

Scientific paper

On Topological Indices of OT[m, n]Octagonal Tillings and TiO_2 Nanotubes

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Abstract

Some well defined connectivity topological indices are Randic index, atom-bond connectivity index, geometric-arithmetic index and Shigehalli & Kanabur indices, brought into light by M. Randic, Estrada $et\ al$, Vukicevic $et\ al$ and V. S. Shigehalli, in their respective research articles. Topological indices preserve the symmetry of molecular structures and provide a mathematical formulation to predict their properties like boiling points, viscosity and the radius of gyrations, mainly their study gets a cover under the category of physical chemistry. Due to its mathematical nature, this idea has caught the attention of many chemists. It has also been reported that these indices are useful in the study of anti-inflammatory activities of certain chemical instances. In this paper, we shall calculate these topological indices of an infinite class of octagonal tilling structures $OT\ [m,\ n]$, which is a molecular graph of a semiconductor allotrope consisting of octagons and rectangles, for all possible values of the parameters m and n. We shall also calculate Shigehalli & Kanabur indices of infinite structure of the titania TiO_2 nanotubes.

Keywords: Randic index; atom-bond connectivity index; octagonal tilling OT[m, n]; Shigehalli & Kanabur indices; TiO_2 nanotubes

1. Introduction

Mathematical chemistry is a branch of theoretical chemistry in which we discuss the chemical structures by using various mathematical techniques. Chemical graph theory is a branch of mathematical chemistry in which we apply techniques of graph theoretic ideas to form the chemical phenomenon mathematically. This theory plays an enigmatic part in different fields of chemical sciences. Primarily, a molecular graph is a simple graph in which vertices denote the atoms and edges denote the chemical bonding in the underlying chemical structure. Let G be a molecular graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set E(G). The order and size of G are denoted by p =|V(G)| and q = |E(G)|, respectively. Where, the order is defined to be number of vertices in G and size is defined to be number of edges in G. Also, an edge in E(G) with end vertices u and v is denoted by uv. A topological index is a molecular graph invariant which correlates the physicchemical properties of a molecular graph with a number.² The first such topological index was introduced by a chemist, Harold Wiener, in 1947 to derive the boiling points of paraffins. This mathematical representation of a molecular graph has shown to be very useful quantity in quantitative structure- property relationship abbreviated as QSPR.³ It has also many applications in communication, networking, coding theory and cryptography that are effectively modeled using a connected graph *G* under certain conditions.⁴ This index was originally derived for tree alike structures to correlate specific physic- chemical properties of alkanes, alcohols, amines and their compounds.

H. Hosoya,⁵ defined the notion of Wiener index for any graph *G* as;

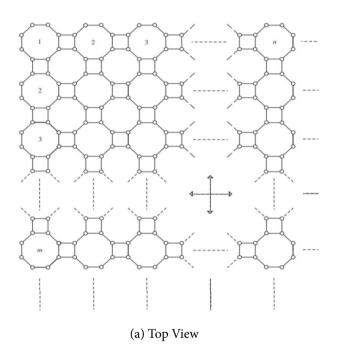
$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v).$$

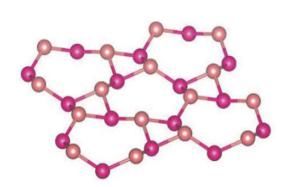
A. Ashrafi *et al*,⁶ calculated the PI, Szeged and edge Szeged indices of some nanostar dendrimers. Recently, authors also investigated *m*- order connectivity indices of nanostar dendrimers.⁷ The atom-bond connectivity index

and geometric-arithmetic index of nanostar dendrimers and some polyomino- chains were studied by S. Hayat *et al.*⁸ The atom-bond connectivity index and geometric-arithmetic index of some fullerenes were studied by M. Baca *et al.*⁹ Rostami *et al.* studied the first kind of geometric- arithmetic index of some nanostar dendrimers.¹⁰ Ghorbani *et al.* ¹¹ did their study on the nullity of an infinite class of nanostar dendrimers.

The elemental two-dimensional 2D materials such as graphene, silicene, germanene, and black phosphorus have pulled considerable attention due to their fascinating physic-chemical attributes. Structurally, they possess the honeycomb, distorted honeycomb and continuous honeycomb lattices, which are composed of six atom rings.

