Available online at http://jprm.sms.edu.pk/
Journal of Prime Research in Mathematics, 17(2) (2021), 123–133

Journal of Prime Research in Mathematics

Sombor index of some nanostructures

Ammar Alsinai[a], B. Basavanagoud[b,*], Mahammadsadiq Sayyed[b], Mohammad Reza Farahani[c]

[a]*Department of Studies in Mathematics, University of Mysore, Manasagangotri Mysuru-570006, India.*
[b]*Department of Mathematics, Karnatak University, Dharwad-580003, Karnataka, India.*
[c]*Department of Mathematics, Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran.*

Abstract

Topological indices are extensively used for establishing relationship between the nanostructure and their physico-chemical properties. The invention of new nanostructures gives a key note to industry, electronics, pharmaceutical, medical treatments, communication, information and food science and so on. In this paper, Sombor index is tested with physico-chemical properties of octane isomers such as entropy, acentric factor, enthalpy of vaporization (HVAP) and standard enthalpy of vaporization (DHVAP) using the linear models. The Sombor index shows excellent correlation with these chemical properties. Specially, high correlation with DHVAP (coefficient of correlation 0.9392673). Further, we obtain Sombor index of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p, q]$ and subdivision graph of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p, q]$.

Keywords: Sombor index, nanostructure and subdivision graph.

1. Introduction

Topological indices are used in the process of correlating the chemical structures with various characteristics such as boiling points and molar heats of formation. Graph theory is used to characterize these chemical structures. In the fields of chemical graph theory, molecular topology and mathematical chemistry, a *topological index* is actually a molecular graph invariant which making matches the physico-chemical properties of a molecular graph with a number. Further-more, in some cases, a topological index known as a *connectivity index* which is a type of a molecular descriptor and is calculated based on the molecular graph of a chemical compound. A molecular graph is a simple graph whose vertices correspond to the atoms and whose edges correspond to the bonds. In science and technology, nanostructures plays a vital role in electronic devices, pharmaceutical and medical treatments, communication and information, food science and so on. Topological indices are such graph invariants. Due to this special property, topological indices are extensively used in chemistry. Several topological indices have found many applications, especially, in

*Corresponding author
Email addresses: aliiammar1985@gmail.com (Ammar Alsinai), b.basavanagoud@gmail.com (B. Basavanagoud), sadiqs26@gmail.com (Mahammadsadiq Sayyed), mrfarahani88@gmail.com (Mohammad Reza Farahani)

Received : 19 March 2021; *Accepted:* 30 September 2021; *Published Online:* 26 October 2021.

QSPR/QSAR study [1, 2, 3, 4, 5, 6, 7, 8, 9]. Let G be a graph with the vertex set $V(G)$ and the edge set $E(G)$. The vertices and the edges of G are used to represent the atoms and the bonds of chemical structures. For a graph G, the degree of a vertex v is the number of edges incident to v and is denoted by $d_G(v)$. The subdivision graph $S(G)$ is the graph obtained from G by replacing each of its edge by a path of length two [10]. For unexplained graph terminology and notation refer [10, 11].

The concept of Sombor index (SO) was recently introduced by Gutman is in [12], which is defined as

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

Let p and q be the number of squares in a row and the number of rows of squares respectively in $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p, q]$. The $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[4, 3]$ is shown in Figure. 1 (a), (b) and (c) respectively. Much of the research work has been done on $TUC_4C_8[p, q]$ nanostructures. For more on nanostruture, one can refer [13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26].

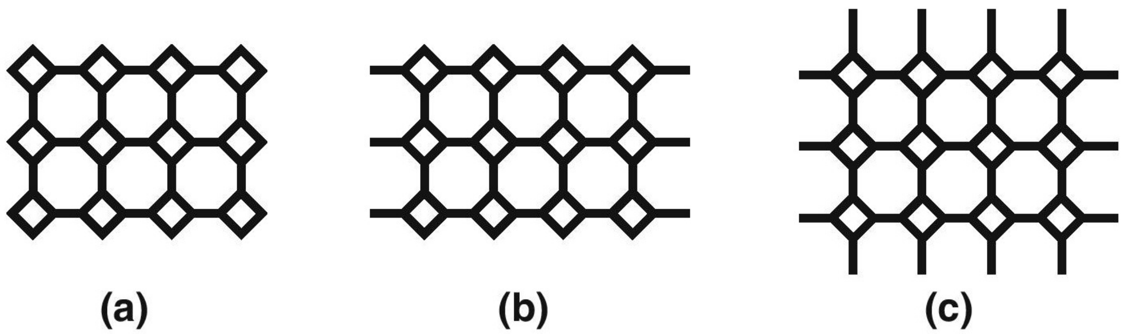

Figure 1: (a) 2D-lattice of $TUC_4C_8[4, 3]$; (b) $TUC_4C_8[4, 3]$ nanotube; (c) $TUC_4C_8[4, 3]$ nanotorus.

