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CHEMICAL APPLICABILITY OF SECOND ORDER SOMBOR INDEX

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Abstract. In this paper, we introduce the higher-order Sombor index of a molecular graph. In addtition, we compute the second order Sombor index of some standard class of graphs and line graph of subdivision graph of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ and also we obtain the expressions of the second order Sombor index of the line graph of subdivision graph of tadpole graph, wheel graph, ladder graph and chain silicate network CS_n. Further, we study the linear regression analysis of the second order Sombor index with the entropy, acentric factor, enthalpy of vaporization and standard enthalpy of vaporization of an octane isomers.

Key words and Phrases: Topological indices, line graph, subdivision graph, nanostructure, tadpole graph.

1. Introduction and Preliminaries

A topological index is a molecular descriptor that is calculated based on the molecular graph of a chemical compound. Chemical graph theory is a branch of mathematical chemistry, which has an major effect on the development of the chemical sciences. In molecular graph, graph is used to represent a molecule by considering the atoms as the vertices and molecular bonds as the edges. A graphical invariant is a number related to a graph. In other words, it is a fixed number under graph automorphisms. In chemical graph theory, these invariants are also called the topological indices. There are several topological indices available today, some of which are used in chemistry. Chemical Data Bases have registered over 3000 topological graph indices. Chemists and mathematicians both investigate this topic. Two-dimensional topological indices have been a successful method in recent years for the discovery of several novel medications, including anticonvulsants, anineoplastics, antimalarials, antiallergics, and silico generation [14, 16]. The use of topological indices and quantitative structure-activity relationships (QSAR) has

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therefore demonstrated that they have evolved from being a promising potential to serving as a cornerstone in the process of drug development and other research fields [10, 11, 12].

Most crucially, three-dimensional molecular characteristics (topographic indices) and molecular chirality are also provided with the further research of chemical indices and drug design and discovery [26]. Studying three-dimensional quantitative structure-activity relationships, such as molecular chirality, is becoming more and more important. Nevertheless, there have only been a few outcomes thus far, with the exception of one related term that is commonly cited in [7]. Boiling points, solubilities, densities, anaesthetics, narcotics, toxicities, resistance etc. are just a few examples of the impressive range of physical, chemical, and biological properties to which higher order topological indices have been successfully applied. These results have been published in more than two books and several hundred scientific journals [14, 15]. The literature has revealed findings about these indices mathematical properties [1, 21].

Let $G = (V, E)$ be such graph with V as vertex set and E as edge set and $|V| = n, |E| = m$. The *degree* $d_G(v)$ of a vertex $v \in V(G)$ is the number of edges incident to it in G. Li and Zhao introduced the first general Zagreb index [17] as follows

$$M_\alpha(G) = \sum_{u \in V(G)} (d_u)^\alpha.$$

The connectivity index (or Randić index) of a graph G , denoted by $\chi(G)$, was introduced by Randić [22] in the study of branching properties of alkanes. It is defined as

$$\chi_\alpha(G) = \sum_{uv \in E_1(G)} \frac{1}{\sqrt{d_G(u) \cdot d_G(v)}}. \tag{1.1}$$

In [14, 13] with the intention of extending the applicability of the connectivity index, Kier, Hall, Murray and Randić considered the higher-order connectivity index of a graph G as

$$^{\alpha}\chi(G) = \sum_{u_1 u_2 \cdots u_{\alpha+1} \in E_\alpha(G)} \frac{1}{\sqrt{d_G(u_1) d_G(u_2) \cdots d_G(u_{\alpha+1})}}. \tag{1.2}$$

The first and second Zagreb [8] indices of a graph G are defined as

$$M_1(G) = \sum_{v \in v(G)} d_G(v)^2,$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_G(u) \cdot d_G(v).$$

The first Zagreb index [18] can be written also as

$$M_1(G) = \sum_{uv \in E(G)} d_G(u) + d_G(v). \tag{1.3}$$

B. Basavanagoud et. al. [3] considered higher-order first Zagreb index as

$$ {}^{\alpha}M_1(G) \quad = \sum_{u_1u_2\cdots u_{\alpha+1}\in E_\alpha(G)} [d_G(u_1)+d_G(u_2)\cdots d_G(u_{\alpha+1})]. \qquad (1.4) $$

B. Basavanagoud et. al. [3] defined the second order first Zagreb index as

$$ {}^{2}M_1(G) \quad = \sum_{u_1u_2u_3\in E_\alpha(G)} [d_G(u_1)+d_G(u_2)+d_G(u_3)]. \qquad (1.5) $$

