_{\text{ve}}(x_1)+\xi_{\text{ve}}(x_2)}$. It is as follows:

$$H_{\text{ve}}(\text{TSCM}_{p,q}) = \frac{9}{10}pq + \frac{4179073}{5290740}p + \frac{11771}{71820}q + \frac{823}{31122}$$

5.10 The sum-connectivity vertex-edge-degree index

We obtain the vertex-edge-degree sum-connectivity index using the values from Table 4 in the equation $\chi_{\text{ve}}(\text{TSCM}_{p,q}) = \sum_{x_1x_2\in E}(\xi_{ve}(x_1) + \xi_{ve}(x_2))^{-\frac{1}{2}}$. It is as follows:

$$\begin{aligned}\chi_{\text{ve}}(\text{TSCM}_{p,q}) &= \left(\sqrt{3} + \frac{2\sqrt{15}}{5}\right)pq \\ &+ \left(\frac{4}{21}\sqrt{42} + \frac{8}{39}\sqrt{39} - \frac{5\sqrt{3}}{6} + \frac{4}{15}\sqrt{5} + \frac{4}{51}\sqrt{51} + \frac{2\sqrt{30}}{15} + \frac{8}{57}\sqrt{57} - \frac{7}{15}\sqrt{15}\right)p \\ &+ \left(\frac{-2\sqrt{15}}{5} + \frac{4}{21}\sqrt{42} + \frac{\sqrt{30}}{15} + \frac{4}{15}\sqrt{5} + \frac{2\sqrt{6}}{9} - \frac{5\sqrt{3}}{6}\right)q \\ &+ \frac{7}{15}\sqrt{15} - 1/3\sqrt{6} - \frac{8}{21}\sqrt{42} + \frac{16}{39}\sqrt{39} - \frac{8}{15}\sqrt{5} + 2/3\sqrt{3}\end{aligned}$$

