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REDUCED SOMBOR COINDEX OF $TUC_4C_8(R)[p,q]$ NANOSTRUCTURES AND ITS CHEMICAL APPLICABILITY

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ABSTRACT: *Nanomaterials possess distinctive chemical, mechanical and physical properties arising from their thin layered structures, strong functionality, anisotropy, large surface area and atomic-scale thickness. Topological indices (TIs) provide numerical descriptions of molecular graphs and support the structural characterization of chemical compounds, networks and nanomaterials. Among Sombor-type descriptors, the Sombor index ($SO(G)$), reduced Sombor index ($RSO(G)$), reverse Sombor index ($rSO(G)$), and the reduced Sombor coindex ($\overline{RSO}(G)$) recently introduced by Rajathagiri et al. have attracted attention because of their mathematical and practical relevance. This paper derives closed-form expressions for $\overline{RSO}(G)$, $SO(G)$, $RSO(G)$ and $rSO(G)$ for the $TUC_4C_8(R)[p,q]$ 2D-lattice, nanotube and nanotorus. It also compares $\overline{RSO}(G)$ with $SO(G)$, $RSO(G)$ and $rSO(G)$ across these structures and evaluates $\overline{RSO}(G)$'s chemical applicability through correlations with experimentally reported physico-chemical properties of selected polycyclic aromatic hydrocarbons (PAHs).*

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1 Introduction

TIs constitute one of the most important graph-theoretical tools for the study of chemical compounds, molecular networks and nanostructures. These indices are numerical descriptors that depend exclusively on the structure of the associated molecular graph. They provide a quantitative representation of molecular structures and are widely applied to correlate the structural features with physico-chemical properties, biological activities and chemical reactivity. Several physico-chemical properties such as toughness, melting point, entropy, rigidity, boiling point, strain energy, enthalpy of formation and enthalpy of vaporization have been shown to be closely associated with the underlying graphical structure of chemical compounds. Therefore, TIs have found widespread application in Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Property Relationship (QSPR) [4, 10, 15, 20] studies and serve as valuable tools in molecular modeling and pharmaceutical design.

Motivated by their broad applicability, numerous TIs have been introduced and systematically investigated in literature. Among the recently introduced degree-based TIs, the Sombor index

($SO(G)$) [9] and its types such as reduced Sombor index ($RSO(G)$) [11] and reverse Sombor index ($rSO(G)$) [18] have gained considerable attention and are extensively studied. These indices are defined as follows:

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

$$RSO(G) = \sum_{uv\in E(G)} \sqrt{(d(u)-1)^2 + (d(v)-1)^2},$$

$$rSO(G) = \sum_{uv\in E(G)} \sqrt{[\Delta + 1 - d(u)]^2 + [\Delta + 1 - d(v)]^2}.$$

While TIs are defined by considering the edge set of a graph, their complementary counterparts, identified as coindices, have also been extensively studied because of their usefulness in characterizing molecular structures. Several coindices have been proposed as extensions of classical TIs, including the first Zagreb coindex ($\overline{M_1}(G)$)[1], second Zagreb coindex ($\overline{M_2}(G)$)[1], Sombor coindex ($\overline{SO}(G)$)[6] and reduced Sombor coindex[19] their definitions are given below:

$$\overline{M_1}(G) = \sum_{uv\notin E(G)} [d(u) + d(v)],$$

$$\overline{M_2}(G) = \sum_{uv\notin E(G)} d(u)d(v),$$

$$\overline{SO}(G) = \sum_{uv\notin E(G)} \sqrt{d(u)^2 + d(v)^2},$$

$$\overline{RSO}(G) = \sum_{uv\notin E(G)} \sqrt{(d(u)-1)^2 + (d(v)-1)^2}.$$

The increasing importance of TIs and coindices has stimulated their application to a variety of molecular and nanostructured systems. In particular, nanoscience deals with the study of materials at the nanoscale i.e., of size 10^{-9} units. Materials and structures within this scale, commonly refereed to as nanomaterials or nanostructures, exhibit remarkable properties such as high strength, stability, conductivity and absorption. These remarkable characteristics have encouraged scientist and researchers from various domains such as physical sciences, material science, electronic devices, pharmaceutical, medical science, communication and information technology, to investigate nanomaterials and employ them as building blocks for more complex systems.

One important class of such nanostructure is $TUC_4C_8(R)[p,q]$ [2, 12, 14], which consist of alternating squares(C_4) and octagons (C_8) arranged in p rows and q columns. This structure can be mathematically modeled as a graph formed by the periodic arrangement of squares and octagons as discussed in [14, 16, 17, 18]. The 2D-lattice, nanotube and nanotorus forms of $TUC_4C_8(R)[p,q]$ are illustrated in Figure 1 for the particular case $p = 6$ and $q = 4$. In recent years, TIs have been gradually applied in the QSPR/QSAR studies of such nanostructures [3, 13]. Within this framework, a nanostructure is represented by a molecular graph whose vertices correspond to atoms and edges correspond to bonds. Such graph-theoretical representation facilitate the investigation of structural characteristics and the computation of various TIs that are useful for predicting physico-chemical properties of nanomaterials.

In the view of growing significance of Sombor-type descriptors in the nanostructure analysis, the present work focuses on reduced Sombor coindex and its relationship with other well-known Sombor-based indices, namely $SO(G)$, $RSO(G)$ and $rSO(G)$. Specifically, we derive closed-form expressions of $\overline{RSO}(G)$, $SO(G)$, $RSO(G)$ and $rSO(G)$ for the studied nanostructures $TUC_4C_8(R)[p,q]$. Also, we present a comparative analysis of $\overline{RSO}(G)$ with $SO(G)$, $RSO(G)$ and $rSO(G)$ for each structure. To demonstrate the chemical applicability of $\overline{RSO}(G)$, we examine its correlation it with the physico-chemical properties of selected PAHs.