The Sombor index was introduced by I. Gutman [9] to be described as

$$ SO(G) \quad = \sum_{uv\in E(G)} \sqrt{d_G(u)^2+d_G(v)^2}. \qquad (1.6) $$

Bearing in mind Eqs. (1.1), (1.2), (1.3), (1.4) and (1.5), we can consider the higher-order Sombor index of Eq. (1.6) as

$$ {}^{\alpha}SO(G) \quad = \sum_{u_1u_2\cdots u_{\alpha+1}\in E_\alpha(G)} \sqrt{d_G(u_1)^2+d_G(u_2)^2\cdots d_G(u_{\alpha+1})^2}. \qquad (1.7) $$

Here, $E_\alpha(G)$ denote the path of length α in a graph G, for example $E_1(G)$ and $E_2(G)$ are path of length 1 and 2 in a graph G respectively.
By Eq. (1.7), it is consistent to define the second order Sombor index as

$$ {}^{2}SO(G) \quad = \sum_{u_1u_2u_3\in E_2(G)} \sqrt{d_G(u_1)^2+d_G(u_2)^2+d_G(u_3)^2}. \qquad (1.8) $$

2. Estimating the second order Sombor index of graphs

In this section, we compute the second order Sombor index of some standard class of graphs viz., path graph P_n, wheel graph W_{n+1}, complete bipartite graph $K_{r,s}$ and $r-regular$ graph. The following Remark, which is needed to prove main results.

Remark 2.1. [4] *For a graph G on m edges, the number of paths of length 2 in G is $-m+\frac{1}{2}M_1(G)$.*

Theorem 2.1. *Let P_n be the path graph on $n\geq 4$ vertices. Then*

$$ {}^{2}SO(P_n) = 2(3+(n-4)\sqrt{3}). $$

Proof. For a path graph P_n on $n\geq 4$ vertices each vertex is of degree either 1 or 2. Based on the degree of vertices on the path of length 2 in P_n we can partition $E_2(P_n)$. In P_n, path $(1,2,2)$ appears 2 times and path $(2,2,2)$ appears $(n-4)$ times. Hence by Eq. (1.8) we get the required result. □

Theorem 2.2. *Let W_{n+1} be the wheel graph $n\geq 4$ vertices. Then*

$$ {}^{2}SO(W_{n+1}) = n3\sqrt{3} + \frac{n^2+3n(\sqrt{n^2+18})}{2}. $$

Proof. For a wheel graph W_{n+1} on $n \geq 4$ vertices each vertex is of degree either 3 or n. Based on the degree of vertices on the path of length 2 in W_{n+1} we can partition $E_2(W_n)$. In W_{n+1}, path $(3,3,3)$ appears n times and path $(3,3,n)$ appears $\frac{n^2+3n}{2}$ times. Therefore by Eq. (1.8), we get the required result. □

Theorem 2.3. *Let $K_{r,s}$ be the complete bipartite graph on $r \geq 2, s \geq 3$, vertices. Then*

$$^2SO(K_{r,s}) = \frac{rs(s-1)}{2}\sqrt{2r^2+s^2} + \frac{sr(r-1)}{2}\sqrt{2s^2+r^2}.$$

Proof. For a complete bipartite graph $K_{r,s}$ with $r+s$ vertices each vertex is of degree either r or s. Based on the degree of vertices on the path of length 2 in $K_{r,s}$ we can partition $E_2(K_{r,s})$. In $K_{r,s}$, path (r,s,r) appears $r\binom{s}{2}$ times and path (s,r,s) appears $s\binom{r}{2}$ times. Therefore by Eq. (1.8), we get the required result. □

Theorem 2.4. *Let G be a $r-regular$ graph on n vertices*

$$^2SO(G) = \frac{nr^2\sqrt{3}(r-1)}{2}.$$

Proof. Since G is a $r-regular$ graph, the path appears $\frac{nr(r-1)}{2}$ times in G. Therefore by Eq. (1.8), we get the required result. □

Corollary 2.5. *For a cycle graph C_n, $n \geq 3$,*

$$^2SO(C_n) = 2n\sqrt{3}.$$

Corollary 2.6. *For a complete graph K_n, $n \geq 4$,*

$$^2SO(K_n) = \frac{n\sqrt{3}(n-2)(n-1)^2}{2}.$$

Lemma 2.7. [5] *Let G be a graph with n vertices and m edges. Then*

$$M_1(G) \quad \leq \quad m\left(\frac{2m}{n-1}+n-2\right). \tag{2.1}$$

Lemma 2.8. [6] *Let G be a graph with n vertices and m edges, $m > 0$. Then the equality*

$$M_1(G) = m\left(\frac{2m}{n-1}+n-2\right).$$

holds if and only if G is isomorphic to star graph S_n or K_n or $K_{n-1} \cup K_1$.