Order and size of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p, q]$ are given in Table 1.

Table 1: Order and Size of graphs

Graph	Order	Size
2D-Lattice of $TUC_4C_8[p, q]$	$4pq$	$6pq - p - q$
$TUC_4C_8[p, q]$ Nanotube	$4pq$	$6pq - p$
$TUC_4C_8[p, q]$ Nonotorus	$4pq$	$6pq$

2. Results for 2D-lattice of $TUC_4C_8[p, q]$

In this section, we obtain explicit formulae for computing Sombor index of 2D-lattice and subdivision graphs of 2D-lattice of $TUC_4C_8[p, q]$. The proof technique used here is partitioning the edge set of nanostructures. Here, we denote p, q are order and size of the underline molecular graph.

In the below table denotes the edge partition of 2D-lattice of $TUC_4C_8[p, q]$.

Table 2: Edge partition of graph G, when $p > 1, q > 1$

$(d_G(u), d_G(v))$	(2, 2)	(2, 3)	(3, 3)
Number of edges	4	$4p + 4q - 8$	$6pq - 5p - 5q + 4$

Theorem 2.1. *Let G be a $2D$-lattice of $TUC_4C_8[p, q]$. Then*

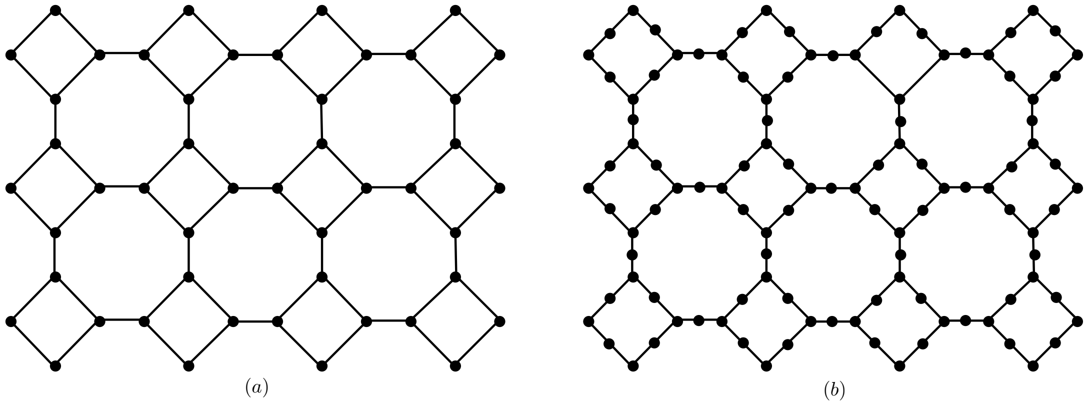

Figure 2: (a) 2D-lattice of $TUC_4C_8[4,3]$; (b) subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$.

Table 3: Edge partition of graph G, when $p>1, q=1$

$(d_G(u), d_G(v))$	(2, 2)	(2, 3)	(3, 3)
Number of edges	4	$4p-4$	$p-1$

$$SO(G)=\begin{cases} \sqrt{13}(4p+4q-8)+\sqrt{2}(18pq-15p-15q+20) & if\ p>1, q>1, \\ \sqrt{13}(4p-4)+\sqrt{2}(3p+5) & if\ p>1, q=1. \end{cases}$$

Proof. The $2D$-lattice of $TUC_4C_8[p,q]$ has $4pq$ vertices and $6pq-p-q$ edges. Let $m_{u,v}$ denote the number of edges connecting the vertices of degrees d_u and d_v. The $2D$-lattice of $TUC_4C_8[p,q]$ (Figure 2) contains only $m_{2,2}$, $m_{2,3}$ and $m_{3,3}$ edges. The number of $m_{2,2}$, $m_{2,3}$ and $m_{3,3}$ edge in each row is mentioned in Table 2 and 3.

Now,

$$\begin{aligned} SO(G) &= \sum_{uv\in E(G)} \sqrt{d_G(u)^2+d_G(v)^2} \\ &= m_{2,2}\big(\sqrt{d_G(u)^2+d_G(v)^2}\big)+m_{2,3}\big(\sqrt{d_G(u)^2+d_G(v)^2}\big)+m_{3,3}\big(\sqrt{d_G(u)^2+d_G(v)^2}\big) \\ &= 4\big(\sqrt{2^2+2^2}\big)+(4p+4q-8)\big(\sqrt{2^2+3^2}\big)+(6pq-5p-5q+4)\big(\sqrt{3^2+3^2}\big) \\ &= 4\big(\sqrt{4+4}\big)+(4p+4q-8)\big(\sqrt{4+9}\big)+(6pq-5p-5q+4)\big(\sqrt{9+9}\big) \\ &= 4\sqrt{8}+(4p+4q-8)\sqrt{13}+(6pq-5p-5q+4)\sqrt{18} \\ &= \sqrt{13}(4p+4q-8)+\sqrt{2}(18pq-15p-15q+12+8) \\ &= \sqrt{13}(4p+4q-8)+\sqrt{2}(18pq-15p-15q+20). \end{aligned}$$

Now consider the following cases.