In this work every graphs considered is finite, simple, connected and undirected. A graph $G = (V, E)$ consisting the vertex set $V(G)$ and the edge set $E(G)$. The degree of a vertex v, denoted by $d(v)$ is the number of edges incident with v. Throughout this article, the symbol $m_{d(u),d(v)}$ denotes the number of edges whose end vertices have degrees $d(u)$ and $d(v)$, whereas $\overline{m}_{d(u),d(v)}$ denotes the number of non-adjacent vertex pairs (u, v) corresponding to each edge in the nanostructure $TUC_4C_8(R)[p,q]$, where the vertices u and v have degrees $d(u)$ and $d(v)$. In [3], some known results on $TUC_4C_8(R)[p,q]$ nanostructurs were established, which are stated as

Theorem 1.1 *Let G be a $TUC_4C_8(R)[p,q]$ 2D-lattice, when $p > 1, q > 1$. Then,*

$$SO(G) = 8\sqrt{2} + [4(p+q) - 8]\sqrt{13} + 3[6pq - 5(p+q) + 4]\sqrt{2}.$$

Theorem 1.2 *Let G be a $TUC_4C_8(R)[p,q]$ nanotube, when $p > 1, q > 1$. Then,*

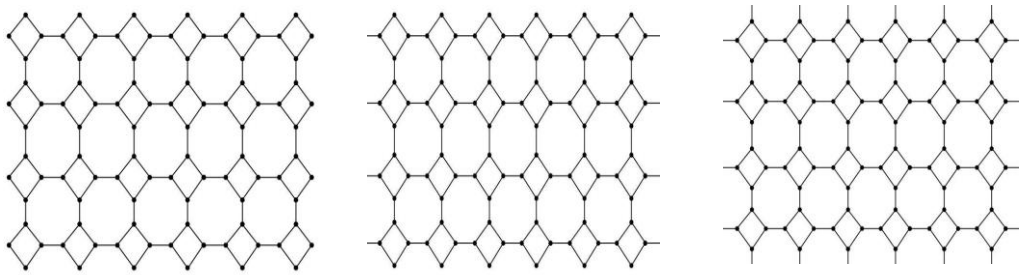
$$SO(G) = 4p\sqrt{13} + (6pq - 5p)3\sqrt{2}.$$

Theorem 1.3 *Let G be a $TUC_4C_8(R)[p,q]$ nanotorus, when $p > 1, q > 1$. Then,*

$SO(G) = 18pq\sqrt{2}$. *In the present work, we use these known results in correlation analysis.*

2 Results and Discussion

In this section, we derive explicit formulae for the indices $\overline{RSO}(G)$, $SO(G)$, $RSO(G)$ and $rSO(G)$ for the studied nanostructures of $TUC_4C_8(R)[p,q]$, consisting of p squares and their q rows. Further, we present a comparative correlation analysis of these indices for each of these nanomaterial. The proofs of the obtained results are based on partitioning the edge sets of corresponding $TUC_4C_8(R)[p,q]$ structures according to the degrees of the vertices incident with each edge.



(a) 2D-lattice (b) Nanotube (c) Nanotorus

Figure 1. $TUC_4C_8(R)[6,4]$ **nanostructures**

Theorem 2.1 *Let* G *be a* $TUC_4C_8(R)[p,q]$ *2D-lattice, when* $p > 1, q > 1$. *Then,*

$$(i)\ \ RSO(G) = 4\sqrt{2} + [4(p+q) - 8]\sqrt{5} + 2(6pq - 5p - 5q + 4)\sqrt{2},$$

$$(ii)\ rSO(G) = 8\sqrt{2} + [4(p+q) - 8]\sqrt{5} + (6pq - 5p - 5q + 4)\sqrt{2}.$$

Proof. (i) The $TUC_4C_8(R)[p,q]$ 2D-lattice graph has $|V(G)| = 4pq$ vertices and $|E(G)| = 6pq - p - q$ edges. The edges can be classified according to the degrees of their end vertices into three categories, namely $(2,2)$, $(2,3)$ and $(3,3)$ edges. The corresponding edge partition is given in Table 1.

Table 1. Edge partition of $TUC_4C_8(R)[p,q]$ **2D-lattice graph**

$(\boldsymbol{d(u)}, \boldsymbol{d(v)})$	$\boldsymbol{m_{d(u),d(v)}}$
(2,2)	4
(2,3)	$4(p+q) - 8$
(3,3)	$6pq - 5(p+q) + 4$

Using Table 1 and by the definition of $RSO(G)$, we obtain

$$RSO(G) = \sum_{uv \in E(G)} \sqrt{(d(u)-1)^2 + (d(v)-1)^2},$$
$$= m_{2,2}\sqrt{1^2+1^2} + m_{2,3}\sqrt{1^2+2^2} + m_{3,3}\sqrt{2^2+2^2}$$

$$= 4\sqrt{2} + [4(p+q) - 8]5 + (6pq - 5p - 5q + 4)3\sqrt{2}$$

$$RSO(G) = 4\sqrt{2} + [4(p+q) - 8]\sqrt{5} + 2(6pq - 5p - 5q + 4)\sqrt{2}.$$

Similarly, (ii) follow by applying the same edge partition together with the definition of $rSO(G)$.

Theorem 2.2 *Let G be a $TUC_4C_8(R)[p,q]$ 2D-lattice. Then*

$$\overline{RSO}(G) = [2(p+q) - 1 \times (p+q)] - 4]\sqrt{2}$$

$$+[(8p-4)q^2 + (8p^2 - 8p - 4)q - (4p^2 + 4p - 8)]\sqrt{5}$$

$$+[(8p^2 - 8p + 2)q^2 + (6 - 4p - 8p^2)q + (2p^2 + 6p - 4)]2\sqrt{2}.$$

Proof. The set of all non-adjacent vertex pairs corresponds to each edge of $TUC_4C_8(R)[p,q]$ 2D-lattice graph are partitioned according to vertex degree pairs $(d(u), d(v))$ of their incident vertices and $\overline{m}_{d(u),d(v)}$ are calculated and is shown in Table 2.