Theorem 2.9. *Let G be a graph with n vertices and m edges. Then*

$$^2SO(G) \quad \leq \quad (n-1)\sqrt{3} \cdot m\left(\frac{m}{n-1}+\frac{n-4}{2}\right). \tag{2.2}$$

the equality holds if and only if G is isomorphic to K_n.

Proof.

$$
\begin{aligned}
{}^2SO(G) &= \sum_{uvw\in E_2(G)} \sqrt{d_G(u)^2+d_G(v)^2+d_G(w)^2} \\
&\leq \sum_{uvw\in E_2(G)} (n-1)\sqrt{3} \qquad (2.3)\\
&= (n-1)\sqrt{3}\left(-m+\frac{1}{2}M_1(G)\right) \\
&\leq (n-1)\sqrt{3}\left(-m+\frac{1}{2}m\left(\frac{2m}{n-1}+n-2\right)\right) \qquad (2.4)\\
&= (n-1)\sqrt{3}\cdot m\left(\frac{m}{n-1}+\frac{n-4}{2}\right).
\end{aligned}
$$

□

Relations (2.3) and (2.4) were obtained by taking into account for each vertices $v \in V(G)$, we have $d_G(v) \leq n-1$ and Eq. (2.1), respectively. Suppose that equality in (2.2) holds. Then inequalities (2.3) and (2.4) become equalities. From (2.3) we conclude that for every vertex v, $d_G(v) = (n-1)$. Then from (2.4) and Lemma 2.8 it follows that G is a complete graph. Conversely, let G be a complete graph. Then it is easily verified that equality holds in (2.2).

Lemma 2.10. *Let G be a graph with n vertices, m edges. Then*

$$M_1(G) \geq 2m(2p+1) - pn(1+p) \text{ where } p = \lfloor \frac{2m}{n} \rfloor.$$

and the equality holds if and only if the difference of the degrees of any two vertices of graph G is at most one.

Theorem 2.11. *Let G be a graph with n vertices, m edges and the minimum vertex degree δ. Then*

$$ {}^2SO(G) \geq \frac{\delta\sqrt{3}}{2}(4mp - pn(p+1)) \text{ where } p = \lfloor \frac{2m}{n} \rfloor. \qquad (2.5)$$

and the equality holds if and only if G is a regular graph.

Proof.

$$\begin{aligned}
{}^2SO(G) &= \sum_{uvw \in E_\alpha(G)} \sqrt{d_G(u)^2 + d_G(v)^2 + d_G(w)^2} \\
&\geq \sum_{uvw \in E_2(G)} \delta\sqrt{3} && (2.6) \\
&= \delta\sqrt{3}\left(-m + \frac{1}{2}M_1(G)\right) \\
&\geq \delta\sqrt{3}\left(-m + \frac{1}{2}(2m(2p+1) - pn(1+p))\right) && (2.7) \\
&= \frac{\delta\sqrt{3}}{2}(4mp - pn(p+1)).
\end{aligned}$$

Relations (2.6) and (2.7) were obtained by taking into accounting for each vertices $v \in V(G)$, we have $d_G(v) \geq \delta$ and Eq. (2.5), respectively. Suppose now that equality in (2.5) holds. Then inequalities (2.6) and (2.7) become equalities. From (2.6) we conclude that for every vertex v, $d_G(v) = \delta$. Then from Eq. (2.7) and Lemma 2.10 it follows that G is a regular graph. Conversely, let G be a regular graph. Then it is easily verified that equality holds in (2.5). □

3. COMPUTING THE THE SECOND ORDER SOMBOR INDEX OF SOME FAMILIES OF GRAPHS

In [19] Nadeem et al. obtained expressions for certain topological indices of the line graphs of subdivision graphs of 2D-lattice, nanotube, and nanotorus of $TUC_4C_8[p,q]$, where p and q denote the number of squares in a row and the number of rows of squares, respectively in 2D-lattice, nanotube and nanotorus as shown in Figure 1 (a), (b) and (c) respectively. The numbers of vertices and edges of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ are given in Table 1.