Case 1: when $p>1$ and $q>1$. Then

$$SO(G)=\sqrt{13}(4p+4q-8)+\sqrt{2}(18pq-15p-15q+20).$$

Case 2: when $p>1$ and $q=1$. Then

$$SO(G)=\sqrt{13}(4p-4)+\sqrt{2}(3p+5).$$

□

Next, we have considered subdivision graph of 2D-lattice of $TUC_4C_8[p,q]$.

In the below table denotes the edge partition of subdivision graph of 2D-lattice of $TUC_4C_8[p,q]$.

Theorem 2.2. *Let G be a subdivision graph of 2D-lattice of $TUC_4C_8[p,q]$. Then*

Table 4: Edge partition of graph G, when $p > 1, q > 1$

$(d_G(u), d_G(v))$	(2, 2)	(2, 3)
Number of edges	$4p + 4q$	$12pq - 6p - 6q$

Table 5: Edge partition of graph G, when $p > 1, q = 1$

$(d_G(u), d_G(v))$	(2, 2)	(2, 3)
Number of edges	$4p + 4$	$6p - 6$

$$SO(G)=\begin{cases} 8p\sqrt{2}+8q\sqrt{2}+12pq\sqrt{13}-6p\sqrt{13}-6q\sqrt{13} & if\ p>1, q>1,\\ (p-1)(8\sqrt{2}+6\sqrt{13}) & if\ p>1, q=1. \end{cases}$$

Proof. The subdivision graph of $2D$-lattice of $TUC_4C_8[p, q]$ has $10pq - p - q$ vertices and $12pq - 2p - 2q$ edges. Let $m_{u,v}$ denote the number of edges connecting the vertices of degrees d_u and d_v. The subdivision graph of $2D$-lattice of $TUC_4C_8[p, q]$ (Figure 2) contains only $m_{2,2}$ and $m_{2,3}$ edges. The number of $m_{2,2}$ and $m_{2,3}$ edges in each row is mentioned in Table 4 and 5.

Now,

$$\begin{aligned} SO(G) &= \sum_{uv\in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \\ &= m_{2,2}\big(\sqrt{d_G(u)^2 + d_G(v)^2}\big) + m_{2,3}\big(\sqrt{d_G(u)^2 + d_G(v)^2}\big) \\ &= (4p+4q)\big(\sqrt{2^2+2^2}\big) + (12pq-6p-6q)\big(\sqrt{2^2+3^2}\big) \\ &= (4p+4q)\big(\sqrt{4+4}\big) + (12pq-6p-6q)\big(\sqrt{4+9}\big) \\ &= (4p+4q)\big(2\sqrt{2}\big) + (12pq-6p-6q)\sqrt{13} \\ &= 8p\sqrt{2}+8q\sqrt{2}+12pq\sqrt{13}-6p\sqrt{13}-6q\sqrt{13}. \end{aligned}$$

Now consider the following cases.

Case 1: when $p > 1$ and $q > 1$. Then

$$SO(G) = 8p\sqrt{2}+8q\sqrt{2}+12pq\sqrt{13}-6p\sqrt{13}-6q\sqrt{13}.$$

Case 2: when $p > 1$ and $q = 1$. Then

$$SO(G) = (p-1)(8\sqrt{2}+6\sqrt{13}).$$

□

3. Results for $TUC_4C_8[p, q]$ nanotube

In this section, we obtain explicit formulae for computing Sombor index of nanotube and subdivision graphs of nanotube of $TUC_4C_8[p, q]$. The proof technique used here is partitioning the edge set of nanostructures. Here, we denote p, q are order and size of the underline molecular graph.