Table 2. Non-adjacent vertex pair partition of the graphical structure of $TUC_4C_8(R)[p,q]$ 2D-lattice

$(d(u), d(v))$	$\overline{m}_{d(u),d(v)}$
(2,2)	$[2(p+q) - 1 \times (p+q)] - 4$
(2,3)	$(8p-4)q^2 + (8p^2 - 8p - 4)q - (4p^2 + 4p - 8)$
(3,3)	$(8p^2 - 8p + 2)q^2 + (6 - 4p - 8p^2)q + (2p^2 + 6p - 4)$

Using Table 2 and by the definition of $\overline{RSO}(G)$, we obtain

$$\overline{RSO}(G) = \sum_{uv \notin E(G)} \sqrt{(d(u)-1)^2 + (d(v)-1)^2},$$

$$= \overline{m}_{2,2}\sqrt{(2-1)^2 + (2-1)^2} + \overline{m}_{2,3}\sqrt{(2-1)^2 + (3-1)^2} + \overline{m}_{3,3}\sqrt{(3-1)^2 + (3-1)^2}$$

$$= [[2(p+q) - 1 \times (p+q)] - 4]\sqrt{1^2 + 1^2}$$

$$+[(8p-4)q^2 + (8p^2 - 8p - 4)q - (4p^2 + 4p - 8)]\sqrt{1^2 + 2^2}$$

$$+[(8p^2 - 8p + 2)q^2 + (6 - 4p - 8p^2)q + (2p^2 + 6p - 4)]\sqrt{2^2 + 2^2}$$

$$\overline{RSO}(G) = [2(p+q) - 1 \times (p+q)] - 4]\sqrt{2}$$

$$+[(8p-4)q^2 + (8p^2 - 8p - 4)q - (4p^2 + 4p - 8)]\sqrt{5}$$

$$+[(8p^2 - 8p + 2)q^2 + (6 - 4p - 8p^2)q + (2p^2 + 6p - 4)]2\sqrt{2}.$$

Theorem 2.3 *Let* G *be a* $TUC_4C_8(R)[p,q]$ *nanotube, when* $p > 1, q > 1$. *Then,*

$$(i) \quad RSO(G) = 4p\sqrt{5} + (6pq - 5p)2\sqrt{2},$$

$$(ii) \quad rSO(G) = 4p\sqrt{5} + (6pq - 5p)\sqrt{2}.$$

Proof. (i) The graphical structure of $TUC_4C_8(R)[p,q]$ nanotube consist of $4pq$ vertices and $6pq - p$ edges. The edges can be classified according to the degrees of their end vertices into two categories, namely $(2,3)$ and $(3,3)$ type edges. The corresponding edge partition is given in Table 3.

Table 3. Edge partition of $TUC_4C_8(R)[p,q]$ nanotube

$(d(u), d(v))$	$m_{d(u),d(v)}$
(2,3)	$4p$
(3,3)	$6pq - 5p$

Using Table 3 and by the definition of $RSO(G)$, we get

$$RSO(G) = \sum_{uv \in E(G)} \sqrt{(d(u)-1)^2 + (d(v)-1)^2},$$

$$= m_{2,3}\sqrt{1^2 + 2^2} + m_{3,3}\sqrt{2^2 + 2^2}$$

$$= 4p\sqrt{5} + (6pq - 5p)2\sqrt{2}$$

$$RSO(G) = 4p\sqrt{5} + (6pq - 5p)2\sqrt{2}.$$

Similarly, (ii) follow by applying the same edge partition together with the definition of $rSO(G)$.

Theorem 2.4 *Let* G *be a* $TUC_4C_8[p,q]$ *nanotube. Then,*

$$\overline{RSO}(G) = p(2p-1)\sqrt{2} + [2p(4pq - 2p - 2)]\sqrt{5} +$$

$$[2p(p+3) + 8pq(pq - p - 1)]2\sqrt{2}.$$

Proof. The set of all non-adjacent vertex pairs corresponds to each edge of $TUC_4C_8(R)[p,q]$ nanotube graph are partitioned according to vertex degree pairs $(d(u), d(v))$ of their incident vertices and $\overline{m}_{d(u),d(v)}$ are calculated and is shown in Table 4.

Table 4. Non-adjacent vertex pair partition of the graphical structure of $TUC_4C_8(R)[p,q]$ nanotube

$(d(u), d(v))$	$\overline{m}_{d(u),d(v)}$
(2,2)	$p(2p-1)$
(2,3)	$2p(4pq-2p-2)$
(3,3)	$2p(p+3)+8pq(pq-p-1)$

Using Table 4 and by the definition of $\overline{RSO}(G)$, we obtain

$$\overline{RSO}(G) = \sum_{uv\notin E(G)} \sqrt{(d(u)-1)^2+(d(v)-1)^2},$$

$$= \overline{m}_{2,2}\sqrt{1^2+1^2} + \overline{m}_{2,3}\sqrt{1^2+2^2} + \overline{m}_{3,3}\sqrt{2^2+2^2}$$

$$= p(2p-1)\sqrt{1^2+1^2} + [2p(4pq-2p-2)]\sqrt{1^2+2^2}$$

$$+[2p(p+3)+8pq(pq-p-1)]\sqrt{2^2+2^2}$$

$$\overline{RSO}(G) = p(2p-1)\sqrt{2} + [2p(4pq-2p-2)]\sqrt{5} +$$

$$[2p(p+3)+8pq(pq-p-1)]2\sqrt{2}.$$

Theorem 2.5 *Let G be a $TUC_4C_8(R)[p,q]$ nanotorus, when $p>1, q>1$. Then,*

$$(i)\ RSO(G) = 12pq\sqrt{2},$$

$$(ii)\ rSO(G) = 6pq\sqrt{2}.$$

Proof. (i) The graph structure of the $TUC_4C_8(R)[p,q]$ nanotorus consists of $4pq$ vertices and $6pq$ edges. It contains only $(3,3)$ type edges. The corresponding edge partition is given in Table 5.