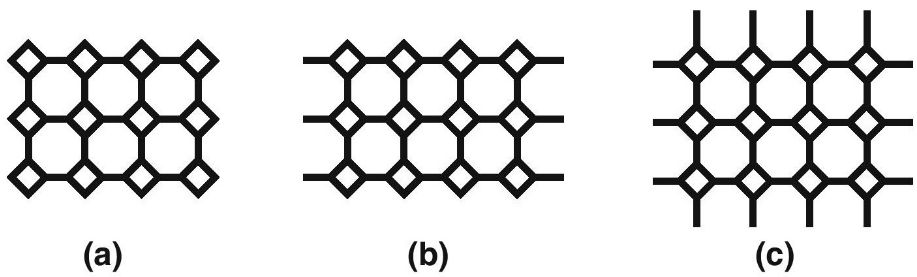

FIGURE 1. (a) 2D-lattice of $TUC_4C_8[4,3]$; (b) $TUC_4C_8[4,3]$ nanotube; (c) $TUC_4C_8[4,3]$ nanotorus.

TABLE 1. Number of vertices and edges.

Graph	Number of vertices	Number of edges
2D-lattices of $TUC_4C_8[p,q]$	$4pq$	$6pq-p-q$
$TUC_4C_8[p,q]$ nanotube	$4pq$	$6pq-p$
$TUC_4C_8[p,q]$ nanotorus	$4pq$	$6pq$

In [23, 24], Ranjini et al. presented explicit formula for computing the Shultz index and Zagreb indices of the subdivision graphs of the tadpole, wheel and ladder graphs. In 2015, Su and Xu [25] calculated the general sum-connectivity index and coindex of the $L(S(T_{n,k}))$, $L(S(W_n))$ and $L(S(L_n))$. In [20], Nadeem et al. derived some exact formulas for ABC_4 and GA_5 indices of the line graphs of the tadpole, wheel and ladder graphs by using the notion of subdivision.

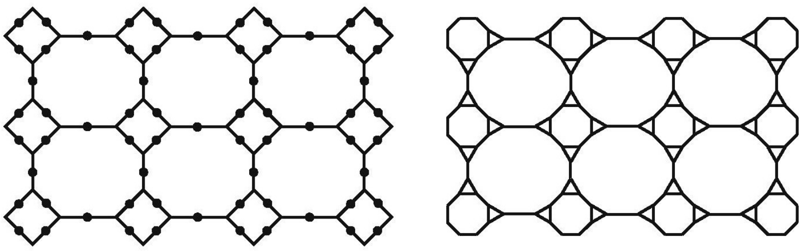

FIGURE 2. (a) Subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$; (b) Line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$.

TABLE 2. Partition of paths of length 2 of the graph X.

$(d_X(u), d_X(v), d_X(w))$ where $uvw \in E_2(X)$	Number of paths of length 2 in X
$(2,2,2)$	8
$(2,2,3)$	$4(p+q-2)$
$(3,3,2)$	$8(p+q-2)$
$(3,3,3)$	$(36pq-26p-26q+16)$

Lemma 3.1. [19] *Let X be the line graph of the subdivision graph of $2D-lattice$ of $TUC_4C_8[p,q]$. Then*

$$M_1(X) = 108pq - 38p - 38q.$$

Theorem 3.2. *Let X be the line graph of the subdivision graph of $2D-lattice$ of $TUC_4C_8[p,q]$. Then*

$${}^2SO(X) = 16\sqrt{3} + 4\sqrt{17}(p+q-2) + 8\sqrt{22}(p+q-2) + 3\sqrt{3}(36pq-26p-26q+16).$$

Proof. The subdivision graph of 2D-lattice of $TUC_4C_8[p,q]$ and the graph X are shown in Fig. 2 (a) and (b), respectively. In X there are total $2(6pq-p-q)$ vertices each vertex is of degree either 2 or 3 and $18pq-5p-5q$ edges. From Remark 2.1 and Lemma 3.1, we get $36pq-14p-14q$ of paths of length 2 in X. Based on the degree of vertices on the path of length 2 in X we can partition $E_2(X)$ as shown in Table 2. Apply Eq. (1.8) to Table 2 and get the required result. □