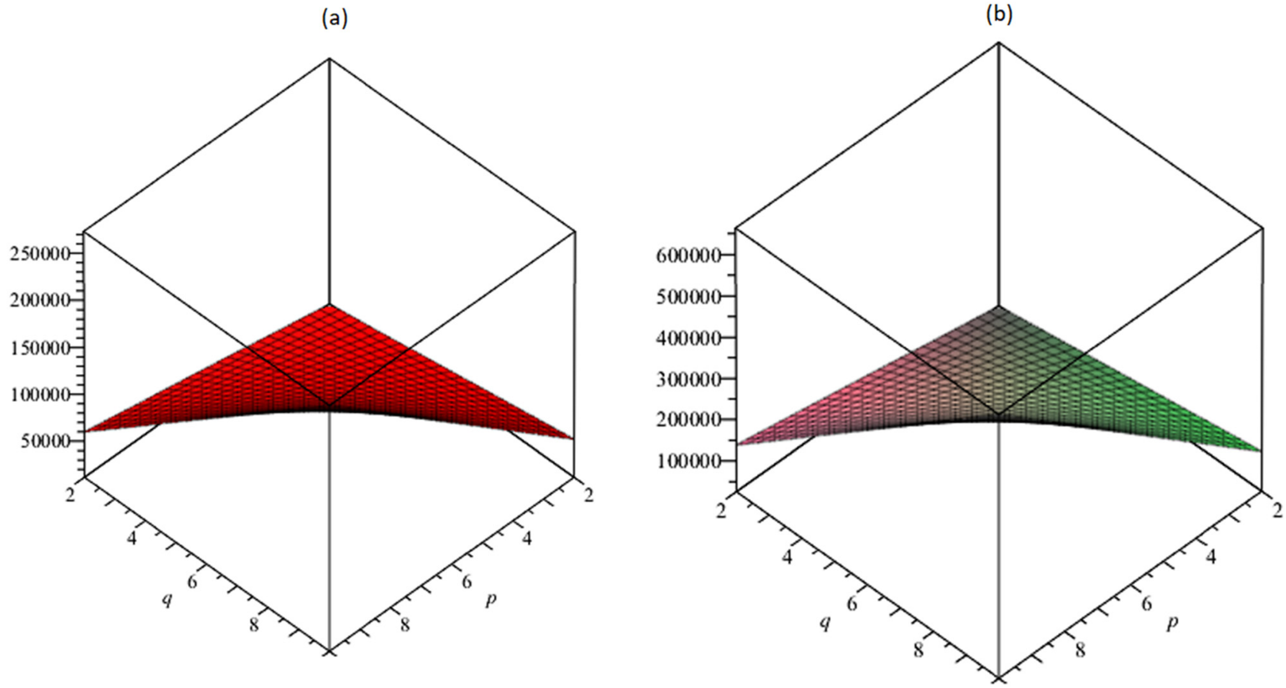

Figure 3: (a) The edge-vertex-degree Zagreb index M_{ev}; (b) the first vertex-edge-degree Zagreb α index $M^1_{\alpha ve}$.

6 Numerical results and discussion of TSCM

In this section, we deliver quantitative examples for the edge-vertex-degree and vertex-edge-degree topological properties of TSCM. We acquired numerical valued tables utilizing various scores of p and q, for all the topological descriptors computed above in our main results section, for the TSCM (Tables 5 and 6).

Furthermore, in Figures 3–7, based on the aforementioned numerical computation, we created the graphical depiction for the TSCM to study the behavior of the above-resulted topological descriptors.

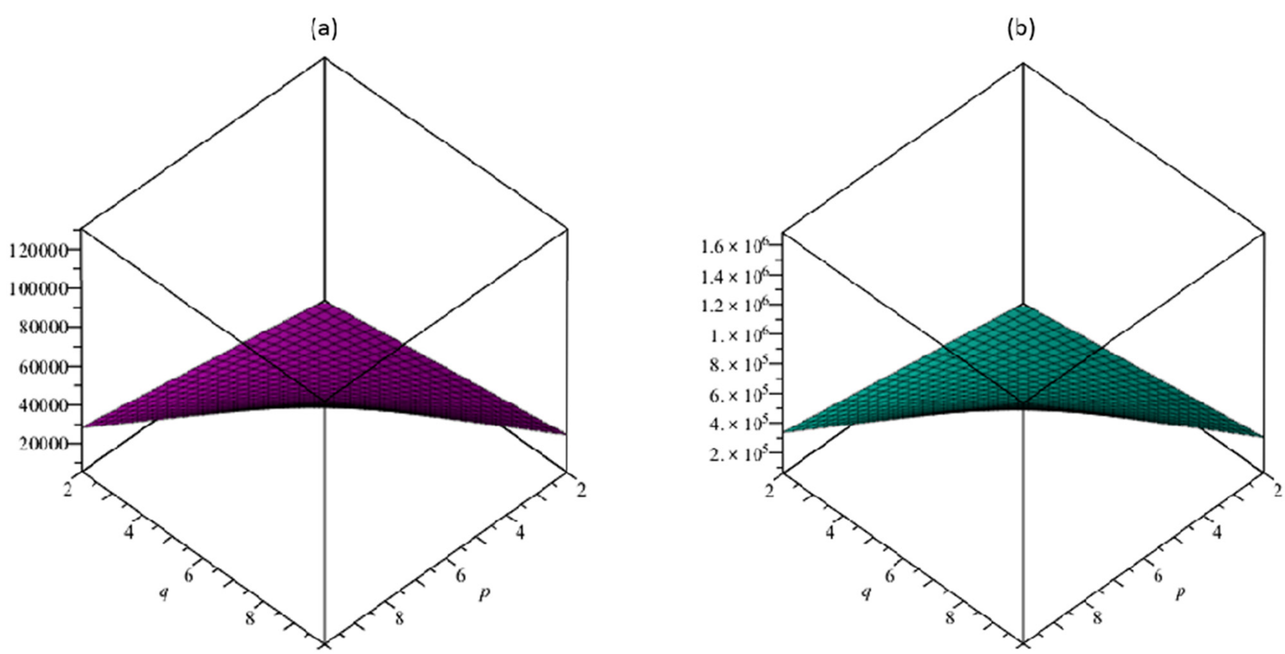

Figure 4: (a) The first vertex-edge-degree Zagreb β index $M^1_{\beta ve}$; (b) the second vertex-edge-degree Zagreb index M^2_{ve}.