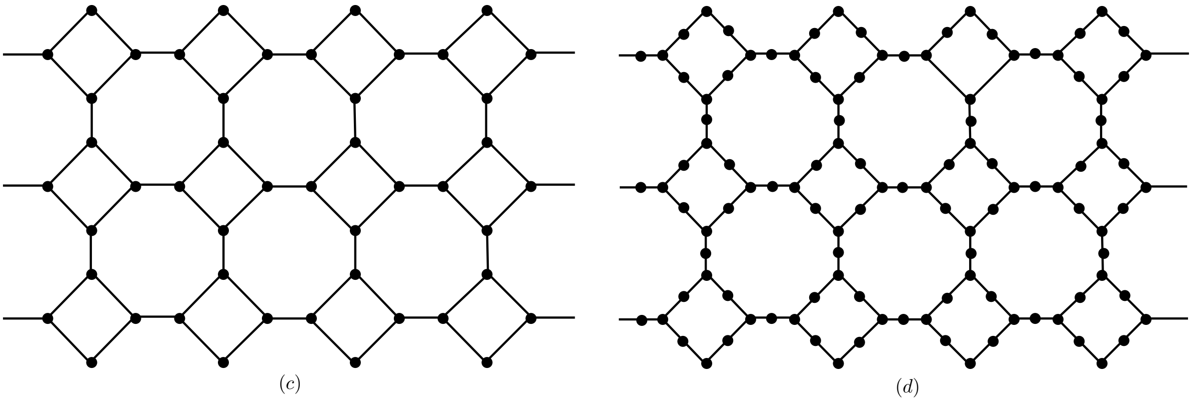

Figure 3: (c) $TUC_4C_8[4,3]$ nanotube; (d) subdivision graph of $TUC_4C_8[4,3]$ nanotube.

In the below table denotes the edge partition of nanotube of $TUC_4C_8[p,q]$.

Table 6: Edge partition of graph G, when $p > 1, q > 1$

$(d_G(u), d_G(v))$	(2, 3)	(3, 3)
Number of edges	$4p$	$6pq - 5p$

Table 7: Edge partition of graph G, when $p > 1, q = 1$

$(d_G(u), d_G(v))$	(2, 3)	(3, 3)
Number of edges	$4p$	p

Theorem 3.1. *Let G be a $TUC_4C_8[p,q]$ nanotube. Then*

$$SO(G)=\begin{cases} 4p\sqrt{13}+18pq\sqrt{2}-15p\sqrt{2} & if\ p>1, q>1,\\ 4p\sqrt{13}+3p\sqrt{2} & if\ p>1, q=1.\end{cases}$$

Proof. The $TUC_4C_8[p,q]$ nanotube has $4pq$ vertices and $6pq-p$ edges. Let $m_{u,v}$ denote the number of edges connecting the vertices of degrees d_u and d_v. The $TUC_4C_8[p,q]$ nanotube (Figure 3) contains only $m_{2,3}$ and $m_{3,3}$ edges. The number of $m_{2,3}$ and $m_{3,3}$ edge in each row is mentioned in Table 6 and 7.

Now,

$$\begin{aligned} SO(G) &= \sum_{uv\in E(G)} \sqrt{d_G(u)^2+d_G(v)^2}\\ &= m_{2,3}\big(\sqrt{d_G(u)^2+d_G(v)^2}\big)+m_{3,3}\big(\sqrt{d_G(u)^2+d_G(v)^2}\big)\\ &= 4p\big(\sqrt{2^2+3^2}\big)+(6pq-5p)\big(\sqrt{3^2+3^2}\big)\\ &= 4p\big(\sqrt{4+9}\big)+(6pq-5p)\big(\sqrt{9+9}\big)\\ &= 4p\sqrt{13}+(6pq-5p)\sqrt{18}\\ &= 4p\sqrt{13}+18pq\sqrt{2}-15p\sqrt{2}. \end{aligned}$$

Now consider the following cases.

Case 1: when $p > 1$ and $q > 1$. Then

$$SO(G) = 4p\sqrt{13}+18pq\sqrt{2}-15p\sqrt{2}.$$

Case 2: when $p > 1$ and $q = 1$. Then

$$SO(G) = 4p\sqrt{13}+3p\sqrt{2}.$$

□

Next, we have considered subdivision graph of $TUC_4C_8[p,q]$ nanotube.
In the below table denotes the edge partition of subdivision graph of $TUC_4C_8[p,q]$ nanotube.

Table 8: Edge partition of graph G, when $p > 1, q > 1$

$(d_G(u), d_G(v))$	(2, 2)	(2, 3)
Number of edges	$4p$	$12pq - 6p$

Table 9: Edge partition of graph G, when $p > 1, q = 1$

$(d_G(u), d_G(v))$	(2, 2)	(2, 3)
Number of edges	$4p$	$6p$

Theorem 3.2. *Let G be a subdivision graph of $TUC_4C_8[p,q]$ nanotube. Then*

$$SO(G)=\begin{cases} 8p\sqrt{2}+12pq\sqrt{13}-6p\sqrt{13} & if\ p>1, q>1, \\ 8p\sqrt{2}+6p\sqrt{13} & if\ p>1, q=1. \end{cases}$$

Proof. The subdivision graph of $TUC_4C_8[p,q]$ nanotube has $10pq - p$ vertices and $12pq - 2p$ edges. Let $m_{u,v}$ denote the number of edges connecting the vertices of degrees d_u and d_v. The subdivision graph of $TUC_4C_8[p,q]$ nanotube (Figure 3) contains only $m_{2,2}$ and $m_{2,3}$ edges. The number of $m_{2,3}$ and $m_{3,3}$ edge in each row is mentioned in Table 8 and 9.