Table 5. Edge partition of $TUC_4C_8(R)[p,q]$ nanotorus

$(d(u), d(v))$	$m_{d(u),d(v)}$
(3,3)	$6pq$

Using Table 5 and by the definition of $RSO(G)$, we have

$$RSO(G) = \sum_{uv\in E(G)} \sqrt{(d(u)-1)^2+(d(v)-1)^2},$$

$$= m_{3,3}\sqrt{2^2+2^2}$$

$$= 6pq(2\sqrt{2})$$

$$RSO(G) = 12pq\sqrt{2}.$$

Similarly, (ii) follow by applying the same edge partition together with the definition of $rSO(G)$.

Theorem 2.6 *Let G be a $TUC_4C_8(R)[p,q]$ nanotorus. Then,*

$$\overline{RSO}(G) = [(2pq-1)(4pq-2)-2]2\sqrt{2}.$$

Proof. The set of all non-adjacent vertex pairs corresponds to each edge of $TUC_4C_8(R)[p,q]$ nanotorus graph can be partitions based on vertex degree pairs $(d(u),d(v))$ and $\overline{m}_{d(u),d(v)}$ are calculated and is shown in Table 6.

Table 6. Non-adjacent vertex pair partition of the graphical structure of $TUC_4C_8(R)[p,q]$ nanotorus

$(d(u),d(v))$	$\overline{m}_{d(u),d(v)}$
(3,3)	$(2pq-1)(4pq-2)-2$

Using Table 6 and by the definition of $\overline{RSO}(G)$, we obtain

$$\overline{RSO}(G) = \sum_{uv\notin E(G)} \sqrt{(d(u)-1)^2+(d(v)-1)^2},$$

$$= \overline{m}_{3,3}\sqrt{2^2+2^2}$$

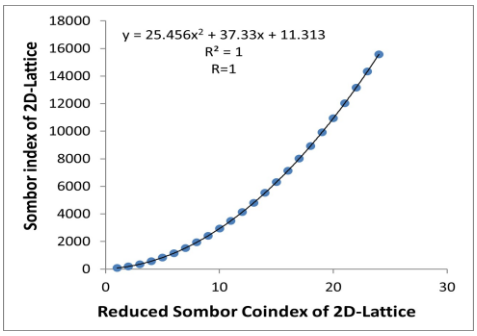
$$= [(2pq-1)(4pq-2)-2]2\sqrt{2}.$$

2.1 Correlation analysis

To examine the relationship between $\overline{RSO}(G)$ and the studied Sombor-type TIs, a correlation analysis has been carried out with the classical TIs $SO(G)$, $RSO(G)$ and $rSO(G)$ for the studied nanostructures of $TUC_4C_8(R)[p,q]$. The analysis is based on the computed values of these indices, where $\overline{RSO}(G)$ as the independent variable (X) and $SO(G)$, $RSO(G)$ and $rSO(G)$ are considered as the dependent variables (Y). The numerical data corresponding to the studied nanostructures of $TUC_4C_8(R)[p,q]$ are provided in Tables 7, 8 and 9 respectively. In this analysis, quadratic regression models have been employed to examine the relationship between the $\overline{RSO}(G)$ and the indices $SO(G)$, $RSO(G)$ and $rSO(G)$ for the studied nanostructures of $TUC_4C_8(R)[p,q]$. The strength of the relationship has been evaluated using the correlation coefficient R. The corresponding regression equations and correlation coefficients (R) are provided presented in Table 10. The resulting correlation plots for the considered nanostructures of $TUC_4C_8(R)[p,q]$ are shown in Figures 2, 3 and 4 respectively

Table 7. Computed values of $\overline{RSO}(G)$, $SO(G)$, $RSO(G)$ and $rSO(G)$ for the $TUC_4C_8(R)[p,q]$ 2D-lattice graph

$[p,q]$	$\overline{RSO}(G)$	$SO(G)$	$RSO(G)$	$rSO(G)$
[2,2]	215.729	74.0992	46.1728	40.516
[3,3]	1397.34	187.796	120.63	86.6888
[4,4]	4848.44	352.405	229.028	149.832
[5,5]	12412.9	567.926	371.367	229.946
[6,6]	26477.5	834.358	547.648	327.031
[7,7]	49972.3	1151.7	757.87	441.086
[8,8]	86370.3	1519.96	1002.03	572.111
[9,9]	1.39688×10^5	1939.13	1280.14	720.107
[10,10]	2.14483×10^5	2409.2	1592.18	885.074
[11,11]	3.15859×10^5	2930.2	1938.17	1067.01
[12,12]	4.49461×10^5	3502.1	2318.09	1265.92
[13,13]	6.21478×10^5	4124.91	2731.96	1481.8
[14,14]	8.38639×10^5	4798.64	3179.77	1714.65
[15,15]	1.10822×10^6	5523.27	3661.52	1964.47
[16,16]	1.43804×10^6	6298.82	4177.21	2231.26
[17,17]	1.83646×10^6	7125.28	4726.85	2515.02
[18,18]	2.31237×10^6	8002.66	5310.42	2815.75
[19,19]	2.87524×10^6	8930.94	5927.94	3133.45
[20,20]	3.53504×10^6	9910.14	6579.39	3468.12
[21,21]	4.30232×10^6	10940.2	7264.79	3819.77
[22,22]	5.18814×10^6	12021.3	7984.13	4188.38
[23,23]	6.20413×10^6	13153.2	8737.41	4573.96
[24,24]	7.36244×10^6	14336	9524.63	4976.52
[25,25]	8.67579×10^6	15569.8	10345.8	5396.04



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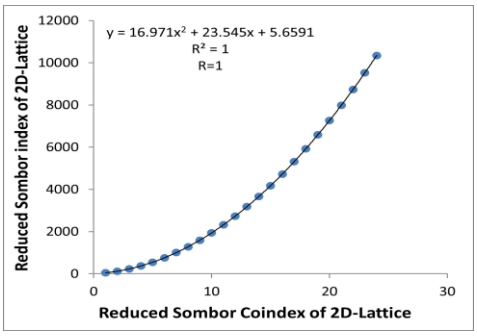