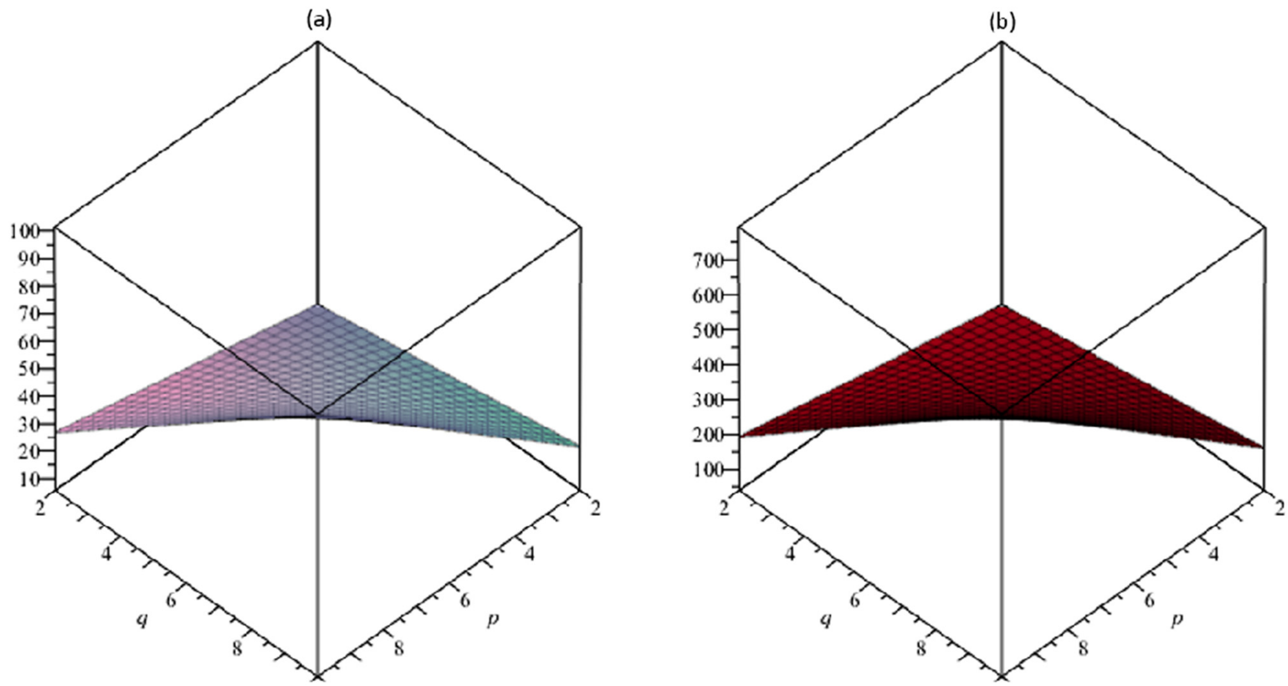

Figure 5: (a) The vertex-edge-degree Randić index R_{ve}; (b) the edge-vertex-degree Randić index R_{ev}.

The resulting topological descriptors for the $TSCM_{p,q}$ increment as p and q rise as shown in Tables 5 and 6 and Figures 3–7.

Throughout the evaluation of the overall π-electron energy of molecules given by Gutman et al. (1975), Zagreb descriptors are implemented, and it is proved that boosting the attributes of p and q rises the total π-electron energy for $TSCM_{p,q}$.