Now,

$$\begin{aligned} SO(G) &= \sum_{uv\in E(G)} \sqrt{d_G(u)^2+d_G(v)^2} \\ &= m_{2,2}\big(\sqrt{d_G(u)^2+d_G(v)^2}\big)+m_{2,3}\big(\sqrt{d_G(u)^2+d_G(v)^2}\big) \\ &= 4p\big(\sqrt{2^2+2^2}\big)+(12pq-6p)\big(\sqrt{2^2+3^2}\big) \\ &= 4p\big(\sqrt{4+4}\big)+(12pq-6p)\big(\sqrt{4+9}\big) \\ &= 4p\sqrt{8}+(12pq-6p)\sqrt{13} \\ &= 8p\sqrt{2}+12pq\sqrt{13}-6p\sqrt{13}. \end{aligned}$$

Now consider the following cases.

Case 1: when $p > 1$ and $q > 1$. Then

$$SO(G) = 8p\sqrt{2} + 12pq\sqrt{13} - 6p\sqrt{13}.$$

Case 2: when $p > 1$ and $q = 1$. Then

$$SO(G) = 8p\sqrt{2} + 6p\sqrt{13}.$$

□

4. Results for $TUC_4C_8[p,q]$ nanotorus

In this section, we obtain explicit formulae for computing Sombor index of nanotorus and subdivision graphs of nanotorus of $TUC_4C_8[p,q]$. The proof technique used here is partitioning the edge set of nanostructures. Here, we denote p, q are order and size of the underline molecular graph.

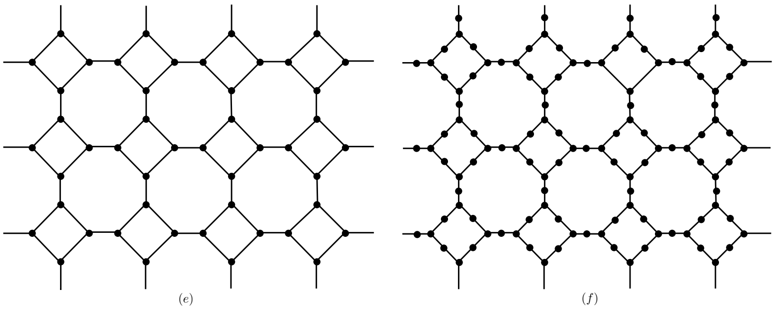

Figure 4: (e) $TUC_4C_8[4,3]$ nanotorus; (f) subdivision graph of $TUC_4C_8[4,3]$ nanotorus.

In the below table denotes the edge partition of nanotorus of $TUC_4C_8[p,q]$.

Table 10: Edge partition of graph G, when $p > 1, q > 1$

$(d_G(u), d_G(v))$	(3, 3)
Number of edges	$6pq$

Theorem 4.1. *Let G be a $TUC_4C_8[p,q]$ nanotorus. Then*

$$SO(G) = 18pq\sqrt{2}.$$

Proof. The $TUC_4C_8[p,q]$ nanotorus has $4pq$ vertices and $6pq$ edges. Let $m_{u,v}$ denote the number of edges connecting the vertices of degrees d_u and d_v. The $TUC_4C_8[p,q]$ nanotorus (Figure 4) contains only $m_{3,3}$ edge. The number of $m_{3,3}$ edge in each row is mentioned in Table 10.

Now,

$$\begin{aligned} SO(G) &= \sum_{uv\in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \\ &= m_{3,3}\big(\sqrt{d_G(u)^2 + d_G(v)^2}\big) \\ &= 6pq\big(\sqrt{3^2+3^2}\big) \\ &= 6pq\sqrt{9+9} \\ &= 6pq\sqrt{18} \\ &= 18pq\sqrt{2}. \end{aligned}$$

□

Next, we have considered subdivision graph of $TUC_4C_8[p,q]$ nanotorus.
In the below table denotes the edge partition of subdivision graph of nanotorus of $TUC_4C_8[p,q]$.