Recently, 12 P. Li and W. Luo have studied a new structure of 2D allotropes of group V elements composed





(b) Birds View (courtesy 12)

Figure 1. General formation of the molecular octagonal tilling structure OT[m, n].

of eight-atom rings, which they termed as octagonal tilling structure, denoted generally by OT. These kinds of allotropes are comprehensively studied in materials sciences. Their findings indicated that these allotropes are dynamically stable and are also thermally stable at temperatures up to $600 \ K$. They also showed, these allotropes are semiconductors with band gaps ranging from 0.3 to $2.0 \ eV$, thus, they are potentially useful in near and mid-infrared devices. The molecular graph of these octagonal tilling structure, OT[m, n], is presented in Figure 1, in which, m denotes the number of octagons in an alternate row and n denotes the number of octagons in an alternate column of OT[m, n].

2. The Randić, ABC and GA Indices of Molecular Octagonal Tilling Structure OT[m, n]

Let H be a simple connected graph with vertex set V(H) and edge set E(H). The degree d_v of a vertex $v \in V(H)$ is the number of edges incident on v and $S_u = \sum_{v \in V(H)} d_v$ $N_H(u) = \{v \in V(H) \mid uv \in E(H)\}$

M. Randic defined the Randic index as follows, 13

$$\chi(H) = \sum_{uv \in E(H)} \frac{1}{\sqrt{dudv}} \tag{1}$$

E. Estrada et al, ¹⁴ defined the atom-bond connectivity index, abbreviated as ABC-index, as:

$$ABC(H) = \sum_{uv \in E(H)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$
 (2)

Another well used connectivity topological descriptor for the molecular graphs is geometric-arithmetic index (GA-index), introduced by Vukicevic and Furtula and is defined by, ¹⁴

$$GA(H) = \sum_{uv \in E(H)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \tag{3}$$

With each edge uv, we associate a pair $(d_w \ d_v)$. The edge partition of octagonal tilling OT[m, n] with respect to the degrees of the end-vertices of edges is presented in Table 1.

Table 1. The (d_u, d_v) - type edge partition of octagonal tilling OT[m, n].

(d_u, d_v) -Partition	Edge Cardinality
(2, 2)	2(m+n+2)
(2, 3)	4(m+n-2)
(3, 3)	4(3mn-2m-2n+1)

Theorem 1. For all m and n, the Randic index χ of the octagonal tilling structure OT[m, n] is

$$\chi(OT[m,n]) = 4mn + (\frac{2\sqrt{6} - 5}{3})(m + n - 2).$$

Proof. The (d_u, d_v) -type edge partition of the graph OT[m, n] is shown in Table 1. We prove the desired result by using partition of Table 1 and the formula of Randic index given by Equation 1 as follows.

$$\chi(OT[m,n]) = 2(m+n+2)\frac{1}{\sqrt{2\times2}} + 4(m+n-2)$$

$$\frac{1}{\sqrt{2\times3}} + 4(3mn-2m-2n+1)\frac{1}{\sqrt{3\times3}}$$

$$= (m+n+2) + (m+n-2)\frac{2\sqrt{2}}{\sqrt{3}} + (3mn-2m-2n+1)\frac{4}{3}$$

$$= m(1+\frac{2\sqrt{2}}{\sqrt{3}} - \frac{8}{3}) + n(1+\frac{2\sqrt{2}}{\sqrt{3}} - \frac{8}{3}) + 4mn + (2-\frac{4\sqrt{2}}{\sqrt{3}} + \frac{4}{3})$$

$$= m(\frac{2\sqrt{6} - 5}{3}) + n(\frac{2\sqrt{6} - 5}{3}) + 4mn + (\frac{10 - 4\sqrt{6}}{3})$$

$$= 4mn + (\frac{2\sqrt{6} - 5}{3})(m+n-2)$$

$$\Rightarrow \chi(OT[m,n]) = 4mn + (\frac{2\sqrt{6} - 5}{3})(m+n-2)$$

Example 1. Consider a 2D structure of allotrope we are discussing called octagonal tilling OT [7, 8] consisting of 448 atoms and 642 chemical bonds, we obtain,

$$\chi(OT[7,8]) = 223.5632.$$

Example 2. The Randić index of 2D allotrope, octagonal tilling OT [m, n], for m = 1, 2, ..., 5 and n = 1, 2, ..., 10 are given as follows