According to the research of isomer chemical compounds (Liu et al., 2019), automatic decision-making,

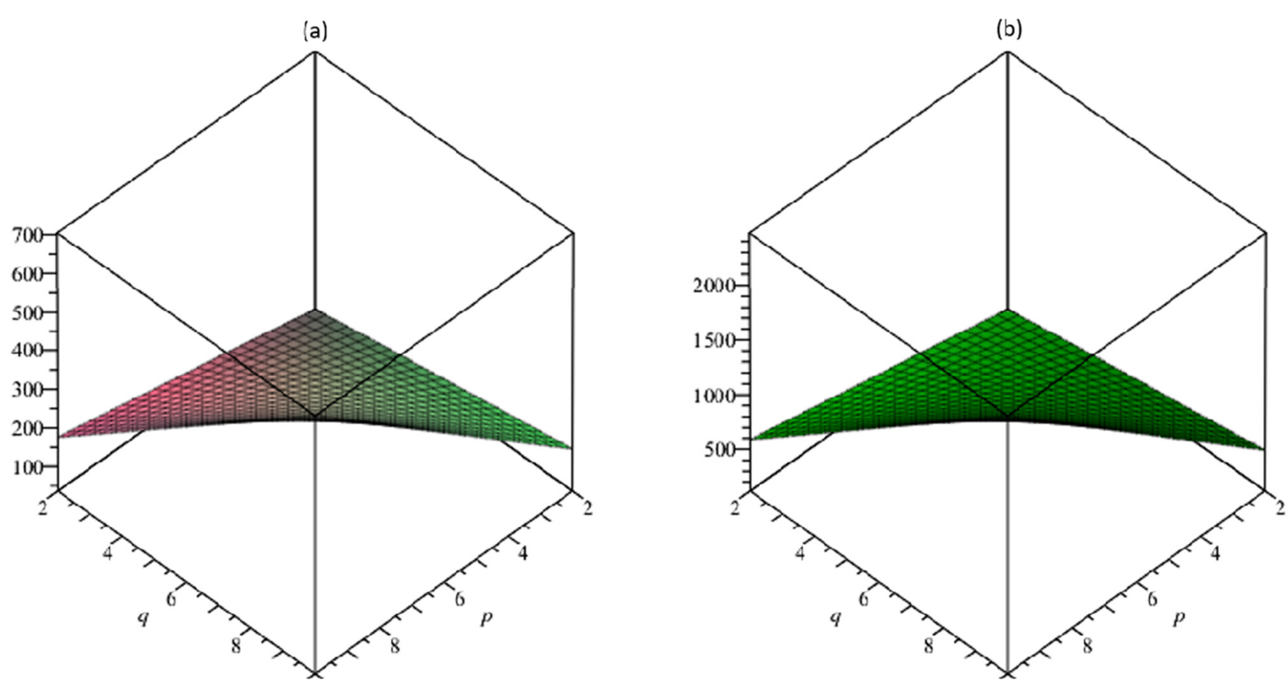

Figure 6: (a) The vertex-edge-degree atom–bond connectivity index ABC_{ve}, (b) the geometric–arithmetic vertex-edge-degree index GA_{ve}.