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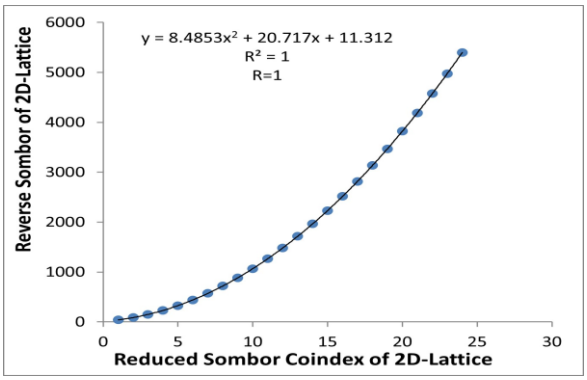


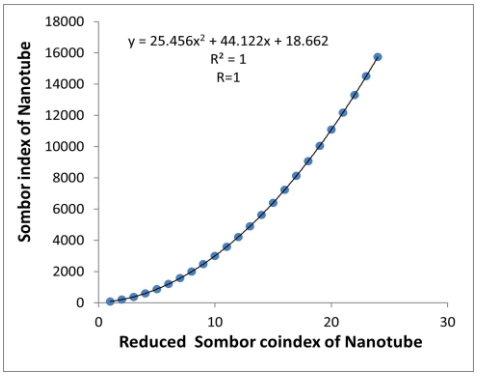
(c)

Figure 2. Correlation graphs corresponding to the $TUC_4C_8(R)[p,q]$ 2D-lattice

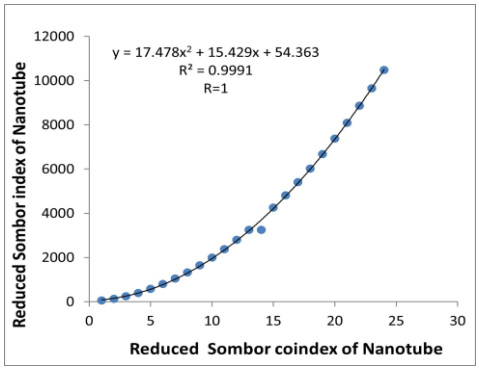
Table 8. Computed values of $\overline{RSO}(G)$, $SO(G)$, $RSO(G)$ and $rSO(G)$ for the $TUC_4C_8(R)[p,q]$ nanotube

$[p,q]$	$\overline{RSO}(G)$	$SO(G)$	$RSO(G)$	$rSO(G)$
[2,2]	245.006	88.2414	57.4865	37.6875
[3,3]	1516.93	208.73	137.141	81.9871
[4,4]	5146.4	380.13	250.738	143.257
[5,5]	13005.7	602.441	398.275	221.498
[6,6]	27510.1	875.664	579.753	316.709
[7,7]	51618.0	1199.8	795.173	428.891
[8,8]	88831.0	1574.85	1044.53	558.044
[9,9]	1.43193×10^5	2000.8	1327.83	704.167

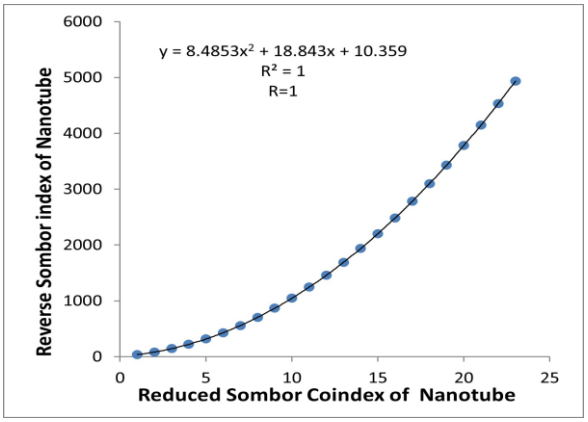
$[p,q]$	$\overline{RSO}(G)$	$SO(G)$	$RSO(G)$	$rSO(G)$
[10,10]	2.19293×10^5	2477.67	1645.08	867.26
[11,11]	3.2226×10^5	3005.46	1996.26	1047.32
[12,12]	4.57768×10^5	3584.15	2381.39	1244.36
[13,13]	6.32035×10^5	4213.75	2800.45	1458.36
[14,14]	8.51819×10^5	4894.27	3253.46	1689.34
[15,15]	1.12442×10^6	5625.7	3253.46	1937.29
[16,16]	1.4577×10^6	6408.04	4261.3	2202.2
[17,17]	1.86002×10^6	7241.29	4816.13	2484.09
[18,18]	2.34034×10^6	8125.46	5404.9	2782.95
[19,19]	2.90812×10^6	9060.53	6027.61	3098.78
[20,20]	3.57337×10^6	10046.5	6684.27	3431.58
[21,21]	4.34667×10^6	11083.4	7374.86	3781.35
[22,22]	5.23912×10^6	12171.2	8099.4	4148.09
[23,23]	6.26236×10^6	13309.9	8857.88	4531.8
[24,24]	7.42858×10^6	14499.6	9650.3	4932.48
[25,25]	8.75053×10^6	15740.1	10476.7	5350.13



(a)



(b)



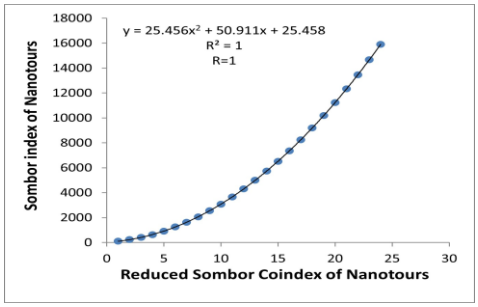
(c)