OT[m, n]	X(OT[m, n])
OT[1, 1]	4
OT[1, 2]	7.9664
OT[1, 3]	11.9328
OT[1, 4]	15.8992
OT[1, 5]	19.8656
OT[1, 6]	23.832
OT[1, 7]	27.7984
OT[1, 8]	31.7648
OT[1, 9]	35.7312
OT[1, 10]	39.6976
OT[2, 1]	7.9664
OT[2, 2]	15.9328
OT[2, 3]	23.8992
OT[2, 4]	31.8656
OT[2, 5]	39.832
OT[2, 6]	47.7984
OT[2, 7]	55.7648
OT[2, 8]	63.7312
OT[2, 9]	71.6976

OT[m, n]	X(OT[m, n])
OT[2, 10]	79.664
OT[3, 1]	11.9328
OT[3, 2]	23.8992
OT[3, 3]	35.8656
OT[3, 4]	47.832
OT[3, 5]	59.7984
OT[3, 6]	71.7648
OT[3, 7]	83.7312
OT[3, 8]	95.6976
OT[3, 9]	107.664
OT[3, 10]	119.6304
OT[4, 1]	15.8992
OT[4, 2]	31.8656
OT[4, 3]	47.832
OT[4, 4]	63.7984
OT[4, 5]	79.7648
OT[4, 6]	95.7312
OT[4, 7]	111.6976
OT[4, 8]	127.664
OT[4, 9]	143.6304
OT[4, 10]	159.5968
OT[5, 1]	19.8656
OT[5, 2]	39.832
OT[5, 3]	59.7984
OT[5, 4]	79.7648
OT[5, 5]	99.7312
OT[5, 6]	119.6976
OT[5, 7]	139.664
OT[5, 8]	159.6304
OT[5, 9]	179.5968
OT[5, 10]	199.5632

Theorem 2. For all m and n, the atom-bond connectivity index of the octagonal tilling structure OT[m, n] is

$$ABC(OT[m,n]) = 8mn + (\frac{9 - 8\sqrt{2}}{3\sqrt{2}})(2m + 2n) + (\frac{8\sqrt{2} - 12}{3\sqrt{2}}).$$

Proof. The (d_w, d_v) -type edge partition of the graph OT[m, n] is shown in Table 1. We prove the desired result by using partition of Table 1 and the formula of atom bond connectivity index given by Equation 2 as:

$$ABC(OT[m,n]) = 2(m+n+2)\sqrt{\frac{2+2-2}{2\times 2}} + 4(m+n-2).$$

$$\sqrt{\frac{2+3-2}{2\times 3}} + 4(3mn-2m-2n+1)\sqrt{\frac{3+3-2}{3\times 3}}$$

$$= 2(m+n+2)\sqrt{\frac{2}{4}} + 4(m+n-2)\sqrt{\frac{3}{6}} + 4(3mn-2m-2n+1)\sqrt{\frac{4}{9}}$$

$$= 2(m+n+2)\frac{1}{\sqrt{2}} + 4(m+n-2)\frac{1}{\sqrt{2}} + (12mn-8m-8n+4)\sqrt{\frac{4}{9}}$$

$$= (2m+2n+4)\frac{1}{\sqrt{2}} + (4m+4n-8)\frac{1}{\sqrt{2}} + (12mn-8m-8n+4)\frac{2}{3}$$

$$= (2m+2n+4)\frac{1}{\sqrt{2}} + (4m+4n-8)\frac{1}{\sqrt{2}} + (12mn-8m-8n+4)\frac{2}{3}$$

$$= (2m+2n+4+4m+4n-8)\frac{1}{\sqrt{2}} + (12mn-8m-8n+4)\frac{2}{3}$$

$$= m(\frac{6}{\sqrt{2}} - \frac{16}{3}) + n(\frac{6}{\sqrt{2}} - \frac{16}{3}) + 8mn + (-\frac{4}{\sqrt{2}} + \frac{8}{3})$$

$$= m(\frac{18 - 16\sqrt{2}}{3\sqrt{2}}) + n(\frac{18 - 16\sqrt{2}}{3\sqrt{2}}) + 8mn + (\frac{8\sqrt{2} - 12}{3\sqrt{2}})$$

$$\Rightarrow ABC(T[m, n]) = 8mn + (\frac{9 - 8\sqrt{2}}{3\sqrt{2}})(2m + 2n) + (\frac{8\sqrt{2} - 12}{3\sqrt{2}})$$