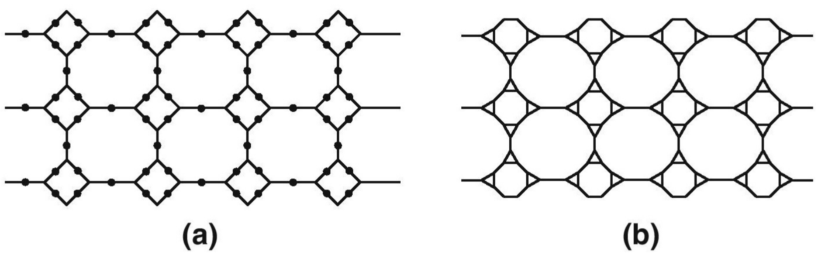

FIGURE 3. (a) Subdivision graph of $TUC_4C_8[4,3]$ of nanotube; (b) line graph of the subdivision graph of $TUC_4C_8[4,3]$ of nanotube.

TABLE 3. Partition of paths of length 2 of the graph Y.

$(d_Y(u), d_Y(v), d_Y(w))$ where $uvw \in E_2(Y)$	Number of paths of length 2 in Y
$(2,2,3)$	$4p$
$(3,3,2)$	$8q$
$(3,3,3)$	$(36pq-26p)$

Lemma 3.3. [19] *Let Y be the line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotube. Then*

$$M_1(Y) = 108pq - 38p.$$

Theorem 3.4. *Let Y be the line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotube. Then*

$$^2SO(Y) = 4p\sqrt{17} + 8p\sqrt{22} + 3\sqrt{2}(36pq - 26p).$$

Proof. The subdivision graph of $TUC_4C_8[p,q]$ nanotube and the graph Y are shown in Fig. 3 (a) and (b), respectively. In Y there are total $12pq-2p$ vertices in which each vertex is of degree either 2 or 3 and $18pq-5p$ edges. From Remark 2.1 and Lemma 3.3, we get $36pq-14p$ number of paths of length 2 in Y. Based on the degree of vertices on the paths of length 2 in Y we can partition $E_2(Y)$ as shown in Table 3. Apply Eq. (1.8) to Table 3 and get the required result. □

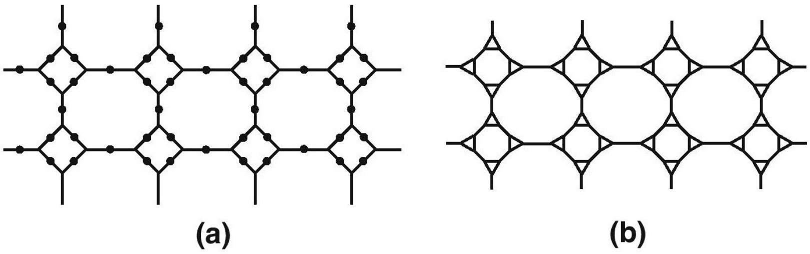

FIGURE 4. (a) Subdivision graph of $TUC_4C_8[4,3]$ of nanotorus; (b) Line graph of the subdivision graph of $TUC_4C_8[4,3]$ of nanotorus.

Theorem 3.5. *Let* Z *be the line graph of the subdivision graph of* $TUC_4C_8[p,q]$ *nanotorus. Then*

$$^2SO(Z) = 9n\sqrt{3}.$$

Proof. The subdivision graph of $TUC_4C_8[p,q]$ nanotorus and the graph Z are shown in Fig. 4 (a) and (b), respectively. Since Z is a 3-regular graph with 12pq vertices and $18pq$ edges. Therefore by Theorem 2.4, we get the required result. □

TABLE 4. Partition of paths of length 2 of the graph $A = L(S(T_{n,k}))$ for $k = 1$.

$(d_A(u), d_A(v), d_A(w))$ where $uvw \in E_2(A)$	Number of paths of length 2 in A
$(1,3,3)$	2
$(2,3,3)$	4
$(2,2,3)$	2
$(3,3,3)$	3
$(2,2,2)$	$2n-4$

TABLE 5. Partition of paths of length 2 of the graph $A = L(S(T_{n,k}))$ for $k > 1$.