Table 11: Edge partition of graph G, when $p > 1, q > 1$

$(d_G(u), d_G(v))$	(2, 3)
Number of edges	$12pq$

Theorem 4.2. *Let G be a subdivision graph of $TUC_4C_8[p,q]$ nanotorus. Then*

$$SO(G) = 12pq\sqrt{13}.$$

Proof. The subdivision graph of $TUC_4C_8[p,q]$ nanotorus has $10pq$ vertices and $12pq$ edges. Let $m_{u,v}$ denote the number of edges connecting the vertices of degrees d_u and d_v. The $TUC_4C_8[p,q]$ nanotorus (Figure 4) contains only $m_{2,3}$ edge. The number of $m_{2,3}$ edge in each row is mentioned in Table 11.

Now,

$$\begin{aligned} SO(G) &= \sum_{uv\in E(G)} \sqrt{d_G(u)^2+d_G(v)^2} \\ &= m_{2,3}\big(\sqrt{d_G(u)^2+d_G(v)^2}\big) \\ &= 12pq\big(\sqrt{2^2+3^2}\big) \\ &= 12pq\sqrt{4+9} \\ &= 12pq\sqrt{13}. \end{aligned}$$

□

5. Chemical applicability of Sombor index on octane isomers

The topological indices with the high correlation factor are of foremost important in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) analysis. In this section we discuss the linear regression analysis of Sombor index (SO) with entropy(S), acentric factor(AcentFac), enthalpy of vaporization(HVAP) and DHVAP of octane isomers. The SO was tested using a dataset of octane isomers found at http://www.moleculardiscriptors.eu/dataset.htm. Interestingly, we have noticed that this index is highly correlated with DHVAP($|r|$=0.9392673). The dataset of octane isomers (columns 1-5 of Table 12) are taken from above web link whereas last column of Table 12 is calculated by definition of Sombor index.

Table 12: Experimental values of the entropy, AcentFac, HVAP, DHVAP and the corresponding value of SO of octane isomers.

Alkane	S	AcentFac	DHVAP	HVAP	SO
n-octane	111.67	0.397898	9.915	73.19	18.614
2-methyl-heptane	109.84	0.377916	9.484	70.3	20.65
3-methyl-heptane	111.26	0.371002	9.521	71.3	20.501
4-methyl-heptane	109.32	0.371504	9.483	70.91	20.501
3-ethyl-hexane	109.43	0.362472	9.476	71.7	20.3532
2,2-dimethyl-hexane	103.42	0.339426	8.915	67.7	24.7342
2,3-dimethyl-hexane	108.02	0.348247	9.272	70.2	22.3993
2,4-dimethyl-hexane	106.98	0.344223	9.029	68.5	22.5394
2,5-dimethyl-hexane	105.72	0.35683	9.051	68.6	22.6886
3,3-dimethyl-hexane	104.74	0.322596	8.973	68.5	24.4909
3,4-dimethyl-hexane	106.59	0.340345	9.316	70.2	22.2503
2-methyl-3-ethyl-pentane	106.06	0.332433	9.209	69.7	22.2503
3-methyl-3-ethyl-pentane	101.48	0.306899	9.081	69.3	22.0116
2,2,3-trimethyl-pentane	101.31	0.300816	8.826	67.3	26.373
2,2,4-trimethyl-pentane	104.09	0.30537	8.402	64.87	26.7714
2,3,3-trimethyl-pentane	102.06	0.293177	8.897	68.1	26.2788
2,3,4-trimethyl-pentane	102.39	0.317422	9.014	68.37	24.2965
2,2,3,3-tetramethylbutane	93.06	0.255294	8.41	66.2	30.3954

The linear regression models for the entropy, acentric factor, DHVAP and HVAP using the data of Table 12 are obtained using the least squares fitting procedure as implemented in R software [27]. The fitted models are:

$$
\begin{aligned}
S &= 138.0306(\pm 3.8656) - 1.4042(\pm 0.1652)SO &(5.1)\\
AcentFac &= 0.596085(\pm 0.027879) - 0.011207(\pm 0.001191)SO &(5.2)\\
DHVAP &= 11.9992(\pm 0.2644) - 0.1237(\pm 0.0113)SO &(5.3)\\
HVAP &= 83.77924(\pm 1.74126) - 0.62924(\pm 0.07441)SO &(5.4)
\end{aligned}
$$