Example 3. Consider a 2D structure of allotrope we are discussing called octagonal tilling OT [7, 9] consisting of 504 atoms and 724 chemical bonds. Then, its atom bond connectivity index is

$$ABC(OT[7,9]) = 486.3887.$$

Example 4. The atom bond connectivity index of 2D allotrope, octagonal tilling OT [m, n], for m = 1, 2, ..., 5 and n = 1, 2, ..., 10 are given as follows:

OT[m, n]	ABC(OT[m, n])
OT[1, 1]	5.6571
OT[1, 2]	12.5665
OT[1, 3]	19.4759
OT[1, 4]	26.3853
OT[1, 5]	33.2947
OT[1, 6]	40.2041
OT[1, 7]	47.1135
OT[1, 8]	54.0229
OT[1, 9]	60.9323
OT[1, 10]	67.8417
OT[2, 1]	12.5665
OT[2, 2]	27.4759
OT[2, 3]	42.3853
OT[2, 4]	57.2947
OT[2, 5]	72.2041
OT[2, 6]	87.1135
OT[2, 7]	102.0229
OT[2, 8]	116.9323
OT[2, 9]	131.8417
OT[2, 10]	146.7511
OT[3, 1]	19.4759
OT[3, 2]	42.3853
OT[3, 3]	65.2947
OT[3, 4]	88.2041
OT[3, 5]	111.1135
OT[3, 6]	134.0229
OT[3, 7]	156.9323
OT[3, 8]	179.8417
OT[3, 9]	202.7511
OT[3, 10]	225.6605
OT[4, 1]	26.3853
OT[4, 2]	57.2947
OT[4, 3]	88.2041
OT[4, 4]	119.1135
OT[4, 5]	150.0229
OT[4, 6]	180.9323
OT[4, 7]	211.8417
OT[4, 8]	242.7511
OT[4, 9]	273.6605
OT[4, 10]	304.5699
OT[5, 1]	33.2947

OT[m, n]	ABC(OT[m, n])
OT[5, 2]	72.2041
OT[5, 3]	111.1135
OT[5, 4]	150.0229
OT[5, 5]	188.9323
OT[5, 6]	227.8417
OT[5, 7]	266.7511
OT[5, 8]	305.6605
OT[5, 9]	344.5699
OT[5, 10]	383.4793

Theorem 3. For all m and n, the geometric-arithmetic connectivity index of the octagonal tilling structure OT[m, n] is

$$GA(OT[m,n]) = 12mn + (\frac{4\sqrt{6} - 15}{5})$$
$$(2m + 2n) + 8(\frac{5 - 2\sqrt{6}}{5}).$$

Proof. The $(d_w \ d_v)$ -type edge partition of the graph OT[m, n] is shown in Table 1. We prove the required result by using partition of Table 1 and the formula geometric-arithmetic connectivity index given by Equation 3 by following calculations:

$$GA(OT[m,n]) = 2(m+n+2)\frac{2\sqrt{2\times2}}{2+2} + (12)$$

$$4(m+n-2)\frac{2\sqrt{2\times3}}{2+3} + 4(3mn-2m-2n+1)\frac{2\sqrt{3\times3}}{3+3}$$

$$= 2(m+n+2)\frac{2\sqrt{4}}{4} + 4(m+n-2)\frac{2\sqrt{6}}{5} + 4(3mn-2m-2n+1)\frac{2\sqrt{9}}{6}$$

$$= 2(m+n+2)\frac{2\cdot2}{4} + 4(m+n-2)\frac{2\sqrt{6}}{5} + 4(3mn-2m-2n+1)\frac{2\cdot3}{6}$$

$$= 2(m+n+2) + (m+n-2)\frac{8\sqrt{6}}{5} + (12mn-8m-8n+4)$$

$$= 12mn + m(2 + \frac{8\sqrt{6}}{5} - 8) + n(2 + \frac{8\sqrt{6}}{5} - 8) + (4 - \frac{16\sqrt{6}}{5} + 4)$$

$$= 12mn + 2(\frac{4\sqrt{6} - 15}{5})(m+n) + 8(\frac{5 - 2\sqrt{6}}{5})$$

$$= 12mn + (\frac{4\sqrt{6} - 15}{5})(2m+2n) + 8(\frac{5 - 2\sqrt{6}}{5})$$

$$\Rightarrow GA(OT[m,n]) = 12mn + (\frac{4\sqrt{6} - 15}{5})(2m+2n) + 8(\frac{5 - 2\sqrt{6}}{5}).$$