$(d_A(u), d_A(v), d_A(w))$ where $uvw \in E_2(A)$	Number of paths of length 2 in A
$(1,2,2)$	1
$(2,3,3)$	6
$(2,2,3)$	3
$(3,3,3)$	3
$(2,2,2)$	$2n+2k-8$

Lemma 3.6. [23, 25] *Let A be the line graph of the subdivision graph of the tadpole graph $T_{n,k}$. Then*

$$M_1(A) = 8n + 8k + 12.$$

Theorem 3.7. *Let A be a line graph of the subdivision graph of the tadpole graph $T_{n,k}$. Then*

$$^2SO(A) = \begin{cases} 2\sqrt{19} + 4\sqrt{22} + 2\sqrt{17} + 9\sqrt{3} + 2(2n-4)\sqrt{3} & \text{for } k = 1. \\ 3(1 + 2\sqrt{22} + \sqrt{17} + 3\sqrt{3}) + 2(2n + 2k - 8)\sqrt{3} & \text{for } k > 1. \end{cases}$$

Proof. First of all, we consider graph A for $n \geq 3$ and $k > 1$. In this graph there are total $2(n+k)$ vertices and $2n + 2k + 1$ edges. From Remark 2.1 and Lemma 3.6, we get $2k+2n+5$ of paths of length 2 in A. Based on the degree of vertices on the paths of length 2 in A we can partition $E_2(A)$ as shown in Table 5. Apply Eq. (1.8) to Table 5 and get the required result. By similar arguments we can obtain the expression of $^2SO(A)$ for k = 1 from Table 4. □

Lemma 3.8. [23] *Let B be a line graph of the subdivision graph of the wheel graph W_{n+1}. Then*

$$M_1(B) = n^3 + 27n.$$

TABLE 6. Partition of paths of length 2 of the graph B.

$(d_B(u), d_B(v), d_B(w))$ where $uvw \in E_2(B)$	Number of paths of length 2 in B
$(3,3,3)$	$7n$
$(3,3,n)$	$2n$
$(3,n,n)$	$n(n-1)$
(n,n,n)	$\frac{n(n-1)(n-2)}{2}$

Theorem 3.9. *Let B be a line graph of the subdivision graph of the wheel graph W_{n+1}. Then*

$$^2SO(B) = 21n\sqrt{3} + 2n\sqrt{18+n^2} + n(n-1)\sqrt{9+2n^2} + \frac{n^2(n-1)(n-2)\sqrt{3}}{2}.$$

Proof. The graph $L(S(W_{n+1}))$ contains $4(n+1)$ vertices and $\frac{n^2+9n}{2}$ edges. From Remark 2.1 and Lemma 3.8, we get $\frac{n^3-n^2+18n}{2}$ number of paths of length 2 in B. Based on the degree of vertices on the paths of length 2 in B we can partition $E_2(B)$ as shown in Table 6. Apply Eq. (1.8) to Table 6 and get the required result. □

Lemma 3.10. [23, 25] *Let C be a line graph of the subdivision graph of a ladder graph with order n. Then*

$$M_1(C) = 54n - 76.$$

TABLE 7. Partition of paths of length 2 of the graph C.

$(d_C(u), d_C(v), d_C(w))$ where $uvw \in E_2(C)$	Number of paths of length 2 in C
$(2,2,2)$	4
$(2,2,3)$	4
$(2,3,3)$	8
$(3,3,3)$	$18n-44$

Theorem 3.11. *Let C be a line graph of the subdivision graph of a ladder graph with order n. Then*

$$^2SO(C) = 8\sqrt{3} + 4\sqrt{17} + 8\sqrt{22} + 3\sqrt{3}(18n-44).$$

Proof. The graph $L(S(L_n)$ contains $6n-4$ vertices and $\frac{18n-20}{2}$ edges. From Remark 2.1 and Lemma 3.10, we get $18n-28$ number of paths of length 2 in C. Based on the degree of vertices on the paths of length 2 in C we can partition $E_2(C)$ as shown in Table 7. Apply Eq. (1.8) to Table 7 and get the required result. □