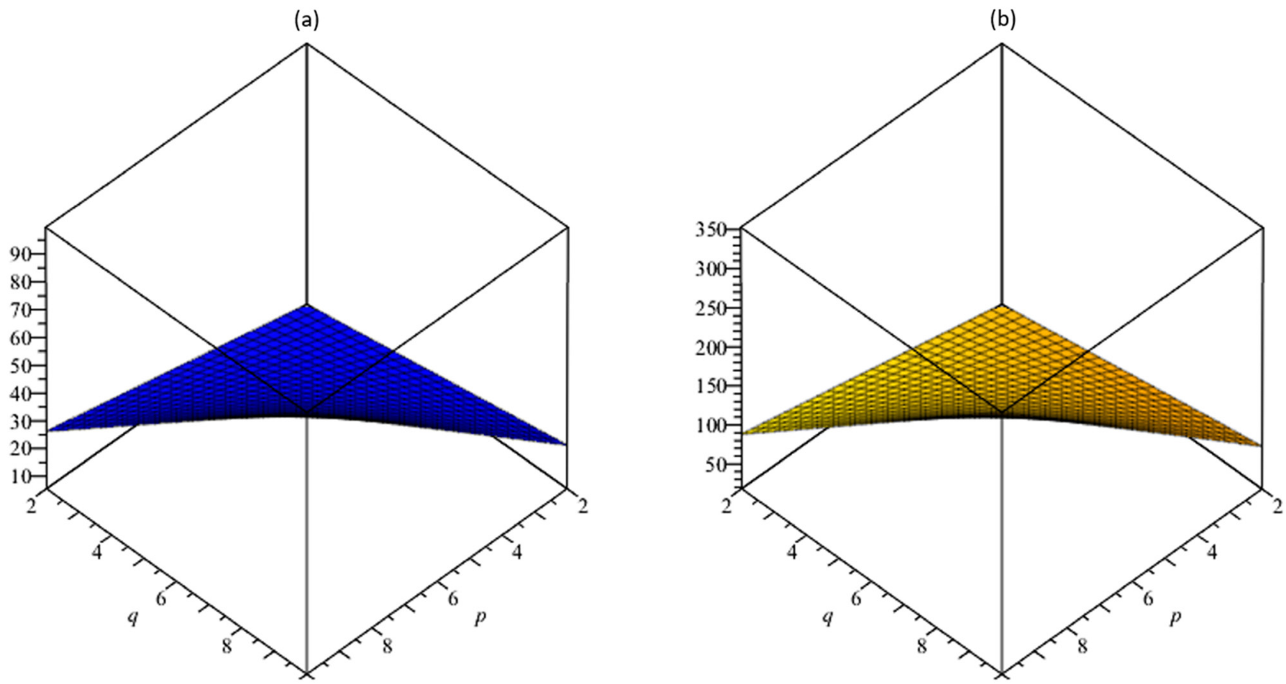

Figure 7: (a) The vertex-edge-degree harmonic index H_{ve}; (b) the sum-connectivity vertex-edge-degree index χ_{ve}.

computation of Kovats constants, and boiling point of molecules, the Randić descriptor is used. It can be observed that raising the quantities of p and q increases the quantities of the Randić characteristics for $TSCM_{p,q}$.

The geometric–arithmetic descriptor outperforms the connectivity descriptor in terms of prediction power, and it is observed that the values of the GA descriptor increase for $TSCM_{p,q}$ as p and q increase.

The stability of linear and branched alkanes given in the research by Gao et al. (2017), also the strain energy of cycloalkanes, comparative to our computational ABC descriptor, provides a very good correlation. The ABC descriptor is increased for the underlying graph $TSCM_{p,q}$ with the increment of p and q.

7 Conclusion

Understanding the underlying topologies of graphs and networks requires the study of topological descriptors. Such studies have a wide spectrum of uses in the fields of cheminformatics, bioinformatics, and biomedicine, where various graph invariant-based assessments are used to deal with a variety of difficult strategies. Graph invariants are important tools for approximating and predicting the properties of biological and chemical compounds in the analysis of QSPRs/ and QSARs.

Rather, more importantly, we have indeed quantified results in this article for the edge-vertex-degree and vertex-edge-degree topological descriptors, namely, sum-connectivity vertex-edge-degree (X_{ve}), vertex-edge-degree harmonic (H_{ve}) index, geometric–arithmetic vertex-edge-degree (GA_{ve}) index, atom–bond connectivity vertex-edge-degree (ABC_{ve}) index, edge-vertex-degree Randić index, vertex-edge-degree Randić index, the second vertex-edge-degree Zagreb index, first vertex-edge-degree Zagreb β index, first vertex-edge-degree Zagreb α index, and Zagreb edge-vertex-degree index, for the TSCM.

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