Example 5. Consider a 2D structure of allotrope we are discussing called octagonal tilling OT [13, 14] consisting of 504 atoms and 724 chemical bonds. Then, its gepmetric arithmetic index is

$$GA(OT[13,14]) = 2127.98.$$
 (13)

Example 6. The geometric-arithmetic index of 2D allotrope, octagonal tilling OT [m, n], for m = 1, 2, ..., 5 and n = 1, 2, ..., 10 are given as:

OT[m, n]	GA(OT[m, n])
OT[1, 1]	8
OT[1, 2]	17.9192
OT[1, 3]	27.8384
OT[1, 4]	37.7576
OT[1, 5]	47.6768
OT[1, 6]	57.596
OT[1, 7]	67.5152
OT[1, 8]	77.4344
OT[1, 9]	87.3536
OT[1, 10]	97.2728
OT[2, 1]	17.9192
OT[2, 2]	39.8384
OT[2, 3]	61.7576
OT[2, 4]	83.6768
OT[2, 5]	105.596
OT[2, 6]	127.5152
OT[2, 7]	149.4344
OT[2, 8]	171.3536
OT[2, 9]	193.2728
OT[2, 10]	215.192
OT[3, 1]	27.8384
OT[3, 2]	61.7576
OT[3, 3]	95.6768
OT[3, 4]	129.596
OT[3, 5]	163.5152
OT[3, 6]	197.4344
OT[3, 7]	231.3536
OT[3, 8]	265.2728
OT[3, 9]	299.192
OT[3, 10]	333.1112
OT[4, 1]	37.7576
OT[4, 2]	83.6768
OT[4, 3]	129.596
OT[4, 4]	175.5152
OT[4, 5]	221.4344
OT[4, 6]	267.3536
OT[4, 7]	313.2728
OT[4, 8]	359.192
OT[4, 9]	405.1112
OT[4, 10]	451.0304
OT[5, 1]	47.6768
OT[5, 2]	105.596
OT[5, 3]	163.5152
OT[5, 4]	221.4344
OT[5, 5]	279.3536
OT[5, 6]	337.2728
OT[5, 7]	395.192
OT[5, 8]	453.1112
OT[5, 9]	511.0304
OT[5, 10]	568.9496

3. The Shigehalli & Kanabur Indices of the TiO₂ Nanotube

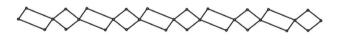
Another well known semiconductor, Titania is comprehensively discussed in materials sciences, which admits many aspects of various technological applications. Titania nanotubes were systematically synthesized in the course of last 10- 20 years using different methods in labs. The growth mechanism for TiO_2 nanotubes has been studied well. ¹⁶ Due to high applicability of the Titania nanotubes, their comprehensive theoretical studies are getting enhanced attention. Also, the TiO_2 sheets with a thickness of a few atomic layers were discovered to be remarkably stable. ¹⁷ In this section, We shall calculate three Shigehalli & Kanabur indices, ¹⁸ of the TiO_2 nanotubes. These expressions for these indices are given as follows:

$$SK(H) = \sum_{uv \in E(H)} \frac{d_u + d_v}{2} \tag{4}$$

$$SK_1(H) = \sum_{uv \in E(H)} \frac{d_u \times d_v}{2} \tag{5}$$

$$SK_2(H) = \sum_{uv \in E(H)} \left(\frac{du + dv}{2}\right)^2$$
 (5)

Further, Figure 2 shows the graph of $TiO_2[m, n]$ nanotubes, where number of octagons represent m in rows and n in columns respectively.



Rird's View

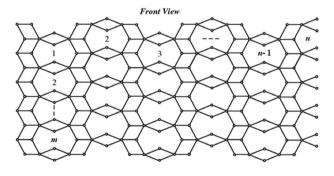


Figure 2. General formation of the molecular graph of titania $TiO_2[m, n]$ nanotubes.