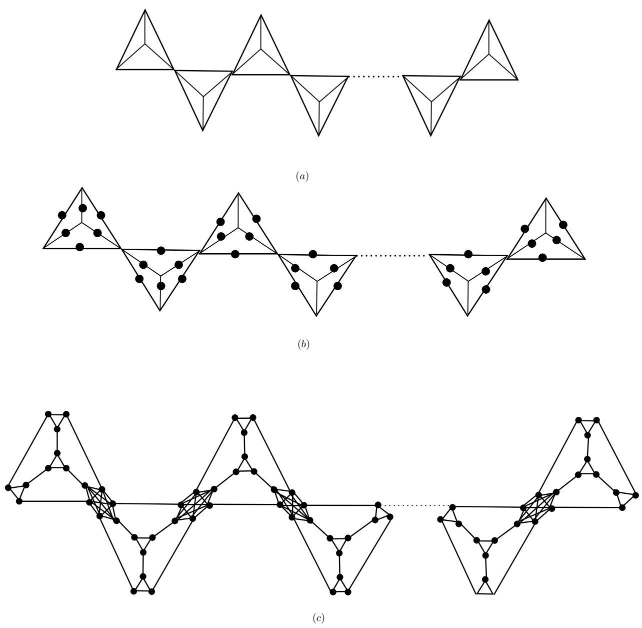

FIGURE 5. (a) CS_n (b) A subdivision graph of CS_n (c) A line graph of subdivision graph of CS_n.

A chain silicate network CS_n of dimension n is obtained by linearly arranging n tetrahedra. The number of vertices and the number of edges in CS_n with $n > 1$ are $3n+1$ and $6n$, respectively [2]. The number of vertices and number of edges in the line graph of the subdivision graph $L(S(CS_n)) = G$ of CS_n are $12n$ and $27n-9$, respectively. Figure 5 shows the line graph of subdivision graph of CS_n.

TABLE 8. Partition of paths of length 2 of the graph $L(S(CS_n)) = G$.

$(d_G(u), d_G(v), d_G(w))$ where $uvw \in E_2(G)$	Number of paths of length 2 in G
$(3,6,6)$	$10(2n-1)$
$(6,6,6)$	$10(7n-8)$
$(3,3,6)$	$4(2n-1)$
$(3,3,3)$	$2(5n+11)$

Lemma 3.12. [2] *Consider the line graph of the subdivision graph G of CS_n. Then*

$$M_\alpha(G) = 2(n+1)\cdot 3^{\alpha+1} + (n-1)6^{\alpha+1}.$$

By substituting $\alpha = 2$ in above Lemma we get the first Zagreb index of $L(S(CS_n))$

$$M_1(G) \quad = \quad 18(15n-9). \tag{3.1}$$

Theorem 3.13. *Let G be the line graph of the subdivision graph of CS_n. Then*

$$^2SO(G) = 90(2n-1) + 10\sqrt{108}(7n-8) + 12\sqrt{6}(2n-1) + 6\sqrt{3}(5n+11).$$

Proof. The graph G contains $12n$ vertices and $27n-9$ edges. From Remark 2.1 and Eq. (3.1), we get $108n-72$ number of paths of length 2 in G. Based on the degree of vertices on the paths of length 2 in G we can partition $E_2(G)$ as shown in Table 8. Apply Eq. (1.8) to Table 8 and get the required result. □

4. CHEMICAL APPLICABILITY OF THE SECOND ORDER SOMBOR INDEX

In this section, a linear regression model of four physical properties is presented for the second order Sombor index $^2SO(G)$. The physical properties such as entropy(S), acentric factor (AF), enthalpy of vaporization (HVAP) and standard enthalpy of vaporization (DHVAP) of octane isomers have shown good correlation with the index considered in the study. The second order Sombor index $^2SO(G)$ is tested for the octane isomers database available at https://www.moleculardescriptors.eu/dataset.htm. $^2SO(G)$ index are computed and tabulated in column 6 of Table 9.

Using the method of least squares, the linear regression models for S, AF, HVAP, and DHVAP are fitted using the data of Table 9. The fitted models for the $^2SO(G)$ index are

$$S \quad = \quad 122.03814(\pm 2.29981) - 0.48111(\pm 0.06483)(^2SO(G)) \tag{4.1}$$
$$Acentric\ Factor \quad = \quad 0.4773309(\pm 0.0114833) - 0.0041000(\pm 0.0003237)(^2SO(G)) \tag{4.2}$$
$$HVAP \quad = \quad 76.20523(\pm 1.20918) - 0.2038(\pm 0.03409)(^2SO(G)) \tag{4.3}$$
$$DHVAP \quad = \quad 10.524133(\pm 0.201277) - 0.040454(\pm 0.005674)(^2SO(G)) \tag{4.4}$$

From Table 10 and Figure 6, it is obvious that the $^2SO(G)$ index highly correlates with the acentric factor and the correlation coefficient $|r|$=**0.9535739.** Also, the

TABLE 9. Experimental values of S, AF, $HVAP$ and $DHVAP$ and the corresponding values of the ^2SO of octane isomers.