Figure 3. Correlation graphs corresponding to the $TUC_4C_8(R)[p,q]$nanotube

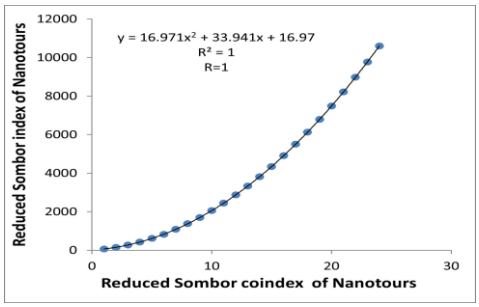
Table 9. Computed values for $\overline{RSO}(G)$, $SO(G)$, $RSO(G)$ and $rSO(G)$ of $TUC_4C_8(R)[p,q]$ nanotorus

$[p,q]$	$\overline{RSO}(G)$	$SO(G)$	$RSO(G)$	$rSO(G)$
[2,2]	271.529	101.823	67.8823	33.9411
[3,3]	1629.17	229.103	152.735	76.3675
[4,4]	5430.58	407.294	271.529	135.765
[5,5]	13576.5	636.396	424.264	212.132
[6,6]	28510.5	916.41	610.94	305.47
[7,7]	53219.7	1247.34	831.558	415.779
[8,8]	91233.7	1629.17	1086.12	543.058
[9,9]	11.46626×10^5	2061.92	1374.62	687.308
[10,10]	2.24011×10^5	2545.58	1697.06	848.528
[11,11]	3.2855×10^5	3080.16	2053.44	1026.72
[12,12]	4.65944×10^5	3665.64	2443.76	1221.88
[13,13]	6.42438×10^5	4302.04	2868.03	1434.01
[14,14]	8.6482×10^5	4989.35	3326.23	1663.12
[15,15]	1.14042×10^6	5727.56	3818.38	1909.19
[16,16]	1.47712×10^6	6516.7	4344.46	2172.23
[17,17]	1.88333×10^6	7356.74	4904.49	2452.25
[18,18]	2.368×10^6	8247.69	5498.46	2749.23
[19,19]	2.94066×10^6	9189.56	6126.37	3063.19
[20,20]	3.61134×10^6	10182.3	6788.23	3394.11

$[p,q]$	$\overline{RSO}(G)$	$SO(G)$	$RSO(G)$	$rSO(G)$
[21,21]	4.39062×10^6	11226	7484.02	3742.01
[22,22]	5.28966×10^6	12320.6	8213.75	4106.88
[23,23]	6.32011×10^6	13466.1	8977.43	4488.71
[24,24]	7.4942×10^6	14662.6	9775.04	4887.52
[25,25]	8.82469×10^6	15909.9	10606.6	5303.3



(a)



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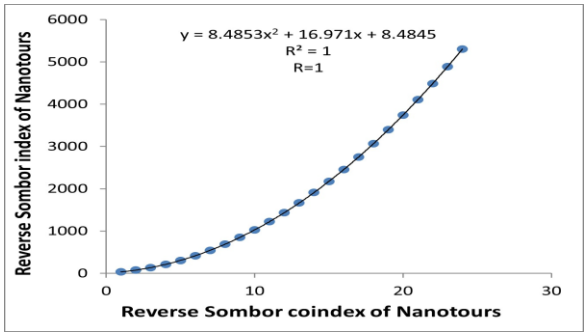


(c)

Figure 4. Correlation graphs corresponding to the $TUC_4C_8(R)[p,q]$ nanotorus

Table 10 presents the quadratic regression models and correlation coefficients (R).

Table 10. Quadratic regression models and their corresponding correlation coefficients of the studied nanomaterials

TIs	Regression model	R
$TUC_4C_8(R)[p,q]$2D-lattice		
$SO(G)$	$SO(G) = (25.456)\overline{RSO}(G)^2 + (37.33)\overline{RSO}(G) + 11.313$	1
$RSO(G)$	$RSO(G) = (16.971)\overline{RSO}(G)^2 + (23.545)\overline{RSO}(G) + 5.6591$	1
$rSO(G)$	$rSO(G) = (8.4853)\overline{RSO}(G)^2 + (20.717)\overline{RSO}(G) + 11.312$	1
$TUC_4C_8(R)[p,q]$ nanotube		
$SO(G)$	$SO(G) = (25.456)\overline{RSO}(G)^2 + (44.122)\overline{RSO}(G) + 18.662$	1
$RSO(G)$	$RSO(G) = (17.478)\overline{RSO}(G)^2 + (15.429)\overline{RSO}(G) + 54.363$	1
$rSO(G)$	$rSO(G) = (8.4853)\overline{RSO}(G)^2 + (18.843)\overline{RSO}(G) + 10.359$	1
$TUC_4C_8(R)[p,q]$ nanotorus		
$SO(G)$	$SO(G) = (25.456)\overline{RSO}(G)^2 + (50.911)\overline{RSO}(G) + 25.458$	1
$RSO(G)$	$RSO(G) = (16.971)\overline{RSO}(G)^2 + (33.943)\overline{RSO}(G) + 16.97$	1
$rSO(G)$	$rSO(G) = (8.4853)\overline{RSO}(G)^2 + (16.971)\overline{RSO}(G) + 8.4845$	1

The analysis shows that the correlation coefficient is approximately $R = 0.98$ in all cases, indicating a very strong positive relationship between $\overline{RSO}(G)$ and the studies indices. The findings suggest that $\overline{RSO}(G)$ has strong association with $SO(G)$, $RSO(G)$ and $rSO(G)$ for the studied nanostructures.