Once again with each edge uv, we correspond a pair (d_u, d_v) . The edge partition of $TiO_2[m, n]$ nanotubes with respect to the degrees of the end-vertices of edges is presented in Table 2.¹⁹

Table 2. The $(d_u\,,\,d_v\,)$ -type edge partition of titania $TiO_2[m,\,n]$ nanotubes

(d_u, d_v) - Partition	Edge Cardinality
(2, 4)	6 <i>n</i>
(2,5)	2 <i>n</i> + 4 <i>mn</i>
(3, 4)	2n
(3, 5)	6mn- 2n

Theorem 4. For all m and n, the 1st Shigehalli & Kanabur index, SK, of the titania $TiO_2[m, n]$ nanotubes is

$$SK(TiO_2[m, n]) = 24n + 38mn.$$

Proof. The (d_w, d_v) -type edge partition of the graph $TiO_2[m, n]$ are shown in Table 2. We prove the desired result by using partition of Table 2 and the formula of the 1st Shigehalli & Kanabur index given by Equation 4 as follows.

$$SK(TiO_{2}[m,n]) = (6n)\left(\frac{2+4}{2}\right) + (2n+4mn)$$

$$\left(\frac{2+5}{2}\right) + (2n)\left(\frac{3+4}{2}\right) + [6mn-2n]\left(\frac{3+5}{2}\right)$$

$$= (6n)(3) + (2n+4mn)\left(\frac{7}{2}\right) + 7n + [6mn-2n]$$

$$= 18n + 2n\left(\frac{7}{2}\right) + 4mn\left(\frac{7}{2}\right) + 7n + 24mn - 8n$$

$$= 18n + 7n + 14mn + 7n + 24mn - 8n$$

$$\Rightarrow SK(TiO_{2}[m,n]) = 24n + 38mn.$$

Example 7. The 1st Shigehalli & Kanabur of the *titania* TiO_2 [8, 9] nanotube consisting of 784 chemical bonds is given as

$$SK(TiO_2[8,9]) = 2928.$$

Theorem 5. For all m and n, the 2^{nd} Shigehalli & Kanabur index, SK_1 , of the titania $TiO_2[m, n]$ nanotubes is

$$SK_1(TiO_2[m,n]) = 31n + 65mn.$$

Proof. The $(d_w \ d_v)$ -type edge partition of the graph $TiO_2[m, n]$ are shown in Table 2. We obtain the required calculation by using partition of Table 2 and the formula of the 2nd Shigehalli & Kanabur index given by Equation 5 as follows.

$$SK_1(TiO_2[m,n]) = (6n)\left(\frac{2\times 4}{2}\right) + (2n + 4mn)\left(\frac{2\times 5}{2}\right)$$

 $\left[+ (2n)\left(\frac{3\times 4}{2}\right) + [6mn - 2n]\left(\frac{3\times 5}{2}\right) \right]$

$$= (6n)(4) + (2n + 4mn)(5) + (2n)(6) + [6mn - 2n] \left(\frac{15}{2}\right)$$

$$= 24n + 10n + 20mn + 12n + [6mn - 2n] \left(\frac{15}{2}\right)$$

$$= 24n + 10n + 20mn + 12n + 45mn - 15n$$

$$\Rightarrow SK_1(TiO_2[m,n]) = 31n + 65mn$$

Example 8. The 2^{nd} Shigehalli & Kanabur index of the titania TiO_2 [10, 12] nanotube consisting of 1280 chemical bonds is given as

$$SK_1(TiO_2[10,12]) = 72440.$$

Theorem 6. For all m and n, the 3^{rd} Shigehalli & Kanabur index, SK_2 , of the titania $TiO_2[m, n]$ nanotubes is

$$SK_2(TiO_2[m, n]) = 71n + 145mn.$$

Proof. The (d_w, d_v) -type edge partition of the graph $TiO_2[m, n]$ are shown in Table 2. We obtain the required calculation by using partition of Table 2 and the formula of the 3rd Shigehalli & Kanabur index given by Equation 6 as follows.