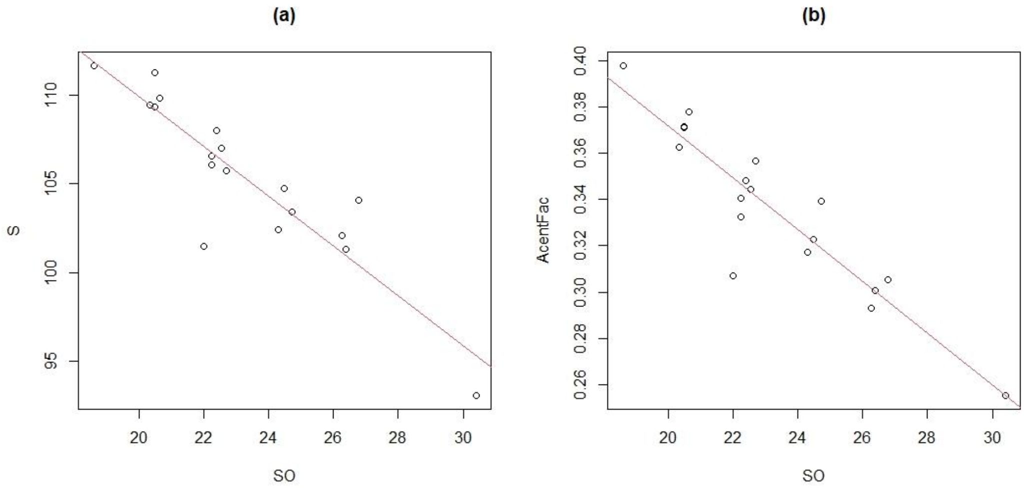

Figure 5: Scatter diagram of (a) S on SO, (b) $AcentFac$ on SO superimposed by the fitted regression line.

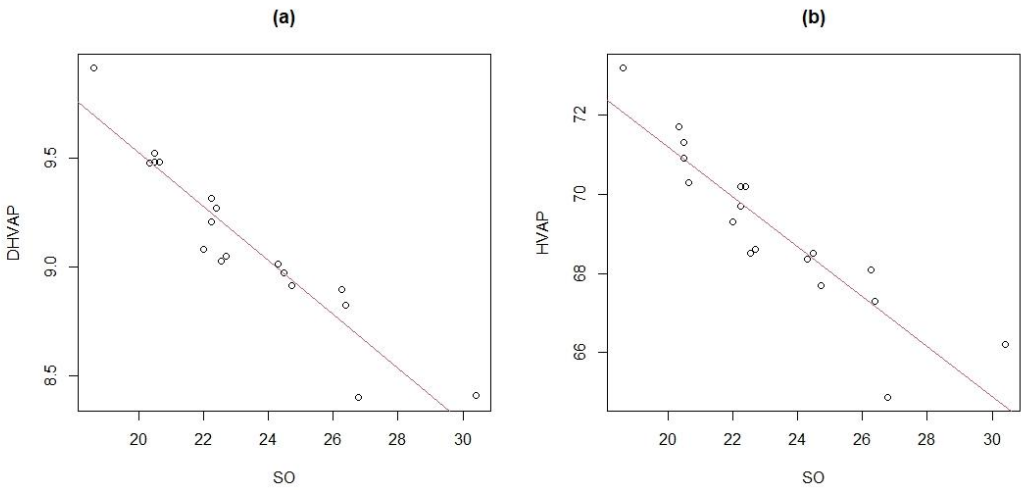

Figure 6: Scatter diagram of (a) $DHVAP$ on SO (b) $HVAP$ on SO, superimposed by the fitted regression line.

Note: The values in the brackets of Eq. (5.1) to (5.4) are the corresponding standard errors of the regression coefficients.

6. Conclusion

Chemical graph theory is an essential tool for studying molecular structure and has an important impact on the development of chemical sciences. The study of topological indices is one of the most active studied

Table 13: Correlation coefficient and residual standard error of regression models

Physical Property	**Absolute value of the correlation coefficient ($\|r\|$)**	**Residual standard error**
Enthalpy	0.9048227	1.983
Acentric Factor	0.920249	0.0143
DHVAP	**0.9392673**	**0.1356**
HVAP	0.903962	0.8931

field in chemical graph theory. In this paper, we have used Sombor index (SO), in the field of mathematical chemistry, it has chemical applicability in determining several physico-chemical properties of octane isomers as it has coefficient of correlation close to 1. Further, we have obtained explicit formulae for Sombor index of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ and subdivision graph of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$.

References

[1] Alsinai, A., Alwardi, A., & Soner, N. D. (2021). On Reciprocals Leap Indices of Graphs. *International Journal of Analysis and Applications, 19*(1), 1-19.

[2] Alsinai, A., Alwardi, A., Farahani, M. R., & Soner, N. D. (2021). On the ψ_k-polynomial of graph. *Eurasian Chemical Communications, 3*(4), 219-226.

[3] Alsinai, A., Alwardi,A., N.D. Soner. Topological Properties of Graphene Using ψ_k polynomial, Proceedings of the Jangjeon Mathematical Society, 24(3), (2021), 375-388.

[4] Alsinai, A., Alwardi, A., & Soner, N. D. (2021). On Reciprocal leap function of graph. *Journal of Discrete Mathematical Sciences and Cryptography, 24*(2), 307-324.