3 Chemical applicability of $\overline{RSO}(G)$

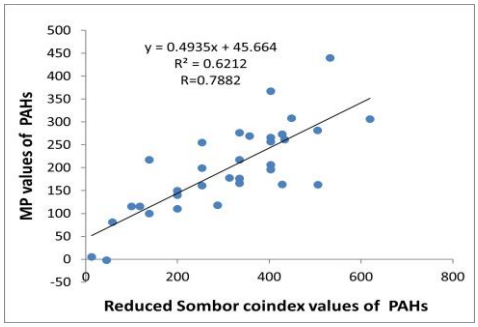
The chemical applicability of the $\overline{RSO}(G)$ is investigated in this section, through a correlation analysis involving the physico-chemical properties of 38 selected PAHs, namely melting point ($MP,\ °C$), Structural complexity (C), polarizability ($PO, 10^{-24}cm^3$), Flash point ($FP,\ °C$), molecular weight ($MW,\ g/mol$), boiling point ($BP,\ °C$), molar refractivity (MR, cm^3) and molar volume (MV, cm^3). These physico-chemical properties are treated as dependent variables (Y), whereas the corresponding $\overline{RSO}(G)$ values of PAHs as the independent variable (X). The strength of the relationship has been evaluated using the correlation coefficient R. The correlation coefficient (R) is a real number ranges from -1 to $+1$ that shows the strength and direction of a link between two variables X and Y. In general, absolute correlation coefficient greater than 0.7 indicates a strong correlation, whereas a value below 0.7 indicates moderate correlation. For every PAHs under consideration, the corresponding $\overline{RSO}(G)$ value was determined. The experimentally determined values of the properties, together with the computed $\overline{RSO}(G)$ values are listed in Table 11, while the

Figure 5 and 6 illustrates corresponding correlation plots. The regression models employed to examine the relationship between the $\overline{RSO}(G)$ of studied PAHs and the physico-chemical properties of PAHs, along with their associated correlation coefficients are reported in Table 12. The obtained results reveal a strong positive correlation between the $\overline{RSO}(G)$ of PAHs and all the selected physico-chemical properties of PAHs. These findings demonstrate the chemical significance and potential applicability of the $\overline{RSO}(G)$.

Table 11. Computed values of $\overline{RSO}(G)$ for selected PAHs and their experimentally reported physico-chemical properties

Name	$\overline{RSO}(G)$	MP	C	PO	FP	MW	BP	MR	MV
Acephenanthrylene	199.7141	140	303	27.4	188.6	202.25	405.7	69.1	162.3
Benzo[a]anthracene	253.19	161	294	31.6	209.1	228.3	436.7	79.8	191.8
Benzene	12.7279	5	15.5	10.4	−11.1	78.11	78.8	26.3	89.4
Anthracene	138.0222	217	154	24.5	146.6	178.23	337.4	61.9	157.7
Benzo[a]pyrene	335.14	176	372	35.8	228.6	252.3	495	90.3	196.1
Phenanthrene	138.2517	100	174	24.6	146.6	178.23	337.4	61.9	157.7
Benzo[b]fluoranthene	335.3669	166	372	35.8	228.6	252.3	467.5	90.3	196.1
Anthanthrene	433.236	261	411	40	247.2	276.3	497.1	100.8	200.4
Benzo[k]fluoranthene	335.1374	217	338	35.8	228.6	252.3	480	90.3	196.1
Benzo[e]pyrene	312.78	177.5	336	35.8	228.6	252.3	467.5	90.3	196.1
Corannulene	356.81	269	303	37.1	210.1	250.3	438	93.5	170.6
Benzo[g, h, i]perylene	428.4	273	411	40	247.2	276.3	501	100.8	200.4
Coronene	532.75	440	376	44.1	265.2	300.4	525.6	111.4	204.7
Chrysene	253.42	255	264	31.6	209.1	228.3	448	79.8	191.8
Biphenylene	99.379	115	339	19.8	187.2	152.19	469.9	50	129.9
Dibenz[a, c]anthracene	403.44	206	361	38.7	264.5	278.3	518	97.6	225.9
Fluoranthene	199.94	110	243	28.7	168.4	202.25	375	72.5	162
Dibenz[a, h]anthracene	403.21	266	361	38.7	264.5	278.3	524.7	97.6	225.9
Dibenz[a, i]anthracene	403.21	196	363	38.7	264.5	278.3	524.7	97.6	225.9
Indene	44.98	−2	124	15.1	58.9	116.16	181.6	38	111.8
Dibenzo[a, h]pyrene	448.47	308	436	42.9	282	302.4	552.3	108.1	230.2
Fluorene	117.99	115	165	21.3	133.1	166.22	293.6	53.8	148.3
Dibenzo[a, i]pyrene	505.42	281.5	436	42.9	282	302.4	552.3	108.1	230.2
perylene	335.37	276	304	35.8	228.6	252.3	467.5	90.3	196.1
Dibenzo[a, l]pyrene	505.65	162.4	480	42.9	282	302.4	552.3	108.1	230.2

Indeno[1, 2, 3-cd]pyrene	428.4	163.6	453	40	247.2	276.3	497.1	100.8	200.4
Rubicene	619.4	306	514	47	298.8	326.4	579	118.7	234.5
s-indacene	98.9204	–	341	19.8	214.4	152.19	525.3	50	129.9
Isochrysene	253.65	199	217	31.6	209.1	228.3	425	79.8	191.8
-Methylchrysene	287.6	118	320	33.5	217.8	242.3	449.4	84.6	208.1
Picene	403.4412	367	361	38.7	264.5	278.3	519	97.6	225.9
Naphthalene	57.9455	81	80.6	17.5	78.9	128.17	221.5	44.1	123.5
Pentalene	33.4448	–	174	38.7	97.2	102	308.9	34.2	96.1
Pentacene	402.75	257	325	38.7	264.5	278.3	524.7	97.6	225.9
Pyrene	199.7141	150	217	28.7	168.8	202.25	404	72.5	162



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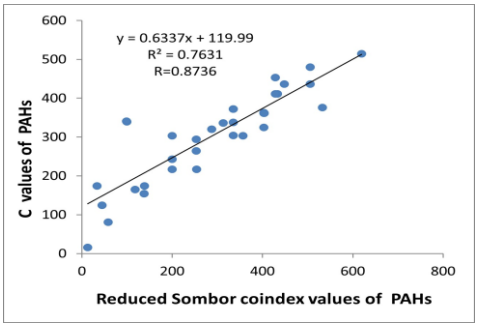