$$SK_{2}(TiO_{2}[m,n]) = (6n)\left(\frac{2+4}{2}\right)^{2} + (2n+4mn)$$

$$\left(\frac{2+5}{2}\right)^{2} + (2n)\left(\frac{3+4}{2}\right)^{2} + [6mn-2n]\left(\frac{3+5}{2}\right)^{2}$$

$$= (6n)\left(\frac{6}{2}\right)^{2} + (2n+4mn)\left(\frac{7}{2}\right)^{2} + (2n)\left(\frac{7}{2}\right)^{2} + [6mn-6n+4n]\left(\frac{8}{2}\right)^{2}$$

$$= (6n)(3)^{2} + (2n+4mn)\left(\frac{49}{4}\right) + (2n)\left(\frac{49}{4}\right) + [6mn-2n](4)^{2}$$

$$= 54n + \frac{49}{2}n + 49mn + \frac{49}{2}n + 96mn - 32n$$

$$\Rightarrow SK_{2}(TiO_{2}[m,n]) = 71n + 145mn.$$

Example 9. The 3rd Shigehalli & Kanabur index of the titania TiO₂ [20, 9] nanotube consisting of 1960 chemical bonds is given as

$$SK_2(TiO_2[10,12]) = 29710.$$

4. Conclusion

In this article, we have calculated some degree based topological indices of an infinite class of molecular graph, termed as octagonal tilling structure OT[m, n]. Precisely, we have studied the Randic index, atom-bond connectivity index and geometric-arithmetic connectivity index of the OT[m, n], defined by M. Randic, ¹³ Estrada *et al.* ¹⁴ and Vukicevic *et al.*, ¹⁵ respectively. Secondly, we

have studied the 1st, 2nd and 3rd Shigehalli & Kanabur indices of the *titania* TiO_2 [m, n] nanotube. These topological indices are mathematical predictors for various chemical properties of molecular structures as boiling point and viscosity, they are also reported to be useful in anti-inflammatory properties of certain chemical instances. They have also been used as branching indices and have several applications in QSPR and QSAR studies. We are confident that these indices will help the researchers and chemists in analyzing various chemical instances of the octagonal tilling 2D allotrope structure OT[m, n], discussed in this article and of the titania TiO_2 nanotubes. From these indices of OT[m, n] and TiO_2 nanotubes, we can observe two strict chains which conclude our research. These chains are:

$$\chi(OT[m,n]) < ABC(OT[m,n]) < GA(OT[m,n])$$
 (1)

$$SK(TiO2) < SK1(TiO2) < SK2(TiO2)$$
 (2)

Graphically, these strict inequality MATLAB comparison is presented in Figures 3 and 4.

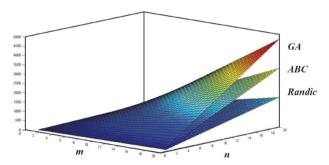


Figure 3. A comparison of *Randic*, *ABC* and *GA* indices of OT[m, n]; $m, n \in \{1, 20\}$.

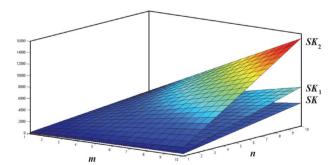


Figure 4. A comparison of SK, SK_1 and SK_2 indices of the titania $TiO_2[m, n]$ nanotubes; where $m, n \in \{1, 10\}$.

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Povzetek

Nekateri dobro definirani povezovalni topološki indeksi so Randićev indeks, povezovalni indeks atom-vez, geometrijsko-aritmetični indeks in Shigehalli & Kanabur indeksi, ki so jih v raziskovalnih člankih razjasnili M. Randic, Estrada et al, Vukicevic et al and V. S. Shigehalli. Topološki indeksi ohranjajo simetrijo molekulske strukture in zagotavljajo matematično formulacijo za napovedovanje lastnosti kot so vrelišča, viskoznost in radiji sukanja;¹ večinoma te študije sodijo v kategorijo fizikalne kemije. Zaradi svoje matematične narave je ta ideja pritegnila pozornost mnogih kemikov. Poročajo tudi, da so ti indeksi uporabni pri študiju protivnetnega delovanja določenih kemičnih primerov. V tem delu smo izračunali topološke indekse za neskončen razred osmerokotne predalčne strukture OT [m, n], ki je molekularni graf polprevodniškega alotropa, sestavljenega iz osmerokotnikov in pravokotnikov, in sicer za vse možne vrednosti parametrov m in n. Uporabili smo Shigehalli & Kanabur indekse neskončne strukture nanocevk TiO_2 .