Alkane	S	AF	$HVAP$	$DHVAP$	$^2SO(G)$
n-Octane	111.700	0.398	73.190	9.915	19.856
2-Methylheptane	109.800	0.378	70.300	9.484	24.851
3-Methylheptane	111.300	0.371	71.300	9.521	25.935
4-Methylheptane	109.300	0.372	70.910	9.483	25.852
3-Ethylhexane	109.400	0.362	71.700	9.476	26.975
2, 2-Dimethylhexane	103.400	0.339	67.700	8.915	37.838
2, 3-Dimethylhexane	108.000	0.348	70.200	9.272	31.948
2, 4-Dimethylhexane	107.000	0.344	68.500	9.029	30.838
2, 5-Dimethylhexane	105.700	0.357	68.600	9.051	29.846
3, 3-Dimethylhexane	104.700	0.323	68.500	8.973	39.953
3, 4-Dimethylhexane	106.600	0.340	70.200	9.316	33.065
2-Methyl-3-ethylpentane	106.100	0.332	69.700	9.209	33.021
3-Methyl-3-ethylpentane	101.500	0.307	69.300	9.081	42.192
2, 2, 3-Trimethylpentane	101.300	0.301	67.300	8.826	45.992
2, 2, 4-Trimethylpentane	104.100	0.305	64.870	8.402	42.660
2, 3, 3-Trimethylpentane	102.100	0.293	68.100	8.897	47.088
2, 3, 4-Trimethylpentane	102.400	0.317	68.370	9.014	37.982
2, 2, 3, 3-Trimethylpentane	93.060	0.255	66.200	8.410	46.053

TABLE 10. Parameters of regression models for the $^2SO(G)$ index.

Physical properties	Value of the correlation coefficient	Residual standard error
Entropy	0.8802677	2.209
Acentric factor	**0.9535739**	0.01103
HVAP	0.8311469	1.161
DHVAP	0.8721235	0.1933

$^2SO(G)$ index has good correlation coefficient $|r| = 0.8802677$ with entropy, $|r| = 0.8311469$ with HVAP, and $|r| = 0.8721235$ with DHVAP.

Note: In equations (4.1) - (4.4), the errors of the regression coefficients are represented within brackets. Table 10 and Figure 6 show the correlation coefficient and residual standard error for the regression models of four physical properties with $^2SO(G)$ index.

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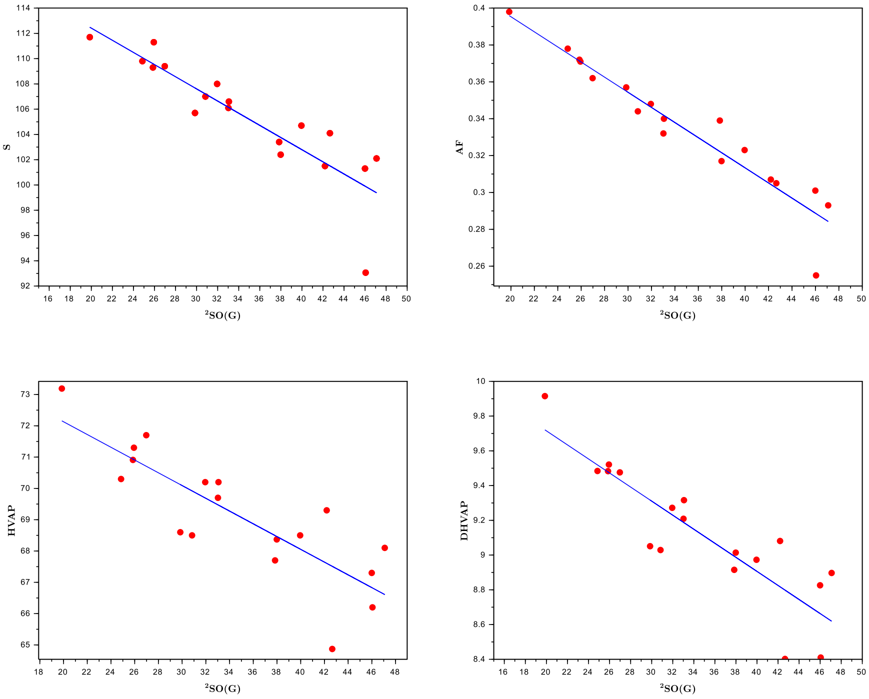

FIGURE 6. Scatter diagram of physical properties $S, AF, HVAP$ and $DHVAP$ with the ${}^2SO(G)$ index.

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