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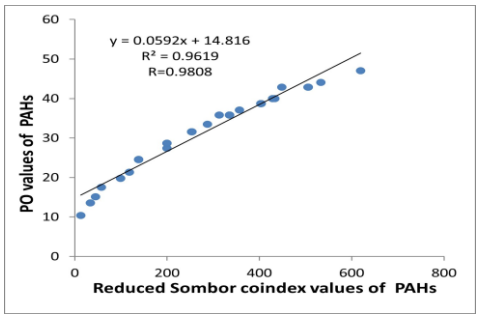

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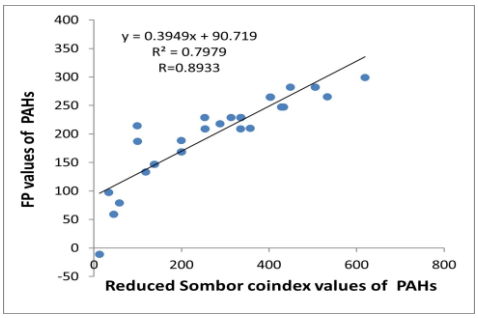

(d)

Figure 5. Correlation plots for PAHs

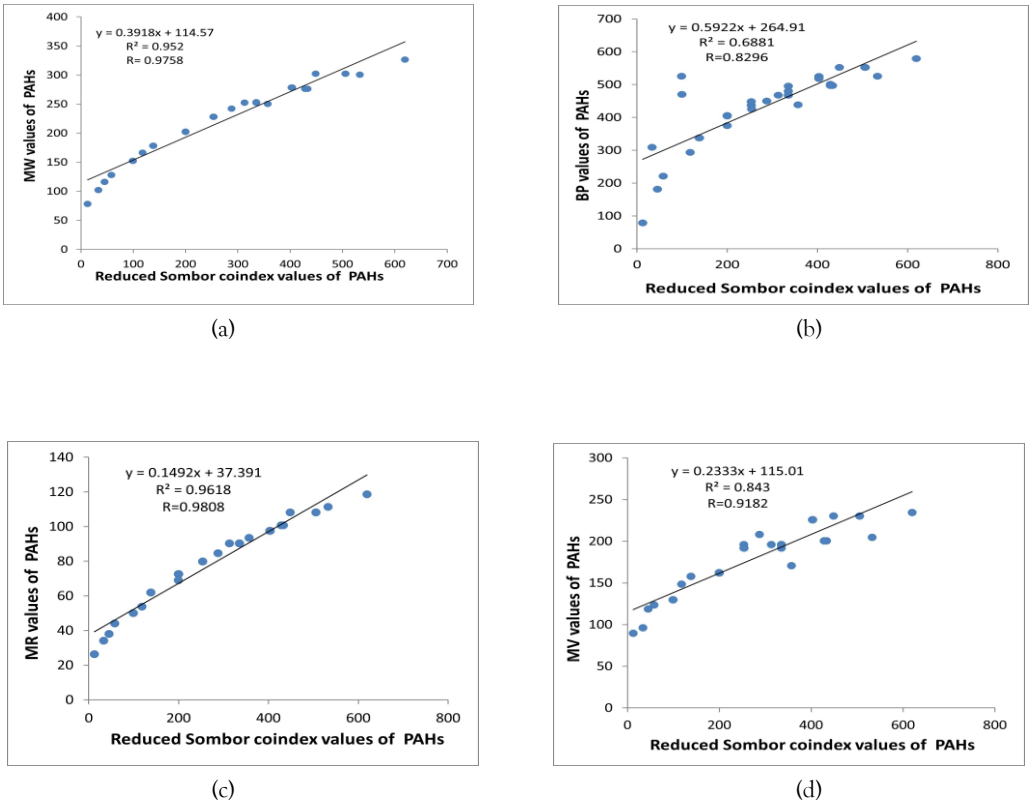

Figure 6. Correlation plots for PAHs

Table 12. Linear regression models and their corresponding correlation coefficients

PAHs Properties	Regression model	***R***
MP	$MP = 0.4935(\overline{RSO}(G)) + 45.664$	0.7882
C	$C = 0.6337(\overline{RSO}(G)) + 119.99$	0.8736
PO	$PO = 0.0592(\overline{RSO}(G)) + 14.816$	0.9808
FP	$FP = 0.3949(\overline{RSO}(G)) + 90.719$	0.8933
MW	$MW = 0.3918(\overline{RSO}(G)) + 114.57$	0.9758
BP	$BP = 0.5922(\overline{RSO}(G)) + 264.91$	0.8296
MR	$MR = 0.1492(\overline{RSO}(G)) + 37.391$	0.9808
MV	$MV = 0.2333(\overline{RSO}(G)) + 115.01$	0.9182

4 Conclusion

In this paper, we have derived explicit formulae of the TIs $\overline{RSO}(G)$, $SO(G)$, $RSO(G)$ and $rSO(G)$ for the considered nanostructures of $TUC_4C_8(R)[p,q]$. The relationship between the $\overline{RSO}(G)$ and $SO(G)$, $RSO(G)$ and $rSO(G)$ have been investigated using quadratic regression models. The analysis has revealed a strong positive correlation between the $\overline{RSO}(G)$ and $SO(G)$, $RSO(G)$ and $rSO(G)$. Furthermore, the chemical applicability of the $\overline{RSO}(G)$ has been examined through a correlation analysis considering the selected physico-chemical properties of selected PAHs. The obtained results reveal a significant positive correlation between the $\overline{RSO}(G)$ of PAHs and selected physico-chemical properties of PAHs. Overall, obtained result demonstrate that $\overline{RSO}(G)$ is an reliable and efficient topological descriptor for characterizing the structural properties for the considered nanostructures of $TUC_4C_8(R)[p,q]$ as well as PAH molecular graphs. Therefore, $\overline{RSO}(G)$ has significant potential for applications in chemical graph theory and QSPR/QSAR studies.

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