[5] Alsinai, A., Alwardi, A., Ahmed, H., & Soner, N. D. (2021). Leap Zagreb indices for the Central graph of graph. *Journal of Prime Research in Mathematics, 17*(2), 73-78.

[6] Gutman, I., & Polansky, O. E. (1986). Graph theory and molecular orbitals. In *Mathematical Concepts in Organic Chemistry* (pp. 42-45). Springer, Berlin, Heidelberg.

[7] Kulli, V. R. (2018). *Multiplicative connectivity indices of nanostructures* (pp. 1-10). Riga: LAP Lambert Academic Publishing.

[8] Javaraju, S., Alsinai, A., Alwardi, A., Ahmed, H., N.D. Soner. Reciprocal leap indices of some wheel related graphs. Journal of Prime Research in Mathematics.17(2),2021, 101-110.

[9] Li, D. X., Liu, J. B., Hosamani, S. M., Basavanagoud, B., & Farahani, M. R. (2017). Zagreb Indices of Semi-Total (Total) Block Graphs of Bridge and Chain Graphs. *J. Comput. Theor. Nanosci, 14*(6), 2692-2695.

[10] F. Harary, *Graph Theory*, Addison-Wesley, Reading, 1969.

[11] V. R. Kulli, *College Graph Theory*, Vishwa International Publications, Gulbarga, India, (2012).

[12] Gutman, I. (2021). Geometric approach to degree-based topological indices: Sombor indices. *MATCH Commun. Math. Comput. Chem, 86*(1), 11-16.

[13] Ashrafi, A. R., & Yousefi, S. (2007). Computing the Wiener index of a $TUSC_4C_8(S)$ nanotorus. *MATCH Commun. Math. Comput. Chem, 57*(2), 403-410.

[14] Basavanagoud, B., Patil, S., & Deng, H. Y. (2017). On the second order first Zagreb index. *Iranian Journal of Mathematical Chemistry, 8*(3), 299-311.

[15] Basavanagoud, B., Desai, V. R., & Patil, S. (2017). (β,α) Connectivity Index of Graphs. *Applied Mathematics and Nonlinear Sciences, 2*(1), 21-30.

[16] Basavanagoud, B., Sunilkumar, M. H., & Anand, P. B. (2018). First neighbourhood Zagreb index of some nanostructures. *Proceedings of the Institute of Applied Mathematics, 7*(2), 178-193.

[17] Farahani, M. R. (2015). The hyper-Zagreb index of $TUSC_4C_8(S)$ nanotubes. *Int. J. Engg. & Tech. Research, 3*(1), 1-6.

[18] Farahani, M. R. (2014). Domination polynomial of Nanotorus by using the 2-variables Generating Function. *Pacific Journal of Applied Mathematics, 6*(1), 79-95.

[19] M.R. Farahani. Zagreb indices of $TUHRC_4(S)$ and $TUSC_4C_8(S)$ Nanotubes. Journal of Advance in Mathematical Science. 2(1), (2015), 98-105.

[20] Farahani, M. R. (2015). Multiplicative versions of Zagreb indices of $TUSC_4C_8(S)$. *Journal of Chemistry and Materials Research, 2*(2), 67-70.

[21] Farahani, M. R., Siddiqui, H. M. A., Baby, S., Imran, M., & Siddiqui, M. K. (2016). The second and second-

sum-connectivity indices of $TUC_4C_8(S)$ nanotubes. *Journal of Optoelectronic and Biomedical Materials, 8*(3), 107-111.

[22] Hosamani, S. M. (2017). Computing Sanskruti index of certain nanostructures. *Journal of Applied Mathematics and Computing, 54*(1), 425-433.

[23] S. M. Hosamani, On Topological Properties of the Line Graphs of Subdivision Graphs of certain nanostructures-II, *Global J. Sci. Frontier Res: Mathematics and Decision Sciences*, **17 (4)** (2017) 9 pages.

[24] Lokesha, V., Shruti, R., & sinan CEVIK, A. (2018). ON CERTAIN TOPOLOGICAL INDICES OF NANOSTRUCTURES USINGQ (G) AND R (G) OPERATORS. Communications Faculty of Sciences University of Ankara Series A1 Mathematics and Statistics, 67(2), 178-187.

[25] Nadeem, M. F., Zafar, S., & Zahid, Z. (2016). On topological properties of the line graphs of subdivision graphs of certain nanostructures. *Applied mathematics and computation, 273*, 125-130.

[26] VETRK, T. (2019). DEGREE-BASED TOPOLOGICAL INDICES OF $TUC_4C_8(S)$ NANOTUBES. *UPB Scientific Bulletin, Series B, 81*(4), 187-96.

[27] R Core Team. R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria. (2016) URL https://www.R-project.org/.